

Isotropic-nematic phase transition in liquid crystals

Some materials consisting of strongly anisotropic colloids or molecules behave as liquid crystals. Liquid crystals possess many of the mechanical properties of a liquid, such as high fluidity, but are similar to crystals in other physical properties. For example, they may be birefringent and may have anisotropic magnetic or electric susceptibilities. Liquid crystals often exhibit a transition between the crystalline phase and the isotropic liquid phase as a function of the temperature or the concentration. In this exercise, we will study a temperature-induced phase transition.

Consider a two-dimensional square grid of anisotropic molecules, each characterized by a unit vector \mathbf{u} . The molecules i and j interact via the potential

$$U(r, \mathbf{u}^{(i)}, \mathbf{u}^{(j)}) = -\varepsilon(r)(\mathbf{u}^{(i)} \cdot \mathbf{u}^{(j)})^2. \quad (1)$$

The function $\varepsilon(r)$ depends on the distance r between the molecules. We do not consider the fluidity of the system, keeping the molecule positions fixed instead.

1. Monte Carlo sampling

- Generate a 10×10 grid of unit vectors and write a script that selects a molecule and rotates its unit vector over an arbitrary angle $0 < \phi < 2\pi$. Does this transition satisfy detailed balance?
- Write a Monte Carlo script that simulates a 10×10 grid of freely rotating molecules interacting only with their nearest neighbours via the potential of Eq. (1). That means that each molecule only interacts with the four molecules on the adjacent grid points in the two perpendicular directions of the square grid. In terms of the interaction potential of Eq. (1), the function $\varepsilon(r)$ is a step function, equal to ε for nearest neighbours and zero otherwise. Use periodic boundary conditions.
- In order to extract meaningful results, run the Monte Carlo algorithm for a number of equilibration steps before starting the production run used for generating a sample. After the equilibration, the system should have converged to a stable configuration. To check for convergence, calculate the interaction energy of the entire grid and plot the result as a function of Monte Carlo steps. Determine the number of necessary equilibration steps by eye.

2. Order parameter

The elements of the two-dimensional nematic order tensor are given by

$$Q_{\alpha\beta} = \frac{1}{N} \sum_{i=1}^N \left(2u_{\alpha}^{(i)}u_{\beta}^{(i)} - \delta_{\alpha\beta} \right), \quad (2)$$

where N is the number of molecules and $\delta_{\alpha\beta}$ is the Kronecker delta. The largest eigenvalue of this tensor equals the nematic order parameter

$$S = \frac{1}{N} \sum_i^N (2 \cos^2 \psi_i - 1),$$

where ψ_i is the angle between the director of molecule i and the *a priori* unknown general director of the nematic. From the latter equation it can be concluded that the order parameter approaches $S = 1$ if all molecules align in the direction of the general director, whereas it approaches zero in the isotropic phase.

- (a) Write a script to calculate the tensor Q and the order parameter S at every Monte Carlo step from Eq. (2).¹ Calculate the distribution of the order parameter S over a large number of Monte Carlo steps. Plot the corresponding histogram both for a temperature $k_B T \ll \varepsilon$ and for a temperature $k_B T \gg \varepsilon$.
- (b) For both temperatures, calculate and plot the autocorrelation function of S as a function of the number of Monte Carlo steps. Calculate the integrated autocorrelation time τ_{int} .² Check your estimate of the autocorrelation time by assuming an exponential decay of the autocorrelation function and plotting your data together with the exponential decay.

3. Phase transition

- (a) At a low temperature, $k_B T \ll \varepsilon$, the liquid crystal is in the nematic phase. Starting at low temperature, slowly increase the temperature and plot the average order parameter $\langle S \rangle$ as a function of the temperature.
- (b) Calculate the standard deviation of the order parameter using your code to calculate τ_{int} from part 2b to make sure that the data used for the estimate are independent and uncorrelated. Plot the order parameter as a function of the temperature including error bars.
- (c) At what temperature does the phase transition take place? What happens to the standard deviation of the order parameter near the phase transition? What is the order of the phase transition?

¹Note that the explicit equation for S and the general director are not necessary for this calculation.

²For the range of integration used to calculate τ_{int} , you can take the region from zero till the first time the autocorrelation function turns negative.