Collective Effects

in

Equilibrium and Nonequilibrium Physics

Website: http://cncs.bnu.edu.cn/mccross/Course/

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Today's Lecture

The simplest magnet: the Ising model

- Calculate a simple *phase transition* from first principles
- Discuss the behavior near this *second order* phase transition
- Clarify the idea of *broken symmetry*
- Introduce *Landau theory*

Equilibrium Statistical Mechanics

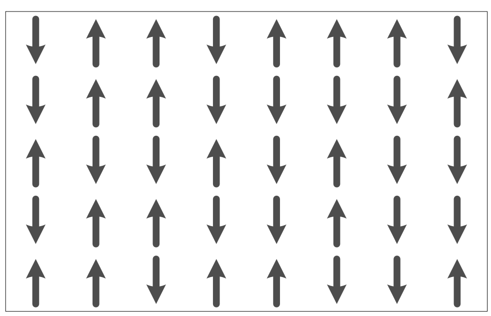
Isolated system (microcanonical ensemble)

- Each accessible (micro)state equally probable
- Thermodynamic potential: entropy $S = k_B \ln \sum_n'$
- Probability of macroscopic configuration C: $P(C) \propto e^{S(C)/k_B}$

System in contact with heat bath at temperature T (canonical ensemble)

- Probability of microstate n proportional to $e^{-\beta E_n}$, with $\beta = (k_B T)^{-1}$
- Thermodynamic potential: free energy $F = -k_B T \ln \sum_n e^{-\beta E_n}$
- Calculate the partition function $Z = \sum_n e^{-\beta E_n}$
- Probability of macroscopic configuration C:
  $P(C) \propto e^{S(C)/k_B} e^{-\beta E(C)} = e^{-\beta F(C)}$

Ising Model



d-dimensional lattice of N "spins" $s_i = \pm 1$

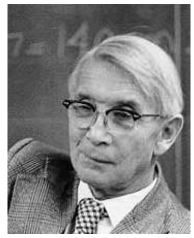
Hamiltonian

$$H = -\frac{1}{2} J \sum_{\substack{i \\ nn\ \delta}} s_i s_{i+\delta} - \mu \sum_i s_i B$$

Partition Function

Canonical partition function

$$Z = \sum_{\{s_i\}} e^{-\beta H\{s_i\}} \qquad .$$



The enumeration of all configurations cannot be done for $d \geq 3$, and although possible in $d = 2$, it is extremely hard there (a problem solved by Onsager). Ising solved the model in one dimension.

We will use an approximate solution technique known as *mean field theory*.

Free Spins in a Field

$$H_0 = -b \sum_i s_i$$

writing b for μB.

This is easy to deal with, since the Hamiltonian is the sum over independent spins.

Average spin on each site is

$$\langle s_i \rangle = \frac{e^{\beta b} - e^{-\beta b}}{e^{\beta b} + e^{-\beta b}} = \tanh(\beta b) \qquad .$$

The partition function is the product of single-spin partition functions

$$Z_0 = [e^{-\beta b} + e^{\beta b}]^N$$

Mean Field Theory

In the mean field approximation we suppose that the ith spin sees an *effective field* b_{eff} which is the sum of the external field and the interaction from the neighbors calculated as if each neighboring spin were fixed at its ensemble average value

$$b_{\text{eff}} = b + J \sum_{\delta} \langle s_{i+\delta} \rangle \qquad .$$

We now look for a self consistent solution where each $\langle s_i \rangle$ takes on the same value s which is given by the result for noninteracting spins

$$s = \tanh[\beta b_{\text{eff}}] = \tanh[\beta(b + 2dJs)] \qquad .$$

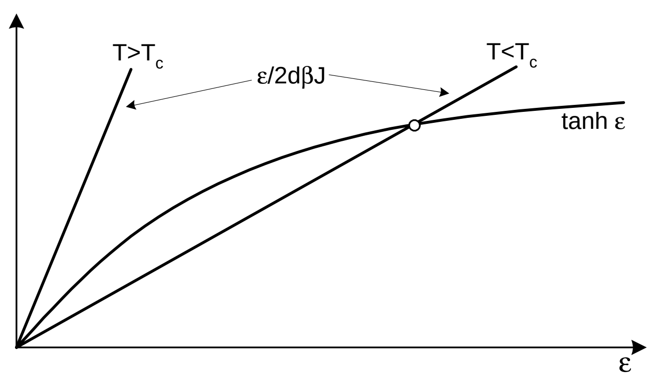
First look at $b = 0$

$$s = \tanh(2d\beta Js) \qquad \text{or} \qquad \varepsilon/2d\beta J = \tanh \varepsilon$$

with $\varepsilon = 2d\beta Js$.

