Chapter 1: Useful definitions

1.1. Cross-sections (review)

The Nuclear and Radiochemistry class, listed as a prerequisite, is a good place to start. The understanding of a cross-section being fundamental in this course, I will review it quickly.

1.1.1. So, what is a cross-section ?

The short story is : “The cross-section represents the probability of an interaction”. Now, that is a quite good story, but it lacks substance, don’t you think ? Well, I agree, which is why I happily refer you to the previously cited class (chapter 3).

As you thus already know, a cross-section can be microscopic, meaning that it is characteristic of an individual target, or macroscopic, meaning that it is characteristic of a material containing a large number of targets.

1.1.2. Microscopic cross-section

It is very important to start by defining some of the vocabulary you’ll have to know when talking of neutron-induced reactions.
First, “scattering”. This refers to any reaction that re-emits a neutron. This can be compared with a bouncing effect of the neutron on the atom.
Second, “absorption”. No surprise here, ladies and gentlemen. This simply indicates that the neutron was absorbed by the atom it collided with.

Now, the absorption has two different consequences. It either induces the “fission” of the atom that absorbed the neutron, i.e. the atom breaks into two smaller atoms and gives away neutrons, or it induces a “capture”, i.e. the atom “accepts” the additional neutron and is transformed into another atom, an isotope of the first atom.
In a mathematical form, we can write :

$$\sigma_a = \sigma_f + \sigma_c,$$

where σ_f and σ_c are respectively the fission and the capture cross-section.

Now, all that means that we have a total microscopic cross-section that can be expressed as the sum of the absorption cross-section and the scattering cross-section. Indeed, the absorption cross-section represents the probability that the neutron is absorbed (and then induces fission or capture), and the scattering cross-section the probability that the neutron is scattered. As those are the only options for the interactions, it represents the total cross-section.
Therefore, we can write :

$$\sigma_t = \sigma_s + \sigma_a,$$

where σ_s and σ_a are respectively the scattering and the absorption cross-section.
The microscopic cross-section can be *considered* as an area of interaction. The larger the area, the higher the probability of interaction. Note that the largeness of this "area" does not depend on the size of the atom itself, no, in fact it takes into account the energy of the incoming particle, neutron in our case, among other factors. As a sort of area, the unit of a microscopic cross-section is m^2. The area we're talking about being very small (of the order of$10^{-24}cm^2$), physicists have created a specific unit, the barn (b), to express those quantities.

$$1\ barn\ = 10^{-28}m^2.$$

1.1.3. Macroscopic cross-section

Now that we have seen the case of an individual target, let's look at a higher level, with a large number of targets. Imagine a neutron travelling in matter, which the neutron "sees" as if it were a vacuum with nuclei here and there, since the neutron is unaware of electrons. It therefore travels in a straight line at a constant speed until it hits a nucleus in its path, very much like a flipper game. For a short path dx, this collision probability is infinitesimal and proportional to the distance dx. This translates into : "the path is twice as long ? Then the probability of interaction is twice as high".
This probability can be written as $\Sigma.dx$ where Σ is the appropriate proportionality coefficient, called macroscopic cross-section. Neutron physicists generally use the centimetre as the unit of length for their calculations (order of magnitude for typical materials), and so macroscopic cross-sections are expressed in cm^{-1}.

Let us calculate the probability relationship that governs the distance x between the starting point of the neutron and the point where it will have its first collision.

So, the first collision takes place between x and x+dx:

- *if* the neutron has had no collision between 0 and x
    - This probability is denoted $Q(x)$,
- *and if* the neutron has a collision$x$ and x+dx
    - by definition, this probability is $\Sigma.dx$

The probability of the collision happening between x and x+dx is therefore :

$$p(x).dx = Q(x) * \Sigma.dx,$$

where $p(x)$ is the probability density function.

Now, we need to calculate $Q(x)$.

