Problem set 3

1. Tensor order parameter and symmetry

Problem.
(a) Define

$$Q_{\alpha\beta} = \langle u_\alpha u_\beta - \frac{1}{3}\delta_{\alpha\beta}\rangle.$$

Show that $Q_{\alpha\beta}$ is symmetric and traceless.
(b) For a uniaxial nematic with director **n**, show that

$$Q_{\alpha\beta} = S\left(n_\alpha n_\beta - \frac{1}{3}\delta_{\alpha\beta}\right).$$

(c) Find the three eigenvalues of Q.
(d) Explain how the largest eigenvalue and corresponding eigenvector are related to the degree and direction of orientational order.

2. Landau–de Gennes expansion

Problem.
Consider a bulk free-energy density written for a uniaxial scalar order parameter S as

$$f(S) = \frac{A}{2}(T - T^*)S^2 - \frac{B}{3}S^3 + \frac{C}{4}S^4, B, C > 0.$$

(a) Show that the cubic term implies a first-order transition.
(b) Find the stationary points of $f(S)$.
(c) Determine the condition for coexistence between isotropic and nematic phases.
(d) Explain the role of T^*: is it the transition temperature or a lower spinodal-like temperature?

3. Response to an external magnetic field

Problem.
(a) Write the lowest-order symmetry-allowed coupling between the tensor order parameter and a magnetic field **H**.
(b) In the isotropic phase, show that the induced order parameter scales as $S \propto H^2$ for weak fields.
(c) Explain why the response becomes very large near the isotropic–nematic transition.
(d) In the ordered phase, distinguish between changing the magnitude of order and rotating the director.

4. Elastic energy and correlation length near a surface

Problem.
Suppose a wall imposes weak orientational ordering on a liquid crystal in the isotropic phase.

(a) Starting from a quadratic Landau–de Gennes free energy with a gradient term, explain why the induced order decays exponentially away from the wall.
(b) Define the correlation length ξ.
(c) Explain qualitatively how ξ behaves as the temperature approaches the transition from above.
(d) What is the physical meaning of a diverging ξ in this context?

5. Frank elastic modes: splay, twist, and bend

Problem.
(a) Write the Frank free-energy density in terms of splay, twist, and bend.
(b) For each deformation, draw or describe a director field realizing that mode.
(c) Give one experimental geometry or boundary condition that tends to favor each mode.
(d) In the one-constant approximation, what information is lost compared with the full Frank description?

6. Onsager theory and the role of excluded volume

Problem.
(a) Explain physically how a system of purely repulsive hard rods can undergo an isotropic–nematic transition.
(b) Why is the transition entropy-driven?
(c) State the limit in which Onsager theory becomes asymptotically exact.
(d) Compare briefly the physical mechanisms behind nematic ordering in Onsager and Maier–Saupe theories.

7. Planar isotropic–nematic interface from Landau–de Gennes theory

Consider a scalar order parameter $S(z)$ varying across a flat interface between an isotropic phase ($S = 0$) and a nematic phase ($S = S_N$). Assume a 1D free-energy density

$$f = \frac{L}{2}\left(\frac{dS}{dz}\right)^2 + \frac{a}{2}(T - T^*)S^2 - \frac{b}{3}S^3 + \frac{c}{4}S^4.$$

Problem.
(a) Derive the Euler–Lagrange equation for $S(z)$.
(b) State the boundary conditions at $z \to \pm\infty$ for a coexistence interface.
(c) Show that the problem can be rewritten as the motion of a fictitious particle in an effective potential.
(d) Obtain an expression for the interfacial tension

$$\gamma = \int_{-\infty}^{\infty} dz\, L\left(\frac{dS}{dz}\right)^2,$$

and explain why $\gamma > 0$.
(e) Estimate how the interface width scales with L and the curvature of the bulk free energy near the minimum.

