
Physics with neutrons 2

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Exercise sheet 2
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EXERCISE 2.1

When investigating an object with small-angle scattering, the Patterson function yields useful statistical information. It is defined by

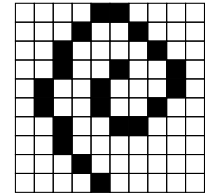
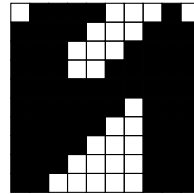
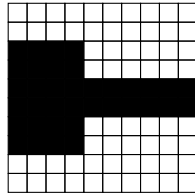
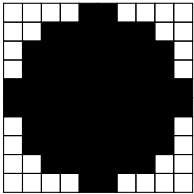
$$P(\mathbf{r}) = \int \rho(\mathbf{r}_1)\rho(\mathbf{r}_2) d\mathbf{V}, \quad \text{with } \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2,$$

where ρ is the scattering-length density function of the object. The correlation function $\gamma(r)$ is the orientational average of the Patterson function $P(\mathbf{r})$, which is in two dimensions

$$\gamma(r) = \frac{1}{2\pi} \int_0^{2\pi} P(\mathbf{r}) d\varphi. \quad (1)$$

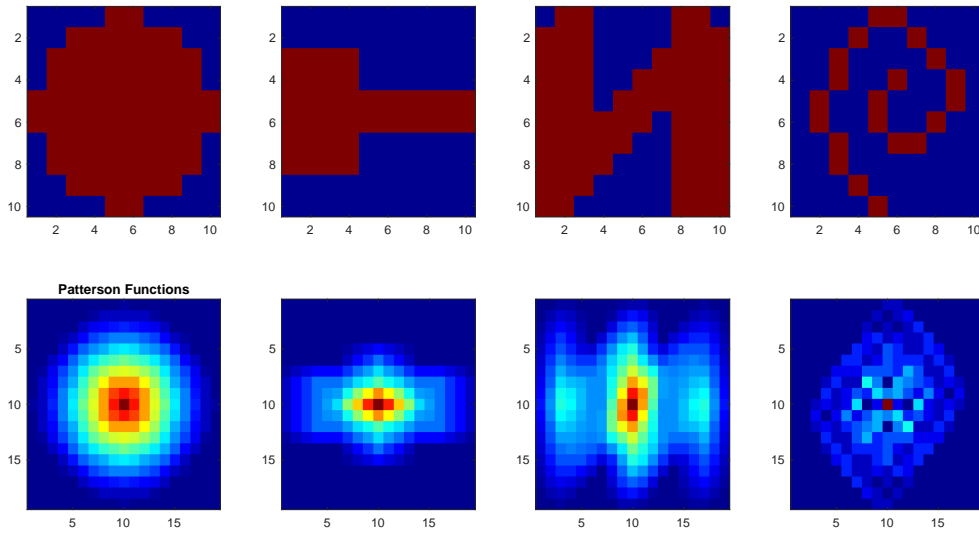
It answers the question: given that there is an atom of the particle at some place, what is the probability that the atoms in the distance r are also situated inside the particle?

Numerically calculate the (two-dimensional) Patterson function and subsequently the characteristic function $\gamma_0(r) = \frac{\gamma(r)}{\gamma(0)}$ of the following objects (black area $\rho = 1$, white area $\rho = 0$)

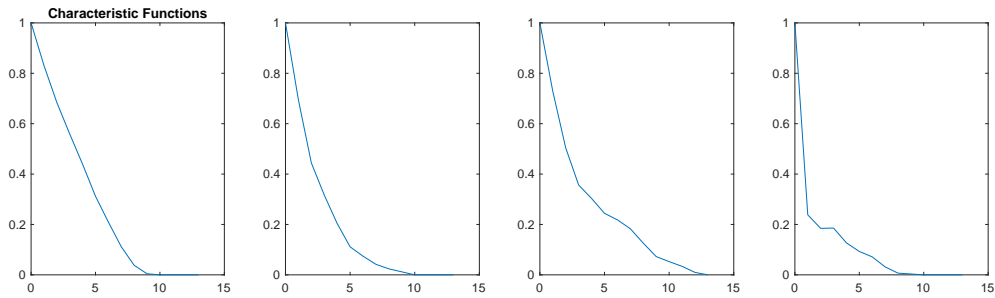


Why is $\gamma(r \geq D) = 0$ when D is the largest possible distance of two atoms inside the particle? What is the connection between Patterson function and scattering signal of the object?

