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8.334 Statistical Mechanics II: Statistical Physics of Fields
Spring 2008

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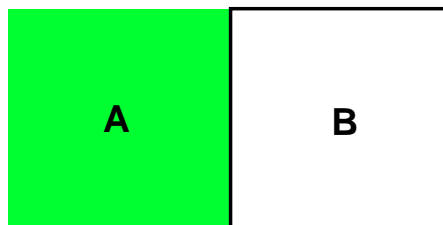
Review Problems & Solutions

The test is ‘closed book,’ but if you wish you may bring a one-sided sheet of formulas. The intent of this sheet is as a reminder of important formulas and definitions, and not as a compact transcription of the answers provided here. If this privilege is abused, it will be revoked for future tests. The test will be composed entirely from a subset of the following problems. Thus if you are familiar and comfortable with these problems, there will be no surprises!

1. The binary alloy: A binary alloy (as in β brass) consists of N_A atoms of type A , and N_B atoms of type B . The atoms form a simple cubic lattice, each interacting only with its six nearest neighbors. Assume an attractive energy of $-J$ ($J > 0$) between like neighbors $A-A$ and $B-B$, but a repulsive energy of $+J$ for an $A-B$ pair.

(a) What is the minimum energy configuration, or the state of the system at zero temperature?

- The minimum energy configuration has as little A-B bonds as possible. Thus, at zero temperature atoms A and B *phase separate*, e.g. as indicated below.



(b) Estimate the total interaction energy assuming that the atoms are randomly distributed among the N sites; i.e. each site is occupied independently with probabilities $p_A = N_A/N$ and $p_B = N_B/N$.

- In a mixed state, the average energy is obtained from

$$\begin{aligned}
 E &= (\text{number of bonds}) \times (\text{average bond energy}) \\
 &= 3N \cdot (-Jp_A^2 - Jp_B^2 + Jp_Ap_B) \\
 &= -3JN \left(\frac{N_A - N_B}{N} \right)^2.
 \end{aligned}$$

(c) Estimate the mixing entropy of the alloy with the same approximation. Assume $N_A, N_B \gg 1$.

- From the number of ways of randomly mixing N_A and N_B particles, we obtain the mixing entropy of

$$S = k_B \ln \left(\frac{N!}{N_A! N_B!} \right).$$

Using Stirling's approximation for large N ($\ln N! \approx N \ln N - N$), the above expression can be written as

$$S \approx k_B (N \ln N - N_A \ln N_A - N_B \ln N_B) = -Nk_B (p_A \ln p_A + p_B \ln p_B).$$

(d) Using the above, obtain a free energy function $F(x)$, where $x = (N_A - N_B)/N$. Expand $F(x)$ to the fourth order in x , and show that the requirement of convexity of F breaks down below a critical temperature T_c . For the remainder of this problem use the expansion obtained in (d) in place of the full function $F(x)$.

- In terms of $x = p_A - p_B$, the free energy can be written as

$$\begin{aligned} F &= E - TS \\ &= -3JNx^2 + Nk_B T \left\{ \left(\frac{1+x}{2} \right) \ln \left(\frac{1+x}{2} \right) + \left(\frac{1-x}{2} \right) \ln \left(\frac{1-x}{2} \right) \right\}. \end{aligned}$$

Expanding about $x = 0$ to fourth order, gives

$$F \simeq -Nk_B T \ln 2 + N \left(\frac{k_B T}{2} - 3J \right) x^2 + \frac{Nk_B T}{12} x^4.$$

Clearly, the second derivative of F ,

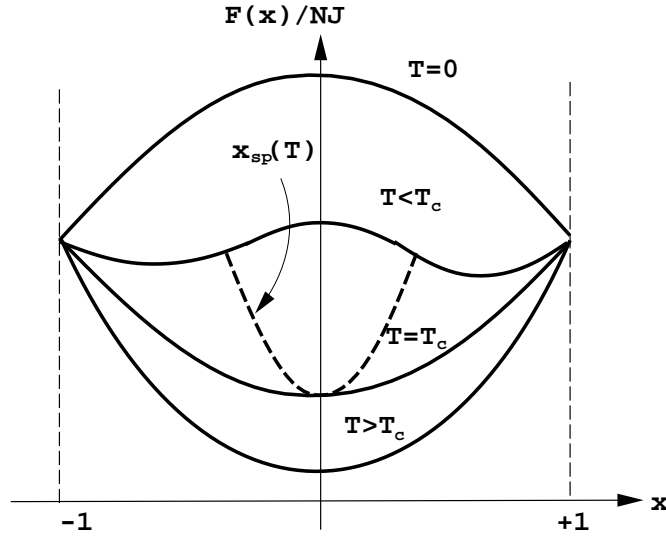
$$\frac{\partial^2 F}{\partial x^2} = N (k_B T - 6J) + Nk_B T x^2,$$

becomes negative for T small enough. Upon decreasing the temperature, F becomes concave first at $x = 0$, at a critical temperature $T_c = 6J/k_B$.

(e) Sketch $F(x)$ for $T > T_c$, $T = T_c$, and $T < T_c$. For $T < T_c$ there is a range of compositions $x < |x_{sp}(T)|$ where $F(x)$ is not convex and hence the composition is locally unstable. Find $x_{sp}(T)$.

- The function $F(x)$ is concave if $\partial^2 F / \partial x^2 < 0$, *i.e.* if

$$x^2 < \left(\frac{6J}{k_B T} - 1 \right).$$



This occurs for $T < T_c$, at the spinodal line given by

$$x_{sp}(T) = \sqrt{\frac{6J}{k_B T} - 1},$$

as indicated by the dashed line in the figure below.

(f) The alloy globally minimizes its free energy by separating into A rich and B rich phases of compositions $\pm x_{eq}(T)$, where $x_{eq}(T)$ minimizes the function $F(x)$. Find $x_{eq}(T)$.

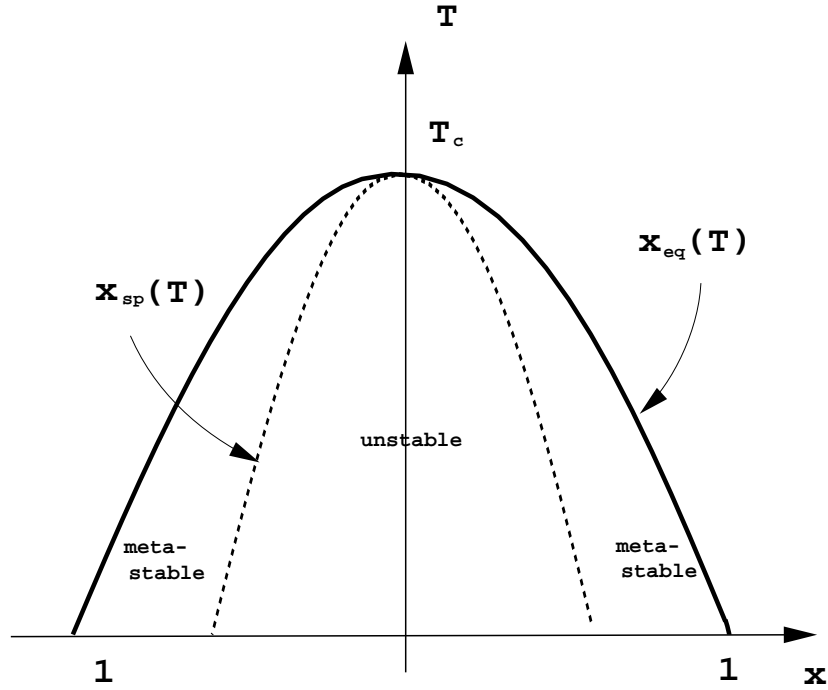
- Setting the first derivative of $dF(x)/dx = Nx \{(k_B T - 6J) + k_B T x^2/3\}$, to zero yields the equilibrium value of

$$x_{eq}(T) = \begin{cases} \pm \sqrt{3} \sqrt{\frac{6J}{k_B T} - 1} & \text{for } T < T_c \\ 0 & \text{for } T > T_c \end{cases}.$$

(g) In the (T, x) plane sketch the phase separation boundary $\pm x_{eq}(T)$; and the so called spinodal line $\pm x_{sp}(T)$. (The spinodal line indicates onset of metastability and hysteresis effects.)

- The spinodal and equilibrium curves are indicated in the figure above. In the interval between the two curves, the system is locally stable, but globally unstable. The formation of ordered regions in this regime requires nucleation, and is very slow. The dashed area is locally unstable, and the system easily phase separates to regions rich in A and B .

2. The Ising model of magnetism: The local environment of an electron in a crystal sometimes forces its spin to stay parallel or anti-parallel to a given lattice direction. As a model of magnetism in such materials we denote the direction of the spin by a single



variable $\sigma_i = \pm 1$ (an Ising spin). The energy of a configuration $\{\sigma_i\}$ of spins is then given by

$$\mathcal{H} = \frac{1}{2} \sum_{i,j=1}^N J_{ij} \sigma_i \sigma_j - h \sum_i \sigma_i \quad ;$$

where h is an external magnetic field, and J_{ij} is the interaction energy between spins at sites i and j .

(a) For N spins we make the drastic *approximation* that the interaction between all spins is the same, and $J_{ij} = -J/N$ (the equivalent neighbor model). Show that the energy can now be written as $E(M, h) = -N[Jm^2/2 + hm]$, with a magnetization $m = \sum_{i=1}^N \sigma_i / N = M/N$.

• For $J_{ij} = -J/N$, the energy of each configuration is only a function of $m = \sum_i \sigma_i / N$, given by

$$\begin{aligned} E(M, h) &= -\frac{J}{2N} \sum_{i,j=1}^N \sigma_i \sigma_j - h \sum_{i=1}^N \sigma_i \\ &= -N \frac{J}{2} \left(\sum_{i=1}^N \sigma_i / N \right) \left(\sum_{j=1}^N \sigma_j / N \right) - Nh \left(\sum_{i=1}^N \sigma_i / N \right) \\ &= -N \left(\frac{J}{2} m^2 + hm \right). \end{aligned}$$

(b) Show that the partition function $Z(h, T) = \sum_{\{\sigma_i\}} \exp(-\beta \mathcal{H})$ can be re-written as

$Z = \sum_M \exp[-\beta F(m, h)]$; with $F(m, h)$ easily calculated by analogy to problem (1). For the remainder of the problem work only with $F(m, h)$ expanded to 4th order in m .

- Since the energy depends only on the *number* of up spins N_+ , and not on their configuration, we have

$$\begin{aligned}
Z(h, T) &= \sum_{\{\sigma_i\}} \exp(-\beta \mathcal{H}) \\
&= \sum_{N_+=0}^N (\text{number of configurations with } N_+ \text{ fixed}) \cdot \exp[-\beta E(M, h)] \\
&= \sum_{N_+=0}^N \left[\frac{N!}{N_+! (N - N_+)!} \right] \exp[-\beta E(M, h)] \\
&= \sum_{N_+=0}^N \exp \left\{ -\beta \left[E(M, h) - k_B T \ln \left(\frac{N!}{N_+! (N - N_+)!} \right) \right] \right\} \\
&= \sum_M \exp[-\beta F(m, h)].
\end{aligned}$$

By analogy to the previous problem ($N_+ \leftrightarrow N_A$, $m \leftrightarrow x$, $J/2 \leftrightarrow 3J$),

$$\frac{F(m, h)}{N} = -k_B T \ln 2 - hm + \frac{1}{2} (k_B T - J) m^2 + \frac{k_B T}{12} m^4 + \mathcal{O}(m^5).$$

(c) By saddle point integration show that the actual free energy $F(h, T) = -kT \ln Z(h, T)$ is given by $F(h, T) = \min[F(m, h)]_m$. When is the saddle point method valid? Note that $F(m, h)$ is an analytic function but not convex for $T < T_c$, while the true free energy $F(h, T)$ is convex but becomes non-analytic due to the minimization.

