Resonance lectures

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November 2023

1 Motivation

As nuclear engineers, we are concerned with the behaviour of neutrons in nuclear reactors due to their influence on reaction rates, criticality, hot spots, burn-up, etc. The governing neutron transport equation that we are most frequently interested in is:

$$\begin{aligned}\boldsymbol{\Omega}\cdot\nabla\psi(\mathbf{r},E,\boldsymbol{\Omega})+\Sigma_{\mathrm{t}}(\mathbf{r},E)\psi(\mathbf{r},E,\boldsymbol{\Omega})=\frac{\chi(E)}{4\pi k_{\mathrm{eff}}}\int_0^\infty \mathrm{d}E'\bar{\nu}\Sigma_{\mathrm{f}}(\mathbf{r},E')\phi(\mathbf{r},E')\\ +\int_0^\infty \mathrm{d}E'\int_{4\pi}\mathrm{d}\Omega'\Sigma_{\mathrm{s}}(\mathbf{r},E'\to E,\boldsymbol{\Omega}'\to\boldsymbol{\Omega})\psi(\mathbf{r},E',\boldsymbol{\Omega}')\ ,\end{aligned} \tag{1}$$

where ψ is the neutron angular flux which depends upon position, $\mathbf{r}$, neutron energy, E, and neutron direction, $\boldsymbol{\Omega}$, Σ_x is a cross section (total, fission, and scattering), χ is the fission neutron energy spectrum, k_{eff} is the criticality eigenvalue, $\bar{\nu}$ is the average neutron production from fission, ϕ is the scalar neutron flux, and $\Sigma_s(\mathbf{r},E'\to E,\boldsymbol{\Omega}'\to\boldsymbol{\Omega})$ is the double-differential scattering cross section. However, no nuclear engineer solves this equation: either we use Monte Carlo where this equation is irrelevant or we solve an approximation of this equation.

The most ubiquitous approximation is the multigroup approximation, i.e., discretisation of the energy variable. We do this by asserting that in a given energy range (or energy group, g) the cross sections and flux are piecewise constant: $\Sigma_{x,g}$, ψ_g. We then define our multigroup flux as the integral of the continuous energy flux over the energy range $E\in[E_g,E_{g-1}]$:

$$\psi_g(\mathbf{r},\boldsymbol{\Omega})=\int_{E_g}^{E_{g-1}}\mathrm{d}E\psi(\mathbf{r},E,\boldsymbol{\Omega})\ ,$$

$$\phi_g(\mathbf{r})=\int_{E_g}^{E_{g-1}}\mathrm{d}E\phi(\mathbf{r},E)\ .$$

Integrating Eq. (1) over each energy group produces a set of equations of the form:

$$\begin{aligned}\boldsymbol{\Omega}\cdot\nabla\psi_g(\mathbf{r},\boldsymbol{\Omega})+\Sigma_{\mathrm{t},g}(\mathbf{r})\psi_g(\mathbf{r},\boldsymbol{\Omega})=\frac{\chi_g}{4\pi k_{\mathrm{eff}}}\sum_{g'}\bar{\nu}\Sigma_{\mathrm{f},g'}(\mathbf{r})\phi_{g'}(\mathbf{r})\\ +\sum_{g'}\int_{4\pi}\mathrm{d}\Omega'\Sigma_{\mathrm{s},g'\to g}(\mathbf{r},\boldsymbol{\Omega}'\to\boldsymbol{\Omega})\psi_{g'}(\mathbf{r},\boldsymbol{\Omega}')\ .\end{aligned} \tag{2}$$

While this equation is an approximation of Eq. (1), it can be valuable provided it preserves the reaction rates that would be obtained by solving Eq. (1). More precisely, we want to ensure:

$$\Sigma_{x,g}\phi_g=\int_{E_g}^{E_{g-1}}\mathrm{d}E\ \Sigma_x(E)\phi(E)\ . \tag{3}$$

*These notes follow from notes produced by Meir Segev, as well as sections of Duderstadt & Hamilton and Knott & Yamamoto.

This requirement in turn tells us exactly how to choose the values of $\Sigma_{x,g}$:

$$\Sigma_{x,g} = \frac{\int_{E_g}^{E_{g-1}} \mathrm{d}E\ \Sigma_x(E)\phi(E)}{\phi_g} = \frac{\int_{E_g}^{E_{g-1}} \mathrm{d}E\ \Sigma_x(E)\phi(E)}{\int_{E_g}^{E_{g-1}} \mathrm{d}E\ \phi(E)}\ . \tag{4}$$

In other words, $\Sigma_{x,g}$ should be a flux-weighted average of $\Sigma_x(E)$. This brings us to one of the central problems of nuclear engineering...

> **"Wait a minute," you ask, "the purpose of solving the transport equation is to get the flux, but I have to know the flux to compute the multi-group constants!"**
>
> **– The NJOY manual**

Life could be worse, however: when neutrons are thermal, the spectrum is essentially Maxwellian. Meanwhile, when neutrons are fast, the fission spectrum is a good approximation and geometry effects are negligible – in LWRs, neutrons do not spend significant time in the fast region anyway. In these two regions, we can (with some approximations or slightly finer energy discretisation) reasonably accurately evaluate cross sections using Eq. (4). In between, however, we do not have this luxury.

In this intermediate range, **cross sections are resonant** and sufficiently large such that **geometry effects** become important. Both of these means that the flux spectrum can be perturbed quite dramatically depending on the particular composition and configuration of a reactor. This is strongly related to the concept of spatial and energy self-shielding. We must somehow account for these resonance and geometry effects.

Despite this, we still manage to have a reasonably low number of energy groups while maintaining good accuracy in LWR calculations. This is illustrated with the WIM69 group structure in Fig. 1.

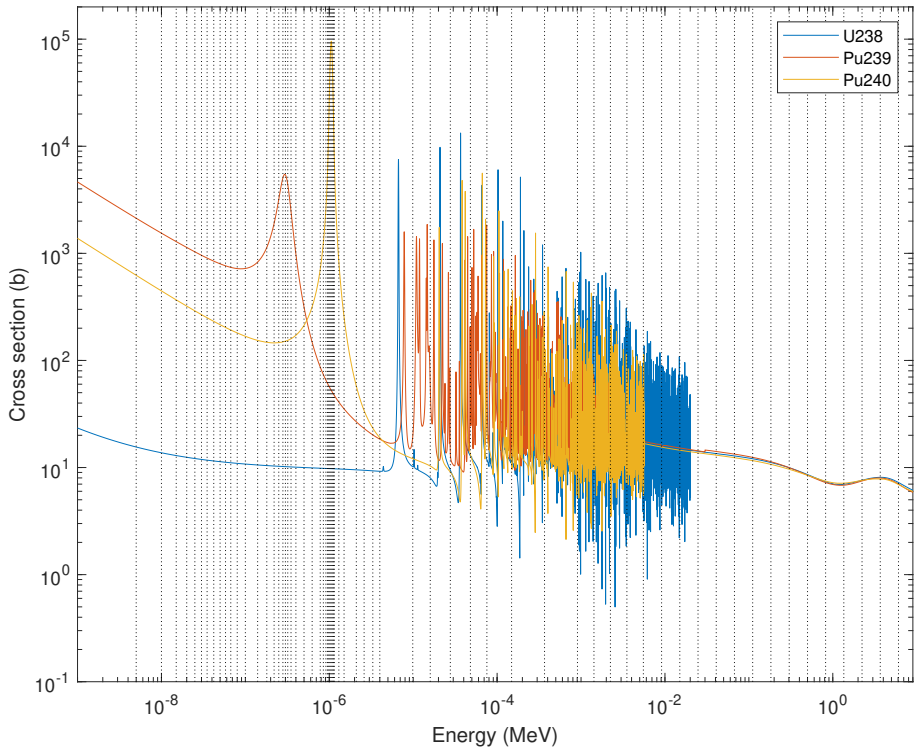


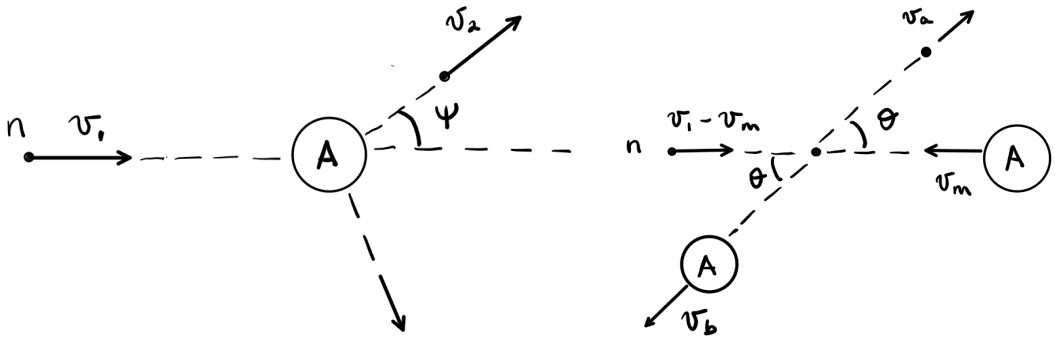
Figure 1: WIMS69 group structure overlaid with some prominent nuclides.

This lecture series aims to partially explain how we can generate multigroup cross sections by coming up with sufficiently good approximations to the flux spectrum in a surprisingly wide number of conditions. The basic principles have been well known for a while, but are not often taught as they sit at the back of proprietary lattice physics code. Most of the content of this lecture series is ultimately about explaining the theoretical basis of the HEAD module in WIMS, for example. While there are several quite simple and important results that allow these codes to produce cross sections which are sufficiently accurate for reactor design, reaching these results is non-trivial. Perhaps the main purpose of this series is to convey that, as Eugene would often say, **"cross sections do not fall from the sky"**.

I should emphasise that the focus is tailored towards thermal reactors; the approximations that feature here were historically deemed acceptably accurate for thermal systems without exceeding the contemporary computational budget – treatments for fast reactors tend to differ significantly. However, it remains an open question how relevant some of these methods will be in the future: many of the treatments described here could be and have been replaced by higher fidelity methods. Several lattice physics codes now employ fine-group slowing down equation solutions, while Monte Carlo is regularly used to generate cross sections for whole-core transport or diffusion simulations. History suggests that computation only becomes cheaper and the cost of conservatism becomes greater, so it will be interesting to see whether the methods discussed will persist for much longer.

2 Neutron kinematics

We are first going to examine the kinematics of a neutron scattering elastically with a stationary target. We will assume scattering is **s-wave**, i.e., **low incoming neutron energy** and **low Z target**, such that this can be treated like the collision of two spheres scattering **isotropically** in a centre of mass reference frame.



(a) Lab frame.

(b) Centre-of-mass (CoM) frame.

Figure 2: Co-ordinate systems/reference frames for elastic collisions.

First we consider the 'lab frame', i.e., how we would see the kinematics occurring as observers in 'the lab', shown in Fig. 2a. Here n is the incoming neutron, v_1 is its initial velocity, and its mass is $M_\mathrm{n} = 1$. The target has a mass $M_\mathrm{target} = A$. On collision, the neutron will deflect at an angle of ψ, travelling at a velocity of v_2. The total momentum in this system is:

$$\sum_i v_i M_i = v_1 \times 1 + 0 \times A = v_1 \ .$$

The kinetic energy of the system is:

$$\mathrm{KE}_\mathrm{Lab} = \frac{1}{2} v_1^2 \ .$$

The centre of mass of the system will move as the neutron moves towards the target. The centre of mass velocity is given as the weighted sum of the particle velocities:

$$v_\mathrm{m} = \frac{v_1 M_\mathrm{n} + 0 \times M_\mathrm{target}}{M_\mathrm{n} + M_\mathrm{target}} = \frac{v_1}{1 + A} \ .$$

From this we can create a simpler reference frame by **fixing the centre of mass to be stationary** – this will be referred to as the Centre of Mass (CoM) system. Given that the CoM does not move, other particles must move relative to it (shown in Fig. 2b). The net neutron velocity before collision then becomes:

$$v_1 - v_\mathrm{m} = v_1 \left(1 - \frac{1}{A+1}\right) = v_1 \frac{A}{A+1} \ ,$$

and its momentum is identically:

$$1 \times (v_1 - v_\mathrm{m}) = v_1 \frac{A}{A+1} \ .$$

The target also has a relative velocity, which is simply $-v_\mathrm{m}$ and a momentum of:

$$-v_\mathrm{m} A = -v_1 \frac{A}{1+A} \ .$$

Hence the total momentum of the system is zero. The kinetic energy of the system is:

$$\mathrm{KE}_\mathrm{CoM} = \frac{1}{2} (v_1 - v_\mathrm{m})^2 + \frac{1}{2} A v_\mathrm{m}^2 = \frac{1}{2} v_1^2 \frac{A}{A+1} \ .$$

We must conserve both energy and momentum in the collision. This will allow us to relate the outgoing velocities to the incoming velocities. Our KE balance is:

$$\frac{1}{2}v_1^2\frac{A}{A+1} = \frac{1}{2}v_\mathrm{a}^2 + \frac{1}{2}Av_\mathrm{b}^2 \; .$$

Given that the total momentum is zero, the momentum balance reduces to:

$$v_\mathrm{a} = v_\mathrm{b}A \; .$$

Solving for the outgoing velocities we get:

$$v_\mathrm{a} = \frac{Av_1}{A+1} \; ,$$
$$v_\mathrm{b} = \frac{v_1}{A+1} \; .$$

But now we need to get back to the lab system in order to work out the neutron energy loss. The two systems move relative to each other with a velocity v_m such that:

$$\vec{v}_2 = \vec{v}_\mathrm{a} + \vec{v}_\mathrm{m} \; .$$

This is illustrated in the diagram in Fig. 3.

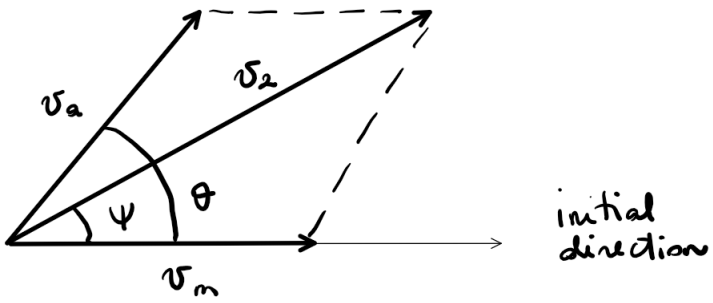


Figure 3: Geometry of the outgoing collision system.

Given the geometry of the problem (or vector addition or the law of cosines where $c^2 = a^2+b^2+2ab\cos\theta$), we can relate the magnitudes of the incoming and outgoing velocities as:

$$v_2^2 = v_1^2\frac{A^2 + 2A\cos\theta + 1}{(A+1)^2}$$

We can rewrite the speed relation in terms of the ratio of energies by dividing by v_1^2:

$$\frac{v_2^2}{v_1^2} = \frac{E_2}{E_1} = \frac{A^2 + 2A\cos\theta + 1}{(A+1)^2} \; .$$

It is common to define a new variable here:

$$\alpha \equiv \left(\frac{A-1}{A+1}\right)^2 \; ,$$

where $\alpha(\mathrm{hydrogen}) = 0$ and $\alpha(M_\mathrm{target} \to \infty) = 1$. This lets us rewrite the energy ratio as:

$$\frac{E_2}{E_1} = \frac{(1+\alpha) + (1-\alpha)\cos\theta}{2} \tag{5}$$

This tells us that our minimum energy loss (or maximum E_2/E_1) must occur when $\theta = 0$ or $\cos\theta = 1$:

$$\max \frac{E_2}{E_1} = \frac{(1+\alpha)+(1-\alpha)}{2} = 1 \, .$$

Conversely, our maximum energy loss occurs if $\theta = \pi$ (a head-on collision and 180° deflection):

$$\min \frac{E_2}{E_1} = \frac{(1+\alpha)-(1-\alpha)}{2} = \frac{2\alpha}{2} = \alpha \, .$$

If our target were hydrogen, $\alpha = 0$, i.e., all energy can be lost in a direct collision.

