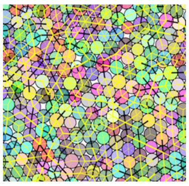

IPA SCHOOL ON DISORDER IN COMPLEX SYSTEMS
INTRODUCTION TO PHASE TRANSITIONS AND CRITICAL PHENOMENA
TUTORIAL 2
PREPARED WITH M. LENZ AND F. VAN WIJLAND

Constructing a Landau functional for liquid crystals

Liquid crystal are small rod-like molecules whose optical properties are used, *e.g.*, in your laptop display. They acquire some of these properties by undergoing a first-order phase transition toward long-range orientational order upon an increase of their density. This so-called isotropic to nematic transition is the prototype of the emergence of order in soft matter systems, and studying it is the occasion for us to train in several powerful statistical mechanical techniques.

We are interested in inhomogeneous solutions, and in deriving the corresponding free energy functional using Landau theory. To this end, we consider a liquid crystal deep in the nematic phase, implying that its nematic order parameter has a fixed, almost constant value. While the corresponding magnitude of the local rod orientation does not vary, its alignment direction can. To estimate the cost of such deformations, we move away from a microscopic description, and attempt to infer a minimal form of the liquid crystal free energy guided only by symmetry considerations. This is the general strategy used in constructing a Landau theory.

The local orientation of the rods is described by the nematic director field $\hat{\mathbf{n}}(\mathbf{r})$, where $\hat{\mathbf{n}}$ is a unit vector and $\mathbf{r}$ denotes the vector of spatial coordinates, which we will restrict to two dimensions for simplicity. Assuming that our rods are up-down symmetric, the system must be invariant under the transformation $\hat{\mathbf{n}} \to -\hat{\mathbf{n}}$. In two dimensions, we can equivalently parametrize our alignment field by the angle $\phi(\mathbf{r})$ between $\hat{\mathbf{n}}$ and the horizontal axis. Considering slow spatial variations, we write the free energy functional of the system as a Taylor expansion in powers of the gradient:

$$F = \int \left[\alpha(\phi) + \beta_i(\phi)(\nabla_i\phi) + \gamma_{ij}(\phi)(\nabla_i\phi)(\nabla_j\phi) + \mathcal{O}(\nabla^3)\right] \mathrm{d}x\mathrm{d}y, \tag{1}$$

were the Einstein summation rule is used and where $\alpha(\phi)$, $\beta_i(\phi)$ and $\gamma_{ij}(\phi)$ are *a priori* unknown functions whose form we set out to determine from the symmetries of the system.

1 Preliminaries

1) Why are we justified in keeping only the lowest terms of the gradient expansion?

2) Considering only the zeroth order term (*e.g.*, in a situation where ϕ is the same everywhere), we consider a solid rotation of the system, *i.e.*, a simultaneous rotation of $\mathbf{n}$ and $\mathbf{r}$ by an angle ϕ_0 (or equivalently a rotation of the coordinate axes leaving the system untouched). How are the new variables ϕ', x', y' related to the old ones (ϕ, x, y)?

3) The free energy of the system should be invariant under such a transformation. Why is that? To order 0, how is the free energy of Eq. (1) transformed under this rotation?

4) Conclude from this that α is a constant and can thus be dropped.

5) Now consider the first order term. How should the free energy transform under the reflection symmetry $\mathbf{r} \to -\mathbf{r}$ (or equivalently a rotation of the system axes by π followed by an inversion of the polarity of each individual molecule)? Deduce from this the form of $\beta_i(\phi)$.

2 Second order terms

1) Equation (1) does not include second order terms of the form $\tilde{\gamma}(\phi)\nabla_i\nabla_j\phi$. Show through an integration by part that this does not restrict its generality.

2) We again consider the same rotation as in question 1.2. How are the new differential operators ∇_i' related to the old? What constraints does the invariance of the free energy put on the functions γ_{ij}?

