8.334: Statistical Mechanics II   Problem Set # 3

Landau theory, susceptibility & fluctuations

1. Ising ferromagnet.

a) Consider the Landau functional for an Ising ferromagnet near transition. Evaluate the free energy by minimizing the functional and find entropy and specific heat near the transition. Compare with the result of Problem #1, PS2.

Starting from

$$F = -\frac{1}{2}a\tau m^2 + bm^4 \tag{1}$$

and minimizing F, obtain

$$m_* = \begin{cases} \pm\frac{1}{2}\sqrt{a\tau/b} & \tau > 0 \\ 0 & \tau < 0 \end{cases} \qquad F(m_*) = \begin{cases} -\frac{1}{16b}a^2\tau^2 & \tau > 0 \\ 0 & \tau < 0 \end{cases} \tag{2}$$

The thermodynamic quantities are:

$$S(m_*) = -\frac{\partial F}{\partial T} = \begin{cases} -\frac{1}{8bT_c}a^2\tau & \tau > 0 \\ 0 & \tau < 0 \end{cases} \tag{3}$$

$$C(m_*) = T\frac{\partial S}{\partial T} = \begin{cases} \frac{1}{8bT_c}a^2 & \tau > 0 \\ 0 & \tau < 0 \end{cases} \tag{4}$$

where we used $d\tau/dT = -1/T_c$. Note that negative entropy is acceptable, because this is just the singular part near T_c, not the full entropy.

b) Using Landau theory of a ferromagnet in an external field, consider magnetization as a function of temperature. Make a plot showing $M(T)$ for different values of magnetic field, positive and negative.

Minimizing $F(m) = -\frac{1}{2}a\tau m^2 + bm^4 - hm$, obtain

$$m^3 - \frac{a\tau}{4b}m = \frac{h}{4b} \tag{5}$$

A schematic plot of the solutions $m(\tau)$ for different h is presented on Fig. 1.

c) Find magnetic susceptibility $\chi = dM/dH$ in zero field separately above and below the transition. Compare the two results.

$$\chi = \frac{dM}{dh} = \frac{1}{F''(m_*)} = \begin{cases} \frac{1}{2a\tau} & \tau > 0 \\ \frac{1}{a\tau} & \tau < 0 \end{cases} \tag{6}$$

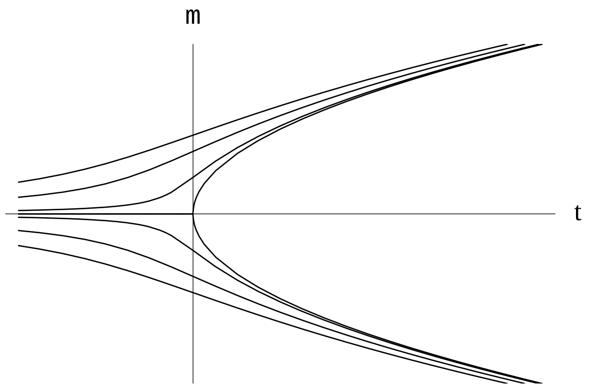

Figure 1: A schematic plot of magnetization of Ising ferromagnet.

2. Ising antiferromagnet, Landau theory.
Antiferromagnet on a cubic lattice is described by spin Hamiltonian with negative exchange interaction between nearest neighbors:

$$\mathcal{H} = \frac{1}{2} J \sum_{|r-r'|=1} \sigma_r \sigma_{r'} \,, \quad J > 0 \tag{7}$$

with $\sigma_r = \pm 1$ *Ising spins. This interaction favors opposite spins on neighboring lattice sites, which results in a ground state with spins opposite on each of the two sublattices. In fact, there are two equivalent ground states related by an overall spin sign change. (Compare with the two ground states in a binary alloy pictured in figure (1), Lecture 2.)*
a) Develop Landau theory for the phase transition in Ising antiferromagnet. Phenomenologically, choose the order parameter to be staggered magnetization, i.e. the difference of magnetization on two sublattices. Derive the form of Landau free energy from a symmetry argument, show that it is the same as for the ferromagnet.
The order parameter for antiferromagnet is $l = m_1 - m_2$, where $m_{1,2}$ are the sublattice magnetizations. The Hamiltonian is invariant under transformation $l \to -l$, hence Landau functional must be a polynomial in l^2, l^4, ...

