Mean Field Theory & the Ising Model

The key approximation made for the van der Waal's gas was an average over the interaction term. What physics is left out by this averaging? To see the answer, it is useful to examine a different model – the Ising Hamiltonian – in which it is more clear what averaging leaves out.

The Ising model appears superficially as a highly simplified model for magnetically ordered materials. It can be used for this, but in fact it serves as a useful model for many systems with the great utility that it is relatively easy to make calculations with. Example systems studied with Ising models include

- magnetically ordered spins
- polymer chains
- compositional alloys
- ferroelectrics
- lattice gases (fermion)
- forest fire & disease spreading
- neural networks

The Ising model hamiltonian is simple:

$$\hat{H} = -\sum_{ij} J_{ij} \hat{S}_{z\,i} \hat{S}_{z\,j}$$

describes a lattice of spins at sites $\{i\}$. The spins interact via a pairwise energy with strength J_{ij}.

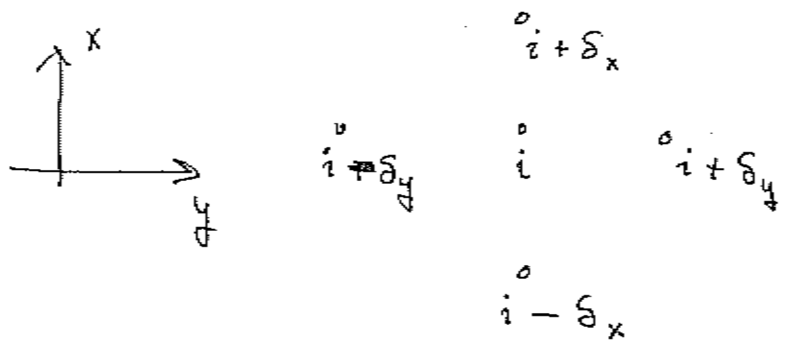
A simple version can be realized with spin $1/2$ particles aligned along the z direction. It is useful to add a magnetic field term in order to examine the case of $J=0$ which reduces to a non-interacting paramagnet model. We then have

field energy $B\mu_B = h$

$$\hat{H} = -J\sum_{\langle i,j\rangle}\hat{\sigma}_{zi}\hat{\sigma}_{zj} - h\sum_i \hat{\sigma}_{zi}$$

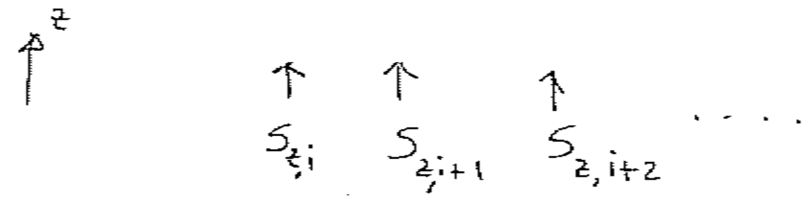
where $\hat{\sigma}_{zi}|\pm\rangle = \pm|\pm\rangle$ and a further simplification has been imposed in the form of $J_{ij}=0$ unless $j=i+\delta$ where δ connects only to neighbouring sites.

On a two dimensional lattice, for example,



The notation $\langle i,j\rangle$ indicates that the sum includes only nearest neighbours, regardless of the geometry.

If $J>0$, then the total energy is lowest for parallel alignment of spins (S_z components).



We allow the collection of spins to be in contact with a heat bath. An excited state would cost energy $\propto J$. An example is

$$\uparrow \uparrow \downarrow \uparrow \uparrow \uparrow \downarrow \downarrow \uparrow \uparrow$$

and so perfect parallel alignment corresponds to the $J>0$ ground state. This is only realized for $T=0$.

If $T \to \infty$, entropy dominates and one arrives at a nearly completely not-parallel state. The average $\langle \sigma_z \rangle$ for $T \to \infty$ must be zero. We define a magnetization m as

$$m = \langle \sigma_z \rangle$$

which is maximum (1) for $T=0$, and zero for $T \to \infty$.