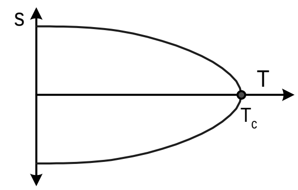
Self Consistency

$$\varepsilon/2d\beta J = \tanh \varepsilon$$



For $T > T_c = 2dJ/k_B$ the only solution is $\varepsilon = 0$

For $T < T_c$ two new solutions develop (equal in magnitude but opposite signs) with $|\varepsilon|$ growing continuously below T_c.



Near T_c we can get the behavior by expanding $\tanh\varepsilon$ in small ε:

$$\varepsilon = 2d\beta J \tanh\varepsilon \qquad \text{with} \qquad \varepsilon = 2d\beta J s,\ k_B T_c = 2dJ$$

becomes

$$\varepsilon = \frac{T_c}{T}(\varepsilon - \frac{1}{3}\varepsilon^3) \qquad \text{or} \qquad \varepsilon^2 = 3(\frac{T_c}{T} - 1)$$

giving to lowest order in small $(1 - T/T_c)$

$$s = \pm\sqrt{3}\left(\frac{T_c - T}{T_c}\right)^{1/2}$$

Order Parameter Exponent

Focus on the *power law* temperature dependence near T_c.

Introduce the small reduced temperature deviation $t = (T - T_c)/T_c$.

We had

$$s = \pm\sqrt{3}\left(\frac{T_c - T}{T_c}\right)^{1/2}$$

Write this for small $t < 0$ as:

$$s \propto |t|^{\beta} \qquad \Rightarrow \qquad \text{order parameter exponent } \beta = 1/2$$

Susceptibility Exponent

The spin susceptibility is $\chi = ds/db|_{b=0}$:

$$s = \tanh[\beta(b + 2Jds)]$$

so that (writing $s' = ds/db$)

$$s' = \mathrm{sech}^2[\beta(b + 2Jds)](\beta + \frac{T_c}{T}s') \qquad .$$

Just above T_c, setting $b = s = 0$

$$\chi = \frac{1}{k_B T_c}\left(\frac{T - T_c}{T_c}\right)^{-1}$$

giving a *diverging* susceptibility as T approaches T_c from above

$$\chi \propto |t|^{-\gamma} \qquad \Rightarrow \qquad \text{susceptibility exponent } \gamma = 1$$

Magnetization Exponent

Exactly at T_c there is a *nonlinear* dependence $s(b)$ of s on b:

$$\begin{aligned} s &= \tanh[\beta_c(b + 2Jds)] \\ &\simeq (\beta_c b + s) - \frac{1}{3}(\beta_c b + s)^3 + \cdots . \end{aligned}$$

The s terms cancel, so we must retain the s^3 term. The linear term in b survives, so we can ignore terms in b^2, bs etc.

This gives

$$s(T = T_c, b) \simeq \left(\frac{3b}{k_B T_c}\right)^{1/3} \mathrm{sgn} b + \cdots .$$

so that

$$s \propto |b|^{1/\delta}\mathrm{sgn} b \qquad \Rightarrow \qquad \text{magnetization exponent } \delta = 3.$$

Internal Energy

With a little more effort we can calculate the internal energy U and other thermodynamic potentials.

We will do this in zero magnetic field only.

In the mean field approximation U is simply given by Nd "bonds" each with energy $-Js^2$ for $T < T_c$:

$$U = -NdJs^2 \simeq -3NdJ\left(\frac{T_c - T}{T_c}\right).$$

For $T > T_c$ the energy is zero in mean field theory (an indication of the limitations of this theory, since clearly there will be some lowering of energy from the correlation of nearest neighbors).

Free Energy

For noninteracting spins in field b we had $F = -k_B T \ln Z_0$ with

$$Z_0 = [e^{-\beta b} + e^{\beta b}]^N.$$

Evaluate (?) the free energy for the interacting spins replacing b by $b_{\text{eff}} = 2Jds$.

This turns out not to be quite right, so call the expression F_I (I for independent)

$$F_I = -Nk_B T \ln\left[e^{-(T_c/T)s} + e^{(T_c/T)s}\right]$$

replacing $2dJ/k_B$ by T_c.

