COOPERATIVE PHENOMENA: ISING MODEL

In this Section, we are discussing various approaches to obtain a mean-field solution to the Ising model. In fact, several of the approaches will yield exactly identical results. The reason they are presented is that they highlight different ways of carrying out the approximation(s) that are commonly referred to as "mean-field approximations". Essentially, they differ by whether:

1-   neglects spin fluctuations around the mean or
2-   considers spins to behave statistically independently and by which part of the system one treats exactly (Bethe-Peierls mean-field theory).

1. PHASE TRANSITIONS OF THE SECOND KIND

Consider ferromagnetic substances, like iron and nickel. Some of the spins of the atoms become spontaneously (without any external field) polarized in the same direction, below the Curie temperature T_c (the critical temperature). This creates a macroscopic magnetic field. As temperature is raised, the thermal energy makes it possible for some of the aligned spins to flip over. This tends to destroy the initial ordered state. For $T > T_c$, the spins get oriented at random and the spontaneous magnetization vanishes. As T_c is approached, from both sides, the heat capacity of the metal approaches ∞. The transition from the non–ferromagnetic state to the ferromagnetic state is called a *phase transition of the second kind*. It is associated with some kind of change in symmetry of the lattice. For example, in ferromagnetism the symmetry of spins is involved. The energy levels of the system are given by

$$E\{\sigma_i\} = -\sum_{i,j}^{N} \varepsilon_{ij}\sigma_i\sigma_j - h\sum_{i}^{N}\sigma_i \tag{1}$$

where, on each lattice site i, the spin quantum number σ_i is +1 or –1, ε_{ij} is the interaction energy (the spin-spin couplings), $h = \mu_B H$ is the interaction energy associated with the external magnetic field H, and μ_B is the magnetic moment associated with the spin. For spontaneous configuration, $h = 0$.

The change of symmetry can also occur due to the change in the ordering of the crystal. For example, in an alloy AB the atoms may be substituted for one another on a set of given lattice sites. Then we can say that a $\sigma_i = +1$ for an atom A on the site i, and $\sigma_i = -1$ for an atom B on that site. At low temperatures the alloy AB is ordered. Above a transition temperature it becomes disordered.

The difference between the nonferromagnetic–ferromagnetic transition and the order-disorder transition is that in the former case 'up' and 'down' spins can be transformed freely into one another, while in the latter case the total number of A type and B type atoms is fixed. However similar theoretical results hold in both the cases.

These transitions come under a large group of phenomena called ***cooperative phenomena***. Certain subsystems, like spins or atoms, cooperate due to exchange interactions to form units below a certain critical point.

Note that a phase transition of the second kind, in contrast to ordinary phase transitions (of the first kind), is continuous in the sense that the state of the body changes continuously. Although the symmetry changes discontinuously at the transition point, at each instant the body belongs to one of the two phases. At a phase transition point of the first kind, the bodies in two different states are in equilibrium, while at a phase transition point of the second kind the states of the two phases are the same.

2. ISING MODEL

The theory of cooperative phenomena is very complicated; especially when all interactions are included and three-dimensional systems are considered.

We assume that in (1) the ε_{ij} acts only between nearest neighbors in the lattice. This is the basic assumption of the *Ising model*. Then (1) is written as

$$E\{\sigma_i\} = -\varepsilon \sum_{\langle i,j \rangle}^{N} \sigma_i \sigma_j - h \sum_i^N \sigma_i \qquad (2)$$

where $\langle i,j \rangle$ means that the sum is over pairs of nearest neighbors, and the interactions are **isotropic**, that is, all ε_{ij} have the same value ε. For $\varepsilon > 0$, the neighboring spins tend to be parallel and ferromagnetism is possible. The spontaneous configuration of least energy is the *completely polarized* (*ordered*) configuration in which all the Ising spins are oriented in the same direction. This configuration is attained at $T = 0$. For $\varepsilon < 0$, the neighboring spins tend to be antiparallel and **antiferromagnetism** results. We will assume $\varepsilon > 0$.

In (2) no distinction is made between $\langle i,j \rangle$ and $\langle j,i \rangle$. The sum over $\langle i,j \rangle$ has $nN/2$ terms, where n is the number of nearest neighbors of a site (*coordination number of the lattice*) and N the number of spins, for example:

$$n = \begin{cases} 2 & \text{in one dimension;} \\ 4 & \text{in two dimensions (square lattice);} \\ 6 & \text{in three dimensions (simple cubic lattice);} \\ 8 & \text{in three dimensions (body-centered cubic lattice);} \\ 12 & \text{in three dimensions (face-centered cubic lattice).} \end{cases}$$

The thermodynamic quantities require the evaluation of the partition function

$$Z(N,h,T) = \sum_{\sigma_1}\sum_{\sigma_2}\cdots\sum_{\sigma_N} e^{-\beta E\{\sigma_i\}} = \sum_{\sigma_1}\sum_{\sigma_2}\cdots\sum_{\sigma_N} e^{\beta \left[\frac{\varepsilon}{2}\sum_{\langle i,j \rangle}^{N} \sigma_i\sigma_j - h\sum_i^N \sigma_i \right]} \qquad (3)$$

where $\beta = 1/k_B T$ and the sum is taken over all the 2^N possible combinations of the N spins.

It is extremely difficult to calculate (3). Several approximate methods have been developed for this. The Weiss theory and Bragg-Williams (BW) approximation are the simplest. More approximations are elaborate, such as: Fowler-Guggenheim approximation and Kirkwood method.

3. Weiss Molecular Field Theory
We start by identifying the order parameter of the magnet which distinguishes the ordered (magnetic) from the disordered (nonmagnetic) phase. For describing a paramagnetic to ferromagnetic transition, the obvious choice is the (local) magnetization

$$m = \langle \sigma_i \rangle = \frac{1}{N} \left\langle \sum_{i=0}^{N} \sigma_i \right\rangle$$

We now focus on a single spin, σ_0, which on a hypercubic lattice in d dimensions has $n = 2d$ nearest neighbors, which we label $\sigma_1, \ldots, \sigma_{2d}$. The scenario considered is shown for the two-dimensional case in Fig. 5.1
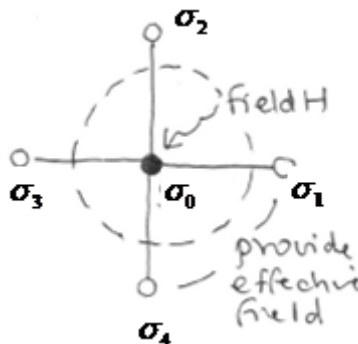

Figure 5.1: A spin σ_0 on a two-dimensional square lattice interacts with its nearest neighbors $\sigma_1, \ldots, \sigma_4$.

