
Neutron and X-ray Scattering of Quantum Materials

PHYS-640

Week 1 solutions

1: Neutron production

(a) Hydrogen as a moderator

Exercise 4.P.1 in the neutron notes.

The final energy of the neutron after the collision is:

$$E_{f,p} = \frac{1}{2}m_n v_{f,n}^2 = \frac{1}{2}m_n v_{i,n}^2 \cos^2 \varphi.$$

Now to average we need to integrate over all possible take-off angles which means first evaluating the average of $\cos^2 \varphi$:

$$\langle \cos^2 \varphi \rangle = \frac{1}{2\pi} \int_0^{2\pi} \cos^2 \varphi d\varphi = \frac{1}{4\pi} [\varphi + \sin \varphi \cos \varphi]_0^{2\pi} = \frac{1}{2}.$$

Plugging in that result and knowing the the initial neutron energy was $E_{i,n} = \frac{1}{2}m_n v_{i,n}^2$, we get:

$$\langle E_{f,p} \rangle = \frac{1}{2}m_n v_{i,n}^2 \langle \cos^2 \varphi \rangle = \frac{1}{2} \left(\frac{1}{2}m_n v_{i,n}^2 \right) = \frac{E_{i,n}}{2}.$$

Do we have to consider the neutron as relativistic particles before the moderation process? What about after?

Typical energies of neutrons right after production are in the MeV range. We can now use the rest mass of the neutron, $m_0 = 939.6 \text{ MeV}/c^2$, to estimate the speed of the neutron. From special relativity we have:

$$m = \frac{m_0}{\sqrt{1 - v^2/c^2}} \rightarrow \frac{v}{c} = \sqrt{1 - m_0^2/m^2} = 0.0461 \approx 5\%.$$

With the neutron travelling only at around 5% of the speed of light, we can safely use classical kinematics. As the neutron is much slower (meV range) after the moderator, this will hold even more. However, the neutron interaction with matter is far from classical and should be considered a quantum mechanical process.

(b) Wavelength distribution

The wavelengths of the neutrons coming from a moderator in thermal equilibrium at a given temperature, T , follow a Maxwell distribution as follows:

$$P(\lambda) \propto \frac{1}{\lambda^2} e^{\frac{-h^2}{2k_B m T \lambda^2}},$$

where λ is the neutron wavelength, h the Planck constant, k_B the Boltzmann constant and m the neutron mass.

- Show that the most probable kinetic energy is $E = k_B T$
- What is the most probable neutron wavelength at room temperature?

To find the most probable energy we need to find the maximum of $P(\lambda)$ with respect to the energy. So first we need to rewrite P in terms of the energy $E = \frac{\hbar^2 k^2}{2m} = \frac{(\frac{h}{2\pi})^2 (\frac{2\pi}{\lambda})^2}{2m} = \frac{h^2}{2m\lambda^2}$. We now see that $P(E) \propto E e^{-\frac{E}{k_B T}}$ and we can look for the maximum:

$$\frac{dP}{d\lambda} = e^{-\frac{E}{k_B T}} + E e^{-\frac{E}{k_B T}} \left(\frac{-1}{k_B T} \right) = \left(1 - \frac{E}{k_B T} \right) e^{-\frac{E}{k_B T}} = 0.$$

By definition $e^{-\frac{E}{k_B T}}$ is always finite and positive so it means that to solve the equation we must have $\left(1 - \frac{E}{k_B T} \right) = 0$ and therefore the most probable energy is $E = k_B T$.

To calculate the wavelength at this energy we simply solve $k_B T = \frac{h^2}{2m\lambda^2}$ which gives $\lambda = \frac{h}{\sqrt{2mk_B T}}$. Plugging in room temperature ($T = 300$ K) then results in $\lambda = 1.78$ Å.

2: Neutron interaction with matter

(a) Scattering cross section

Exercise 2.P.1 in the neutron notes.