This is not quite correct, because we have *double counted* the interaction energy. So we need to subtract off a term U to correct for this

$$F = F_I - U = -Nk_B T \ln\left[e^{-(T_c/T)s} + e^{(T_c/T)s}\right] + NdJs^2.$$

Near T_c expand this in small s

$$F_I = -Nk_B T \ln 2 - \frac{Nk_B T_c}{2}\left[\left(\frac{T_c - T}{T}\right)s^2 - \frac{1}{6}\left(\frac{T_c}{T}\right)^3 s^4 \cdots\right].$$

Specific Heat Exponent

$$F = -Nk_B T \ln 2 - NJd\left[\left(\frac{T_c - T}{T}\right)s^2 - \frac{1}{6}\left(\frac{T_c}{T}\right)^3 s^4 \cdots\right]$$

Minimize F with respect to s gives, as before

$$s = \begin{cases} \pm\sqrt{3}\left(\frac{T_c - T}{T_c}\right)^{1/2} & \text{for } T < T_c \\ 0 & \text{for } T \geq T_c \end{cases}$$

and the reduction in F below T_c for nonzero s

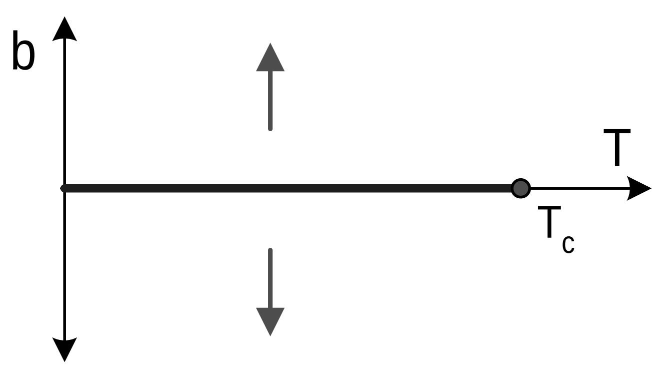
$$\delta F = -\frac{3}{2}NdJ\left(\frac{T_c - T}{T_c}\right)^2 + \cdots .$$

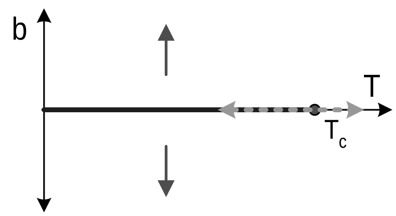
The power law dependence of δF near T_c is used to define the *specific heat exponent*

$$\delta F \propto |t|^{2-\alpha} \qquad \Rightarrow \qquad \text{specific heat exponent } \alpha = 0$$

Specific heat is $C = -Td^2F/dT^2$ is *zero* above T_c, and *jumps* to $3Nk_B/2$ at T_c

Summary

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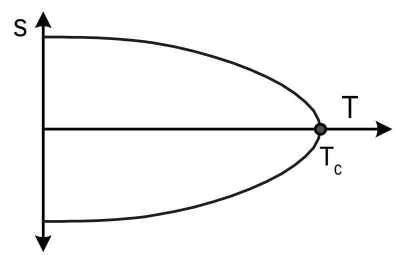
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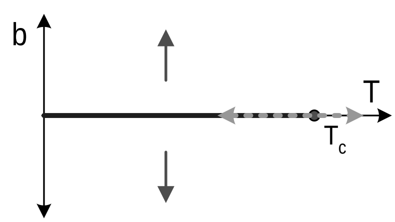
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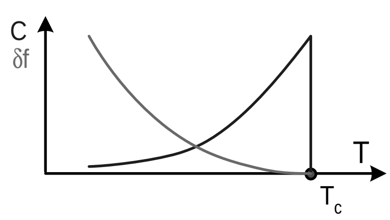
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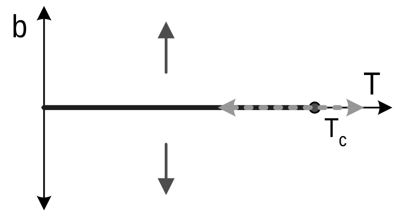
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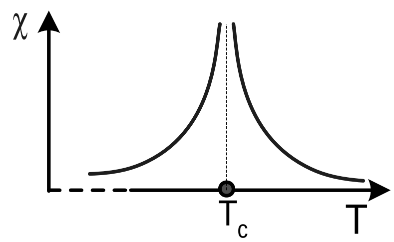
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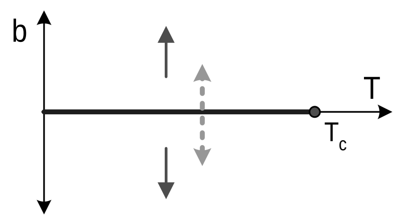
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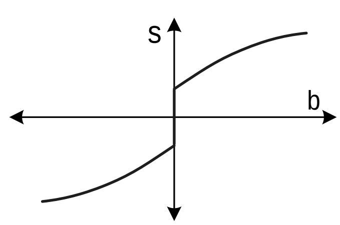
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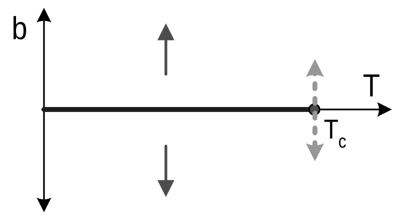
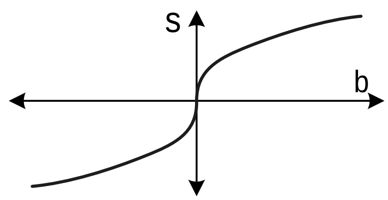




