Neutron and X-ray Scattering of Quantum Materials

PHYS-640

Week 3 exercises

1: The time-of-flight experiment

(a) Derive Eq. (5.15) in the notes. What can be done to improve the wavelength resolution at an instrument?

The fastest and slowest neutrons arrive at the detector position, L, at $t_1 = \alpha L \lambda_1$ and $t_2 = \alpha L \lambda_2$, respectively, see Fig. 1. Now we require that $\Delta t < T$ to avoid frame overlap and this yields the following:

$$\Delta t = t_2 - t_1 = \alpha L(\lambda_2 - \lambda_1) = \alpha L \Delta\lambda < T,$$

when recognising $\Delta\lambda = \lambda_2 - \lambda_1$.

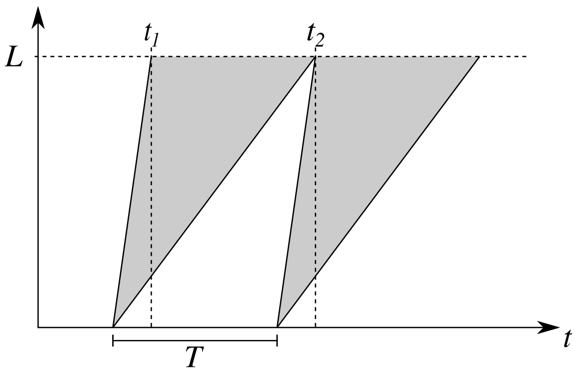

Figure 1: Time-of-flight diagram for a diffraction experiment with the detector positioned at L. The fastest neutron arrives at the detector at time t_1 and the slowest one at t_2. The period between neutron pulses is T.

(b) As seen from Eq. (5.14), we will need long guides to transport neutrons to the sample position. Calculate the critical angle for a guide with a single Ni layer and neutrons with energy, $E = 5$ meV.

The critical angle can be found using Eq. (5.1) where it is given that $q_{c,\mathrm{Ni}} = 0.0217\,\text{Å}^{-1}$:

$$q_c = 4\pi\frac{\theta_c}{\lambda} \quad \Leftrightarrow \quad \theta_c = \frac{q_c \lambda}{4\pi},$$

where we use $E = \frac{\hbar^2 k^2}{2m}$ and $k = \frac{2\pi}{\lambda}$ to find $\lambda = 4.045\,\text{Å}$ and then $\theta_{c,\mathrm{Ni}} = 0.40°$.

(c) The Spallation Neutron Source at the Oak Ridge National Laboratory in Tennessee, US, has neutron pulse frequency of 60 Hz. The SEQUOIA instrument is placed $L = 25$ m from the moderator and a wavelength band of $[0.2, 0.7]$ Å is needed for an experiment. Is frame overlap going to be a problem in this experiment?

Using Eq (5.15), we have $\Delta\lambda = 0.7 - 0.2 = 0.5\,\text{Å}$, $\alpha = 252.7\,\mu\text{s/m/Å}$ and thus $\alpha L \Delta\lambda = 3.16\,\text{ms}$. With $f = 60\,\text{Hz}$ we have $T = 16.7\,\text{ms}$ and thus $\alpha L \Delta\lambda < T$ is fulfilled and frame overlap will not be an issue in this experiment.

(d) Exercise 5.P.3 in the neutron notes.

From the de Broglie equation we can find the speed of a neutron with wavelength, λ:

$$\lambda = \frac{h}{p} = \frac{h}{mv} \quad \Leftrightarrow \quad v = \frac{h}{m\lambda}.$$

The time, t, it takes the neutron to travel through the velocity selector with length, L, is then:

$$v = \frac{L}{t} \quad \Leftrightarrow \quad t = \frac{L}{v} = \frac{mL\lambda}{h}.$$