Solution. The Patterson function corresponds to a convolution of the scattering length density $\rho(r)$ with $\rho(-r)$. This operation is called Autocorrelation and it describes the correlation of a function with itself translated by a distance r' . In our case, the function corresponds to the particle shape. We get the following Patterson functions (Matlab function `conv2`)



Certain characteristics of the particle shape are still visible in this representation. In the next step we perform the radial integration around the centre to get the characteristic function of the particle

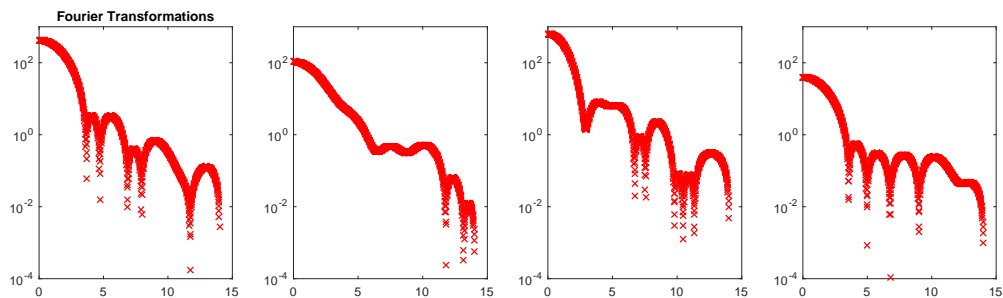


The characteristic function is important for interpreting scattering data, since the Wiener-Khinchin theorem states that the Fourier transform of the patterson function is equal the squared Fourier transform of the scattering length density, e.g. the scattering signal

$$|\mathcal{F}(\rho)|^2 = |\mathcal{F}(P)|.$$

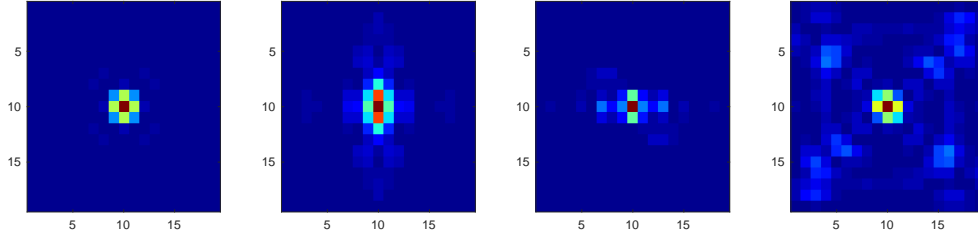
Consequently, we can calculate the radial averaged scattering signal by performing the radial Fourier transform of the characteristic

$$I(Q) = 4\pi \int_0^D \gamma(r) \frac{\sin(Qr)}{Q} r dr.$$

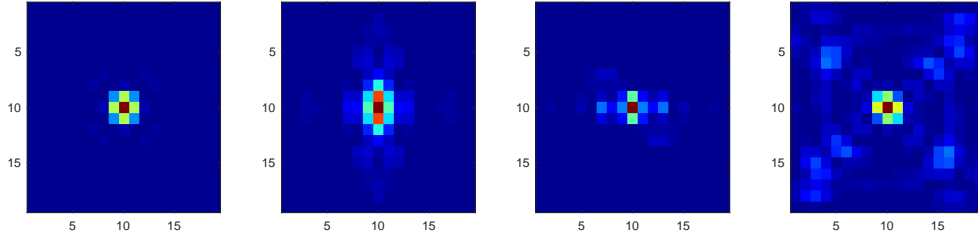


As a cross check we calculate the scattering signal in both ways, from the Patterson function and the squared Fourier transform of the scattering length density

