

# Physics with Neutrons I

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## Exercise sheet 4

<https://wiki.mlz-garching.de/n-lecture06:index>

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**Due on 23.11.2017**

### 1. 1D Reciprocal Lattice

For the scattering computations from a simple cubic lattice, so far, we have simplified the crystal to a 1 dimensional lattice, with point-like atoms at equal distance. Instead of computing the scattering pattern by summing up over all scattered waves, we have learned in the lecture, that the scattering function is also given by the Fourier transform of the scattering structure in real space.

Assume a 1D chain of point-like atoms (delta functions) with distance  $d$  and follow the steps below.

- Express the linear chain of Atoms in form of a function  $f(r)$ .
- Form the Fourier transform of this function and evaluate it by assuming an infinite number of atoms. What is the meaning of  $k$ ?

$$FT(f(r)) = f(k) = \frac{1}{\sqrt{2\pi}} \int f(r) \exp(-ikr) dr$$

- The Fourier transform will have the same general form as the real space function with a different spacing  $p$ . How are  $d$  and  $p$  related?
- (optional) Compute the Fourier transform for limited numbers of Atoms in the chain and compare it to the results previously obtained by Bragg scattering.

### 2. Ambiguity of the Scattering Intensity

In a scattering experiment, we can only measure the scattering intensity  $I(k) = |f(k)|^2$ . Since  $f(k)$  is complex, we lose a part of the information contained in it, i.e. the imaginary part (or phase). To illustrate this, we take a look at a small chain of 4 atoms which have a gaussian shape:

$$f_l(x) = \frac{1}{\sqrt{2\pi\sigma_l^2}} \exp\left(-\frac{(x-r_l)^2}{2\sigma_l^2}\right)$$

where each atom  $l$  has a position  $r_l$  and a standard deviation  $\sigma_l$ . The scattering pattern is again given by the Fourier transform  $FT(f(x)) = f(k)$ , with the the Fourier transform of a single gaussian:

$$FT(f_l(x)) = f_l(k) = \exp(-ikr_l) \exp\left(-\frac{1}{2}\sigma_l^2 k^2\right)$$

Compute the scattering function  $f(k)$  and visualize the Intensity, real part and imaginary part and compare them for the following cases:

- All 4 atoms are equidistant with  $d = 3\text{\AA}$  and have the same shape  $\sigma_l = 0.5$ .
- As before, but shift all atoms by  $1\text{\AA}$ .
- All atoms are equidistant, but have a different shape  $\sigma_l = [0.1, 0.2, 0.3, 0.4]\text{\AA}$ .
- As before, but reverse the order of  $\sigma_l$

### 3. 2D Reciprocal Lattice

Now, we go a step further and consider a two dimensional rectangular lattice of point-like atoms (delta functions) with lattice distances  $d_x = 2\text{\AA}$  in x-direction and  $d_y = 3\text{\AA}$  in y-direction. The positions of all atoms are now  $r_l = m_l\vec{a}_1 + n_l\vec{a}_2$  with integers  $m_l, n_l$  and the basis vectors of the lattice  $\vec{a}_1$  and  $\vec{a}_2$ :

$$\vec{a}_1 = \begin{pmatrix} d_x \\ 0 \end{pmatrix}, \vec{a}_2 = \begin{pmatrix} 0 \\ d_y \end{pmatrix}$$

Analogous to the 1D case, this 2D lattice can be formulated as a function  $f(\vec{r})$  and Fourier transformed to obtain the scattering function  $f(\vec{k})$ . The result is again a regular structure which is called the reciprocal lattice of the crystal. The basis vectors of the reciprocal lattice  $\vec{b}_1$  and  $\vec{b}_2$  are then defined such that:

$$\vec{a}_l \cdot \vec{b}_m = 2\pi\delta_{lm}$$

- Draw the real and reciprocal lattice.
- What does the crystal unit cell and first Brillouin zone look like?
- In the real lattice, each point represents the position of an atom. What is the meaning of each point in the reciprocal lattice?
- Repeat the previous steps for a hexagonal lattice with lattice distance  $d = 3\text{\AA}$ .

### 4. Internal Structure

The previous example of a 2D crystal lattice assumed point like atoms, which is reasonable if we only consider the size of a nucleus (and its interaction potential) compared to the neutron wavelength. However, in real materials this assumption is typically not correct. Possible reasons might be a crystal with more than one Atom per unit cell or scatterers which are not atoms at all, e.g. larger molecules or magnetic structures. Similarly, thermal motion of the atoms can be described by an effective gaussian shape which is normally accounted for by the Debye-Waller factor.

Consider the rectangular 2D lattice from the previous exercise, but now with three Atoms per unit cell. Atom 1 is positioned directly at the lattice points  $\vec{u}_1 = 0$ , while atoms 2 and 3 are at the relative positions  $\vec{u}_2 = 0.4\vec{a}_1$  and  $\vec{u}_3 = 0.6\vec{a}_2$ .

- The real space lattice is now given by the convolution of two functions  $f(\vec{r}) = S(\vec{r}) \otimes F(\vec{r})$ .  $S(\vec{r})$  describes the periodic structure of the lattice and is identical to lattice described in exercise 3.  $F(\vec{r})$  describes the arrangement of atoms in a single unit cell (the positions of the atoms 1, 2 and 3 ). Draw the real space lattice and formulate the functions  $S(\vec{r})$  and  $F(\vec{r})$
- How are the Fourier transforms  $S(\vec{k})$  and  $F(\vec{k})$  related in the scattering function  $f(\vec{k})$ ?
- How is the intensity measured in an experiment (qualitatively) changed in comparison to exercise 3?