Neutron and X-ray Scattering
of
Quantum Materials

PHYS-640

Week 5 exercises

1: The small angle neutron scattering experiment

(a) Exercise 7.P.2 in the neutron notes.

1.
The general formula for the form factor is:

$$P(\mathbf{q}) = \left| \frac{1}{V} \int dV e^{i\mathbf{q}\cdot\mathbf{r}} \right|^2 .$$

The volume of a sphere with radius, R, is $V = \frac{4}{3}\pi R^3$. The volume integral is evaluated using spherical coordinates and the Debye formula $\langle e^{i\mathbf{q}\cdot\mathbf{r}} \rangle = \frac{\sin(qr)}{qr}$:

$$\begin{aligned}
\int dV e^{i\mathbf{q}\cdot\mathbf{r}} &= \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta \, d\theta \int_0^R r^2 dr \, e^{i\mathbf{q}\cdot\mathbf{r}}, \\
&= 2\pi \left[-\cos\theta \right]_0^{\pi} \int_0^R dr \, \frac{r\sin(qr)}{q}, \\
&= \frac{4\pi}{q} \left[\frac{\sin(qr) - qr\cos(qr)}{q^2} \right]_0^R , \\
&= \frac{4\pi}{q^3} \Big(\sin(qR) - qR\cos(qR) \Big).
\end{aligned}$$

Combing everything we get:

$$P(\mathbf{q}) = \left| \frac{3}{4\pi R^3} \frac{4\pi}{q^3} \Big(\sin(qR) - qR\cos(qR) \Big) \right|^2 = \left(3\frac{\sin(qR) - qR\cos(qR)}{(qR)^3} \right)^2 .$$

2.
Figure **??**(a) shows the form factor obtained in 1. for $R = 20, 40, 60$ and 80 Å as a function of q. The larger particle, the more dips in the form factor.

3.
Figure **??**(b) shows the effect of 1 and 10% width of a uniform size distribution. The features are smeared out with the particles have different sizes. For fun I did it also for a Gaussian distribution – see Fig. **??**(c) – which is probably a more realistic distribution of particle sizes.

(b) Exercise 7.P.4 in the neutron notes.

1.
A sketch of the setup is shown in Fig. **??**. The range of scattering angles is given by the diameter of the PSD as well as the beamstop with the lowest angle at $2\theta_{\text{min}} = \tan^{-1}\left(\frac{d_{\text{beamstop}}}{2R_d}\right)$ and the largest angle at $2\theta_{\text{max}} = \tan^{-1}\left(\frac{d_{\text{PSD}}}{2R_d}\right)$. We have $q = 2k\sin\theta$ where $k = \frac{2\pi}{\lambda}$. This means that

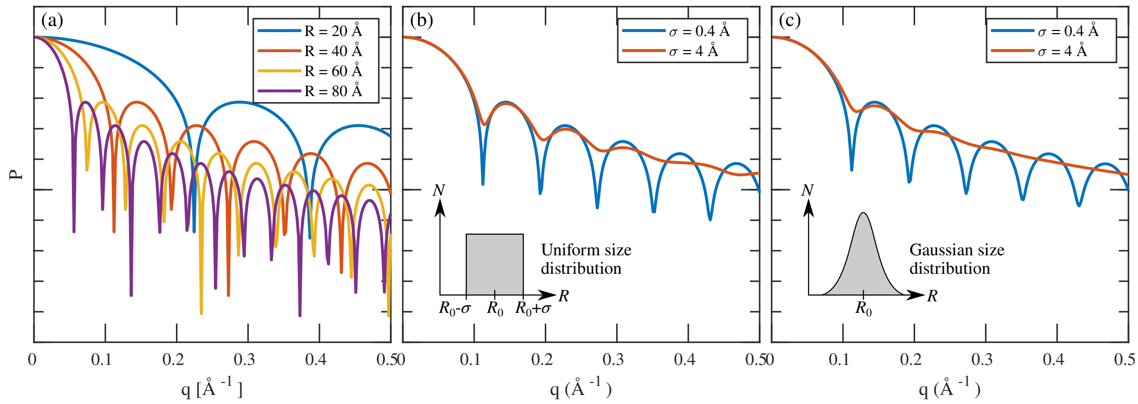

Figure 1: (a) The form factor for dilute spherical particles, $P(q)$ a function of q for different particle radii. (b)-(c) Same as in (a) but now for different particle size distributions with mean size $R_0 = 40$ Å and standard deviations (or width) $\sigma = 0.4$ and 4.0 Å using uniform and Gaussian size distributions.