$$F(l) = -\frac{1}{2} a\tau l^2 + b l^4 \tag{8}$$

that gives a type II phase transition.
b) Now, describe an antiferromagnet near the phase transition in the presence of an external magnetic field. Using symmetry argument, show that there is no coupling of uniform field to the staggered magnetization linear in the order parameter.
The Hamiltonian is invariant under permutation of the sublattices, $m_1 \leftrightarrow m_2$. Under this transformation l changes sign, therefore terms like lh are excluded. The lowest order term in l and h allowed by the symmetry is $l^2 h^2$. Therefore Landau functional is

$$F(l) = -\frac{1}{2} a\tau l^2 + b l^4 + \frac{1}{2} c l^2 h^2 + \frac{1}{2} \chi_0 h^2 \tag{9}$$

where χ_0 is susceptibility of the other degrees of freedom.

The magnetization is $M = dF/dh = (cl^2 + \chi_0)h$ with $l(\tau)$ obtained by minimizing (9):

$$l^2(\tau) = \begin{cases} 0 & \tau < 0 \\ \dfrac{a\tau}{4b} & \tau > 0 \end{cases} \tag{10}$$

The resulting susceptibility $\chi(\tau) = cl^2(\tau) + \chi_0$ has a cusp at the transition — a weak singularity compared to the ferromagnetic case.

c) Generalize this approach by including the average magnetization in the Landau functional. Write the most general free energy form, allowed by symmetry, in the presence of an external field. Find magnetic susceptibility χ above and below the transition. Determine the form of singularity in $\chi(T)$ at $T = T_c$.

If the average magnetization $m = m_1 + m_2$ is included in F, the two symmetries of the microscopic Hamiltonian, the spin reversal and the lattice permutation, allow to change the signs of l and m independently. Thus, all the possible invariant terms of orders up to l^2 and m^2 are

$$F(m,l) = -\frac{1}{2}a\tau l^2 + bl^4 + \frac{1}{2}\left(U_1 + U_2 l^2\right)m^2 + \frac{1}{2}cl^2h^2 + \frac{1}{2}\chi_0 h^2 - mh \tag{11}$$

The coefficients U_1 and U_2 are regular near T_c. Thus one can minimize $F(m,l)$ in m:

$$m_* = \frac{h}{U_1 + U_2 l^2} \tag{12}$$

which gives the free energy

$$F(l) = -\frac{1}{2}a\tau l^2 + bl^4 + \frac{1}{2}\chi(l)h^2 \tag{13}$$

where

$$\chi(l) = \chi_0 + cl^2 - \frac{1}{U_1 + U_2 l^2} \tag{14}$$

For small l, near the transition,

$$\chi(l) = \chi_0 - \frac{1}{U_1} + \left(c + \frac{U_2}{U_1^2}\right)l^2 + O(l^4) \tag{15}$$

The results for susceptibility and all the other thermodynamic quantities are the same as in part b), up to a change of constants: $\chi_0 \to \chi_0 - 1/U_1$, $c \to c + U_2/U_1^2$.

3. Curie and Neel susceptibilities.

Here we consider ferromagnet and antiferromagnet in magnetic field, starting with the microscopic hamiltonian and solving the problem using the mean field approach.

a) From the mean field equation for the Ising and Heisenberg ferromagnet magnetization derived in class (Eqs.(11),(17), Lecture 2), derive susceptibility in zero field at $T > T_c$. Express the resulting $\chi(T)$ in terms of T/T_c (Curie law).

For Ising ferromagnet $M = \tanh(\beta JM + \beta h)$. For small h and M (above $T_c = \beta J$), this yields $M = \beta JM + \beta h$ or $M = \beta h/(1 - \beta J)$. Hence we obtain Curie law

$$\chi = \frac{1}{T - T_c} \tag{16}$$

For Heisenberg ferromagnet above $T_c = \beta J/3$

$$M = \coth(\beta JM + \beta h) - \frac{1}{\beta JM + \beta h} \tag{17}$$

Linearizing, we obtain $M = (\beta JM + \beta h)/3$ and

$$\chi = \frac{\beta/3}{1 - \beta J/3} = \frac{1}{3(T - T_c)} \tag{18}$$

b) From the mean field approach, find the zero field susceptibility of an Ising antiferromagnet at $T > T_c$ (Neel law).

