8.334: Statistical Mechanics II   Problem Set # 5

Fluctuations. Scaling. Gaussian statistics.

1. The fluctuation region width.

Thermodynamic fluctuations control the behavior near the critical point. However, the size of the temperature interval, in which fluctuations are large, depends on microscopic details, and in some cases can be quite narrow. In Lecture 5 we discussed the mean field theory validity criterion, and used it to estimate the critical region. It is interesting to look a bit closer at several examples.

a) For the Ising ferromagnet in space dimension $d = 3$, described by the mean field theory developed in Problem 1, PS#2 (see also Lecture 2), estimate the width of the temperature interval near critical point, $\tau = (T_c - T)/T_c$, where the contribution of fluctuations to the thermodynamic quantities is dominant.

Fluctuations in $F = \int(-a\tau m^2/2 + bm^4 + K(\nabla m)^2/2)d^3x$ are strong when

$$T_c b(a\tau)^{3/2-2} \gg K^{3/2} \tag{1}$$

for $d = 3$ (see Lecture 5). Therefore the critical region is $\tau \ll \tau_* = abT_c/K^3$. In a ferromagnet (see Problem 1, PS2) $a, b \approx T_c$, $K = 1/6\sum_r J(r)r^2$

(i) For nearest neighbor interaction, $K \approx T_c$. In this case $\tau_* = 1$, i.e. the fluctuation region width is of the order of T_c

(ii) For interaction of large radius, $K \approx T_c N^2$ where N is the number of spins within the interaction radius. Then $\tau_* = 1/N^6$, i.e. the fluctuation region is narrow.

b) Consider a weakly interacting Bose gas (space dimension $d = 3$) with density n, particle mass m, and a short-range interparticle interaction

$$U(\mathbf{r} - \mathbf{r}') = g\delta(\mathbf{r} - \mathbf{r}'), \quad g = 4\pi\hbar^2 a/m \tag{2}$$

The interaction is called weak, when atom scattering length a, related to the interaction constant by[1] *Eq.(2, is much less then the interparticle distance, $a \ll n^{-1/3}$.*

In this weakly nonideal gas, the Bose-Einstein condensation transition temperature T_c is accurately described by the ideal Bose gas theory. The mean field energy for the condensate amplitude ψ can be written in the form of Eq.(1), PS#1, with n being the temperature-dependent condensate density of an ideal gas. Estimate the fluctuation region τ_* for this system, using the parameters for magnetically trapped Rubidium from the experiment in JILA: $n \approx 10^{14}\,\mathrm{cm}^{-3}$, $a \approx 100\,a_B$, where $a_B = 0.5\times10^{-8}\,\mathrm{cm}$ is Bohr's radius.

In a superfluid above T_{BEC}, $a\tau = \mu$, the chemical potential, and $b = g$, the interaction. The constant K is $\hbar^2/2m$ and $a \approx T_{BEC}$ since at $\tau = 1$ $\mu \approx T_{BEC}$. Using $\tau_* = abT_c/K^3$ obtain $\tau_* = T_{BEC}^2 g/(\hbar^2/2m)^3$. Replacing T_{BEC} by $\hbar^2 n^{2/3}/(2m)$ and g by $4\pi\hbar^2 a/m$. obtain

$$\tau_* = an^{1/3} = 0.5 \cdot 10^{-6}\ \mathrm{cm}\ 10^{14/3}\ \mathrm{cm}^{-1} \approx 2 \cdot 10^{-2} \tag{3}$$

[1] This corresponds to the low energy limit of particle scattering. Although the real interaction between atoms is certainly not short-ranged, at low energy it can be effectively replaced by a δ–function *pseudopotential* expressed in terms of the scattering length by Eq.(2 — this is discussed in more detail, e.g., in "Statistical Mechanics," by Parthia.

