Problem Set 10 – Statistical Physics B

Problem 1: Inhomogeneous Landau-de Gennes theory

An inhomogeneous nematic liquid crystal is modelled by the Landau-de Gennes free energy $F_{\text{LdG}}[\boldsymbol{\mathcal{Q}}] = \int d\mathbf{r} f(\boldsymbol{\mathcal{Q}}(\mathbf{r}))$. The form of the free energy density within the one-constant approximation at a given temperature T is

$$f(\boldsymbol{\mathcal{Q}}(\mathbf{r})) = \frac{L_1}{2}\partial_\alpha \mathcal{Q}_{\beta\gamma}(\mathbf{r})\partial_\alpha \mathcal{Q}_{\beta\gamma}(\mathbf{r}) + A(T-T^*)\text{Tr}[\boldsymbol{\mathcal{Q}}(\mathbf{r})^2] - B\text{Tr}[\boldsymbol{\mathcal{Q}}(\mathbf{r})^3] + C\{\text{Tr}[\boldsymbol{\mathcal{Q}}(\mathbf{r})^2]\}^2,$$

with Einstein summation convention implied and constants $A, B, C, L_1, T^* > 0$. The symmetric traceless tensorial order-parameter *density* $[\boldsymbol{\mathcal{Q}}]_{\alpha\beta} =: \mathcal{Q}_{\alpha\beta}$ is given by the ensemble average

$$\mathcal{Q}_{\alpha\beta}(\mathbf{r}) = \left\langle \frac{3}{2N}\sum_{i=1}^{N}\left(\hat{u}_{i\alpha}\hat{u}_{i\beta} - \frac{1}{3}\delta_{\alpha\beta}\right)\delta(\mathbf{r}-\mathbf{r}_i)\right\rangle,$$

with $(\mathbf{r}_1, ..., \mathbf{r}_N)$ and $(\hat{\mathbf{u}}_1, ..., \hat{\mathbf{u}}_N)$ the centre-of-mass positions and orientations of the particles in the liquid crystal (the mesogens), respectively, and N the number of particles. Tr(...) denotes the trace of a tensor, e.g, $\text{Tr}[\boldsymbol{\mathcal{Q}}(\mathbf{r})^2] = \mathcal{Q}_{\alpha\beta}(\mathbf{r})\mathcal{Q}_{\beta\alpha}(\mathbf{r})$.

(a) Within the uniaxial approximation, the order parameter is given by

$$\mathcal{Q}_{\alpha\beta}(\mathbf{r}) = \frac{3}{2}S(\mathbf{r})\left(\hat{n}_\alpha(\mathbf{r})\hat{n}_\beta(\mathbf{r}) - \frac{1}{3}\delta_{\alpha\beta}\right),$$

with $S(\mathbf{r})$ the scalar order parameter and $\hat{\mathbf{n}}(\mathbf{r})$ the director with $|\hat{\mathbf{n}}(\mathbf{r})|^2 = \hat{n}_\alpha(\mathbf{r})\hat{n}_\alpha(\mathbf{r}) = 1$. What do these quantities physically represent? Derive an expression for $S(\mathbf{r})$ that connects this quantity to the one-body distribution function $\rho(\mathbf{r}, \hat{\mathbf{u}}) = \langle\sum_{i=1}^{N}\delta(\mathbf{r}-\mathbf{r}_i)\delta(\hat{\mathbf{u}}-\hat{\mathbf{u}}_i)\rangle$.

(b) Show that within the uniaxial approximation and under the assumption of a spatially constant director field that $F_{\text{LdG}}[\boldsymbol{\mathcal{Q}}]$ reduces to

$$F_{\text{LdG}}[S] = \int d\mathbf{r}\,\left[\frac{m}{2}|\nabla S(\mathbf{r})|^2 + a(T-T^*)S(\mathbf{r})^2 - bS(\mathbf{r})^3 + cS(\mathbf{r})^4\right],$$

and give the expressions for m, a, b, and c. Why is the cubic term absent for a ferromagnet?

(c) Take the inhomogeneous system at coexistence $T = T_{\text{IN}}$ with $S(\mathbf{r}) = S(z)$ and boundary conditions $S(z \to -\infty) = S_{\text{IN}}$ and $S(z \to \infty) = 0$. Show from the Euler-Lagrange equation $\delta F_{\text{LdG}}[S]/\delta S(\mathbf{r}) = 0$ that the order-parameter profile is determined by,

$$S(z) = \frac{S_{\text{IN}}}{2}\left[1 - \tanh\left(\frac{z}{2\xi}\right)\right].$$

You may fix the order-parameter profile such that $S(z=0) = S_{\text{IN}}/2$. Give the expression for ξ and explain the physical meaning of this quantity.

Problem 2: Equal-constant approximation of Frank elastic free energy

Consider the Frank elastic free energy

$$F_{\text{E}} = \frac{1}{2}\int d\mathbf{r}\,\left\{K_1(\nabla\cdot\hat{\mathbf{n}})^2 + K_2[\hat{\mathbf{n}}\cdot(\nabla\times\hat{\mathbf{n}})]^2 + K_3|\hat{\mathbf{n}}\times(\nabla\times\hat{\mathbf{n}})|^2\right\},$$

with $\hat{\mathbf{n}} = \hat{\mathbf{n}}(\mathbf{r})$ the nematic director and K_i elastic constants.

(a) What deformation modes do each of the terms represent?

(b) Show that for $K := K_1 = K_2 = K_3$, the so-called equal-constant approximation that

$$F_{\mathrm{E}} = \frac{K}{2} \int d\mathbf{r} \, \left[(\nabla \cdot \hat{\mathbf{n}})^2 + |\nabla \times \hat{\mathbf{n}}|^2 \right].$$

Problem 3: Size of a defect line in a nematic

Consider a cylindrical region of radius R and length L filled with a nematic with a radial director field $\hat{\mathbf{n}} = \hat{\boldsymbol{\rho}}$ in cylindrical coordinates.

(a) Calculate the Frank free energy for such a structure. Explain why it is necessary to introduce a cutoff near the center of the cylinder.

(b) We can associate with this cutoff the core of the defect line, which we presume to contain molten nematic, i.e., isotropic phase. Calculate the size of the core of the defect given that the free energy densities are f_{iso} and f_{nem}, for an isotropic and nematic phase, respectively.

(c) Argue why in reality a line defect tends to be a loop, and calculate the tension on such loops. What can be said about the speed at which the loop reduces in size?