The part of the Ising Hamiltonian containing spin σ_0 reads as follows, where we decompose the spins σ_j into their mean value (the magnetization), and fluctuations around it, $\sigma_j = m + \underbrace{(\sigma_j - m)}_{\text{fluctuations}}$:

$$H_{\sigma_0} = -\sigma_0 \left(\varepsilon \sum_{j=1}^{n} \sigma_j + H \right) = -\sigma_0 (\varepsilon nm + H) - \sigma_0 \varepsilon \sum_{j=1}^{n} (\sigma_j - m)$$

The fundamental assumption of mean-field theory is now to set the fluctuations to 0, i.e. $(\sigma_j - m) = (\sigma_j - \langle \sigma_j \rangle) \to 0$, such that the resulting Hamiltonian reads:

$$H_{\sigma_0} = -\sigma_0 (\varepsilon nm + H)$$

This represents a non-interacting spin in an effective field $H_{eff} = \varepsilon nm + H$. This Hamiltonian allows us to calculate $\langle \sigma_j \rangle$. The second step of mean-field theory is to argue that the chosen spin is not special at all, hence its mean must be identical to the magnetization. This gives us a *self-consistency condition* $\langle \sigma_j \rangle = m$. As

$$\langle \sigma_0 \rangle = \frac{\text{tr}\,\sigma_0 e^{\beta \sigma_0 (\varepsilon nm + H)}}{\text{tr}\, e^{\beta \sigma_0 (\varepsilon nm + H)}} = \frac{e^{\beta \sigma_0 (\varepsilon nm + H)} - e^{-\beta \sigma_0 (\varepsilon nm + H)}}{e^{\beta \sigma_0 (\varepsilon nm + H)} + e^{-\beta \sigma_0 (\varepsilon nm + H)}} = \tanh \left[\beta (\varepsilon nm + H) \right]$$

we obtain the following self-consistent equation for the magnetization:

$$m = \tanh \left[\beta (\varepsilon nm + H) \right]$$

While this equation cannot be solved analytically, the main features can be extracted anyways. For a finite field $H \neq 0$, we see for example that solutions change sign with the field: $m(T, H) = -m(T, -H)$.

H.W. Mathematica program to plot equation $m = \tanh \left[\beta (\varepsilon nm + H) \right], H = 0$

Plot the one-dimensional lattice, $n = 2$, $m = \tanh(m/t)$, $t = k_B T / \varepsilon$.

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In[8]:= Plot[FindRoot[m == Tanh[1 m / T], {m, .5}][[1, 2]], {T, 0, 1}, PlotRange → All,
        Frame → True, PlotLabel → " Plot m versus T", FrameLabel → {t, m}]
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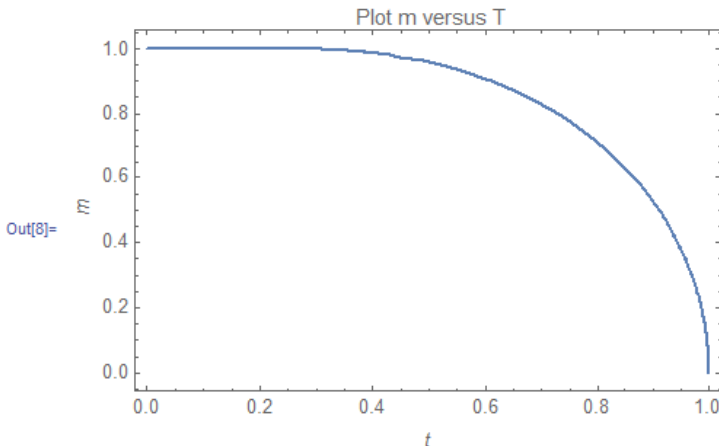

The field-free case $H = 0$ is more interesting. First of all, $m = 0$ is always a solution, which corresponds to the paramagnetic regime. But if we draw both sides of the equation $m = \tanh[\beta \varepsilon nm]$ as a function of m (see Fig. 5.2), we see that there are two more solutions $\pm m_0$ if the slope of the hyperbolic tangent at $m = 0$ exceeds slope 1. Now the slope of the hyperbolic tangent is given by

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$$\frac{d}{dm}\tanh[\beta\varepsilon nm]\Big|_{m=0} = \frac{1}{\cosh^2[\beta\varepsilon nm]}[\beta\varepsilon n] = \beta\varepsilon n$$

Hence, if $\beta\varepsilon n > 1$, there are 3 solutions, $m = 0$ and $m = \pm m_0$, which corresponds to the two Z_2-ymmetry breaking solutions of an Ising magnet. The critical temperature is given by

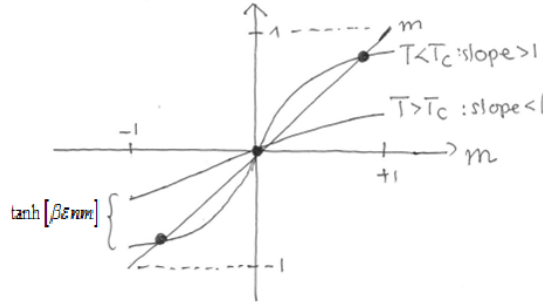$$\boxed{\beta_c\varepsilon n = 1 \quad \Rightarrow \quad k_B T_c = \varepsilon n}$$

Figure 5.2: Graphical representation of the self-consistency equation for the magnetization in the Weiss mean field approximation.

For the hypercubic lattices, this means:

➢ There is a phase transition at $k_B T_c = 2$ ε in the one-dimensional case. In fact, we will see from an entropy argument due to Peierls and from an exact calculation in see next chapter that this is wrong; there is no phase transition in 1D. Of course, omitting all fluctuations is a serious approximation, but we will have to see why our theory fails even qualitatively.

➢ There is a phase transition at $k_B T_c = 4$ ε in the two-dimensional case. We will see from exact calculations in next chapter that there is indeed a phase transition, so our mean field theory is qualitatively right, but it is quantitatively wrong: the true transition temperature is at $k_B T_c = 2.269$ ε, hence overestimated. This is a typical feature of mean-field theories, because their neglect of fluctuations makes them overestimate the tendency to order.

➢ In three and more transitions, mean-field theory continues to predict (correctly) the existence of phase transitions, and the estimates for T_c get increasingly better ($k_B T_c = 6$ ε versus numerical $k_B T_c = 4.511$ ε). This can be understood qualitatively: in higher dimensions, spin s0 is coupled to more and more neighbors, whose fluctuations around the mean (i.e. the magnetization) will increasingly tend to cancel each other (cf. the growth as $1/\sqrt{N}$ of the relative fluctuations for N independent identically distributed random variables with the proviso that the neighboring spins are not acting independently). This means that on average σ_0 indeed is coupled to an effective field $H_{eff} = \varepsilon nm + H$.

