1 Lecture 5. Fluctuations near phase transition. Renormalization group.

1.1 Critical exponents

There are several quantities that have singular behavior, typically of a power law divergence form, near a type II phase transition. For reference we list the most often used scaling relations with a standard notation for the critical indices:

- Specific heat $C_V \propto |\tau|^{-\alpha}$;
- Susceptibility $\chi \propto |\tau|^{-\gamma}$;
- Order parameter $\langle m\rangle_{\tau>0} \propto |\tau|^{\beta}$ $(\langle m\rangle_{\tau>0} = 0)$;
- Correlation radius $\xi \propto |\tau|^{-\nu}$;
- Correlation function $G(\mathbf{x}) \propto |\mathbf{x}|^{-d+2-\eta}$ for $|\mathbf{x}| \ll \xi$.

$(\tau = (T_c - T)/T_c)$. Several other scaling relations arise for thermodynamic quantities vs. ordering field h at the transition, $\tau = 0$:

- Specific heat $C_V \propto |h|^{-\epsilon}$;
- Susceptibility $\chi \propto |h|^{-1/\delta-1}$;
- Order parameter $\langle m\rangle \propto |h|^{-1/\delta}$;
- Correlation radius $\xi \propto |h|^{-\mu}$.

The experimentally measured values of critical indices are typically different from the mean field values. They depend on system universality class (space dimension, the number of order parameter components, and the symmetry class). The same is true for the indices found numerically. For reference, we list the results found from simulation of the 3D Ising model on a computer[1]:

$$\alpha = 0.104 \pm 0.003,\ \beta = 0.325,\ \gamma = 1.2385 \pm 0.0015,\ \nu = 0.632 \pm 0.025,\ \eta = 0.039 \pm 0.004. \tag{1}$$

[1] L. P. Kadanoff, Chap. 11, §8, p.244, Statistical Physics. Statics, Dynamics, and Renormalization. (World Scientific, 1999)

and the exponents obtained from Onsager's exact solution of the 2D Ising model

$$\alpha = +0,\ \beta = 1/8,\ \gamma = 7/4,\ \nu = 1,\ \eta = 1/4. \tag{2}$$

are also totally different from the mean field theory prediction. (We write $\alpha = +0$ to indicate the logarithmic singularity of the specific heat, $C \propto \ln(1/|\tau|)$.)

However, in some experimental situations, such as ferroelectrics and superconductors, the agreement with the mean field theory is nearly perfect. To understand this, we need to analyze the role of fluctuations.

1.2 When mean field theory fails. Upper critical dimension

Whether the mean field theory[2] is consistent can be verified by estimating the magnitude of fluctuations. There are many ways of doing this. We first present a simple argument due to Ginzburg.

The correlation function or order parameter fluctuations is

$$C_2(\mathbf{r}-\mathbf{r}') = \langle(\sigma_r - m)(\sigma_{r'} - m)\rangle = \int e^{\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} C_2(\mathbf{q}) \frac{d^d q}{(2\pi)^d}\,, \quad C_2(\mathbf{q}) = \frac{T}{K(\mathbf{q}^2 + \xi^{-2})} \tag{3}$$

with the correlation length $\xi \propto |\tau|^{-1/2}$. For the sake of generality we consider a system of arbitrary dimension d. The dependence of the results on d will be quite interesting.

The Fourier transform $C_2(q)$ was obtained in Lecture 4 from equipartition theorem applied to fluctuations at $T > T_c$. One can derive a very similar expression at $T < T_c$ (see homework problem 4, PS#3). The integral in (3) can be estimated from a dimensional argument by setting $|\mathbf{q}| \simeq |\mathbf{r}-\mathbf{r}'|^{-1}$:

$$C_2(\mathbf{r}-\mathbf{r}') \simeq \exp\left(-\frac{|\mathbf{r}-\mathbf{r}'|}{\xi}\right) \frac{a^{d-2}}{|\mathbf{r}-\mathbf{r}'|^{d-2}} \tag{4}$$

with $a = T/K$. This expression, correct up to a numerical factor, is all we need now. (In fact, one can evaluate the integral exactly — see problem 4, PS#3.)

