1 Lecture 4. Universality classes. Susceptibility and fluctuations.

1.1 Isomorphic phase transitions

One useful consequence[1] of the symmetry approach is that it allows to identify *isomorphic phase transitions* in which the symmetry change is the same. Isomorphic transitions may take place in very different systems, and despite that, they have the same macroscopic characteristics.

Our reason to emphasize symmetry is that the change of the state that occurs at phase transition is macroscopic. The characteristic length scale for thermodynamic fluctuations near the phase transition, as well as below it in the ordered state, is large. (This will be discussed below.) The microscopic origin of the degrees of freedom participating in the transition plays a relatively minor role, since on relevant length scales, much larger than interparticle or lattice spacing, a *coarse grained* picture emerges.

For concreteness, let us talk now about a magnetic system. The order parameter variable used to describe the ordering is magnetization $\mathbf{m}(\mathbf{x})$, representing microscopic magnetic moments coarse grained from lattice length scale up to a large length scale at which thermodynamic fluctuations take place. In that, we treat $\mathbf{x}$ as a continuous variable with the understanding that the function $\mathbf{m}(\mathbf{x})$ exhibit variations on length scales larger than the lattice spacing a.

The free energy expansion in powers of $\mathbf{m}$ near the transition, known as Landau functional, has a universal form dictated solely by symmetry:

$$\mathcal{H} = \int \left[-\frac{1}{2} a\tau \mathbf{m}^2 + b\mathbf{m}^4 + \frac{1}{2} K(\nabla \mathbf{m})^2 + O(\mathbf{m}^6) \right] d^3x \,, \quad \tau = (T_c - T)/T_c \qquad (1)$$

$(a, b > 0)$. Compared to the discussion in Lecture 3, we added a gradient term $\frac{1}{2}K(\nabla \mathbf{m})^2$, sometimes called Lifshits term. On phenomenological grounds, this term gives the energy associated with spatially nonuniform fluctuations. The *rigidity constant* in this term is positive, $K > 0$. Such a term can also be derived from the microscopic mean field approach, as we saw in Lecture 1.

There are many phase transition varieties described by the free energy (1). In general, $\mathbf{m}$ is an n component vector. One can relate phase transitions in different systems which are described by the same symmetry change, and hence by an order parameter with the same number of components:

- $n = 1$ describes liquid-gas critical point, binary mixtures (e.g., alloys), as well as uniaxial magnets (e.g. Ising model);

[1] Moved here from Lec. 3 and expanded.

- $n = 2$ describes superfluidity, superconductivity, planar magnets (i.e. Heisenberg magnets with the the so-called easy plane anisotropy);
- $n = 3$ corresponds to Heisenberg ferromagnets, etc.

There are many other transitions not included in this brief list. For instance, the problem (1) in the limit of zero number of components, $n = 0$, is used to describe disordered systems.

Another important characteristic is space dimension. It turns out that the behavior near transition, and even the mere existence of the transition, is very sensitive to the dimensionality of the problem. Most of the systems of interest have $d = 3$, but it is very useful to consider different space dimensions, $d = 1$, 2 and even $d = 4$ and higher. The transitions in the same space dimension, described by the same order parameter symmetry are said to belong to the same *universality class*. Many universality classes are possible, not limited to the above three varieties.

To illustrate how the correspondence between the systems of the same universality class can be established, let us discuss the first item in the above list, $n = 1$. The Ising phase transition, the liquid-gas critical point, and the binary alloy, have already been described in Lecture 2. In all three cases, the ordering is describes by a scalar order parameter. The symmetry is exact in the case of the Ising problem ($m \to -m$), and in the case of a binary alloy ($a \leftrightarrow b$), but only approximate near the liquid-gas critical point (however, it becomes exact asymptotically right at this point). For convenience, we list analogous quantities in a table:

