Physics with neutrons 1

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Exercise sheet 12
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Exercise 12.1

We are interested in $\mathbf{Q}$, but we measure $\mathbf{k_i}$ and $\mathbf{k_f}$ (all measured in $^{-1}$) which are connected via

$$\mathbf{Q} = \mathbf{k_f} - \mathbf{k_i} \ . \tag{1}$$

1. Draw some possible scattering triangles for both elastic and inelastic scattering. What is the meaning of the direction of the $\mathbf{k}$ and $\mathbf{Q}$? Which experimental constraints do you expect?
2. Which absolute values $|\mathbf{Q}|$ can be reached in a scattering experiment as a function of $|\mathbf{k_i}|$, $|\mathbf{k_f}|$, and the scattering angle 2θ?
3. Show that this relation reduces to Bragg's law in the case of elastic scattering.
4. Basically, there are two classes of spectrometers: some fix $\mathbf{k_i}$, others $\mathbf{k_f}$ during an experiment. (It can also be varied which however requires a reconfiguration of the instrument.) Two examples at the FRM II are the time-of-flight spectrometer TOFTOF which works with a fixed $\mathbf{k_i}$ and the triple axis spectrometer PUMA which fixes $\mathbf{k_f}$. What are the consequences for the scattering triangles that can be realized during an experiment?
5. The energy change of the neutron is defined as $\Delta E = E_f - E_i$ (all measured in meV) with

$$E_{i/f} = \frac{\hbar^2 k_{i/f}^2}{2m_n} \ .$$

Which are the limits of ΔE for TOFTOF and PUMA, respectively?

Solution. 1. The direction of $\vec{k}$ is indeed the direction in which the neutrons propagate and therefore quite fixed (because, for example, the neutron source is always at the sample place). However, it is possible by turning the sample to have $\vec{Q}$ pointing in different directions in the reciprocal lattice of the crystal. As the crystal has to be mounted somehow, it will not be possible to turn it in *every* direction, therefore limiting the regions in reciprocal space that can be accessed by $\vec{Q}$. Also the scattering angle is limited: it cannot be 0° because the signal drowns there in the direct beam and it cannot be 180° because that would require to place the detector in the incoming beam.

2.

$$\vec{Q} = \vec{k_f} - \vec{k_i}$$

$$|Q|^2 = |\vec{k_f} - \vec{k_i}|^2 = |k_{f,x} - k_{i,x}|^2 + |k_{f,y} - k_{i,y}|^2 = |k_f|^2 + |k_i|^2 - 2|k_f||k_i| \cdot \cos(2\theta)$$

3.

$$
\begin{aligned}
|Q|^2 &= 2|k|^2 - 2|k|^2 \cdot \cos(2\theta) \\
&= \frac{2 \cdot 4\pi}{\lambda^2} \left(1 - \cos(2\theta)\right) \\
&= \frac{2 \cdot 4\pi}{\lambda^2} \left(1 - 2\sin^2\left(\frac{2\theta}{2}\right)\right) \\
&= \frac{16\pi^2}{\lambda^2} \sin^2\left(\frac{2\theta}{2}\right)
\end{aligned}
$$

4. When the initial wavevector (and therefore the initial energy) of the neutron is fixed, the maximal energy it can possibly lose is this initial energy. In contrast, the energy it can gain is unlimited.

   When the final energy of the neutron is fixed, the maximal energy it can gain is this final energy – and the energy it can lose is unlimited.

   a) TOFTOF: $\Delta E \in [-E_i, \infty[$

   b) PUMA: $\Delta E \in]-\infty, E_i]$.

5. TOFTOF:

$$
\begin{aligned}
|Q|^2 &= |k_f|^2 + |k_i|^2 - 2|k_f||k_i|\cos(2\theta) \\
&= \frac{2mE_f}{\hbar^2} + \frac{2mE_i}{\hbar^2} - 2\sqrt{\frac{2mE_f}{\hbar^2}}\sqrt{\frac{2mE_i}{\hbar^2}}\cos(2\theta) \\
&= \frac{2m}{\hbar^2}\left(2E_i + \Delta E - 2\sqrt{E_i(E_i + \Delta E)}\cos(2\theta)\right)
\end{aligned}
$$

   PUMA:

$$
\begin{aligned}
|Q|^2 &= |k_f|^2 + |k_i|^2 - 2|k_f||k_i|\cos(2\theta) \\
&= \dots \\
&= \frac{2m}{\hbar^2}\left(2E_f - \Delta E - 2\sqrt{E_f(E_f - \Delta E)}\cos(2\theta)\right)
\end{aligned}
$$

   There are effectively two variables: the length of the unit cell, a, and the slope at low k, which is the sound velocity.

□

Exercise 12.2

Most neutron experiments measure the scattering function $S(\mathbf{Q}, \omega)$. Neutron Spin-Echo (NSE) was introduced by Ferenc Mezei in the 1970s as a means of directly measuring $I(\mathbf{Q}, \tau)$, i.e. the Fourier-transform of the scattering function, the intermediate scattering function.
Derive the spin-echo condition for (quasi-)elastic scattering at a sample which links a change in the neutron energy to a change of the polarisation phase. Why is it possible to use a broad wavelength band $\delta\lambda/\lambda \sim 10^{-1}$ of incoming neutrons?

Solution. The fundamental idea of NSE is to follow the energy change of each individual neutron in the scattering process. The existence of the neutron spin allows us, recording information on its trajectory.

