Hand-in sheet 1 – Statistical Physics B

- *Please hand in your solution before Thursday 23 October 2025, 16:15. This can be done during the lectures or tutorials or in mailbox 50 (J. Everts) located close to the secretariat of the Institute of Theoretical Physics on the 5th floor.*
- *We only accept hand-written or printed solutions. Digital format, such as pdf, will not be accepted.*
- *Please do not forget to write your name and student number.*
- *Make sure to answer every question as completely as possible. When you do calculations, provide sufficient explanation for all steps. Unless stated otherwise, saying that you used Mathematica (or equivalent) does not count as an explanation!*
- *In total 100 points can be earned.*

Landau-de Gennes model for a nematic liquid crystal

We consider a collection of N rods with orientations $\hat{\mathbf{u}}_i \in \mathcal{S}^2$, for $i = 1, ..., N$, where $\mathcal{S}^2$ is the two-dimensional unit sphere. The rods are apolar, i.e. $\hat{\mathbf{u}}_i$ is equivalent to $-\hat{\mathbf{u}}_i$, a property which is also reflected in the (anisotropic) interactions between the particles. This system can undergo a phase transition from a disordered "isotropic" phase to a so-called nematic phase where the particles are on average aligned in a specific direction, as we will explore in this exercise. We define the components of the tensor $\mathbf{Q}$ –which will act as an order parameter– as

$$Q_{\alpha\beta} = \left\langle \frac{3}{2N} \sum_{i=1}^{N} \left(\hat{u}_{i,\alpha}\hat{u}_{i,\beta} - \frac{1}{3}\delta_{\alpha\beta} \right) \right\rangle, \quad \alpha, \beta = x, y, z.$$

Because $\mathbf{Q}$ is traceless and symmetric, it can be diagonalised. We denote the largest eigenvalue by S and the corresponding (unit) eigenvector by $\hat{\mathbf{n}}$.

(a) (*15 points*) Show that $S = \langle P_2(\hat{\mathbf{u}} \cdot \hat{\mathbf{n}}) \rangle_\Omega$. Here, $\langle ... \rangle_\Omega$ denotes an average using the orientational distribution function of the system at a given state point, and $P_2(x) = (3x^2 - 1)/2$ is the second order Legendre polynomial. Give an interpretation for S and $\hat{\mathbf{n}}$ and explain why S is a good order parameter for the isotropic-nematic phase transition.

Even without writing an explicit microscopic model, we can make some predictions on the phase transition using symmetry arguments. We consider the so-called Landau-de Gennes free energy for an uniaxial nematic liquid crystal (i.e. only the largest eigenvalue is taken into account),

$$f_\mathrm{L}(S) := \frac{F_\mathrm{L}(S)}{V} = f_0 + a(T - T^*)S^2 - bS^3 + cS^4.$$

Here, a, b, c are positive material constants and T^* is a temperature to be interpreted in this exercise. Furthermore, f_0 is a constant independent of S.

(b) (*10 points*) What does f_0 physically represent? Explain the occurrence of the cubic term and why this term would be absent in, for example, the description of the paramagnet to ferromagnet phase transition.

(c) (*15 points*) This free energy models the transition from an isotropic liquid ($S = 0$) to a nematic state ($S \neq 0$). Show that the condition $\partial f_\mathrm{L}(S)/\partial S = 0$ gives rise to three branches. Determine the stability of each branch.

(e) (*15 points*) Show that the *global* minimum condition for $f_{\mathrm{L}}(S)$ results in

$$S(T) = \begin{cases} \dfrac{3b}{8c}\left[1+\sqrt{1-\dfrac{8(T-T_*)}{9(T_{\mathrm{IN}}-T_*)}}\right], & (T < T_{\mathrm{IN}}), \\ 0, \quad (T > T_{\mathrm{IN}}). \end{cases}$$

What is the order of the phase transition?

(f) (*15 points*) Denote the nematic spinodal temperature by T_+ and the corresponding order-parameter value by S_+. Plot all stable, unstable and metastable solutions S/S_+ as a function of $(T-T_*)/(T_+-T_*)$. Indicate also in your plot the spinodal and binodal points. Why are they given by points and not lines?

(g) (*10 points*) Consider an isotropic liquid ($T > T_{\mathrm{IN}}$) that we quench into the nematic phase ($T < T_{\mathrm{IN}}$). What is the difference when we quench into a system with temperature $T_* < T < T_{\mathrm{IN}}$ compared to $T < T_*$?

(h) (*10 points*) The simplest microscopic model describing the transition to a nematic phase is a lattice model where each lattice site is occupied by a rod with orientation $\hat{\mathbf{u}}_i \in \mathcal{S}^2$. The energy of a rod configuration is given by

$$E(\{\hat{\mathbf{u}}_i\}) = -\varepsilon \sum_{\langle i,j\rangle} P_2(\hat{\mathbf{u}}_i \cdot \hat{\mathbf{u}}_j),$$

with nearest-neighbour interaction strength $\varepsilon > 0$. Show that the free energy within the mean-field approximation is

$$\frac{\beta F}{N} = \frac{1}{2} z\beta\varepsilon S^2 - \ln\left[\int_{\mathcal{S}^2} \mathrm{d}^2\hat{\mathbf{u}}\, e^{\beta z\varepsilon S P_2(\hat{\mathbf{n}}\cdot\hat{\mathbf{u}})}\right].$$

Hint: Define $q_{i,\alpha\beta} = (3\hat{u}_{i,\alpha}\hat{u}_{i,\beta} - \delta_{\alpha\beta})/2$ *and express* $E(\{\hat{\mathbf{u}}_i\})$ *in terms of this quantity.*

(i) (*10 points*) Show that the free energy within the mean-field approximation reproduces $f_{\mathrm{L}}(S)$ including the correct signs of the coefficients. Express the Landau coefficients in terms of parameters of the model, such as the coordination number z.