The mean field result for magnetization of Ising antiferromagnet is the same as for ferromagnetic case, but with $J < 0$. For Ising antiferromagnet this leads to Neel law

$$\chi = \frac{1}{T + T_c} \tag{19}$$

with $T_c = |\beta J|$.

c) Using the mean field approach, find the zero field susceptibility χ of an Ising antiferromagnet at $T < T_c$. Does the behavior near T_c agree with the Landau theory result of Problem 2?

To apply the mean field theory to AFM, consider an ordered state with magnetization different on two sublattices. The free energy of the sublattices is

$$F_1 = \frac{1}{2} J m_1 m_2 - T \ln\left[2\cosh\beta(Jm_2 + h)\right] \tag{20}$$

$$F_2 = \frac{1}{2} J m_1 m_2 - T \ln\left[2\cosh\beta(Jm_1 + h)\right] \tag{21}$$

The total free energy per spin is $F = (F_1 + F_2)/2$. Minimizing it with respect to m_1 and m_2, we obtain

$$m_1 = \tanh\beta(Jm_2 + h) \tag{22}$$

$$m_2 = \tanh\beta(Jm_1 + h) \tag{23}$$

Since J is negative, the ground state for $h = 0$ is $m_0 = m_1 = -m_2$. The susceptibility is

$$\chi = \frac{1}{2}\frac{\partial(m_1 + m_2)}{\partial h}\Big|_{h\to 0} = \frac{1}{2}\frac{\beta}{\cosh^2\beta(Jm_0)}\left(2 + J\frac{\partial(m_1 + m_2)}{\partial h}\Big|_{h\to 0}\right) \tag{24}$$

Hence

$$\chi(T < T_c) = \frac{1}{T\cosh^2(\beta Jm) - J} = \frac{1 - m^2(\tau)}{T + T_c(1 - m^2(\tau))} \tag{25}$$

where $m(\tau)$ is the solution to $m = \tanh(\beta|J|m)$. The function $\chi(\tau)$ is continuous at T_c, since $\chi(T_c) = 1/2T_c$ is equal to the value of (19) at T_c. In the ordered state $m^2(\tau) \propto \tau$ near T_c, hence $\chi(\tau)$ has a cusp at T_c (see Fig. 2).

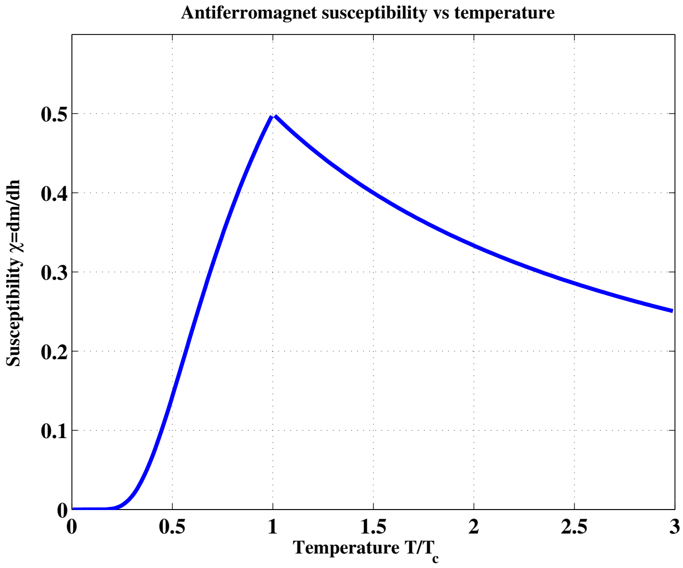

Figure 2: Susceptibility of Ising antiferromagnet

4. Ornstein-Zernicke formula.

a) Use Landau theory to study the correlation function $\langle m(\mathbf{x})m(\mathbf{x}')\rangle$ in an Ising ferromagnet near T_c. For the order parameter Fourier harmonics $m_{\mathbf{k}} = \int e^{-i\mathbf{k}\cdot\mathbf{x}} m(\mathbf{x}) d^3x$, derive the formula

$$\langle m_{\mathbf{k}} m_{-\mathbf{k}}\rangle = \frac{A}{\xi^2\mathbf{k}^2 + 1} \tag{26}$$

