Physics with Neutrons I

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Exercise sheet 8

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

Solutions

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 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:

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

Solution

The generic definition of a Fourier transform is typically given in cartesian coordinates:

$$FT\left(g(r)\right) = \int g(r) e^{i\vec{q}\vec{r}} d^3 r$$

,

In order to better suit the symmetry of our problem, we switch to spherical coordinates. The differentials and vector product are then defined as following:

$$\int d^3 r = \int_{-\inf}^{-\inf} \int_{-\inf}^{-\inf} \int_{-\inf}^{-\inf} dx dy dz = \int_0^{-\inf} \int_0^{2\pi} \int_0^{\pi} r^2 \sin(\theta) d\theta d\phi dr$$

$$\vec{q}\vec{r} = qr \cos(\theta)$$

We choose (without loss of generality) θ as the angle between the vectors. The equation now looks like:

$$FT\left(g(r)\right) = \int_0^{-\inf} \int_0^{2\pi} \int_0^{\pi} g(r) e^{iqr\cos(\theta)} r^2 \sin(\theta) d\theta d\phi dr$$

,

where we introduce a variable substitution to get rid of the trigonometric functions:

$$\alpha = \cos(\theta) \rightarrow d\alpha = -\sin(\theta) d\theta$$

The angular integrals can now be easily solved and we arrive at the expression given in the exercise.

$$FT\left(g(r)\right) = -\int_0^{-\inf}\int_0^{2\pi}\int_0^{\pi} g(r)r^2 e^{iqr\alpha}d\alpha d\phi dr$$

$$= -2\pi\int_0^{-\inf} g(r)r^2 \int_0^{\pi} e^{iqr\alpha}d\alpha dr$$

$$= -2\pi\int_0^{-\inf} g(r)r^2 \left[\frac{1}{iqr}e^{iqr\alpha}\right]_1^{-1} dr$$

$$= 2\pi\int_0^{-\inf} g(r)r^2 \frac{1}{iqr}\left(e^{iqr} - e^{iqr}\right) dr$$

$$= 4\pi\int_0^{-\inf} g(r)r^2 \frac{\sin(qr)}{qr}dr$$

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)
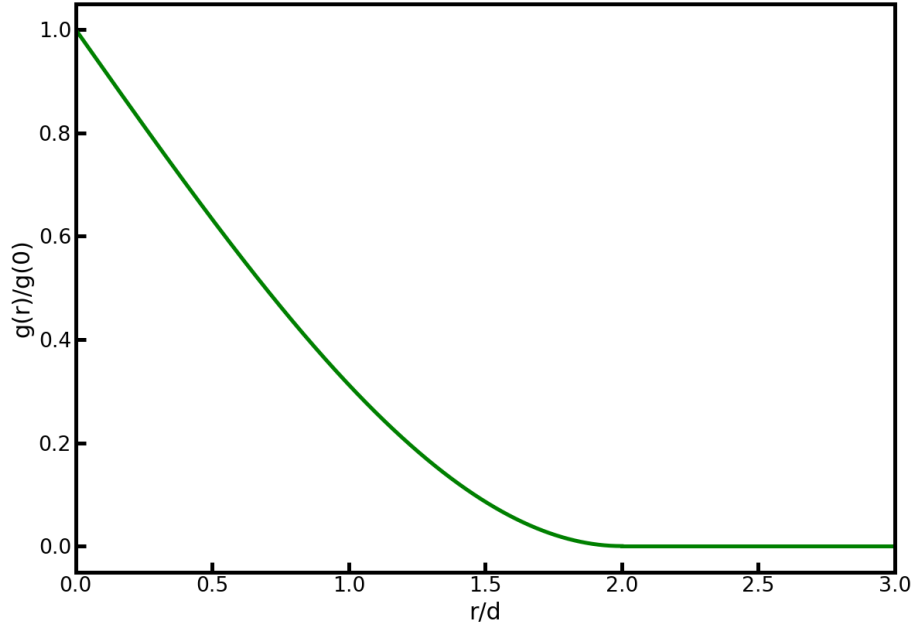
Solution
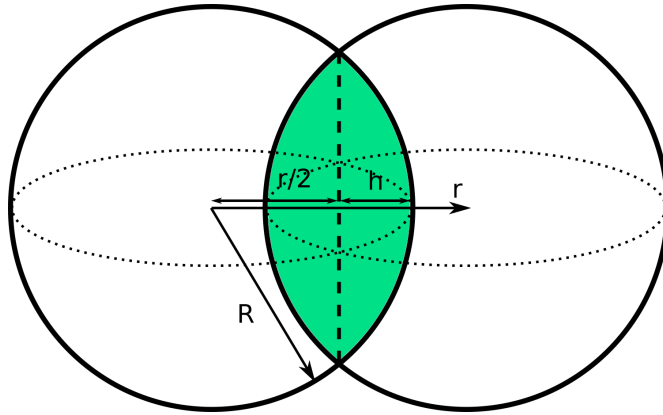
The overlap of two spheres consists of two identical spherical caps which make up the shaded area in the image above. The separation between the spheres is r, their radius d and the hight of one cap is $h = d - r/2$:

$$g^{(1)}(r) = \rho^2 2V_{cap} = \rho^2 \frac{\pi h^2}{3}(3d - h)$$

$$= \frac{4\pi d^3}{3}\left(1 - \frac{3}{4}\left(\frac{r}{d}\right) + \frac{1}{16}\left(\frac{r}{d}\right)^3\right)$$

The separation is limited to $0 \leq r \leq 2d$. The normalized result is shown below.

The scattering cross section can be calculated using the result from the first exercise:

$$\frac{d\sigma}{d\Omega} = \frac{16\pi^2 d^3}{3} \int_0^{2d} \left(1 - \frac{3}{4}\left(\frac{r}{d}\right) + \frac{1}{16}\left(\frac{r}{d}\right)^3\right) r^2 \frac{sin[qr]}{qr} dr$$

which is solvable using the following trigonometric integral:

$$\int x^n sin(ax)dx = -\sum_{j=0}^{n} \frac{x^{n-j}}{a^{1+j}} \frac{n!}{(n-j)!} \cos(ax + j\frac{\pi}{2})$$

From these integrals, a total of nine terms, containing sine and cosine functions, emerges which require tedious calculations until we arrive at the desired short form of the formula.

$$\frac{d\sigma}{d\Omega} = 16\pi \left(\frac{\sin(qd - qd\cos(qd))}{q^3}\right)^2$$

These steps are omitted here and instead another way of arriving at the same result is shown. This other way is to start from the radial scattering length density $\rho(r)$ and directly do the Fourier transform:

$$\frac{d\sigma}{d\Omega} \propto |\int \rho(r)\frac{r}{q}\sin(qr)dr|^2$$

which is simpler because $\rho(r)$ is just a stepfunction. Still we need the solution of the integral, which can be looked up. Depending on the particles, one or he other way might be easier.

Of course, for most real applications, the analytical approach is not viable because the particles are too complex. Then, the result is most often obtained by numerical integration, which, of course gives the same result as well.