From the same trigonometry as before, we can obtain the cosine of ψ:

$$\cos\psi = \frac{A\cos\theta + 1}{\sqrt{A^2 + 1 + 2A\cos\theta}} \, .$$

This implies that:

$$\lim_{A\to\infty} \cos\psi = \cos\theta \, ,$$

i.e., (elastic) scattering becomes more isotropic for heavier nuclei.

Note that an angular element over the unit sphere is given as $\mathrm{d}\Omega = \sin\theta \mathrm{d}\theta\mathrm{d}\varphi$, where θ is a polar angle and φ is an azimuthal angle. This would be integrated from $\varphi = 0, 2\pi$ and $\theta = 0, \pi$ to give the surface area of the unit sphere, 4π radians. If we assert (from observing physics) that outgoing collision directions tend to depend only on the cosine between the incoming and outgoing direction, we can define the collision angular co-ordinate system such that the cosine is over θ and therefore scattering is independent of the azimuthal angle (or equi-probable). This reduces our angular element to $\mathrm{d}\Omega = 2\pi\sin\theta\mathrm{d}\theta$. This is visualised in Fig. 4.

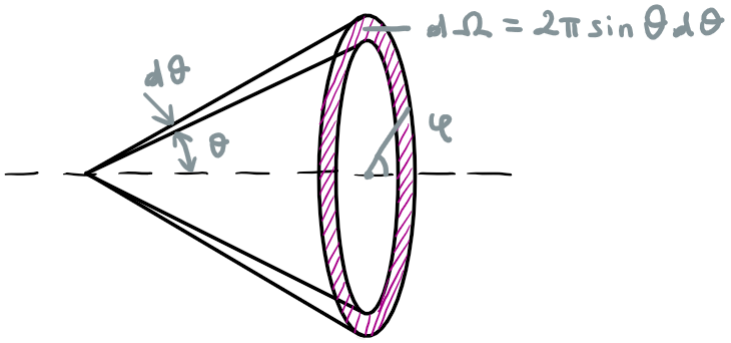


Figure 4: Differential angular element for the scattering system with azimuthal symmetry.

Given the definition of the differential angular element and s-wave isotropy, the average scattering cosine in the CoM system is 0. For the lab system, this is:

$$\overline{\cos\psi} = \frac{\int_0^\pi \mathrm{d}\theta \ \sin\theta\cos\psi}{\int_0^\pi \mathrm{d}\theta \sin\theta} = \frac{2}{3A} \, .$$

Once again we can see that $\lim_{A\to\infty} \overline{\cos\psi} = 0$.

Now we can calculate probabilities of scattering from one angle and energy to another angle and energy. Due to isotropy in CoM for s-wave scattering, the probability of scattering to an angle $\mathrm{d}\theta$ about θ is simply:

$$P(\theta)\mathrm{d}\theta = \frac{\mathrm{d}\Omega}{4\pi} = \frac{2\pi\sin\theta\mathrm{d}\theta}{4\pi} = \frac{1}{2}\sin\theta\mathrm{d}\theta \, .$$

From Eq. (5), we also know that θ maps directly to a value of E_2, i.e., $E_2 = f(\theta)$, and so we can construct a relationship between the probability density functions (PDFs) of θ and E_2. This relationship will be of the form (given that probability in a differential area must be the same under a change of variables):

$$|P(E_2)\mathrm{d}E_2| = |P(\theta)\mathrm{d}\theta| \, .$$

As standard PDFs must be everywhere positive, this implies that:

$$P(E_2) = P(\theta) \left| \frac{\mathrm{d}\theta}{\mathrm{d}E_2} \right| \ . \tag{6}$$

If we differentiate Eq. (5) with respect to θ we get:

$$\mathrm{d}E_2 = \frac{1-\alpha}{2} E_1 \ \mathrm{d}\left(\cos\theta\right) = -\frac{1-\alpha}{2} E_1 \sin\theta \mathrm{d}\theta \ ,$$

giving:

$$\frac{\mathrm{d}\theta}{\mathrm{d}E_2} = -\frac{2}{(1-\alpha)E_1 \sin\theta} \ .$$

Inserting this relationship into Eq. (6) gives:

$$P(E_2) = \frac{1}{2}\sin\theta \times \frac{2}{(1-\alpha)E_1\sin\theta} = \frac{1}{(1-\alpha)E_1} \ . \tag{7}$$

With this, we can finalise the construction of a PDF for our outgoing energy. The resulting outgoing energy must be between E_1 and αE_1 (from Eq. (5)) and the probability of a given energy is uniform over this range (from Eq. (7), there is no dependence on the outgoing energy). Hence, our probability of scattering from E_1 to some E_2 is:

$$P(E_1 \rightarrow E_2)\mathrm{d}E_2 = \begin{cases} \frac{\mathrm{d}E_2}{E_1(1-\alpha)} \ ; \ E_2 \in [\alpha E_1, E_1] \\ 0 \ ; \ \text{otherwise} \end{cases} \ .$$

This is illustrated in Fig. 5. This is an extremely useful result. Note, that this is only true for elastic scattering in light nuclei and for heavier nuclei there will tend to be other angular dependencies from other scattering channels creeping in. In LWRs, however, water is dominant in the physics and this distribution describes the interaction of neutrons and hydrogen very well.

Finally, we can calculate our average energy loss per collision as:

$$\overline{\Delta E} = E_1 - \overline{E_2} = E_1 - \int_{\alpha E_1}^{E_1} \frac{E_2 \mathrm{d}E_2}{E_1(1-\alpha)} = \frac{1-\alpha}{2} E_1 \ .$$

On average, neutrons will lose half their energy on collision with hydrogen.

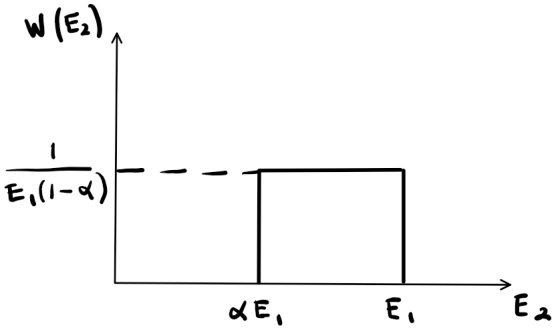


Figure 5: Probability density function for the outgoing neutron energy from elastic collisions.

2.1 Lethargy

We do not have to work explicitly in terms of neutron energy – other quantities can be useful in doing the maths too. Often we use the neutron lethargy, defined as:

$$u = \ln \frac{E_0}{E} \ ,$$

where u is lethargy, E is the corresponding neutron energy, and E_0 is some reference neutron energy which should be larger than E. Rather than speaking in terms of energy loss per collision, we can speak in terms of lethargy gain per collision. To do this, we need to relate changes in energy to changes in lethargy, the same as we did for angles. This would give:

$$|P(u_1 \to u_2)\mathrm{d}u_2| = |P(E_1 \to E_2)\mathrm{d}E_2| \ ,$$

or

$$P(u_1 \to u_2) = P(E_1 \to E_2) \left| \frac{\mathrm{d}E_2}{\mathrm{d}u_2} \right| \ .$$

Given the definition of lethargy, this is very easy to construct:

$$u = \ln \frac{E_0}{E} \to E = E_0 e^{-u} \ ,$$

and so

$$\mathrm{d}u = -\frac{\mathrm{d}E}{E} \to \mathrm{d}E = -E \ \mathrm{d}u \ .$$

Hence our probability density function is:

$$P(u_1 \to u_2) = E_2 P(E_1 \to E_2) = \frac{E_2}{E_1(1-\alpha)} \ ,$$

or

$$P(u_1 \to u_2)\mathrm{d}u_2 = \begin{cases} \frac{e^{u_1-u_2}}{1-\alpha}\mathrm{d}u_2 \ ; \ u_2 \in [u_1, u_1 + \ln(1/\alpha)] \\ 0 \ ; \ \text{otherwise} \end{cases} \ .$$

Here $\ln(1/\alpha)$ is the maximum lethargy a particle can gain in a collision. Arguably, this may appear to just complicate things, but the value of lethargy becomes more apparent when we start having to integrate many things in energy which look like $\mathrm{d}E/E = -\mathrm{d}u$.

One important lethargy quantity which we will see is the average lethargy gain per collision. This is defined as:

$$\xi = \int_{\alpha E'}^{E'} \mathrm{d}E \ln\left(\frac{E'}{E}\right) P(E' \to E) = 1 + \frac{\alpha}{1-\alpha} \ln \alpha \ .$$

Note, lethargy becomes a bit more painful to work with when dealing with hydrogen and $\alpha = 0$.

3 Neutron slowing down

We want to understand the energy spectrum of neutrons slowing down. We will start by assuming there is only hydrogen around, then we will add in other materials, and finally include heterogeneity in the system. By the end, we should have a pretty good estimate of the neutron spectrum in an LWR geometry.

First, let's define some of the familiar variables in nuclear engineering.

- The scalar flux, $\phi(\mathbf{r}, E)$ (where $\mathbf{r}$ is the position and E is the energy), the total track length of neutrons per unit volume or the neutron density times speed $\phi = n \times v$. It has units of neutrons $\mathrm{cm}^{-2}\mathrm{eV}^{-1}\mathrm{s}^{-1}$.
- Macroscopic cross sections, $\Sigma_x(\mathbf{r}, E)$, for some reaction type x. These are the probability per unit path length that a neutron will undergo some reaction. They have units of cm^{-1}. The common reaction types are fission (f), scattering (s), capture (c), absorption (a = f + c), and total (t = a + s). The total cross section is sometimes denoted as simply Σ.
- Microscopic cross sections, $\sigma_x(E)$. These are the target size that a given nucleus presents to a neutron for a given reaction type, with units of cm^2. Multiplying by the local density of its corresponding nuclide will give that nuclide's macroscopic cross section, $\Sigma_x = \sigma_x \times N$.

With these, we can define other quantities. Reaction rates $[\mathrm{s}^{-1}]$ in a given volume and energy range are defined as:

$$R_x = \int_V \mathrm{d}V \int_{E_2}^{E_1} \mathrm{d}E\, \Sigma_x(E)\phi \,.$$

For the purposes of our present analysis, we will use reaction rate **densities**, i.e., not integrated over any part of phase space. For example, the collision rate density (or just the collision density) [collisions cm^{-3} s^{-1} eV^{-1}] is given as:

$$F(\mathbf{r}, E) = \Sigma_\mathrm{t}(\mathbf{r}, E)\phi(\mathbf{r}, E) \,.$$

With this we can start analysing slowing down from a simple case and then build up complexity.

3.1 Case 1: slowing down on hydrogen

Assumptions:

- There is **no absorption**, $\Sigma_\mathrm{a} = 0$.
- **Infinite medium**, no leakage.
- **Homogeneous medium**, no dependence of variables on $\mathbf{r}$ (or $\mathbf{\Omega}$).
- **Homogeneously distributed source** $S(E)$ [neutrons cm^{-3} s^{-1} eV^{-1}].
- **Elastic scattering on hydrogen** only and $P(E_1 \to E_2) = 1/E_1$ ($\alpha = 0$). This also implies no up-scattering.

Some of these assumptions aren't too bad. For example, in hydrogen, the ratio of the absorption cross section to the scattering is about 0.014. However, there are usually more materials nearby which do indeed absorb neutrons.

If we plug all of these assumptions into the transport equation (or just compare our reaction rates) we would end up with:

$$\Sigma_\mathrm{s}(E)\phi(E) = \int_E^\infty \mathrm{d}E'\, \Sigma_\mathrm{s}(E' \to E)\phi(E') + S(E) \,. \tag{8}$$

Our differential scattering cross section can be divided into its cross section component, $\Sigma_\mathrm{s}(E')$ and its scattering distribution component, $P(E' \to E)$. From kinematics we had that

$$P(E' \to E)\mathrm{d}E = \frac{\mathrm{d}E}{E'(1-\alpha)} \,,$$

so our slowing down equation becomes:

$$\Sigma_{\mathrm{s}}(E)\phi(E) = \int_E^\infty \mathrm{d}E' \, \frac{\Sigma_{\mathrm{s}}(E')\phi(E')}{E'} + S(E) \, .$$

We can also think about this distribution as the probability that a neutron born at E' will scatter into some interval $\mathrm{d}E$ between E' and $\alpha E'$, shown in Fig. 6. Due to the uniform probability distribution, the probability that a neutron will scatter into a given $\mathrm{d}E$ about E within the range $\alpha E'$ to E' can be thought of as the ratio of these two areas:

$$P(E' \to E)\mathrm{d}E = \frac{A}{B} = \frac{\mathrm{d}E}{E' - \alpha E'} \, .$$

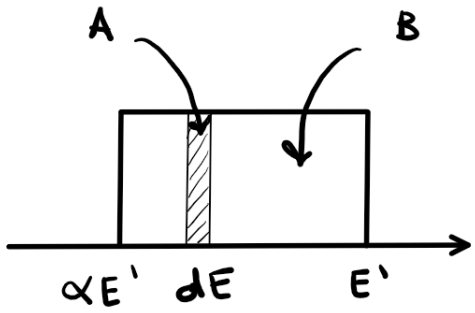


Figure 6: Probability that a neutron scatters into a given energy interval.

Next, we will assert that our neutron source is **monoenergetic**, i.e., $S(E) = S_0\delta(E - E_0)$, where $\delta(...)$ is the Dirac delta distribution and E_0 is the source energy. We will also introduce the **collision rate density** $F(E) = \Sigma_{\mathrm{s}}(E)\phi(E)$ to make things more compact. Thus the slowing down equation becomes:

$$F(E) = \int_E^{E_0} \mathrm{d}E' \, \frac{F(E')}{E'} + S_0\delta(E - E_0) \, , \tag{9}$$

where the upper bound of neutron energy is now E_0, because neutrons cannot reach higher energies than the source.

The following is hand-wavy, but it's the only way I know how to solve this without resorting to integral equation theory – what we will do is essentially rewrite Eq. (9) to remove neutrons that haven't collided and get rid of the delta source. Let's consider the balance of neutrons that make it into some energy interval $\mathrm{d}E$ about energy E. These can have come from two sources:

- **Source neutrons that have undergone one collision**. These neutrons are born at energy E_0 at a rate of S_0 and then scatter once. Since $P(E_0 \to E)\mathrm{d}E = \mathrm{d}E/E_0$, we have this source as:

$$\text{Contribution from first-collided neutrons} = \frac{S_0 \, \mathrm{d}E}{E_0}$$

- **Source neutrons that have undergone more than one collision**. The source of neutrons is $F(E')\mathrm{d}E'$ for $E' > E$. The number of these neutrons undergoing collisions in an interval $\mathrm{d}E'$ about E' and slowing down to E is:

$$\text{Contribution from previously collided neutrons} = \frac{F(E')\mathrm{d}E' \, \mathrm{d}E}{E'} \, .$$

  This squared differential expression represents neutrons in the differential width $\mathrm{d}E'$ about E' scattering into the differential width $\mathrm{d}E$ about E.

