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T VI: Soft Matter and Biological Physics
(Prof. E. Frey)

Problem set 6

Problem 6.1 *effective free energy of a fluid*

In terms of the canonical ensemble, a fluid is characterized by a temperature T as conjugate variable to the energy, as well as the two macro-variables volume V, and particle number N.

Here we want to achieve a proper description of the fluid that includes small fluctuations of the temperature $T(\vec{r}) = T + \delta T(\vec{r})$ and the local particle densities $n(\vec{r}) = n + \delta n(\vec{r})$ close to their equilibrium values. Up to quadratic order an effective hamiltonian is given by

$$\mathcal{H}_{\text{eff}} = \frac{1}{2}\int \mathrm{d}^d\vec{r}\left[\frac{C_V}{VT}\delta T(\vec{r})^2 + \frac{1}{n^2\kappa_T}\delta n(\vec{r})^2\right],$$

where C_V denotes the heat capacity at constant volume, and κ_T is the isothermal compressibility.

1. Introduce discrete Fourier modes in the finite box $V = L^d$,

$$\delta n_{\vec{k}} = \frac{1}{V}\int_V \mathrm{d}^d\vec{r}\,\mathrm{e}^{-\mathrm{i}\vec{k}\cdot\vec{x}} n(\vec{r}), \qquad \delta n(\vec{r}) = \sum_{\vec{k}} \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{x}} n_{\vec{k}}$$

   and similarly for $\delta T(\vec{r})$ to obtain a representation of $\mathcal{H}_{\text{eff}}$ in Fourier space.

2. Calculate thermal averages of the density, temperature modes, e.g. $\langle n_{\vec{k}} n_{\vec{q}}\rangle$ using the equipartition theorem.

3. Use thermodynamic arguments to argue that the effective hamiltonian gives a faithful representation of the macroscopic properties of a fluid. In particular, corroborate that $\mathcal{H}_{\text{eff}}$ should not contain mixed terms $\delta T(\vec{r})\delta n(\vec{r})$.

Problem 6.2 *tricritical point*

Consider the partition sum for a single scalar order parameter field $m(\vec{x})$,

$$Z = \int \mathcal{D}[m(\vec{x})] \exp(-\beta\mathcal{H}[m(\vec{x})]),$$

for the Ginzburg-Landau functional

$$\beta\mathcal{H}[m(\vec{x})] = \int \mathrm{d}\vec{x}\left\{\frac{a}{2}m(\vec{x})^2 + \frac{c}{2}(\vec{\nabla}m(\vec{x}))^2 + \frac{u}{4}m(\vec{x})^4 + \frac{v}{6}m(\vec{x})^6\right\},$$

where now the phenomenological parameters a, u may take either sign, whereas stability is guaranteed by the inequalities $c > 0$ and $v > 0$.

1. Perform a functional derivative of $\beta\mathcal{H}$ to derive an equation for the configuration $m(\vec{x})$ that minimizes $\beta\mathcal{H}$.

2. Consider now only homogeneous solutions $m(x) = const.$. Make a sketch of the effective free energy and show that there may be five extremal points. Discuss their respective stability and distinguish a continuous and discontinuous phase transition scenario. Make a sketch of the phase diagram in the a–v plane and indicate the nature of the phase boundaries.

3. The *tricritical* point $(a, u) = (0, 0)$ is a special point in the phase diagram. Extend the Ginzburg-Landau functional by a coupling to some space-varying external field $h(\vec{x})$,

$$\beta\mathcal{H}[m(\vec{x})] = \int \mathrm{d}\vec{x} \left\{ \frac{a}{2} m(\vec{x})^2 + \frac{c}{2} (\vec{\nabla} m(\vec{x}))^2 + \frac{u}{4} m(\vec{x})^4 + \frac{v}{6} m(\vec{x})^6 - h(\vec{x}) m(\vec{x}) \right\} .$$

Assuming a linear temperature dependence for $a = a'\tau$, and $u = u'\tau$ with the reduced temperature $t = (T - T_c)/T_c$, discuss the critical behavior close to the tricritical point. In particular, determine the critical exponents

   (a) for the low-temperature phase behavior of the order parameter $m \sim (-\tau)^{\beta_t}$,

   (b) the zero-field susceptibility $\chi \sim |\tau|^{-\gamma_t}$,

   (c) and the divergence of the correlation length $\xi \sim |\tau|^{-\nu_t}$.

   (d) Furthermore show that at the tricritical point the order parameter depends singularly on the field $m \sim h^{1/\delta_t}$.