II Phase Transitions and Critical Behavior:

A. Phenomenology (ibid., Chapter 10)
B. mean field theory (ibid., Chapter 11)
C. Failure of MFT
D. Phenomenology Again (ibid., Chapter 12) //

Phenomenology

Given either a classical or a quantum system there are several qualitatively different situations or "phases" possible

1. Normal Phase: Let us define this phase of natural systems by saying that all the average properties of the measure able quantitates in the system depend smoothly (analytically) upon all the parameters in the Hamiltonian. This dull phase of matter is what we see much of the time. In systems which obey classical physics, this is the behavior of any finite system with finite interactions, and of most infinite ones. In QM there is an extra requirement that one be in a non-degenerate state. In these cases, all derivatives with respect to parameters (like temperature, interaction strength, h) are finite. There is no broken symmetry, all systems have the same basic symmetry as their Hamiltonian.

Proof: look at z. It is a finite sum of positive smooth terms, exponentials, .. all derivatives of its logs are harmless. By varying the parameters in the system one can usually reduce the system to a non-interacting one-- changing nothing along the way

2. “First order” transition point. A situation in which a system can jump from one phase to another. In the jump some quantity, called an order parameter, jumps discontinuously. Example a single-domain ferromagnet, which then has a non-zero magnetization. Usually if the magnetization can point in one direction, it can equally well point in exactly the opposite direction. This example has two-fold symmetry. Higher symmetries of rotation invariance in two or three dimensions are also possible. Superconductors have a full two-dimensional symmetry of a rotation of the phase of their order parameter. Another example is a liquid gas phase transition. Order parameter is density. There is no exact symmetry between liquid and vapor. Nonetheless system does jump between the two phases, as when you boil water.

3. “second order” transition point. System is between order and disorder. Limit of 1st order as order parameter goes to zero. System becomes confused. Large portions of system choose one ordering, other portions another pick another ordering. Interesting decision-making process is involved. Typically the mass goes to zero (□ goes to infinity) as second order transition is approached.

Start with a Simple Model of a Phase Transition called

"Mean Field Theory"

e.g. apply to Ising Model, $\sigma = \pm 1$

Spin in a magnetic field d-dimensions:

$$-\beta H\{\sigma\} = \sum_{<n.n.>} K\sigma_r\sigma_s + \sum_r h_r\sigma_r$$

"Mean Field Theory" assume the spin at r sits in the average field produced by its neighboring spins

$$-\beta H_{eff}(\sigma_r) = \sum_{<\mathbf{s}\ n.n.\ to\ \mathbf{r}>} K\sigma_r <\sigma_s> + h\sigma_r + const$$

$$= \sigma_r\, h_{eff}$$

$$h_{eff} = h + \sum_{s\ n.n.\ to\ r} K <\sigma_s> = h + zK <\sigma>$$

$$<\sigma_r> = \tanh h_{eff} \qquad h_{eff} = h_r + \sum_{s\ n.n.\ to\ r} K <\sigma_s>$$