From the equation for the magnetization at nonzero field, the exponent δ is obtained as follows:

$$m = \tanh\{\beta(n\varepsilon m + H)\} \quad \Rightarrow \quad \beta(n\varepsilon m + H) = \tanh^{-1}(m) = m + \frac{m^3}{3} + \cdots$$

where we used the expansion of the inverse hyperbolic tangent about $m = 0$. Rearrange, we have:

$$H = k_B T\left(m + \frac{m^3}{3} + \cdots\right) - n\varepsilon m = (k_B T - n\varepsilon)m + \frac{kT}{3}m^3 = mk_B\underbrace{(T - T_c)}_{\sim 0 \text{ at } (T=T_c)} + \frac{k_B T}{3}m^3$$

Here, we used the critical value, $k_B T_c = n\varepsilon$, in the third line. At the critical temperature, this becomes

$$H \sim m^3 \quad \Rightarrow \quad \delta = 3 .$$

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Compared with the equation $H \sim m^{\delta}$. **Note that**: At $H = 0$, one finds ($mk(T - T_c) + \dfrac{kT}{3} m^3 = 0$):

$$m^2 = \begin{cases} 0 & T > T_c \\ \dfrac{3}{T}(T_c - T) & T < T_c \end{cases} \quad \Rightarrow \quad m \approx (T_c - T)^{1/2} \qquad T < T_c$$

Finally, the susceptibility, which is given by

$$\chi = \frac{\partial m}{\partial H} = \frac{1}{\partial H / \partial m}$$

but, near $m = 0$,

$$H = mk(T - T_c) + \frac{kT}{3} m^3$$

$$\frac{\partial H}{\partial m} = k(T - T_c) + kTm^2$$

$$\chi = \frac{1}{k_B(T - T_c) + k_B Tm^2} \sim \begin{cases} \chi_- = \chi = (t \to 0^+) = \dfrac{1}{k_B(T - T_c)} \sim (T - T_c)^{-1} & T > T_c \\ \chi_+ = \chi(t \to 0^-) = \dfrac{1}{k_B(T - T_c) + k_B T \dfrac{3}{T}(T_c - T)} \sim \dfrac{1}{2}(T_c - T)^{-1} & T < T_c \end{cases}$$

As the critical temperature is approached, $m \to 0_+ = 0$ and

$$\chi_+ \sim |T - T_c|^{-1} \qquad \Rightarrow \quad \gamma = 1.$$

The MFT exponents for the Ising model are, therefore

$$\beta = 1/2, \quad \gamma = 1, \quad \delta = 3$$

which are exactly the same exponents that the van der Waals theory! predict for the fluid system. The fact that two (or more) dissimilar systems have the same set of critical exponents (at least at the MFT level) is a consequence of a more general phenomenon known as *universality*, which was alluded to in the introduction.

3-   BRAGG-WILLIAMS APPROXIMATION

In this approach, the approximation made will again lead to an effective single spin problem; instead of solving a self-consistency equation, we will minimize the resulting approximate free energy. The appeal of this approach is not any improved result, but a first insight into a very generic form of mean-field free energies.

Bragg and Williams assume that the distribution of spins is random. So, we start by rewriting the Hamiltonian in terms of the number of nearest neighbor bonds with both spins up (N_{++}), both spins down (N_{--}) and one up and one down (N_{+-}). For a hypercubic lattice in d dimensions with $n = 2d$ nearest neighbors, the total number of bonds for N sites is $Nd = Nn/2$ (assuming periodic boundary conditions). We also use N_{+} (N_{-}) be the number of spins for which σ_i is +1 (−1); $N = N_{+} + N_{-}$. Then the Hamiltonian can be expressed exactly as

$$H = -\varepsilon \left[N_{++} + N_{--} - N_{+-} \right] - h \left(N_{+} - N_{-} \right) \tag{1}$$

we have taken $N_{+} > N_{-}$ in the last term.

As magnetization per site $m = \dfrac{(N_{+} - N_{-})}{N}$, m is called **long-range order parameter**, therefore magnetization $M = Nm = (N_{+} - N_{-})$, we can express $N_{\pm}$ in terms of m :

$$\frac{N_{\pm}}{N} = \frac{1}{2}(1 \pm m) \tag{2}$$

The approximation now consists in a *decoupling assumption*: the spin states on different sites are statistically independent, and we have site-independent probabilities for $\sigma = \pm 1$ as

$$p_{\pm} = \frac{N_{\pm}}{N} \tag{3}$$

The number N_{+} / N is a measure of the *long-range order*, as it requires no correlation between nearest neighbors. It only requires that in the entire lattice a fraction N_{+} / N of all the spins are up. If N_{+} / N is known in the neighborhood of a given spin, then the same average value is likely to occur everywhere on the entire lattice.
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Another Look: With μ_{B}, the total magnetic moment is

$$M = \mu_{B} \left(N_{+} - N_{-} \right) \tag{4}$$

Using $N = N_{+} + N_{-}$,

$$\frac{N_{\pm}}{N} = \frac{1}{2}(1 \pm m), \quad m \equiv \frac{M}{N \mu_{B}}, \tag{5}$$

$$U = -\frac{1}{2} n \varepsilon N m^2 - N m \mu_{B} H \tag{6}$$

****

The order parameter m may be magnetization in a ferromagnetic system, the dielectric polarization in a ferroelectric system, the fraction of neighbor A—B bonds to total bonds in an alloy AB, or the fraction of superconducting electrons in a superconductor. In transitions, where the atoms are displaced from their positions in the symmetrical phase, m can be taken as the amount of this displacement.

The number of arrangements of spins over the N sites is given by the number of ways we can pick N_{+} things out of N ,

$$W_{BW} = \binom{N}{N_+} = \frac{N!}{N_+!(N-N_+)!} \tag{7}$$

Someone can use the entropy in the form $S = Nk_B \ln W_{BW}$, or, using the von Neumann expression $S = -k_B \sum p_i \ln p_i$. As the entropy is simply additive for independent subsystems (i.e. individual spins), we have:

$$S = -Nk_B \sum p_i \ln p_i = -Nk_B \left(\frac{N_+}{N} \ln \frac{N_+}{N} + \frac{N_-}{N} \ln \frac{N_-}{N} \right), \quad p_i = \frac{N_i}{N} \tag{8}$$

Under the decoupling assumption, N_{++}; N_{--}; N_{+-} can be traced back to $N_\pm$. There are $Nn/2$ bonds. The probability that both spins are up is p_+^2 due to statistical independence. Then

$$N_{++} = \frac{Nn}{2} p_+^2 = n \frac{N_+^2}{2N}, \quad N_{--} = \frac{Nn}{2} p_-^2 = n \frac{N_-^2}{2N}, \quad N_{+-} = n \frac{N_+ N_-}{N}. \tag{9}$$