1. The neutron flux is $\Psi = \frac{N}{A}$.
2. The situation is sketched in Fig. (a). The probability for one neutron to hit the nucleus is $P = \frac{4\pi b^2}{A} N$ where $4\pi b^2$ is the area of the nucleus.
3. To get the cross section we have to normalize with respect to the neutron flux: $\sigma = \frac{P}{\Psi} = 4\pi b^2$.

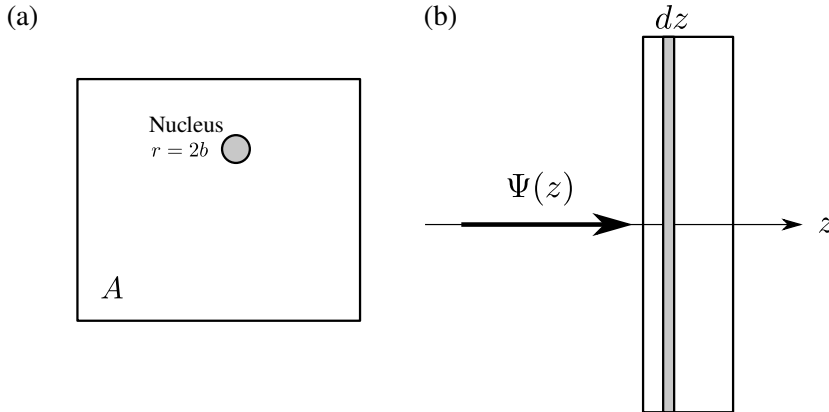


Figure 1: (a) A single nucleus with radius $r = 2b$ sitting inside the area A . (b) Neutrons hitting a material and getting absorbed.

(b) Attenuation

Exercise 2.P.2 in the neutron notes.

1. The number of neutron absorbed or scattered in a small portion of the slab, dz , is $\Psi(z)\Sigma_t Adz$. This corresponds to the difference the number of neutrons at z and $z + dz$, $-Ad\Psi(z)$. The minus sign reflects the fact that the neutron flux decreases. We therefore end up with the following differential equation:

$$\frac{d\Psi(z)}{dz} = -\Sigma_t \Psi(z) \Rightarrow \Psi(z) = \Psi_0 e^{-\Sigma_t z}$$

2. The volume specific cross section is given by the sum of the absorption and scattering cross sections, $\Sigma_t = \Sigma_s + \Sigma_a$, which means that the number of neutrons absorbed or scattering can be

written as $\Psi(z)(\Sigma_s + \Sigma_a)Adz$ leading to:

$$\frac{d\Psi(z)}{dz} = -(\Sigma_s + \Sigma_a)\Psi(z) \quad \Rightarrow \quad \Psi(z) = \Psi_0 e^{-(\Sigma_s + \Sigma_a)z}.$$

This means that the attenuation coefficient is also just simply a sum of the two contributions, $\mu = \Sigma_s + \Sigma_a$.

(c) Incoherent cross section

Exercise 2.P.4 in the neutron notes

First we evaluate the absolute square of the sum of the two exponential functions (assuming that the scattering lengths are real) in Eq. (2.35) of the neutron notes:

$$\begin{aligned} \left\langle \frac{d\sigma}{d\Omega} \right\rangle &= \left\langle \left| b_j e^{i\mathbf{q} \cdot \mathbf{r}_j} + b_{j'} e^{i\mathbf{q} \cdot \mathbf{r}_{j'}} \right|^2 \right\rangle \\ &= \left\langle (b_j e^{i\mathbf{q} \cdot \mathbf{r}_j} + b_{j'} e^{i\mathbf{q} \cdot \mathbf{r}_{j'}}) (b_j e^{-i\mathbf{q} \cdot \mathbf{r}_j} + b_{j'} e^{-i\mathbf{q} \cdot \mathbf{r}_{j'}}) \right\rangle \\ &= \left\langle b_j^2 + b_j b_{j'} e^{i\mathbf{q} \cdot (\mathbf{r}_j - \mathbf{r}_{j'})} + b_{j'} b_j e^{i\mathbf{q} \cdot (\mathbf{r}_{j'} - \mathbf{r}_j)} + b_{j'}^2 \right\rangle \\ &= \left\langle b_j^2 + b_{j'}^2 + 2b_j b_{j'} \cos(\mathbf{q} \cdot (\mathbf{r}_{j'} - \mathbf{r}_j)) \right\rangle \\ &= \langle b_j^2 \rangle + \langle b_{j'}^2 \rangle + 2 \langle b_j b_{j'} \rangle \cos(\mathbf{q} \cdot (\mathbf{r}_{j'} - \mathbf{r}_j)). \end{aligned}$$

