

Lecture 10

(10/13)

Mean Field Approximation

$$F(m, T) = \alpha_0(T) + \alpha_2(T)m^2 + \alpha_4(T)m^4 - hm$$

m is Magnetisation

α_4 = constant near T_c

$$\alpha_2 = t\alpha_2^0 \rightarrow t = \frac{T - T_c}{T_c}$$

$$\frac{\partial F}{\partial m} = 0 = 2t\alpha_2^0 m + 4\alpha_4 m^3$$

$$m = \begin{cases} \pm \sqrt{\frac{2t\alpha_2^0}{4\alpha_4}} & t < 0 \\ 0 & t > 0 \end{cases}$$

$$m \sim |t|^{1/2} \quad t < 0$$

$$C \propto |t|^{-\alpha}$$

$$m \propto (-t)^\beta$$

$$x \propto |t|^{-\gamma}$$

$$@T_c, t=0$$

$$m \propto |h|^{1/\delta}$$

$\alpha, \beta, \gamma, \delta$ are critical exponent

MF

$$\beta = 1/2$$

$$\gamma = 1$$

$$\delta = 3$$

$$\left. \frac{\partial F}{\partial m} \right|_{T=T_c} = 0 = 4\alpha_4 m^3 - h$$

$$m = \left(\frac{h}{4\alpha_4} \right)^{1/3}$$

$$\frac{\partial F}{\partial m} = 0 = 2\alpha_2^0 t m + 4\alpha_4 m^3 - h = 0$$

$$\frac{\partial m}{\partial h}$$

$$h = (2\alpha_2^0 t + 4\alpha_4 m^2) m$$

$$1 = (2\alpha_2^0 t + 4\alpha_4 m^2) m/h$$

$$x = \frac{m}{h} = \frac{1}{2\alpha_2^0 t + 4\alpha_4 m^2} \propto \frac{1}{t}$$

$$t > 0 \quad m^2 = 0$$

$$t < 0 \quad m^2 \propto t$$

Heat capacity

$$T > T_c \quad C_p = C_p^0$$

$$T < T_c \quad C_p = C_p^0 + \text{constant}$$

$$\left. \begin{array}{l} \gamma = \beta(\delta - 1) \\ 2\beta + \delta = 2 - \alpha \end{array} \right\} \rightarrow \text{Mean Field model}$$

	2D Ising	3D Ising	3D Heisenberg
C	0	0.1106	-0.1336
m	1/8	0.3264	0.3689
χ	7/4	1.2365	1.3960
at T_c ; $t=0$ m	15	4.7883	4.783

Heat capacity

$C \propto T^3$	AF magnons
$C \propto T^{3/2}$	F magnons

$$G^2(\vec{r}) = (\vec{s}_i \cdot \vec{s}_j) \quad ; \text{ if } G \text{ is 2 point correlation function}$$

$$r = |\vec{r}_i - \vec{r}_j|$$

$$G_C^2(r) = \langle \vec{s}_i \cdot \vec{s}_j \rangle - \langle \vec{s}_i \rangle \langle \vec{s}_j \rangle ; \text{ connected 2 point}$$

$$@ T_c \quad G_C^2(r) \propto \frac{1}{r^{d-\nu}} \quad d \text{ is dimensionality}$$

ν is critical exponent

$$\text{near } T_c \quad G_C^2(r) \propto e^{-r/\xi} \quad \xi \text{ correlation length}$$