Find the correlation length ξ and the constant A at $T > T_c$.

$$F = \int \left(-\frac{1}{2}a\tau m^2 + bm^4 + \frac{1}{2}K(\nabla m)^2\right) d^3x \tag{27}$$

Above T_c F has minimum at $\bar{m} = 0$. Expanding F in fluctuations δm we obtain

$$F(\delta m) = \int \left(\frac{1}{2}a|\tau|(\delta m)^2 + \frac{1}{2}K(\nabla\,\delta m)^2\right) d^3x = \sum_q \frac{a|\tau| + Kq^2}{2}|\delta m_q|^2 \tag{28}$$

Equipartition theorem gives

$$\langle|\delta m_q|^2\rangle = \frac{T}{a|\tau| + Kq^2} = \frac{A}{\xi^2 q^2 + 1} \tag{29}$$

with $A = T/a|\tau|$ and $\xi^2 = K/a|\tau|$

b) What is the relationship of this correlator with the susceptibility χ?

The susceptibility is $\chi = dm/dh = 1/a|\tau|$. Therefore $A = T\chi$. This agrees with the general theorem about fluctuations and linear response.

c) Consider the correlation function $C_2(\mathbf{x} - \mathbf{x}') = \langle\delta m(\mathbf{x})\delta m(\mathbf{x}')\rangle$ in real space. Find its functional form in $D = 3$ using the above formula.

$$C_2(x-x') = \int \frac{e^{iq(x-x')}A}{1+\xi^2q^2}\frac{d^3q}{(2\pi)^3} = \frac{A}{4\pi^2}\int_0^\infty\int_0^\pi \frac{e^{iq(x-x')\cos\theta}}{1+\xi^2q^2}q^2d\,q\,d\cos\theta =$$
$$= \frac{A}{2\pi^2}\frac{1}{x-x'}\int_0^\infty \frac{\sin q(x-x')}{1+\xi^2q^2}q\,dq = -\frac{A}{2\pi^2(x-x')}\frac{\partial}{\partial x}\int_0^\infty \frac{\cos q(x-x')}{1+\xi^2q^2}d\,q =$$
$$= -\frac{A}{2\pi^2(x-x')}\frac{\partial}{\partial x}\left(\frac{\pi}{2\xi}e^{-|x-x'|/\xi}\right) = \frac{A}{4\pi\xi^2}\frac{e^{-|x-x'|/\xi}}{|x-x'|} \quad (30)$$

d) Consider the correlation function $C_2(\mathbf{x}-\mathbf{x}')$ in the ordered state, at $T<T_c$. Use equipartition theorem to show that the structure factor form (26) does not change (up to numerical factors in A and ξ). From that, derive a real space form of C_2.

In the ordered state ($\tau>0$) $\bar{m}=(a\tau/4b)^{1/2}$ and for fluctuations $m=\bar{m}+\delta m$ the free energy is

$$F(\delta m) = \int\left(\left(6b\bar{m}^2-\frac{1}{2}a\tau\right)\delta m^2+\frac{1}{2}K(\nabla\,\delta m)^2\right)d^3x = \int\left(\frac{1}{2}2a\tau\delta m^2+\frac{1}{2}K(\nabla\,\delta m)^2\right)d^3x \quad (31)$$

Therefore C_2 has the same form as in part c) with $a\to 2a$, $\xi\to\xi/\sqrt{2}$, $A\to A/2$.