Hence, our balance in the interval $\mathrm{d}E$ about E becomes:

$$F(E)\mathrm{d}E = \frac{S_0\,\mathrm{d}E}{E_0} + \int_E^{E_0} \frac{F(E')\mathrm{d}E'\,\mathrm{d}E}{E'} \,,$$

or

$$F(E) = \frac{S_0}{E_0} + \int_E^{E_0} \frac{F(E')\mathrm{d}E'}{E'} \,. \tag{10}$$

Differentiating both sides gives:

$$\frac{\mathrm{d}F(E)}{\mathrm{d}E} = -\frac{F(E)}{E} \,,$$

which has the solution:

$$F(E) = \frac{C}{E} \,,$$

for some constant C. Inserting this solution into the governing equation at $E = E_0$ gives:

$$\frac{C}{E_0} = \frac{S_0}{E_0} + \underbrace{\int_{E_0}^{E_0} \frac{F(E')}{E'}\,dE'}_{=0} = \frac{S_0}{E_0} \,,$$

so $C = S_0$ and hence:

$$F(E) = \frac{S_0}{E} \,,$$

$$\phi(E) = \frac{S_0}{\Sigma_\mathrm{s}(E)E} \,. \tag{11}$$

We can also write this in terms of lethargy. Noting that $u = \ln(E_0/E)$, $\mathrm{d}u = -\mathrm{d}E/E$, and that $|F(u)\mathrm{d}u| = |F(E)\mathrm{d}E|$ we would get:

$$F(u) = F(E)\left|\frac{\mathrm{d}E}{\mathrm{d}u}\right| = EF(E) \,,$$

or

$$\phi(u) = \phi(E)E = \frac{S_0}{\Sigma_\mathrm{s}(u)} \,.$$

This is why when producing an energy-integrated or multi-group flux (either by deterministic methods or Monte Carlo) the spectrum will tend to be approximately flat in the resonance region.

If we were to be more thorough, we would also obtain an additional $S_0\delta(E - E_0)$ term, i.e., the flux spectrum is strongly influenced by the source close to source energies. However, far from the source, Eq. (11) holds and is known as the **Fermi spectrum** or the **asymptotic spectrum**.

This might appear an unfriendly equation still due to the dependence upon $\Sigma_\mathrm{s}(E)$. However, in hydrogen, the scattering cross section is a relatively weak function of energy across a large energy range of interest. This is because the cross section is dominated by 'potential scattering', i.e., elastic scattering where the cross section corresponds to an effective nuclear radius of the nucleus in question – which should be constant. The cross section of hydrogen is shown in Fig. 7, where the potential scattering's dominance can be seen in the wide range over which the cross section is roughly constant.

Assuming this constant cross section, this implies the spectrum should look like $\phi(E) \propto 1/E$. This is a remarkably good approximation in reactors far (in energy) from neutron sources. By way of proof, I present in Fig. 8 a spectrum produced by a Monte Carlo code, SCONE, with a source of neutrons at 2 MeV, slowing down in water, as well as the $1/E$ line. For a quite large energy range there appears to be considerable agreement!

But, naturally, the better we approximate the spectrum, the more accurate our final cross sections will be and there are many effects yet to be considered. Cynics might also suggest that you can hide an elephant inside a log-log plot!

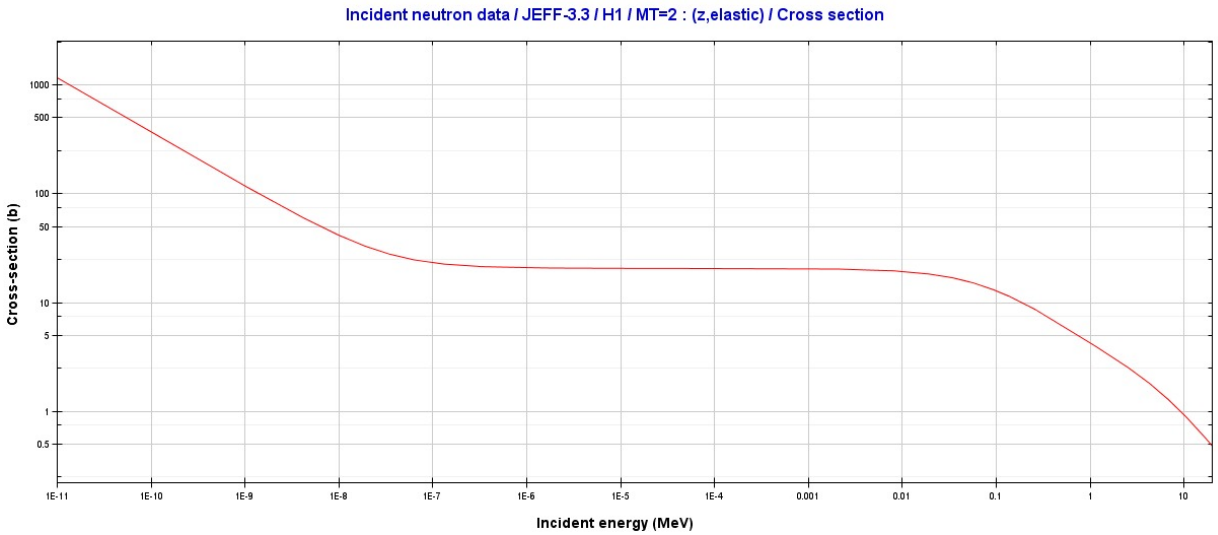


Figure 7: The hydrogen microscopic cross section.

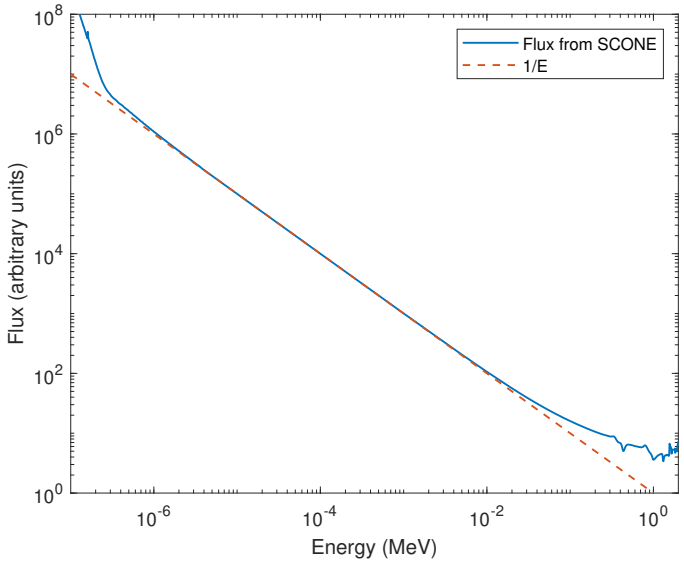


Figure 8: The spectrum produced by a Monte Carlo code compared to the asymptotic spectrum.

Before proceeding, it's useful to investigate the **neutron slowing down density**, $q(E)$. This is the rate at which neutrons slow down below energy E. Formally, this can be calculated as:

$$q(E) = \int_E^{E_0} \left[\int_0^E \mathrm{d}E'' \, \Sigma_\mathrm{s}(E' \to E'')\phi(E') \right] \mathrm{d}E' \, .$$

Less formally, we can calculate this as the total number of neutrons from the source which slow down below E plus the neutrons between E and E_0 which then collide to end up below E. This can be aided by looking at the probability distribution of collided neutrons, shown in Fig. 9. For a given neutron at some energy $E' > E$, the probability of slowing down below E must be:

$$P(\text{of slowing down below } E) = \frac{\text{reachable energies } < E}{\text{energies } \leq E'} \, .$$

Because, on scattering in hydrogen, the reachable energies from any starting energy are a uniform distribution below that energy, this probability is simply the geometric ratio of areas:

$$P(\text{of slowing down below } E) = \frac{\text{reachable energies } < E}{\text{energies } \leq E'} = \frac{E-0}{E'-0} = \frac{E}{E'} \, .$$

Hence, for neutrons freshly born from the source, the slowing down density contribution is:

$$S_0 \times P = S_0 \times \frac{E}{E_0} \, ,$$

while for previously scattered neutrons it is:

$$\int_E^{E_0} \mathrm{d}E' F(E') \times \frac{E}{E'} \, ,$$

giving:

$$q(E) = \frac{S_0 E}{E_0} + E \int_E^{E_0} \mathrm{d}E' \frac{F(E')}{E'} \, .$$

Using Eq. (10), this turns into:

$$q(E) = EF(E) \, ,$$

and using the definition of $F(E) = S_0/E$ we finally get:

$$q(E) = S_0 \, .$$

What this tells us is that at any energy E **there is no accumulation or loss of neutrons**: all neutrons that are born continually slow down. Obviously this is not entirely physical: in reality things like absorption and up-scattering will start to bite!

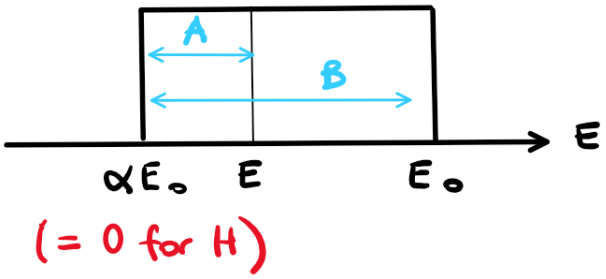


Figure 9: Illustration of the probability of slowing down below energy E.

3.2 Case 2: slowing down on moderator with $A > 1$

If we take the most straightforward next step, things immediately become a bit more complicated. If $A > 1$, $\alpha \neq 0$, so a neutron cannot lose all of its energy in a single collision. If we have our neutron source with strength S_0 producing neutrons at energy E_0, then the lowest energy a neutron can reach after one collision is αE_0. After two collisions, the minimum energy is $\alpha^2 E_0$, and so on for n collisions where the energy would be $\alpha^n E_0$. We are going to define and work with the collision density for neutrons which have undergone n collisions, $F_n(E)$. Our logic will be helped by the diagram in Fig. 10.

We will do this by once again splitting the collision density into its components and we can recover the collision density as $F(E) = \sum_{n=1}^{\infty} F_n(E)$.

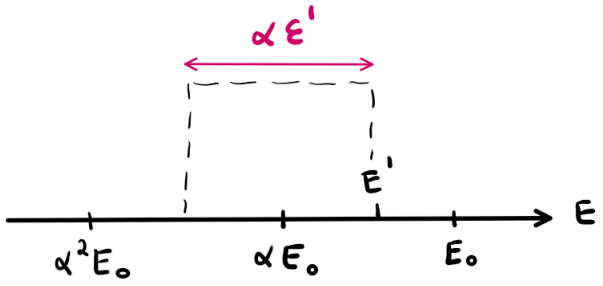


Figure 10: Illustration of the intervals into which a neutron can slow down into given a number of scattering events.

- **Neutrons having undergone 1 collision.** These neutrons will be born with energy E_0 and will scatter according to the usual scattering law, but with a different lower energy bound. Hence we would get (multiplying $S_0\delta(E - E_0)$ by $P(E_0 \to E)$ and integrating):

$$F_1(E) = \begin{cases} \frac{S_0}{E_0(1-\alpha)} \; ; \; \alpha E_0 < E < E_0 \\ 0 \; ; \; E < \alpha E_0 \end{cases} .$$

  This function is obviously discontinuous about αE_0 and E_0.

- **Neutrons having undergone 2 collisions.** These are the neutrons which result from the collision of neutrons produced by $F_1(E)$. They have two possibilities in their lives: scatter and remain in the energy range $\alpha E_0 < E < E_0$ or scatter into the next energy range down, $\alpha^2 E_0 < E < \alpha E_0$. **Neutrons that remain in the same energy range** can scatter anywhere from E_0 down to the energy of interest $E(> \alpha E_0)$:

$$F_2(E) = \int_E^{E_0} \frac{F_1(E')\mathrm{d}E'}{E'(1-\alpha)} = \frac{S_0}{E_0(1-\alpha)^2} \int_E^{E_0} \frac{\mathrm{d}E'}{E'} = \frac{S_0}{E_0(1-\alpha)^2} \ln\left(\frac{E_0}{E}\right) \; ; \; \alpha E_0 < E < E_0 \; .$$

  Neutrons that scatter into the lower range $\alpha^2 E_0 < E < \alpha E_0$ must have a maximum energy of $E' = E/\alpha$. However, from $F_1(E)$, they cannot have an energy lower than αE_0. Therefore, we obtain an integral like:

$$F_2(E) = \int_{\alpha E_0}^{E/\alpha} \frac{F_1(E')\mathrm{d}E'}{E'(1-\alpha)} = \frac{S_0}{E_0(1-\alpha)^2} \int_{\alpha E_0}^{E/\alpha} \frac{\mathrm{d}E'}{E'} = \frac{S_0}{E_0(1-\alpha)^2} \ln\left(\frac{E}{\alpha^2 E_0}\right) \; ; \; \alpha^2 E_0 < E < \alpha E_0 \; .$$

  Below $\alpha^2 E_0$, no neutrons can go after only two scatters. So $F_2(E) = 0$ for $E < \alpha^2 E_0$. Therefore, $F_2(E)$ is:

$$F_2(E) = \begin{cases} \frac{S_0}{E_0(1-\alpha)^2} \ln\left(\frac{E_0}{E}\right) \; ; \; \alpha E_0 < E < E_0 \\ \frac{S_0}{E_0(1-\alpha)^2} \ln\left(\frac{E}{\alpha^2 E_0}\right) \; ; \; \alpha^2 E_0 < E < \alpha E_0 \\ 0 \; ; \; E < \alpha^2 E_0 \end{cases} .$$

  While the function is now continuous at all points, it now has a discontinuous derivative at $E = \alpha E_0$.

- As you can imagine, the general expressions for collision densities become even more complicated for $n > 2$ collisions...

Fortunately, not only does $F_n(E)$ become more smooth as $n \to \infty$, but, far from the source, $F(E)$ once again obtains a $1/E$ shape! Solving a fixed source graphite problem in SCONE, the first few of these collision densities (or Placzek distributions) are shown in Fig. 11. The usual approximation is to say for $E < \alpha^3 E_0$ we can solve the following equation by asserting that the source has little influence:

$$F(E) \approx \int_E^{E/\alpha} \frac{F(E')\mathrm{d}E'}{E'(1-\alpha)} .$$

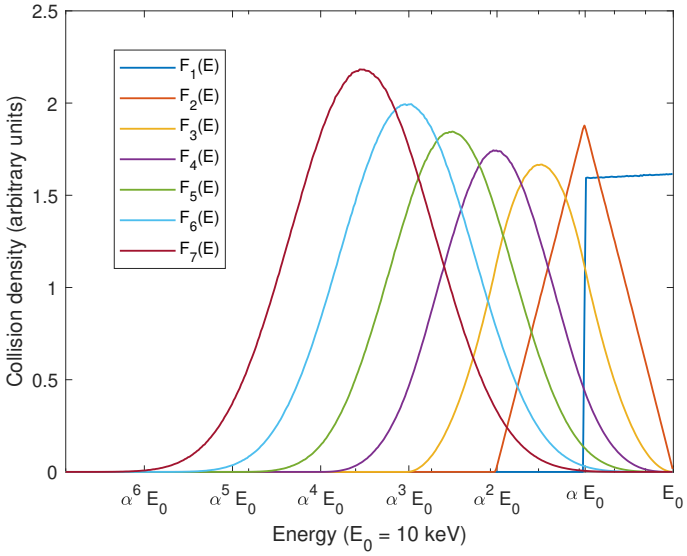


Figure 11: The first few collision densities produced from a 10 keV fixed neutron source in graphite (the tilt in F_1 is due to some scattering anisotropy).