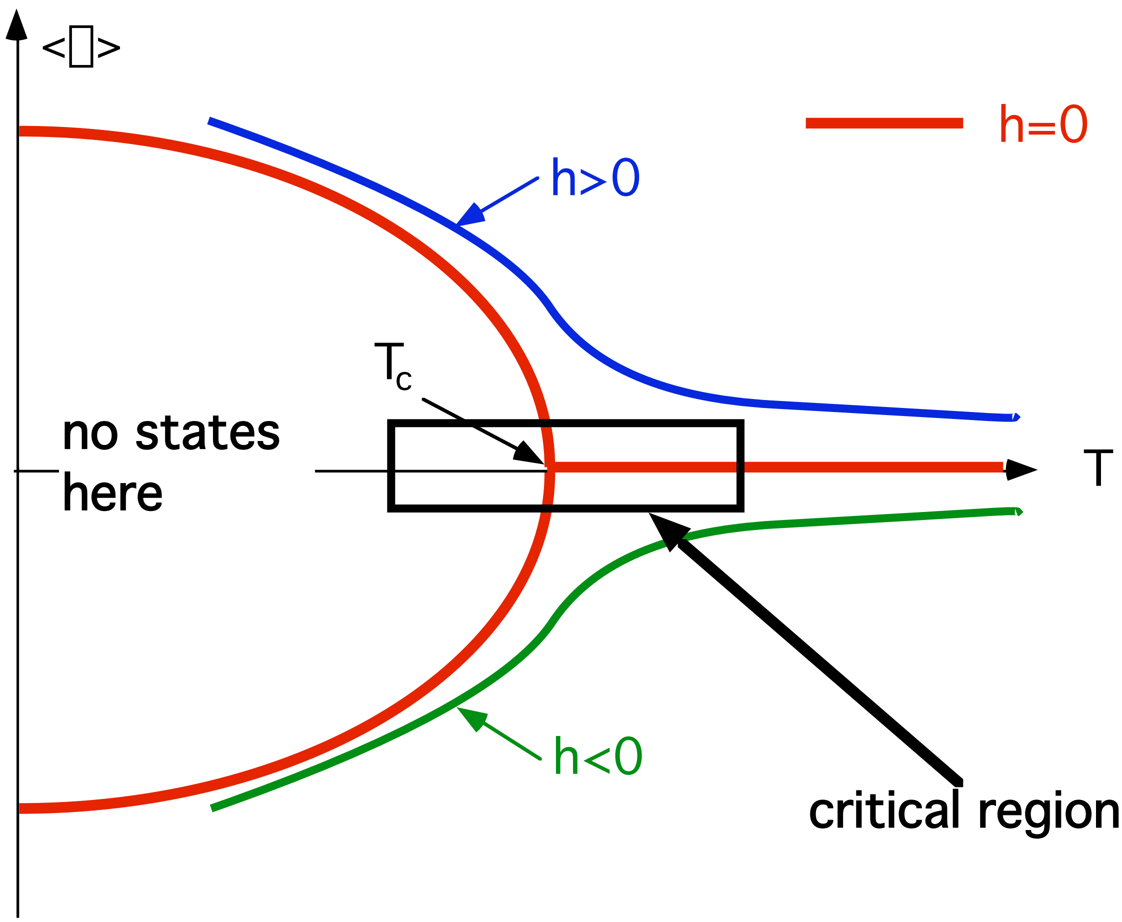
no space dependence

••• $<\sigma> = \tanh(h + z K <\sigma>)$ •••

phase diagram:

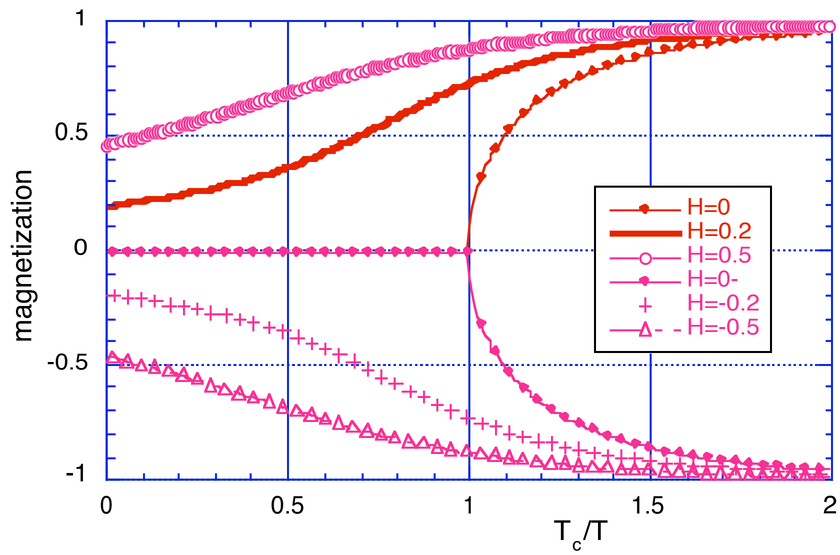
look at magnetization versus temperature for various values of K (or better T)