5. Goldstone mode fluctuation suppressed by an external field.

a) Scattering of light in a dielectric medium takes place due to spatial fluctuations of refraction index, i.e. the dielectric permeability $\delta\epsilon_{ij}$. The angular distribution of scattered light is determined by the correlator $\langle\delta\epsilon_{ij}\delta\epsilon_{i'j'}\rangle$ of the fluctuating part of permeability. This quantity is called the scattering tensor[1]. Show that when an electromagnetic plane wave with wavevector $\mathbf{q}$ and polarization $\mathbf{E}$ is scattered on the fluctuations in the medium, the scattered field $\mathbf{E}'$ is determined by the correlator of permeability $\delta\epsilon$ Fourier harmonics

$$\langle E_i'(E_j')^*\rangle \propto V\langle\delta\epsilon_{im}(\mathbf{k})\delta\epsilon^*_{jn}(-\mathbf{k})\rangle E_mE_n^*,\quad \mathbf{k}=\mathbf{q}'-\mathbf{q} \quad (32)$$

where V is the system volume, $\delta\epsilon_{ij}(\mathbf{k})=\int\delta\epsilon_{ij}(\mathbf{x})e^{-i\mathbf{k}\cdot\mathbf{x}}d^3x$ and $\mathbf{q}'$ is the wavevector of a scattered wave.

In the scattering medium $D_i=(\epsilon_{ij}+\delta\epsilon_{ij})E_j$. Starting with the wave equation $\nabla\times\nabla\times\mathbf{E}=\omega^2/c^2\mathbf{D}$, obtain

$$\nabla\times\nabla\times E_i-\frac{\omega^2}{c^2}\epsilon_{ij}E_j=\frac{\omega^2}{c^2}\delta\epsilon_{ij}E_j \quad (33)$$

The radiation field with wave vector k' at a point far away from the scattering region is

$$E'=\frac{\omega^2}{4\pi c^2}\frac{e^{ik'R}}{R}\int_{x\in V}(\delta\epsilon_{ij}E_j(x))d^3x \quad (34)$$

For plane wave $\mathbf{E}(x)=\mathbf{E}\exp(ikx)$, the radiation field

$$E'\propto\frac{e^{ik'R}}{R}\int_{x\in V}\delta\epsilon_{ij}e^{-iqx}d^3x \quad (35)$$

[1] Definition and discussion of the scattering tensor can be found in: Landau & Lifshits, Electrodynamics of Continuous Media, §117

where $q = k' - k$. The integral over scattering region of size much larger than EM wavelength is the Fourier harmonic of ϵ_{ij}. The field intensity is

$$\langle E_i'(E_j')^*\rangle \propto \sum_{k'k_1'} \int\int \langle \delta\epsilon_{in}(x)\delta\epsilon_{jm}(x')\rangle e^{-iqx+iq_1x_1} d^3x d^3x_1 \tag{36}$$

where $q = k' - k$, $q_1 = k_1' - k_1$. Change the variables to $X = (x + x_1)/2$, $y = x - x_1$. Then

$$\sum_{k'k_1'} \int\int \langle \delta\epsilon_{in}(x)\delta\epsilon_{jm}(x')\rangle e^{-iqx+iq_1x_1} d^3x d^3x_1 = \sum_{k'k_1'} \int\int \langle \ldots\rangle e^{i(q_1-q)X+iy(q_1+q)/2} d^3X d^3y =$$

$$= \sum_{k'k_1'} (2\pi)^3 \int \langle \ldots\rangle e^{iy(q_1+q)/2} \delta(q_1 - q) d^3y = \int \sum_k e^{iqy} \langle \ldots\rangle d^3y \tag{37}$$

Therefore

$$\langle E_i'(E_j')^*\rangle \propto \int \sum_k e^{iqy} \langle \delta\epsilon_{ii'}(y)\delta\epsilon_{jj'}(0)\rangle E_{i'}E_{j'} d^3y = V\langle \delta\epsilon_{ii'}(q)\delta\epsilon_{jj'}(-q)\rangle E_{i'}E_{j'} \tag{38}$$