When is mean field theory exact?

Mean field theory is a useful first approach giving a qualitative prediction of the behavior at phase transitions.

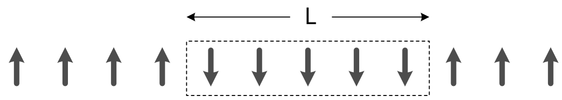
It becomes exact when a large number of neighbors participate in the interaction with each spin:

- in high enough spatial dimension d;
- for long range interactions.

In other cases it is only an approximate theory, and fluctuations are important.

Fluctuations May Destroy the Order

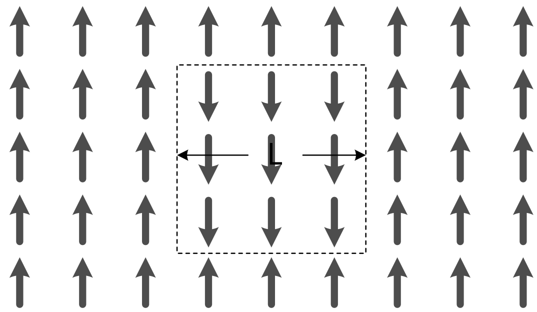
One dimension



- Energy cost to flip a cluster of length L is $4J$
- Probability of flipping cluster $\propto e^{-4\beta J}$

No ordering at any nonzero temperature (the problem Ising solved)

Fluctutations in 2d Ising Model



- Energy to flip cluster of size L grows as roughly $8JL$

Ordering occurs at nonzero transition temperature

Fluctuations Change Exponents

Exponents for the Ising model

Quantity	Dependence	MF	2d	3d
Order parameter	$\lvert s\rvert \propto \lvert t\rvert^{\beta}$, $t < 0$	$\beta = \frac{1}{2}$	$\beta = \frac{1}{8}$	$\beta = 0.33$
Susceptibility	$\chi \propto \lvert t\rvert^{-\gamma}$	$\gamma = 1$	$\gamma = \frac{7}{4}$	$\gamma = 1.25$
Free energy	$\delta F \propto \lvert t\rvert^{2-\alpha}$	$\alpha = 0$	$\alpha = 0$	$\alpha = 0.12$
Order parameter at T_c	$s \propto \lvert b\rvert^{1/\delta}\mathrm{sgn} b$	$\delta = 3$	$\delta = 15$	$\delta = 4.8$

General Remarks

- A new state grows continuously out of the previous one: for $T \to T_c$ the two states become quantitatively the same.
- For $T < T_c$ equally good but macroscopically different states exist. This is a *broken symmetry*—the thermodynamic states do not have the full symmetry of the Hamiltonian. Instead the different thermodynamic states below T_c are related by this symmetry operation.
- The thermodynamic potentials $F, U, S \ldots$ are continuous at T_c but not necessarily smooth (analytic).
- Fluctuations involving admixtures of the other states become important as $T \to T_c$, so that mean field theory will *not in general be a good approximation* near T_c.
- Thermodynamic potentials show *power law* behavior in $\lvert 1 - T/T_c\rvert$ near T_c. The *derivatives* of the potentials (specific heat, susceptibility etc.) similarly show power laws, and will *diverge* at T_c if the power is negative. The exponents are different than the values calculated in mean field theory, and are usually no longer rationals.
- It is not possible to classify phase transitions into higher orders (second, third etc.) according to which derivative of the free energy is discontinuous (Ehrenfest).