Drawing



System chooses for itself at h=0, $T<T_c$

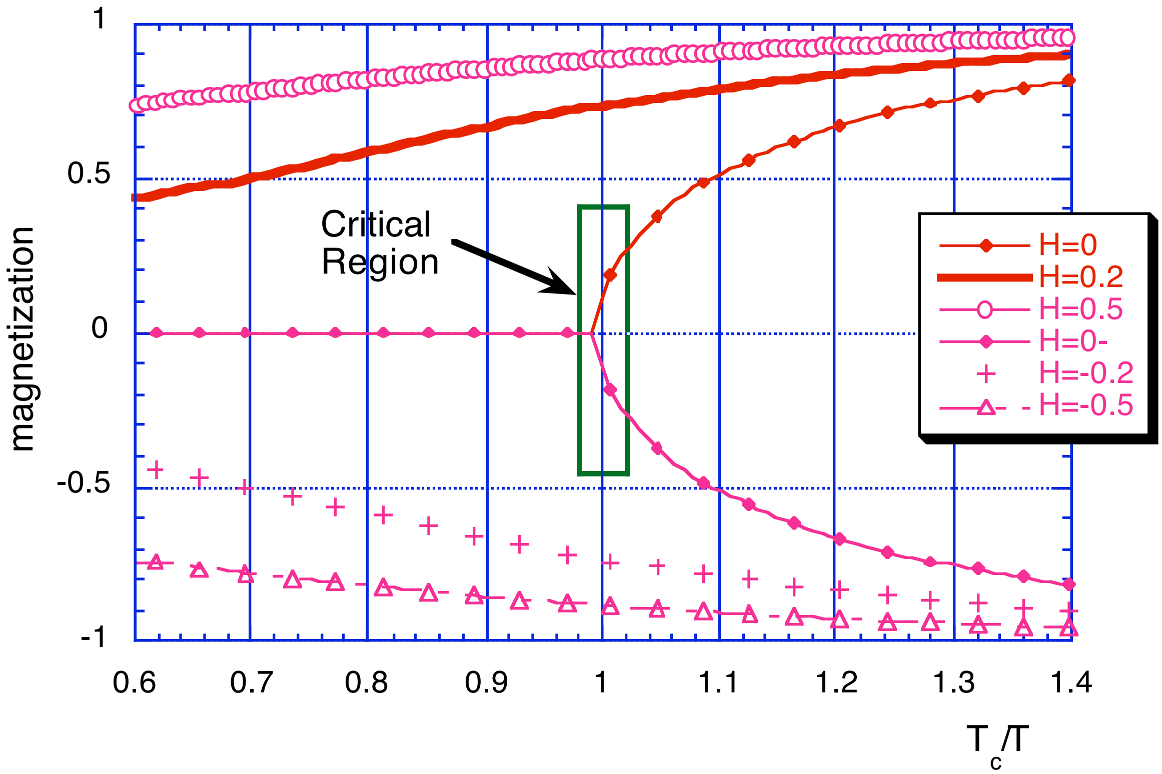
Computer Plot of Phase Diagram



Note left-right flip in comparison to last picture

So below the critical point, we can have a first order phase transition at h=0. At the critical point h=0,T=T_C we have a second order transition.

Focus on Critical Region



We know that there is something wrong with the model. It seems to apply to all dimensions and to systems which might as well be finite. The model shows phase transitions. However, there are no phase transitions in either the finite system or the on-dimensional one. Nonetheless we press on to explore the model's consequences.

Algebra

Note that interesting things are happening around $\langle \square \rangle=0$ where h is close to 0 and Kz is close to 1.

We wish to get the qualitative behavior in the neighborhood of the transition by expanding about $h=0$, $\langle \square \rangle=0$, $T_C/T=zK=1$. It is important for us to identify the terms that can be neglected because they are of smaller relative order compared to the terms which dominate this neighborhood. These left-out terms are called irrelevant.