$$\phi \propto |t|^{-\nu}$$

NF	2D Ising	3D Ising	Heisenberg
η	0	$1/4$	0.0366
ν	$1/2$	1	0.6298

$$\boxed{\nu_d = 2 - \alpha}$$
$$\boxed{\nu(2 - \eta) = \delta}$$

2. Magnetic phase transitions - single layer

2.1 Say hello to infinity - *Phase transitions in the thermodynamic limit*

A magnetic phase diagram is easy to draw, which is exemplified in Fig. 2.1, but the basic mechanisms behind the behavior were mysterious for a long time. The critical temperature (T_c) can be defined in many ways, but the easiest phrasing is that it corresponds to the temperature where the zero-field magnetization vanishes. The phase transition is also accompanied by a diverging magnetic susceptibility (χ), which is infinitely large at T_c . Both theoretical and experimental work has proven that, close to the critical temperature, the magnetic quantities follow simple power laws of the form $a = |t|^b$, where $t \equiv T/T_c - 1$ is the reduced temperature and b represents any critical exponent. A number of critical exponents, together with their definitions are found in Table 2.1. The physical quantities are described in later sections.

An expression often encountered in the phase transition community is "the thermodynamic limit", the meaning of which might be hard to comprehend. The essence is however not complicated, it means that the system size is infinitely large. The term comes from the fact that the energy of a system fluctuates, but as the system size goes to infinity these instabilities becomes negligible (except at the critical temperature) [1].

Quantity	Definition	Conditions
Specific heat	$C_H \propto t ^{-\alpha}$	$h = 0, T \rightarrow T_c$
Magnetization	$m \propto (-t)^\beta$	$h = 0, T < T_c, T \rightarrow T_c$
Susceptibility	$\chi \propto t ^{-\gamma}$	$h = 0, T \rightarrow T_c$
Critical isotherm	$m \propto h ^{1/\delta}$	$T = T_c$
Connected two-point correlation function	$G_c^2(r) \propto 1/r^{d-2+\eta}$	$h = 0, r \text{ large}, T = T_c$
Correlation length	$\xi \propto t ^{-\nu}$	$h = 0, T \rightarrow T_c$

Table 2.1. Definition of the critical exponents, from Binney et. al [1]. The reduced temperature is defined as $t \equiv T/T_c - 1$. The physical quantities are described in later sections.

An interesting hypothesis states that the exponents only depend on the spatial and spin dimensionalities of the material. This is called *universality* and gives a correct picture in many cases, but fails to capture what happens when interactions are long-ranged and when the spatial dimension is ambiguous. A

where $t = T/T_c - 1$ and α_2^0 is a constant. This makes it possible to evaluate the temperature dependence of m in zero field by minimizing the free energy,

$$\frac{\partial F}{\partial m} = 2t\alpha_2^0 m + 4\alpha_4 m^3 = 0 \quad (2.4)$$

and finding the two solutions:

$$m = \begin{cases} \pm \sqrt{\frac{2|t|\alpha_2^0}{4\alpha_4}} & t < 0 \\ 0 & t > 0 \end{cases} \quad (2.5)$$

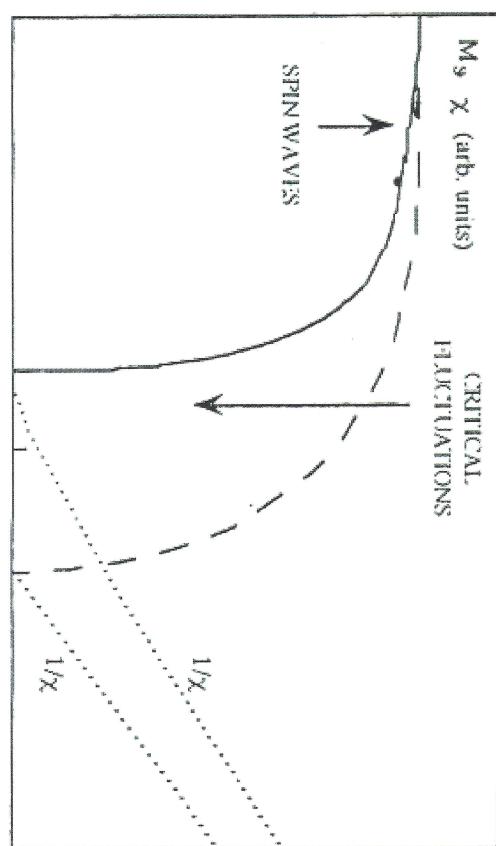
which allows us to identify $m \propto |t|^{1/2}$ and therefore $\beta = 1/2$.