The Helmholtz free energy $F(T,H) = U - TS$ where

$$U = \langle E \rangle = -\frac{1}{2} n\varepsilon N \left[\left(\frac{N_+}{N} \right)^2 + \left(\frac{N_-}{N} \right)^2 - 2 \left(\frac{N_+ N_-}{N^2} \right) \right] - \mu_B H (N_+ - N_-)$$

is

$$F(T,H) = -\frac{1}{2} n\varepsilon N m^2 - Nm\mu_B H + Nk_B T \left[-\ln 2 + \frac{1}{2}(1-m)\ln(1-m) + \frac{1}{2}(1+m)\ln(1+m) \right] \tag{10}$$

The dependence on T is implicit in m. Passing to the intensive Helmholtz free energy per site $f = F/N$, we now determine m by minimizing f, setting $\frac{\partial f}{\partial m} = 0$. The result is

$$-n\varepsilon m - \mu_B H + k_B T \left[-\frac{1}{2}\ln(1-m) + \frac{1}{2}\ln(1+m) + \frac{1}{2} \right] = 0$$

$$\Rightarrow \quad -n\varepsilon m - \mu_B H + \frac{1}{2} k_B T \ln \left[\frac{(1+m)}{(1-m)} \right] = 0 \tag{11}$$

This looks new, but isn't, because $\tanh^{-1} m = \frac{1}{2} \ln \left[\frac{(1+m)}{(1-m)} \right]$. Hence, we recover $m = \tanh[\beta(n\varepsilon m + \mu_B H)]$, and the same predictions for T_c and $m(T)$. The advantage of this approach is that we get an idea of the form of the free energy expressed in the order parameter m.

Let us focus on the field-free case $H = 0$. Then

$$f(T,0) = -\frac{n\varepsilon}{2} m^2 + \frac{1}{2} k_B T \left[-2\ln 2 + (1-m)\ln(1-m) + (1+m)\ln(1+m) \right] \tag{12}$$

Expanding the logarithm up to fourth order,

$$\ln(1 \pm x) \simeq \pm x - \frac{x^2}{2} \pm \frac{x^3}{3} - \frac{x^4}{4},$$

we find that

$$f(T,0) = -k_B T \ln 2 + \frac{1}{2}(k_B T - n\varepsilon)m^2 + \frac{1}{12} k_B T m^4 + O(m^6) \tag{13}$$

Looking at the structure of the expansion of the logarithm, one sees that there are only even powers of m present. This is as it should be, as the Hamiltonian is invariant under reflection $\sigma_i \to -\sigma_i$, hence the sign of m

may not appear. One can also see from the prefactors of the powers of m in the expansion that all higher orders m^6, m^8, etc. will have *positive* prefactors.

Using a more generic form and recognizing that $\frac{1}{2}(k_B T - n\varepsilon) = \frac{k_B}{2}(T - T_c)$, we have

$$f(T,0) = a(T) + \frac{b(T)}{2}m^2 + \frac{c(T)}{4}m^4 + O(m^6) \tag{14}$$

where

- $a(T)$ is an irrelevant constant

- $b(T) \equiv \begin{cases} > 0 & T > T_c \\ < 0 & T < T_c \end{cases} \Rightarrow$ a sign change occurs at $T = T_c$
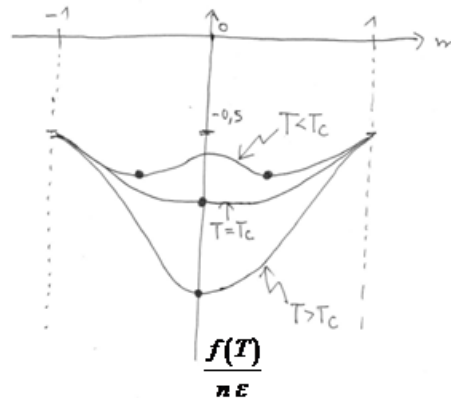

Figure A: Helmholtz free energy g from Eq. (13) as a function of m ($|m| \leq 1$) for temperatures above, at and below the critical temperature. Dots indicate the magnetization that minimizes energy. At $T = T_c$, at the minimum the second (and third) derivative(s) vanish too, making the energy curve very flat.

- $b(T)$ is linear in $(T - T_c)$
- $c(T) > 0$

We encountered this form in the framework of Landau's theory of phase transitions, where it emerged as the minimum instance of the description of a continuous phase transition. The prefactors are for later convenience. Fig. A shows f above, at and below T_c. For symmetry reasons, $f(m) = f(-m)$. The shape depends on the sign of $b(T)$: above T_c it is positive, so there is a global minimum at $m = 0$. For $T < T_c$ it is negative, such that a double-well structure emerges, where the minima sit at finite magnetization.

The exponent α, which describes the temperature dependence of the specific heat at zero-field, follows from differentiating the free energy twice. In either case (C_h or C_m), we have, for $T > T_c$, where $m = 0$,

$$F = -NkT \ln(2)$$

so

$$C_h = -T \left(\frac{\partial^2 F}{\partial T^2} \right) = 0$$

from which is it clear that $\alpha = 0$. For $T < T_c$, C_h approaches a different value as $T \to T_c$, however, the dependence on $|T - T_c|$ is the same, so that $\Rightarrow$ $\alpha = 0$ is still obtained.

$$\ln \frac{1+m}{1-m} = 2x, \quad x \equiv \frac{n\varepsilon m + \mu_B H}{k_B T} = \beta(n\varepsilon m + \mu_B H) \tag{11}$$

It gives the well-known result of the Weiss theory,

$$m \equiv \frac{M}{N\mu_B} = \frac{e^{2x} - 1}{e^{2x} + 1} = \tanh x \tag{12}$$

For $H = 0$, the spontaneous magnetic moment is

$$M_s = N\mu_B \tanh \frac{n\varepsilon M_s}{N\mu_B k_B T},$$

$$m_s = \tanh\left(\frac{T_c m_s}{T} \right), \quad T_c \equiv \frac{n\varepsilon}{k_B}, \quad m_s = \frac{M_s}{N\mu_B} \tag{13}$$