It is easy to show that $F(E) = C/E$ is a solution by plugging it in – it is much harder to show that it is the only solution! Finding the constant, C, takes a little bit of work. One way to do this is to use our previous knowledge that, in a non-absorbing problem, $q(E) = S_0$; we then need to find what $q(E)$ is for $\alpha \neq 0$. We do this in a similar manner as before by phrasing the problem in terms of slowing down from one energy and reaching another:

$$P\,(\text{slow down below } E) = \frac{E - \alpha E'}{E' - \alpha E'} = \frac{A}{B}\,.$$

This is illustrated in Fig. 12.

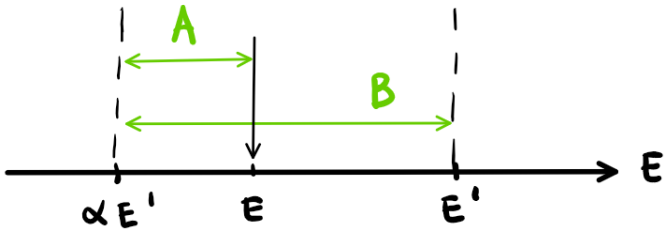


Figure 12: Illustration of the probability of slowing down below energy E given limits on maximum energy loss.

From before, our definition of $q(E)$ is:

$$q(E) = \int_E^{E/\alpha} \mathrm{d}E' F(E') P(\text{slow down below } E) = \int_E^{E/\alpha} \mathrm{d}E' \frac{C}{E'} \frac{E - \alpha E'}{E' - \alpha E'} = C\left(1 + \frac{\alpha}{1-\alpha} \ln \alpha\right) = C\xi = S_0\,.$$

Here we remember ξ as the average lethargy gain per collision. Hence:

$$F(E) = \frac{S_0}{\xi E}\,;\, \phi(E) = \frac{S_0}{\xi \Sigma_s E}\,.$$

Hence, once again, the Fermi spectrum holds.

3.3 Case 3: Non-monenergetic source

Sources in nuclear reactors are not monoenergetic and this will affect the validity of the equations we obtain, but thankfully not too much.

Recall that the equations we have from before,

$$\phi(E) = \frac{S_0}{\Sigma_\mathrm{s} E} \text{ for } A = 1 \,,$$

and

$$\phi(E) = \frac{S_0}{\xi \Sigma_\mathrm{s} E} \text{ for } A > 1 \,,$$

are the solutions for the slowing down source $S_0\delta(E - E_0)$ – otherwise known as Green's functions. This means that the generalisation is simply to integrate over whatever source distribution we have, $S(E)$, giving:

$$\phi(E) = \frac{1}{\Sigma_\mathrm{s} E} \int_{E_\mathrm{cut}}^{\infty} \mathrm{d}E' \; S(E') \text{ for } A = 1 \,,$$

and

$$\phi(E) = \frac{1}{\xi \Sigma_\mathrm{s} E} \int_{E_\mathrm{cut}}^{\infty} \mathrm{d}E' \; S(E') \text{ for } A > 1 \,.$$

Usually we do not integrate between 0 and ∞, but rather from some lower bound, E_cut. This is often taken to be about 50 keV. Below this value only about 1% of fission neutrons are produced and we would expect the asymptotic spectrum to be reached due to the weak source.

3.4 Case 4: Slowing down in a mixture of nuclides

Let's denote a given nuclide with index i such that we can define:

$$F^{(i)}(E) \text{: collision density on nuclide } i$$

$$\Sigma_\mathrm{s}^{(i)}(E) \text{: scattering cross section of nuclide } i$$

This lets us write:

$$F^{(i)}(E) = \Sigma_\mathrm{s}^{(i)} \phi(E) \times \frac{\Sigma_\mathrm{s}(E)}{\Sigma_\mathrm{s}(E)} = \frac{\Sigma_\mathrm{s}^{(i)}(E)}{\Sigma_\mathrm{s}(E)} \times F(E) \,.$$

We also have that the equation for $F(E)$ is simply:

$$F(E) = \sum_i \int_E^{E/\alpha_i} \frac{\mathrm{d}E' F^{(i)}(E')}{E'(1 - \alpha_i)} \,.$$

We will look for solutions of the form $F^{(i)}(E) = C_i/E$ – this should satisfy the previous equation, but it does not tell us the value of C_i. Lacking absorption, we still have that $q(E) = S$ where $S = S_0$ for a point energy source or $S = \int \mathrm{d}E S(E)$ for a spectrum. The expression for $q(E)$ is:

$$\begin{aligned} q(E) = \sum_i \int_E^{E/\alpha_i} F^{(i)}(E) \times \frac{E - \alpha_i E'}{E' - \alpha_i E'} \mathrm{d}E' &= \sum_i \int_E^{E/\alpha_i} \frac{C_i}{E} \times \frac{E - \alpha_i E'}{E' - \alpha_i E'} \mathrm{d}E' \\ &= \sum_i C_i \left(1 + \frac{\alpha_i}{1 - \alpha_i} \ln \alpha_i \right) = \sum_i C_i \xi_i = S \,. \end{aligned}$$

We also have another expression for C_i, which we can insert, namely $C_i = F^{(i)} E$:

$$S = \sum_i C_i \xi_i = E \sum_i F^{(i)} \xi_i = E F(E) \sum_i \frac{\Sigma_\mathrm{s}^{(i)}(E)}{\Sigma_\mathrm{s}(E)} \xi_i \,.$$

If we define

$$\bar{\xi}(E) = \frac{\sum_i \xi_i \Sigma_{\mathrm{s}}^{(i)}(E)}{\Sigma_{\mathrm{s}}(E)} \ ,$$

then:

$$S = EF(E)\bar{\xi}(E) \ ,$$

$$F(E) = \frac{S}{\bar{\xi}(E)E} \ ; \ \phi(E) = \frac{S}{\bar{\xi}(E)\Sigma_{\mathrm{s}}(E)E} \ .$$

3.5 Case 5: Slowing down with absorption

We'll revert back to a point energy source, $S_0\delta(E - E_0)$, where E_0 is above the resonance region such that there is no absorption on first collision. Suppose we have a mix of purely scattering hydrogen and heavy absorber with $A \to \infty$ (so we can drop α from our scattering energy distributions).

The balance of neutrons becomes:

$$F(E)\mathrm{d}E = \text{neutrons arriving in } \mathrm{d}E \text{ after 1 collision} + \text{neutrons arriving into } \mathrm{d}E \text{ after } > 1 \text{ collision} \ .$$

From before, the first term is going to be simply:

$$\text{Neutrons arriving into } \mathrm{d}E \text{ after 1 collision} = S_0 \frac{\mathrm{d}E}{E_0} \ ,$$

while the second term will be produced from $F(E')\mathrm{d}E'$ which then **survive the collision** and **get scattered to** E. The probability of surviving a collision is given by:

$$\frac{\Sigma_{\mathrm{s}}(E)}{\Sigma_{\mathrm{t}}(E)} = \frac{\Sigma_{\mathrm{s}}(E)}{\Sigma_{\mathrm{s}}(E) + \Sigma_{\mathrm{a}}(E)} \ ,$$

while getting redistributed to E is the usual $\mathrm{d}E/E'$. Hence:

$$\text{Neutrons arriving into } \mathrm{d}E \text{ after } > 1 \text{ collision} = \int_E^{E_0} F(E') \frac{\Sigma_{\mathrm{s}}(E')}{\Sigma_{\mathrm{s}}(E') + \Sigma_{\mathrm{a}}(E')} \frac{\mathrm{d}E'}{E'} \mathrm{d}E \ .$$

Hence, the equation for the collision density is:

$$F(E) = \frac{S_0}{E_0} + \int_E^{E_0} F(E') \frac{\Sigma_{\mathrm{s}}(E')}{\Sigma_{\mathrm{s}}(E') + \Sigma_{\mathrm{a}}(E')} \frac{\mathrm{d}E'}{E'} \ . \tag{12}$$

As before, we will differentiate to get:

$$\frac{\mathrm{d}F(E)}{\mathrm{d}E} = -\frac{F(E)}{E} \frac{\Sigma_{\mathrm{s}}(E)}{\Sigma_{\mathrm{s}}(E) + \Sigma_{\mathrm{a}}(E)} \ .$$

Using the balance of probabilities, we can convert the scatter probability into $1-$ absorption probability:

$$\frac{\Sigma_{\mathrm{s}}(E)}{\Sigma_{\mathrm{s}}(E) + \Sigma_{\mathrm{a}}(E)} = 1 - \frac{\Sigma_{\mathrm{a}}(E)}{\Sigma_{\mathrm{s}}(E) + \Sigma_{\mathrm{a}}(E)} \ .$$

This allows us to rewrite the collision density differential equation to give:

$$\frac{\mathrm{d}F(E)}{F(E)} = -\frac{\mathrm{d}E}{E} + \frac{\Sigma_{\mathrm{a}}(E)}{\Sigma_{\mathrm{s}}(E) + \Sigma_{\mathrm{a}}(E)} \frac{\mathrm{d}E}{E} \ ,$$

giving, when integrating from E to E_0:

$$\ln\left(\frac{F(E_0)}{F(E)}\right) = -\ln\frac{E_0}{E} + \int_E^{E_0} \frac{\Sigma_{\mathrm{a}}(E')}{\Sigma_{\mathrm{s}}(E') + \Sigma_{\mathrm{a}}(E')} \frac{\mathrm{d}E'}{E'},$$

and:

$$F(E) = \frac{F(E_0)E_0}{E} \exp\left(- \int_E^{E_0} \frac{\Sigma_\mathrm{a}(E')}{\Sigma_\mathrm{s}(E') + \Sigma_\mathrm{a}(E')} \frac{\mathrm{d}E'}{E'} \right) .$$

This means that $q(E)$ is no longer uniform across energy because $q(E) = F(E)E \neq F(E_0)E_0$. This is because of absorption. The expression for $q(E)$ in this case is:

$$q(E) = \frac{S_0 E}{E_0} + E \int_E^{E_0} \frac{\Sigma_\mathrm{s}(E')}{\Sigma_\mathrm{s}(E') + \Sigma_\mathrm{a}(E')} \frac{F(E')\mathrm{d}E'}{E'} .$$

Note that from this we can equate $F(E_0)E_0 = S_0$ with the integral reducing to 0. Also recall $q(E)$ is the number of neutrons that survived slowing down to energy E. Hence we can speak of a probability of not being absorbed:

$$p(E) = \frac{q(E)}{S} = \exp\left(- \int_E^{E_0} \frac{\Sigma_\mathrm{a}(E')}{\Sigma_\mathrm{s}(E') + \Sigma_\mathrm{a}(E')} \frac{\mathrm{d}E'}{E'} \right) . \tag{13}$$

This is the **resonance escape probability**. To say anything more useful, we need to understand something about how $\Sigma_\mathrm{a}(E)$ and $\Sigma_\mathrm{s}(E)$ look, in particular with respect to resonant behaviour.

4 Resonances

To describe the complicated behaviour of cross sections, we must use some model for their behaviour. The classical model is the **Single Level Breit-Wigner** (SLBW) formalism. This is sufficient for our purposes, but has now been largely superseded by the Multi Level Breit-Wigner or Reich-Moore (pronounced Rich-More) formalism in practical applications.

We will begin by making some definitions. Resonances can be characterised by their location in energy, E_0, the peak value for the total cross section, σ_0, and their 'channel width', Γ, or the energy interval it spans between the two points at half the maximum values (otherwise known as the Full Width at Half Maximum, FWHM). The main components of a SLBW resonance are illustrated in Fig. 13.

For the (n,γ) reaction, SLBW gives:

$$\sigma_\gamma(E_{\rm CM}) = \sigma_0 \frac{\Gamma_\gamma}{\Gamma} \left(\frac{E_0}{E_{\rm CM}}\right)^{\frac{1}{2}} \frac{1}{1+y^2} \ ,$$

where:

$$E_{\rm CM} \equiv \text{neutron energy in Centre of Mass frame} \ ,$$

(note $E = E_{\rm LAB} = \frac{A+1}{A} E_{\rm CM}$)

$$E_0 \equiv \text{energy of the resonance} \ ,$$

$$y = \frac{2}{\Gamma}(E_{\rm CM} - E_0) \ ,$$

(at the resonance peak $E_{\rm CM} = E_0$ giving $\sigma_\gamma = \sigma_0 \frac{\Gamma_\gamma}{\Gamma}$),

$$\Gamma \equiv \text{total resonance width (FWHM)} \ ,$$

(this also has the quantum mechanical definition of $\Gamma = \hbar/\tau$, where τ is the average lifetime of a compound nucleus).

$$\Gamma_\gamma \equiv \text{radiative line width (partial width)} \ ,$$

$$\frac{\Gamma_\gamma}{\Gamma} \equiv \text{probability of decaying through the (n,}\gamma\text{) channel} \ ,$$

$$\sigma_0 \equiv \text{total cross section at } E_{\rm CM} = E_0 \ .$$

There is also an equation for σ_0 which is:

$$\sigma_0 = 4\pi \lambda\!\!\!^{-2}_0 \frac{\Gamma_{\rm n}}{\Gamma} g \ ,$$

where:

$$\Gamma_{\rm n} \equiv \text{neutron emission line width} \propto E_{\rm CM}^{\frac{1}{2}} \ ,$$

$$\lambda\!\!\!^{-}_0 \equiv \text{reduced wave length corresponding to } E_0 = \frac{\hbar}{\sqrt{2\mu E_0}} \ ,$$

$$\mu \equiv \text{reduced mass} = \frac{A}{A+1} = \frac{mM}{m+M} \ ,$$

$$g \equiv \text{statistical factor} = \frac{2J+1}{(2S+1)(2I+1)} \ ,$$

where $S = \frac{1}{2}$ is the neutron spin, I is the target nucleus spin ($I = 0$ for even-even nuclides), and J us the spin of the compound nucleus ($J = I - \frac{1}{2}$ or $J = I + \frac{1}{2}$). Note that if $E_{\rm CM} << E_0$ and $A \to \infty$ (or $E << E_0$) then

$$\sigma(E) \sim \frac{1}{\sqrt{E}} \sim \frac{1}{v} \ .$$

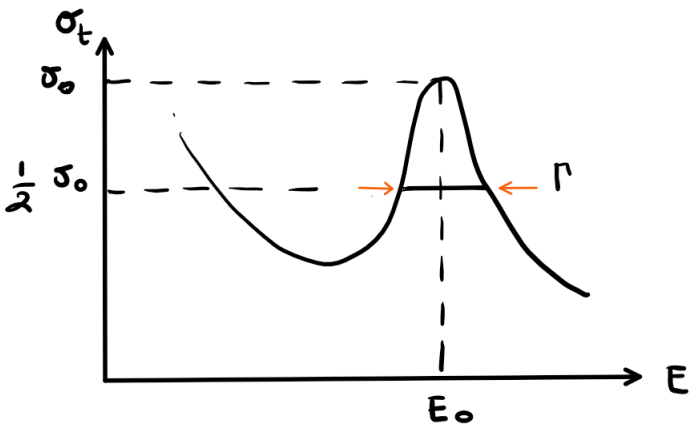


Figure 13: Illustration of a Single-Level Breit Wigner resonance.

