Physics with Neutrons I

Alexander Backs
alexander.backs@frm2.tum.de

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Exercise sheet 9 https://wiki.mlz-garching.de/n-lecture06:index

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Solutions

1. Guinier Approximation

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

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

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:

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

  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.

Solution

First of all, the taylor expansion of the exponential starts out as :

$$e^{i\,\vec{q}\,\vec{r}} = 1 + i\,\vec{q}\,\vec{r} - \frac{1}{2}(\vec{q}\,\vec{r})^2 + \ldots$$

If we only consider the constant term and all special cases mentioned in the exercise, the calculation of the differential scattering cross section becomes quite simple. The orientational average can be omitted (there are no terms depending on the orientation) and the absolute is trivial as well because there are only positive real quantities involved.

$$\frac{d\sigma}{d\Omega}\Big|_{q=0} = \Big\langle \Big| \int_{V_p} \Delta\rho_b d^3r \Big|^2 \Big\rangle_\Theta = (\Delta\rho_b V_p)^2$$

This is the value exactly at $q = 0$. For the q-dependence at low q we add the cubic term of the expansion and start by rearranging the integration, absolute square and average.

$$\frac{d\sigma}{d\Omega} = \Big\langle \Big| \int_{V_p} \Delta\rho_b (1 - \frac{1}{2}(\vec{q}\,\vec{r})^2) d^3r \Big|^2 \Big\rangle_\Theta = \Big\langle \Big| \int_{V_p} \Delta\rho_b d^3r - \int_{V_p} \Delta\rho_b \frac{1}{2}(\vec{q}\,\vec{r})^2 d^3r \Big|^2 \Big\rangle_\Theta$$

The first integral is again the $q = 0$ expression we just calculated and the absolute square can be approximated in the following way. Again, we use, that all quantities involved are real. Additionally we make a further approximation by dropping the square of the second integral, which is a very small quantity.

$$\Big| a - b \Big|^2 = (a - b)^2 = a^2 - 2ab + b^2 \approx a^2 - 2ab$$

Using this and the fact, that we can calculate the average for both terms separately we arrive at:

$$\frac{d\sigma}{d\Omega} = \Big(\Delta\rho_b V_p\Big)^2 - \Big\langle \Delta\rho_b V_p \int_{V_p} \Delta\rho_b (\vec{q}\,\vec{r})^2 d^3r \Big\rangle_\Theta$$

For the second part we actually have to perform the orientation average, where we use spherical coordinates due to the symmetry of the problem.

$$\Big\langle \int_{V_p} V_p\, \Delta\rho_b^2 (\vec{q}\,\vec{r})^2 d^3r \Big\rangle_\Theta =$$

$$\int_0^{2\pi} \int_0^{\pi} \sin(\theta) \int_{V_p} V_p\, \Delta\rho_b^2 (\vec{q}\,\vec{r})^2 d^3r \, d\theta \, d\phi =$$

$$\int_0^{2\pi} \int_0^{\pi} \sin(\theta) \int_{V_p} V_p\, \Delta\rho_b^2 (q\, r\cos(\theta))^2 d^3r \, d\theta \, d\phi =$$

$$\frac{1}{4\pi} V_p\, \Delta\rho_b^2 q^2 \int_0^{2\pi} d\phi \int_0^{\pi} \sin(\theta)\cos^2(\theta)\, d\theta \int_{V_p} r^2 d^3r =$$

$$\frac{1}{4\pi} V_p\, \Delta\rho_b^2 q^2 2\pi \big[\frac{-1}{3}\cos(\theta)\big]_0^{\pi} \int_{V_p} r^2 d^3r$$

$$\frac{1}{3} V_p^2\, \Delta\rho_b^2 q^2\, \frac{1}{V_p} \int_{V_p} r^2 d^3r =$$

$$\frac{d\sigma}{d\Omega}\Big|_{q=0} \frac{q^2}{3} \Big(\frac{1}{V_p} \int_{V_p} r^2 d^3r \Big)$$

Together with the constant term of the approximation we arrive at the given expression.

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

And with the definition for the radius of gyration:

$$\frac{d\sigma}{d\Omega} = \frac{d\sigma}{d\Omega}\Big|_{q=0}\Big(1 - \frac{q^2 R_g^2}{3}\Big)$$

In classical mechanics, the radius of gyration is used for rotating objects and it describes at which distance to the rotation axis a mass point of the same mass as the real object would have to be to have the same moment of inertia. For an object with constant density, it is defined as:

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

In contrast to the classical case, the R_g used for scattering is averaged over the rotation in all directions instead of just one axis. There is no good analogy to the moment of inertia but the radius of gyration still gives an estimate of the size of an object. However, this 'size' strongly depends no the geometry of the particles. For a sphere the calculation is easily done in spherical coordinates.

