Physics with neutrons 2

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Exercise sheet 1
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EXERCISE 1.1

1. With which part of matter do neutrons and photons interact, respectively? What are the differences between light and neutron scattering?

2. What gives rise to coherent / incoherent scattering? Which information can be extracted from each of them?

3. Recall the most important facts about the structure factor $|S|^2$ and the form factor $|F|^2$.

Solution. 1. Whereas photons are scattered by the electrons, neutrons interact with the nuclei (and magnetic moments). Due to the mass of the neutron, the accessible momentum transfers are very different in an experiment (important for phonons).

2. The scattering of one scatterer is per se neither coherent nor incoherent. The part with a modulated intensity reflecting the internal structure of the sample is termed coherent. If the scatterers in the sample have different scattering cross sections (which is especially for neutrons the normal case as the cross section depends on the relative alignment of the spins), a part of the scattering does not completely destructively interfere so that it yields a Q independent term, the incoherent scattering.

   In elastic scattering, the incoherent term does not carry any information – this changes in inelastic scattering where the coherent term yields information about the pair correlation function and the incoherent term about the auto correlation function.

3. Both have in common that only the square of the absolute value can be measured.

   The structure factor $|S|^2$ describes the alignment of the unit cells.

   - It peaks at each reciprocal lattice vector. The corresponding peaks are called *Bragg peaks*.
   - Their height is $\propto N^2$, their width $\propto \frac{1}{N_k}$.
   - From the peak positions, one can determine
     - crystal system
     - Bravais lattice (from systematic extinctions)
     - macro-strain

- lattice constants.

- From the peak width, one obtains information about
  - particle size
  - shape of the particle
  - internal micro-strain.

The form factor $|F|^2$ describes the interior of the unit cell.

- It can only be measured as intensity of the reflections at the reciprocal lattice vectors (where the structure factor is not zero).
- It is the squared Fourier transform of the scattering potential.
- If the scattering results from a non-point-like particle (e. g. electrons for photons or magnetic moments for neutrons), the form factor diminishes with increasing Q, rendering only a few peaks at low Q observable (Fourier transform of unlike δ-function).
- The fact that the phases cannot be measured is called the *phase problem*. There are several methods to tackle it but it is never possible to completely resolve them.

□

EXERCISE 1.2

Verify the diffraction patterns of Fig. 1. The atomic positions of NaH and NaD in the fcc unit cell are defined by

$$\mathbf{b}_{Na} = a(0,0,0), a(1/2,1/2,0), a(1/2,0,1/2), a(0,1/2,1/2)$$
$$\mathbf{b}_{H/D} = a(1/2,0,0), a(0,1/2,0), a(0,0,1/2), a(1/2,1/2,1/2)$$

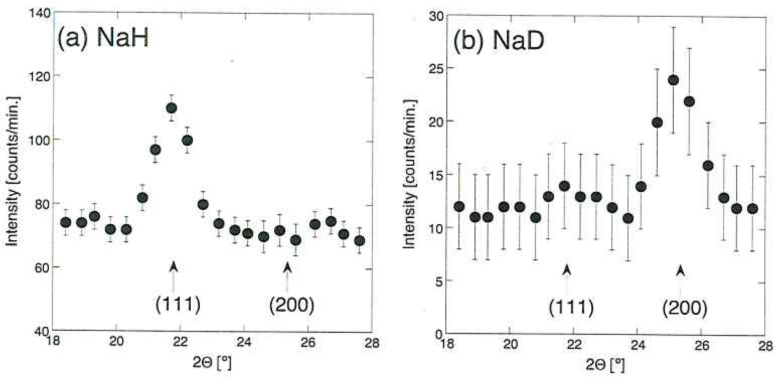

Figure 1: Neutron diffraction patterns obatined for NaH and NaD at room temperature (Shull *et al.*, 1948)

Solution. [1] The structure factor is given as

$$S_\tau = \sum_{\mathbf{d}} b_{\mathbf{d}} e^{i\tau\mathbf{d}}$$

Therefore,

$$\begin{aligned} S_{111} &= b_{\text{Na}} e^{i\tau_{111}\cdot\mathbf{d}_{\text{Na}}} + b_{\text{H/D}} e^{i\tau_{111}\cdot\mathbf{d}_{\text{H/D}}} \\ &= b_{\text{Na}}\left(1 + e^{2\pi i}\right) + 4b_{\text{H/D}} e^{i\pi} = 4(b_{\text{Na}} - b_{\text{H/D}}) \end{aligned}$$

and

$$S_{200} = b_{\text{Na}}\left(2 + 2e^{2\pi i}\right) + b_{\text{H/D}}\left(2 + 2e^{2\pi i}\right) = 4(b_{\text{Na}} + b_{\text{H/D}}).$$

Calculating the structure factor using the scattering lengths as given in e.g. Furrer et al. leads to

$\lvert S_{hkl}\rvert^2$	NaH	NaD
$\lvert S_{111}\rvert^2$	$8.69 \cdot 10^{-24}\,\text{cm}^2$	$1.48 \cdot 10^{-24}\,\text{cm}^2$
$\lvert S_{200}\rvert^2$	$0.002 \cdot 10^{-24}\,\text{cm}^2$	$17.11 \cdot 10^{-24}\,\text{cm}^2$

□

[1] Furrer A. et al., Neutron scattering in condensed matter physics, Singapore: World Scientific, 2009