

## Phase transitions, Mean-field and Ginzburg-Landau formulations

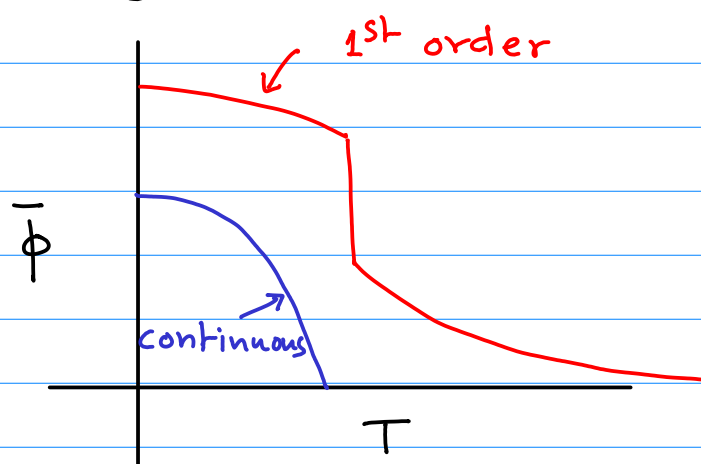
A phase transition upon changing external parameters ( $T$ ,  $P$ , couplings) takes the system from one phase to a macroscopically distinguishable phase.

Here are some examples:

- ① Melting of a crystal into a liquid. The crystal has atoms (on average) in certain positions relative to each other, and has nonzero shear modulus. The liquid has full translation symmetry and zero shear modulus.
- ② Demagnetization of a permanent magnet upon heating beyond  $T_c$ . For  $T < T_c$  there is a macroscopic magnetic moment while for  $T > T_c$  there isn't.
- ③ The  $\lambda$ -transition of  $^4\text{He}$  at  $T_\lambda = 2.6 \text{ K}$  from a normal fluid for  $T > T_\lambda$  with nonzero viscosity to a superfluid with zero viscosity.
- ④ Boiling of a liquid into gas. No symmetries distinguish the two phases but a discontinuous change in the density occurs at the transition.

Different phases of matter are usually (but not always) distinguishable by an order parameter, which is typically zero on one side. For melting the shear modulus is an order parameter, for the magnet it is the magnetization density. For the superfluid it is not so obvious what the order parameter is, and we will need some technology to describe it. The density serves as an order parameter for boiling.

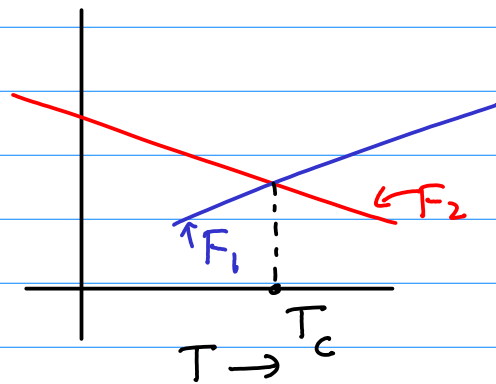
If the order parameter (we will call it  $\phi$  for convenience) changes discontinuously the transition is 1<sup>st</sup> order. If it smoothly vanishes the transition is continuous.



Consider the Free energy of the system  $F(\phi, T)$ . The macroscopic average of  $\phi$  will be whatever minimizes  $F$ . Clearly,  $F$  must be non-analytic (not describable by a convergent Taylor series) at the transition

Let the thermodynamic average of  $\phi$  be  $\bar{\phi}$

For a 1st order transition, plotting  $F(\bar{\phi}(T), T)$  one gets



$T < T_c$  the system is in phase 1 with  $F \equiv F_1(T)$  while for  $T > T_c$   $F \equiv F_2(T)$

and, of course  $F_1(T_c) = F_2(T_c)$

The reason this is called 1st order is that the 1st derivative of  $F$  shows a singularity at  $T_c$ .