$$(R_g^{sphere})^2 = \frac{1}{V_p}\int_{V_p} r_\perp^2 d^3r = \frac{1}{V_p}\int_0^{2\pi}\int_0^{\pi}\sin(\theta)\int_0^R r^2\, r^2 dr\, d\theta\, d\phi =$$
$$\frac{2\pi}{V_p}\int_0^{\pi}\sin(\theta)d\theta\int_0^R r^4\, dr = \frac{4\pi R^5}{5V_p} = \frac{3}{5}R^2$$

For the logarithmic form of Guinier's law we use the following approximation for small x,

$$\ln(1-x) \approx -x - \frac{x^2}{2}$$

and the standard logarithmic identities. This form is mainly used because data is most often shown on a logarithmic scale.

$$\ln\left(\frac{d\sigma}{d\Omega}\right) = \ln\left(\frac{d\sigma}{d\Omega}\Big|_{q=0}\Big(1 - \frac{q^2}{3}\Big(\frac{1}{V_p}\int_{V_p} r^2 d^3r\Big)\Big)\right) =$$
$$\ln\left(\frac{d\sigma}{d\Omega}\Big|_{q=0}\right) + \ln\left(1 - \frac{q^2}{3}\Big(\frac{1}{V_p}\int_{V_p} r^2 d^3r\Big)\right) \approx$$
$$\ln\left(\frac{d\sigma}{d\Omega}\Big|_{q=0}\right) - \left(\frac{q^2}{3}\Big(\frac{1}{V_p}\int_{V_p} r^2 d^3r\Big)\right) =$$
$$\ln\left(\frac{d\sigma}{d\Omega}\Big|_{q=0}\right) - \left(\frac{q^2}{3}\Big(\frac{1}{V_p}\int_{V_p} r^2 d^3r\Big)\right) =$$

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):

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

- 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.

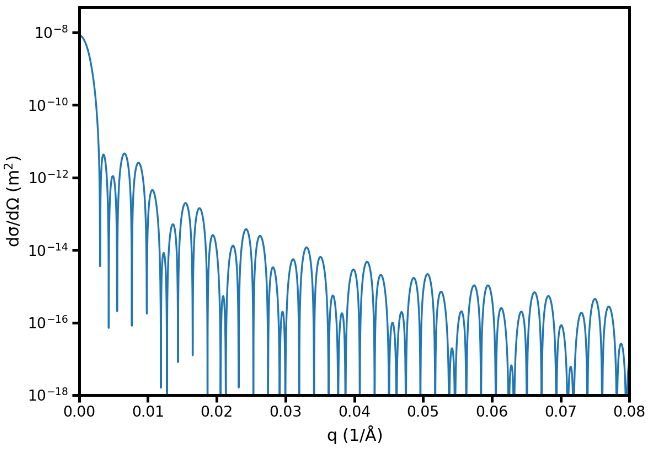
Solution

The scattering cross section of the described particle can be calculated analogous to a simple sphere, just with two different regions.

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

$$16\pi^2 \Big| \Big[(\rho_i - \rho_s) \frac{\sin(qr) - qr\sin(qr)}{q^2} \Big]_0^{R_i} + \Big[(\rho_o - \rho_s) \frac{\sin(qr) - qr\sin(qr)}{q^2} \Big]_{R_i}^{R_o} \Big|^2$$

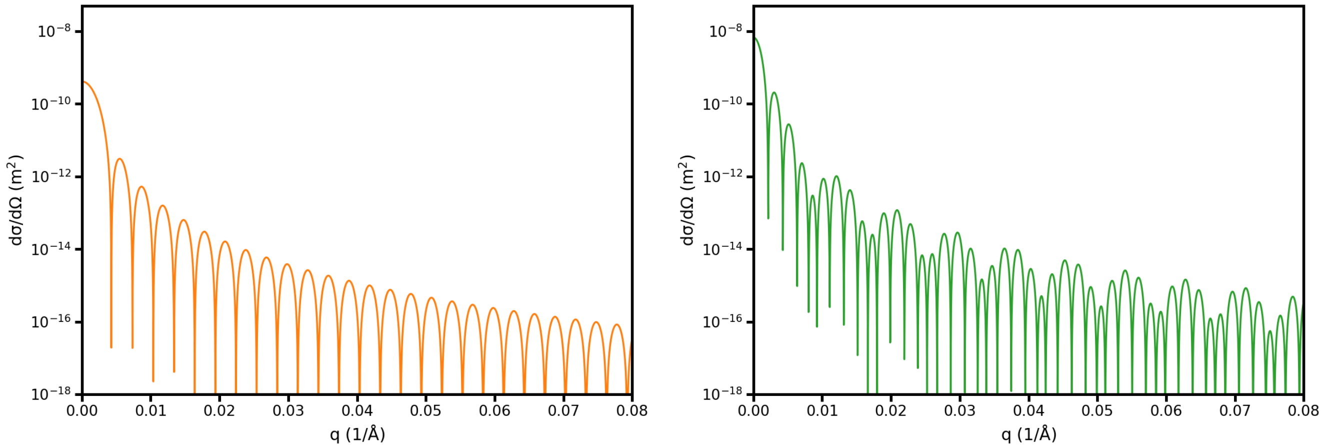
Note that $\Delta\rho$ is in both cases the difference to the solution, not the difference between the two particle regions. The result is plotted below (blue curve). The oscillations in this pattern have a more complex structure than we know it from the simple sphere (changing width of the oscillations and a kind of beating pattern). This is of course due to the different parts and sizes in the particle.