First expand in h

$$\langle \square \rangle = h /\cosh^2(z K\langle \square \rangle) +\tanh(z K\langle \square \rangle)$$

and then in $\langle \square \rangle$

$$\langle \square \rangle = h /[1+0.5(z K\langle \square \rangle)^2] +(z K\langle \square \rangle) -(z K\langle \square \rangle)^3/6$$

so that

$$\langle \square \rangle [1-z K]= h \quad -(z K\langle \square \rangle)^3/6$$

Note that coefficient of $\langle \square \rangle$ goes to zero at critical point. That's the reason we hold on to cubic term. Since zK is close to one we can set it equal to one in the last term and get our final result

••• $\langle \square \rangle [1-T_C/T]= h \quad - \langle \square \rangle^3/6$ •••

Spontaneous Magnetization

let h=0.

$<\square> [1-T_C/T]= \quad -<\square>^3/6$

Define $zK=T_C/T$. Here T_C is a critical temperature which will play a crucial role in what follows Focus on $zK=T_C/T$ very close to 1. Then,

$<\square> [T-T_C]/T= \quad -(<\square>)^3/6$

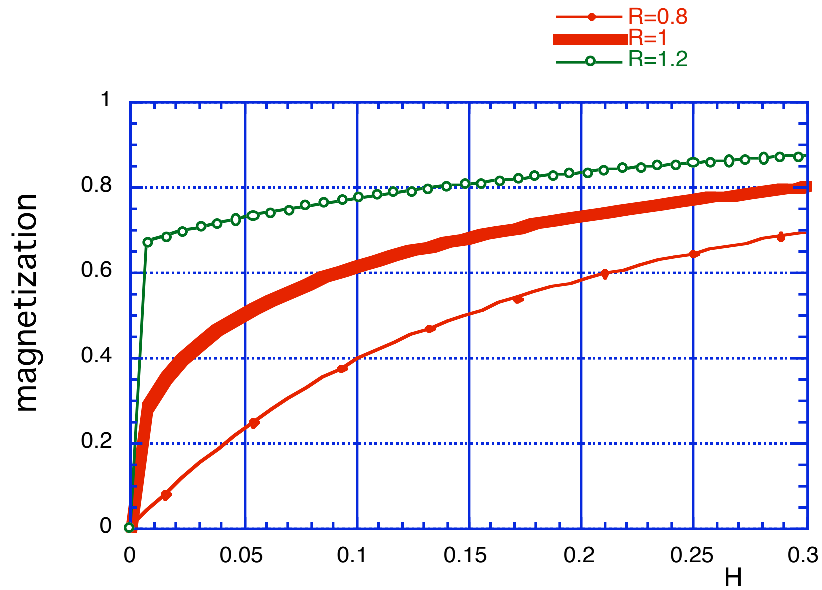
Note that we always have one solution $<\square>=0$, which gives the system zero magnetization. We look for additional solutions which have non-zero magnetization. We must have $[T-T_C]/T=-(<\square>)^2/6$

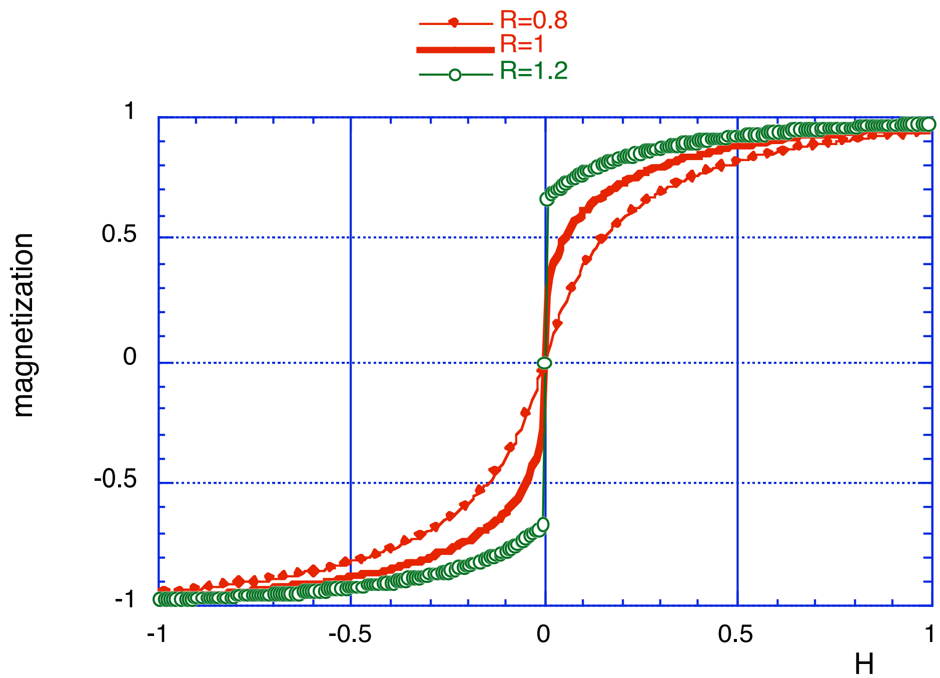
To get real magnetization we must have T below T_C and then