- Let $m^*(h, T)$ minimize $F(m, h)$, *i.e.* $\min[F(m, h)]_m = F(m^*, h)$. Since there are N terms in the sum for Z , we have the bounds

$$\exp(-\beta F(m^*, h)) \leq Z \leq N \exp(-\beta F(m^*, h)),$$

or, taking the logarithm and dividing by $-\beta N$,

$$\frac{F(m^*, h)}{N} \geq \frac{F(h, T)}{N} \geq \frac{F(m^*, h)}{N} + \frac{\ln N}{N}.$$

Since F is extensive, we have therefore

$$\frac{F(m^*, h)}{N} = \frac{F(h, T)}{N}$$

in the $N \rightarrow \infty$ limit.

(d) For $h = 0$ find the critical temperature T_c below which spontaneous magnetization appears; and calculate the magnetization $\overline{m}(T)$ in the low temperature phase.

- From the definition of the *actual* free energy, the magnetization is given by

$$\overline{m} = -\frac{1}{N} \frac{\partial F(h, T)}{\partial h},$$

i.e.

$$\overline{m} = -\frac{1}{N} \frac{dF(m, h)}{dh} = -\frac{1}{N} \left\{ \frac{\partial F(m, h)}{\partial h} + \frac{\partial F(m, h)}{\partial m} \frac{\partial m}{\partial h} \right\}.$$

Thus, if m^* minimizes $F(m, h)$, *i.e.* if $\partial F(m, h)/\partial m|_{m^*} = 0$, then

$$\overline{m} = -\frac{1}{N} \left. \frac{\partial F(m, h)}{\partial h} \right|_{m^*} = m^*.$$

For $h = 0$,

$$m^{*2} = \frac{3(J - k_B T)}{k_B T},$$

yielding

$$T_c = \frac{J}{k_B},$$

and

$$\overline{m} = \begin{cases} \pm \sqrt{\frac{3(J - k_B T)}{k_B T}} & \text{if } T < T_c \\ 0 & \text{if } T > T_c \end{cases}.$$

(e) Calculate the singular (non-analytic) behavior of the response functions

$$C = \left. \frac{\partial E}{\partial T} \right|_{h=0}, \quad \text{and} \quad \chi = \left. \frac{\partial \overline{m}}{\partial h} \right|_{h=0}.$$

- The heat capacity is given by

$$C = \left. \frac{\partial E}{\partial T} \right|_{h=0, m=m^*} = -\frac{NJ}{2} \frac{\partial m^{*2}}{\partial T} = \begin{cases} \frac{3NJ T_c}{2T^2} & \text{if } T < T_c \\ 0 & \text{if } T > T_c \end{cases},$$

i.e. $\alpha = 0$, indicating a discontinuity. To calculate the susceptibility, we use

$$h = (k_B T - J) \overline{m} + \frac{k_B T}{3} \overline{m}^3.$$

Taking a derivative with respect to h ,

$$1 = (k_B T - J + k_B T \bar{m}^2) \frac{\partial \bar{m}}{\partial h},$$

which gives

$$\chi = \left. \frac{\partial \bar{m}}{\partial h} \right|_{h=0} = \begin{cases} \frac{1}{2k_B (T_c - T)} & \text{if } T < T_c \\ \frac{1}{k_B (T - T_c)} & \text{if } T > T_c \end{cases}.$$

From the above expression we obtain $\gamma_{\pm} = 1$, and $A_+/A_- = 2$.

3. The lattice-gas model: Consider a gas of particles subject to a Hamiltonian

$$\mathcal{H} = \sum_{i=1}^N \frac{\vec{p}_i^2}{2m} + \frac{1}{2} \sum_{i,j} \mathcal{V}(\vec{r}_i - \vec{r}_j), \quad \text{in a volume } V.$$

(a) Show that the grand partition function Ξ can be written as

$$\Xi = \sum_{N=0}^{\infty} \frac{1}{N!} \left(\frac{e^{\beta\mu}}{\lambda^3} \right)^N \int \prod_{i=1}^N d^3 \vec{r}_i \exp \left[-\frac{\beta}{2} \sum_{i,j} \mathcal{V}(\vec{r}_i - \vec{r}_j) \right].$$

• The grand partition function is calculated as

$$\begin{aligned} \Xi &= \sum_{N=0}^{\infty} \frac{e^{N\beta\mu}}{N!} Z_N \\ &= \sum_{N=0}^{\infty} \frac{e^{N\beta\mu}}{N!} \int \prod_{i=1}^N \frac{d^3 p_i d^3 r_i}{h^3} e^{-\beta \mathcal{H}} \\ &= \sum_{N=0}^{\infty} \frac{e^{N\beta\mu}}{N!} \left(\prod_{i=1}^N \int \frac{d^3 p_i}{h^3} e^{-\beta p_i^2 / 2m} \right) \int \prod_{i=1}^N d^3 r_i \exp \left(-\frac{\beta}{2} \sum_{i,j} \mathcal{V}_{ij} \right) \\ &= \sum_{N=0}^{\infty} \frac{1}{N!} \left(\frac{e^{N\beta\mu}}{\lambda^3} \right)^N \int \prod_{i=1}^N d^3 r_i \exp \left(-\frac{\beta}{2} \sum_{i,j} \mathcal{V}_{ij} \right), \end{aligned}$$

where $\lambda^{-1} = \sqrt{2\pi m k_B T} / h$.

(b) The volume V is now subdivided into $\mathcal{N} = V/a^3$ cells of volume a^3 , with the spacing a chosen small enough so that each cell α is either empty or occupied by one particle; i.e. the

cell occupation number n_α is restricted to 0 or 1 ($\alpha = 1, 2, \dots, \mathcal{N}$). After approximating the integrals $\int d^3\vec{r}$ by sums $a^3 \sum_{\alpha=1}^{\mathcal{N}}$, show that

$$\Xi \approx \sum_{\{n_\alpha=0,1\}} \left(\frac{e^{\beta\mu} a^3}{\lambda^3} \right)^{\sum_\alpha n_\alpha} \exp \left[-\frac{\beta}{2} \sum_{\alpha,\beta=1}^{\mathcal{N}} n_\alpha n_\beta \mathcal{V}(\vec{r}_\alpha - \vec{r}_\beta) \right].$$

• Since

$$\int \prod_{i=1}^N d^3 r_i \exp \left(-\frac{\beta}{2} \sum_{i,j} \mathcal{V}_{ij} \right) \approx a^{3N} \sum' \exp \left\{ -\frac{\beta}{2} \sum_{\alpha,\beta=1}^{\mathcal{N}} n_\alpha n_\beta \mathcal{V}(\vec{r}_\alpha - \vec{r}_\beta) \right\} \cdot N!,$$

where the primed sum is over the configurations $\{n_\alpha = 0, 1\}$ with fixed N , and

$$N = \sum_{\alpha=1}^{\mathcal{N}} n_\alpha,$$

we have

$$\Xi \approx \sum_{\{n_\alpha=0,1\}} \left(\frac{e^{\beta\mu} a^3}{\lambda^3} \right)^{\sum_\alpha n_\alpha} \exp \left\{ -\frac{\beta}{2} \sum_{\alpha,\beta=1}^{\mathcal{N}} n_\alpha n_\beta \mathcal{V}(\vec{r}_\alpha - \vec{r}_\beta) \right\}.$$

(c) By setting $n_\alpha = (1 + \sigma_\alpha)/2$ and approximating the potential by $\mathcal{V}(\vec{r}_\alpha - \vec{r}_\beta) = -J/\mathcal{N}$, show that this model is identical to the one studied in problem (2). What does this imply about the behavior of this imperfect gas?

• With $n_\alpha = (1 + \sigma_\alpha)/2$, and $\mathcal{V}(\vec{r}_\alpha - \vec{r}_\beta) = -J/\mathcal{N}$,

$$\Xi = \sum_{\{n_\alpha=0,1\}} \exp \left\{ \left(\beta\mu + 3 \ln \frac{a}{\lambda} \right) \sum_{\alpha=1}^{\mathcal{N}} \left(\frac{1 + \sigma_\alpha}{2} \right) + \frac{\beta J}{2\mathcal{N}} \sum_{\alpha,\beta=1}^{\mathcal{N}} \left(\frac{1 + \sigma_\alpha}{2} \right) \left(\frac{1 + \sigma_\beta}{2} \right) \right\}.$$

Setting $m \equiv \sum_\alpha \sigma_\alpha / \mathcal{N}$, $h' = \frac{1}{2} \left(\mu + \frac{3}{\beta} \ln \frac{a}{\lambda} + \frac{J}{2} \right)$, and $J' = J/4$, the grand partition function is written

$$\Xi = \text{const.} \sum_{\{n_\alpha=0,1\}} \exp \{ \mathcal{N} \beta (J' m^2 / 2 + h' m) \}.$$

The phase diagram of the lattice-gas can thus be mapped onto the phase diagram of the Ising model of problem 2. In particular, at a chemical potential μ such that $h' = 0$, there is a continuous “condensation” transition at a critical temperature $T_c = J/4k_B$. (Note that

$$m = \sum_\alpha \sigma_\alpha / \mathcal{N} = \sum_\alpha (2n_\alpha - 1) / \mathcal{N} = 2a^3 \rho - 1,$$

where $\rho = N/V$ is the density of the gas.)

- The manifest equivalence between these three systems is a straightforward consequence of their mapping onto the same (Ising) Hamiltonian. However, there is a more subtle equivalence relating the critical behavior of systems that cannot be so easily mapped onto each other due to the Universality Principle.

4. Surfactant condensation: N surfactant molecules are added to the surface of water over an area A . They are subject to a Hamiltonian

$$\mathcal{H} = \sum_{i=1}^N \frac{\vec{p}_i^2}{2m} + \frac{1}{2} \sum_{i,j} \mathcal{V}(\vec{r}_i - \vec{r}_j),$$

where \vec{r}_i and \vec{p}_i are two dimensional vectors indicating the position and momentum of particle i .

(a) Write down the expression for the partition function $Z(N, T, A)$ in terms of integrals over \vec{r}_i and \vec{p}_i , and perform the integrals over the momenta.

- The partition function is obtained by integrating the Boltzmann weight over phase space, as

$$Z(N, T, A) = \int \frac{\prod_{i=1}^N d^2\vec{p}_i d^2\vec{q}_i}{N! h^{2N}} \exp \left[-\beta \sum_{i=1}^N \frac{p_i^2}{2m} - \beta \sum_{i<j} \mathcal{V}(\vec{q}_i - \vec{q}_j) \right],$$

with $\beta = 1/(k_B T)$. The integrals over momenta are simple Gaussians, yielding

$$Z(N, T, A) = \frac{1}{N!} \frac{1}{\lambda^{2N}} \int \prod_{i=1}^N d^2\vec{q}_i \exp \left[-\beta \sum_{i<j} \mathcal{V}(\vec{q}_i - \vec{q}_j) \right],$$

where as usual $\lambda = h/\sqrt{2\pi m k_B T}$ denotes the thermal wavelength.

The inter-particle potential $\mathcal{V}(\vec{r})$ is infinite for separations $|\vec{r}| < a$, and attractive for $|\vec{r}| > a$ such that $\int_a^\infty 2\pi r dr \mathcal{V}(r) = -u_0$.

(b) Estimate the total non-excluded area available in the positional phase space of the system of N particles.

- To estimate the joint phase space of particles with excluded areas, add them to the system one by one. The first one can occupy the whole area A , while the second can explore only $A - 2\Omega$, where $\Omega = \pi a^2$. Neglecting three body effects (i.e. in the dilute limit), the area available to the third particle is $(A - 2\Omega)$, and similarly $(A - n\Omega)$ for the n -th particle. Hence the joint excluded volume in this dilute limit is

$$A(A - \Omega)(A - 2\Omega) \cdots (A - (N - 1)\Omega) \approx (A - N\Omega/2)^N,$$

where the last approximation is obtained by pairing terms m and $(N - m)$, and ignoring order of Ω^2 contributions to their product.

(c) Estimate the total *potential* energy of the system, *assuming a uniform density* $n = N/A$. Using this potential energy for all configurations allowed in the previous part, write down an approximation for Z .