Fourier transform of the Patterson function



Squared Fourier transform of the scattering length density



□

EXERCISE 2.2

To obtain *Porod's law*, an intermediate step is to integrate the central formula for the scattered intensity I as a function of the absolute value of the scattering vector Q ,

$$I(Q) = 4\pi \int_0^D \gamma(r) \frac{\sin(Qr)}{Q} r \, dr . \quad (2)$$

Solve the integral.

Solution. The integration has to be done in parts,

$$I(Q) = 4\pi \int_0^D \underbrace{\gamma(r)r}_u \underbrace{\frac{\sin(Qr)}{Q}}_{v'} \, dr \quad (3)$$

yielding

$$I(Q) = 4\pi \left\{ \underbrace{\left[\gamma(r)r \left(\frac{-\cos(Qr)}{Q^2} \right) \right]_0^D}_{=0} - \int_0^D (\gamma'(r)r + \gamma(r)) \left(\frac{-\cos(Qr)}{Q^2} \right) \, dr \right\} . \quad (4)$$

The first term is zero because $\gamma(D) = 0$. One step further, one arrives at

$$I(Q) = -4\pi \left\{ \frac{-\gamma'(D)D \sin(QD)}{Q^3} + \int_0^D \gamma''(r)r \frac{\sin(Qr)}{Q^3} \, dr + 2 \int_0^D \gamma'(r) \frac{\sin(Qr)}{Q^3} \, dr \right\} . \quad (5)$$

In the last step, we use that

$$(r\gamma(r))''' = 3\gamma''(r) + r\gamma'''(r) \quad (6)$$

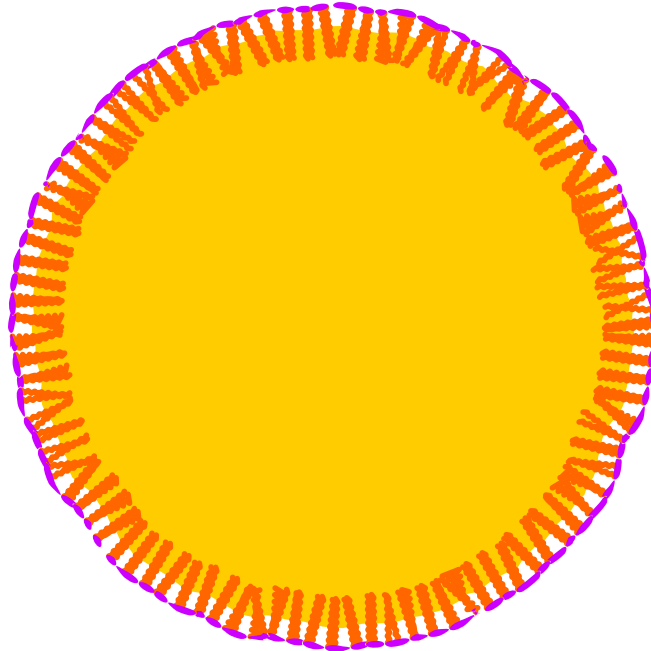
to obtain

$$\begin{aligned}
 I(Q) = & -\frac{8\pi}{Q^4}\gamma'(0) + \frac{4\pi}{Q^3}D\gamma'(D)\sin(QD) \\
 & + \frac{4\pi}{Q^4}[2\gamma'(D) + D\gamma''(D)]\cos(QD) \\
 & - \frac{4\pi}{Q^4}\int_0^D (r\gamma(r))''' \cos(Qr) dr . \quad (7)
 \end{aligned}$$

□

EXERCISE 2.3

Consider an emulsion of hexane droplets (diameter about 100 nm) in water, stabilized by the (protonated) phospholipid DMPC. Hexane (C_6H_{14}) has a density of 659 kg/m^3 , Hexane-d₁₄ (C_6D_{14}) 767 kg/m^3 , water (H_2O) 1000 kg/m^3 , and heavy water (D_2O) 1105 kg/m^3 .