2. A relation between scaling dimensions of a field and an operator.
Consider an RG transformation of a hamiltonian near critical point, $\mathcal{H} = \mathcal{H}_0 + \delta\mathcal{H}$, where the hamiltonian $\mathcal{H}_0$ is invariant under renormalization, $\mathcal{R}(\mathcal{H}_0) = \mathcal{H}_0$, and $\delta\mathcal{H}$ is a perturbation. Suppose that $\delta\mathcal{H}$ is of the form

$$\delta\mathcal{H} = \int h(\mathbf{x})\phi(\mathbf{x})d^3x \tag{4}$$

where $\phi(\mathbf{x})$ is some density-type variable associated with the system (e.g. spin density, energy, charge or current density, etc.) and h is a field conjugate to ϕ. Suppose also that ϕ is a scaling variable. This means that the RG transforms the ϕ into itself,

$$\phi'(\mathbf{x}') = b^{y_\phi}\phi(\mathbf{x})\,, \quad \mathbf{x}' = \mathbf{x}/b, \tag{5}$$

i.e. the perturbation $\delta\mathcal{H} \propto \int \phi(\mathbf{x})d^dx$ is an eigenvector of the RG transformation linearized at the fixed point $\mathcal{H}_0$.
a) Show that the scaling dimensions of ϕ and h are related as

$$y_h + y_\phi = d \tag{6}$$

For partition function to be invariant under the transformations $h \to h' = b^{y_h}h$, $\phi \to \phi' = b^{y_\phi}\phi$ and $x \to x' = x/b$, the term

$$\int h(x)\phi(x)\,d^dx = b^{-y_h-y_\phi+d}\int h'(x')\phi'(x')\,d^dx' \tag{7}$$

must be invariant. Hence $y_h + y_\phi = d$.
b) For the Ising model, by choosing ϕ and h to be spin density and magnetic field, and using Eq.(6), derive the RG equation for the pair spin correlation function (Eq.(17), Lecture 7) and the scaling form (Eq.(21), Lecture 7).

$$C_2(r,\tau) = \langle\phi(0)\phi(r)\rangle_\tau = b^{-2y_\phi}\langle\phi(0)\phi(r/b)\rangle = b^{-2y_\phi}C_2(r/b,\tau') \tag{8}$$

with $y_\phi = d - y_h$ and $\tau' = b^{y_t}\tau$ — renormalized temperature perturbation. This agrees with Eq. (18), Lecture 7. At $\tau = 0$ (exactly at the transition) for any n

$$C_2(r) = b^{-2y_\phi}C_2(r/b) = b^{-2ny_\phi}C_2(r/b^n) \tag{9}$$

Therefore $C_2(r) \propto r^{-2y_\phi} = r^{-2(d-y_h)}$
c) How can one use the result (6), with properly chosen ϕ and h, to obtain the scaling equation for the free energy (Eqs.(5,6), Lecture 7)?

The singular part of the free energy contributes[2] $\delta H = \int f_s(\tau,h)d^dx$ to the hamiltonian. Hence the scaling dimension of f_s is d. This gives the following RG scaling relations

$$f_s(h,\tau) = b^{-d}f_s(h/b^{y_h},\tau/b^{y_t}) = b^{-nd}f_s(h/b^{ny_h},\tau/b^{ny_t}) \tag{10}$$

[2]Formally, the field conjugated to f is unity.

valid for any n. This means that

$$f_s(h,\tau) = \tau^{d/y_t}\Phi(h/\tau^{y_h/y_t}). \tag{11}$$

3. Gaussian statistics.

Prove the basic facts about gaussian statistics of one variable, many variables, and fields (Eqs.(5,6,7,8), Lecture 8).