In order to do that, we must realize that $Q(x+dx)$ -- the probability of no collision over the distance $x+dx$-- is the product of :

- the probability of no collision between 0 and x, i.e. $Q(x)$;
    - Indeed, the neutron has to not collide before that point
- the probability of no collision between x and $x+dx$, i.e., by definition, $1-\Sigma.dx$.
    - Indeed, the neutron must not collide before $x+dx$ but is assumed to collide at $x+dx$

This gives :

$$Q(x+dx) = Q(x) * (1 - \Sigma.dx)$$

We can notice that $Q(0) = 1$ by definition. Indeed, it is given that the neutron has not collided at its exact starting point, because, well, we say so by defining 0 as the starting point. This allows us to simplify the previous equation and obtain :

$$Q(x) = e^{-\Sigma x},$$

Question n°1 : ✪

Please demonstrate why $Q(x) = e^{-\Sigma x}$.

Rewriting the previous equation with the explicit expression of $Q(x)$, we find that :

$$p(x).dx = Q(x) * \Sigma.dx = e^{-\Sigma x} * \Sigma.dx$$

We have thus calculated the probability of the collision happening between x and $x+dx$, $p(x).dx$.

This allows us to calculate the mean free path of the neutrons λ, i.e. the average value of the distance x at which the first collision occurs. This is the inverse of the macroscopic cross-section :

$$\lambda = \frac{1}{\Sigma}$$

Question n°2 : ✪✪✪

Please demonstrate why $\lambda = \frac{1}{\Sigma}$. *(Hint : $\lambda = \langle x \rangle$, "the average value of the distance x at which the first collision occurs")*

Finally, one can express the macroscopic cross-section as a function of the density of obstacles (nuclei) on the way and the probability of interacting with a specific obstacle (microscopic cross-section).

Indeed, the probability element $\Sigma.dx$ of interaction with matter for a path dx is quite obviously proportional to the number of obstacles the neutron is likely to encounter, and therefore to the number N of nuclei per unit volume ($\#.cm^{-3}$). Once again, one can try to visualize that by comparing with a flipper game. The proportionality coefficient is the probability of interaction with a specific target, the microscopic cross-section σ ($10^{24}\ barns = cm^2$).

We can thus write :

$$\Sigma = N.\sigma$$

1.2. Neutron density, neutron flux, reaction rate

In a nuclear reactor, the population of neutron is very small compared to the population of atoms (there is something like a 10^{15} factor !) . But that does not mean that it is a small population in and by itself, no. Indeed, there are of the order of 10^{14}neutrons per cubic meter in a nuclear reactor. This is why we use the concept of density and statistic to describe their behavior.

1.2.1. So, let's define the neutron density

Imagine a small cube, in the region of interest, whose edges length is dr, centered at a point $\vec{r}$. Its volume is therefore $dr * dr * dr$, that is d^3r. Then, consider you take a picture of that scene, and look at it later (indeed, everything is moving quite fast in there !). Then the average number of neutron found in this little cube is :

$$n(\vec{r}).d^3r,$$

where n is the density (number of neutrons observed per unit volume). Keep in mind that this is an average.

1.2.2. Reaction rate

Let's say that $n$does not depend on $\vec{r}$, (homogeneous repartition) for the sake of simplicity, and let's call v the speed of the neutrons. During a time interval dt, a neutron travels a path dx. A very simple and well-known formula gives us :

$$dx = v.dt$$

If we recall the previous section (macroscopic cross-section), we can remember that the probability of interaction of one neutron with matter over a path dx is $\Sigma.dx$.
This then translates to :

$$\Sigma.dx = \Sigma.v.dt$$

Note that the only thing done there was to inject the new expression of dx into the equation.

If you want to know the number of neutron-matter interactions taking place in the little cube we were considering -- in more mathematical terms in the volume element d^3r -- we just have to multiply the probability that one neutron interacts with matter by the average number of neutrons in that volume.
Thus, the number of neutron-matter interactions taking place in the volume element d^3r during a time dt is :

$$\Sigma.v.dt * n.d^3r$$

From that expression, we can obtain what is called the ***reaction rate*** R, which is the number of interactions per unit volume $d^3r$and unit time dt:

$$R = \Sigma . n . v$$

1.2.3. Neutron flux

If we look at the units of the product $n.v$, we can see that it is :

$$\#.m^{-3} * m.s^{-1} = \#.m^{-2}.s^{-1} ,$$

thus apparently a number of neutron going through a surface area during a given time. This has the dimension of a flux, doesn't it ? Yes, but it isn't a flux as we are used to see them. It has no connection to a surface, it is a volumetric quantity. We'll go ahead and call that a flux anyway, the ***angular flux***. Why do this if it isn't an actual flux ? Well, that's a historical definition, and things are really hard to change.