• Assuming a *uniform density* $n = N/A$, an average attractive potential energy, \bar{U} , is estimated as

$$\begin{aligned}\bar{U} &= \frac{1}{2} \sum_{i,j} \mathcal{V}_{\text{attr.}}(\vec{q}_i - \vec{q}_j) = \frac{1}{2} \int d^2\vec{r}_1 d^2\vec{r}_2 n(\vec{r}_1) n(\vec{r}_2) \mathcal{V}_{\text{attr.}}(\vec{r}_1 - \vec{r}_2) \\ &\approx \frac{n^2}{2} A \int d^2\vec{r} \mathcal{V}_{\text{attr.}}(\vec{r}) \equiv -\frac{N^2}{2A} u_0.\end{aligned}$$

Combining the previous results gives

$$Z(N, T, A) \approx \frac{1}{N!} \frac{1}{\lambda^{2N}} (A - N\Omega/2)^N \exp \left[\frac{\beta u_0 N^2}{2A} \right].$$

(d) The surface tension of water without surfactants is σ_0 , approximately independent of temperature. Calculate the surface tension $\sigma(n, T)$ in the presence of surfactants.

• Since the work done in changing the surface area is $dW = \sigma dA$, we have $dF = -TdS + \sigma dA + \mu dN$, where $F = -k_B T \ln Z$ is the free energy. Hence, the contribution of the surfactants to the surface tension of the film is

$$\sigma_s = - \left. \frac{\partial \ln Z}{\partial A} \right|_{T,N} = - \frac{N k_B T}{A - N\Omega/2} + \frac{u_0 N^2}{2A^2},$$

which is a two-dimensional variant of the familiar van der Waals equation. Adding the (constant) contribution in the absence of surfactants gives

$$\sigma(n, T) = \sigma_0 - \left. \frac{\partial \ln Z}{\partial A} \right|_{T,N} = - \frac{N k_B T}{A - N\Omega/2} + \frac{u_0 N^2}{2A^2}.$$

(e) Show that below a certain temperature, T_c , the expression for σ is manifestly incorrect. What do you think happens at low temperatures?

• Thermodynamic stability requires $\delta\sigma\delta A \geq 0$, i.e. σ must be a monotonically increasing function of A at any temperature. This is the case at high temperatures where the first term in the equation for σ_s dominates, but breaks down at low temperatures when the term

from the attractive interactions becomes significant. The critical temperature is obtained by the usual conditions of $\partial\sigma_s/\partial A = \partial^2\sigma_s/\partial A^2 = 0$, i.e. from

$$\left\{ \begin{array}{l} \frac{\partial\sigma_s}{\partial A}\Big|_T = \frac{Nk_B T}{(A - N\Omega/2)^2} - \frac{u_0 N^2}{A^3} = 0 \\ \frac{\partial^2\sigma_s}{\partial A^2}\Big|_T = -\frac{2Nk_B T}{(A - N\Omega/2)^3} + \frac{3u_0 N^2}{A^4} = 0 \end{array} \right.,$$

The two equations are simultaneously satisfied for $A_c = 3N\Omega/2$, at a temperature

$$T_c = \frac{8u_0}{27k_B\Omega}.$$

As in the van der Waals gas, at temperatures below T_c , the surfactants separate into a high density (liquid) and a low density (gas) phase.

(f) Compute the heat capacities, C_A and write down an expression for C_σ without explicit evaluation, due to the surfactants.

- The contribution of the surfactants to the energy of the film is given by

$$E_s = -\frac{\partial \ln Z}{\partial \beta} = 2N \times \frac{k_B T}{2} - \frac{u_0 N^2}{2A}.$$

The first term is due to the kinetic energy of the surfactants, while the second arises from their (mean-field) attraction. The heat capacities are then calculated as

$$C_A = \frac{dQ}{dT}\Big|_A = \frac{\partial E}{\partial T}\Big|_A = Nk_B,$$

and

$$C_\sigma = \frac{dQ}{dT}\Big|_\sigma = \frac{\partial E}{\partial T}\Big|_\sigma - \sigma \frac{\partial A}{\partial T}\Big|_\sigma.$$

5. Cubic invariants: When the order parameter m , goes to zero discontinuously, the phase transition is said to be first order (discontinuous). A common example occurs in systems where symmetry considerations do not exclude a cubic term in the Landau free energy, as in

$$\beta\mathcal{H} = \int d^d\mathbf{x} \left[\frac{K}{2}(\nabla m)^2 + \frac{t}{2}m^2 + cm^3 + um^4 \right] \quad (K, c, u > 0).$$

(a) By plotting the energy density $\Psi(m)$, for uniform m at various values of t , show that as t is reduced there is a discontinuous jump to $\bar{m} \neq 0$ for a positive \bar{t} in the saddle-point approximation.

• To simplify the algebra, let us rewrite the energy density $\Psi(m)$, for uniform m , in terms of the rescaled quantity

$$m_r = \frac{u}{c} m.$$

In this way, we can eliminate the constant parameters c , and u , to get the expression of the energy density as

$$\Psi_r(m_r) = \frac{1}{2} t_r m_r^2 + m_r^3 + m_r^4,$$

where we have defined

$$\Psi_r = \left(\frac{c^4}{u^3} \right) \Psi, \quad \text{and} \quad t_r = \left(\frac{u}{c^2} \right) t.$$

To obtain the extrema of Ψ_r , we set the first derivative with respect to m_r to zero, i.e.

$$\frac{d\Psi_r(m_r)}{dm_r} = m_r (t_r + 3m_r + 4m_r^2) = 0.$$

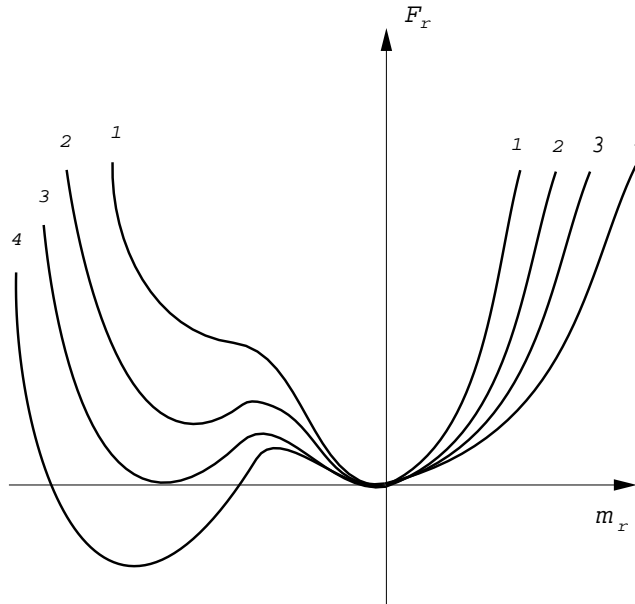
The trivial solution of this equation is $m_r^* = 0$. But if $t_r \leq 9/16$, the derivative vanishes also at $m_r^* = (-3 \pm \sqrt{9 - 16t_r})/8$. Provided that $t_r > 0$, $m_r^* = 0$ is a minimum of the function $\Psi_r(m_r)$. In addition, if $t_r < 9/16$, $\Psi_r(m_r)$ has another minimum at

$$m_r^* = -\frac{3 + \sqrt{9 - 16t_r}}{8},$$

and a maximum, located in between the two minima, at

$$m_r^* = \frac{-3 + \sqrt{9 - 16t_r}}{8}.$$

The accompanying figure depicts the behavior of $\Psi_r(m_r)$ for different values of t_r .



1. For $t_r > 9/16$, there is only one minimum $m_r^* = 0$.
2. For $0 < \bar{t}_r < t_r < 9/16$, there are two minima, but $\Psi_r(m_r^*) > \Psi_r(0) = 0$.
3. For $0 < t_r = \bar{t}_r$, $\Psi_r(m_r^*) = \Psi_r(0) = 0$.
4. For $0 < t_r < \bar{t}_r$, $\Psi_r(m_r^*) < \Psi_r(0) = 0$.

The discontinuous transition occurs when the local minimum at $m_r^* < 0$ becomes the absolute minimum. There is a corresponding jump of m_r , from $m_r^* = 0$ to $m_r^* = \bar{m}_r$, where $\bar{m}_r = m_r^*(t_r = \bar{t}_r)$.

(b) By writing down the two conditions that \bar{m} and \bar{t} must satisfy at the transition, solve for \bar{m} and \bar{t} .

- To determine \bar{m}_r and \bar{t}_r , we have to simultaneously solve the equations

$$\frac{d\Psi_r(m_r)}{dm_r} = 0, \quad \text{and} \quad \Psi_r(m_r) = \Psi_r(0) = 0.$$

Excluding the trivial solution $m_r^* = 0$, from

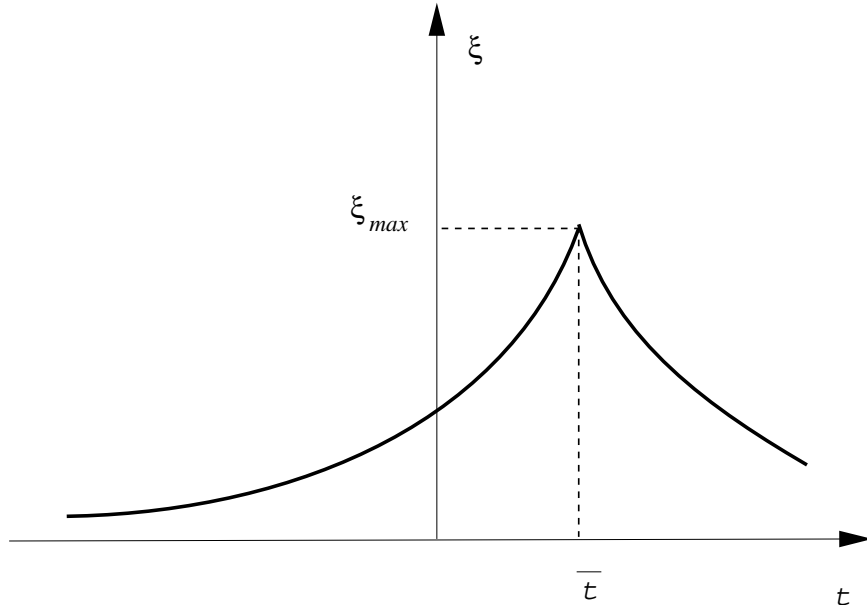
$$\begin{cases} t_r + 3m_r + 4m_r^2 = 0 \\ \frac{t_r}{2} + m_r + m_r^2 = 0 \end{cases},$$

we obtain $\bar{t}_r = -\bar{m}_r = 1/2$, or in the original units,

$$\bar{t} = \frac{c^2}{2u}, \quad \text{and} \quad \bar{m} = -\frac{c}{2u}.$$

(c) Recall that the correlation length ξ is related to the curvature of $\Psi(m)$ at its minimum by $K\xi^{-2} = \partial^2\Psi/\partial m^2|_{eq.}$. Plot ξ as a function of t .

•



Likewise, the equilibrium value of $m = m_{eq}$ in the original units equals to

$$m_{eq} = \begin{cases} 0 & \text{for } t > \bar{t} = \frac{c^2}{2u}, \\ -\left(\frac{c}{u}\right) \frac{3 + \sqrt{9 - 16ut/c^2}}{8} & \text{for } t < \bar{t}. \end{cases}$$

The correlation length ξ , is related to the curvature of $\Psi(m)$ at its equilibrium minimum by

$$K\xi^{-2} = \left. \frac{\partial^2 \Psi}{\partial m^2} \right|_{m_{eq}} = t + 6cm_{eq} + 12um_{eq}^2,$$

which is equal to

$$\xi = \begin{cases} \left(\frac{K}{t}\right)^{1/2} & \text{if } t > \bar{t}, \\ \left(-\frac{K}{2t + 3cm_{eq}}\right)^{1/2} & \text{if } t < \bar{t}. \end{cases}$$

(To arrive to the last expression, we have used $d\Psi(m)/dm|_{m=m_{eq}} = 0$.)

$$\xi_{max} = \xi(\bar{t}) = \frac{\sqrt{2Ku}}{c}.$$

A plot of ξ as a function of t is presented here. Note that the correlation length ξ , is finite at the discontinuous phase transition, attaining a maximum value of

6. Tricritical point: By tuning an additional parameter, a second order transition can be made first order. The special point separating the two types of transitions is known as a tricritical point, and can be studied by examining the Landau–Ginzburg Hamiltonian

$$\beta\mathcal{H} = \int d^d\mathbf{x} \left[\frac{K}{2}(\nabla m)^2 + \frac{t}{2}m^2 + um^4 + vm^6 - hm \right],$$

where u can be positive or negative. For $u < 0$, a positive v is necessary to ensure stability.