where T_c is the Curie temperature (phase transition points of the second kind). We can solve (13) graphically (Fig. 1 a) to obtain m_s as a function of T in the BW approximation (Fig. lb). For this, plot the right and left sides separately as functions m_s. The intercepts of the two curves give the value of m at the temperature of interest. Clearly the solution is such that $m_s = 0$ for $T_c/T < 1$ and $m_s = m, 0, -m$, for $T_c/T > 1$. In the latter case the root $m_s = 0$ is not acceptable because it corresponds to a maximum of F, instead of minimum. Thus, $m_s = 0$ for $T > T_c$ and $\pm m$ for $T < T_c$, where m is the root of (13) that is greater than zero. The degeneracy $m_s = \pm m$ occurs because for $H = 0$ there is no intrinsic difference between 'up' and 'down'. This degeneracy does not affect F as it is an even function of m (for example take $m = 1$ or -1 in Eq. 10). In general, m is obtained numerically to yield Fig. l b.
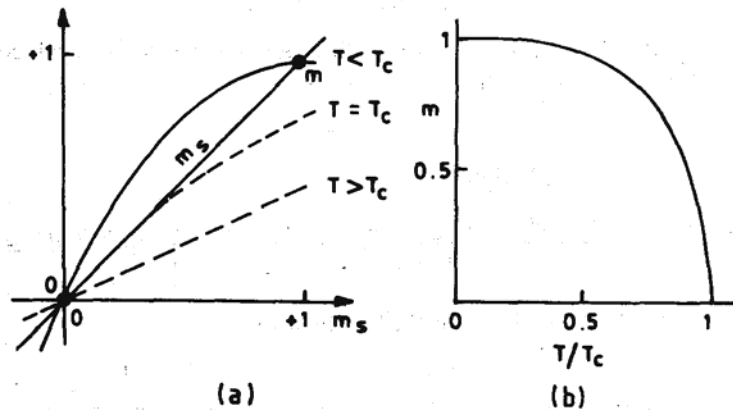

(a)   (b)

Fig. 1 (a) Graphical solution $m_s = \tanh\left(T_c m_s / T\right)$. The intersection point m moves up to $m_s = 1$ as $T \to 0$. All the magnetic moments are lined up at $T = 0$. (b) The spontaneous magnetic moment in the Bragg-Williams approximation. The order parameter m varies smoothly in a second-order phase transition.

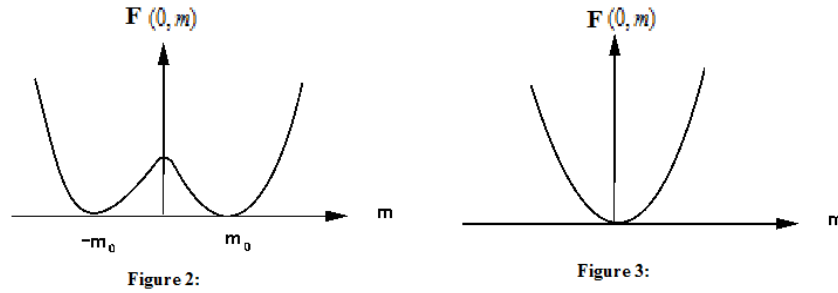Allowing $h \to 0$, one finds a transcendental equation for m

$$m = \tanh(\beta m \varepsilon)$$

which can be solved graphically as we mentioned earlier.

To see the physical meaning of the various cases, consider expanding the free energy about $m = 0$ at zero-field $\left(h = 0\right)$. The expansion gives

$$F(0, m) = \text{ constant} + \varepsilon(1 - \beta \varepsilon)m^2 + c\, m^4$$

where c is a (possibly temperature dependent) constant with $c > 0$. For $\beta \varepsilon > 1$, the sign of the quadratic term is negative and the free energy as a function of m looks like figure (2). Thus, there are two stable minima at $\pm m_0$, corresponding to the two possible states of magnetization. Since a large portion of the spins will be aligned below the critical temperature, the magnetic phase is called an *ordered phase*. For $\beta \varepsilon > 1$, the sign of the quadratic term is positive and the free energy plot looks like figure (3) i.e., a single minimum function at $m = 0$, indicating no net magnetization above the critical temperature at $h = 0$.

Figure 2:   Figure 3:

The exponent β (*this for the scaling of the magnetization $m \sim |t|^{\beta}$*) can be obtained directly from this expression for the free energy. For $T < T_c$, the value of the magnetization is given by:

$$\left.\frac{\partial F}{\partial m}\right|_{m=m_o} = 0$$

which gives

$$\frac{2\varepsilon}{T}\left(T - T_c\right)m_o + 4cm_o^3 = 0$$

$$m_o \sim \left(T_c - T\right)^{1/2} \qquad \Rightarrow \quad \beta = 1/2.$$

where we used in the parenthesis the critical value, $kT_c = n\varepsilon$. The third roots, $m = 0$, is unstable in case $T < T_c$.

From the equation for the magnetization at nonzero field, the exponent δ is obtained as follows:

$$m = \tanh\left\{\beta\left(\varepsilon m + h\right)\right\} \quad \Rightarrow \quad \beta\left(\varepsilon m + h\right) = \tanh^{-1}(m) = m + \frac{m^3}{3} + \cdots$$

where we used the expansion of the inverse hyperbolic tangent about $m = 0$. Rearrange, we have:

$$h = kT\left(m + \frac{m^3}{3} + \cdots\right) - \varepsilon m = \left(kT - \varepsilon\right)m + \frac{kT}{3}m^3 = mk(T - T_c) + \frac{kT}{3}m^3$$

Here, we used the critical value, $kT_c = \varepsilon$, in the third line. At the critical temperature, this becomes

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$$h \sim m^3 \quad \Rightarrow \quad \delta = 3.$$

Compared with the equation $H \sim m^\delta$. **Note that**: At $h = 0$, one finds ($mk(T - T_c) + \dfrac{kT}{3}m^3 = 0$):

$$m^2 = \begin{cases} 0 & T > T_c \\ \dfrac{3}{T}(T_c - T) & T < T_c \end{cases} \quad \Rightarrow \quad m \approx (T_c - T)^{1/2} \qquad T < T_c$$

The exponent α, which describes the temperature dependence of the specific heat at zero-field, follows from differentiating the free energy twice. In either case (C_h or C_m), we have, for $T > T_c$, where $m = 0$,

$$F = -NkT \ln(2)$$

so

$$C_h = -T\left(\frac{\partial^2 F}{\partial T^2}\right) = 0$$

from which is it clear that $\alpha = 0$. For $T < T_c$, C_h approaches a different value as $T \to T_c$, however, the dependence on $\left|T - T_c\right|$ is the same, so that $\Rightarrow \quad \alpha = 0$ is still obtained.