Recalling

$$S = - \left( \frac{\partial F}{\partial T} \right)_{V, N} \quad (1)$$

We see that the two phases have different entropy at  $T_c$  (3)

$$S_1 = - \lim_{T \rightarrow T_c^-} \left( \frac{\partial F}{\partial T} \right)_{V, N} \quad (2)$$

$$S_2 = - \lim_{T \rightarrow T_c^+} \left( \frac{\partial F}{\partial T} \right)_{V, N} \quad (3)$$

Thus there is a Latent Heat at the transition.

$$T_c \Delta S \quad (4)$$

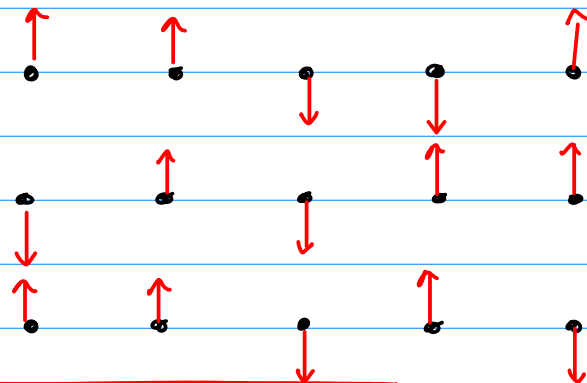
For a continuous transition,  $F$  is still nonanalytic but its 1st derivative is continuous. If some 2nd derivative shows singularities then the transition is 2nd order.

Generally, the system can be put in a field which couples linearly to the order parameter in which case the energy becomes

$$E\{\phi\} \rightarrow E\{\phi\} - \int h \phi d^d x \quad (5)$$

I am using a continuous notation, though the coupling could well be a lattice sum.

A very powerful method of analyzing phase transitions is known as Mean Field Theory. To illustrate, let us go back to the Ising Model in 2 dimensions on a square lattice



One possible Ising configuration

Let  $\vec{x} = a(m\hat{i} + n\hat{j}) \quad (6) \quad m, n \in \mathbb{Z} \quad (7)$

$$E(\{\mathcal{S}(\vec{x})\}) = -J \sum_{\vec{x}} (\mathcal{S}(\vec{x})\mathcal{S}(\vec{x}+a\hat{i}) + \mathcal{S}(\vec{x})\mathcal{S}(\vec{x}+a\hat{j})) - h \sum_{\vec{x}} \mathcal{S}(\vec{x})$$

The exact partition function is

$$Z = \sum_{\{s(\bar{x})\}} e^{-E(\{s(\bar{x})\})/kT} \quad (8)$$

It is possible to do this by sophisticated tricks in 2D (but not in 3D) but we want to approximately solve it and see if there is a phase transition.

Let us assume that  $\langle s(\bar{x}) \rangle = m$ . By translation invariance this must be indep of  $\bar{x}$ . The Mean-Field approximation consists of replacing all neighbors of a particular site  $\bar{x}$  by their average  $m$ . The single site feels the average, or mean, field of its neighbors.

$$E(\bar{x}) = -4Jm s(\bar{x}) - h s(\bar{x}) \quad (10)$$

Now we let this  $s(\bar{x}) = \pm 1$  fluctuate and find its partition  $f^n z(\bar{x})$  (11)

$$z(\bar{x}) = \sum_{s=\pm 1} e^{\frac{s}{kT}(4Jm+h)} = 2 \operatorname{ch} \left( \frac{4Jm+h}{kT} \right)$$

define  $\beta = \frac{1}{kT}$  (12)

$$z(\bar{x}) = 2 \operatorname{ch} [\beta(4Jm+h)] \quad (13)$$

Now the thermodynamic average magnetization of  $\mathcal{S}(\vec{x})$  is

$$\langle \mathcal{S}(\vec{x}) \rangle = \frac{1}{Z(\vec{r})} \left[ e^{\beta(4Jm+h)} - e^{-\beta(4Jm+h)} \right]$$