largest scattering angle together with the smallest wavelength gives the largest value of q. Likewise, the smallest scattering angle together with the longest wavelength gives the smallest value of q. Concretely we find the following lower and upper limit of the length of the scattering vector, q:

$$
\begin{aligned}
q_{\min}(\lambda = 20\,\text{Å}, R_c = 20\,\text{m}) &= \frac{4\pi}{20\,\text{Å}} \sin\left[\frac{1}{2}\tan^{-1}\left(\frac{20\,\text{mm}}{20\,\text{m}}\right)\right] = 3.14 \times 10^{-4}\,\text{Å}^{-1}, \\
q_{\max}(\lambda = 20\,\text{Å}, R_c = 20\,\text{m}) &= \frac{4\pi}{20\,\text{Å}} \sin\left[\frac{1}{2}\tan^{-1}\left(\frac{0.5\,\text{m}}{20\,\text{m}}\right)\right] = 7.85 \times 10^{-3}\,\text{Å}^{-1}, \\
q_{\min}(\lambda = 4\,\text{Å}, R_c = 1\,\text{m}) &= \frac{4\pi}{4\,\text{Å}} \sin\left[\frac{1}{2}\tan^{-1}\left(\frac{20\,\text{mm}}{1\,\text{m}}\right)\right] = 3.14 \times 10^{-2}\,\text{Å}^{-1}, \\
q_{\max}(\lambda = 4\,\text{Å}, R_c = 1\,\text{m}) &= \frac{4\pi}{4\,\text{Å}} \sin\left[\frac{1}{2}\tan^{-1}\left(\frac{0.5\,\text{m}}{1\,\text{m}}\right)\right] = 0.72\,\text{Å}^{-1}.
\end{aligned}
$$

2.
The divergence between the two pinholes can be expressed as follows:

$$
\delta\theta = \tan^{-1}\left(\frac{d_f + d_s}{2R_c}\right),
$$

where $d_f = 20$ mm and $d_s = 10$ mm are the diameters of the two pinholes, respectively (see also Fig. ??). Plugging in $R_c = 1$ and 20 m yields a range of divergence of $\delta\theta = 0.86° = 51'$ for

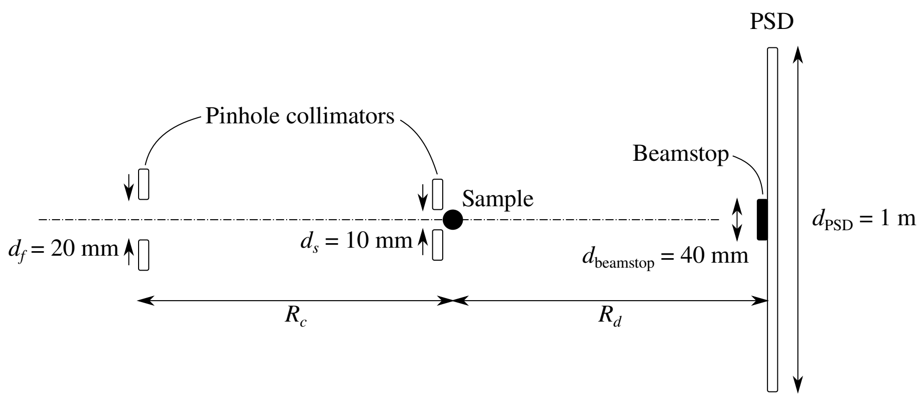

Figure 2: Sketch of the SANS setup described in the collimation exercise.

$R_c = 1\,\mathrm{m}$ and $\delta\theta = 0.043° = 2.6'$ for $R_c = 20\,\mathrm{m}$.

3.
The uncertainty in $q = \frac{4\pi}{\lambda}\sin\theta$ can be found as follows:

$$(\delta q)^2 = \left(\frac{\partial q}{\partial\lambda}\right)^2 (\delta\lambda)^2 + \left(\frac{\partial q}{\partial\theta}\right)^2 (\delta\theta)^2,$$
$$= (4\pi)^2 \left[\left(\frac{-\sin\theta}{\lambda^2}(\delta\lambda)\right)^2 + \left(\frac{\cos\theta}{\lambda}(\delta\theta)\right)^2\right].$$

If we then divide through by q^2 we get the relative uncertainty:

$$\left(\frac{\delta q}{q}\right)^2 = \left(\frac{\delta\lambda}{\lambda}\right)^2 + (\cot\theta\ \delta\theta)^2.$$

Assuming $\frac{\delta\lambda}{\lambda}$ is small we have $\frac{\delta q}{q} \approx \cot\theta\ \delta\theta$ which means that the relative uncertainty in q is directly proportional to the beam divergence, $\delta\theta$. Since we are generally dealing with small angles $\cot\theta$ is a rather large number and this means the beam divergence becomes a very important factor for the uncertainty in q in SANS experiments.