In order to get additional information, we perform sld matched experiments. In the first case we set $\rho_s = \rho_o$ (orange) and in the second one $\rho_s = \rho_i$ (green).

$$\frac{d\sigma}{d\Omega}_{Case1} = 16\pi^2 \Big| \Big[(\rho_i - \rho_o) \frac{\sin(qr) - qr\sin(qr)}{q^2} \Big]_0^{R_i} \Big|^2$$

$$\frac{d\sigma}{d\Omega}_{Case2} = 16\pi^2 \Big| \Big[(\rho_o - \rho_i) \frac{\sin(qr) - qr\sin(qr)}{q^2} \Big]_{R_i}^{R_o} \Big|^2$$



Using the Guinier approximation from above, we can calculate a value for $q = 0$:

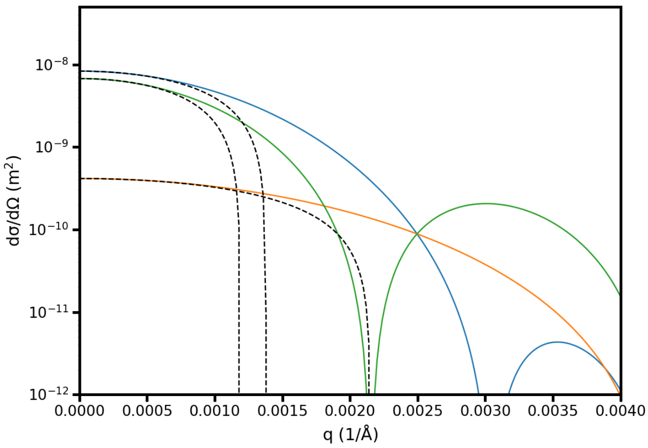
$$\left.\frac{d\sigma}{d\Omega}\right|_{q=0} = ((\rho_i - \rho_s)_b V_i + (\rho_o - \rho_s)_b V_o)^2 = 8.319 \cdot 10^{-9} m^2$$

$$\left.\frac{d\sigma}{d\Omega}\right|_{q=0,Case1} = ((\rho_i - \rho_o)_b V_i)^2 = 4.148 \cdot 10^{-10} m^2$$

$$\left.\frac{d\sigma}{d\Omega}\right|_{q=0,Case2} = ((\rho_o - \rho_i)_b V_o)^2 = 6.763 \cdot 10^{-9} m^2$$

The radius of gyration is strictly only valid for a homogeneous SLD, so a calculation for the whole particle is questionable, but for the separate shells we get $R_{g,Case1} = 81.33$nm and $R_{g,Case2} = 150.4$nm

The image below shows the low q region for all three cases (same colors as above) with Guinier fits (black dotted lines). The fit was performed only at very low $q < 0.0003/\AA$. The values obtained are given as well and match the calculated values very good.



calculated

both shell : $\left.\frac{d\sigma}{d\Omega}\right|_{q=0} = 8.319 \cdot 10^{-9} m^2$

inner shell : $\left.\frac{d\sigma}{d\Omega}\right|_{q=0} = 4.148 \cdot 10^{-10} m^2$, $R_g = 81.33$nm

outer shell : $\left.\frac{d\sigma}{d\Omega}\right|_{q=0} = 6.763 \cdot 10^{-9} m^2$, $R_g = 150.4$nm

fits

both shell : $\left.\frac{d\sigma}{d\Omega}\right|_{q=0} = 8.313 \cdot 10^{-9} m^2$, $R_g = 125.4$nm

inner shell : $\left.\frac{d\sigma}{d\Omega}\right|_{q=0} = 4.147 \cdot 10^{-10} m^2$, $R_g = 80.51$nm outer shell : $\left.\frac{d\sigma}{d\Omega}\right|_{q=0} = 6.754 \cdot 10^{-9} m^2$, $R_g = 145.5\text{nm}$

Just from the Guinier fit, the whole particle can of course be interpreted as a homogeneous sphere. The values derived from the fit would then be $R = 161.9\text{nm}$ and $\rho = 46 \cdot 10^{-6}/\text{Å}^2$. However, as we can also measure the high q scattering, we see, that this is not a fitting model.