Finally, the susceptibility, which is given by

$$\chi = \frac{\partial m}{\partial h} = \frac{1}{\partial h / \partial m}$$

but, near $m = 0$,

$$h = mk(T - T_c) + \frac{kT}{3}m^3$$

$$\frac{\partial h}{\partial m} = k(T - T_c) + kTm^2$$

$$\chi = \frac{1}{k_B(T - T_c) + k_B Tm^2} \sim \begin{cases} \chi_- = \chi = (t \to 0^+) = \dfrac{1}{k_B(T - T_c)} \sim (T - T_c)^{-1} & T > T_c \\[4mm] \chi_+ = \chi(t \to 0^-) = \dfrac{1}{k_B(T - T_c) + k_B T \dfrac{3}{T}(T_c - T)} \sim \dfrac{1}{2}(T_c - T)^{-1} & T < T_c \end{cases}$$

As the critical temperature is approached, $m \to 0_+ = 0$ and

$$\chi_+ \sim \left|T - T_c\right|^{-1}$$
$$\Rightarrow \quad \gamma = 1.$$

The MFT exponents for the Ising model are, therefore

$$\alpha = 0, \quad \beta = 1/2, \quad \gamma = 1, \quad \delta = 3$$

which are exactly the same exponents that the van der Waals theory predict for the fluid system. The fact that two (or more) dissimilar systems have the same set of critical exponents (at least at the MFT level) is a consequence of a more general phenomenon known as *universality*, which was alluded to in the introduction.

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4-   Mean field theory and the calculation of magnetic exponents

The calculation of critical exponents is nontrivial, even for simple models such as the Ising model. Here, we will introduce an approximate technique known as *mean field theory*. The approximation that is made in the mean field theory (MFT) is that fluctuations can be neglected. Clearly, this is a severe approximation, the consequences of which we will see in the final results.
Consider the Hamiltonian for the Ising model:

$$H = -\frac{1}{2}\sum_{\langle i,j \rangle} \varepsilon_{ij}\sigma_i\sigma_j - h\sum_i \sigma_i$$

where $\langle i,j \rangle$ indicates restriction of the sum to nearest neighbor pairs only. The variables σ_i can take on the values ± 1 only. The ε_{ij} represent the spin-spin couplings and h describes a uniaxial ferromagnetic system in external magnetic field. The parameters T and h are experimental control parameters.

The partition function is given by

$$Z(N,h,T) = \sum_{\sigma_1}\sum_{\sigma_2}\cdots\sum_{\sigma_N} e^{-\beta H} = \sum_{\sigma_1}\sum_{\sigma_2}\cdots\sum_{\sigma_N} e^{\beta\left[\frac{1}{2}\sum_{\langle i,j \rangle}^{N}\varepsilon_{ij}\sigma_i\sigma_j - h\sum_{i=0}^{N}\sigma_i\right]}$$

This sum is nontrivial to carry out.
In the MFT approximation, one introduces the magnetization

$$m = \langle \sigma_i \rangle = \frac{1}{N}\left\langle \sum_{i=0}^{N}\sigma_i \right\rangle$$

explicitly into the partition function by using the identity

$$\sigma_i\sigma_j = (\sigma_i - m + m)(\sigma_j - m + m) = m^2 + m(\sigma_i - m) + m(\sigma_j - m) + (\sigma_i - m)(\sigma_j - m)$$

The last term is quadratic in the spins and is of the form $(\sigma_i - \langle\sigma_i\rangle)(\sigma_j - \langle\sigma_j\rangle)$, the average of which measures the spin fluctuations. Thus, this term is neglected in the MFT. If this term is dropped, then

$$\sigma_i\sigma_j \approx m^2 + m(\sigma_i + \sigma_j) - 2m^2 = -m^2 + m(\sigma_i + \sigma_j)$$

and the spin-spin interaction term in the Hamiltonian becomes:

$$\frac{1}{2}\sum_{\langle i,j \rangle}^{N}\varepsilon_{ij}\sigma_i\sigma_j = \frac{1}{2}\sum_{\langle i,j \rangle}^{N}\varepsilon_{ij}\left[-m^2 + m(\sigma_i + \sigma_j)\right]$$

We will restrict ourselves to isotropic magnetic systems, for which $\sum_j \varepsilon_{ij}$ is independent of i (all sites are equivalent). Define

$$\sum_j \varepsilon_{ij} = n\varepsilon,$$

where n is the number of nearest neighbors of each spin. This number will depend on the number of spatial dimensions. Since this dependence on spatial dimension is a trivial one, we can absorb the n factor into the coupling constant and redefine. $\varepsilon \equiv n\varepsilon = kT_c$ Then,

$$\frac{1}{2}\sum_i \varepsilon = \frac{1}{2}N\varepsilon$$

where N is the total number of spins. Finally,

$$\frac{1}{2}\sum_{\langle i,j \rangle}^{N} \varepsilon_{ij}\left[m\left(\sigma_i + \sigma_j\right)\right] = \varepsilon m \sum_i \sigma_i$$

and the Hamiltonian now takes the form

$$\frac{1}{2}\sum_{\langle i,j \rangle}^{N} \varepsilon_{ij}\sigma_i\sigma_j + h\sum_i \sigma_i \rightarrow -\frac{1}{2}N\varepsilon m^2 + (\varepsilon m + h)\sum_i \sigma_i$$

and the partition function becomes

$$Z(N,h,T) = e^{-\frac{1}{2}\beta N\varepsilon m^2}\sum_{\sigma_1}\sum_{\sigma_2}\cdots\sum_{\sigma_N} e^{-\beta(\varepsilon m+h)\sum_i \sigma_i} = e^{-\frac{1}{2}\beta N\varepsilon m^2}\left(\sum_{\sigma=\pm 1} e^{-\beta(\varepsilon m+h)\sigma}\right)^N$$

$$= e^{-\frac{1}{2}\beta N\varepsilon m^2}\left[2\cosh\left\{\beta\left(\varepsilon m+h\right)\right\}\right]^N$$

The free energy per spin $g(h,t) = G(h,t)/N$ is then given by

$$g(h,t) = -\frac{1}{N\beta}\ln\left[Z(N,h,T)\right] = \frac{1}{2}\varepsilon m^2 - \frac{1}{\beta}\ln\left[2\cosh\left\{\beta\left(\varepsilon m+h\right)\right\}\right]$$

The magnetization per spin can be computed from

$$m = -\left(\frac{\partial g}{\partial h}\right)_h = \tanh\left\{\beta\left(\varepsilon m+h\right)\right\}$$

Allowing $h \rightarrow 0$, one finds a transcendental equation for m

$$m = \tanh(\beta m \varepsilon)$$

which can be solved graphically as we mentioned earlier.