Landau Theory of Second Order Phase Transitions

Landau theory formalizes these ideas for any second order phase transition.

Landau Theory of Second Order Phase Transitions

- Second order phase transitions occur when a new state of *reduced symmetry* develops continuously from the disordered (high temperature) phase.
- The ordered phase has a *lower symmetry* than the Hamiltonian — *spontaneously broken symmetry*.
- There will therefore be a number (sometimes infinite) of equivalent symmetry related states (e.g., equal free energy).
- These are macroscopically different, and so thermal fluctuations will not connect one to another in the thermodynamic limit.
- To describe the ordered state we introduce a macroscopic *order parameter* ψ that describes the *character* and *strength* of the broken symmetry.
- The order parameter ψ is an additional thermodynamic variable

Free Energy Expansion

Since the order parameter grows continuously from zero at the transition temperature, Landau suggested an expansion of the free energy:

- Taylor expansion in order parameter ψ (i.e., analytic)
- The free energy must be invariant under all symmetry operations of the Hamiltonian, and the terms in the expansion are restricted by these symmetry considerations.
- The order parameter may take on different values in different parts of the system $\psi(\mathbf{r})$, and so we introduce the free energy density f

$$F = \int d^d x \; f(\psi, T)$$

and expand the free energy density f in the local order parameter $\psi(\mathbf{r})$ for small ψ.

Expansion for the Ising Model

For the Ising ferromagnet, use $\psi = m(\vec{r})$, with $m(\vec{r})$ the magnetization per unit volume averaged over some reasonably macroscopic volume.

The free energy is invariant under spin inversion, and so the Taylor expansion contains only even powers of m

$$f(m,T) \simeq f_o(T) + \alpha(T)m^2 + \frac{1}{2}\beta(T)m^4 + \gamma(T)\vec{\nabla}m \cdot \vec{\nabla}m \qquad .$$

The last term in the expansion gives a free energy cost for a nonuniform $m(\vec{r})$. A positive γ ensures that the spatially uniform state gives the lowest value of the free energy.

Higher order terms could be retained, but are not usually necessary for the important behavior near T_c.

Minimum Free Energy

$$f(m,T) - f_o(T) \simeq \alpha(T)m^2 + \frac{1}{2}\beta(T)m^4 + \gamma(T)\vec{\nabla}m \cdot \vec{\nabla}m \qquad .$$

If fluctuations are small, the state that minimizes the free energy will be the physically realized state. This is not always the case, and Landau's theory corresponds to a mean field theory that ignores these fluctuations.

For the Ising magnet the minimum of F is given by a uniform $m(\vec{r}) = \bar{m}$ satisfying

$$\alpha\bar{m} + \beta\bar{m}^3 = 0 \qquad .$$

giving

$$\bar{m} = \begin{cases} \pm\sqrt{-\alpha/\beta} & \text{for} \quad \alpha < 0 \\ 0 & \text{for} \quad \alpha > 0 \end{cases} \qquad .$$

Identify $\alpha = 0$ as where the temperature passes through T_c, and expand near here

$$\begin{aligned} \alpha(T) &\simeq a(T - T_c) + \cdots \\ \beta(T) &\simeq b + \cdots \\ \gamma(T) &\simeq \gamma + \cdots \end{aligned}$$

Exponents etc.

$$\begin{aligned} f - f_o &\simeq \alpha(T)m^2 + \frac{1}{2}\beta(T)m + \gamma(T)(\vec{\nabla}m)^2 \\ &\simeq a(T - T_c)m^2 + \frac{1}{2}bm^4 + \gamma(\vec{\nabla}m)^2 \end{aligned}$$

and the value $m = \bar{m}$ minimizing f

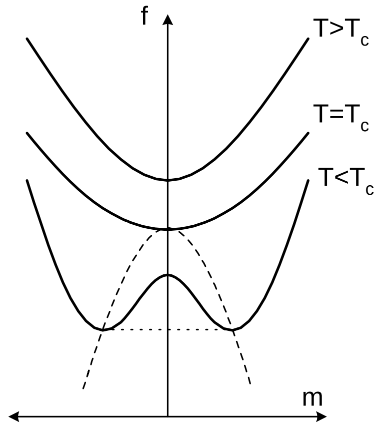
$$\bar{m} \simeq \left(\frac{a}{b}\right)^{1/2}(T_c - T)^{1/2} \quad \text{for } T < T_c \qquad .$$