System described by Ising model	Curie point of a ferromagnet	Liquid-gas critical point of a one component liquid	Critical point of a binary mixture
Density-like variable	Magnetization $M = -(\partial\Phi/\partial H)_T$	Density $\rho = -(\partial P/\partial\mu)_T$	Concentration $x = -(\partial\mu_1/\partial\mu^*)_T$
Field-like variable	Magnetic field $H = -(\partial F/\partial\mu_1)_T$	Chemical potential $\mu = F + PV = [\partial(\rho F)/\partial\rho]_T$	The difference of the chemical potentials of the components, $\mu^* = \mu_2 - \mu_1 = (\partial F/\partial x)_T$
Thermodynamic potential for the density variable	$F(T, M) = \Phi + Mh$, $dF = -SdT + hdM$	$\rho F(T, \rho) = -P + \rho\mu$, $d(\rho F) = -\rho SdT + \mu d\rho$	$F(T, x) = \mu_1 + \mu^* x$, $dF = -SdT + \mu^* dx$
Thermodynamic potential for the field variable	$\Phi(T, h) = F - Mh$, $d\Phi = -SdT - Mdh$	$-P(T, \rho)$, $-dP = \rho SdT - \rho d\mu$	$\mu_1(T, \mu^*) = F - \mu^* x$, $d\mu_1 = -SdT - xd\mu^*$
Order parameter ϕ	M	$(\rho - \rho_c)/\rho_c$	$x - x_c$
Ordering field h	h	$(\mu - \mu(\rho_c, T))/T_c$	$(\mu^* - \mu^*(\rho_c, T))/T_c$
Susceptibility $(\partial\phi/\partial h)_T$	$(\partial M/\partial h)_T$	$(T_c/\rho_c)(\partial\rho/\partial\mu)_T$	$T_c(\partial x/\partial\mu^*)_T$
Specific heat C_ϕ	$C_M = -T(\partial^2 F/\partial T^2)_M$	$\rho C_V = -T(\partial^2 \rho F/\partial T^2)_V$	$C_x = -T(\partial^2 \rho F/\partial T^2)_x$

1.2 Susceptibility

An efficient probe of the physics near transition is provided by susceptibility of the order parameter to various external fields. It is particularly illuminating to introduce the so called ordering field that couples to the order parameter linearly:

$$\mathcal{H}(\mathbf{m}) = \mathcal{H}_0(\mathbf{m}) - \int \mathbf{h}\cdot\mathbf{m}\, d^3x \tag{2}$$

where $\mathcal{H}_0$ is the field independent functional (1). In magnetic systems, the field $\mathbf{h}$ is just the ordinary magnetic field. In other problems it may have a different meaning (see Table above).

Susceptibility is defined as

$$\chi = d\mathbf{M}/d\mathbf{h}\,, \quad \mathbf{M} = \langle \mathbf{m} \rangle \tag{3}$$

Here $\langle ... \rangle$, as usual, stands for thermodynamic averaging $\frac{1}{Z}\mathrm{tr}\,(...e^{-\beta\mathcal{H}})$.

For illustration, let us consider the Landau theory for an Ising ferromagnet, ignoring the effects of fluctuations:

$$\mathcal{H}(m) = -\frac{1}{2}a\tau m^2 + bm^4 - hm \tag{4}$$

(here $\tau = (T_c - T)/T_c$). The average $\langle m \rangle$ in this case is simply given by the extremal m value. At $h = 0$,

$$m_0 = \langle m \rangle = \begin{cases} 0, & \text{at } \tau < 0 \\ (a\tau/4b)^{1/2} & \text{at } \tau > 0 \end{cases} \tag{5}$$

In a small field h, the extremal value changes:

$$m = m_0 + \delta m\,, \quad \delta m = \frac{h}{\mathcal{H}''(m_0)} = \begin{cases} h/(-a\tau), & \text{at } \tau < 0 \\ h/(2a\tau) & \text{at } \tau > 0 \end{cases} \tag{6}$$

where $\mathcal{H}'' = \partial^2\mathcal{H}/\partial m^2$. Hence the susceptibility χ diverges as $1/\tau$ near the transition.

Similar result comes from the mean field theory. Indeed, above T_c one can linearize the selfconsistent equation for magnetization, $m = \tanh(\beta J m + \beta h)$, derived in Lecture 2. This gives a linear relationship, $m = h/(T - T_c)$, which yields the Curie law $\chi = 1/(T - T_c)$.

Comparison with experiment. A power law divergence is seen, but the form of singularity is often somewhat different: $1/\tau^\gamma$ with $\gamma > 1$. To understand this, we need to look into the role of fluctuations.