$$\langle \mathcal{S}(\vec{x}) \rangle = \text{th}[\beta(4Jm+h)] \quad (14)$$

But there is nothing special about  $\vec{r}$ , so

$$\langle \mathcal{S}(\vec{x}) \rangle = m$$

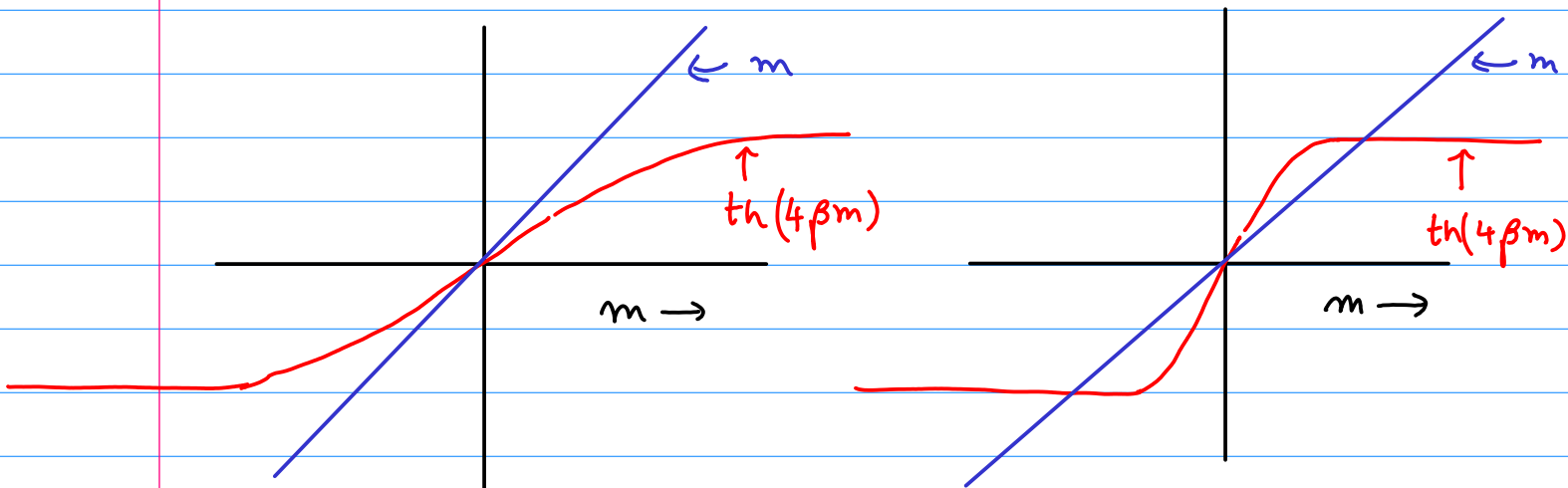
This leads to the self-consistency condition

$$m = \text{th}[\beta(4Jm+h)] \quad (15)$$

For  $h > 0$   $m$  is always nonzero. The crucial question is whether there is a spontaneous order parameter even when  $h=0$ .

$$m = \text{th}(4\beta Jm) \quad (16)$$

The  $\text{th}$  function goes between  $-1$  and  $1$  and its maximum slope is at the origin



In the 1<sup>st</sup> picture the only solution to (16) is  $m=0$ , while there are two (equal and opposite) solutions in the 2<sup>nd</sup> picture. The transition occurs when the slope of the RHS of (16) at  $m=0$  becomes 1

$$(17) \quad 1 = 4\beta_c J \Rightarrow T_c = \frac{4J}{k} \quad (18)$$

How does  $m$  behave for  $T < T_c$ , near  $T_c$ ?

$$\beta = \frac{1}{T} = \frac{1}{T_c + (T - T_c)} \approx \frac{1}{T_c} - \frac{(T - T_c)}{T_c^2} + \dots \quad (19)$$

Now  $\text{th } x = x - \frac{x^3}{3} + \dots \quad (20) \quad x \ll 1$

For  $T - T_c \ll T_c$   $4\beta J m$  will be  $\ll 1$  and we get from (16)

$$m = \frac{4Jm}{kT_c} \left[ 1 - \frac{T - T_c}{T_c} + \dots \right] - \frac{1}{3} \left( \frac{4Jm}{kT_c} \right)^3 + \dots \quad (21)$$

However  $\frac{4J}{kT_c} = 1$

$$\Rightarrow \frac{4J}{kT_c} \frac{(T - T_c)}{T_c} m \approx -\frac{1}{3} \left( \frac{4J}{kT_c} \right)^3 m^3 \quad (22)$$

$$\Rightarrow m = \text{Const} \sqrt{T_c - T} \quad (23) \quad T < T_c$$

Clearly a continuous transition.