Evaluating f at $\bar{m}$ gives

$$\bar{f} - f_0 \simeq -\frac{a^2(T - T_c)^2}{2b} \qquad .$$

These are the same results for the exponents we found directly from mean field theory.

$$f - f_o = a(T - T_c)m^2 + \frac{1}{2}bm^4$$



Coupling to Magnetic Field

$$f(m, T, B) = f_0(T) + a(T - T_c)m^2 + \frac{1}{2}bm^4 + \gamma(\vec{\nabla}m)^2 - mB.$$

The magnetic field couples directly to the order parameter and is a *symmetry breaking* field.

Minimizing f with respect to m gives a susceptibility diverging at T_c, e.g., for $T > T_c$

$$\chi = \left.\frac{\bar{m}}{B}\right|_{B=0} = \frac{1}{2a}(T - T_c)^{-1},$$

and at $T = T_c$ for small B

$$\bar{m} = \left(\frac{1}{2b}\right)^{1/3} B^{1/3}.$$

Again the exponents are the same as we found in from mean field theory.

First Order Transitions

We can also encounter first order broken-symmetry transitions.

For example the liquid solid transition is described by the strength of density waves $\rho e^{i\vec{q}\cdot\vec{r}}$.

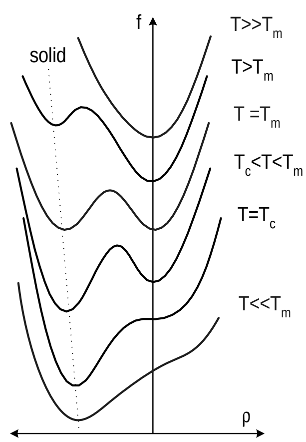
In three dimensions we need three density waves with wave vectors that prescribe the reciprocal lattice; we will suppose all three components have the same magnitude ρ.

Since the density perturbation is added to the uniform density of the liquid, there is no symmetry under changing sign of the density wave, and so the free energy expansion now may have a cubic term

$$f - f_0 = a(T - T_c)\rho^2 + c\rho^3 + \frac{1}{2}b\rho^4$$

(suppose uniform ρ for simplicity).

$$f - f_0 = a(T - T_c)\rho^2 + c\rho^3 + \frac{1}{2}b\rho^4$$

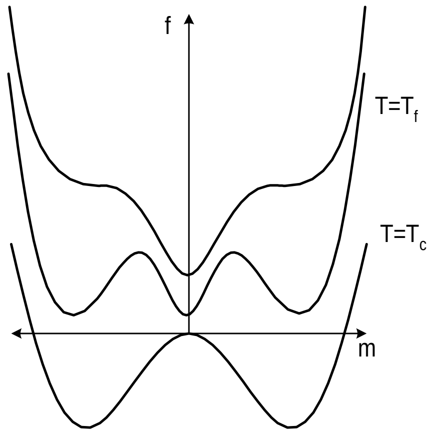


- At high temperatures there is a single minimum at $\rho = 0$ corresponding to the liquid phase.
- As the temperature is lowered a second minimum develops, but at a free energy that remains higher than the liquid.
- At T_m the new free energy becomes equal: this is the melting temperature where the liquid and solid have the same free energy.
- Below T_m the solid has the lower free energy. There is a jump in ρ at T_m, not a continuous variation as at a second order transition.
- The temperature T_c at which the minimum in the free energy at $\rho = 0$ disappears (i.e. the liquid state no longer exists) is not of great physical significance.
- The Landau expansion technique may not be accurate at a first order transition: the jump in ρ at the transition means there is no guarantee that the truncated expansion in ρ is a good approximation.

Another way a first order transition can occur is if the coefficient of the quartic term turns out to be *negative*. Then we must extend the expansion to *sixth* order to get finite results (otherwise the free energy is unbounded below):

$$f - f_0 = a(T - T_c)m^2 - \frac{1}{2}|b|\, m^4 + \frac{1}{3}cm^6.$$

$$f - f_0 = a(T - T_c)m^2 - \frac{1}{2}|b|\, m^4 + \frac{1}{3}cm^6$$



Next Lecture

- Magnets with continuous symmetry (XY model)
  - ◇ Spin waves and the Mermin-Wagner theorem
  - ◇ Topological defects
  - ◇ Kosterlitz-Thouless transition