Scattering resonances are slightly more complicated. They have two additional terms: one due to potential scattering (nuclides behaving like hard spheres) and one due to interference effects – we will leave it as quantum weirdness without further explanation.

$$\sigma_{\mathrm{s}}(E_{\mathrm{CM}}) = \underbrace{\sigma_0 \frac{\Gamma_{\mathrm{n}}}{\Gamma}\left(\frac{E_0}{E_{\mathrm{CM}}}\right)^{\frac{1}{2}} \frac{1}{1+y^2}}_{\text{resonance scattering}} + \underbrace{\sigma_0 \frac{2R}{\lambda\!\!\!^{-}_0} \frac{y}{1+y^2}}_{\text{interference scattering}} + \underbrace{4\pi R^2}_{\text{potential scattering}} .$$

Here Γ_{n} is the scattering channel width (or neutron width in literature) and R is the nuclear radius $\sim r_0 A^{\frac{1}{3}} = 1.25 \times 10^{-13} \times A^{\frac{1}{3}}$ cm.

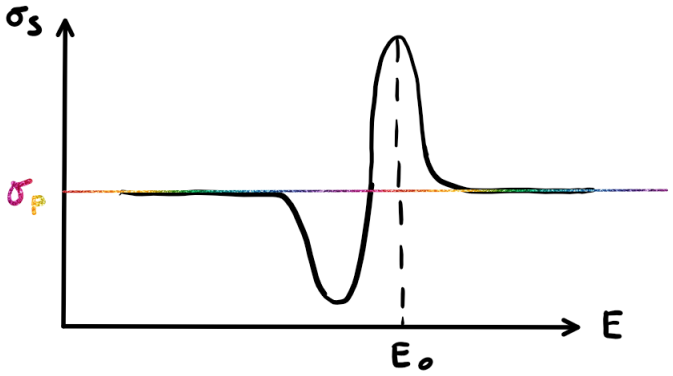


Figure 14: Illustration of a scattering resonance.

Potential scattering is independent of energy. In a mixture, the sum of the potential scattering cross sections of all nuclides results in a 'background' cross section. If this background cross section is sufficiently high, it will drown out resonances – they will be submerged under this background cross section. This is important with respect to determining how strongly a resonance affects the flux spectrum. We will examine the relative strength of a resonance at its peak versus the total background cross section in the presence of a moderator. We will use p to denote the potential scatter cross section, A to denote an absorber, and H to denote the moderator (hydrogen). Given that $\Sigma_{\mathrm{A,peak}} = N_{\mathrm{A}}\sigma_{\mathrm{A},0}$, this can be written as:

$$\frac{\Sigma_{\mathrm{A,peak}}}{\Sigma_{\mathrm{p}}} = \frac{N_{\mathrm{A}}\sigma_{\mathrm{A},0}}{N_{\mathrm{A}}\sigma_{\mathrm{A,p}} + N_{\mathrm{H}}\sigma_{\mathrm{H,p}}} = \frac{\sigma_{\mathrm{A},0}}{\sigma_{\mathrm{A,p}} + \frac{N_{\mathrm{H}}}{N_{\mathrm{A}}}\sigma_{\mathrm{H,p}}} .$$

The quantity $\frac{N_{\mathrm{H}}}{N_{\mathrm{A}}}$ is referred to as the dilution. As $\frac{N_{\mathrm{H}}}{N_{\mathrm{A}}} \to \infty$, the relative importance of $\sigma_{\mathrm{A},0}$ (or the resonance) goes to 0. This case is commonly referred to as infinite dilution and means that the resonance does not perturb the neutron flux. More generally, dilution refers to the ratio of the resonance nuclide density to that of all other nuclides. Perhaps, more usefully, one also talks about the 'background cross section', $\sigma_{\mathrm{b}} = \frac{\sigma_{\mathrm{H,p}} N_{\mathrm{H}}}{N_{\mathrm{A}}}$. Then one can phrase things in terms of the relative sizes of microscopic cross sections – if there is a high background or a low background.

4.1 Evaluating the resonance escape probability

With this, we can evaluate the resonance escape probability we saw previously in Eq. (13) if we assume an SLBW form of the resonance and say that our absorber is infinitely dilute. Initially, this probability has the form:

$$p(E) = \exp\left(-\int_E^{E_0} \frac{\Sigma_{\mathrm{a}}(E')}{\Sigma_{\mathrm{s}}(E') + \Sigma_{\mathrm{a}}(E')} \frac{\mathrm{d}E'}{E'}\right) = \exp\left(-\int_E^{E_0} \frac{N_{\mathrm{A}}\sigma_\gamma^{\mathrm{A}}(E')}{N_{\mathrm{H}}\sigma_{\mathrm{s}}^{\mathrm{H}} + N_{\mathrm{A}}\sigma_\gamma^{\mathrm{A}}(E')} \frac{\mathrm{d}E'}{E'}\right).$$

We will make two approximations. First, we will say the absorber is infinitely dilute, i.e., $N_{\mathrm{H}}\sigma_{\mathrm{s}}^{\mathrm{H}} >> N_{\mathrm{A}}\sigma_\gamma^{\mathrm{A}}(E')$. Second, we will say contributions to the integral are small far away from the resonance (above or below), i.e., we are evaluating the integral in the small vicinity about E_0, the resonance energy, so we can write $\int_{E_0} \mathrm{d}E'$. This allows us to use the filthy trick that the $1/E'$ term can be approximated as $1/E_0$ and extracted from the integral. This gives us:

$$p_{E_0}^{\infty} \approx \exp\left(-\frac{N_{\mathrm{A}}}{N_{\mathrm{H}}\sigma_{\mathrm{s}}^{\mathrm{H}} E_0} \int_{E_0} \sigma_\gamma^{\mathrm{A}}(E')\mathrm{d}E'\right).$$

Now we need to insert the SLBW definition of σ_γ. Despite what we said earlier, we will evaluate the integral from $-\infty$ to ∞ (but still assuming contributions are negligible at the wings of the resonance and assuming that $\frac{E_0}{E_{\mathrm{CM}}} \approx 1$). We also note that:

$$y = \frac{2}{\Gamma}(E - E_0),$$

$$\mathrm{d}y = \frac{2}{\Gamma}\mathrm{d}E,$$

$$\mathrm{d}E = \frac{\Gamma}{2}\mathrm{d}y.$$

Making this insertion gives:

$$p_{E_0}^{\infty} \approx \exp\left(-\frac{\sigma_0 N_{\mathrm{A}}\Gamma_\gamma}{2N_{\mathrm{H}}\sigma_{\mathrm{s}}^{\mathrm{H}} E_0} \int_{-\infty}^{\infty} \frac{\mathrm{d}y}{1+y^2}\right) = \exp\left(-\frac{\sigma_0 N_{\mathrm{A}}\Gamma_\gamma \pi}{2N_{\mathrm{H}}\sigma_{\mathrm{s}}^{\mathrm{H}} E_0}\right).$$

Unfortunately, if we don't have infinity dilution then life becomes more complicated. However, this equation nevertheless lets us observe some interesting effects, e.g., examining aspects of the moderator temperature coefficient. Increasing moderature temperature decreases N_{H}, decreasing $p_{E_0}^{\infty}$, increasing the resonance absorption probability $(1 - p_{E_0}^{\infty})$, decreasing k_{eff}.

We also see that low energy resonances are more important – as E_0 decreases, so does the resonance escape probability by similar logic as above. This can be justified because the collision rate is $F(E) \sim 1/E$, i.e., there are more collisions at low energies.

5 Resonance Integrals

If we cast our minds back to the problem that motivates these lectures, we want to estimate multigroup cross sections of the form:

$$\Sigma_{\mathrm{a},g} = \frac{\int_{E_g}^{E_{g-1}} \mathrm{d}E\ \Sigma_{\mathrm{a}}(E)\phi(E)}{\int_{E_g}^{E_{g-1}} \mathrm{d}E\ \phi(E)}\ .$$

If we define the **resonance integral** for resonance i as:

$$I_i = \int_{E_i} \mathrm{d}E\ \sigma_{\mathrm{a}}^{\mathrm{A}}(E)\phi(E)\ ,$$

and assert that the resonances are narrow compared to the width of an energy group, ΔE_g, such that $\phi(E) \approx \frac{1}{E}$ (giving $\int_{E_g}^{E_{g-1}} \mathrm{d}E\phi(E) \approx \ln \frac{E_{g-1}}{E_g}$), then we can write the cross section as:

$$\Sigma_{\mathrm{a},g} = \frac{N_{\mathrm{A}} \sum_{i\in g} I_i}{\ln \frac{E_{g-1}}{E_g}} = \frac{N_{\mathrm{A}} \sum_{i\in g} I_i}{\Delta u_g}\ .$$

This means that the problem of calculating cross sections becomes a problem of calculating resonance integrals. This generalises straightforwardly when there is more than one absorbing nuclide. However, this also assumes there is no interference effect between these resonances. We will go through some of the methods used to approximate these integrals in various conditions. This will start from solving the slowing down equation:

$$\Sigma_{\mathrm{t}}(E)\phi(E) = \int_E^{E/\alpha_{\mathrm{M}}} \frac{\Sigma_{\mathrm{s}}^{\mathrm{M}}\phi(E')\mathrm{d}E'}{E'(1-\alpha_{\mathrm{M}})} + \int_E^{E/\alpha_{\mathrm{A}}} \frac{\Sigma_{\mathrm{s}}^{\mathrm{A}}(E')\phi(E')\mathrm{d}E'}{E'(1-\alpha_{\mathrm{A}})}\ , \tag{14}$$

where we use M to refer to the moderator and A to refer to the resonant absorber. We make a few approximations:

- No absorption in moderator: $\Sigma_{\mathrm{t}}^{\mathrm{M}}(E) = \Sigma_{\mathrm{s}}^{\mathrm{M}}$.
- Only potential scattering in moderator: $\Sigma_{\mathrm{s}}^{\mathrm{M}}(E) = \Sigma_{\mathrm{s}}^{\mathrm{M}} = \Sigma_{\mathrm{p}}^{\mathrm{M}}$.
- The absorber cross section can be decomposed as: $\Sigma_{\mathrm{t}}^{\mathrm{A}}(E) = \Sigma_{\mathrm{a}}^{\mathrm{A}}(E) + \Sigma_{\mathrm{s}}^{\mathrm{A}}(E) + \Sigma_{\mathrm{p}}^{\mathrm{A}}$.

We can make one further approximation in one of two ways, which will affect our results.

5.1 Narrow resonance approximation

In this case we first assume that resonances are "narrow" for collisions with moderator, i.e., $\Gamma_{\mathrm{prac}} << \Delta E_{\mathrm{M}} = \frac{1}{2}(1-\alpha_{\mathrm{M}})E_0$, or the practical resonance width is much smaller than the average energy loss per collision with moderator. If we make the same assertion for the absorber ($\Gamma_{\mathrm{prac}} << \Delta E_{\mathrm{M}} = \frac{1}{2}(1-\alpha_{\mathrm{A}})E_0$), this allows us to approximate the flux in the integrals as unperturbed from the asymptotic, i.e., $\phi(E) \sim 1/E$. If we also say the contribution of scattering resonances are also small, then the absorber's scattering cross section is just composed of the potential cross section. Hence, our equations becomes:

$$\Sigma_{\mathrm{t}}(E)\phi_{\mathrm{NR}}(E) = \int_E^{E/\alpha_{\mathrm{M}}} \frac{\Sigma_{\mathrm{s}}^{\mathrm{M}}\mathrm{d}E'}{E'^2(1-\alpha_{\mathrm{M}})} + \int_E^{E/\alpha_{\mathrm{A}}} \frac{\Sigma_{\mathrm{p}}^{\mathrm{A}}\mathrm{d}E'}{E'^2(1-\alpha_{\mathrm{A}})} = \frac{\Sigma_{\mathrm{p}}^{\mathrm{M}} + \Sigma_{\mathrm{p}}^{\mathrm{A}}}{E}\ ,$$

giving:

$$\phi_{\mathrm{NR}}(E) = \frac{\Sigma_{\mathrm{p}}^{\mathrm{M}} + \Sigma_{\mathrm{p}}^{\mathrm{A}}}{\Sigma_{\mathrm{t}}(E)}\frac{1}{E} = \frac{\sigma_{\mathrm{p}}^{\mathrm{A}} + \sigma_{\mathrm{b}}}{\sigma_{\mathrm{t}}^{\mathrm{A}}(E) + \sigma_{\mathrm{b}}}\frac{1}{E}\ ,$$

where $\sigma_{\mathrm{b}} = \frac{\Sigma_{\mathrm{p}}}{N^{\mathrm{A}}}$ is the background cross section. This expression for the flux is known as the narrow-resonance approximation flux – one thing it implies is that the perturbation due to a resonance depends strongly on the background cross section. This lets us evaluate the resonance integral as:

$$I_{\mathrm{NR}} = \int_{E_0} \mathrm{d}E\sigma_{\mathrm{a}}^{\mathrm{A}}(E)\phi_{\mathrm{NR}}(E) = \int_{E_0} \frac{\mathrm{d}E}{E}\sigma_{\mathrm{a}}^{\mathrm{A}}(E)\frac{\sigma_{\mathrm{p}}^{\mathrm{A}} + \sigma_{\mathrm{b}}}{\sigma_{\mathrm{t}}^{\mathrm{A}}(E) + \sigma_{\mathrm{b}}}$$

This can be integrated numerically given we should know how the microscopic cross sections look – or looked up from a precomputed table given an input background cross section.

We expect the NR approximation to be more valid for higher energy resonances due to the increased average energy loss per collision.