The square root is an example of a critical exponent. Many exponents are defined for a continuous transition.

$\alpha$  = specific heat exponent (24)

Recall

$$E = F + TS = F - T \left( \frac{\partial F}{\partial T} \right)_{V,N} \quad (25)$$

$$C_V = \left( \frac{\partial E}{\partial T} \right)_{V,N} = -T \left( \frac{\partial^2 F}{\partial T^2} \right)_{V,N} \quad (26)$$

Near  $T_c$ ,  $C_V \sim |T - T_c|^{-\alpha}$  defines  $\alpha$  (27)

$\beta$  = order parameter exponent (28)

Near  $T_c$   $\bar{\phi} \sim (T_c - T)^\beta$  (29)

$\gamma$ : susceptibility exponent. (30)

Recall that for  $T > T_c$  the magnetization is proportional to  $h$  as  $h \rightarrow 0$

$$m(h) = \chi(T)h + \text{higher orders in } h \quad (31)$$

as  $T \rightarrow T_c$

$$\chi(T) \sim (T - T_c)^{-\gamma} \quad (32)$$

$\nu$  = correlation length exponent. (33)

For  $T \neq T_c$  the correlation function



$$\langle \phi(\bar{x}) \phi(0) \rangle - \langle \phi(0) \rangle^2 \sim e^{-|\bar{x}|/\xi(T)} \quad (34)$$

as  $T \rightarrow T_c$   $\xi(T) \sim |T - T_c|^{-\nu}$  (35)

To make further progress we turn to a more sophisticated formulation of MFT developed by Ginzburg and Landau.

There will always be fluctuations around the thermodynamic average. The idea is to "coarse-grain" the microscopic degrees of freedom (here  $\phi(\bar{x}) = \pm 1$ ) into continuous fields  $\phi(\bar{x})$ . One way to imagine the coarse-graining is to take some volume and find the average of the microscopic degrees of freedom in that volume.

What should the action (Energy) for  $\phi$  be? Go back to (22) and define

$$r = \frac{4J}{kT_c} \frac{(T - T_c)}{T_c} \quad (36)$$

and

$$\lambda = \frac{1}{3} \left( \frac{4J}{kT_c} \right)^3 m^3 \quad (37)$$

The (22) is the result of minimizing

$$\frac{r}{2} m^2 + \frac{\lambda}{4} m^4 \quad (38)$$

We want to replace  $m$  by  $\phi(\bar{x})$  and allow  $\phi(\bar{x})$  to vary in space. We should not forget that there is a cost to the variation of  $\phi$ .

$$-J \mathcal{L}(\bar{x}) \mathcal{L}(\bar{x}+\bar{a}) = \frac{J}{2} \left[ \mathcal{L}(\bar{x})^2 + \mathcal{L}(\bar{x}+\bar{a})^2 - (\mathcal{L}(\bar{x}+\bar{a}) - \mathcal{L}(\bar{x}))^2 \right]$$

$$\rightarrow \frac{J}{2} \left[ \phi(\bar{x})^2 + \phi(\bar{x}+\bar{a})^2 - (\phi(\bar{x}+\bar{a}) - \phi(\bar{x}))^2 \right] \quad (39)$$

For slow variations of  $\phi$

$$(\phi(\bar{x}+\bar{a}_1) - \phi(\bar{x}))^2 + (\phi(\bar{x}+\bar{a}_2) - \phi(\bar{x}))^2 \approx a^2 (\vec{\nabla} \phi(\bar{x}))^2 \quad (40)$$

For  $\hbar=0$  we arrive at

$$E \{ \phi(\bar{x}) \} = \int d^d x \left[ \frac{1}{2} (\vec{\nabla} \phi)^2 + \frac{r}{2} \phi^2 + \frac{\lambda}{4} \phi^4 \right] \quad (41)$$

where  $\phi$  has been normalized to make the coefficient of the  $(\vec{\nabla} \phi)^2$  term  $\frac{1}{2}$ . Note that we are ignoring higher-derivative terms, and terms like  $\phi^6$ ,  $\phi^8$  etc, which we will justify soon.