(a) By sketching the energy density $\Psi(m)$, for various t , show that in the saddle-point approximation there is a first-order transition for $u < 0$ and $h = 0$.

• If we consider $h = 0$, the energy density $\Psi(m)$, for uniform m , is

$$\Psi(m) = \frac{t}{2}m^2 + um^4 + vm^6.$$

As in the previous problem, to obtain the extrema of Ψ , let us set the first derivative with respect to m to zero. Again, provided that $t > 0$, $\Psi(m)$ has a minimum at $m^* = 0$. But

the derivative also vanishes for other nonzero values of m as long as certain conditions are satisfied. In order to find them, we have to solve the following equation

$$t + 4um^2 + 6vm^4 = 0,$$

from which,

$$m^{*2} = -\frac{u}{3v} \pm \frac{\sqrt{4u^2 - 6tv}}{6v}.$$

Thus, we have real and positive solutions provided that

$$u < 0, \quad \text{and} \quad t < \frac{2u^2}{3v}.$$

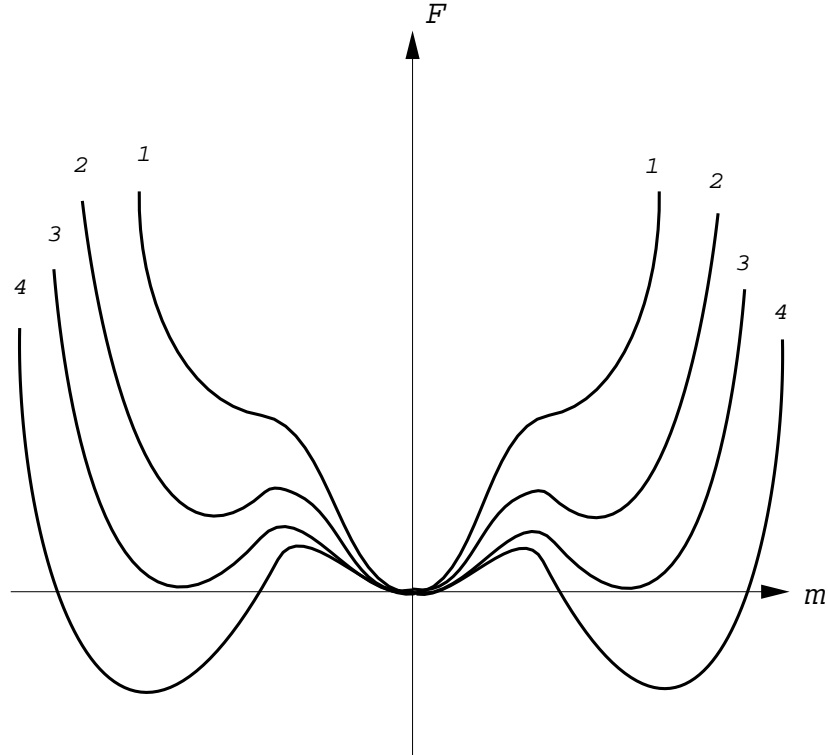
Under these conditions $\Psi(m)$ has another two minima at

$$m^{*2} = \frac{|u|}{3v} + \frac{\sqrt{4u^2 - 6tv}}{6v},$$

and two maxima at

$$m^{*2} = \frac{|u|}{3v} - \frac{\sqrt{4u^2 - 6tv}}{6v},$$

as depicted in the accompanying figure.



The different behaviors of the function $\Psi(m)$ are as follows:

1. For $t > 2u^2/3v$, there is only one minimum $m^* = 0$.
2. For $0 < \bar{t} < t < 2u^2/3v$, there are three minima, but $\Psi(\pm m^*) > \Psi(0) = 0$.
3. For $0 < t = \bar{t}$, $\Psi(\pm m^*) = \Psi(0) = 0$.
4. For $0 < t < \bar{t}$, $\Psi(\pm m^*) < \Psi(0) = 0$.

There is a thus discontinuous phase transition for $u < 0$, and $t = \bar{t}(u)$.

(b) Calculate \bar{t} and the discontinuity \bar{m} at this transition.

- To determine \bar{t} , and $\bar{m} = m^*(t = \bar{t})$, we again have to simultaneously solve the equations

$$\frac{d\Psi(m)}{dm^2} = 0, \quad \text{and} \quad \Psi(m^2) = \Psi(0) = 0,$$

or equivalently,

$$\begin{cases} \frac{t}{2} + 2um^2 + 3vm^4 = 0 \\ \frac{t}{2} + um^2 + vm^4 = 0 \end{cases},$$

from which we obtain

$$\bar{t} = \frac{u^2}{2v}, \quad \text{and} \quad \bar{m}^2 = -\frac{u}{2v} = \frac{|u|}{2v}.$$

(c) For $h = 0$ and $v > 0$, plot the phase boundary in the (u, t) plane, identifying the phases, and order of the phase transitions.

- In the (u, t) plane, the line $t = u^2/2v$ for $u < 0$, is a first-order phase transition boundary. In addition, the line $t = 0$ for $u > 0$, defines a second-order phase transition boundary, as indicated in the accompanying figure.

(d) The special point $u = t = 0$, separating first- and second-order phase boundaries, is a *tricritical* point. For $u = 0$, calculate the tricritical exponents β , δ , γ , and α , governing the singularities in magnetization, susceptibility, and heat capacity. (Recall: $C \propto t^{-\alpha}$; $\bar{m}(h = 0) \propto t^\beta$; $\chi \propto t^{-\gamma}$; and $\bar{m}(t = 0) \propto h^{1/\delta}$.)

- For $u = 0$, let us calculate the tricritical exponents α , β , γ , and δ . In order to calculate α and β , we set $h = 0$, so that

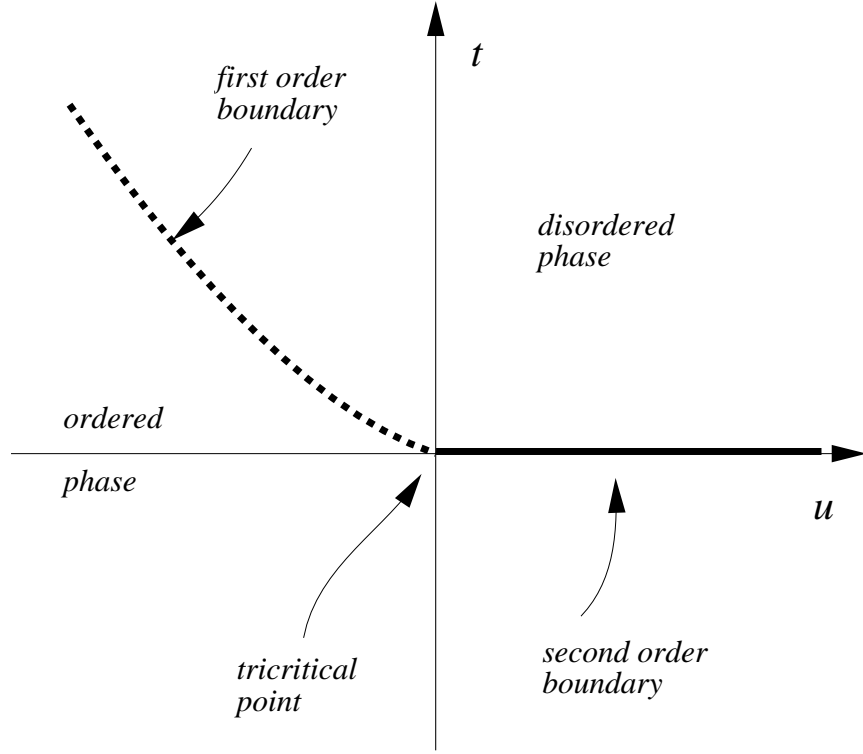
$$\Psi(m) = \frac{t}{2}m^2 + vm^6.$$

Thus from

$$\left. \frac{\partial \Psi}{\partial m} \right|_{\bar{m}} = \bar{m} (t + 6v\bar{m}^4) = 0,$$

we obtain,

$$\bar{m} = \begin{cases} 0 & \text{for } t > \bar{t} = 0, \\ \left(-\frac{t}{6v}\right)^{1/4} & \text{for } t < 0 \end{cases},$$



resulting in,

$$\overline{m}(h=0) \propto t^\beta, \quad \text{with} \quad \beta = \frac{1}{4}.$$

The corresponding free energy density scales as

$$\Psi(\overline{m}) \sim \overline{m}^6 \propto (-t)^{3/2}.$$

The tricritical exponent α characterizes the non-analytic behavior of the heat capacity $C \sim (\partial^2 \Psi / \partial T^2)|_{h=0, \overline{m}}$, and since $t \propto (T - T_c)$,

$$C \sim \left. \frac{\partial^2 \Psi}{\partial t^2} \right|_{h=0, \overline{m}} \propto t^{-\alpha}, \quad \text{with} \quad \alpha = \frac{1}{2}.$$

To calculate the tricritical exponent δ , we set $t = 0$ while keeping $h \neq 0$, so that

$$\Psi(m) = vm^6 - hm.$$

Thus from

$$\left. \frac{\partial \Psi}{\partial m} \right|_{\overline{m}} = 6v\overline{m}^5 - h = 0,$$

we obtain,

$$\overline{m} \propto h^{1/\delta}, \quad \text{with} \quad \delta = 5.$$

Finally, for $h \neq 0$ and $t \neq 0$,

$$\left. \frac{\partial \Psi}{\partial m} \right|_{\bar{m}} = t\bar{m} + 6v\bar{m}^5 - h = 0,$$

so that the susceptibility scales as

$$\chi = \left. \frac{\partial \bar{m}}{\partial h} \right|_{h=0} \propto |t|^{-1}, \quad \text{for both } t < 0 \quad \text{and} \quad t > 0,$$

i.e. with the exponents $\gamma_{\pm} = 1$.

7. Transverse susceptibility: An n -component magnetization field $\vec{m}(\mathbf{x})$ is coupled to an external field \vec{h} through a term $-\int d^d \mathbf{x} \vec{h} \cdot \vec{m}(\mathbf{x})$ in the Hamiltonian $\beta \mathcal{H}$. If $\beta \mathcal{H}$ for $\vec{h} = 0$ is invariant under rotations of $\vec{m}(\mathbf{x})$; then the free energy density ($f = -\ln Z/V$) only depends on the absolute value of \vec{h} ; i.e. $f(\vec{h}) = f(h)$, where $h = |\vec{h}|$.

(a) Show that $m_{\alpha} = \langle \int d^d \mathbf{x} m_{\alpha}(\mathbf{x}) \rangle / V = -h_{\alpha} f'(h)/h$.