In the previous equation, I wrote Σ. This corresponded to the total macroscopic cross-section. One can notice that we can separate this total macroscopic cross-section into several interaction cross-sections (Σ_a for absorption, Σ_s for scattering), which yields to a specific reaction rate R per interaction. Just wanted to clarify that.

Thus, we finally obtain :

$$R = \Sigma . \Psi ,$$

where Σ represents the matter (as in "the cross-section depends on the matter density and other variables") and Ψ represents the neutron population.

1.3. The phase space

We have to use seven independent variables to describe the neutron population behavior in space and time :

- Space : (x, y, z)
- Velocity : (v_x, v_y, v_z)
- Time : t

One has to notice that this Cartesian coordinate system can be translated into a spherical one (you can see the "translation graph" on figure 1)

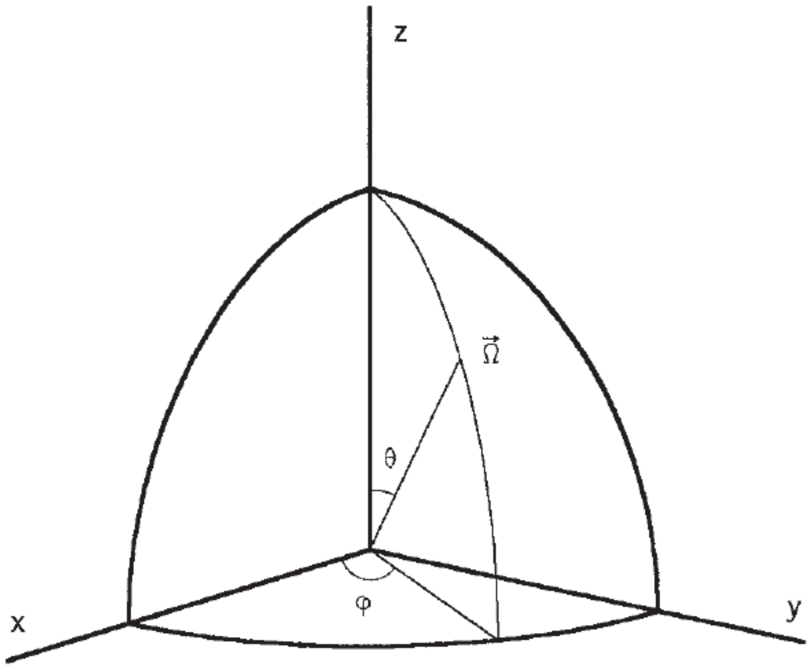

fig. 1

The materials inside the reactor are theoretically isotropic, which means that no matter which angle they're seen from, they have the same properties. Cross-sections are thus not dependent on the direction of the incident neutron, but only on its speed, and by speed I mean energy. Indeed, instead of velocity, we use kinetic energy (E) and direction ($\hat{\Omega}$) :

$$\vec{v} = v.\hat{\Omega} = \sqrt{\frac{2E}{m}}\hat{\Omega},$$

with the unit velocity vector $\hat{\Omega}$, identified by the two angles of the spherical coordinates (θ, φ) :

$$\hat{\Omega} = \frac{\vec{v}}{v}$$

We can keep in mind several useful formulas concerning $\hat{\Omega}$:

$$\Omega_x = sin(\theta)$$
$$\Omega_y = sin(\theta).sin(\varphi)$$
$$\Omega_z = cos(\theta)$$
$$d^2\Omega = sin(\theta).d\theta.d\varphi$$

So, that's all good and stuff, but what next ? Well, this takes us to the notion of ***angular density***, the n that we have talked about earlier. When I introduced this density, I did not consider speed nor time. This angular density depends on $(\vec{r}, \vec{v}, t)$.
So, $n(\vec{r}, \vec{v}, t).d^3r.d^3v$ is the number of neutrons in the volume d^3r around $\vec{r}$ and with their velocity in the "volume" (velocity space) d^3v around $\vec{v}$, at time t.
If, as we said earlier, we use E and $\hat{\Omega}$ instead of $\vec{v}$, we obtain $n(\vec{r}, E, \hat{\Omega}, t)$ instead of $n(\vec{r}, \vec{v}, t)$.