A very important aspect of coarse-graining is that it preserves the symmetry of the order parameter. The Ising model with  $\hbar=0$  has the global symmetry

$$\mathcal{L}(\bar{x}) \rightarrow -\mathcal{L}(\bar{x}) \quad (42) \quad \text{for all } \bar{x}$$

Now the partition function of the coarse grained theory can be written as an integral over all configurations of  $\phi(\bar{x})$ . This is a Euclidean version of the Path-Integral of Quantum Mechanics.

$$\mathcal{Z} = \int \mathcal{D}\phi(\bar{x}) e^{-\mathcal{S}} \quad (43) \quad \mathcal{S} = \text{Action}$$

$$\mathcal{S} = \frac{1}{kT} \int d^d x \left[ \frac{1}{2} (\vec{\nabla} \phi)^2 + \frac{r}{2} \phi^2 + \frac{\lambda}{4} \phi^4 \right] \quad (44)$$

where  $r$  is proportional to  $T - T_c$ . If we are interested in the vicinity of  $T_c$ , we might as well rescale the variables to remove the  $\frac{1}{kT}$  prefactor  $\Rightarrow$

$$\mathcal{S} = \int d^d x \left[ \frac{1}{2} (\vec{\nabla} \phi)^2 + \frac{r}{2} \phi^2 + \frac{\lambda}{4} \phi^4 \right] \quad (45)$$

We are using  $\mathcal{S}$  for the action. Don't confuse this with  $S$  for entropy or  $s$  for spin!!

Adding the coupling to the external field  $h$  we finally get

$$\mathcal{S} = \int d^d x \left[ \frac{1}{2} (\vec{\nabla} \phi)^2 + \frac{r}{2} \phi^2 - h\phi + \frac{\lambda}{4} \phi^4 \right] \quad (46)$$

Now we are ready to compute the critical exponents in the Ginzburg-Landau approximation. The approximation consists of replacing the partition function by the contribution of the minimum action configuration.

Why is this justified? Remember that the sample is large with of the order of an Avogadro number of constituents.

So  $S \propto \text{Number of constituents} = N$  (47)

Now suppose, for a configuration

$$\phi(\bar{x}) = \phi_{\min}(\bar{x}) + \delta\phi(\bar{x}) \quad (48)$$

$$S[\phi] = S[\phi_{\min}] + \delta S \quad (49)$$

$\delta S$  is also proportional to  $N$  (50)

$$\Rightarrow e^{-\delta S} \rightarrow 0 \quad \text{as } N \rightarrow \infty$$

So deviations from the minimum action configuration can be ignored.

What is the minimum  $S$  configuration?  
 $\phi_{\min}$  should satisfy the Euler-Lagrange eq's

$$\text{If } \mathcal{S} = \int d^d x \mathcal{L}[\phi] \quad (51)$$

Then

$$\vec{\nabla} \left[ \frac{\partial \mathcal{L}}{\partial (\vec{\nabla} \phi)} \right] = \frac{\partial \mathcal{L}}{\partial \phi} \quad (52)$$

$$\text{For our case } \mathcal{L} = \frac{1}{2} (\vec{\nabla} \phi)^2 + \frac{r}{2} \phi^2 + \frac{\lambda}{4} \phi^4 \quad (53)$$

$$\frac{\partial \mathcal{L}}{\partial \vec{\nabla} \phi} = \vec{\nabla} \phi \quad (54)$$

$$\frac{\partial \mathcal{L}}{\partial \phi} = r\phi + \lambda\phi^3 \quad (55)$$

$$\Rightarrow \vec{\nabla}^2 \phi = r\phi + \lambda\phi^3 \quad (56)$$

The natural solution is  $\phi = \text{constant}$ , because a variation of  $\phi(\vec{x})$  costs energy and increases  $\mathcal{S}$  due to the  $\frac{1}{2} (\vec{\nabla} \phi)^2$  term.