Now consider the hamiltonian for a single spin. For simplicity, locate the spin at $i=0$. Then

$$\hat{H}_0 = -J \sum_{\langle 0j \rangle} \hat{\sigma}_{z0} \hat{\sigma}_{zj} - h \hat{\sigma}_{z0}$$

Call $z \equiv$ # nearest neighbours, and suppose a lattice that is periodic so that z is the same for all spins. Then

$$\hat{H}_0 = -J \sum_{\langle 0,j \rangle} \hat{\sigma}_{z0} \hat{\sigma}_{zj} - h \hat{\sigma}_{z0}$$

can be written as

$$\hat{H}_0 = -J \sum_{\langle 0,j\rangle} \hat{\sigma}_{z0}(\hat{\sigma}_{zj} - m) - J \sum_{\langle 0,j\rangle} \hat{\sigma}_{z0}\, m - h\,\hat{\sigma}_{z0}$$

$$= -J \sum_{\langle 0,j\rangle} \hat{\sigma}_{z0}(\hat{\sigma}_{zj} - m) - zJ\hat{\sigma}_{z0}\, m - h\,\hat{\sigma}_{z0}$$

$$= -J \sum_{\langle 0,j\rangle} \hat{\sigma}_{z0}(\hat{\sigma}_{zj} - m) - \hat{\sigma}_{z0}(zJm + h)$$

The first term represents energy <u>fluctuations</u> due to interactions with spins that do not equal m. The second term represents the interaction of $\hat{\sigma}_{z0}$ with the <u>average</u> m.

Keeping only the second term, and neglecting the first is called the "mean field approximation". The form of the interaction of S_{0z} with the average $m = \langle \sigma_z \rangle$ is of the form of S_{0z} in an "effective" magnetic field:

$$h_{eff} = h + zJm$$

so the mean field hamiltonian is

$$\hat{H}_{M.F.} = -\, h_{eff}\, \hat{\sigma}_{z,0}$$

The canonical density matrix is

$$\hat{\rho}_{M.F.} = \frac{e^{+\beta h_{eff} \hat{\sigma}_{z,0}}}{\mathrm{Tr}\left(e^{-\beta h_{eff} \hat{\sigma}_{z0}}\right)}$$

The average $\langle \sigma_{z0} \rangle$ is then

$$\langle \sigma_{z0} \rangle = \langle \hat{\rho}\, \hat{\sigma}_{z0} \rangle = \frac{e^{+\beta h_{eff}} - e^{-\beta h_{eff}}}{e^{\beta h_{eff}} + e^{-\beta h_{eff}}}$$

since

$$\langle + | e^{\beta h_{eff} \hat{\sigma}_{z0}} | + \rangle = e^{\beta h_{eff}}$$

$$\langle - | e^{\beta h_{eff} \hat{\sigma}_{z0}} | - \rangle = e^{-\beta h_{eff}} .$$

We can therefore write

$$m = \tanh(\beta h_{eff}) = \tanh(\beta(h + zJm))$$

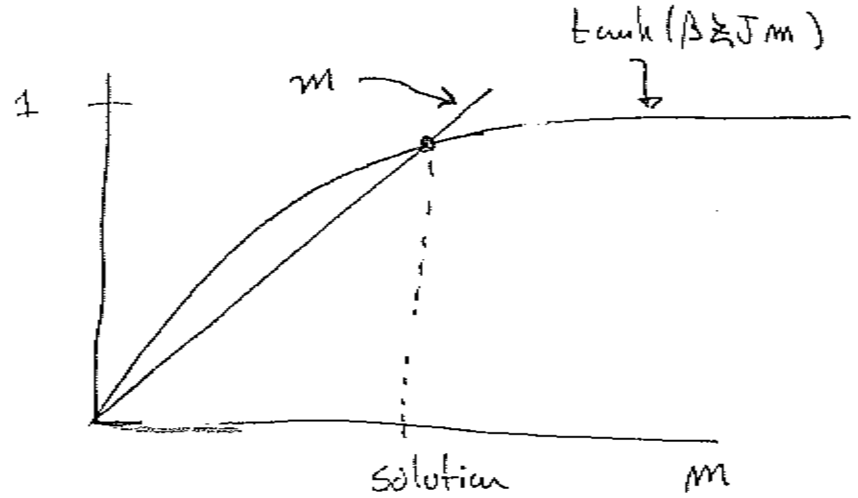
In the limit $J = 0$, $m = \tanh(\beta h)$ which is the result for non interacting spins in a field $h = \mu_B B$.