Then, the number of neutrons in the volume d^3r around $\vec{r}$, with energy between E and $E + dE$, and with their direction between $\hat{\Omega}$ and $\hat{\Omega} + d^2\Omega$, at time t, is :

$$n(\vec{r}, E, \hat{\Omega}, t). d^3r. dE. d^2\Omega$$

Consequently, the relationship between $n(\vec{r}, \vec{v}, t)$ and $n(\vec{r}, E, \hat{\Omega}, t)$ is given by the change of variables :

$$n(\vec{r}, \vec{v}, t). d^3r. d^3v = n(\vec{r}, E, \hat{\Omega}, t). d^3r. dE. d^2\Omega$$

Let us quickly come back to the fluxes for a moment. After all, it will be the main focus of our work later on.
We've seen that we can write the ***angular flux*** (not a "real" flux) as the product of the neutron density and their velocity, i.e. :

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

From there, it is also possible to define what we'll call the ***scalar flux***, $\phi(\vec{r}, E, t)$. The scalar flux is the angular flux integrated over all angles :

$$\phi(\vec{r}, E, t) = \int_{4\pi} d^2\,\Omega. \Psi(\vec{r}, E, \hat{\Omega}, t)$$

In a similar way, integrating over all angles the angular density gives us the energy dependent density :

$$n(\vec{r}, E, t) = \int_{4\pi} d^2\,\Omega. n(\vec{r}, E, \hat{\Omega}, t)$$

1.4. Concept of current

We've seen that neutron physicists used the term "flux" to describe something that, despite having the unit of a flux, was not a flux. And they've been consistent in this notation changes. That's why the term "current" is used, in neutronics, to denote what is known as "flux" in other branches of physics : the number of neutrons passing through a surface area, normalized per unit surface and unit time.

1.4.1. Angular current density

We can first define the ***angular current density*** $\vec{j}(\vec{r}, E, \hat{\Omega}, t)$, which is the angular flux $\Psi(\vec{r}, E, \hat{\Omega}, t)$ multiplied by the unit velocity vector $\hat{\Omega}$.

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

1.4.2. Neutron current

Now, consider a surface element $\overrightarrow{dS} = \widehat{n_s}.dS$, with surface area dS and located perpendicular to the unit vector $\widehat{n_s}$ (normal). Let's examine the neutrons with a given direction between $\hat{\Omega}$ and $\hat{\Omega} + d^2\Omega$. The situation can be seen on figure 2 below.

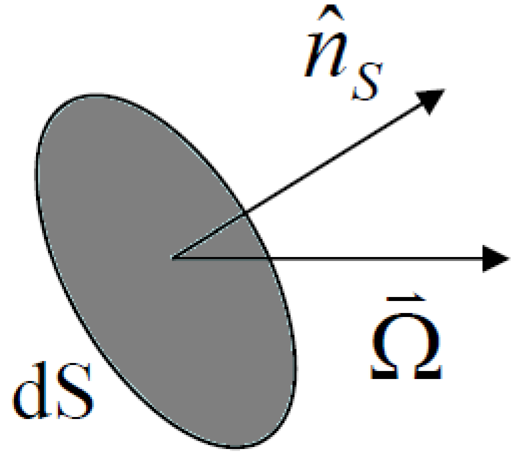

fig. 2

We can define the ***neutron current***, i.e. the number of neutrons with energy E and direction $\hat{\Omega}$ which cross the surface $\overrightarrow{dS}$ per unit time :

$$\widehat{n_s}.\vec{j}(\vec{r}, E, \hat{\Omega}, t).\overrightarrow{dS}.dE.d^2\Omega$$