$$\Rightarrow r\phi_{\min} + \lambda\phi_{\min}^3 = 0 \quad (57)$$

$$\begin{array}{ll} \text{for } r > 0 \quad (T > T_c) & \phi_{\min} = 0 \\ \text{for } r < 0 \quad (T < T_c) & \phi_{\min} = \sqrt{\frac{-r}{\lambda}} \end{array} \quad (58)$$

This is merely a recasting of (22), (23).

However, we can now find all the exponents in a straightforward manner.

Consider  $\alpha$ : We need to find  $F$

$$Z = e^{-\beta F}$$

$$\Rightarrow F = S_{\min} = \begin{cases} 0 & T > T_c \\ L^d \left[ \frac{r}{2} \phi_{\min}^2 + \frac{\lambda}{4} \phi_{\min}^4 \right] & T < T_c \end{cases} \quad (59)$$

$$S_{\min} = - \textcircled{H} (T_c - T) \frac{r^2}{4\lambda} = - \textcircled{H} (T_c - T) \text{const} \cdot (T_c - T)^2 \quad (60)$$

$$\Rightarrow C_v = - \frac{\partial^2 F}{\partial T^2} = \textcircled{H} (T_c - T) \cdot \text{const.} \quad (61)$$

There is a discontinuity of  $C_v$ , which corresponds to  $\alpha = 0$  (62)

We already know  $\beta = \frac{1}{2}$  (63)

To find  $\gamma$  we need to solve for  $\phi_{\min}$  with  $h \neq 0$ .

$$\Rightarrow r \phi_{\min} - h + \frac{\lambda}{4} \phi_{\min}^3 = 0 \quad (64)$$

$$\Rightarrow \phi_{\min} \approx \frac{h}{r} \sim \frac{h}{T - T_c} \quad (65)$$

$$\Rightarrow \chi \sim \frac{1}{T - T_c} \quad \Rightarrow \gamma = 1 \quad (66) \quad (67)$$

To find  $\nu$  we need the correlation function of fluctuations around  $\phi_{\min}$ .

let  $\phi(\bar{x}) = \phi_{\min} + \psi(\bar{x})$  (68)  $\phi_{\min}$  independent of  $\bar{x}$

$$S = \int d^d x \left\{ \frac{1}{2} (\bar{\nabla} \psi)^2 + \frac{r}{2} \phi_{\min}^2 + r \phi_{\min} \psi + \frac{r}{2} \psi^2 \right. \\ \left. + \frac{\lambda}{4} [\phi_{\min}^4 + 4 \phi_{\min}^3 \psi + 6 \phi_{\min}^2 \psi^2 + 4 \phi_{\min} \psi^3 + \psi^4] \right\} \quad (69)$$

The terms linear in  $\phi_{\min}$  vanish because  $S$  is a minimum there. The terms quadratic in  $\psi$  are

$$\frac{1}{2} (\bar{\nabla} \psi)^2 + \frac{\psi^2}{2} (r + 3 \phi_{\min}^2 \lambda) \quad (70)$$

$$r + 3 \phi_{\min}^2 \lambda = \begin{cases} r & T > T_c \\ -2r & T < T_c \end{cases} \quad (71)$$

$$\tilde{r} = r + 3 \phi_{\min}^2 \lambda > 0 \quad \text{both for } T > T_c \text{ and } T < T_c$$

$$\tilde{r} \sim |T - T_c| \quad (72)$$

Now Fourier transform  $\psi$

$$\psi(\bar{x}) = \int \frac{d^d k}{(2\pi)^d} e^{i\bar{k} \cdot \bar{x}} \psi(\bar{k}) \quad (73)$$

