Université Paris Cité

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M2 PCS — Statistical field theory and soft matter

TD n°2 : Liquid crystals

1 Diagrammatic way for the nematic–isotropic Hamiltonian

The quadratic term $T_2 = a_{ijk\ell}\, q_{ij} q_{k\ell}$ in the expansion of the effective Hamiltonian in power series of the field q_{ij} is obtained by searching for the most general isotropic rank 4 tensor $a_{ijk\ell}$. Since such a tensor must be constructed only with Kronecker deltas, it is convenient to use a diagrammatic method where the sum over repeated indices is represented by a curved line joining the positions of these indices, a "contraction".

1. Find how this method works, and show that $T_2 = a\, q_{ij} q_{ij}$ is obtained from the diagram $q\,q$ and this one only.
2. Use the diagrammatic method to construct $T_3 = c\, q_{ij} q_{jk} q_{ki}$.
3. Construct likewise the two independent quartic terms $T_{41} = d_1 (q_{ij} q_{ij})^2$ and $T_{42} = d_2\, q_{ij} q_{jk} q_{k\ell} q_{\ell i}$.
4. Use the diagrammatic method to show that there are three independent terms that are quadratic in the gradient $q_{ij,k}$ of the nematic field.
5. Show that they reduce to only two bulk terms $T'_{21} = L_1\, q_{ij,k} q_{ij,k}$ and $T'_{22} = L_2\, q_{ij,k} q_{kj,i}$.

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2 Fluctuations in a weakly first-order nematic

Close to a weakly first-order nematic–isotropic transition, the director exhibits large fluctuations that are clearly visible under the microscope using crossed polarizers. Neglecting the biaxial character of the nematic fluctuation[1], we assume

$$\boldsymbol{q}(\boldsymbol{r}) = s(\boldsymbol{r}) \left(\boldsymbol{\nu}(\boldsymbol{r}) \otimes \boldsymbol{\nu}(\boldsymbol{r}) - \frac{1}{3} \boldsymbol{I} \right) \qquad (\boldsymbol{\nu}^2 = 1), \tag{1}$$

[1] This is reasonable when the coarse-graining length is much larger than molecular dimensions since the phase is uniaxial

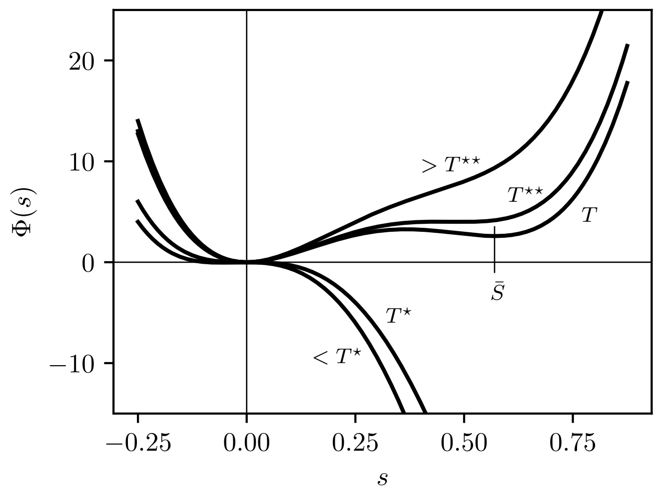

Figure 1: Hamiltonian density (4).

with, perturbatively,

$$s(\boldsymbol{r}) = \bar{S} + \sigma(\boldsymbol{r}), \tag{2}$$

$$\boldsymbol{\nu}\,(\boldsymbol{r}) = \left(\alpha, \beta, \sqrt{1-\alpha^2-\beta^2}\right)^t, \tag{3}$$

where σ, α and β are small quantities, of order ϵ. In this problem, we shall systematically neglect terms that are of order higher than ϵ^2. The expansion in (2) is made around the value $\bar{S}(T)$ that corresponds to the local nematic minimum of the Hamiltonian density $\Phi(s)$ (see Fig. 1). The full nematic Hamiltonian density has the form

$$f(\boldsymbol{q}) = \Phi(s) + \frac{1}{2}L_1 q_{ij,k}q_{ij,k}, \qquad \Phi(s) = A(T-T^\star)s^2 - Cs^3 + Ds^4, \tag{4}$$

where for the sake of simplicity we have neglected the second gradient term.

