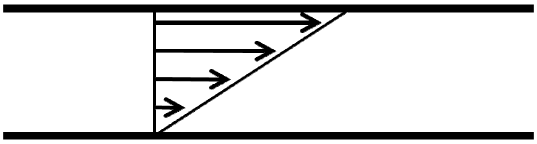
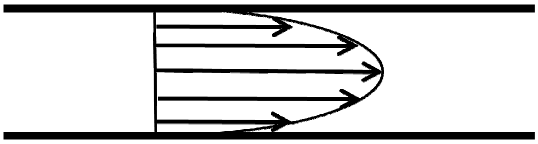
Exercise 1 – Two flow fields

We assume two parallel plates which extend in the (x,y)-plane and have a distance d in z-direction. In between there is a Newtonian fluid. Only linear effects are considered. We assume two flow fields and look for the shear rate as a function of the characteristic velocity.

a) The top plate moves with a speed v_{top}. What is the speed of the fluid as a function of the z-coordinate? What is the shear rate $\partial v/\partial z$?
b) Both plates rest. The speed profile of the fluid is assumed to be parabolic, according to $v(z) = z\cdot(d-z)\cdot v_{max}\cdot 4/d^2$. What is the average speed v_{av} of the fluid? What is the shear rate at the plate surfaces as a function of the average speed v_{av}?





Exercise 2 – Fourier-transformation of a lamellar structure

We assume a symmetric lamellar structure which shall be Fourier-transformed in discrete space. We use the function $f(x) = \begin{cases} +1 \text{ for } 0 \le x < \pi \\ -1 \text{ for } \pi \le x \le 2\pi \end{cases}$. The Fourier Integrals are $F_n = \int_0^{2\pi} f(x)\sin(nx)dx$.

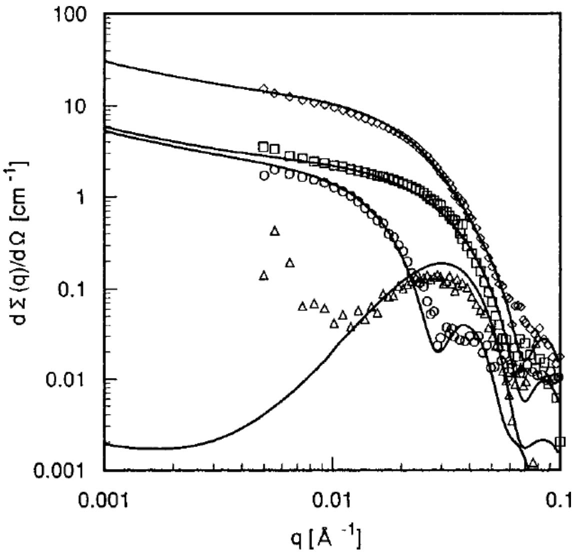
The intensities are proportional to the amplitude squared, i.e. $I_n=F_n^2$. Calculate I_n and F_n! How would the Fourier-transformation be interpreted for a continuous variable q instead of n? How does the 3-dimensional Fourier-transformed lamellar structure look like?

Exercise 3 – reciprocal lattice of a hexagonal structure

We define three vectors to describe the structure of a hexagonal cylinder structure, which read $\vec{r}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \vec{r}_2 = \begin{pmatrix} 1/2 \\ \sqrt{3/4} \\ 0 \end{pmatrix}, \vec{r}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$. In the (x,y)-plane the structure is hexagonal according to the two vectors $\vec{r}_1, \vec{r}_2$. In the z-direction the cylinders should be infinitely long.

Calculate the vectors of the reciprocal lattice, according to $\vec{g}_1 = \vec{r}_2 \times \vec{r}_3$ (and rotating indices). For simplicity we leave the vectors of the reciprocal lattice not normalized. Visualize the real space and reciprocal space picture! What happens for the z-direction in reciprocal space according to the infinitely long cylinders?

Exercise 4 – Scattering of Micelles (Contrast Variation)



The three symbols □, ○, and △ indicate the characteristic small angle scattering of spherical polymer micelles under different important contrast conditions. There are three conditions called: shell contrast, core contrast and zero average contrast. What do these terms specify? Which condition can be connected to which symbol (or curve)? Why?