5.2 Wide resonance approximation

Also known as the Narrow Resonance-Infinite Mass approximation. This is the other extreme from NR: we say that the average energy loss per collision with an absorber is much less than the practical resonance width, $\frac{1}{2}(1-\alpha_{\mathrm{A}})E_0 << \Gamma_{\mathrm{prac}}$. This is illustrated in Fig. 15. As $A \to \infty$, $\alpha_{\mathrm{A}} \to 1$. If we apply this limit to the absorber integral we get:

$$\lim_{\alpha_{\mathrm{A}}\to 1} \int_E^{E/\alpha_{\mathrm{A}}} \frac{\mathrm{d}E' \Sigma_{\mathrm{s}}^{\mathrm{A}}(E')\phi(E')}{(1-\alpha_{\mathrm{A}})E'} \to \Sigma_{\mathrm{s}}^{\mathrm{A}}(E)\phi(E) \lim_{\alpha_{\mathrm{A}}\to 1} \frac{1}{E} \int_E^{E/\alpha_{\mathrm{A}}} \frac{\mathrm{d}E'}{1-\alpha_{\mathrm{A}}} = \Sigma_{\mathrm{s}}^{\mathrm{A}}(E)\phi(E) \ .$$

We use the same $1/E$ treatment for the moderator flux and insert this into the slowing down equation to give:

$$\Sigma_{\mathrm{t}}(E)\phi_{\mathrm{WR}}(E) = \Sigma_{\mathrm{s}}^{\mathrm{A}}(E)\phi_{\mathrm{WR}}(E) + \frac{\Sigma_{\mathrm{s}}^{\mathrm{M}}}{E} \ ,$$

resulting in:

$$\phi_{\mathrm{WR}}(E) = \frac{\Sigma_{\mathrm{s}}^{\mathrm{M}}}{\Sigma_{\mathrm{t}}(E) - \Sigma_{\mathrm{s}}^{\mathrm{A}}(E)} \frac{1}{E} = \frac{\sigma_{\mathrm{b}}}{\sigma_{\mathrm{a}}^{\mathrm{A}}(E) + \sigma_{\mathrm{b}}} \frac{1}{E} \ .$$

Once again, this can be used to evaluate resonance integrals, dependent on the background cross section.

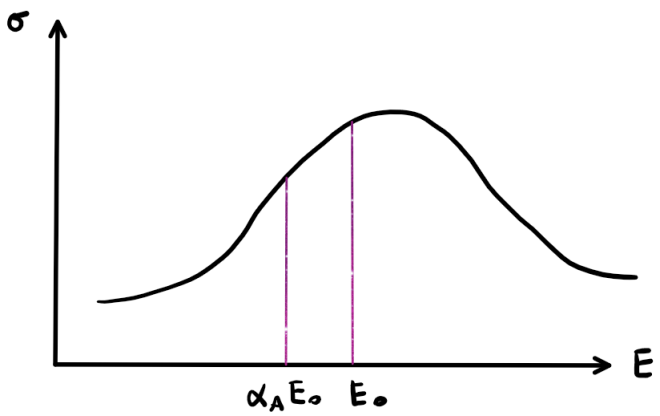


Figure 15: Illustration of the wide resonance approximation.

From both the NR and WR approximations, if the background cross section (or dilution) is very high, we would obtain the infinite dilution resonance integral:

$$I^{\infty} = \int_{E_0} \mathrm{d}E \sigma_{\mathrm{a}}^{\mathrm{A}}(E) \frac{1}{E} \ .$$

Note that $I^{\infty} > I_{\mathrm{NR}}$ and $I^{\infty} > I_{\mathrm{WR}}$. This is the effect of self-shielding!

5.3 Intermediate resonance approximation

The difference between the NR and WR approximations is ultimately whether we include contributions from the scattering cross section of the resonant nuclide. This suggests that we can do something part-way, i.e., have an **intermediate** resonance approximation where we only include part of the scattering cross section. This is done with a parameter λ such that we have:

$$\phi_{\mathrm{IR}}(E) = \frac{\lambda\sigma_{\mathrm{p}}^{\mathrm{A}} + \sigma_{\mathrm{b}}}{\sigma_{\mathrm{a}}^{\mathrm{A}}(E) + \lambda\sigma_{\mathrm{p}}^{\mathrm{A}} + \sigma_{\mathrm{b}}} \frac{1}{E} \ ,$$

where λ is a parameter deciding the importance of the scattering cross section for a particular resonance; $\lambda = 1$ corresponds to NR, $\lambda = 0$ corresponds to WR. This model tends to produce significantly better results in intermediate energy ranges where neither the narrow nor wide approaches are very accurate. As such, it is commonly used in many lattice physics codes. However, the determination of the λ parameters for a given system is not elegant – this is usually done numerically and fixed for future use.

6 Collision probabilities

So far, we have only dealt with homogeneous systems and the effect of energy self-shielding. However, spatial self-shielding is extremely important and we need a means to account for spatial heterogeneity of reactors. We are going to do this via the integral transport equation, or, in particular, the collision probabilities method. This is a convenient formalism because it works very well in general geometries – ultimately what we want to produce are expressions describing how likely it is that a neutron will collide in one material region given it was born in another.

6.1 Integral transport equation

Let's say we have some volume of space with a boundary from which no neutrons enter. We want to know how many neutrons are within some $\mathrm{d}V$ about a point $\mathbf{r}$. These neutrons come to $\mathbf{r}$ from the volumes about other point, $\mathrm{d}V'$ about $\mathbf{r}'$. This is illustrated in Fig. 16.

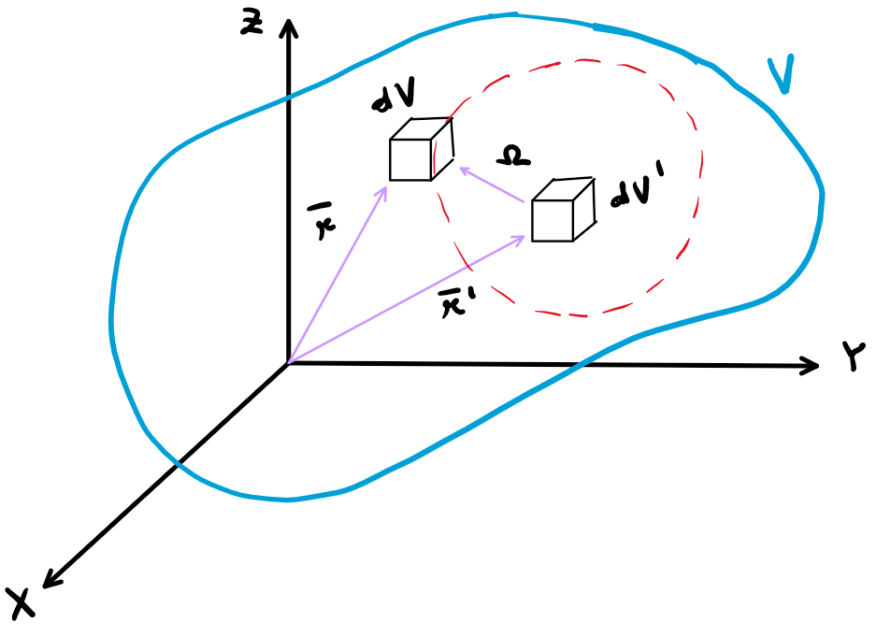


Figure 16: Geometry for deriving the integral transport equation.

To reach $\mathbf{r}$ from $\mathbf{r}'$, it will take some time. To arrive at $\mathbf{r}$ at time t, neutrons would have to leave $\mathbf{r}'$ at a time:

$$t' = t - \frac{|\mathbf{r} - \mathbf{r}'|}{v} \ ,$$

where v is the neutron speed.

The number of neutrons coming from $\mathrm{d}V'$ about $\mathbf{r}'$ is from scattering, fission and other sources. The total number of neutrons produced at this point at the appropriate time is:

$$q(\mathbf{r}')\mathrm{d}V'\mathrm{d}t' \ ,$$

where $q(\mathbf{r}')$ is the local source rate density. We assume production is isotropic – otherwise the equations become nightmarish.

The probability that a neutron will fly the appropriate distance $|\mathbf{r} - \mathbf{r}'|$ without colliding along the way is:

$$e^{-\Sigma_\mathrm{t}|\mathbf{r}-\mathbf{r}'|} \ ,$$

where Σ_t is the total cross section and we have assumed the medium is homogeneous. If the medium is not homogeneous, we would have to work in terms of the medium's optical depth, giving:

$$e^{-\int_0^{|\mathbf{r}-\mathbf{r}'|}\mathrm{d}R\,\Sigma_\mathrm{t}(\mathbf{r}'+\mathbf{\Omega}R)}\ ,$$

where $\mathbf{\Omega}$ is the neutron's flight direction and R is the distance along that direction. We also often rewrite the exponentiated term simply as $\tau(\mathbf{r},\mathbf{r}')$, referred to as the optical distance between the two points.

For neutrons that have been produced by the source, after some time $t-t'$ or after they have travelled a distance $|\mathbf{r}-\mathbf{r}'|$, they will form a spherical shell around the source. This shell will have a volume:

$$4\pi|\mathbf{r}-\mathbf{r}'|^2 v\mathrm{d}t'\ .$$

Putting these expressions all together, the neutron density about $\mathrm{d}V$ due to neutrons about $\mathrm{d}V'$ will be:

$$n(\mathbf{r},\mathbf{r}') = \frac{q(\mathbf{r}')e^{-\Sigma_\mathrm{t}|\mathbf{r}-\mathbf{r}'|}\mathrm{d}V'\mathrm{d}t'}{4\pi|\mathbf{r}-\mathbf{r}'|^2 v\mathrm{d}t'}\ .$$

To obtain the actual density of neutrons at the point $\mathbf{r}$, we need to integrate this equation over all of space, giving:

$$n(\mathbf{r}) = \int_V q(\mathbf{r}')\frac{e^{-\Sigma_\mathrm{t}|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|^2 v}\mathrm{d}V'\ ,$$

or, more conventionally, the flux is:

$$\phi(\mathbf{r}) = \int_V q(\mathbf{r}')\frac{e^{-\Sigma_\mathrm{t}|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|^2}\mathrm{d}V'\ . \tag{15}$$

6.2 Discretisation

To be able to solve this problem numerically, we need to discretise it. We do so by asserting that space is split up into several homogeneous regions, where region i has volume V_i. In each region, we will also have a uniform flux and source (and cross sections), defined as:

$$\phi_i = \frac{1}{V_i}\int_{V_i}\mathrm{d}V\phi(\mathbf{r})\ ,$$

$$q_i = \frac{1}{V_i}\int_{V_i}\mathrm{d}V q(\mathbf{r})\ .$$

If we integrate Eq. (15) over volume V_i and multiply by $\Sigma_{\mathrm{t},i}$ we obtain:

$$\begin{aligned}\Sigma_{\mathrm{t},i}\int_{V_i}\mathrm{d}V\phi(\mathrm{r}) = \Sigma_{\mathrm{t},i}\phi_i V_i &= \Sigma_{\mathrm{t},i}\int_{V_i}\mathrm{d}V\int_V\mathrm{d}V'\frac{q(\mathbf{r}')e^{-\tau(\mathbf{r},\mathbf{r}')}}{4\pi|\mathbf{r}-\mathbf{r}'|^2}\\ &= \Sigma_{\mathrm{t},i}\sum_j q_j\int_{V_i}\mathrm{d}V\int_{V_j}\mathrm{d}V'\frac{e^{-\tau(\mathbf{r},\mathbf{r}')}}{4\pi|\mathbf{r}-\mathbf{r}'|^2} = \sum_j q_j V_j P_{ij}\ ,\end{aligned} \tag{16}$$

where we have introduced P_{ij}, the collision probability, or the probability that a particle produced in region i will collide in region j, defined as:

$$P_{ij} = \frac{\Sigma_{\mathrm{t},i}}{V_j}\int_{V_i}\mathrm{d}V\int_{V_j}\mathrm{d}V'\frac{e^{-\tau(\mathbf{r},\mathbf{r}')}}{4\pi|\mathbf{r}-\mathbf{r}'|^2}\ . \tag{17}$$

Hence we can write the transport problem as, simply:

$$\Sigma_{\mathrm{t},i}\phi_i V_i = \sum_j q_j V_j P_{ij}\ , \tag{18}$$

which states that the collision rate in a region is due to the contributions of neutrons born in all regions in the problem. This can be written simply as a matrix multiplication, where P_{ij} is a matrix, acting on the vector $(qV)_j$.

The problem, of course, comes with how to calculate P_{ij}. In self-shielding calculations, this is done very approximately as we shall see.

6.3 Digression on the common use of the collision probability method

We will be using collision probabilities as a formalism without much meaningful numerics, but the more complete method is important in reactor physics. In particular, after we have done all of our self-shielding calculations, we want to account for spatial effects – usually this is done on a pin cell level with many groups, followed by calculations on an assembly level with fewer groups.

Where the collision probabilities method (CPM) is most common in reactor physics is in that second step: spatial calculations for single pin cells, for each pin cell type in the reactor. These calculations are often performed with a major approximation: the pins are 'circularised' or a Wigner-Seitz cell is constructed, preserving fuel and moderator volumes. This also results in the need to use 'white' boundary conditions, rather than the more common reflective or periodic. The reason for this is that calculating collision probabilities in a circular geometry is much more straightforward as the geometry is essentially 1D.

CPM tends not to be applied to larger problems, despite its geometric flexibility. This is due to it producing dense matrices that must be inverted to obtain the flux. Matrix inversion operations are $\mathcal{O}(n^3)$ in time complexity, making the method become intractable as the geometry becomes larger. However, the ray tracing procedures devised for CPM were put to good usage afterwards; they are used by the method of characteristics, which can perform a transport sweep, rather than a direct matrix inversion, and this is now the method of choice for assembly-level lattice physics.

7 Cell homogenisation and equivalence theory

Now, armed with the language of collision probabilities, we return to slowing down. But this time, we will assert that there is heterogeneity, namely, a cylindrical fuel region and a surrounding moderator region.

We will use the following notation:

- f: fuel
- m: moderator
- 0: absorber nuclide in fuel
- 1: moderator nuclide in fuel
- 2: moderator nuclide in the moderator

In a given region and for a given nuclide, our scattering source will look like:

$$I_i(\phi_z) \equiv \int_E^{E/\alpha_i} \frac{\mathrm{d}E'}{(1-\alpha_i)E'} \Sigma_{\mathrm{s},i} \phi_z(E') \ ,$$

where i refers to the nuclide, z refers to the zone.

We will make some additional notation:

- $P_{\mathrm{f}\to\mathrm{m}}(E)$: probability for a neutron born in the moderator with energy E to enter the fuel and collide there for the first time.
- $P_{\mathrm{m}\to\mathrm{f}}(E)$: the same, but in the other direction
- V_{m}, V_{f}: the volumes of the moderator and fuel.
- ϕ_{m}, ϕ_{f}: zone average fluxes in the moderator and fuel.

Given this, in our heterogeneous system, the neutron balance equation in the fuel looks like:

$$V_{\mathrm{f}} \phi_{\mathrm{f}}(E) \Sigma_{\mathrm{t,f}}(E) = V_{\mathrm{f}}(1 - P_{\mathrm{f}\to\mathrm{m}}(E)) \times (I_0(\phi_{\mathrm{f}}) + I_1(\phi_{\mathrm{f}})) + V_{\mathrm{m}} P_{\mathrm{m}\to\mathrm{f}}(E) I_2(\phi_{\mathrm{m}}) \ .$$

For the moment, we will assume that **if a neutron escapes the fuel, it will collide in the moderator with 100% certainty**. We will hence refer to $P_{\mathrm{f}\to\mathrm{m}}$ as the escape probability, P_{escape}, or P_{esc}. This is obviously wrong but we will correct it later.

The path forward from here is:

1. Calculate P_{esc}
2. Connect P_{esc} to $P_{\mathrm{m}\to\mathrm{f}}$
3. Solve the 2-zone slowing down equation
4. Relax the "isolated rod" assumption, generalising to tight lattices
5. Produce estimates for $\phi_{\mathrm{f}}(E)$ and $\phi_{\mathrm{m}}(E)$ to calculate cross sections

7.1 Estimating the escape probability

We need to calculate the probability that a neutron leaves the fuel (given we have assumed an isolated system – if it weren't, we would need to account for it colliding in another fuel element beyond the moderator).