(74)

$$\delta S = \int d^d \bar{x} \frac{d^d k_1 d^d k_2}{(2\pi)^{2d}} e^{i(\bar{k}_1 + \bar{k}_2) \cdot \bar{x}} \psi(\bar{k}_1) \psi(\bar{k}_2) [-\bar{k}_1 \cdot \bar{k}_2 + \tilde{r}]$$

$$\int d^d x e^{i(\vec{k}_1 + \vec{k}_2) \cdot \vec{x}} = (2\pi)^d \delta^d(\vec{k}_1 + \vec{k}_2)$$

(75)

$$\Rightarrow \mathcal{S} = \frac{1}{2} \int \frac{d^d k}{(2\pi)^d} |\psi(\vec{k})|^2 [k^2 + \tilde{r}]$$

(76)

where I have used the reality of  $\psi(\vec{x})$  to infer

$$\psi(-\vec{k}) = \psi^*(\vec{k})$$

(77)

So

$$\langle \psi(\vec{k}_1) \psi(\vec{k}_2) \rangle = \frac{(2\pi)^d \delta^d(\vec{k}_1 + \vec{k}_2)}{k^2 + \tilde{r}}$$

(78)

and thus

$$\langle \psi(\vec{x}) \psi(0) \rangle = \int \frac{d^d k_1 d^d k_2}{(2\pi)^{2d}} e^{i\vec{k}_1 \cdot \vec{x}} \langle \psi(\vec{k}_1) \psi(\vec{k}_2) \rangle$$

(79)

$$= \int \frac{d^d k}{(2\pi)^d} \frac{e^{i\vec{k} \cdot \vec{x}}}{k^2 + \tilde{r}}$$

rescale

$$\vec{k} = \sqrt{\tilde{r}} \vec{p}$$

$$= \tilde{r}^{\frac{d}{2}-1} \int \frac{d^d p}{(2\pi)^d} \frac{e^{i\vec{p} \cdot \vec{x} \sqrt{\tilde{r}}}}{\vec{p}^2 + 1}$$

$$\langle \psi(\vec{x}) \psi(0) \rangle = \tilde{r}^{\frac{d}{2}-1} f(|\vec{x}| \sqrt{\tilde{r}})$$

(80)

by rotational invariance



Since the argument of  $f$  is  $|\bar{x}|\sqrt{\tilde{r}}$   
 we can identify the correlation length  
 as

$$\frac{|\bar{x}|}{\xi} = |\bar{x}| \sqrt{\tilde{r}} \quad (81)$$

$$\Rightarrow \xi \sim |T - T_c|^{-\frac{1}{2}} \quad \Rightarrow \nu = \frac{1}{2} \quad (82) \quad (83)$$

The correlation function at the critical  
 point is a power law, and the  
 anomalous exponent  $\eta$  of  $\phi$  is defined as

$$T = T_c \quad \langle \phi(\bar{x}) \phi(0) \rangle = \frac{\text{Const}}{|\bar{x}|^{d-2+\eta}} \quad (84)$$

In GL theory at  $T = T_c$   $\tilde{r} = 0$

$$\langle \phi(\bar{x}) \phi(0) \rangle = \int \frac{d^d k}{(2\pi)^d} \frac{e^{i\bar{k} \cdot \bar{x}}}{k^2} \sim \frac{1}{|\bar{x}|^{d-2}} \quad (85)$$

$$\Rightarrow \eta = 0 \quad (86)$$

Finally the exponent  $\delta$ . At  $T_c$

$$\frac{d}{d\phi} \left( \frac{\lambda \phi^4}{4} - h\phi \right) = 0 \quad \Rightarrow \quad \phi_{\min} = h^{1/3} \quad (87)$$

$$\delta = 3 \quad (88)$$

So we have a full collection of critical exponents in Landau-Ginzburg theory

$$\alpha=0 \quad \beta=\frac{1}{2} \quad \gamma=1 \quad \delta=3 \quad \nu=\frac{1}{2} \quad \eta=0$$

This explains universality, the fact that systems which are microscopically different show the same critical exponents.

Now the question is, Is this what actually happens in real life?

The answer is a resounding NO!

The actual exponents are (i) different from LG and (ii) depend on dimension/symmetry. We will start with the 2D Ising Model, which can be exactly solved to see that the exact exponents are quite different.