Let us suppose that the crucial fluctuations occur at the characteristic length scale ξ. According to the above, the characteristic size of the fluctuation is

$$\langle \delta\sigma_r \delta\sigma_{r'} \rangle \sim |\tau|^{d/2-1} \tag{5}$$

This fluctuation should be compared with the average value

$$\langle \sigma_r \rangle \sim |\tau|^{1/2} \tag{6}$$

[2] All the same is true for Landau theory. In fact, in the discussion of the effects of fluctuations, the distinction between these two theories – one being microscopic, the other purely phenomenological, based on symmetry, – is totally unimportant. You can often see in the texts on critical phenomena both of these theories discussed under the same name.

To see which is bigger, we divide fluctuations by the mean magnetization:

$$\frac{\langle \delta\sigma_r \delta\sigma_{r'} \rangle}{\langle \sigma_r \rangle \langle \sigma_{r'} \rangle} \sim |\tau|^{d/2-2} \tag{7}$$

Near the transition, at small τ, the relative size of the two terms will depend on whether the exponent $d/2-2$ is positive or negative. If it is negative, the fluctuations diverge and make the mean field picture invalid near the transition. This is the case in the space dimension d is less than 4. The space dimension above which the fluctuations can be ignored is called *the upper critical dimension.*

A more explicit relation between the effects of fluctuations and thermodynamic quantities can be obtained. Let us revisit the mean field estimate of the free energy near the transition (Lecture 2) and study fluctuation corrections. For that, we estimate the contribution to the free energy of the term

$$\delta\mathcal{H} = -\sum_{r\neq r'} J(r-r')\delta\sigma_r \delta\sigma_{r'}\,, \quad \delta\sigma_r = \sigma_r - \langle \sigma_r \rangle, \tag{8}$$

which was neglected in the mean field calculation.

Taking the average of $\delta\mathcal{H}$, express the result through spin correlation function defined

$$\langle \delta\mathcal{H} \rangle = -\sum_{r\neq r'} J(r-r')\langle \delta\sigma_r \delta\sigma_{r'} \rangle = -\sum_{r\neq r'} J(r-r') C_2(r-r') \tag{9}$$

The correlation function $C_2(r-r')$ was defined in Lecture 4. Using its Fourier transform $G(\mathbf{q}) = a/(\mathbf{q}^2 + \xi^{-2})$ and the correlation length $\xi \propto |\tau|^{-1/2}$, we obtain

$$\langle \delta\mathcal{H} \rangle = -\int_{\mathrm{BZ}} J(\mathbf{q}) \frac{a}{\mathbf{q}^2 + \xi^{-2}} \frac{d^d q}{(2\pi)^d} \tag{10}$$

where the integral is taken over the Brillouin zone of the lattice, i.e. over the period of the reciprocal lattice. Here again we consider a lattice of arbitrary dimension d.

We have to extract the contribution of the long wavelength modes with $q \simeq \xi^{-1}$. A convenient way to do this is to subtract and add an expression for $\langle \delta\mathcal{H} \rangle$ with $\xi^{-1} = 0$, which gives

$$\langle \delta\mathcal{H} \rangle = \mathrm{const} + \frac{Ja}{(2\pi)^d \xi^2} \int \frac{d^d q}{\mathbf{q}^2(\mathbf{q}^2 + \xi^{-2})} \tag{11}$$

Here we note that the integral is determined by small $q \simeq \xi^{-1}$, much smaller than lattice spacing, allows to replace $J(q)$ by a constant $J = J(0)$ and to extend integration limits to infinity. For $d < 4$ the integral can be estimated by setting $q \sim \xi^{-1}$, which gives $a\xi^{2-d} \approx (\tau/K)^{d/2-1}/K$. Using this result, let us find the correction to the specific heat:

$$\delta C = d\langle \delta\mathcal{H} \rangle / dT \approx a\tau^{d/2-2}/K^{d/2} \tag{12}$$

This expression should be compared with the mean field specific heat, which has a finite jump at the transition (Lecture 3). The fluctuation correction is significant when

$$a\tau^{d/2-2}/K^{d/2} \gg 1 \quad \text{or} \quad a\xi^{4-d} > K^2 \tag{13}$$

(we recall that $\xi \propto (K/\tau)^{1/2}$). We conclude that at $d < 4$ the effect of fluctuations dominates near the critical point, while at $d > 4$ the role of fluctuations at the transition is small. Thus in $d = 3, 2, 1$ the mean field treatment is inadequate near T_c.