To see the physical meaning of the various cases, consider expanding the free energy about $m = 0$ at zero-field $(h = 0)$. The expansion gives

$$g(0,m) = \text{constant} + \varepsilon(1 - \beta\varepsilon)m^2 + c\,m^4$$

where c is a (possibly temperature dependent) constant with $c > 0$. For $\beta\varepsilon > 1$, the sign of the quadratic term is negative and the free energy as a function of m looks like figure (2). Thus, there are two stable minima at $\pm m_0$, corresponding to the two possible states of magnetization. Since a large portion of the spins will be aligned below the critical temperature, the magnetic phase is called an *ordered phase*. For $\beta\varepsilon > 1$, the sign of the quadratic term is positive and the free energy plot looks like figure (3) i.e., a single minimum function at $m = 0$, indicating no net magnetization above the critical temperature at $h = 0$.
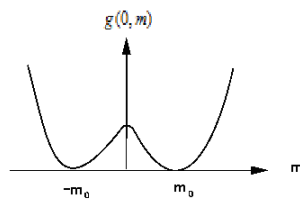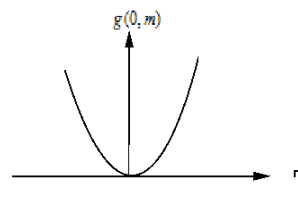

Figure 2:   Figure 3:

The exponent β (*this for the scaling of the magnetization* $m \sim |t|^{\beta}$) can be obtained directly from this expression for the free energy. For $T < T_c$, the value of the magnetization is given by:

$$\left.\frac{\partial g}{\partial m}\right|_{m=m_o} = 0$$

which gives

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$$\frac{2\varepsilon}{T}(T-T_c)m_o + 4cm_o^3 = 0$$

$$m_o \sim (T_c - T)^{1/2} \qquad \Rightarrow \quad \beta = 1/2 .$$

where we used in the parenthesis the critical value, $kT_c = \varepsilon$. The third roots, $m = 0$, is unstable in case $T < T_c$.

From the equation for the magnetization at nonzero field, the exponent δ is obtained as follows:

$$m = \tanh\{\beta(\varepsilon m + h)\} \quad \Rightarrow \quad \beta(\varepsilon m + h) = \tanh^{-1}(m) = m + \frac{m^3}{3} + \cdots$$

where we used the expansion of the inverse hyperbolic tangent about $m = 0$. Rearrange, we have:

$$h = kT\left(m + \frac{m^3}{3} + \cdots\right) - \varepsilon m = (kT - \varepsilon)m + \frac{kT}{3}m^3 = mk(T - T_c) + \frac{kT}{3}m^3$$

Here, we used the critical value, $kT_c = \varepsilon$, in the third line. At the critical temperature, this becomes

$$h \sim m^3 \quad \Rightarrow \quad \delta = 3 .$$

Compared with the equation $H \sim m^\delta$. **Note that**: At $h = 0$, one finds ($mk(T - T_c) + \frac{kT}{3}m^3 = 0$):

$$m^2 = \begin{cases} 0 & T > T_c \\ \dfrac{3}{T}(T_c - T) & T < T_c \end{cases}$$

The exponent α, which describes the temperature dependence of the specific heat at zero-field, follows from differentiating the free energy twice. In either case (C_h or C_m), we have, for $T > T_c$, where $m = 0$,

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$$\frac{\partial h}{\partial m} = k(T - T_c) + kTm^2$$

$$\chi = \frac{1}{k(T - T_c) + kTm^2} \sim \begin{cases} \chi(t \to 0^+) = \dfrac{1}{k(T - T_c)} \sim (T - T_c)^{-1} & T > T_c \\[4mm] \chi(t \to 0^-) = \dfrac{1}{k(T - T_c) + kT\dfrac{3}{T}(T_c - T)} \sim \frac{1}{2}(T_c - T)^{-1} & T < T_c \end{cases}$$

As the critical temperature is approached, $m \to 0_+ = 0$ and

$$\chi_+ \sim \left| T - T_c \right|^{-1}$$
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The MFT exponents for the Ising model are, therefore

$$\alpha = 0, \quad \beta = 1/2, \quad \gamma = 1, \quad \delta = 3$$

which are exactly the same exponents that the van der Waals theory predict for the fluid system. The fact that two (or more) dissimilar systems have the same set of critical exponents (at least at the MFT level) is a consequence of a more general phenomenon known as *universality*, which was alluded to in the introduction.

H.W. Prove that: $\chi_+ \sim \dfrac{1}{2} \left| T - T_c \right|^{-1}$

The Mean Field Approximation (Schroeder page 343)

This is a very crude approximation, which can be used to "solve" the Ising model in any dimensionality. This approximation won't be very accurate, but it does give some qualitative insight into what's happening and why the dimensionality matters. Let's concentrate on just a single dipole, somewhere in the middle of the lattice and label it "i" (see Figure 1), so its alignment is s_i which:

$$s_i = \begin{cases} +1 & \text{when the dipole is pointing up} \\ -1 & \text{when the dipole is pointing down} \end{cases}.$$

Let n be the number of nearest neighbors that this dipole has.

Figure 1. The four neighbors of this particular dipole have an average $\overline{s}$ value of $\frac{(1-3)}{4} = -\frac{1}{2}$. If the central

dipole points up, the energy due to its interactions with its neighbors is $n\overline{s} = +2\varepsilon$, while if it points down, the energy is -2ε.
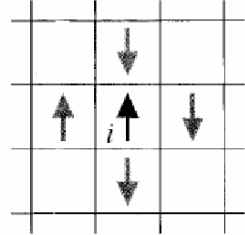
Imagine that the alignments of these neighboring dipoles are temporarily frozen, but that our dipole "i" is free to point up or down. If it points up, then the interaction energy between this dipole and its neighbors is

$$E_\uparrow = -\epsilon \sum_{\text{neighbors}} s_{\text{neighbor}} = -\epsilon n \overline{s}, \tag{8.46}$$

where $\overline{s}$ is the *average* alignment of the neighbors and "ε" is a positive quantity represents the dipole-dipole interaction. Similarly, if dipole i points down, then the interaction energy is

$$E_\downarrow = +\epsilon n \overline{s}. \tag{8.47}$$

The partition function for just this dipole is therefore ($Z_i = \sum_i e^{-\beta E_i}$)

$$Z_i = e^{\beta \epsilon n \overline{s}} + e^{-\beta \epsilon n \overline{s}} = 2\cosh(\beta \epsilon n \overline{s}), \tag{8.48}$$

and the average expected value of its spin alignment is ($\overline{s}_i = \frac{1}{Z_i}\sum_i s_i e^{-\beta E_i}$)

$$\overline{s}_i = \frac{1}{Z_i}\left[(1)e^{\beta \epsilon n \overline{s}} + (-1)e^{-\beta \epsilon n \overline{s}}\right] = \frac{2\sinh(\beta \epsilon n \overline{s})}{2\cosh(\beta \epsilon n \overline{s})} = \tanh(\beta \epsilon n \overline{s}). \tag{8.49}$$

Now look at both sides of this equation (8.49). On the left is $\overline{s}_i$, the thermal average value of the alignment of any typical dipole (except those on the edge of the lattice, which we'll neglect). On the right is $\overline{s}$, the average of the actual instantaneous alignments of this dipole's n neighbors. The idea of the mean field approximation is to assume (or pretend) that these two quantities are the same: $\overline{s}_i = \overline{s}$. In other words, we assume that at every moment, the alignments of all the dipoles are such that every neighborhood is "typical"- there are no fluctuations that cause the magnetization in any neighborhood to be more or less than the expected thermal average. (This approximation is similar to the one that used to derive the Van der Waals equation. There it was the density, rather than the spin alignment, whose average value was not allowed to vary from place to place within the system.)