(i) One variable

$$\int_{-\infty}^{\infty} e^{iJx-ax^2/2}d\,x = e^{-\frac{J^2}{2a}}\int_{-\infty}^{\infty} e^{-a(x')^2/2}d\,x' \tag{12}$$

Therefore the average is

$$\langle e^{iJx}\rangle = \frac{\int_{-\infty}^{\infty} e^{iJx-ax^2/2}d\,x}{\int_{-\infty}^{\infty} e^{-ax^2/2}d\,x} = \exp\left(-\frac{J^2}{2a}\right) \tag{13}$$

The gaussian integral in eq. 12 can be evaluated as follows:

$$\int_{-\infty}^{\infty} e^{-ax^2/2}d\,x = \left(\iint \exp\left[-\frac{1}{2}a(x^2+y^2)\right]d\,x\,d\,y\right)^{1/2} = \left(2\pi\int_0^{\infty} e^{-r^2/2a}r\,d\,r\right)^{1/2} = (2\pi a)^{1/2} \tag{14}$$

(ii) in case of many variables, one needs to evaluate

$$\int\ldots\int e^{iJ_nx_n - x_ix_jA_{ij}/2}\prod d\,x_n. \tag{15}$$

where the summation over repeated indices is assumed. To integrate (15), diagonalize A_{nm} using rotation $x_n = U_{nm}x'_m$. Then the integral becomes

$$\int\ldots\int e^{iJ_nx_n - x_ix_jA_{ij}/2}\prod d\,x_n = \int\ldots\int e^{iJ'_nx'_n - x'_nx'_na_n/2}\det U\prod d\,x'_n =$$
$$= \prod_n\left(\int e^{iJ'_nx' - x'x'a_n/2}d\,x'\right) = \prod_n (2\pi a_n)^{1/2}\exp\left(-\frac{(J'_n)^2}{2a_n}\right) \tag{16}$$

where $J'_n = J_mU_{mn}$. Using $U^{-1} = U^T$ and

$$\sum_n \frac{(J'_n)^2}{a_n} = \sum_{i,j,n} J_iU_{in}\frac{1}{a_n}U^T_{nj}J_j = J_i(A^{-1})_{ij}J_j, \tag{17}$$

find the average

$$\langle e^{iJ_nx_n}\rangle = \frac{\exp\left(-\frac{1}{2}J^TA^{-1}J\right)\prod_n(2\pi a_n)^{1/2}}{\prod_n(2\pi a_n)^{1/2}} = \exp\left(-\frac{1}{2}J^TA^{-1}J\right) \tag{18}$$

(iii) Field average can be performed by discreetizing the space, replacing integrals by sums and using the above results

$$\langle e^{i\int J(x)\phi(x)d\,x}\rangle = \langle e^{i\sum_{x_i}J(x_i)\phi(x_i)}\rangle = \exp\left(-\frac{1}{2}\sum_{x,x'}J(x)\tilde{A}(x,x')J(x')\right) \tag{19}$$

Taking the limit of zero grid spacing gives

$$\langle e^{i\int J(x)\phi(x)dx}\rangle = \exp\left(-\frac{1}{2}\iint J(x)\tilde{A}(x,x')J(x')\,dx\,dx'\right) \tag{20}$$

4. RG for quadratic hamiltonians.
a) Apply the field-theoretic RG transformation described in Lecture 8 (coarse grain + rescale + renormalize hamiltonian) to a gaussian field problem with a quadratic hamiltonian

$$\mathcal{H} = \int \frac{1}{2}K\left(\partial_\mu\phi\right)^2 d^dx \tag{21}$$

Show that, depending on the dimensionality d, the rigidity constant K grows or decreases upon RG transformation, with the critical dimension $d = 2$.