For a neutron in the fuel, flying in direction $\mathbf{\Omega}$, with a distance of s to the surface of the fuel, the probability of travelling that distance is $\exp\left(-\Sigma_{\mathrm{t,f}}(E)s\right)$. The small volume surrounding the neutron can be expressed as $(\mathbf{n}\cdot\mathbf{\Omega})\mathrm{d}S\mathrm{d}s$, where $\mathrm{d}S$ is a small surface element of the total surface, S, and $\mathbf{n}$ is the inward normal vector from that surface element. The geometry of this setup is shown in Fig. 17. For a fixed

direction, if we sum over all surfaces and distances to the surface, we would estimate the escape probability as:

$$P_{\text{esc}}(E,\mathbf{\Omega}) = \frac{1}{V_{\text{f}}}\int_S \mathrm{d}S\,(\mathbf{n}\cdot\mathbf{\Omega})\int_0^l \mathrm{d}s\exp\left(-\Sigma_{\text{t,f}}(E)s\right) = \frac{1}{\Sigma_{\text{t,f}}(E)V_{\text{f}}}\int_S \mathrm{d}S\,(\mathbf{n}\cdot\mathbf{\Omega})\times\left(1-\exp\left(-\Sigma_{\text{t,f}}(E)l\right)\right)\ ,$$

where l is the chord length, or distance from one surface to another in a given direction. We also want to average over angle, so we need integrate over that as well:

$$P_{\text{esc}}(E) = \frac{1}{4\pi}\int_{\mathbf{n}\cdot\mathbf{\Omega}>0}\mathrm{d}\Omega P_{\text{esc}}(E,\mathbf{\Omega}) = \frac{1}{4\pi\Sigma_{\text{t,f}}(E)V_{\text{f}}}\int_{\mathbf{n}\cdot\mathbf{\Omega}>0}\mathrm{d}\Omega\int_S \mathrm{d}S\,(\mathbf{n}\cdot\mathbf{\Omega})\times\left(1-\exp\left(-\Sigma_{\text{t,f}}(E)l\right)\right)\ .$$

To resolve this integral, we need to know how the chord length, l, is distributed. Even if we did, the result for evaluating this integral is complicated and (at least historically) painful to evaluate. For example, for a slab of width a, this would produce:

$$P_{\text{esc}}(E) = \frac{1}{\Sigma_{\text{t,f}}(E)a}\left[\frac{1}{2}-E_3(\Sigma_{\text{t,f}}(E)a)\right]\ ,$$

where E_3 is an exponential integral:

$$E_3(y) = \int_1^\infty \mathrm{d}x x^{-3}\exp\left(-yx\right)\ . \tag{19}$$

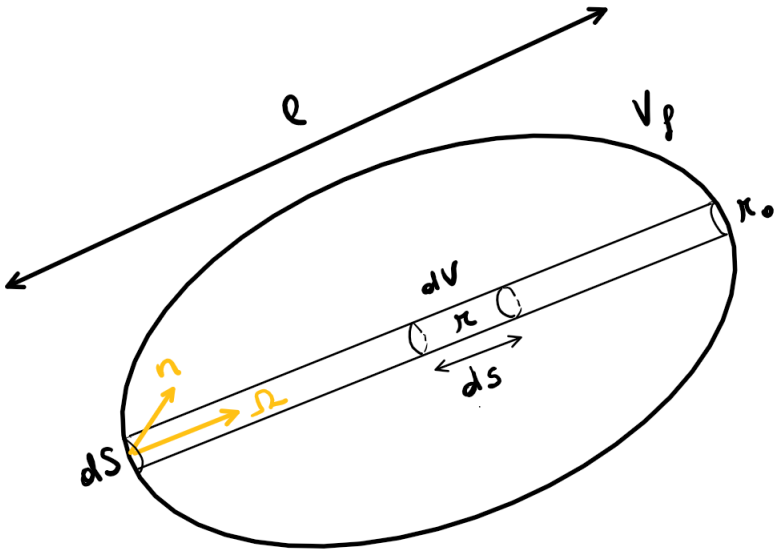


Figure 17: Geometry for estimating the escape probability.

7.2 Wigner's rational approximation

Generally, we can say some things about the chord length and escape probability. For a convex body, it is known (from Dirac) that the average chord length, $\bar{l}$ is simply

$$\bar{l} = \frac{4V}{A}\ ,$$

where V is the volume of the region and A is the surface area. We will try to obtain P_{esc} in terms of this quantity.

From physical intuition, we can reason that as bodies become small/optically thin (or $\Sigma_{\mathrm{t,f}}\bar{l} \to 0$), $P_{\mathrm{esc}} \to 1$. We can show what happens as bodies become large, or $\Sigma_{\mathrm{t,f}}\bar{l} \to \infty$. In this scenario, $e^{-\Sigma_{\mathrm{t,f}}l} << 1$, so, $1 - e^{-\Sigma_{\mathrm{t,f}}l} \approx 1$. This reduces our escape probability to:

$$P_{\mathrm{esc}} \approx \frac{1}{4\pi V_{\mathrm{f}}\Sigma_{\mathrm{t,f}}} \int_S \mathrm{d}S \int_{\mathbf{n}\cdot\mathbf{\Omega}>0} \mathrm{d}\Omega(\mathbf{n}\cdot\mathbf{\Omega}) \ .$$

The term $(\mathbf{n}\cdot\mathbf{\Omega})$ approaches the cosine with respect to the surface, μ, as the body becomes very large. Hence we can evaluate the angular integral as:

$$\int_{\mathbf{n}\cdot\mathbf{\Omega}>0} \mathrm{d}\Omega(\mathbf{n}\cdot\mathbf{\Omega}) = \int_0^{2\pi} \mathrm{d}\varphi \int_0^1 \mu \mathrm{d}\mu = \pi \ ,$$

where the cosine integral is between 0 and 1 due to the constraint of the cosine being positive. Evaluating the S integral results in the surface area, A, giving:

$$P_{\mathrm{esc}} = \frac{A}{4V\Sigma_{\mathrm{t,f}}} = \frac{1}{\Sigma_{\mathrm{t,f}}\bar{l}} \ .$$

Based on these observations, Wigner introduced his rational approximation for the escape probability, satisfying both conditions:

$$P_{\mathrm{esc}} = \frac{1}{1 + \Sigma_{\mathrm{t,f}}\bar{l}} \ .$$

This obviously works very well in the extremes, but under-predicts the escape probability in between.

'Then why would we use it?' I hear you ask. 'We can work out the exact answer and it's a bit wrong for our basic range of interesting values'. Well, it happens to be good enough for most purposes but there is also something very convenient about the use of a rational approximation to represent the escape probability... But we will come back to this shortly.

7.3 Reciprocity

Given we have an expression for P_{esc}, we want to eliminate the remaining $P_{\mathrm{m}\to\mathrm{f}}$ term. It happens that collision probabilities allow us to express $P_{\mathrm{m}\to\mathrm{f}}$ in terms of $P_{\mathrm{f}\to\mathrm{m}}$ (or P_{esc}).

Once again, a collision probability from region m to region f is written as:

$$P_{\mathrm{m}\to\mathrm{f}} = \frac{\Sigma_{\mathrm{t,f}}}{V_{\mathrm{m}}} \int_{V_{\mathrm{f}}} \mathrm{d}V \int_{V_{\mathrm{m}}} \mathrm{d}V' \frac{e^{-\tau(\mathbf{r},\mathbf{r}')}}{4\pi|\mathbf{r}-\mathbf{r}'|^2} \ .$$

The expression for the opposite probability is:

$$P_{\mathrm{f}\to\mathrm{m}} = \frac{\Sigma_{\mathrm{t,m}}}{V_{\mathrm{f}}} \int_{V_{\mathrm{m}}} \mathrm{d}V \int_{V_{\mathrm{f}}} \mathrm{d}V' \frac{e^{-\tau(\mathbf{r},\mathbf{r}')}}{4\pi|\mathbf{r}-\mathbf{r}'|^2} \ .$$

We note a similarity in the expressions such that we may write:

$$\frac{V_{\mathrm{m}}P_{\mathrm{m}\to\mathrm{f}}}{\Sigma_{\mathrm{t,f}}} = \frac{V_{\mathrm{f}}P_{\mathrm{f}\to\mathrm{m}}}{\Sigma_{\mathrm{t,m}}} = \int_{V_{\mathrm{m}}} \mathrm{d}V \int_{V_{\mathrm{f}}} \mathrm{d}V' \frac{e^{-\tau(\mathbf{r},\mathbf{r}')}}{4\pi|\mathbf{r}-\mathbf{r}'|^2} \ ,$$

where the order of integration does not matter, i.e., the integrated optical depth or attenutation from $\mathbf{r}$ to $\mathbf{r}'$ is the same as from $\mathbf{r}'$ to $\mathbf{r}$. This relationship between collision probabilities is known as the reciprocity relation.

Given the reciprocity relation, we can rewrite $P_{\mathrm{m}\to\mathrm{f}}$ as:

$$P_{\mathrm{m}\to\mathrm{f}} = \frac{V_{\mathrm{f}}P_{\mathrm{f}\to\mathrm{m}}\Sigma_{\mathrm{t,f}}}{V_{\mathrm{m}}\Sigma_{\mathrm{t,m}}} = \frac{V_{\mathrm{f}}P_{\mathrm{esc}}\Sigma_{\mathrm{t,f}}}{V_{\mathrm{m}}\Sigma_{\mathrm{t,m}}} \ .$$

Inserting this into our 2-zone slowing down equation gives:

$$V_{\mathrm{f}}\phi_{\mathrm{f}}(E)\Sigma_{\mathrm{t,f}}(E) = V_{\mathrm{f}}(1 - P_{\mathrm{esc}}(E)) \times (I_0(\phi_{\mathrm{f}}) + I_1(\phi_{\mathrm{f}})) + V_{\mathrm{f}}P_{\mathrm{esc}}(E)\frac{\Sigma_{\mathrm{t,f}}(E)}{\Sigma_{\mathrm{t,m}}(E)}I_2(\phi_{\mathrm{m}}) \ .$$

7.4 Equivalence theory

Now we make some final simplifications to this equation. As usual, we will assume that the moderator has only potential scattering such that

$$\Sigma_{\mathrm{t,m}}(E) = \Sigma_{\mathrm{p,m}} \ .$$

Additionally, we will make the narrow resonance approximation for collisions in the moderator in the fuel and moderator zones, i.e.,

$$I_i = \frac{\Sigma_{\mathrm{p},i}}{E} \ , \ i \in [1,2] \ .$$

This leaves us with:

$$\Sigma_{\mathrm{t,f}}(E)\phi_{\mathrm{f}}(E) = (1 - P_{\mathrm{esc}}(E))I_0(\phi_{\mathrm{f}}) + (1 - P_{\mathrm{esc}}(E))\frac{\Sigma_{\mathrm{p},1}}{E} + P_{\mathrm{esc}}\frac{\Sigma_{\mathrm{t,f}}(E)}{E} \ .$$

The escape probability is:

$$P_{\mathrm{esc}} = \frac{1}{1 + \Sigma_{\mathrm{t,f}}(E)\bar{l}} \ ,$$

but if we define an 'escape' cross section of $\Sigma_{\mathrm{e}} \equiv \frac{1}{\bar{l}}$ then the escape probability can be written as:

$$P_{\mathrm{esc}} = \frac{1/\bar{l}}{1/\bar{l} + \Sigma_{\mathrm{t,f}}(E)} = \frac{\Sigma_{\mathrm{e}}}{\Sigma_{\mathrm{e}} + \Sigma_{\mathrm{t,f}}(E)} \ ,$$

and we can also write:

$$1 - P_{\mathrm{esc}}(E) = \frac{\Sigma_{\mathrm{t,f}}(E)}{\Sigma_{\mathrm{e}} + \Sigma_{\mathrm{t,f}}(E)} \ .$$

Thus our slowing down equation becomes:

$$\Sigma_{\mathrm{t,f}}(E)\phi_{\mathrm{f}}(E) = \frac{\Sigma_{\mathrm{t,f}}(E)}{\Sigma_{\mathrm{e}} + \Sigma_{\mathrm{t,f}}(E)}I_0(\phi_{\mathrm{f}}) + \frac{\Sigma_{\mathrm{t,f}}(E)}{\Sigma_{\mathrm{e}} + \Sigma_{\mathrm{t,f}}(E)}\frac{\Sigma_{\mathrm{p},1}}{E} + \frac{\Sigma_{\mathrm{e}}}{\Sigma_{\mathrm{e}} + \Sigma_{\mathrm{t,f}}(E)}\frac{\Sigma_{\mathrm{t,f}}(E)}{E} \ ,$$

or:

$$\phi_{\mathrm{f}}(E) = \frac{1}{\Sigma_{\mathrm{e}} + \Sigma_{\mathrm{t,f}}(E)}I_0(\phi_{\mathrm{f}}) + \frac{1}{\Sigma_{\mathrm{e}} + \Sigma_{\mathrm{t,f}}(E)}\frac{\Sigma_{\mathrm{p},1}}{E} + \frac{\Sigma_{\mathrm{e}}}{\Sigma_{\mathrm{e}} + \Sigma_{\mathrm{t,f}}(E)}\frac{1}{E} \ ,$$

or:

$$\phi_{\mathrm{f}}(E) = \frac{I_0(\phi_{\mathrm{f}}) + \Sigma_{p,1}/E + \Sigma_{\mathrm{e}}/E}{\Sigma_{\mathrm{e}} + \Sigma_{\mathrm{t,f}}(E)} \ .$$

We can evaluate I_0 using the narrow or wide resonance approximations, giving either:

$$\phi_{\mathrm{f,NR}}(E) = \frac{\Sigma_{\mathrm{p},0} + \Sigma_{\mathrm{p},1} + \Sigma_{\mathrm{e}}}{\Sigma_{\mathrm{e}} + \Sigma_{\mathrm{t,f}}(E)}\frac{1}{E} = \frac{\sigma_{\mathrm{p},0} + \sigma_{\mathrm{b}} + \sigma_{\mathrm{e}}}{\sigma_{\mathrm{b}} + \sigma_{\mathrm{e}} + \sigma_{\mathrm{t},0}(E)}\frac{1}{E} \ ,$$

or

$$\phi_{\mathrm{f,WR}}(E) = \frac{\sigma_{\mathrm{b}} + \sigma_{\mathrm{e}}}{\sigma_{\mathrm{b}} + \sigma_{\mathrm{e}} + \sigma_{\mathrm{a},0}(E)}\frac{1}{E} \ ,$$

where we have defined a slightly different background cross section from before which is only in the fuel. In general, for a mixture of nuclides, this would be written as $\sigma_{\mathrm{b}} = \sum_{i \neq 0} N_i \sigma_{\mathrm{p},i}/N_0$, where the i nuclides are in the fuel.