• The magnetic work is the product of the magnetic field and the magnetization density, and appears as the argument of the exponential weight in the (Gibbs) canonical ensemble. We can thus “lower” the magnetization $M = \int d^d \mathbf{x} m_{\alpha}(\mathbf{x})$ “inside the average” by taking derivatives of the (Gibbs) partition function with respect to h_{α} , as

$$\begin{aligned} m_{\alpha} &= \frac{1}{V} \left\langle \int d^d \mathbf{x} m_{\alpha}(\mathbf{x}) \right\rangle = \frac{1}{V} \frac{\int \mathcal{D}\mathbf{m}(\mathbf{x}) \left(\int d^d \mathbf{x}' m_{\alpha}(\mathbf{x}') \right) e^{-\beta \mathcal{H}}}{\int \mathcal{D}\mathbf{m}(\mathbf{x}) e^{-\beta \mathcal{H}}} \\ &= \frac{1}{V} \frac{1}{Z} \frac{1}{\beta} \frac{\partial}{\partial h_{\alpha}} \int \mathcal{D}\mathbf{m}(\mathbf{x}) e^{-\beta \mathcal{H}} = \frac{1}{\beta V} \frac{\partial}{\partial h_{\alpha}} \ln Z = -\frac{\partial f}{\partial h_{\alpha}}. \end{aligned}$$

For an otherwise rotationally symmetric system, the (Gibbs) free energy depends only on the magnitude of \mathbf{h} , and using

$$\frac{\partial h}{\partial h_{\alpha}} = \frac{\partial \sqrt{h_{\beta} h_{\beta}}}{\partial h_{\alpha}} = \frac{1}{2} \frac{2\delta_{\alpha\beta} h_{\beta}}{\sqrt{h_{\beta} h_{\beta}}} = \frac{h_{\alpha}}{h},$$

we obtain

$$m_{\alpha} = -\frac{\partial f}{\partial h_{\alpha}} = -\frac{df}{dh} \frac{\partial h}{\partial h_{\alpha}} = -f' \frac{h_{\alpha}}{h}.$$

(b) Relate the susceptibility tensor $\chi_{\alpha\beta} = \partial m_{\alpha} / \partial h_{\beta}$, to $f''(h)$, \vec{m} , and \vec{h} .

• The susceptibility tensor is now obtained as

$$\begin{aligned} \chi_{\alpha\beta} &= \frac{\partial m_{\alpha}}{\partial h_{\beta}} = \frac{\partial}{\partial h_{\beta}} \left(-\frac{h_{\alpha}}{h} f'(h) \right) = -\frac{\partial h_{\alpha}}{\partial h_{\beta}} \frac{1}{h} f' - \frac{\partial h^{-1}}{\partial h_{\beta}} h_{\alpha} f' - \frac{h_{\alpha}}{h} \frac{\partial f'}{\partial h_{\beta}} \\ &= -\left(\delta_{\alpha\beta} - \frac{h_{\alpha} h_{\beta}}{h^2} \right) \frac{f'}{h} - \frac{h_{\alpha} h_{\beta}}{h^2} f''. \end{aligned}$$

In order to express f' in terms of the magnetization, we take the magnitude of the result of part (a),

$$m = |f'(h)| = -f'(h),$$

from which we obtain

$$\chi_{\alpha\beta} = \left(\delta_{\alpha\beta} - \frac{h_\alpha h_\beta}{h^2} \right) \frac{m}{h} + \frac{h_\alpha h_\beta}{h^2} \frac{dm}{dh}.$$

(c) Show that the transverse and longitudinal susceptibilities are given by $\chi_t = m/h$ and $\chi_\ell = -f''(h)$; where m is the magnitude of \vec{m} .

• Since the matrix $(\delta_{\alpha\beta} - h_\alpha h_\beta/h^2)$ removes the projection of any vector along the magnetic field, we conclude

$$\begin{cases} \chi_\ell = -f''(h) = \frac{dm}{dh} \\ \chi_t = \frac{m}{h} \end{cases}.$$

Alternatively, we can choose the coordinate system such that $h_i = h\delta_{i1}$ ($i = 1, \dots, d$), to get

$$\begin{cases} \chi_\ell = \chi_{11} = \left(\delta_{11} - \frac{h_1 h_1}{h^2} \right) \frac{m}{h} - \frac{h_1 h_1}{h^2} f''(h) = \frac{dm}{dh} \\ \chi_t = \chi_{22} = \left(\delta_{11} - \frac{h_2 h_2}{h^2} \right) \frac{m}{h} - \frac{h_2 h_2}{h^2} f''(h) = \frac{m}{h} \end{cases}.$$

(d) Conclude that χ_t diverges as $\vec{h} \rightarrow 0$, whenever there is a spontaneous magnetization. Is there any similar a priori reason for χ_ℓ to diverge?

• Provided that $\lim_{h \rightarrow 0} m \neq 0$, the transverse susceptibility clearly diverges for $h \rightarrow 0$. There is no similar reason, on the other hand, for the longitudinal susceptibility to diverge. In the saddle point approximation of the Landau–Ginzburg model, for example, we have

$$tm + 4um^3 + h = 0,$$

implying (since $4um^2 = -t$ at $h = 0$, for $t < 0$) that

$$\chi_\ell|_{h=0} = \left(\frac{dh}{dm} \right)^{-1} \Big|_{h=0} = (t - 3t)^{-1}, \quad i.e. \quad \chi_\ell = \frac{1}{2|t|},$$

at zero magnetic field, in the ordered phase ($t < 0$).

NOTE: Another, more pictorial approach to this problem is as follows. Since the Hamiltonian is invariant under rotations about \mathbf{h} , \mathbf{m} must be parallel to \mathbf{h} , *i.e.*

$$m_\alpha = \frac{h_\alpha}{h} \varphi(h),$$

where φ is some function of the magnitude of the magnetic field. For simplicity, let $\mathbf{h} = h\mathbf{e}_1$, with \mathbf{e}_1 a unit vector, implying that

$$\mathbf{m} = m\mathbf{e}_1 = \varphi(h)\mathbf{e}_1.$$

The longitudinal susceptibility is then calculated as

$$\chi_\ell = \left. \frac{\partial m_1}{\partial h_1} \right|_{\mathbf{h}=h\mathbf{e}_1} = \frac{dm}{dh} = \varphi'(h).$$

To find the transverse susceptibility, we first note that if the system is perturbed by a small external magnetic field $\delta h\mathbf{e}_2$, the change in m_1 is, by symmetry, the same for $\delta h > 0$ and $\delta h < 0$, implying

$$m_1(h\mathbf{e}_1 + \delta h\mathbf{e}_2) = m_1(h\mathbf{e}_1) + \mathcal{O}(\delta h^2).$$

Hence

$$\left. \frac{\partial m_1}{\partial h_2} \right|_{\mathbf{h}=h\mathbf{e}_1} = 0.$$

Furthermore, since \mathbf{m} and \mathbf{h} are parallel,

$$\frac{m_1(h\mathbf{e}_1 + \delta h\mathbf{e}_2)}{h} = \frac{m_2(h\mathbf{e}_1 + \delta h\mathbf{e}_2)}{\delta h},$$

from which

$$m_2(h\mathbf{e}_1 + \delta h\mathbf{e}_2) = \frac{m_1(h\mathbf{e}_1)}{h}\delta h + \mathcal{O}(\delta h^3),$$

yielding

$$\chi_t = \left. \frac{\partial m_2}{\partial h_2} \right|_{\mathbf{h}=h\mathbf{e}_1} = \frac{m}{h}.$$

8. Spin waves: In the XY model of $n = 2$ magnetism, a unit vector $\vec{s} = (s_x, s_y)$ (with $s_x^2 + s_y^2 = 1$) is placed on each site of a d -dimensional lattice. There is an interaction that tends to keep nearest-neighbors parallel, i.e. a Hamiltonian

$$-\beta\mathcal{H} = K \sum_{\langle ij \rangle} \vec{s}_i \cdot \vec{s}_j \quad .$$

The notation $\langle ij \rangle$ is conventionally used to indicate summing over all *nearest-neighbor* pairs (i, j) .

(a) Rewrite the partition function $Z = \int \prod_i d\vec{s}_i \exp(-\beta\mathcal{H})$, as an integral over the set of angles $\{\theta_i\}$ between the spins $\{\vec{s}_i\}$ and some arbitrary axis.

- The partition function is

$$Z = \int \prod_i d^2 \vec{s}_i \exp \left(K \sum_{\langle ij \rangle} \vec{s}_i \cdot \vec{s}_j \right) \delta(\vec{s}_i^2 - 1).$$

Since $\vec{s}_i \cdot \vec{s}_j = \cos(\theta_i - \theta_j)$, and $d^2 \vec{s}_i = ds_i d\theta_i s_i = d\theta_i$, we obtain

$$Z = \int \prod_i d\theta_i \exp \left(K \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) \right).$$

(b) At low temperatures ($K \gg 1$), the angles $\{\theta_i\}$ vary slowly from site to site. In this case expand $-\beta\mathcal{H}$ to get a quadratic form in $\{\theta_i\}$.

- Expanding the cosines to quadratic order gives

$$Z = e^{N_b K} \int \prod_i d\theta_i \exp \left(-\frac{K}{2} \sum_{\langle ij \rangle} (\theta_i - \theta_j)^2 \right),$$

where N_b is the total number of bonds. Higher order terms in the expansion may be neglected for large K , since the integral is dominated by $|\theta_i - \theta_j| \approx \sqrt{2/K}$.

(c) For $d = 1$, consider L sites with periodic boundary conditions (i.e. forming a closed chain). Find the normal modes θ_q that diagonalize the quadratic form (by Fourier transformation), and the corresponding eigenvalues $K(q)$. Pay careful attention to whether the modes are real or complex, and to the allowed values of q .

- For a chain of L sites, we can change to Fourier modes by setting

$$\theta_j = \sum_q \theta(q) \frac{e^{iqj}}{\sqrt{L}}.$$

Since θ_j are real numbers, we must have

$$\theta(-q) = \theta(q)^*,$$

and the allowed q values are restricted, for periodic boundary conditions, by the requirement of

$$\theta_{j+L} = \theta_j, \quad \Rightarrow \quad qL = 2\pi n, \quad \text{with } n = 0, \pm 1, \pm 2, \dots, \pm \frac{L}{2}.$$

Using

$$\theta_j - \theta_{j-1} = \sum_q \theta(q) \frac{e^{iqj}}{\sqrt{L}} (1 - e^{-iq}),$$

the one dimensional Hamiltonian, $\beta\mathcal{H} = \frac{K}{2} \sum_j (\theta_j - \theta_{j-1})^2$, can be rewritten in terms of Fourier components as

$$\beta\mathcal{H} = \frac{K}{2} \sum_{q,q'} \theta(q) \theta(q') \sum_j \frac{e^{i(q+q')j}}{L} (1 - e^{-iq}) (1 - e^{-iq'}).$$

Using the identity $\sum_j e^{i(q+q')j} = L\delta_{q,-q'}$, we obtain

$$\beta\mathcal{H} = K \sum_q |\theta(q)|^2 [1 - \cos(q)].$$

(d) Generalize the results from the previous part to a d -dimensional simple cubic lattice with periodic boundary conditions.

- In the case of a d dimensional system, the index j is replaced by a vector

$$j \mapsto \mathbf{j} = (j_1, \dots, j_d),$$

which describes the lattice. We can then write

$$\beta\mathcal{H} = \frac{K}{2} \sum_{\mathbf{j}} \sum_{\alpha} (\theta_{\mathbf{j}} - \theta_{\mathbf{j}+\mathbf{e}_{\alpha}})^2,$$

where \mathbf{e}_{α} 's are unit vectors $\{\mathbf{e}_1 = (1, 0, \dots, 0), \dots, \mathbf{e}_d = (0, \dots, 0, 1)\}$, generalizing the one dimensional result to

$$\beta\mathcal{H} = \frac{K}{2} \sum_{\mathbf{q}, \mathbf{q}'} \theta(\mathbf{q}) \theta(\mathbf{q}') \sum_{\alpha} \sum_{\mathbf{j}} \frac{e^{i(\mathbf{q}+\mathbf{q}') \cdot \mathbf{j}}}{L^d} (1 - e^{-i\mathbf{q} \cdot \mathbf{e}_{\alpha}}) (1 - e^{-i\mathbf{q}' \cdot \mathbf{e}_{\alpha}}).$$

Again, summation over \mathbf{j} constrains \mathbf{q} and $-\mathbf{q}'$ to be equal, and

$$\beta\mathcal{H} = K \sum_{\mathbf{q}} |\theta(\mathbf{q})|^2 \sum_{\alpha} [1 - \cos(q_{\alpha})].$$

(e) Calculate the contribution of these modes to the free energy and heat capacity. (Evaluate the *classical* partition function, i.e. do not quantize the modes.)