1.4.3. Current density

As with the angular and scalar flux, one can integrate the ***angular current density*** $\vec{j}(\vec{r}, E, \hat{\Omega}, t)$ over all angle in order to obtain the ***current density*** $\vec{J}(\vec{r}, E, t)$.

$$\vec{J}(\vec{r}, E, t) = \int_{4\pi} d^2\Omega \, .\vec{j}(\vec{r}, E, \hat{\Omega}, t)$$

1.4.4. Partial currents

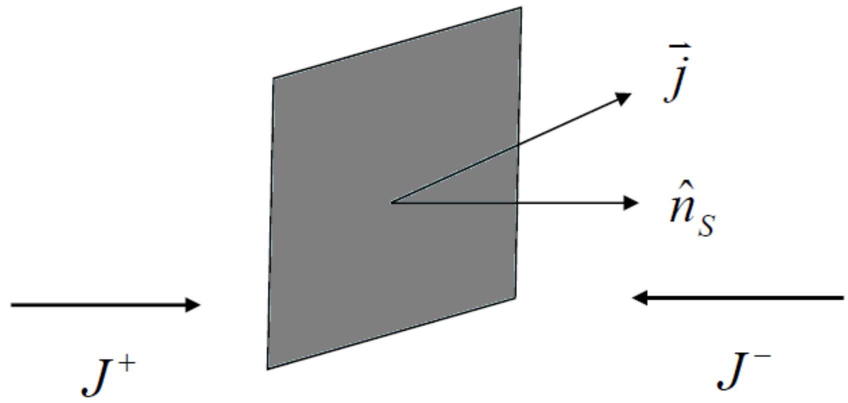

fig. 3

The current considers both neutrons going in a direction (following $\hat{n}_s$) and in the opposite direction ($-\widehat{n_s}$). Therefore, we can further define partial currents, J_+ and J_-.

$$J_+(\vec{r},E,t) = \int_{\widehat{n_s}.\vec{\Omega}>0} d^2\Omega \,.\widehat{n_s}.\vec{j}(\vec{r},E,\hat{\Omega},t)$$

$$J_-(\vec{r},E,t) = \int_{\widehat{n_s}.\vec{\Omega}<0} d^2\Omega \,.\widehat{n_s}.\vec{j}(\vec{r},E,\hat{\Omega},t)$$

It is useful to note that $\widehat{n_s}.\hat{\Omega} > 0$ indicates that the direction of the neutron projected on the normal is positive. This means that, if we look at figure 3 (or figure 2), the neutron with such direction $\hat{\Omega}$ is going from left to right, hence, J_+. Of course, $\widehat{n_s}.\hat{\Omega} < 0$ represents the opposite, hence J_-.

If the flux is isotropic, i.e. if it doesn't have a privileged direction (independent of $\hat{\Omega}$), then :

$$J_+(\vec{r},E,t) = J_-(\vec{r},E,t) = \frac{\phi(\vec{r},E,t)}{4}$$

<u>*Question n°3 :*</u> ✪✪

Please demonstrate why $J_+(\vec{r},E,t) = J_-(\vec{r},E,t) = \frac{\phi(\vec{r},E,t)}{4}$ in the case of an isotropic flux.

Well, this ends the first lecture. If you have any question, please let me know directly or post a thread in the dedicated subreddit. Do not forget, and I can't stress this enough : if you have a question, then someone else in the class is wondering the same thing, or should be. Therefore, asking it will help you and others.

The homework #1 (which will be the three questions that I've written in this lecture in order to give you context, as well as a bonus problem) can be difficult if you are not familiar with the mathematics involved. If you have any difficulty (it's definitely okay not to know how to integrate a "hidden" multiple integral), once again, use the discussion platform (refer to previous link) or email me directly.

There is another thing that I should say. If you do not understand something, do not feel like it's your fault, and do not give up. It merely means that my explanations were not good enough. I will gladly upgrade the class by taking into account your suggestions and remarks.