What is remarkable about these formulae is that they are nearly identical to those for the homogeneous case – they only differ by the presence of the escape cross section. Zeroing the escape cross section would lead to the same results as before. Hence equivalence theory – the addition of an extra cross section, can force equivalence between a homogeneous and a heterogeneous problem. Practically, this means that, when calculating resonance integrals, **the effect of heterogeneity can be accounted for by the presence of additional scattering**.

7.5 Improving the escape probability

The escape probability was approximate in two ways. First, Wigner's rational approximation is simply inaccurate for intermediate values of the average optical distance. Second, it does not account for the presence of other fuel pins – we were assuming an isolated fuel pin.

There are several ways to improve upon Wigner. The classical approach is by the use of the 'Bell factor'. This is a factor to correct the rational approximation, written as a_{B}, and applied as:

$$P_{\mathrm{esc}} = \frac{a_{\mathrm{B}}}{\Sigma_{\mathrm{t}}\bar{l} + a_{\mathrm{B}}} = \frac{a_{\mathrm{B}}\Sigma_{\mathrm{e}}}{\Sigma_{\mathrm{t}} + a_{\mathrm{B}}\Sigma_{\mathrm{e}}} \ .$$

In principle, this factor can be calculated by an accurate method – but that is typically too expensive to do. Instead, the value is usually fixed at about ~ 1.2 and this proves sufficiently accurate for the values of $\Sigma_{\mathrm{t}}l$ representative of LWR pins, though it will induce a 20% bias in the optically thick limit.

More modern approaches (e.g., CASMO-5) simply use a slightly more elaborate rational approximation, e.g., with two terms rather than one. This complicates the algebra of creating an escape cross section, but notably improves accuracy. Further improvements to accuracy tend to be made by relaxing the two-region assumption, although this also adds significant complications.

7.6 Dancoff correction

Finally, the other assumption that is relaxed is that the fuel is isolated in an infinite sea of moderator, or that no other fuel surrounds the fuel region. In reality, fuel sits in a lattice and there is a non-zero probability that a neutron will not collide in the moderator but in another fuel pin. This means that the isolated rod escape probability is overestimated. This effect is particularly noticeable in tight fuel lattices.

From before, the probability of colliding in the same fuel rod is:

$$P_{\mathrm{collide}}^{\text{same rod}} = (1 - P_{\mathrm{esc}}) = \frac{\Sigma_{\mathrm{t,f}}}{\Sigma_{\mathrm{e}} + \Sigma_{\mathrm{t,f}}} \ .$$

We define the Dancoff factor as:

$$\gamma \equiv \text{probability for an escaping neutron to collide in the moderator before another fuel rod}$$

We also define the 'sticking probability':

$$G \equiv \text{probability for a neutron entering the fuel to collide there}$$

Finally we distinguish between $P_{\mathrm{esc}}^{\mathrm{lattice}}$, the quantity that we want to obtain for a whole lattice system, and $P_{\mathrm{esc}}^{\mathrm{rod}} = P$, the probability of escaping from any given fuel pin.

Given these, the probability for a neutron born in fuel to collide in fuel is:

$$\begin{aligned} P_{\mathrm{collide}}^{\mathrm{lattice}} = & \underbrace{1-P}_{\text{collide in the same rod}} + \underbrace{P(1-\gamma)G}_{\text{reach the next rod and collide}} + P(1-\gamma)(1-G)(1-\gamma)G + ... \\ & = 1 - P + P(1-\gamma)G\left[1 + (1-\gamma)(1-G) + ((1-\gamma)(1-G))^2 + ...\right] \\ & = 1 - P + P(1-\gamma)G\frac{1}{1-(1-\gamma)(1-G)} \\ & = 1 - P + \frac{P(1-\gamma)G}{\gamma + (1-\gamma)G} = \frac{\gamma(1-P) + (1-\gamma)G}{\gamma + (1-\gamma)G} \ . \end{aligned}$$

However, we need to somehow link G and P. This will be done with respect to Fig. 18.

The probability that a neutron, born uniformly along a chord through a pin, will not collide when travelling across a fuel region in a given direction is given as:

$$P(\mathbf{\Omega}, R) = \frac{1}{R}\int_0^R \exp\left(-\Sigma_{\mathrm{t,f}}r\right)\mathrm{d}r = \frac{1}{\Sigma_{\mathrm{t,f}}R}\left(1 - \exp\left(-\Sigma_{\mathrm{t,f}}R\right)\right) \ ,$$

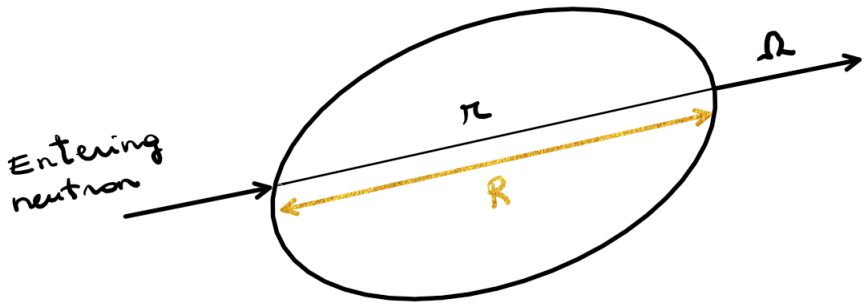


Figure 18: Geometry for estimating the sticking probability from the escape probability.

while the probability that a neutron, entering from the outside, will collide in the fuel along its way through is:

$$G(\mathbf{\Omega}, R) = 1 - \exp\left(-\Sigma_{\mathrm{t,f}} R\right) \ ,$$

so we know that:

$$G(\mathbf{\Omega}, R) = \Sigma_{\mathrm{t,f}} R P(\mathbf{\Omega}, R) \ .$$

It can be proven that this relationship also holds for the average values:

$$\langle G \rangle = \Sigma_{\mathrm{t,f}} \langle R \rangle \langle P \rangle = \Sigma_{\mathrm{t,f}} \bar{l} \langle P \rangle \tag{20}$$

Hence, if we equate $P = \frac{a_{\mathrm{B}}}{a_{\mathrm{B}} + \Sigma_{\mathrm{t,f}} \bar{l}}$, we get

$$\begin{aligned} P_{\text{collide}}^{\text{lattice}} &= \frac{\gamma(1-P) + (1-\gamma)\Sigma_{\mathrm{t,f}} \bar{l} P}{\gamma + (1-\gamma)\Sigma_{\mathrm{t,f}} \bar{l} P} = \frac{\frac{\gamma \Sigma_{\mathrm{t,f}} \bar{l}}{a_{\mathrm{B}} + \Sigma_{\mathrm{t,f}} \bar{l}} + (1-\gamma)\frac{a_{\mathrm{B}} \Sigma_{\mathrm{t,f}} \bar{l}}{a_{\mathrm{B}} + \Sigma_{\mathrm{t,f}} \bar{l}}}{\gamma + (1-\gamma)\frac{a_{\mathrm{B}} \Sigma_{\mathrm{t,f}} \bar{l}}{a_{\mathrm{B}} + \Sigma_{\mathrm{t,f}} \bar{l}}} \\ &= \frac{\gamma \Sigma_{\mathrm{t,f}} \bar{l} + (1-\gamma) a_{\mathrm{B}} \Sigma_{\mathrm{t,f}} \bar{l}}{\gamma a_{\mathrm{B}} + \gamma \Sigma_{\mathrm{t,f}} \bar{l} + (1-\gamma) a_{\mathrm{B}} \Sigma_{\mathrm{t,f}} \bar{l}} = \frac{\gamma + (1-\gamma) a_{\mathrm{B}}}{\gamma \frac{a_{\mathrm{B}}}{\Sigma_{\mathrm{t,f}} \bar{l}} + \gamma + (1-\gamma) a_{\mathrm{B}}} \\ &= \frac{1}{\frac{\gamma a_{\mathrm{B}}}{\Sigma_{\mathrm{t,f}} \bar{l} (\gamma + (1-\gamma) a_{\mathrm{B}})} + 1} = \frac{\Sigma_{\mathrm{t,f}}}{\frac{\gamma a_{\mathrm{B}} \Sigma_{\mathrm{e}}}{\gamma + a_{\mathrm{B}}(1-\gamma)} + \Sigma_{\mathrm{t,f}}} = \frac{\Sigma_{\mathrm{t,f}}}{\Sigma_{\mathrm{t,f}} + \frac{\Sigma_{\mathrm{e}}}{1/a_{\mathrm{B}} + 1/\gamma - 1}} \ . \end{aligned}$$

This means that the Dancoff correction is another 'straightforward' modification to our equivalence theory procedure where our escape cross section takes on a slightly modified form.

The procedure to calculate γ can be involved. In modern codes, this is often done with ray tracing, e.g., through the method of characteristics.

8 Conclusions

We have developed equivalence theory, the approach used in most lattice physics codes to estimate cross sections in the resonance region of the spectrum for reactor calculations.

Despite being popular and widely used, equivalence theory has several deficiencies. For example, it does not account for resonance overlap (this can be significant for Sm149 and U238, for example), nor does it account for inelastic scattering (which is very significant in fast reactor physics and leads to significant energy loss). These can be accounted for with semi-empirical means (like resonance interference tables) or by more sophisticated (and more expensive) approaches.

There are several alternatives to equivalence theory: at the extreme end, the full slowing down equation could be solved in many groups and is done increasingly commonly, but this can be extremely slow. Likewise, it is common to simply generate cross sections via Monte Carlo – while also slow, this is easier to implement and use than a lattice physics code and exactly treats geometry. These approaches tend not to be necessary unless the spectrum is fast (e.g., the common use case for ECCO), there is significant burn-up occurring or, for Monte Carlo in particular, the geometry deviates significantly from a large LWR.

There are several important topics which have not been covered in these lectures which are also very important for cross section generation. One is scattering anisotropy: we typically perform transport simulations approximating scattering as isotropic – but this is not the case. The way around this is to perform a 'transport correction', accounting for the (mainly hydrogen-induced) linear anisotropy by having neutrons fly further before colliding (reducing the total cross section) while retaining an isotropic scattering kernel. Choosing how to do this correction is a subject of some interest, although there seems to be increasing concensus about how best to do it for LWRs at least. Another important topic is leakage correction: lattice physics works by assuming that the spectra of pins and assemblies are essentially only determined by their local surroundings, and not their position within the reactor core. This is done by imposing reflective boundaries, i.e., there is no net leakage from an assembly. In a real reactor, there is of course net leakage from certain assemblies to their neighbours (giving the cosine/Bessel shape) or even strongly dissimilar neighbours, which will induce a change in the spectrum from the reflected system. There are techniques to account for this in the generation of cross sections also.

Following such calculations, what next? This is shown in Fig. 19. In the typical LWR calculation sequence, equivalence theory calculations will have been performed for however many pin cells are present in a given assembly type, producing shielded cross sections in the group structure of the code's library. This tends to be $\mathcal{O}(100)$ groups these days. However, to account more accurately for spatial self-shielding, additional calculations are done where the inter-pin effects are accounted for. These tend to take the form of a series of collision probability calculations to condense the group structure down further, followed by method of characteristics calculations to evaluate the assembly-level spatial effects. At the conclusion of this, these cross sections are condensed to produce assembly-averaged cross sections for nodal codes. This process is repeated for all temperature, density, and burn-up conditions to which an assembly might reasonably be subjected.

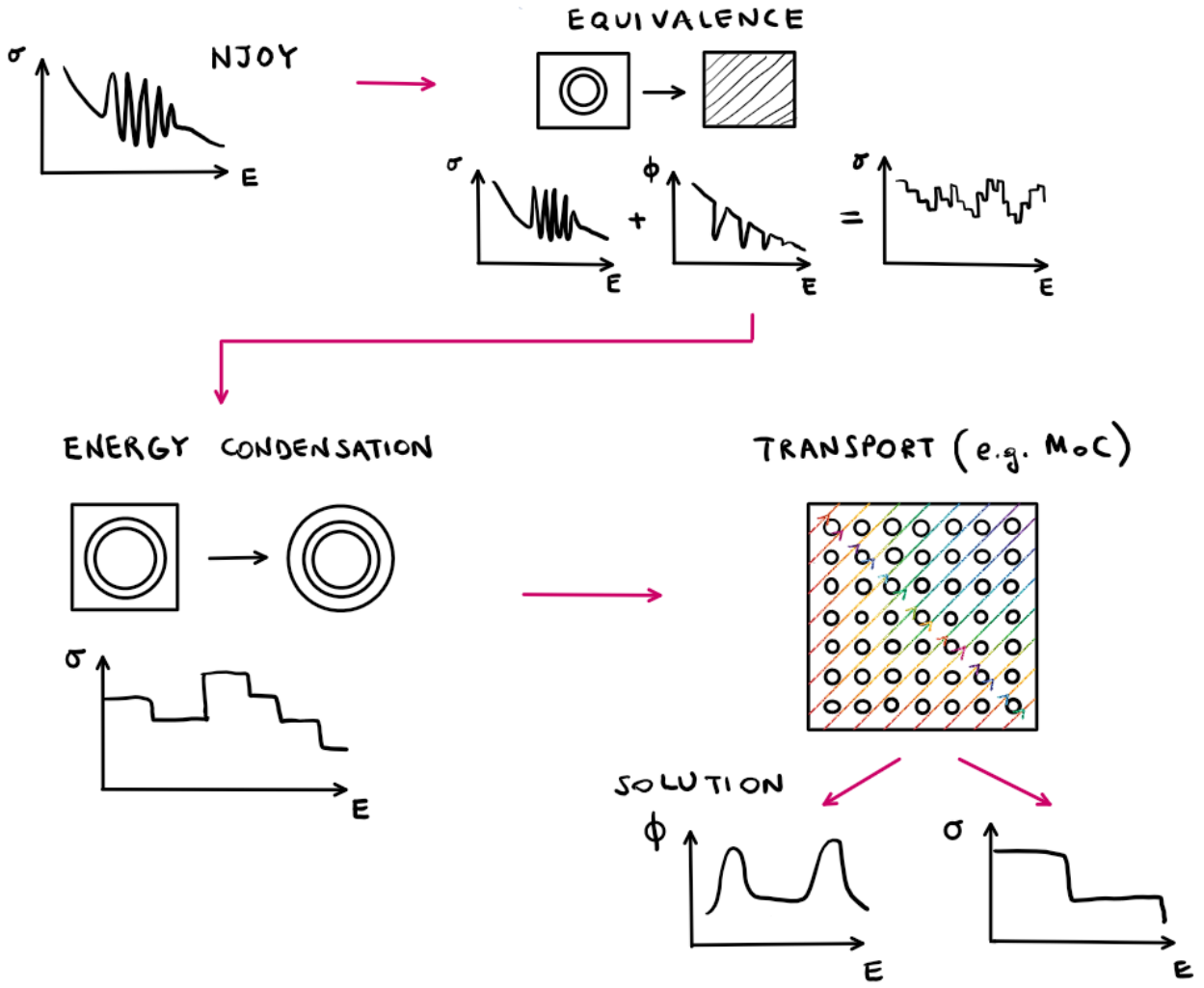


Figure 19: The usual flow of modern LWR lattice physics codes. NJOY provides processed nuclear data. Equivalence theory is applied to all pin cells to produce self-shielded cross sections in the library fine multi-group structure. Energy condensation is performed at a pin cell level using a collision probabilities solver. Assembly-level transport is performed using a transport solver, producing cross sections for a nodal code, or producing the final solution in some cases.