1.3 Fluctuations. Structure factor.

The appearance of a long range order is associated with the change in the behavior of the correlation function

$$C_2(\mathbf{x} - \mathbf{x}') \equiv \langle m(\mathbf{x}) m(\mathbf{x}') \rangle = \frac{1}{Z}\mathrm{tr}\,\left(m(\mathbf{x}) m(\mathbf{x}') e^{-\beta\mathcal{H}}\right) \tag{7}$$

Here, for simplicity, we discuss the case of one component order parameter, $n = 1$. Generalization to other forms of order parameter will be straightforward.

Above the transition, fluctuations of m at different points are practically uncorrelated, and thus the correlation function (7) falls of rapidly as a function of the distance $|\mathbf{x} - \mathbf{x}'|$. As the temperature approaches the transition, the range in which the fluctuations of m are correlated increases, typically as a power law in $1/\tau$. At the transition, the order proliferates making the range of correlations infinite. One can use, as an illustration of this behavior, the Landau theory (1), and show that

$$C_2(\mathbf{x} - \mathbf{x}') \propto \exp\left(|\mathbf{x} - \mathbf{x}'|/\xi\right), \quad \xi(\tau) \propto 1/|\tau|^{1/2} \tag{8}$$

This behavior is analyzed in more detail in the homework problem 4, PS#3.

Fluctuations can be easily measured experimentally in a scattering experiment. Remind of the liquid-gas system becoming opaque near the critical point. (This phenomenon is called *critical opalescence.*) Magnetic ordering is usually probed by neutron scattering: unlike light, neutrons have spin which couples to electron spins (via dipole interaction) and to to nuclear spins (via exchange interaction).

There are two characteristics that one can look for in a scattering experiment, the intensity and the angular distribution of scattered light (or other waves used in the experiment). To illustrate the relation of these characteristics with the correlation function, let us consider neutron scattering in an Ising magnetic system, with a contact interaction $\mathcal{H}_{\rm int} = \gamma \int \sigma_n m(\mathbf{x})\, d^3x$. Taking the incident neutron state to be a plane wave with momentum $\mathbf{p}$, assuming the scattering to be elastic, and using Born scattering approximation, the angular distribution of scattered neutrons is

$$dN(\theta) \propto \gamma^2 \langle |\int e^{-i\mathbf{k}\cdot\mathbf{x}} m(\mathbf{x})\, d^3x|^2\rangle, \quad |\mathbf{k}| = 2\sin(\theta/2)|\mathbf{p}| \tag{9}$$

where $\mathbf{k} = \mathbf{p}' - \mathbf{p}$ is the momentum change at scattering, $|\mathbf{p}'| = |\mathbf{p}|$. This expression can be rewritten in terms of Fourier harmonics $m_{\mathbf{k}} = \int e^{-i\mathbf{k}\cdot\mathbf{x}} m(\mathbf{x})\, d^3x$ as

$$dN(\theta) \propto \gamma^2 \langle |m_{\mathbf{k}}|^2\rangle \tag{10}$$

Also, Eq.(9) can be brought to the form where the relation with the correlation function (7) is more explicit. For that, we change the integration variables $\mathbf{x}$ and $\mathbf{x}'$ in (9) to $\mathbf{X} = \frac{1}{2}(\mathbf{x} + \mathbf{x}')$ and $\mathbf{y} = \mathbf{x} - \mathbf{x}'$:

$$\iint e^{-i\mathbf{k}\cdot\mathbf{x} + i\mathbf{k}\cdot\mathbf{x}'} \langle m(\mathbf{x}) m(\mathbf{x}')\rangle\, d^3x d^3x' \tag{11}$$

$$= \iint e^{-i\mathbf{k}\cdot\mathbf{y}} \langle m(\mathbf{x}) m(\mathbf{x}')\rangle\, d^3y d^3X = V \int e^{-i\mathbf{k}\cdot\mathbf{y}} C_2(\mathbf{y})\, d^3y \tag{12}$$

where V is the volume of the system. We see that in the scattering measurement one can probe the so-called *structure factor*, defined as a Fourier transform of the correlation function (7).