Two plots of the result are shown below(note the different scales). The high q region is indicated in the first plot with a red dotted line, which represents a power law decay proportional to q^{-4}. The low q region in the second plot is scetched by a red dotted line as well, which is a parabola (q^2). We will later learn that these are the Porod and Guinier regimes respectively.
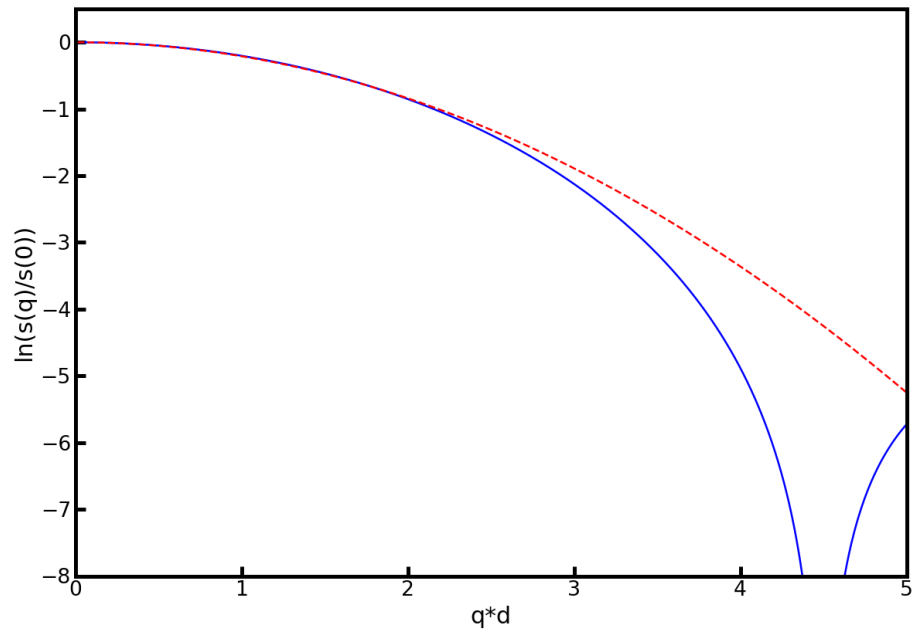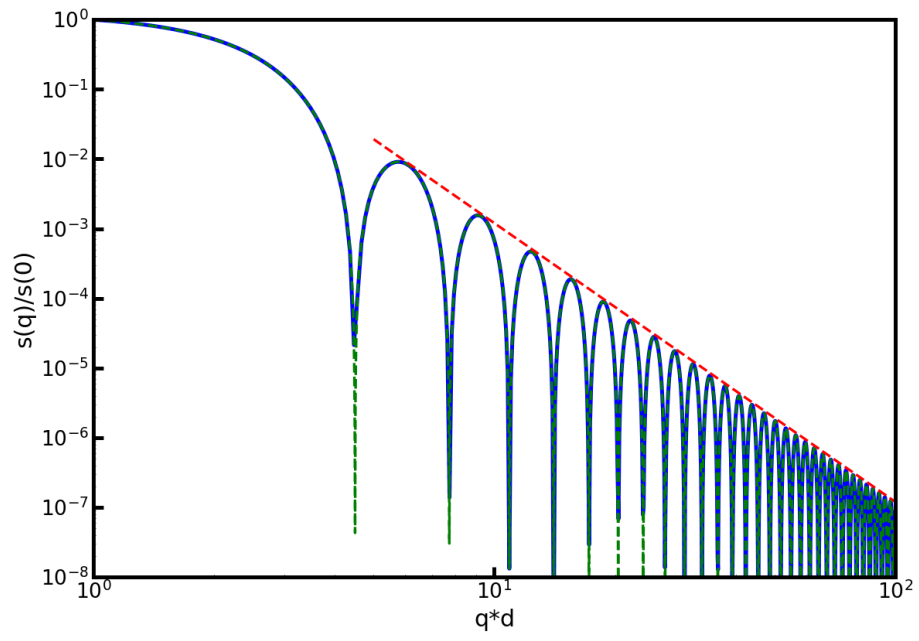
3. 1D Liquid

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 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.

Solution

The different plots show the pair correlation function (including self correlation) for different numbers of iteration N. The extreme case $N = 1$ gives essentially just the positions of each sphere. For high N (in this case several 1000) , we arrive at the true correlations function for a 1D liquid of hard spheres. Due to the chosen possibilities how the particles can be placed, the oscillation is very well visible even for high distances. Still the high distance limit shows the density of particles, like expected. In a real 3D liquid, the function would be slightly different (especially the oscillations would die away much quicker) , because new possible positions become available, but the overall shape is very similar.

N=1

N=10

N=100

N=1000

N=10000