$$<\square>=\pm\sqrt{\square 6\ (1 \square T_c/T)}$$

Note the square root. It indicates a singularity in magnetization versus temperature at T_C. This behavior is only possible in an infinite system.

Magnetization versus Field





$R=T_C/T$

Free Energy Formulation

There is an elegant alternative formulation of the problem due to Lev Landau, imagine that we have a relatively slowly varying $<\sigma_r>$. We want to understand the effects of relatively long-wave length fluctuations in this magnetization density. To do this imagine that we calculate a partition function based upon an effective Hamiltonian or free energy $F\{<\sigma_r>\}$. We assume that the spatial dependence is derived from a term in which a magnetic field vies in space and gives a contribution to -F which is

$$\sum_r h_r \sigma_r = (a_0)^{-d} \int dr \;\; h_r \sigma_r$$

the remaining terms in the free energy density are assumed to be expandable in a series in the magnetization density, based upon the idea that the density is small. The first term is independent of the density. We assume that this term is large but unimportant for our analysis. The remaining terms must be even in the magnetization density, since a parity transformation flips the sign of that density without changing anything else. An appropriate expansion might be that -F has terms of the form

$$-(a_0)^{-d} \int dr \;\; [a \; \sigma_r^{\;2} / 2 + b \; \sigma_r^{\;4} / 4 + c \;\; (\nabla \sigma_r) \circ \; (\nabla \sigma_r) / 2]$$

The gradient term is the simplest such term consistent with rotational and translational invariance.

To get an equation obeyed by the magnetization density, use the concept from thermodynamics that all the internal parameters of the system adjust themselves to minimize the free energy. In this way we find

$$h_r = a\square_r + b\square_r^{\ 3} \square c\square^2\square_r$$

This is our mean field equation extended to include spatial variation. The coefficient a is to be identified with $1\text{-}T_c/T$, to make the critical temperature be a point of singularity. The only other difference is that of notation. Here we write $\square_r$, previously we wrote $<\square_r>$.

Universality

We have just found a mean field theory result of the form

$$h_r = A(1 - T_c / T)\phi_r + b\phi_r^{\,3} - c\nabla^2\phi_r$$

where A, b, and c are some coefficients describing how an order parameter, ϕ_r, might depend upon a symmetry breaking field h and a deviation from the critical temperature. This result, with different coefficients can equally well be applied to a wide variety of phase transitions--indeed almost any one with a scalar order parameter. The consequences are then "universal" in that they apply equally to a whole variety of phase transitions. These consequences include the conclusion that at h=0, the order parameter varies as the square root of $(1-T_C/T)$, while at $T=T_C$ it varies as the 1/3 power of h, and that the coherence length, i.e. the range of important correlations diverges as $\xi \sim (|1 - T_c / T|)^{-1/2}$ both above and below the critical temperature. In this and many other respects the behavior is, expect for a few dimensional coefficients, expected to be model independent.

