

Physics with Neutrons I

Alexander Backs
alexander.backs@frm2.tum.de

WS 18/19
13.11.2018

Exercise sheet 8

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

Due on 19.12.2018

1. Isotropic Scattering

For amorphous materials or liquids, mathematical treatment gets a lot easier, if the material can be assumed to be isotropic. This means there are no preferential directions, molecules align with, or preferred alignments between them. Vectorial functions $f(\vec{r})$ can then be reduced to a radial dependence $f(r)$.

Assume, we know the radial distribution function of an isotropic liquid $g(r)$. Proof, that the Fourier transformation (yielding the differential scattering cross section) can be reduced to the following expression:

$$\frac{d\sigma}{d\Omega} = FT(g(r)) = 4\pi \int g(r)r^2 \frac{\sin(qr)}{qr} dr$$

2. Isolated Hard Sphere

Liquids and amorphous solids have no long range order, which prevents Bragg scattering. However, they exhibit local structure which is described by the radial distribution function. It tells us about the shape of atoms or molecules (self correlation) and the short range order (pair correlation).

Calculate the self correlation function $g^{(1)}(r)$ for a homogeneous hard sphere with diameter d and the scattering length density ρ inside its volume. (this can still be calculated analytically). Calculate or compute the corresponding scattering cross section using the formula from exercise 1. (This can still be done analytically, however it gets quite extensive.) Take a look at the high- q and low- q part of the scattering cross section and see if you can find any asymptotic behaviors. (It might be helpful to plot the function with single or double logarithmic scales)

3. 1D Liquid

Assume a 1D liquid of hard spheres as described above. Compute the pair correlation function and associated scattering cross section.

The pair correlation function $g^{(2)}(r)$ is defined as the overlap of a particle with all its neighbors, when displaced by the distance r . Mathematically this is a convolution of the liquid with itself (compare to the Patterson function!). For computation a slightly different approach might be easier:

- Generate a list of positions for the spheres.
- Add up the self correlation function of each sphere at its position. Use the function calculated in the previous exercise.
- Generate several of these pair correlation functions and add them up, to account for statistics.
- Compute the Fourier transform from the result.

Some notes and hints: For this simple computation, we are restricted to the integer positions available in a list (or pixels in the plot). To achieve a good result make your sphere large enough ($R \approx 20$ entries / pixels). In order to see the whole range of interest, calculate a chain consisting of $N \approx 50$ spheres. For a good statistical result calculate more than 100 repetitions.