PS 1 Nematic Liquid Crystal

1 Nematic order parameter

Quadrupolar tensor $\langle \boldsymbol{q} \rangle_{T,P,N} = \left\langle |w\rangle\langle w| - \frac{1}{3}I \right\rangle_{T,P,N}$. Establish the following points:

a) $\operatorname{tr} \langle \boldsymbol{q} \rangle = 0$;

b) $\langle \boldsymbol{q} \rangle$ is symmetric: $\langle \boldsymbol{q} \rangle^t = \langle \boldsymbol{q} \rangle$;

c) compute the eigen values and vectors $|\ell\rangle, |m\rangle, |n\rangle$ of $\langle \boldsymbol{q} \rangle$;

d) $\langle \boldsymbol{q} \rangle = Q(T)(|n\rangle\langle n| - \frac{1}{3}I)$ where $Q(T)$ is a scalar function;

e) $\langle \boldsymbol{q} \rangle = 0$ in isotropic phase.

2 Landau – de Gennes theory

a) Show that the Landau free energy can be written, up to $O(Q^5)$,

$$f(T,Q) = f_0(T) + \frac{1}{3}a_0(T - T^*)Q^2 - \frac{2}{27}b\,Q^3 + \frac{1}{9}c\,Q^4$$

where T^* is the spinodal temperature.

b) Find the equilibrium state(s) minimising the free energy for the various temperatures T.

c) Determine the coordinates, T_c, $Q_c = Q(T_c)$, of the isotropic-nematic phase transition and the order of the transition.

3 Variational mean field theory [Maier-Saupe 1958]

For each molecule $\alpha = 1, \ldots, N$, denote w^α the director and $\boldsymbol{q}(w^\alpha)$ the quadrupolar tensor. The Hamiltonian (potential energy) is

$$H = \frac{1}{2}\sum\nolimits_{\alpha \neq \alpha'} \operatorname{tr} \boldsymbol{q}(w^\alpha)\boldsymbol{q}(w^{\alpha'})U(\boldsymbol{x}^\alpha - \boldsymbol{x}^{\alpha'}),$$

where U is an even integrable function. Verify the following points.

a) For any one particle density function ρ, the variational mean field free energy is

$$F(\rho) = \tfrac{1}{2}N(N-1)\operatorname{tr}\int \mathrm{d}^3x\,\mathrm{d}^3x'\mathrm{d}^2w\,\mathrm{d}^2w'\rho(\boldsymbol{x},w)\rho(\boldsymbol{x'},w')\,\boldsymbol{q}(w)\boldsymbol{q}(w')U(\boldsymbol{x}-\boldsymbol{x'})$$
$$+\; Nk_{\mathrm{B}}T\int \mathrm{d}^3x\mathrm{d}^2w\,\rho(\boldsymbol{x},w)\log\rho(\boldsymbol{x},w).$$

b) The optimal solution is

$$\rho(\boldsymbol{x}, w) = Z^{-1} \exp\bigl(-\beta U^e(\boldsymbol{x}, w)\bigr)$$

with $\beta = (k_\mathrm{B}T)^{-1}$ and $U^e(\boldsymbol{x}, w) = (N{-}1)\,\mathrm{tr}\int \mathrm{d}^3x' U(\boldsymbol{x}{-}\boldsymbol{x'})\boldsymbol{q}(w) \int \mathrm{d}^2w'\, \rho(\boldsymbol{x'}, w')\boldsymbol{q}(w')$.

c) For a homogeneous uni-axial nematic, the average moment density

$$\langle \boldsymbol{q}(\boldsymbol{x})\rangle = N \int \mathrm{d}^2w\, \rho(\boldsymbol{x}, w)\boldsymbol{q}(w) = \frac{N}{V}\,\langle \boldsymbol{q}\rangle$$

has the form $\langle \boldsymbol{q}\rangle = Q\left(|n\rangle\langle n| - \frac{1}{3}I\right)$ where $|n\rangle$ is the Frank director. The scalar amplitude Q satisfies

$$\tfrac{2}{3}Q = \bigl\langle \cos^2\theta - \tfrac{1}{3}\bigr\rangle = Z_a^{-1} \int_0^{\pi/2} \mathrm{d}(\cos\theta)\exp\bigl(-\beta Q U_0(\cos^2\theta - \tfrac{1}{3})\bigr)\left(\cos^2\theta - \tfrac{1}{3}\right)$$

with $U_0 = (N/V)\int \mathrm{d}^3x\, U(\boldsymbol{x})$.

d) Expand the free energy in powers of Q, for small Q, and get the Landau – de Gennes formula.