The channels in the velocity selector are twisted by the angle φ as shown in Fig. 2. In order for the neutron to reach the other side without getting absorbed in the channel walls, the rotation angle, θ, completed during the time, t, must equal the twisting angle. From uniform circular motion we know that $\theta = \omega t$ where $\omega = 2\pi f$ is the angular frequency and f is the rotation frequency we are after. Putting all this together yields:

$$\theta = \omega t \quad \Rightarrow \quad \varphi = 2\pi f \frac{mL\lambda}{h} \quad \Leftrightarrow \quad f = \frac{h\varphi}{2\pi mL\lambda} = \frac{\hbar\varphi}{mL\lambda}.$$

Plugging in the numbers gives $f = 212.3\,\mathrm{Hz}$ or 12738 rpm (the unit most often used).

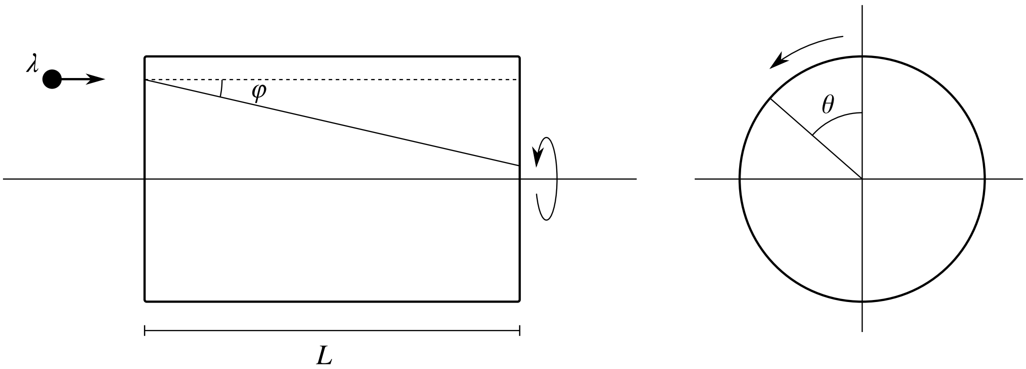

Figure 2: Sketch showing the side and end views of the velocity selector of length, $L = 0.25\,\mathrm{m}$, and twisting angle, $\varphi = 48.3°$, and the neutron travelling through the selector with wavelength, $\lambda = 10\,\text{Å}$.

2: Critical magnetic scattering of MnF_2

Do the McStass simulation exercise Tasks 0-5. We will save the analysis of the data (Task 6) for next week.

Solutions to the McStas entire exercise will follow next week.

3: The Be filter

Exercise 5.P.5 in the neutron notes.

1.
The shortest allowed reciprocal lattice vector, q_{cut}, or corresponding longest lattice plane distance, d_{cut}, limits the wavelength for which scattering can happen in the powder. Since $|\sin\theta| \leq 1$ then $\lambda_{\mathrm{cut}} = 2d_{\mathrm{cut}}$. This means that any neutron with longer wavelength than λ_{cut} goes straight through the powder without getting scattered.

2.
The shortest possible reciprocal lattice vector is for Be $(10\bar{1}0)$ (space group $P6_3/mmc$ no. 194). Using the formula for hexagonal closed packed structure, $\frac{1}{d^2} = \frac{4}{3}\left(\frac{H^2+HK+K^2}{a^2}\right) + \frac{L^2}{c^2}$, and with $H = 1$, $K = L = 0$, we get $d_{\mathrm{cut}} = 1.966\,\text{Å}$. Now $\lambda_{\mathrm{cut}} = 2d_{\mathrm{cut}} = 3.93$ Å and that corresponds to an energy of $E = \frac{h^2}{2m\lambda^2} = 5.29$ meV.

3.
Wavelengths above the cut-off are transmitted through the filter whereas the ones below get scattered and are therefore blocked from reaching the detector. Hence, a wavelength just above the cut-off (such as $\lambda = 4.05\,\text{Å}$ corresponding to $E = 5\,\text{meV}$) will go through the filter whereas the $\lambda/2$ contribution will get blocked.