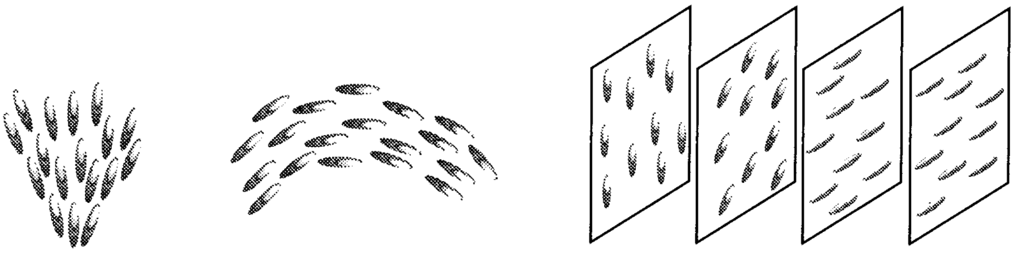

Figure 1: The three independent types of deformation for the nematic order parameter, know as splay (a), bend (b) and twist (c). Adapted from Chaikin and Lubensky, *Orinciples of Condensed Matter Physics*, CUP.

3) Using an infinitesimal rotation $\phi_0 \ll 1$, show that these conditions yield the system of equations:

$$\begin{aligned}
\partial_\phi \gamma_{11} &= -\gamma_{12} - \gamma_{21} && \text{(2a)}\\
\partial_\phi \gamma_{12} &= \gamma_{11} - \gamma_{22} && \text{(2b)}\\
\partial_\phi \gamma_{21} &= \gamma_{11} - \gamma_{22} && \text{(2c)}\\
\partial_\phi \gamma_{22} &= \gamma_{12} + \gamma_{21} && \text{(2d)}
\end{aligned}$$

4) Solve Eqs. (2) to show that F takes the following form:

$$\begin{aligned}
F = \int \{\, C\,(\nabla\phi)^2 + (A\cos 2\phi + B\sin 2\phi)\ \left[(\nabla_x\phi)^2 - (\nabla_y\phi)^2\,\right] \\
+ (2A\sin 2\phi - 2B\cos 2\phi)\,(\nabla_x\phi)\,(\nabla_y\phi)\,\}\,\mathrm{d}x\mathrm{d}y, \qquad (3)
\end{aligned}$$

where A, B and C are undetermined constants.

5) Use reflection symmetry to kill a few more terms.

6) Show that the resulting free energy can be rewritten in terms of the two quantities $\nabla \cdot \hat{\mathbf{n}}$ and $\hat{\mathbf{n}} \times (\nabla \times \hat{\mathbf{n}})$ only.

7) This free energy is known as the Frank free energy. Its more general, three-dimensional form is

$$F = \int \left\{ \frac{K_1}{2}(\nabla \cdot \hat{\mathbf{n}})^2 + \frac{K_2}{2}[\hat{\mathbf{n}} \cdot (\nabla \times \hat{\mathbf{n}})]^2 + \frac{K_3}{2}[\hat{\mathbf{n}} \times (\nabla \times \hat{\mathbf{n}})]^2 \right\} \mathrm{d}\mathbf{r}. \qquad (4)$$

The constants K_1, K_2 and K_3 are associated with the three types of deformation illustrated in Fig. 1. Which is which? Why is one of these terms missing in 2D? What is their sign? For PAA at 120°C $K_1 = 7\,\mathrm{pN}$, $K_2 = 4.3\,\mathrm{pN}$ and $K_3 = 17\,\mathrm{pN}$. Can you rationalize this order of magnitude from dimensional analysis?

8) Why could we assume that the magnitude of the nematic order parameter was fixed in this analysis?

The Frank free energy derived above is widely used as the basis for many studies of liquid crystals where the spatial structure of the nematic field plays a role. One such example is the discussion of the turbidity of nematics included in your homework assignment. Another one, the Fréedericksz transition, forms the basis of liquid crystal displays and will be studied by students of the Soft Matter and Biophysics in their Soft Matter course. Anticipating on the next tutorial, we can also note that in two dimensions the case $K_1 = K_3$ gives $F \propto \int(\nabla\phi)^2$, which is the energy functional of the XY model. This illustrates the broad relevance of the symmetry considerations developed here.