1. Assuming that σ, α and β are independent Gaussian random variables, calculate the actual scalar order parameter S and the director $\boldsymbol{n}$ of this nematic phase.

2. Show that the gradient term $T_1 = \frac{1}{2}L_1 q_{ij,k}q_{ij,k}$ takes the form

$$T_1 = \frac{1}{3}L_1\left(\nabla\sigma\right)^2 + L_1 S^2\left(\nabla\alpha\right)^2 + L_1 S^2\left(\nabla\beta\right)^2 + O(\epsilon^3) \tag{5}$$

3. Because $s = \bar{S}$ is a minimum of $\Phi(s)$, we have $\Phi(s) = \Phi_0 + \frac{1}{2}\lambda(T)\sigma^2 + O(\epsilon^3)$. Show that σ, ν_1 and ν_2 are independent random Gaussian variables

4. A simple analysis of the polynomial $\Phi(s)$ gives $\lambda(T) \sim (T^{\star\star} - T)^{1/2}$. Using your knowledge of the Gaussian model, show that the correlation length of the scalar order-parameter diverges as $(T^{\star\star} - T)^{-\nu}$ with $\nu = 1/4$.

5. Likewise, show (in 3D) that the angular fluctuations of the director are given by

$$\langle\theta^2\rangle = \frac{k_{\rm B}T\Lambda}{(2\pi)^2 L_1 S^2}, \tag{6}$$

where θ is α or β, and Λ is the upper wavevector cutoff.

6. What happens near a weakly first-order nematic–isotropic transition?

7. What happens in two dimensions? Do you recognize a theorem?

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3 Frank elasticity of the nematic phase

Deep in the nematic phase, for $T \ll T_{NI}$, the scalar-order parameter S can be considered constant. However, the director field $\boldsymbol{n}(\boldsymbol{r})$ can easily be distorted on large scales by external boundary forces[2]. This is a form of elasticity, since the nematic will relax to a uniform state if the external constraints are relaxed. F. C. Frank showed that the elastic free energy deformation has the form

$$F[\boldsymbol{n}] = \int d^3r \left[\frac{1}{2}K_1\,(\mathrm{div}\,\boldsymbol{n})^2 + \frac{1}{2}K_2\,(\boldsymbol{n}\cdot\mathrm{rot}\,\boldsymbol{n})^2 + \frac{1}{2}K_3\,(\boldsymbol{n}\times\mathrm{rot}\,\boldsymbol{n})^2\right], \tag{7}$$

where the K_i's are three independent elastic constants. The aim of this exercice is to derive this form of the free energy density f above.

1. Justify in a simple way that the three terms in the Frank elasticity correspond to deformations of the type "splay", "twist" and "bend", respectively.

For small distorsions, f can be expanded in power series of the gradient $n_{i,j} \equiv \partial n_i/\partial r_j$ of the director. Each term must be scalar (R1) and invariant under the symmetries of a uniform nematic (R2). Also, since in the ground state a nematic is uniform, the lowest-order terms must be quadratic:

$$f = A_{ijk\ell}\, n_{i,j}\, n_{k,\ell}. \tag{8}$$

The tensor $\boldsymbol{A}$ must thus have the symmetry of a uniform nematic phase (R2). Therefore it must be a linear combination of terms constructed with δ_{ij} and $n_i n_j$ only (a basis of the tensors with $D_{\infty h}$ symmetry). Thus there will be 0, 2 or 4 occurrences of n_i in $A_{ijk\ell}$.