This procedure consists of the following steps:

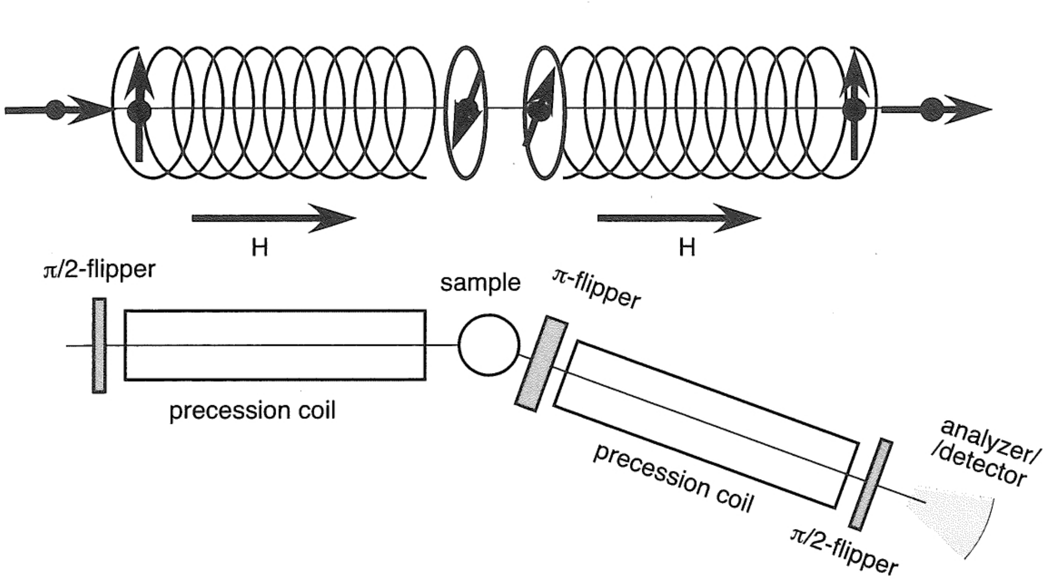

Figure 1: Schematic layout of a spin-echo spectrometer.

1. $\pi/2$ flip: The neutron beam, initially polarised parallel to the magnetic guide field (which stretches over the whole spectrometer) impinges on a flat flipper coil placed perpendicular to the beam. Inside this coil the spin of each neutron will be turned to 900 with respect to the guide field. This $\pi/2$ flip thus initiates Larmor precessions, which act as clocks keeping track of the time elapsed since the neutron hit the $\pi/2$ flipper.

2. Inside a magnetic field of variable strength the Larmor precession angle ϕ is proportional to the time the neutron spends traversing the field, i.e. it is a record of the individual neutron velocity v:

$$\phi = \gamma_L \cdot \frac{LH}{v}$$

   where the Larmor constant $\gamma_L = 2.916kHz/Oe$, H is the average strength of the magnetic field of length L.

3. π flip: One of the two components of the neutron spin in the plane of precession is inverted, the other one is left unchanged by a 180 turn around a properly chosen axis. This has the effect that the spin angle ϕ is transformed into $-\phi$ with respect to this axis.

4. Scattering on the sample results in an energy change of the neutron

$$\hbar\omega = mv'^2/2 - mv^2/2 \cong mv(v' - v) \qquad (2)$$

   with a probability described by the dynamic structure factor $S(Q, \omega)$ of the sample. Here m is the neutron mass and v' the final neutron velocity. The relative velocity change is assumed to be small. The momentum transfer Q is

$$\hbar Q = mv' - mv.$$

5. Larmor precessions in a second field region will add another angle ϕ' to the apparent precession angle $-\phi$ up to the flipper at the sample:

$$-\phi + \phi' = -\frac{\gamma_L HL}{v} + \frac{\gamma_L H'L'}{v'}.$$

This can provide us with a measure of the change of neutron energy if $HL = H'L'$, i.e.

$$-\phi + \phi' = -\gamma_L HL \left(\frac{1}{v'} - \frac{1}{v} \right) \approx \gamma_L HL \frac{1}{v}(v' - v) \approx \frac{\gamma_L H'L'}{mv^3} \hbar\omega$$

where the approximation again applies to small velocity changes and we made use of Eq. (2).

6. $\pi/2$ flip and analyser: The 90 flip turns one (say x) component of the precessing polarisation parallel to the guide field direction (say z). The neutron polarisation is determined by supermirror analysers or polarized ^{3}He filter cells. The transmission coefficient of the analyser strongly depends on the P_z component of the beam polarisation. This allows us to determine

$$P = \frac{\int S(Q,\omega)\cos(\omega t) d\omega}{\int S(Q,\omega) d\omega}.$$

The nominator is just the cosine Fourier transform of $S(Q,\omega)$, which is the real part of the time dependent intermediate scattering function $I(Q,\omega)$. The denominator is just the static structure factor $S(Q)$, thus the directly observed result of a NSE experiment is

$$P = s(Q,t) = \frac{\Re(I(Q,t))}{S(Q)}$$

which by definition obeys the $s(Q, t = 0) = 1$ relation, and the normalized inter- mediate scattering function $s(Q,t)$ is basically identical with the so-called Kubo relaxation function.

Due to the velocity spread the beam suffers a depolarization in the precession coil, resulting in an average polarization

$$P = \langle \cos\phi \rangle = \int f(v) \cos(\phi(v)) dv.$$

However, the depolarization is reverted when traversing the second, identical coil with opposite direction of precession. Therefore, a relatively broad neutron wavelength band of the order $\delta\lambda/\lambda \sim 10^{-1}$ can be used, whereas in backscattering $\delta\lambda/\lambda \sim 10^{-4}$ is generally required. □