ICFP M2 – SOFT MATTER PHYSICS
Tutorial 11. The isotropic-nematic transition

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We revisit here the Maier-Saupe mean-field model for the isotropic-nematic transition in liquid crystals. The N constitutive molecules are slender rigid objects, whose centers of mass are distributed as in a liquid phase, at temperature T, and whose symmetry axes tend to align with each other – thus favouring a low-temperature ordered "nematic" phase. We invoke the usual spherical-coordinate angles (θ_i, ϕ_i) to describe the orientations of the molecular axes around the spontaneously chosen nematic direction z.

I Hamiltonian

1 Show that $s = \langle s_i \rangle$, where $s_i = (3\cos^2\theta_i - 1)/2$, is a relevant order parameter.

2 We consider a pair Hamiltonian $H_{ij} = n_{ij}\, s_i s_j$. What is the sign of the interaction constants n_{ij} for the nematic order to be favoured ?

3 Assuming only nearest-neighbour interactions, with $n_{ij} = n$, between a given molecule and its p close neighbours, and neglecting the highest-order fluctuation terms, show that the mean-field (orientational) Hamiltonian reads :

$$H = \frac{\lambda}{2} \sum_{i=1}^{N} s\,(s - 2\,s_i)\ , \tag{1}$$

and provide the expression of the factor λ.

II Free energy

1 Express the canonical (orientational) partition function of one molecule, involving the function [1] $I(m) = \int_0^1 \mathrm{d}u\ \mathrm{e}^{mu^2}$.

2 Assuming the total partition function is factorable into two parts, the orientational one and the kinetic one, provide its expression.

3 Deduce the free energy $F(s,T)$.

4 What is the excess free energy $\Delta F(s,T)$ with respect to the isotropic phase ?

1. Near $m = 0$, one has the Taylor expansion :

$$\ln[I(m)] = \frac{1}{3}m + \frac{2}{45}m^2 + \frac{8}{2835}m^3 - \frac{4}{14175}m^4 + o(m^4)\,.$$

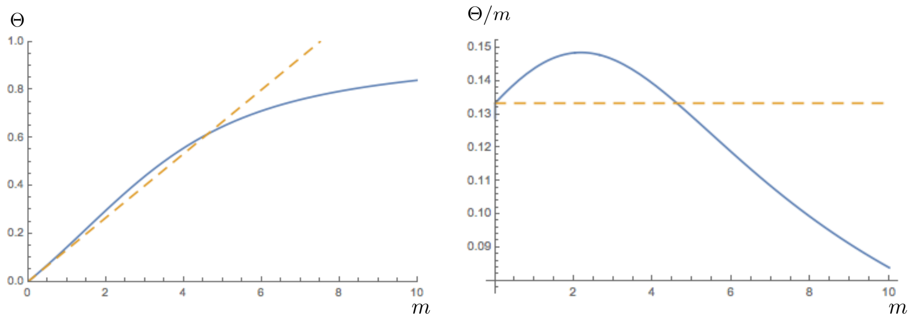

Figure 1 – Plots of $\Theta(m)$ and $\Theta(m)/m$. The dashed lines indicate $m\Theta'(0)$ (left) and $\Theta'(0)$ (right).

III Solutions

1 Obtain an implicit equation on the possible equilibrium values of s, invoking the function :

$$\Theta(m) = \frac{3}{2}\frac{I'(m)}{I(m)} - \frac{1}{2} \; . \tag{2}$$

One can use two different methods.

2 Using Fig. 1, discuss the different solutions (no matter their stability) as a function of temperature. What is the order of the transition ?

3 Discuss the stability of these solutions. In particular, provide the value of the temperature T_c at which the isotropic phase becomes unstable.

4 From what precedes, represent qualitatively $\Delta F(s,T)$ as a function of s for different relevant temperatures. Define the coexistence temperature T_NI.

5 Near T_c, provide a Landau-like development of ΔF at order 4 in s.

6 With this approximation, estimate both the reduced coexistence temperature $k_\mathrm{B}(T_\mathrm{NI} - T_\mathrm{c})/\lambda$ and the nematic order parameter at coexistence. Comment.