- With $K(\mathbf{q}) \equiv 2K \sum_{\alpha} [1 - \cos(q_{\alpha})]$,

$$Z = \int \prod_{\mathbf{q}} d\theta(\mathbf{q}) \exp \left[-\frac{1}{2} K(\mathbf{q}) |\theta(\mathbf{q})|^2 \right] = \prod_{\mathbf{q}} \sqrt{\frac{2\pi}{K(\mathbf{q})}},$$

and the corresponding free energy is

$$F = -k_B T \ln Z = -k_B T \left[\text{constant} - \frac{1}{2} \sum_{\mathbf{q}} \ln K(\mathbf{q}) \right],$$

or, in the continuum limit (using the fact that the density of states in \mathbf{q} space is $(L/2\pi)^d$),

$$F = -k_B T \left[\text{constant} - \frac{1}{2} L^d \int \frac{d^d q}{(2\pi)^d} \ln K(\mathbf{q}) \right].$$

As $K \sim 1/T$ at $T \rightarrow \infty$, we can write

$$F = -k_B T \left[\text{constant}' - \frac{1}{2} L^d \ln T \right],$$

and the heat capacity per site is given by

$$C = -T \frac{\partial^2 F}{\partial T^2} \cdot \frac{1}{L^d} = \frac{k_B}{2}.$$

This is because there is one degree of freedom (the angle) per site that can store potential energy.

(f) Find an expression for $\langle \vec{s}_0 \cdot \vec{s}_{\mathbf{x}} \rangle = \Re \langle \exp[i\theta_{\mathbf{x}} - i\theta_0] \rangle$ by adding contributions from different Fourier modes. Convince yourself that for $|\mathbf{x}| \rightarrow \infty$, only $\mathbf{q} \rightarrow \mathbf{0}$ modes contribute appreciably to this expression, and hence calculate the asymptotic limit.

- We have

$$\theta_{\mathbf{x}} - \theta_0 = \sum_{\mathbf{q}} \theta(\mathbf{q}) \frac{e^{i\mathbf{q} \cdot \mathbf{x}} - 1}{L^{d/2}},$$

and by completing the square for the argument of the exponential in $\langle e^{i(\theta_{\mathbf{x}} - \theta_0)} \rangle$, *i.e.* for

$$-\frac{1}{2} K(\mathbf{q}) |\theta(\mathbf{q})|^2 + i\theta(\mathbf{q}) \frac{e^{i\mathbf{q} \cdot \mathbf{x}} - 1}{L^{d/2}},$$

it follows immediately that

$$\langle e^{i(\theta_{\mathbf{x}} - \theta_0)} \rangle = \exp \left\{ -\frac{1}{L^d} \sum_{\mathbf{q}} \frac{|e^{i\mathbf{q} \cdot \mathbf{x}} - 1|^2}{2K(\mathbf{q})} \right\} = \exp \left\{ -\int \frac{d^d q}{(2\pi)^d} \frac{1 - \cos(\mathbf{q} \cdot \mathbf{x})}{K(\mathbf{q})} \right\}.$$

For x larger than 1, the integrand has a peak of height $\sim x^2/2K$ at $q = 0$ (as it is seen by expanding the cosines for small argument). Furthermore, the integrand has a first node, as q increases, at $q \sim 1/x$. From these considerations, we can obtain the leading behavior for large x :

- In $d = 1$, we have to integrate $\sim x^2/2K$ over a length $\sim 1/x$, and thus

$$\left\langle e^{i(\theta_{\mathbf{x}} - \theta_0)} \right\rangle \sim \exp \left(-\frac{|x|}{2K} \right).$$

- In $d = 2$, we have to integrate $\sim x^2/2K$ over an area $\sim (1/x)^2$. A better approximation, at large x , than merely taking the height of the peak, is given by

$$\begin{aligned} \int \frac{d^d q}{(2\pi)^d} \frac{1 - \cos(\mathbf{q} \cdot \mathbf{x})}{K(\mathbf{q})} &\approx \int \frac{dq d\varphi q}{(2\pi)^2} \frac{1 - \cos(qx \cos \varphi)}{Kq^2} \\ &= \int \frac{dq d\varphi}{(2\pi)^2} \frac{1}{Kq} - \int \frac{dq d\varphi}{(2\pi)^2} \frac{\cos(qx \cos \varphi)}{Kq}, \end{aligned}$$

or, doing the angular integration in the first term,

$$\int \frac{d^d q}{(2\pi)^d} \frac{1 - \cos(\mathbf{q} \cdot \mathbf{x})}{K(\mathbf{q})} \approx \int^{1/|x|} \frac{dq}{2\pi} \frac{1}{Kq} + \text{subleading in } x,$$

resulting in

$$\left\langle e^{i(\theta_{\mathbf{x}} - \theta_0)} \right\rangle \sim \exp \left(-\frac{\ln |x|}{2\pi K} \right) = |x|^{-\frac{1}{2\pi K}}, \quad \text{as } x \rightarrow \infty.$$

- In $d \geq 3$, we have to integrate $\sim x^2/2K$ over a volume $\sim (1/x)^3$. Thus, as $x \rightarrow \infty$, the x dependence of the integral is removed, and

$$\left\langle e^{i(\theta_{\mathbf{x}} - \theta_0)} \right\rangle \rightarrow \text{constant},$$

implying that correlations don't disappear at large x .

The results can also be obtained by noting that the fluctuations are important only for small q . Using the expansion of $K(\mathbf{q}) \approx Kq^2/2$, then reduces the problem to calculation of the Coulomb Kernel $\int d^d \mathbf{q} e^{i\mathbf{q} \cdot \mathbf{x}}/q^2$, as described in the preceding chapter.

(g) Calculate the transverse susceptibility from $\chi_t \propto \int d^d \mathbf{x} \langle \vec{s}_0 \cdot \vec{s}_{\mathbf{x}} \rangle_c$. How does it depend on the system size L ?

- We have

$$\left\langle e^{i(\theta_{\mathbf{x}} - \theta_0)} \right\rangle = \exp \left\{ - \int \frac{d^d q}{(2\pi)^d} \frac{1 - \cos(\mathbf{q} \cdot \mathbf{x})}{K(\mathbf{q})} \right\},$$

and, similarly,

$$\langle e^{i\theta_{\mathbf{x}}} \rangle = \exp \left\{ - \int \frac{d^d q}{(2\pi)^d} \frac{1}{2K(\mathbf{q})} \right\}.$$

Hence the connected correlation function

$$\langle \vec{s}_{\mathbf{x}} \cdot \vec{s}_{\mathbf{0}} \rangle_c = \left\langle e^{i(\theta_{\mathbf{x}} - \theta_{\mathbf{0}})} \right\rangle_c = \left\langle e^{i(\theta_{\mathbf{x}} - \theta_{\mathbf{0}})} \right\rangle - \langle e^{i\theta_{\mathbf{x}}} \rangle \langle e^{i\theta_{\mathbf{0}}} \rangle,$$

is given by

$$\langle \vec{s}_{\mathbf{x}} \cdot \vec{s}_{\mathbf{0}} \rangle_c = e^{-\int \frac{d^d q}{(2\pi)^d} \frac{1}{K(\mathbf{q})}} \left\{ \exp \left[\int \frac{d^d q}{(2\pi)^d} \frac{\cos(\mathbf{q} \cdot \mathbf{x})}{K(\mathbf{q})} \right] - 1 \right\}.$$

In $d \geq 3$, the x dependent integral vanishes at $x \rightarrow \infty$. We can thus expand its exponential, for large x , obtaining

$$\langle \vec{s}_{\mathbf{x}} \cdot \vec{s}_{\mathbf{0}} \rangle_c \sim \int \frac{d^d q}{(2\pi)^d} \frac{\cos(\mathbf{q} \cdot \mathbf{x})}{K(\mathbf{q})} \approx \int \frac{d^d q}{(2\pi)^d} \frac{\cos(\mathbf{q} \cdot \mathbf{x})}{K q^2} = \frac{1}{K} C_d(x) \sim \frac{1}{K |x|^{d-2}}.$$

Thus, the transverse susceptibility diverges as

$$\chi_t \propto \int d^d x \langle \vec{s}_{\mathbf{x}} \cdot \vec{s}_{\mathbf{0}} \rangle_c \sim \frac{L^2}{K}.$$

(h) In $d = 2$, show that χ_t only diverges for K larger than a critical value $K_c = 1/(4\pi)$.

• In $d = 2$, there is no long range order, $\langle \vec{s}_{\mathbf{x}} \rangle = 0$, and

$$\langle \vec{s}_{\mathbf{x}} \cdot \vec{s}_{\mathbf{0}} \rangle_c = \langle \vec{s}_{\mathbf{x}} \cdot \vec{s}_{\mathbf{0}} \rangle \sim |x|^{-1/(2\pi K)}.$$

The susceptibility

$$\chi_t \sim \int^L d^2 x |x|^{-1/(2\pi K)},$$

thus converges for $1/(2\pi K) > 2$, for K below $K_c = 1/(4\pi)$. For $K > K_c$, the susceptibility diverges as

$$\chi_t \sim L^{2-2K_c/K}.$$

9. Capillary waves: A reasonably flat surface in d -dimensions can be described by its height h , as a function of the remaining $(d-1)$ coordinates $\mathbf{x} = (x_1, \dots, x_{d-1})$. Convince yourself that the generalized “area” is given by $\mathcal{A} = \int d^{d-1} \mathbf{x} \sqrt{1 + (\nabla h)^2}$. With a surface tension σ , the Hamiltonian is simply $\mathcal{H} = \sigma \mathcal{A}$.

(a) At sufficiently low temperatures, there are only slow variations in h . Expand the energy to quadratic order, and write down the partition function as a functional integral.

- For a surface parametrized by the height function

$$x_d = h(x_1, \dots, x_{d-1}),$$

an area element can be calculated as

$$dA = \frac{1}{\cos \alpha} dx_1 \cdots dx_{d-1},$$

where α is the angle between the d^{th} direction and the normal

$$\vec{n} = \frac{1}{\sqrt{1 + (\nabla h)^2}} \left(-\frac{\partial h}{\partial x_1}, \dots, -\frac{\partial h}{\partial x_{d-1}}, 1 \right)$$

to the surface ($n^2 = 1$). Since, $\cos \alpha = n_d = [1 + (\nabla h)^2]^{-1/2} \approx 1 - \frac{1}{2} (\nabla h)^2$, we obtain

$$\mathcal{H} = \sigma \mathcal{A} \approx \sigma \int d^{d-1}x \left\{ 1 + \frac{1}{2} (\nabla h)^2 \right\},$$

and, dropping a multiplicative constant,

$$Z = \int \mathcal{D}h(\mathbf{x}) \exp \left\{ -\beta \frac{\sigma}{2} \int d^{d-1}x (\nabla h)^2 \right\}.$$

(b) Use Fourier transformation to diagonalize the quadratic Hamiltonian into its normal modes $\{h_{\mathbf{q}}\}$ (capillary waves).

- After changing variables to the Fourier modes,

$$h(\mathbf{x}) = \int \frac{d^{d-1}q}{(2\pi)^{d-1}} h(\mathbf{q}) e^{i\mathbf{q} \cdot \mathbf{x}},$$

the partition function is given by

$$Z = \int \mathcal{D}h(\mathbf{q}) \exp \left\{ -\beta \frac{\sigma}{2} \int \frac{d^{d-1}q}{(2\pi)^{d-1}} q^2 |h(\mathbf{q})|^2 \right\}.$$

(c) What symmetry breaking is responsible for these Goldstone modes?

- By selecting a particular height, the ground state breaks the translation symmetry in the d^{th} direction. The transformation $h(\mathbf{x}) \rightarrow h(\mathbf{x}) + \xi(\mathbf{x})$ leaves the energy unchanged if $\xi(\mathbf{x})$ is constant. By continuity, we can have an arbitrarily small change in the energy by varying $\xi(\mathbf{x})$ arbitrarily slowly.

(d) Calculate the height–height correlations $\langle (h(\mathbf{x}) - h(\mathbf{x}'))^2 \rangle$.