8. Wetting by a nematic layer at a wall above the bulk transition

A substrate favors nematic alignment. The bulk is at $T > T_{NI}$, so the stable bulk phase is isotropic. Let $S(z)$satisfy a Landau–de Gennes free energy with a surface term

$$F = \int_0^\infty dz \left[\frac{L}{2}(S')^2 + \frac{a}{2}(T - T^*)S^2 + \frac{c}{4}S^4\right] - h_1 S(0).$$

Problem.
(a) Derive the bulk equation and the boundary condition at the wall.
(b) In the weak-order limit, show that $S(z)$ decays exponentially away from the wall and identify the decay length.
(c) Explain the physical meaning of this induced near-wall order.
(d) Under what conditions would you expect complete wetting by a nematic film as $T \to T_{NI}^+$?
(e) How would the answer change if the wall favored homeotropic rather than planar alignment?

9. Binary mixture with coupled concentration and nematic order

Consider a simple model for an isotropic–nematic mixture in terms of concentration $\phi(\mathbf{r})$ and scalar nematic order parameter $S(\mathbf{r})$:

$$f(\phi, S) = \frac{A}{2}\phi^2 + \frac{B}{4}\phi^4 + \frac{\alpha}{2}(T - T^*)S^2 - \frac{\beta}{3}S^3 + \frac{\gamma}{4}S^4 - \lambda\phi S^2.$$

Here ϕ measures composition relative to a reference mixture, and $\lambda > 0$ means that increasing ϕ promotes nematic order.

Problem.
(a) Explain physically the meaning of the coupling term $-\lambda\phi S^2$.
(b) For spatially uniform states, derive the stationarity conditions for ϕ and S.
(c) Show that nematic ordering shifts the effective chemical tendency of the mixture to demix.
(d) Conversely, show that composition fluctuations shift the effective quadratic coefficient controlling nematic order.
(e) Discuss qualitatively how this coupling can generate coexistence between an isotropic phase poor in rods and a nematic phase rich in rods.

10. Interfacial anchoring in an isotropic–nematic mixture

In many isotropic–nematic mixtures, the nematic director at the interface tends to align either parallel or perpendicular to the interface normal. Let $\phi(\mathbf{r})$ be the composition field and $\mathbf{n}$ the director. Consider the interfacial coupling

$$f_{\text{int}} = K_\phi(\nabla\phi)^2 + w\,(\mathbf{n}\cdot\nabla\phi)^2.$$

Problem.
(a) Explain why $\nabla\phi$ is locally normal to the interface.
(b) Show that for $w > 0$, the free energy is minimized by planar anchoring ($\mathbf{n} \perp \nabla\phi$).
(c) Show that for $w < 0$, the preferred alignment is homeotropic ($\mathbf{n} \parallel \nabla\phi$).
(d) Discuss how this anchoring contribution competes with bulk Frank elasticity near a curved droplet.
(e) For a circular nematic droplet in 2D, explain why anchoring may force the presence of topological defects.

11. Stability of a nematic droplet dispersed in an isotropic fluid

Consider a nematic droplet of radius R inside an isotropic phase. Assume strong planar anchoring at the droplet surface.

Problem.
(a) Explain why a spatially uniform director field inside the droplet is incompatible with strong planar anchoring on a closed surface.
(b) Using topology, determine the total topological charge required inside a 2D circular droplet.
(c) Compare qualitatively two possible configurations: a central $+1$ defect and a pair of $+1/2$ defects.
(d) Explain why elasticity usually favors splitting a $+1$ defect into two $+1/2$ defects.
(e) Discuss how the preferred defect structure should depend on droplet size R and anchoring strength.

12. Onsager picture for isotropic–nematic coexistence in rod–polymer or rod–solvent mixtures

A suspension contains long hard rods mixed with a non-adsorbing polymer or a solvent species. The rods can form isotropic and nematic phases with different rod concentrations.

Problem.
(a) Using Onsager's argument, explain why orientational ordering of rods can increase translational entropy at high density.
(b) Why do the coexisting isotropic and nematic phases generally have different rod concentrations?
(c) Explain qualitatively how adding a depletant (or an effective attraction) can widen the coexistence gap.
(d) Discuss the difference between "purely entropy-driven" isotropic–nematic separation and a demixing transition in a truly multicomponent mixture.
(e) Give one experimental signature that would help distinguish concentration-driven demixing from orientational ordering.