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Exercise sheet 9

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

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1. Guinier Approximation

In the lecture, the expression for the differential scattering cross section was given for the case of several assumptions:

$$\frac{d\sigma}{d\Omega} = \left\langle \left| \int_{V_p} \Delta \rho_b \, e^{i\vec{q}\cdot\vec{r}} d^3r \right|^2 \right\rangle_{\Theta}$$

Each particle was assumed to be spherically symmetric and independent from all other particles (thus excluding positional or orientational correlations). The scattering length density $\Delta \rho_b$ is constant inside the particle and measured relative to the solvent (which is thus effectively set to 0) and the integration can be restricted to the particle volume V_p .

For small q, the exponential function in the integral can be expanded in a Taylor series to obtain Guinier's law.

- First only consider the constant term of the expansion and calculate $d\sigma/d\Omega(q=0)$.
- Now add the cubic term (in q) as well. The linear contribution vanishes due to the spherical symmetry we chose. Derive the following equation:

$$\frac{d\sigma}{d\Omega} = \frac{d\sigma}{d\Omega}(q=0) \left(1 - \frac{q^2}{3}\frac{1}{V_p}\int_{V_p} r^2 d^3r\right)$$

You will need to make another approximation where you only take the two lowest order contributions of the absolute square into account.

• In neutron scattering, the radius of gyration is defined as:

$$R_g^2 = \frac{1}{V_p} \int_{V_p} r^2 d^3 r$$

What is the meaning and definition in classical mechanics and how do both quantities differ? Calculate the (neutron) radius of Gyration for a homogeneous sphere.

• Guinier's law is most often written in a way which resembles a single logarithmic plot. Rewrite the equation that it looks like:

$$\ln(\frac{d\sigma}{d\Omega}) = f(q)$$

You will encounter another approximation for low q in this step.

2.Spherical shells

Consider sphere-like particles which consist of an inner and an outer shell. The inner shell has a radius $0 \le r \le R_i = 105$ nm and a homogeneous sld $\rho_i = 65 \cdot 10^{-6}/\text{Å}^2$ while the outer shell has a radius $R_i \le r \le R_o = 180$ nm and a homogeneous sld $\rho_o = 23 \cdot 10^{-6}/\text{Å}^2$. The particles are very dilute in a solution with $\rho_s = -6 \cdot 10^{-6}/\text{Å}^2$.

Starting from the expression for spherical symmetric scattering cross section (reference sheet 8):

$$\frac{d\sigma}{d\Omega} = 16\pi^2 \left| \int \rho(r) \frac{r \sin(qr)}{q} dr \right|^2$$

- Calculate and plot the scattering function for the values given above.
- From the plot, retrieve the values obtained by the approximations from exercise 1 (i.e. q=0 and Guinier's law) and check if they are correct. Omit all normalization factors N/V.
- Can the same scattering cross section be obtained from a simple spherical particle with radius R_x and sld ρ_x ?
- Can the same small q approximative values be obtained from such a sphere?
- Repeat the first two steps in the cases where ρ_s of the solution is matched to either the inner or outer shell sld.