Exercise 5 – Helfrich energies

The simplest structures for microemulsions are spherical, cylindrical droplets and the lamellar phase. Rationalize the principal curvatures c_1 and c_2 for these structures – they are the extreme curvatures for the considered geometry. The Helfrich free energy reads (assuming the equilibrium curvature c_0 being zero):

$$F = \int dS \cdot \left(\tfrac{1}{2}\kappa(c_1 + c_2)^2 + \bar{\kappa} \cdot c_1 c_2\right)$$

Since for the considered geometries, the principal curvatures are constant, the normalized free energy is even simpler, and reads:

$$f = \tfrac{1}{2}\kappa(c_1 + c_2)^2 + \bar{\kappa} \cdot c_1 c_2$$

Calculate *f* for the three cases!

Solutions

Exercise 1

a) $v(z) = z \cdot v_{top}/d$, $\partial v/\partial z = v_{top}/d$ all over the slit, unit of shear rate is [s^{-1}].

b) $v_{av} = v_{max} \cdot 4/d^2 \int_0^d z(d-z)dz \Big/ \int_0^d dz = \frac{2}{3} v_{max}$, $\qquad \left.\frac{\partial v}{\partial z}\right|_{z=0} = 4\frac{v_{max}}{d} = 6\frac{v_{av}}{d}$

Comment to a) The average speed is ½v_{top}, and so the ratio of the shear rates with respect to the average speed is 3.

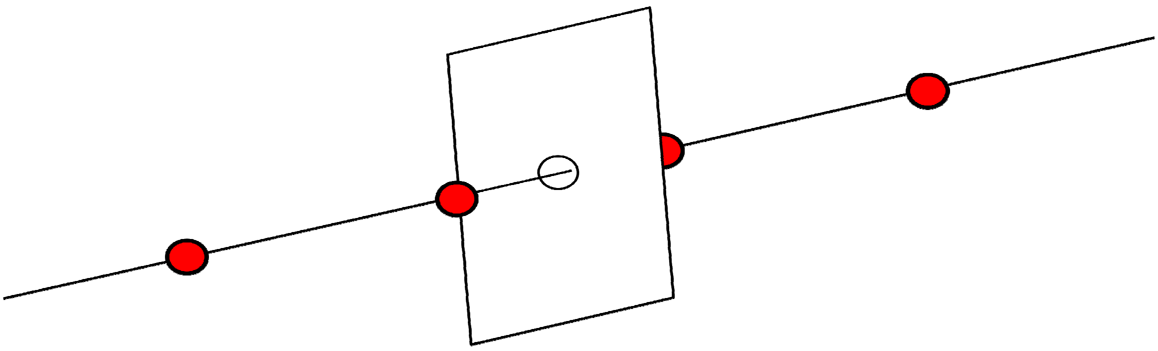
Exercise 2

If n is an even number, the symmetry yields $F_{2i} = 0$. So we assume n to be odd.

$$F_n = 2\int_0^{\pi} 1 \cdot \sin(nx)dx = 2 \cdot \left[-\frac{1}{n}\cos(nx)\right]_0^{\pi} = \frac{4}{n}; \qquad I_n = \frac{16}{n^2}$$

For a continuous variable q, the function would have Delta-peaks at $q = \frac{2\pi}{d} n$ with n being odd.

The three dimensional structure in reciprocal space would have Delta-peaks along the q_z-axis.