The aim is to obtain as much information as possible about the structure of the emulsion using small angle neutron scattering.

1. Which typical distances can be found in the sample and which of them should be observable by SANS? Assume in the following that the concentration of the emulsion droplets is very small.
2. What are the contributions of coherent and incoherent scattering, respectively?
3. In which range can you vary the scattering length density (SLD) of water and hexane by mixing protonated and deuterated substances?
4. How would you choose the scattering length densities if you would like to determine the thickness of the stabilizer layer?

Solution. 1. In water: O–H, H–(–O)–H, H_2O – H_2O .

In hexane: C–H, C–C, H–(–C)–H, H–(–C–C)–H, . . . , hexane–hexane

In the emulsifier: many intramolecular, length of molecule (*), molecule–molecule

In the emulsion: size of the droplets (*), distance of the droplets (*)

The distances with a (*) are in the nm– μ m range, therefore candidates for SAS.

2. Coherent: structure, incoherent: no structural information, Q -independent background

3. The SLD is calculated as

$$\text{SLD} = b_{\text{coh}} \left[\frac{\text{fm}}{\text{molecule}} \right] \cdot \frac{6.022 \cdot 10^{23} \left[\frac{\text{molecules}}{\text{mol}} \right]}{M \left[\frac{\text{g}}{\text{mol}} \right]} \cdot \frac{\rho \left[\frac{\text{kg}}{\text{m}^3} \right]}{10^{-3} \left[\frac{\text{kg}}{\text{g}} \right]}. \quad (8)$$

For b_{coh} , we set the sum over all coherent scattering lengths of the atoms inside the molecule. With the chemical composition $\text{C}_{36}\text{H}_{72}\text{NO}_8\text{P}$ for DMPC we obtain

molecule	$\rho \left[\frac{\text{kg}}{\text{m}^3} \right]$	$M \left[\frac{\text{g}}{\text{mol}} \right]$	$b_{\text{coh}} \left[\frac{\text{fm}}{\text{molecule}} \right]$	SLD(n) $\left[10^{-7} \text{ \AA}^{-2} \right]$
C_6H_{14}	659	86.1759	-12.4924	-5.753
C_6D_{14}	767	100.2544	133.27	61.400
DMPC	1000	677.9362	30.8468	2.740
H_2O	1000	18.0153	-1.6782	-5.610
D_2O	1105	20.0265	19.145	63.614

As a side note: to obtain the scattering length for X-rays, one would sum over all electrons in the molecule each of which has the classical electron radius $r_e = 2.81 \text{ fm}$ as scattering length.

There are three main possibilities:

1. In = Out \neq DMPC

Achieved by In: 100% C_6D_{14} , Out: 3.2% H_2O & 96.8% D_2O

2. In = Out = 0

Achieved by In: 91.4% C_6H_{14} & 8.6% C_6D_{14} , Out: 91.9% H_2O & 8.1% D_2O

3. In = DMPC \neq Out...

Achieved by: In: 87.4% C_6H_{14} & 12.6% C_6D_{14} , Out: 100% D_2O

... and a second measurement with In \neq DMPC = Out

Achieved by: In: 100% C_6D_{14} , Out: 87.9% H_2O & 12.1% D_2O

The first possibility is pretty much straight-forward, only avoiding an additional signal from the inner sphere by choosing its SLD equal to the outside. The second avoids any coherent scattering from the uninteresting phases. This can be advantageous if they exhibit inner structures which are on the same length scale as the sample. The third procedure has the advantage that one measures two times a very simple geometric form (a sphere) instead of one time a complicated (a spherical shell) and makes the data evaluation easier. \square