To go further we need to figure out what is $\langle b_j \rangle$ and $\langle b_j b_{j'} \rangle$. For the latter, we can immediately write $\langle b_j b_{j'} \rangle = \langle b_j \rangle \langle b_{j'} \rangle$ since the variation in scattering lengths on two sites is not correlated. From Eq. (2.35) in the neutron notes, we have $b_j = \langle b_j \rangle + \delta b_j$ which means that $b_j^2 = \langle b_j \rangle^2 + (\delta b_j)^2 + 2 \langle b_j \rangle \delta b_j$. Now, b_j and δb_j are not correlated and $\langle \delta b_j \rangle = 0$ per definition. Therefore, we can write $\langle b_j^2 \rangle = \langle b_j \rangle^2 + \langle (\delta b_j)^2 \rangle$. Putting all that together, the differential cross section becomes:

$$\left\langle \frac{d\sigma}{d\Omega} \right\rangle = \langle b_j \rangle^2 + \langle (\delta b_j)^2 \rangle + \langle b_{j'} \rangle^2 + \langle (\delta b_{j'})^2 \rangle + 2 \langle b_j \rangle \langle b_{j'} \rangle \cos(\mathbf{q} \cdot (\mathbf{r}_{j'} - \mathbf{r}_j)),$$

which is then basically Eq. (2.36).

Now instead of just two nuclei, we put N of them and perform the same derivation:

$$\begin{aligned} \left\langle \frac{d\sigma}{d\Omega} \right\rangle &= \left\langle \left| \sum_{j=1}^N b_j e^{i\mathbf{q} \cdot \mathbf{r}_j} \right|^2 \right\rangle \\ &= \left\langle (b_1 e^{i\mathbf{q} \cdot \mathbf{r}_1} + b_2 e^{i\mathbf{q} \cdot \mathbf{r}_2} + b_3 e^{i\mathbf{q} \cdot \mathbf{r}_3} + \dots) (b_1 e^{-i\mathbf{q} \cdot \mathbf{r}_1} + b_2 e^{-i\mathbf{q} \cdot \mathbf{r}_2} + b_3 e^{-i\mathbf{q} \cdot \mathbf{r}_3} + \dots) \right\rangle \\ &= \left\langle \left(b_1^2 + b_1 b_2 e^{i\mathbf{q} \cdot (\mathbf{r}_1 - \mathbf{r}_2)} + b_1 b_3 e^{i\mathbf{q} \cdot (\mathbf{r}_1 - \mathbf{r}_3)} + \dots \right) + \left(b_2^2 + b_2 b_1 e^{i\mathbf{q} \cdot (\mathbf{r}_2 - \mathbf{r}_1)} + b_2 b_3 e^{i\mathbf{q} \cdot (\mathbf{r}_2 - \mathbf{r}_3)} + \dots \right) \right. \\ &\quad \left. + \left(b_3^2 + b_3 b_1 e^{i\mathbf{q} \cdot (\mathbf{r}_3 - \mathbf{r}_1)} + b_3 b_2 e^{i\mathbf{q} \cdot (\mathbf{r}_3 - \mathbf{r}_2)} + \dots \right) + \dots \right\rangle \\ &= \left\langle \sum_{n=1}^N b_j^2 + 2 \sum_{j,j'}^N b_j b_{j'} e^{i\mathbf{q} \cdot (\mathbf{r}_j - \mathbf{r}_{j'})} \right\rangle. \end{aligned}$$