b) It is interesting to apply this result to scattering in a nematic liquid crystal[2] *caused by fluctuations of the nematic order parameter* $\mathbf{n}$*. In this case, the fluctuating part of dielectric permeability* $\delta\epsilon_{ij}$ *is proportional to the traceless tensor* $n_i(\mathbf{x})n_j(\mathbf{x}) - \frac{1}{3}\delta_{ij}$*.*
Consider a liquid crystal in the presence of a uniform static electric field. The polarizability of anisotropic rod-like molecules is much higher along the molecule axis than in the transverse direction, $\alpha_\parallel \gg \alpha_\perp$*. Hence the field is trying to align the molecules, which is described by adding a term* $-\frac{\alpha}{2}(\mathbf{E}\cdot\mathbf{n})^2$ *to the liquid crystal free energy (Eq.(13), lecture 1). (Here* $\alpha = \alpha_\parallel - \alpha_\perp$ *is a positive constant.) Show that with the field applied, the lowest energy state is indeed* $\mathbf{n} \parallel \mathbf{E}$*.*
c) Consider the fluctuations $\mathbf{n} = \mathbf{n}^{(0)} + \delta\mathbf{n}$*, with* $\delta\mathbf{n} \perp \mathbf{n}^{(0)}$*, by expanding the free energy to the lowest nonvanishing order in* $\delta\mathbf{n}$*. Find the correlator* $\langle \delta\mathbf{n_k}\delta\mathbf{n_{-k}}\rangle$ *and show that applied electric field suppresses scattering. The possibility to change the medium from opaque to transparent by an external field has various practical applications (such as the liquid crystal displays).*
Expand $\mathbf{n} = \mathbf{n}_0(1 - \delta n^2)^{1/2} + \delta\mathbf{n}$, $\delta\mathbf{n}\cdot\mathbf{n} = 0$. To order $O(\delta n^2)$, obtain

$$H(\delta n) = \frac{1}{2}\int \left(K_1(\mathrm{div}\,\delta\mathbf{n})^2 + K_2(\mathbf{n}_0\cdot\mathrm{curl}\,\delta\mathbf{n})^2 + K_3(\mathbf{n}_0\times\mathrm{curl}\,\delta\mathbf{n})^2 + \frac{1}{2}\alpha E^2\delta n^2 \right) d^3x =$$

$$= \frac{1}{2}\sum_q \left(K_1|\mathbf{q}\cdot\delta\mathbf{n}_q|^2 + K_2|\mathbf{n}_0\cdot(\mathbf{q}\times\delta\mathbf{n}_q)|^2 + K_3|\mathbf{n}_0\times(\mathbf{q}\times\delta\mathbf{n}_q)|^2 + \frac{1}{2}\alpha E^2|\delta n_q|^2 \right) \tag{39}$$

since $\mathbf{n}_0\times(\mathbf{q}\times\delta\mathbf{n}) = \mathbf{q}(\mathbf{n}_0\cdot\delta\mathbf{n}) - \delta\mathbf{n}(\mathbf{q}\cdot\mathbf{n}_0) = -\delta\mathbf{n}(\mathbf{q}\cdot\mathbf{n}_0)$, H can be simplified as

$$H(\delta n) = \frac{1}{2}\sum_q K_{ij}(q)\delta n_{q,i}\delta n_{-q,j} + \frac{1}{2}\alpha E^2 \delta\mathbf{n}_q\cdot\delta\mathbf{n}_{-q} \tag{40}$$

[2] Scattering in nematic liquid crystals is discussed in: Landau & Lifshits, Electrodynamics of Continuous Media, §122

where

$$K_{ij}(q) = K_1 q_i q_j + K_2 (\mathbf{n}_0 \times \mathbf{q})_i (\mathbf{n}_0 \times \mathbf{q})_j + K_3 (\mathbf{n}_0 \cdot \mathbf{q})^2 \delta_{ij} \tag{41}$$

It follows from the equipartition theorem that

$$\langle \delta n_{q,i} \delta n_{-q,j} \rangle = \left(K_{ij}(q) + \frac{1}{2} \alpha E^2 \delta_{ij} \right)^{-1} \tag{42}$$

At zero field, $E = 0$, the fluctuations $\langle |\delta n_q|^2 \rangle \propto 1/q^2$ diverge at $q \to 0$. Finite field suppresses $\langle |\delta n_q|^2 \rangle$ at $q = 0$ to $2/\alpha E^2$