Scaling

We have just found a mean field theory result of the form $h_r = A(1 \square T_c / T)\square_r + b\square_r^{\ 3} \square c\square^2\square_r$. In the critical region, all three of the variables in this equation are small and the spatial variation occurs over a long distance in comparison to the lattice size. How can we characterize this smallness? One way of doing this is to describe all variables by their relative sizes in comparison to appropriate powers of $(1 \square T_c / T)$. To do this write

R=r[A$(1 \square T_c / T)$/c]$^{1/2}$

H=h A$^{-3/2}$ b$^{-1/2}$ $(1 \square T_c / T)^{-3/2}$

M= $\square$ (A/b)$^{-1/2}$ $(1 \square T_c / T)^{-1/2}$

In terms of these scaled variables the mean field equation reads $H_R = M_R + M_R^{\ 3} \square \square_R^{\ 2} M_R$, a completely universal form. We describe this situation by saying that we have rescaled distances magnetizations and magnetic fields by the appropriate powers of $(1 \square T_c / T)$, and thereby generated a scaled equation for the local magnetization.

Triumphs and Failures

The approach outlined here has had its major triumphs. Its first appearance was in van der Waals work on the liquid-gas phase transition. A similar set of equations was used by Weiss to describe ferromagnetism, for order-disorder transitions and for many others. In 1937, Landau produced the free-energy argument which unified these and many others studies.

These arguments had a very considerable success. They described the qualitative properties of phase diagram quite well. They got all the gross physics right. But near the critical point, where Landau's expansion was believed to be particularly good there was trouble. But the trouble only appeared in parts of Landau's results.

Comparison with Other Results

Many studies have verified that near the critical point, there is scaling and have shown aspects of the universality described here. Specifically

a. Numerical studies of phase transitions in Ising models showed a very considerable similarity among all three dimensional problems as well as among two dimensional problems. However, the actual behavior was rather different in that for example the three dimensional model had magnetization going roughly as a one third power of the temperature deviation from criticality instead of the one half power described here.

b. Onsager developed an analytical theory of the two dimensional model, universal with respect to lattice, with was shown to have universality and scaling, however with different scaling indices than those given above.

c. Three-dimensional experiments showed scaling behavior which rather closely agreed with the numerical studies and hence differed considerably from the van-der Waals-Landau results. A first set of such experiments were carried out by van der Waals himself. Something new is needed.

physical quantity	name of index	mean field theory	index value $d = 3$	index value $d = 2$
specific heat	α	0 (discontinuity)	0.104 ± 0.003	0 (log singularity)
susceptibility	γ	1	1.2385 ± 0.0015	7/4
susceptibility	γ'	1	1.23	7/4
magnetization	β	1/2	0.325	1/8
magnetization	δ	3	5.2 ± 0.15	15
correlation length	ν	1/2	$0.632 \pm 0.001 \pm 0.025$	1
correlation functions	η	0	0.039 ± 0.004	1/8

Maybe the assumption that one could expand the free energy in the order parameter was as error. Maybe one needs a different starting point.

Fluctuations Can Dominate

V.Ginzburg constructed an argument which suggested that the assumption of a fluctuation-free mean field could be in error near the critical point. Then he looked at the fluctuations in magnetization by studying the correlation function

$G(r)=\langle\sigma_r\sigma_0\rangle$

at criticality where $0 = b\sigma_r^{3} - c\nabla^{2}\sigma_r$ so that $\nabla^{2}G(r) = 0$, with the condition that at r of order the lattice constant the correlated fluctuations are of order unity. The solution is $G(r) \sim (a_0/r)^{d-2}$ at least up to r of order the correlation length.

Substitute this length into the estimate and find $\langle\sigma_r\sigma_0\rangle \sim (T_c-T)^{(d-2)/2}$ which then makes the fluctuations in the magnetization of order

$(T_c-T)^{(d-2)/4}$.

We conclude that the fluctuations are of order

$$□□ \sim (T_c - T)^{(d-2)/4}$$

A comparison with the average magnetization, which has

$$< □ > \sim (T_c - T)^{1/2}$$

implies that when $(d-2)/4 > 1/2$ the fluctuations can be neglected. This inequality says that we need $d>4$ for mean field theory to be valid near the critical point.

So mean field theory can be expected to fail near the critical point in our three-dimensional world.