Using again $\langle b_j^2 \rangle = \langle b_j \rangle^2 + \langle (\delta b_j)^2 \rangle$ and $\langle b_j b_{j'} \rangle = \langle b_j \rangle \langle b_{j'} \rangle$ yields:

$$\left\langle \frac{d\sigma}{d\Omega} \right\rangle = \sum_{n=1}^N \langle (\delta b_j)^2 \rangle + \left| \sum_{j=1}^N \langle b_j \rangle e^{i\mathbf{q} \cdot \mathbf{r}_j} \right|^2,$$

where the two terms correspond to incoherent and coherent scattering respectively.

(d) Material selection

Exercise 2.P.5 in the neutron notes

1. The incoherent scattering cross section for hydrogen (^1H) is $\sigma_{\text{inc},^1\text{H}} = 80.27$ barn whereas for deuterium (^2H) it is $\sigma_{\text{inc},^2\text{H}} = 2.05$. This means that using deuterated organic samples would reduce the incoherent background significantly.

. Vanadium has incoherent scattering cross section $\sigma_{\text{inc},\text{V}} = 5.08$ barn and almost no coherent scattering cross section. This metal is therefore well suited for detector efficiency measurements.

3. The incoherent scattering from hydrogen is strong so any hydrogen-containing material also works well. Of these plastics are easily accessible.

4. Cadmium and gadolinium have large absorption cross sections ($\sigma_{\text{a,Cd}} = 2520$ barn and $\sigma_{\text{a,Gd}} = 49700$ barn) so they would serve well for neutron shielding. Ignoring the scattering cross section (which in both cases is much much smaller than the absorption) we can express the attenuation coefficient as $\mu = n \sigma_{\text{a}}$ where the number density is given as $n = \frac{1}{16 \text{Å}^3}$ (this number you can calculate from the molar and mass densities but it will be in that order for metals). The penetration depth is then $d = \frac{1}{\mu}$. Plugging in the numbers for cadmium and gadolinium we get $d_{\text{Cd}} = 63.5 \mu\text{m}$ and $d_{\text{Gd}} = 3.2 \mu\text{m}$.

5. The absorption cross sections for boron and nitrogen are $\sigma_{\text{a,B}} = 1.90$ barn and $\sigma_{\text{a,N}} = 767$ barn, respectively. The unit cell volume is given as $V_0 = 11.81 \text{Å}^3$ so that $n = \frac{1}{V_0}$ assuming one boron and one nitrogen atom per unit cell. That means the attenuation coefficient is $\mu = \frac{\sigma_{\text{a,B}} + \sigma_{\text{a,N}}}{V_0} \approx \frac{\sigma_{\text{a,N}}}{V_0}$. Again we ignore the scattering cross sections and the boron absorption is by far dominating the attenuation processes in the system. To find where the transmission is reduced to 10^{-6} of the incoming beam flux we need to solve the following equation:

$$10^{-6} = e^{-\mu z} \Rightarrow \ln(10^{-6}) = -\mu z \Rightarrow z = \frac{-\ln(10^{-6})}{\mu} = \frac{6V_0 \ln(10)}{\sigma_{\text{a,N}}} = 2.1 \text{ cm}.$$

This number is for 5 meV neutrons but since the absorption cross section scale with $\sqrt{E}$, that number increases to 4.3 cm for 20 meV neutrons and 9.5 cm for 180 meV neutrons.

6. Aluminium is cheap, relatively strong as well as easy to shape and then it has weak incoherent scattering ($\sigma_{\text{inc,Al}} = 0.0082$ barn) and weak absorption ($\sigma_{\text{a,Al}} = 0.231$ barn).