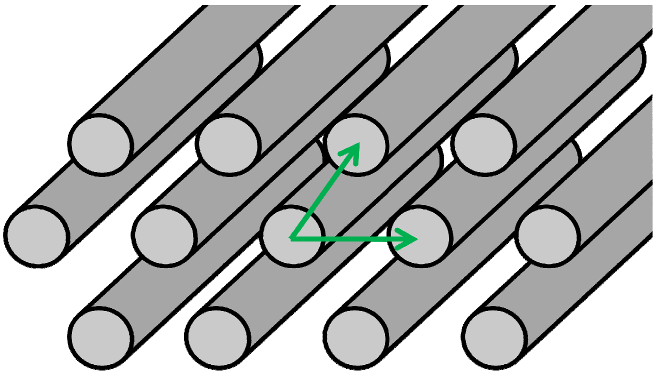
Exercise 3

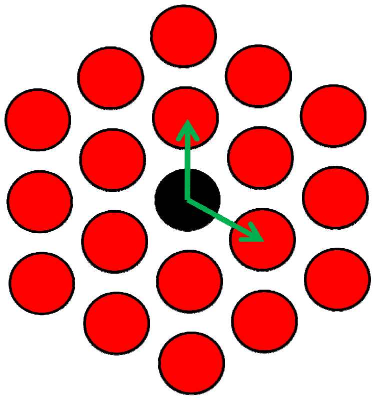
$$\vec{g}_1 = \vec{r}_2 \times \vec{r}_3 = \begin{pmatrix} 1/2 \\ \sqrt{3/4} \\ 0 \end{pmatrix} \times \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \sqrt{3/4} \cdot 1 - 0 \cdot 0 \\ 0 \cdot 0 - 1/2 \cdot 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \sqrt{3/4} \\ -1/2 \\ 0 \end{pmatrix}$$

$$\vec{g}_2 = \vec{r}_3 \times \vec{r}_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \times \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

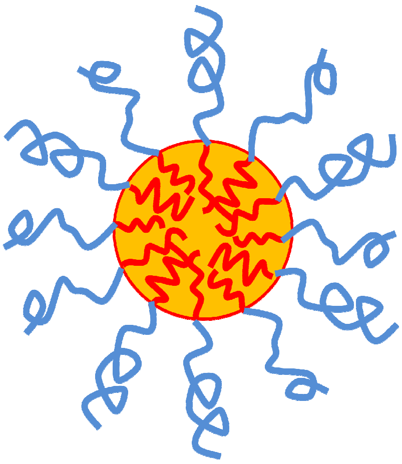
$$\vec{g}_3 = \vec{r}_1 \times \vec{r}_2 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \times \begin{pmatrix} 1/2 \\ \sqrt{3/4} \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \sqrt{3/4} \end{pmatrix}$$

The infinitely long cylinders cause a Delta-like peak in z-direction in reciprocal space.





Exercise 4



The term core contrast specifies the condition where the inner part of the micelle is visible only. For water as solvent, the core is hydrophobic. It is rather compact, because water is expelled. One realization is: deuterated core, and normal shell and water.

The shell contrast highlights the water soluble shell. The polymer is swelled, due to the solubility. Thus the corona is rather dilute and large. One realization is: deuterated core, normal protonated shell, and D_2O.

The zero average contrast is achieved, when the weighted contrast of the polymer (average contrast) is exactly that of the solvent. The structure of the micelle appears as some excitation of the scattering length density SLD (as a fluctuation) while the average SLD is the same everywhere.

Usually, the core is rather compact and small. Therefore, the Guinier behavior bends down at rather large Q. This is found for the curve with the symbol □.

The shell is rather dilute and large. The Gunier behavior bends down at smaller Q. This is found for the symbol ○. Oscillations is both cases arise from a rather monodisperse size. Every Fourier transformation contains oscillations at higher Q. Only polydispersity and resolution effects smear out such oscillations.

The ideal zero average contrast leads to a homogenous sample on large length scales. This means that the intensity at small Q is ideally zero. The maximum indicates some structure on a specific length scale. (It is a maximum because: (a) the intensity is positive, (b) because the structure water-shell-core-shell-water means an oscillation of the scattering length density. This oscillation corresponds to a peak of the intensity.) The length scale is connected to the mean distance of the core and shell. Again further oscillations of the intensity are found (Fourier transformation of monodisperse particles). The symbol for zero average contrast is △.

Exercise 5

Sphere: There is only one radius R, and so the principal curvatures are $c_1 = c_2 = R^{-1}$.

$$f = (2\kappa + \bar{\kappa}) \cdot \frac{1}{R^2}$$

Cylinder: There are extreme curvatures given by the radius R, and by the flat line along the cylinder. Thus $c_1 = R^{-1}$, and $c_2 = 0$.

$$f = \frac{\kappa}{2} \cdot \frac{1}{R^2}$$

Lamellar: The lamellar structure is flat in all directions, thus $c_1 = c_2 = 0$.

$$f = 0$$