• From

$$h(\mathbf{x}) - h(\mathbf{x}') = \int \frac{d^{d-1}q}{(2\pi)^{d-1}} h(\mathbf{q}) \left(e^{i\mathbf{q}\cdot\mathbf{x}} - e^{i\mathbf{q}\cdot\mathbf{x}'} \right),$$

we obtain

$$\langle (h(\mathbf{x}) - h(\mathbf{x}'))^2 \rangle = \int \frac{d^{d-1}q}{(2\pi)^{d-1}} \frac{d^{d-1}q'}{(2\pi)^{d-1}} \langle h(\mathbf{q}) h(\mathbf{q}') \rangle \left(e^{i\mathbf{q}\cdot\mathbf{x}} - e^{i\mathbf{q}\cdot\mathbf{x}'} \right) \left(e^{i\mathbf{q}'\cdot\mathbf{x}} - e^{i\mathbf{q}'\cdot\mathbf{x}'} \right).$$

The height-height correlations thus behave as

$$\begin{aligned} G(\mathbf{x} - \mathbf{x}') &\equiv \langle (h(\mathbf{x}) - h(\mathbf{x}'))^2 \rangle \\ &= \frac{2}{\beta\sigma} \int \frac{d^{d-1}q}{(2\pi)^{d-1}} \frac{1 - \cos[\mathbf{q} \cdot (\mathbf{x} - \mathbf{x}')] }{q^2} = \frac{2}{\beta\sigma} C_{d-1}(\mathbf{x} - \mathbf{x}'). \end{aligned}$$

(e) Comment on the form of the result (d) in dimensions $d = 4, 3, 2$, and 1 .

• We can now discuss the asymptotic behavior of the Coulomb Kernel for large $|\mathbf{x} - \mathbf{x}'|$, either using the results from problem 1(f), or the exact form given in lectures.

• In $d \geq 4$, $G(\mathbf{x} - \mathbf{x}') \rightarrow \text{constant}$, and the surface is *flat*.

• In $d = 3$, $G(\mathbf{x} - \mathbf{x}') \sim \ln |\mathbf{x} - \mathbf{x}'|$, and we come to the surprising conclusion that there are no asymptotically flat surfaces in three dimensions. While this is technically correct, since the logarithm grows slowly, very large surfaces are needed to detect appreciable fluctuations.

• In $d = 2$, $G(\mathbf{x} - \mathbf{x}') \sim |\mathbf{x} - \mathbf{x}'|$. This is easy to comprehend, once we realize that the interface $h(x)$ is similar to the path $x(t)$ of a random walker, and has similar ($x \sim \sqrt{t}$) fluctuations.

• In $d = 1$, $G(\mathbf{x} - \mathbf{x}') \sim |\mathbf{x} - \mathbf{x}'|^2$. The transverse fluctuation of the ‘point’ interface are very big, and the approximations break down as discussed next.

(f) By estimating typical values of ∇h , comment on when it is justified to ignore higher order terms in the expansion for \mathcal{A} .

• We can estimate $(\nabla h)^2$ as

$$\frac{\langle (h(\mathbf{x}) - h(\mathbf{x}'))^2 \rangle}{(\mathbf{x} - \mathbf{x}')^2} \propto |\mathbf{x} - \mathbf{x}'|^{1-d}.$$

For dimensions $d \geq d_\ell = 1$, the typical size of the gradient decreases upon coarse-graining. The gradient expansion of the area used before is then justified. For dimensions $d \leq d_\ell$, the whole idea of the gradient expansion fails to be sensible.

10. Gauge fluctuations in superconductors: The Landau–Ginzburg model of superconductivity describes a complex superconducting order parameter $\Psi(\mathbf{x}) = \Psi_1(\mathbf{x}) + i\Psi_2(\mathbf{x})$, and the electromagnetic vector potential $\vec{A}(\mathbf{x})$, which are subject to a Hamiltonian

$$\beta\mathcal{H} = \int d^3\mathbf{x} \left[\frac{t}{2} |\Psi|^2 + u |\Psi|^4 + \frac{K}{2} D_\mu \Psi D_\mu^* \Psi^* + \frac{L}{2} (\nabla \times A)^2 \right].$$

The gauge-invariant derivative $D_\mu \equiv \partial_\mu - ieA_\mu(\mathbf{x})$, introduces the coupling between the two fields. (In terms of Cooper pair parameters, $e = e^*c/\hbar$, $K = \hbar^2/2m^*$.)

(a) Show that the above Hamiltonian is invariant under the *local gauge symmetry*:

$$\Psi(\mathbf{x}) \mapsto \Psi(x) \exp(i\theta(\mathbf{x})), \quad \text{and} \quad A_\mu(\mathbf{x}) \mapsto A_\mu(\mathbf{x}) + \frac{1}{e} \partial_\mu \theta.$$

• Under a local gauge transformation, $\beta\mathcal{H} \mapsto$

$$\int d^3x \left\{ \frac{t}{2} |\Psi|^2 + u |\Psi|^4 + \frac{K}{2} [(\partial_\mu - ieA_\mu - i\partial_\mu \theta) \Psi e^{i\theta}] [(\partial_\mu + ieA_\mu + i\partial_\mu \theta) \Psi^* e^{-i\theta}] + \frac{L}{2} \left(\nabla \times \vec{A} + \nabla \times \frac{1}{e} \nabla \theta \right)^2 \right\}.$$

But this is none other than $\beta\mathcal{H}$ again, since

$$(\partial_\mu - ieA_\mu - i\partial_\mu \theta) \Psi e^{i\theta} = e^{i\theta} (\partial_\mu - ieA_\mu) \Psi = e^{i\theta} D_\mu \Psi,$$

and

$$\nabla \times \frac{1}{e} \nabla \theta = 0.$$

(b) Show that there is a saddle point solution of the form $\Psi(\mathbf{x}) = \bar{\Psi}$, and $\vec{A}(\mathbf{x}) = 0$, and find $\bar{\Psi}$ for $t > 0$ and $t < 0$.

• The saddle point solutions are obtained from

$$\frac{\delta\mathcal{H}}{\delta\Psi^*} = 0, \quad \implies \quad \frac{t}{2} \Psi + 2u\Psi |\Psi|^2 - \frac{K}{2} D_\mu D_\mu \Psi = 0,$$

and

$$\frac{\delta\mathcal{H}}{\delta A_\mu} = 0, \quad \implies \quad \frac{K}{2} (-ie\Psi D_\mu^* \Psi^* + ie\Psi^* D_\mu \Psi) - L\epsilon_{\alpha\beta\mu}\epsilon_{\alpha\gamma\delta}\partial_\beta\partial_\gamma A_\delta = 0.$$

The ansatz $\Psi(\mathbf{x}) = \bar{\Psi}$, $\vec{A} = 0$, clearly solves these equations. The first equation then becomes

$$t\bar{\Psi} + 4u\bar{\Psi}|\bar{\Psi}|^2 = 0,$$

yielding (for $u > 0$) $\bar{\Psi} = 0$ for $t > 0$, whereas $|\bar{\Psi}|^2 = -t/4u$ for $t < 0$.

(c) For $t < 0$, calculate the cost of fluctuations by setting

$$\begin{cases} \Psi(\mathbf{x}) = (\bar{\Psi} + \phi(\mathbf{x})) \exp(i\theta(\mathbf{x})), \\ A_\mu(\mathbf{x}) = a_\mu(\mathbf{x}), \quad (\text{with } \partial_\mu a_\mu = 0 \text{ in the Coulomb gauge}) \end{cases}$$

and expanding $\beta\mathcal{H}$ to quadratic order in ϕ , θ , and \vec{a} .

• For simplicity, let us choose $\bar{\Psi}$ to be real. From the Hamiltonian term

$$D_\mu \Psi D_\mu^* \Psi^* = [(\partial_\mu - ie a_\mu)(\bar{\Psi} + \phi) e^{i\theta}] [(\partial_\mu + ie a_\mu)(\bar{\Psi} + \phi) e^{-i\theta}],$$

we get the following quadratic contribution

$$\bar{\Psi}^2 (\nabla\theta)^2 + (\nabla\phi)^2 - 2e\bar{\Psi}^2 a_\mu \partial_\mu \theta + e^2 \bar{\Psi}^2 |\vec{a}|^2.$$

The third term in the above expression integrates to zero (as it can be seen by integrating by parts and invoking the Coulomb gauge condition $\partial_\mu a_\mu = 0$). Thus, the quadratic terms read

$$\begin{aligned} \beta\mathcal{H}^{(2)} = \int d^3x \left\{ \left(\frac{t}{2} + 6u\bar{\Psi}^2 \right) \phi^2 + \frac{K}{2} (\nabla\phi)^2 + \frac{K}{2} \bar{\Psi}^2 (\nabla\theta)^2 \right. \\ \left. + \frac{K}{2} e^2 \bar{\Psi}^2 |\vec{a}|^2 + \frac{L}{2} (\nabla \times \vec{a})^2 \right\}. \end{aligned}$$

(d) Perform a Fourier transformation, and calculate the expectation values of $\langle |\phi(\mathbf{q})|^2 \rangle$, $\langle |\theta(\mathbf{q})|^2 \rangle$, and $\langle |\vec{a}(\mathbf{q})|^2 \rangle$.

• In terms of Fourier transforms, we obtain

$$\begin{aligned} \beta\mathcal{H}^{(2)} = \sum_{\mathbf{q}} \left\{ \left(\frac{t}{2} + 6u\bar{\Psi}^2 + \frac{K}{2} q^2 \right) |\phi(\mathbf{q})|^2 + \frac{K}{2} \bar{\Psi}^2 q^2 |\theta(\mathbf{q})|^2 \right. \\ \left. + \frac{K}{2} e^2 \bar{\Psi}^2 |\vec{a}(\mathbf{q})|^2 + \frac{L}{2} (\mathbf{q} \times \vec{a})^2 \right\}. \end{aligned}$$

In the Coulomb gauge, $\mathbf{q} \perp \vec{a}(\mathbf{q})$, and so $[\mathbf{q} \times \vec{a}(\mathbf{q})]^2 = q^2 |\vec{a}(\mathbf{q})|^2$. This diagonal form then yields immediately (for $t < 0$)

$$\begin{aligned} \langle |\phi(\mathbf{q})|^2 \rangle &= \left(t + 12u\bar{\Psi}^2 + Kq^2 \right)^{-1} = \frac{1}{Kq^2 - 2t}, \\ \langle |\theta(\mathbf{q})|^2 \rangle &= \left(K\bar{\Psi}^2 q^2 \right)^{-1} = -\frac{4u}{Ktq^2}, \\ \langle |\vec{a}(\mathbf{q})|^2 \rangle &= 2 \left(Ke^2 \bar{\Psi}^2 + Lq^2 \right)^{-1} = \frac{2}{Lq^2 - Ke^2 t/4u} \quad (\vec{a} \text{ has 2 components}). \end{aligned}$$

Note that the gauge field, “mass-less” in the original theory, acquires a “mass” $Ke^2t/4u$ through its coupling to the order parameter. This is known as the Higgs mechanism.

11. Fluctuations around a tricritical point: As shown in a previous problem, the Hamiltonian

$$\beta\mathcal{H} = \int d^d\mathbf{x} \left[\frac{K}{2}(\nabla m)^2 + \frac{t}{2}m^2 + um^4 + vm^6 \right],$$

with $u = 0$ and $v > 0$ describes a tricritical point.

(a) Calculate the heat capacity singularity as $t \rightarrow 0$ by the saddle point approximation.