As an illustration, consider again the $n = 1$ problem (1). Above the transition, at $\tau > 0$, the mean value $m_0 = \langle m \rangle = 0$. Expanding (1) to the second order in the fluctuations $m = m_0 + \delta m$, we have

$$\mathcal{H}(\delta m) = \int \left[-a\tau(\delta m)^2 + \frac{1}{2}K(\nabla\delta m)^2 \right] d^3x = \sum_{\mathbf{k}} \frac{1}{2} \left(K\,\mathbf{k}^2 + a|\tau| \right) |\delta m_{\mathbf{k}}|^2 \qquad (13)$$

Here we use the standard notation $\sum_{\mathbf{k}} = \int ... d^3k/(2\pi)^3$

From that, using equipartition theorem, obtain

$$\langle |\delta m_{\mathbf{k}}|^2 \rangle = \frac{T}{K\,\mathbf{k}^2 + a|\tau|} \qquad (14)$$

Thus, the scattering intensity in this system will have angular distribution given by a Lorentz function of the width $\propto \tau^{1/2}$. In a more general situation, the width of the scattering distribution is given by the inverse correlation radius $1/\xi = \sqrt{a|\tau|/K}$.

1.4 An intuitive meaning of $C_2(\mathbf{x} - \mathbf{x}')$.

Let us discuss here the properties of the correlation function $C_2(\mathbf{x} - \mathbf{x}')$. Although it was defined in a somewhat formal way, we now show that one can think of it in terms of linear response to an external field. To build the relation with linear response, let us consider $C_2(\mathbf{x} - \mathbf{x}')$ for the Ising model:

$$C_2(\mathbf{x} - \mathbf{x}') = \langle \sigma_x \sigma_{x'} \rangle = \mathrm{tr} \left(\sigma_x \sigma_{x'} e^{-\beta\mathcal{H}(\sigma)} \right) \qquad (15)$$

Let us note that, in the absence of external magnetic field, the Hamiltonian is invariant under changing signs of all spins, $\sigma_x \to -\sigma_x$. Since the function $C_2(\mathbf{x} - \mathbf{x}')$ is also invariant under a global sign change, we can rewrite (15) as

$$C_2(\mathbf{x} - \mathbf{x}') = \mathrm{tr} \left(\sigma_x e^{-\beta\mathcal{H}(\sigma)} \right)_{\sigma_{x'} = +1} \qquad (16)$$

(we changed the sign of all spins so that $\sigma_{r'} = +1$). The result (16) can be interpreted as the magnetization at the point $\mathbf{x}$ due to a spin at the point $\mathbf{x}'$ polarized by an external field. Thus the correlation function $C_2(\mathbf{x} - \mathbf{x}')$ has a meaning of a nonlocal response function.

This interpretation of the correlation function in terms of nonlocal response yields a useful relation between fluctuations and the susceptibility χ in a uniform field. One can prove a theorem:

$$\chi = \beta \int C_2(\mathbf{y})\, d^3y \quad \text{(which is just } C_2(\mathbf{k} = 0)) \qquad (17)$$

This result is completely general. It is related to the fluctuation-dissipation theorem[2].

[2]see: §124, Chap. XII, Landau & Lifshits, Statistical Physics, part I

Proof:

$$\chi = dM/dh = \frac{1}{V}\frac{\partial^2 \ln(Z(h))}{\partial^2 h} = \frac{\beta}{V}\iint \mathrm{tr}\,\left(m(\mathbf{x})m(\mathbf{x}')e^{-\beta\mathcal{H}}\right) d^3x d^3x' - \beta\left(\int m(\mathbf{x})d^3x\right)^2$$
$$= \frac{\beta}{V}\iint \mathrm{tr}\,\left[(m(\mathbf{x}) - \langle m\rangle)(m(\mathbf{x}') - \langle m\rangle)e^{-\beta\mathcal{H}}\right] d^3x d^3x' = \beta\int C_2(\mathbf{y})\, d^3y \qquad (18)$$

Here we used the partition function in magnetic field $Z(h) = \mathrm{tr}\ \exp\left(-\beta\mathcal{H} + \beta\int m(\mathbf{x})hd^3x\right)$
Q.E.D.

This theorem has numerous applications in the theory of critical phenomena and beyond.

1.5 Summarize

- **Isomorphic phase transitions** correspond to the same symmetry change. They are described by order parameter with the same symmetry and the same coarse grained free energy (Landau functional).
- **Susceptibility** characterizes the response of the order parameter to an external field. It diverges near type II transition due to fluctuations of soft modes with long wavelengths.
- **Correlation function** of the order parameter has a finite range (correlation radius) in the disordered state. The correlation radius increases as we approach the transition and ordering takes place. The correlation function is measurable in a scattering experiment.