For the setup with $R_c = R_d = 1$ m, we have a range of scattering angles $2\theta \in [1.15°, 26.6°]$ which together with the divergence of $\delta\theta = 0.86°$ gives a relative uncertainty ranging from $\frac{\delta q}{q} = 1.5$ for the smallest angles to $\frac{\delta q}{q} = 0.064$ for the largest angles.

For the setup with $R_c = R_d = 20$ m, the corresponding scattering angle range is $2\theta \in [0.029°, 0.72°]$ and the divergence is $\delta\theta = 0.043°$. The relative uncertainty then ranges from $\frac{\delta q}{q} = 1.5$ for the smallest angles to $\frac{\delta q}{q} = 0.060$ for the largest angles. Thus it seems that with this $R_c = R_d$ setup, the relative uncertainty in q is independent on the choice of collimation tightness but of course the accessible q range changes with R_c (R_d). Let us have a closer look at this postulate.

For small angles we have $\tan(2\theta) \approx 2\theta$, $\tan(\delta\theta) \approx \delta\theta$ and $\cot\theta \approx \frac{1}{\theta}$. The relative uncertainty is then for the smallest possible scattering angle:

$$\frac{\delta q}{q_{\mathrm{min}}} \approx \left(\frac{4R_d}{d_{\mathrm{beamstop}}}\right)\left(\frac{d_f + d_s}{2R_c}\right) = 2\frac{d_s + d_f}{d_{\mathrm{beamstop}}} = 1.5.$$

Likewise for the largest possible scattering angles we have:

$$\frac{\delta q}{q_{\mathrm{max}}} \approx \left(\frac{4R_d}{d_{\mathrm{PSD}}}\right)\left(\frac{d_f + d_s}{2R_c}\right) = 2\frac{d_s + d_f}{d_{\mathrm{PSD}}} = 0.060,$$

and we see that these expressions are independent on the choice of R_c and R_d and long as they are equal.

2: The neutron reflectometry experiment

A time-of-flight reflectometer with a wavelength range of [0.5, 6.5] Å is used to study the surface of a dilute solution of molecules in deuterated water, D_2O. Calculate the critical wavevector transfer q_c of D_2O and suggest a suitable incident angle to use.

The critical scattering vector is given by $q_c = \sqrt{16\pi\left(\rho_2\bar{b}_2 - \rho_1\bar{b}_1\right)}$, where $\rho_{1,2}$ and $\bar{b}_{1,2}$ are the number density and average scattering length for medium 1 and 2, respectively. In our case, the medium 1 is vacuum which means $\rho_1\bar{b}_1 = 0$.

The molar mass of heavy water is $M = 20\,\frac{\mathrm{g}}{\mathrm{mole}}$ which means that one formula unit of D_2O has a mass of $m = \frac{M}{N_A}$ with N_A the Avogadro's number. The mass density of heavy water is

$\rho_m = 1107\,\frac{\text{kg}}{\text{m}^3}$ so the volume of one formula unit is then $V = \frac{m}{\rho_m} = \frac{M}{N_A \rho_m}$ and hence the atomic number density is $\rho_{\text{D}_2\text{O}} = 1/V = \frac{\rho_m}{M} = 3.3332 \times 10^{28}\,\frac{1}{\text{m}^3}$.

The scattering length of deuterium is $b_\text{D} = 6.671$ fm and that for natural oxygen is $b_\text{O} = 5.803$ barn. Therefore, the average scattering length density per D_2O unit is $\bar{b}_2 = \frac{1}{3}\left(2b_D + b_0\right) = 6.382$ fm.

Putting all these numbers together then yields:

$$q_c = 4\sqrt{\pi \;\cdot\; 3.3332 \times 10^{28}\,\frac{1}{\text{m}^3} \;\cdot\; 6.382 \times 10^{-15}\,\text{m}} = 1.034 \times 10^{8}\,\frac{1}{\text{m}} = 1.034 \times 10^{-2}\,\frac{1}{\text{Å}}.$$

For the wavelength interval $[0.5, 6.5]$ Å results in $\theta_c \in [0.024°, 0.31°]$.

3: The beamtime proposal

Imagine that you have discovered a new mineral, magnificite. It is a strong ferromagnet and superconducting simultaneously. Now, you would like to characterize the magnetic structure in the compound as a function of temperature and magnetic field using neutron diffraction. Find a suitable instrument and write a beamtime proposal to perform the experiment. Some potentially helpful questions:

- Why is it important to do this experiment?
- In which form is the sample? (powder, crystal, liquid?)
- How did you characterize the sample already?
- Which temperature and field range do you need?
- Which scattering plane are you planning to use?
- How much time do you think is needed?

We will discuss this exercise in class.