ICFP M2 – SOFT MATTER PHYSICS
Tutorial 6. Neutron scattering

Jean-Marc Di Meglio and Thomas Salez

The development of neutron scattering was a key step in the experimental determination of the inner structure of materials. Here, we would like to describe its principle and understand how it allows to extract the structure factor of liquids in general before examining the case of ideal polymer chains. We consider a collimated beam of "thermal" neutrons oriented along the unit vector $\mathbf{u_x}$ and we describe it by a monochromatic plane wave of wave vector $\mathbf{k} = k\,\mathbf{u_x}$ and with a real and positive amplitude A_0. This beam interacts with a sample of volume V containing N target atomic nuclei – considered punctual – located at positions $\mathbf{r}_j$ in space, with $1 \leq j \leq N$. The origin of coordinates O is chosen to belong to a zero-phase plane of reference of the incoming wave, just before entering the sample.

I Scattered intensity

The neutron-matter interaction is described through elastic collisions with each target being a secondary source re-emitting a monochromatic spherical ("s") wave. For a nucleus j, the amplitude of the s wave is multiplied by the (positive or negative) scattering length b_j that encompasses the probability of interaction and the details of the composition and internal state of the nucleus. We consider a detection point $\mathbf{r}$ in the far field, and we define the secondary wave vector $\mathbf{k}' = \mathbf{k}+\mathbf{q} = k\mathbf{r}/r$, making an angle θ with $\mathbf{k}$.

1 Estimate the (thermal) energy and the velocity of the incoming neutrons, and deduce their wavelength λ through the de Broglie relation.

2 What are the wavelengths of the re-emitted s-waves ?

3 Show that the norm $q = ||\mathbf{q}||$ of the vector $\mathbf{q}$ reads :

$$q = \frac{4\pi}{\lambda}\sin\left(\frac{\theta}{2}\right) \ .$$

4 Show that a good approximation for the scattered amplitude ψ_j by the object j is :

$$\psi_j = A_0\,\frac{b_j}{r}\,\mathrm{e}^{ikr}\,\mathrm{e}^{-i\mathbf{q}\cdot\mathbf{r_j}} \ . \tag{1}$$

5 Calculate the scattered intensity $I(\mathbf{q})$ per unit solid angle and per unit A_0^2 for the whole sample.

6 What is the spatial resolution of the technique ?

II Link with pair-distribution function

We assume an homogeneous liquid-like state of the sample, and we assume all the constitutive nuclei to be identical, with their scattering lengths being $b_j = b$. We further recall the definition of the pair-distribution function :

$$g(\mathbf{r}, \mathbf{r}') = \frac{< \rho(\mathbf{r})\, \rho(\mathbf{r}') > - < \rho(\mathbf{r}) > \delta(\mathbf{r} - \mathbf{r}')}{< \rho(\mathbf{r}) >< \rho(\mathbf{r}') >} \ , \tag{2}$$

where we introduced the local density $\rho(\mathbf{r})$, the Dirac distribution δ, and the average $\langle \cdot \rangle$ over all possible configurations of the sample.

1 The "structure factor" is defined as $\mathcal{S}(\mathbf{q}) = \langle I(\mathbf{q}) \rangle / (Nb^2)$. Explain why :

$$\mathcal{S}(\mathbf{q}) = \frac{1}{N} \sum_{m,n} \left\langle \mathrm{e}^{i\mathbf{q}\cdot(\mathbf{r}_m - \mathbf{r}_n)} \right\rangle \ .$$

2 Relate the local density $\rho(\mathbf{r})$ of nuclei to their positions $\mathbf{r}_j$. What is the average density $< \rho(\mathbf{r}) >$?

3 Simplify $g(\mathbf{r}, \mathbf{r}')$ using the assumption of homogeneity.

4 Express $\mathcal{S}(\mathbf{q})$ using the Fourier transform of the density correlator $< \rho(\mathbf{0}) \rho(\mathbf{r}) >$.

5 Deduce the relation between the structure factor and the pair-distribution function.

III Application to polymers

We now consider a large volume V containing an ideal polymer chain made of N monomers, each with size a.

1 Calculate the quantity $\left\langle \mathrm{e}^{i\mathbf{q}\cdot(\mathbf{r}_m - \mathbf{r}_n)} \right\rangle$ for the two monomers indexed by m and n.

2 Show that the structure factor satisfies the Debye formula :

$$\frac{\mathcal{S}}{N} = \frac{2}{u} \left[1 - \frac{1}{u} \left(1 - \mathrm{e}^{-u} \right) \right] \ , \tag{3}$$

where :

$$u = \frac{4\pi^2}{3} \frac{Na^2}{\lambda^2} \left(1 - \cos\theta \right) \ . \tag{4}$$

3 Study the small-wavelength and large-wavelength limits, and explain how neutron scattering allows to measure the monomer size a and the polymerization index N.