However, even for $d < 4$, the region where fluctuations dominate can be small when the rigidity K is large. This is the case for superconductors and ferroelectrics, where the discrepancy with the mean field theory can be detected only extremely close to the transition, at $\tau = (T_c - T)/T_c \sim 10^{-4} - 10^{-8}$.

1.3 The renormalization group idea.

The renormalization group is a framework for analyzing problems where strong interactions happen on a range of length scales. Although the RG will be discussed here mainly in the framework of the theory of phase transitions, we point out that nowdays these ideas are being applied much more broadly.

Comment on history and (unfortunate) terminology. The word 'group' is misleading, the underlying mathematical structure is certainly not a group, rather a nonlinear dynamical flow in a parameter space. The word 'renormalization' indicates that in the high energy physics, where prehistoric forms of renormalization group ideas were developed, it was believed that numerical values of physical constants are determined by fundamental symmetries, rather than by dynamical effects. Thus, when dynamical effects change a value of a physical constant (e.g. corrections to electron mass in QED vacuum fluctuations), it should be rescaled back to the physical value, i.e. the value observed in a low energy experiment. The renormalization group ideas were initially brought in statistical mechanics by K. Wilson, L. Kadanoff and M. Fisher in early 70's, and then rapidly evolved and transformed.

Even the article 'the' is misleading, because the renormalization group is not a rigid framework or definite prescription, but rather a loose system of concepts, a flexible framework (a philosophy, in contrast with ideology). Whether or not a RG approach is quantitatively successful depends on the nature of the problem. However, even when the RG approach is not too accurate quantitatively, it can provide a useful qualitative picture.

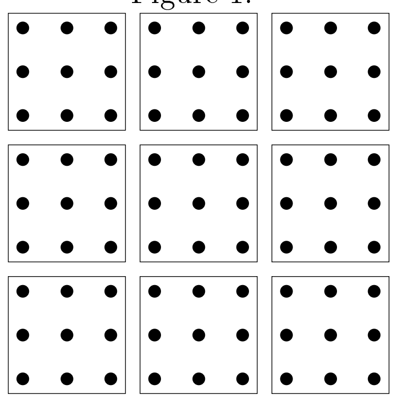
All RG studies have in common the idea of re-expressing the parameters which define the problem in terms of some other, perhaps simpler, set, while keeping unchanged those physical aspects of the problem which are of interest. In the theory of critical phenomena this is accomplished by coarse-graining of the short-distance degrees of freedom. [comment on other situations: many-body quantum problems, turbulence in fluid dynamics, multiscale dynamics, etc.]

We shall start with the example of *real space renormalization* for spin systems on a lattice. This situation is particularly illuminating conceptually, although not always the best from a quantitative point of view. The approximations made in a real space RG sometimes are difficult to control. Later we shall discuss other varieties of RG, more field theory-based, where renormalization is carried out in *momentum space*. In such approaches, one can develop methods, such as the $4 - \epsilon$, $2 + \epsilon$ and $1/n$ expansion, using small parameters to yield systematically improvable quantitative results.

1.4 Block spin transformation

Consider coarse-graining in the Ising model on a 2D square lattice. Divide lattice in blocks, say 3×3, each containing 9 spins (Fig. 1). To each block assign a new variable $\sigma' = \pm 1$, depending on whether the spins in the block are predominantly up or down. The simplest way to do it is by the 'majority rule': $\sigma' = \pm 1$ if there are more spins down than up, and vice versa.

Figure 1:



After defining block variables, we rescale the whole picture by a factor of 3 so that one block is of the same size as original squares. If we start from a spin configuration at the Ising model critical point $T = T_c$, we observe that the new picture is statistically equivalent to the old one, as long as the behavior at large distances (in this case, larger than 3 lattice periods) is concerned. We can continue this blocking procedure, and at all pictures will look pretty much the same. This observation illustrates the *scale invariance* at the critical point.