It is also easy to calculate δ of the critical isotherm at $t = 0$, since it follows that $h + 4\alpha_4 m^3 = 0$, giving $m \propto h^{1/3}$ and $\delta = 3$. The other exponents are also possible to evaluate with this approach. However, the results of the calculations agree very badly with experimental findings. The reason is that the Landau theory fails to acknowledge fluctuations and correlations in the zero-field magnetization close to the critical temperature.

2.1.2 Fluctuations gone wild - *Statistical mechanics*

The continuous phase transition in magnetic materials is often referred to as the order-disorder transition. A common misunderstanding is that all magnetic ordering disappears above the critical temperature, but spins are correlated in blocks also at higher temperatures. The difference is that below T_c one can follow a path of ordered spins throughout the whole system, while above T_c the ordered blocks are much smaller. Statistical mechanics provides the tools needed to understand the concepts of fluctuations and correlations that play a crucial role in the vicinity of the critical point and are the reason why mean-field theories fail to quantitatively describe phase transitions. The fluctuations are not only something turning up in equations and simulations, but can be observed by the naked eye in some binary fluid mixtures, like methanol and n-hexane [1]. In these fluids the solubility is a function of temperature and at high temperatures the fluid forms a single phase, but at low temperatures the two solutions are immiscible and separated into two phases. In-between there is a critical temperature separating the two conditions. When this temperature is approached, density fluctuations scatter the light and the initially transparent liquid becomes opaque. This phenomenon is called critical opalescence and is also observed *e.g.* in carbon dioxide around the critical point where gas and liquid become indistinguishable [7]. Similar fluctuations arise in the magnetization in magnetic materials and with the right tools they are observable. Neutron scattering allows probing of the so called *two-point correlation function* (G^2) [1]. It is a measure of the degree of correlation between different parts of the system and is defined by:

4.4 Critical behaviour



There is a large discrepancy between T_c calculated from the exchange constants J , deduced from spin-wave dispersion relations and the measured value.

$$G(r_{ij}) = \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle - \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle$$

$$G(r) \sim \exp(-r/\xi)$$

ξ is the correlation length

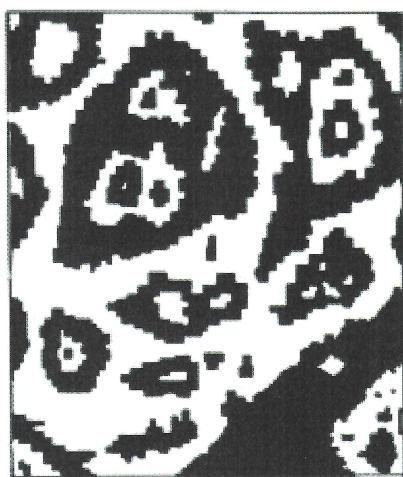
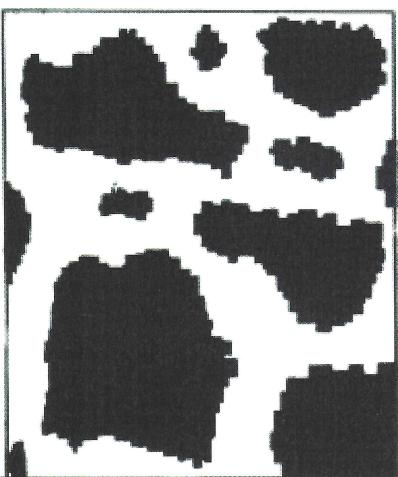


Table 5, 6 More critical exponents for a mean-field ferromagnet

Correlation length	$\xi \approx T - T_c ^{-\nu}$
Correlations at T_c	$G(r) \approx r ^{-(1+\eta)}$
	$\eta = 0$