• As already calculated in a previous problem, the saddle point minimum of the free energy $\vec{m} = \bar{m}\hat{e}_\ell$, can be obtained from

$$\left. \frac{\partial \Psi}{\partial m} \right|_{\bar{m}} = \bar{m} (t + 6v\bar{m}^4) = 0,$$

yielding,

$$\bar{m} = \begin{cases} 0 & \text{for } t > \bar{t} = 0 \\ \left(-\frac{t}{6v}\right)^{1/4} & \text{for } t < 0 \end{cases}.$$

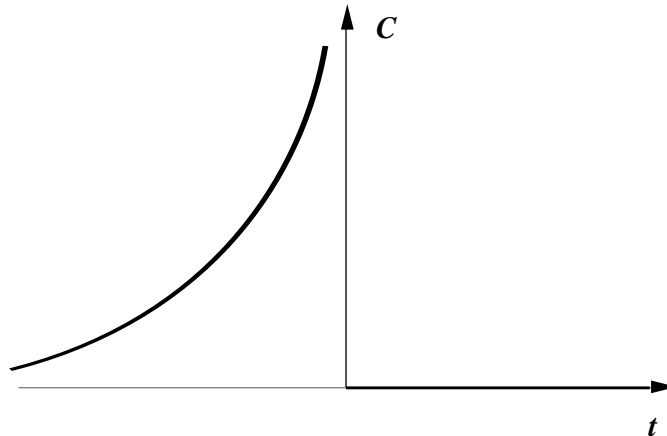
The corresponding free energy density equals to

$$\Psi(\bar{m}) = \frac{t}{2}\bar{m}^2 + v\bar{m}^6 = \begin{cases} 0 & \text{for } t > 0 \\ -\frac{1}{3} \frac{(-t)^{3/2}}{(6v)^{1/2}} & \text{for } t < 0 \end{cases}.$$

Therefore, the singular behavior of the heat capacity is given by

$$C = C_{s.p.} \sim -T_c \left. \frac{\partial^2 \Psi}{\partial t^2} \right|_{\bar{m}} = \begin{cases} 0 & \text{for } t > 0 \\ \frac{T_c}{4} (-6vt)^{-1/2} & \text{for } t < 0 \end{cases},$$

as sketched in the figure below.



(b) Include both longitudinal and transverse fluctuations by setting

$$\vec{m}(\mathbf{x}) = (\bar{m} + \phi_\ell(\mathbf{x}))\hat{e}_\ell + \sum_{\alpha=2}^n \phi_t^\alpha(\mathbf{x})\hat{e}_\alpha,$$

and expanding $\beta\mathcal{H}$ to quadratic order in ϕ .

• Let us now include both longitudinal and transversal fluctuations by setting

$$\vec{m}(\mathbf{x}) = (\bar{m} + \phi_\ell(\mathbf{x}))\hat{e}_\ell + \sum_{\alpha=2}^n \phi_t^\alpha(\mathbf{x})\hat{e}_\alpha,$$

where \hat{e}_ℓ and \hat{e}_α form an orthonormal set of n vectors. Consequently, the free energy $\beta\mathcal{H}$ is a function of ϕ_ℓ and ϕ_t . Since $\bar{m}\hat{e}_\ell$ is a minimum, there are no linear terms in the expansion of $\beta\mathcal{H}$ in ϕ . The contributions of each factor in the free energy to the quadratic term in the expansion are

$$\begin{aligned} (\nabla \vec{m})^2 &\Rightarrow (\nabla \phi_\ell)^2 + \sum_{\alpha=2}^n (\nabla \phi_t^\alpha)^2, \\ (\vec{m})^2 &\Rightarrow (\phi_\ell)^2 + \sum_{\alpha=2}^n (\phi_t^\alpha)^2, \\ (\vec{m})^6 &= ((\vec{m})^2)^3 = (\bar{m}^2 + 2\bar{m}\phi_\ell + \phi_\ell^2 + \sum_{\alpha=2}^n (\phi_t^\alpha)^2)^3 \Rightarrow 15\bar{m}^4(\phi_\ell)^2 + 3\bar{m}^4 \sum_{\alpha=2}^n (\phi_t^\alpha)^2. \end{aligned}$$

The expansion of $\beta\mathcal{H}$ to second order now gives

$$\begin{aligned} \beta\mathcal{H}(\phi_\ell, \phi_t^\alpha) &= \beta\mathcal{H}(0,0) + \int d^d\mathbf{x} \left\{ \left[\frac{K}{2}(\nabla \phi_\ell)^2 + \frac{\phi_\ell^2}{2} (t + 30v\bar{m}^4) \right] \right. \\ &\quad \left. + \sum_{\alpha=2}^n \left[\frac{K}{2}(\nabla \phi_t^\alpha)^2 + \frac{(\phi_t^\alpha)^2}{2} (t + 6v\bar{m}^4) \right] \right\}. \end{aligned}$$

We can formally rewrite it as

$$\beta\mathcal{H}(\phi_\ell, \phi_t^\alpha) = \beta\mathcal{H}(0,0) + \beta\mathcal{H}_\ell(\phi_\ell) + \sum_{\alpha=2}^n \beta\mathcal{H}_{t_\alpha}(\phi_t^\alpha),$$

where $\beta\mathcal{H}_i(\phi_i)$, with $i = \ell, t_\alpha$, is in general given by

$$\beta\mathcal{H}_i(\phi_i) = \frac{K}{2} \int d^d\mathbf{x} \left[(\nabla \phi_i)^2 + \frac{\phi_i^2}{\xi_i^2} \right],$$

with the inverse correlation lengths

$$\xi_\ell^{-2} = \begin{cases} \frac{t}{K} & \text{for } t > 0 \\ \frac{-4t}{K} & \text{for } t < 0 \end{cases},$$

and

$$\xi_{t_\alpha}^{-2} = \begin{cases} \frac{t}{K} & \text{for } t > 0 \\ 0 & \text{for } t < 0 \end{cases}.$$

As shown in the lectures for the critical point of a magnet, for $t > 0$ there is no difference between longitudinal and transverse components, whereas for $t < 0$, there is no restoring force for the Goldstone modes ϕ_t^α due to the rotational symmetry of the *ordered* state.

(c) Calculate the longitudinal and transverse correlation functions.

- Since in the harmonic approximation $\beta\mathcal{H}$ turns out to be a sum of the Hamiltonians of the different fluctuating components ϕ_ℓ , ϕ_t^α , these quantities are independent of each other, i.e.

$$\langle \phi_\ell \phi_t^\alpha \rangle = 0, \quad \text{and} \quad \langle \phi_t^\gamma \phi_t^\alpha \rangle = 0 \quad \text{for } \alpha \neq \gamma.$$

To determine the longitudinal and transverse correlation functions, we first express the free energy in terms of Fourier modes, so that the probability of a particular fluctuation configuration is given by

$$\mathcal{P}(\{\phi_\ell, \phi_t^\alpha\}) \propto \prod_{\mathbf{q}, \alpha} \exp \left\{ -\frac{K}{2} (q^2 + \xi_\ell^{-2}) |\phi_{\ell, \mathbf{q}}|^2 \right\} \cdot \exp \left\{ -\frac{K}{2} (q^2 + \xi_{t_\alpha}^{-2}) |\phi_{t, \mathbf{q}}^\alpha|^2 \right\}.$$

Thus, as it was also shown in the lectures, the correlation function is

$$\langle \phi_\alpha(\mathbf{x}) \phi_\beta(0) \rangle = \frac{\delta_{\alpha, \beta}}{VK} \sum_{\mathbf{q}} \frac{e^{i\mathbf{q} \cdot \mathbf{x}}}{(q^2 + \xi_\alpha^{-2})} = -\frac{\delta_{\alpha, \beta}}{K} I_d(\mathbf{x}, \xi_\alpha),$$

therefore,

$$\langle \phi_\ell(\mathbf{x}) \phi_\ell(0) \rangle = -\frac{1}{K} I_d(\mathbf{x}, \xi_\ell),$$

and

$$\langle \phi_t^\alpha(\mathbf{x}) \phi_t^\beta(0) \rangle = -\frac{\delta_{\alpha, \beta}}{K} I_d(\mathbf{x}, \xi_{t_\alpha}).$$

(d) Compute the first correction to the saddle point free energy from fluctuations.

- Let us calculate the first correction to the saddle point free energy from fluctuations. The partition function is

$$\begin{aligned}
Z &= e^{-\beta\mathcal{H}(0,0)} \int \mathcal{D}\phi(\mathbf{x}) \exp \left\{ -\frac{K}{2} \int d^d\mathbf{x} [(\nabla\phi)^2 + \xi^{-2}\phi^2] \right\} \\
&= e^{-\beta\mathcal{H}(0,0)} \int \prod_{\mathbf{q}} d\phi_{\mathbf{q}} \exp \left\{ -\frac{K}{2} \sum_{\mathbf{q}} (q^2 + \xi^{-2}) \phi_{\mathbf{q}} \phi_{\mathbf{q}}^* \right\} , \\
&= \prod_{\mathbf{q}} [K (q^2 + \xi^{-2})]^{-1/2} = \exp \left\{ -\frac{1}{2} \sum_{\mathbf{q}} (Kq^2 + K\xi^{-2}) \right\}
\end{aligned}$$

and the free energy density equals to

$$\beta f = \frac{\beta\mathcal{H}(0,0)}{V} + \begin{cases} \frac{n}{2} \int \frac{d^d\mathbf{q}}{(2\pi)^d} \ln(Kq^2 + t) & \text{for } t > 0 \\ \frac{1}{2} \int \frac{d^d\mathbf{q}}{(2\pi)^d} \ln(Kq^2 - 4t) + \frac{n-1}{2} \int \frac{d^d\mathbf{q}}{(2\pi)^d} \ln(Kq^2) & \text{for } t < 0 \end{cases} .$$

Note that the first term is the saddle point free energy, and that there are n contributions to the free energy from fluctuations.

(e) Find the fluctuation correction to the heat capacity.

- As $C = -T(d^2 f/dT^2)$, the fluctuation corrections to the heat capacity are given by

$$C - C_{s.p.} \propto \begin{cases} \frac{n}{2} \int \frac{d^d\mathbf{q}}{(2\pi)^d} (Kq^2 + t)^{-2} & \text{for } t > 0 \\ \frac{16}{2} \int \frac{d^d\mathbf{q}}{(2\pi)^d} (Kq^2 - 4t)^{-2} & \text{for } t < 0 \end{cases} .$$

These integrals change behavior at $d = 4$. For $d > 4$, the integrals diverge at large \mathbf{q} , and are dominated by the upper cutoff $\Delta \simeq 1/a$. That is why fluctuation corrections to the heat capacity add just a constant term on each side of the transition, and the saddle point solution keeps its qualitative form. On the other hand, for $d < 4$, the integrals are proportional to the corresponding correlation length ξ^{4-d} . Due to the divergence of ξ , the fluctuation corrections diverge as

$$C_{fl.} = C - C_{s.p.} \propto K^{-d/2} |t|^{d/2-2} .$$

(f) By comparing the results from parts (a) and (e) for $t < 0$ obtain a Ginzburg criterion, and the upper critical dimension for validity of mean-field theory at a tricritical point.

- To obtain a Ginzburg criterion, let us consider $t < 0$. In this region, the saddle point contribution already diverges as $C_{s.p.} \propto (-vt)^{-1/2}$, so that

$$\frac{C_{fl.}}{C_{s.p.}} \propto (-t)^{\frac{d-3}{2}} \left(\frac{v}{K^d} \right)^{1/2}.$$

Therefore at $t < 0$, the saddle point contribution dominates the behavior of this ratio provided that $d > 3$. For $d < 3$, the mean field result will continue being dominant far enough from the critical point, i.e. if

$$(-t)^{d-3} \gg \left(\frac{K^d}{v} \right), \quad \text{or} \quad |t| \gg \left(\frac{K^d}{v} \right)^{1/(d-3)}.$$

Otherwise, i.e. if

$$|t| < \left(\frac{K^d}{v} \right)^{1/(d-3)},$$

the fluctuation contribution to the heat capacity becomes dominant. The upper critical dimension for the tricritical point is then $d = 3$.

(g) A generalized multicritical point is described by replacing the term vm^6 with $u_{2n}m^{2n}$. Use simple power counting to find the upper critical dimension of this multicritical point.

- If instead of the term vm^6 we have a general factor of the form $u_{2n}m^{2n}$, we can easily generalize our results to

$$\overline{m} \propto (-t)^{1/(2n-2)}, \quad \Psi(\overline{m}) \propto (-t)^{n/(n-1)}, \quad C_{s.p.} \propto (-t)^{n/(n-1)-2}.$$

Moreover, the fluctuation correction to the heat capacity for any value of n is the same as before

$$C_{fl.} \propto (-t)^{d/2-2}.$$

Hence the upper critical dimension is, in general, determined by the equation

$$\frac{d}{2} - 2 = \frac{n}{n-1} - 2, \quad \text{or} \quad d_u = \frac{2n}{n-1}.$$