On the other hand, let us start from the spin configuration with temperature a little bit above or below T_c. In this case, even though the initial configuration is very similar to the first one, the result of the blocking repeated several times, looks very different. At $T \neq T_c$ the system is not scale invariant.

These qualitative observations are the essential basis of the renormalization group approach. More quantitatively, the renormalization procedure is built by introducing a block Hamiltonian. The initial configurations are drawn prom the probability distribution $p \propto e^{-\beta\mathcal{H}}$ defined by the Ising model Hamiltonian $\mathcal{H}(\sigma)$. We can try to interpret the statistics of the block spin configurations in terms of some new Hamiltonian $\mathcal{H}'(\sigma')$. Of course, this can always be achieved by choosing a sufficiently complicated form of $\mathcal{H}'(\sigma')$, perhaps including not only nearest neighbor, but also long-range interactions, as well as various 3-spin, 4-spin, and higher order interactions, characterized by a set of couplings K_i.

Except some special cases, the block Hamiltonian looks very different from the initial Hamiltonian. The underlying idea, however, will be to focus on dominant interactions and replace the exact Hamiltonian by an approximate form, perhaps close algebraically to the initial Hamiltonian, and leave out all unimportant interactions. This is the scheme we will use in practice.

However, before considering examples, it is worthwhile to discuss the renormalization method in a general form, without making any approximations. Let us consider the initial partition function

$$Z = \mathrm{tr}_{\,\sigma} e^{-\mathcal{H}(\sigma)} \tag{14}$$

where the factor β is absorbed in $\mathcal{H}$. (Redefining $\mathcal{H}$ in this way is convenient, because it allows to deal with dimensionless coupling constants, such as spin exchange $J^* = \beta J$ and magnetic field $h^* = \beta h$.)

To go from initial spin configurations to block spins, we insert a projection operator under the trace in (14) as follows. Suppose the block spins are given by a majority rule, as discussed above. We define

$$T(\sigma'; \sigma_1, ...\sigma_9) = \begin{cases} 1, & \text{if } \sigma' \left(\sum_i \sigma_i\right) > 0; \\ 0, & \text{otherwise.} \end{cases} \tag{15}$$

The block Hamiltonian is defined by

$$e^{-\mathcal{H}'(\sigma')} \equiv \mathrm{tr}_{\,\sigma} \prod_{\text{blocks}} T(\sigma'; \sigma_i) e^{-\mathcal{H}(\sigma)} \tag{16}$$

We note that, because of the identity $\sum_{\sigma'} T(\sigma'; \sigma_i) = 1$ (unity decomposition), the partition functions for $\mathcal{H}$ and $\mathcal{H}'$ are the same:

$$\mathrm{tr}_{\,\sigma'} e^{-\mathcal{H}'(\sigma')} = \mathrm{tr}_{\,\sigma} e^{-\mathcal{H}(\sigma)} \tag{17}$$

Moreover, all correlation functions that depend on the block spin variables σ', σ'', σ''', ... at higher levels of blocking will be left invariant. Thus all macroscopic properties remain unchanged under the blocking procedure. The only difference is that the quantities have to be expressed in terms of blocked, or renormalized, spins, rather than the original, or bare, spins.

It is useful to think of all couplings in the reduced Hamiltonian $\mathcal{H}'$ as a multicomponent vector $\{K\} \equiv (K_1, K_2, ...)$. In the original Hamiltonian one may have only one nearest neighbor coupling, say K_1, with all other $K_i = 0$. But the RG procedure will in principle generate all other possibilities. We may therefore think of the RG transformation as acting in the space of all couplings:

$$\{K'\} = \mathcal{R}\{K\} \tag{18}$$

The problem is thereby reduced to the problem of understanding the mapping (18). In practice, since the sums involved in the trace in (16) are usually intractable, one has to make approximations by identifying the relevant couplings and leaving out irrelevant ones.

1.5 Summarize

- **Fluctuations** invalidate the mean field theory in the space dimension $d < 4$. Understanding phase transitions for $d < 4$ requires tackling a nontrivial problem of interaction of fluctuations.

- **The renormalization group** is a mathematical framework for expressing scale invariance at the critical point. It allows to coarse-grain physical variables (spins) and their interactions.