In the mean field approximation $\left(\text{when } \overline{s}_i \to \overline{s}\right)$, then, we have the relation

$$\overline{s} = \tanh(\beta \epsilon n \overline{s}), \tag{8.50}$$

where $\overline{s}$ is now the average dipole alignment over the entire system. This is a transcendental equation, so we can't just solve for $\overline{s}$ in terms of $\beta \varepsilon n$.

The best approach is to plot both sides of the equation and look for a graphical solution (see Figure 2). Notice that the larger the value of $\beta\varepsilon n$, the steeper the slope of the hyperbolic tangent function near $\bar{s}=0$. This means that our equation can have either one solution or three, depending on the value of $\beta\varepsilon n$.
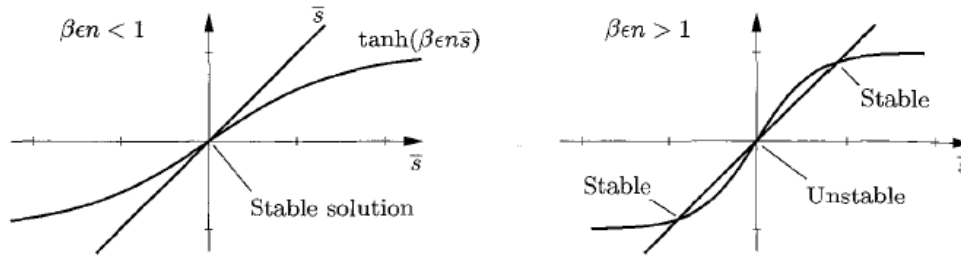

Figure 2. Graphical solution of equation 8.50. The slope of the tanh function at the origin is $\beta\varepsilon n$. When this quantity is less than 1, there is only one solution, at $\bar{s}=0$; when this quantity is greater than 1, the $\bar{s}=0$ solution is unstable but there are also two nontrivial stable solutions.

H.W. Write a MATHEMATICA program to plot Figure 2.

When $\beta\varepsilon n < 1$, that is, when $kT > n\varepsilon$ (high temperature), the only solution is at $\bar{s}=0$; there is no net magnetization. If a thermal fluctuation were to momentarily increase the value of $\bar{s}$, then the hyperbolic tangent function, which dictates what $\bar{s}$ *should* be, would be less than the current value of $\bar{s}$, so $\bar{s}$ would tend to decrease back to zero. The solution $\bar{s}=0$ is stable.

When $\beta\varepsilon n > 1$, that is, when $kT < n\varepsilon$ (low temperature), we still have a solution at $\bar{s}=0$ and we also have two more solutions, at positive and negative values of $\bar{s}$. But *the solution at $\bar{s}=0$ is unstable*: A small positive fluctuation of $\bar{s}$ would cause the hyperbolic tangent function to exceed the current value of $\bar{s}$, driving $\bar{s}$ to even higher values. The stable solutions are the other two, which are symmetrically located because the system has no inherent tendency toward positive or negative magnetization. Thus, the system will acquire a net nonzero magnetization, which is equally likely to be positive or negative. When a system has a built-in symmetry such as this, yet must choose one state or another at low temperatures, we say that the symmetry is **spontaneously broken**.

The critical temperature T_c below which the system becomes magnetized is

$$\beta_c n\varepsilon = 1 \quad \Rightarrow \quad kT_c = n\varepsilon \tag{8.51}$$

proportional to both the neighbor-neighbor interaction energy and to the number of neighbors. This result is no surprise: The more neighbors each dipole has, the greater the tendency of the whole system to magnetize. Notice, though, that even a one-dimensional Ising model should magnetize below a temperature of $2\varepsilon/k$, according to this analysis. Yet we already saw from the exact solution that there is no abrupt transition in the behavior of a one-dimensional Ising model; it magnetizes only as the temperature goes to zero. Apparently, the mean field approximation is no good at all in one dimension. * Fortunately, the accuracy improves as the dimensionality increases.

*There do exist more complicated versions of the mean field approximation that lack this fatal flaw, predicting correctly that the one-dimensional Ising model magnetizes only at $T = 0$. See, for example, Pathria (1996).

An *order parameter* is defined as follows:

Suppose the Hamiltonian H_o of a system is invariant under all the transformations of a group G. If two phases can be distinguished by the appearance of a thermodynamic average $\langle \phi \rangle$, which is not invariant under G, then $\langle \phi \rangle$ is an *order parameter* for the system.

The Ising system, for which H_o is given by

$$H_o = -\frac{1}{2}\left\langle \sum_{\langle i,j \rangle} J_{ij} \sigma_i \right\rangle$$

is invariant under the group Z_2, which is the group that contains only two elements, an identity element and a spin reflection transformation: $Z_2 = 1, -1$. Thus, under Z_2, the spins transform as

$$\sigma_i \to \sigma_i \qquad \sigma_i \to -\sigma_i$$

From the form of H_o it can be seen that $H_o \to H_o$ under both transformations of Z_2, so that it is invariant under Z_2. However, the magnetization

$$m = \frac{1}{N}\left\langle \sum_{i=0}^{N} \sigma_i \right\rangle$$

is not invariant under a spin reflection for $T < T_c$, when the system is magnetized. In a completely ordered state, with all spins aligned, under a spin reflection $m \to -m$. Thus, m is an order parameter for the Ising model, and, since it is a scalar quantity, its dimension is 1.

Thus, the Ising model defines a universality class known as the *Ising universality class*, characterized by d=3, n=1 in three dimensions. Note that the fluid system, which has the same MFT critical exponents as the Ising system, belongs to the same universality class. The order parameter for this system, by the analogy table defined in the last lecture, is the volume difference between the gas and the liquid phases, $V_L - V_G$, or equivalently, the density difference, $\rho_L - \rho_G$. Although the solid phase is the truly ordered phase, while the gas phase is disordered, the liquid phase is somewhere in between, i.e., it is a *partially* ordered phase. The Hamiltonian of a fluid is invariant under rotations of the coordinate system. Ordered and partially ordered phases break this symmetry. Note also that a true magnetic system, in which the spins can point in any spatial direction, need an order parameter that is the vector generalization of the magnetization:

$$m = \frac{1}{N}\left\langle \sum_{i=0}^{N} \sigma_i \right\rangle$$

Since the dimension of the vector magnetization is 3, the true magnetic system belongs to the d=3, n=3 universality class.