Starting with

$$H = \frac{1}{2}\int K(\partial_\mu\phi)^2\,d^dx = \frac{1}{2}\sum_q Kq^2\phi_q\phi_{-q} \tag{22}$$

divide ϕ into fast and slow harmonics, $\phi = \phi_{smooth} + \delta\phi$,

$$H = \frac{1}{2}\left(\sum_{q<\Lambda'} + \sum_{\Lambda'<q<\Lambda}\right)Kq^2\phi_q\phi_{-q}. \tag{23}$$

Then integrating out $\Lambda' < q < \Lambda$ and rescaling $x \to x(\Lambda/\Lambda')$, obtain

$$H'(\phi') = \frac{1}{2}(\Lambda/\Lambda')^{d-2}\int K(\partial_\mu\phi)^2\,d^dx \tag{24}$$

or $K' = (\Lambda/\Lambda')^{d-2}K$. K grows for $d > 2$ and decreases for $d < 2$.

b) Consider thermal fluctuations of the variable $\delta\phi_{12} = \phi(\mathbf{x}_1) - \phi(\mathbf{x}_2)$. Show that the distribution is gaussian and relate its variance to the correlator

$$\langle\delta\phi_{12}^2\rangle = \langle(\phi(\mathbf{x}_1) - \phi(\mathbf{x}_2))^2\rangle \tag{25}$$

To show that $\Phi_{xy} = \phi(x) - \phi(y)$ has a gaussian distribution, note that the distribution of $\phi(x)$ and $\phi(y)$ are gaussian and that the sum of two gaussian variables is also a gaussian varibale.
Consider $\langle\exp(iJ\Phi_{xy})\rangle$. Using results of Problem 3, obtain

$$\langle\exp(iJ\Phi_{xy})\rangle = \exp\left(-\frac{1}{2}J^2\int\left(\delta(x-x') - \delta(y-x')\right)G(x',x'')\left(\delta(x-x'') - \delta(y-x'')\right)\,d^2x\,d^2y\right) \tag{26}$$

where

$$G(x',x'') = (K\nabla^2)^{-1}_{x',x''} = \sum_q \frac{e^{iq(x'-x'')}}{Kq^2}. \tag{27}$$

Therefore the average becomes

$$\langle \exp(iJ\Phi_{xy})\rangle = \exp\left(-\frac{1}{2}J^2\sum_q \frac{2-e^{iq(x-y)}-e^{-iq(x-y)}}{Kq^2}\right) \tag{28}$$

Comparing this to the gaussian average, conclude that

$$\langle \Phi_{xy}^2\rangle = \sum_q \frac{2-e^{iq(x-y)}-e^{-iq(x-y)}}{Kq^2} \tag{29}$$

c) How does the quantity (25) depend on the points 1 and 2 separation at $|\mathbf{x}_1-\mathbf{x}_2|\to\infty$*?*
In $d=1$,

$$\frac{1}{2\pi K}\int \frac{2-e^{iq(x-y)}-e^{-iq(x-y)}}{q^2}\,dq = \frac{1}{K}|x-y| \tag{30}$$

In $d=2$,

$$\sum_q \frac{2-e^{iq(x-y)}-e^{-iq(x-y)}}{Kq^2} = \sum_{|x-y|^{-1}\le|q|\le a^{-1}} \frac{1}{Kq^2}+C = \frac{1}{2\pi K}\ln\frac{|x-y|}{a'}+C, \tag{31}$$

where a is the lattice spacing. Here $C\approx 1$ is the constant obtained by summing over $0\le q\le 1/|x-y|$, and $a'=ae^{-C}$.
In $d=3$,

$$\sum_q \frac{1}{Kq^2}\approx\frac{1}{Ka} \tag{32}$$

and

$$\sum_q \frac{e^{iq(x-y)}}{Kq^2}\approx\frac{1}{K|x-y|.}\to 0 \text{ at large } |x-y| \tag{33}$$

Hence

$$\langle \Phi_{xy}^2\rangle\Big|_{|x-y|\to\infty} = \sum_q \frac{1}{Kq^2} = Const \tag{34}$$

Note the difference between $d=1,2$ and $d=3$. In $d=1,2$ fluctuations grow at increasing $|x-y|$, while in $d=3$ they are bounded.