2. Using the diagrammatic method (Kronecker contractions), show that the terms involving 0 occurrences of n_i yield only two independent bulk terms

$$f_0 = \frac{1}{2}K\, n_{i,i}\, n_{j,j} + \frac{1}{2}K'\, n_{i,j}\, n_{i,j} \tag{9}$$

[2] This is because $\boldsymbol{n}(\boldsymbol{r})$ is a "massless" field with Goldstone modes, contrary to $S(\boldsymbol{r})$, as can be seen in the previous exercice.

3. Using the diagrammatic method introduced in the first exercice, show that the terms involving 2 occurrences of n_i yields only

$$f_2 = \frac{1}{2} K'' n_j \, n_{i,j} \, n_\ell \, n_{i,\ell}. \tag{10}$$

4. Show that the contributions to $A_{ijk\ell}$ involving 4 occurrences of n_i vanish.

5. Using the relation $\epsilon_{ijk} \, \epsilon_{k\ell m} = \delta_{i\ell}\delta_{jm} - \delta_{im}\delta_{j\ell}$ calculate $(\mathrm{rot}\,\boldsymbol{n} \times \boldsymbol{n})_i$ and write f_2 using rot $\boldsymbol{n}$.

6. Show that $a^2 = (\boldsymbol{a} \cdot \boldsymbol{n})^2 + (\boldsymbol{a} \times \boldsymbol{n})^2$ for any vector $\boldsymbol{a}$.

7. Using the relation $\epsilon_{ijk} \, \epsilon_{k\ell m} = \delta_{i\ell}\delta_{jm} - \delta_{im}\delta_{j\ell}$ show that

$$(\mathrm{rot}\,\boldsymbol{n})^2 = n_{k,j} \, n_{k,j} - n_{k,j} \, n_{j,k}. \tag{11}$$

8. Deduce that the Frank form holds, with $K_1 = K + K'$, $K_2 = K'$ and $K_3 = K + K''$.

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4 Weak anchoring

A nematic liquid crystal is filled between two glass plates (Fig. 2). The upper surface is treated so as to set a "strong anchoring" of the director in the direction perpendicular to the surface. The lower surface favors the director parallel to the surface, by means of a "weak anchoring". We wish to study the elastic deformation of the nematic in the cell as a function of its thickness H. The director $\boldsymbol{n}(z)$ is assumed to lie in the (x, z) plane, such that $n_x = \cos\theta(z)$ and $n_z = \sin\theta(z)$. For the bulk elasticity, we take the Frank elasticity with $K_1 = K_2 = K_3 = K$. The upper surface sets $\theta = \pi/2$. For the weak anchoring energy density at the lower surface, we take $F_0 = \frac{1}{2} W\theta^2$, which favors $\theta = 0$.

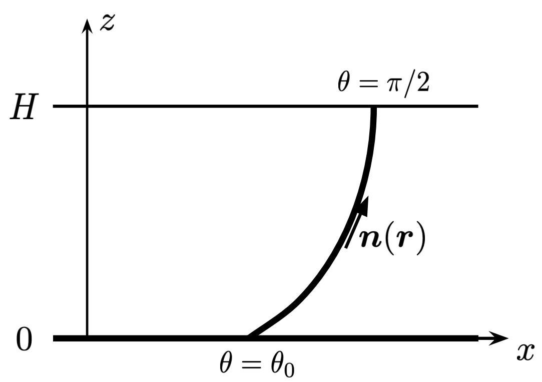

Figure 2: Nematic cell with hybrid anchoring.

1. Show that the bulk elastic energy density reduces to $\frac{1}{2} K(\partial_z\theta)^2$.

2. Show that the minimum of the free energy is obtained for

$$\partial_z^2\theta = 0 \quad (\forall z), \qquad \ell\,\partial_z\theta = \theta \quad (z=0), \tag{12}$$

3. Find the solution $\theta(z)$ and determine the boundary angle θ_0. Discuss the situations $H \ll \ell$ and $H \gg \ell$.

4. Show that the angle θ goes to 0 if one extrapolates the director profile to $z = -\ell$.