The case $J \neq 0$ is still not solved since (set $h = 0$ now)

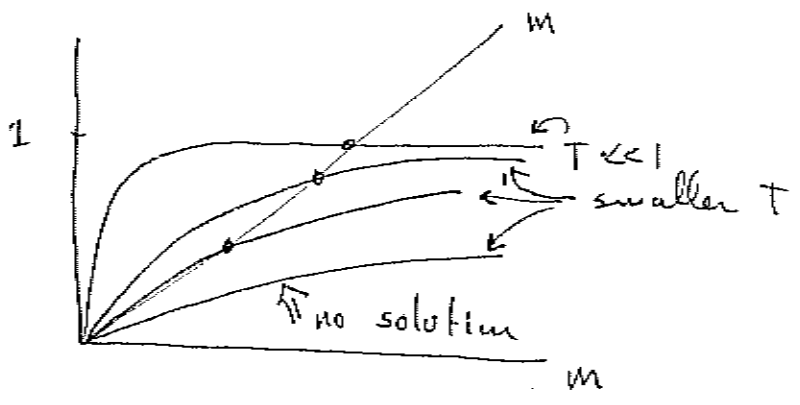
$$m = \tanh(\beta z J m)$$

does not give m explicitly. We can solve this numerically, but can also get some insight using a graphical argument.

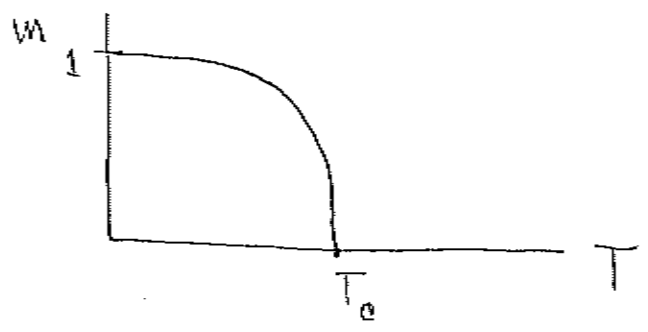
We can plot $\tanh(\beta J Z m)$ vs m together with m vs m. A solution exists wherever the two curves cross:



We find that solutions exist only for a range of temperatures below some cut-off T_c:



The solutions can be plotted against T as



As in the van der Waal's gas, a critical temperature exists where a phase transition occurs.

We can summarize the main points of mean field theory as follows. Interactions between particles can produce phases characterized by some average value of a parameter describing the phase. For the Ising model this parameter is $m = \langle \sigma_z \rangle$. The mean field approximation replaces the actual pair wise interactions with an average effective interaction. This approximation ignores local fluctuations of spins away from the average m value.

Free Energy

We have calculated $\langle \sigma_z \rangle$ using a density matrix for a single spin at site 0. This is justified as representing any spin since we assume that with parallel ferromagnetic order, all spins are equivalent.

We can be a bit more careful and and come up with the N spin $\hat{\rho}_{M.F.}$ by writing

$$\hat{\sigma}_{zi}\hat{\sigma}_{zj} = (m + \hat{\sigma}_{zi} - m)(m + \hat{\sigma}_{zj} - m)$$

$$\doteq m^2 + m(\hat{\sigma}_{zj} - m)$$
$$+ (\hat{\sigma}_{zi} - m)m$$
$$+ \underbrace{(\hat{\sigma}_{zi} - m)(\hat{\sigma}_{zj} - m)}_{\text{neglect}}$$

$$\cong m^2 + m(\hat{\sigma}_{zi} + \hat{\sigma}_{zj}) - 2m^2$$

$$= -m^2 + m(\hat{\sigma}_{zi} + \hat{\sigma}_{zj})$$

The mean field hamiltonian for N spins is then

$$\hat{H}_{M.F.} = +m^2 J \sum_{\langle i,j \rangle} - mJ \sum_{\langle i,j \rangle} (\hat{\sigma}_{zi} + \hat{\sigma}_{zj})$$
$$- h \sum_i \hat{\sigma}_{zi}$$

or

$$\hat{H}_{M.F.} = m^2 J z N - 2 z J m \sum_i \hat{\sigma}_{zi} - h \sum_i \hat{\sigma}_{zi}$$

In keeping with tradition, we define a new interaction energy parameter

$$\mathcal{J} = 2 z J$$

so

$$\hat{H}_{M.F.} = \frac{1}{2} N \mathcal{J} m^2 - \sum_i \hat{\sigma}_{zi} (\mathcal{J}m + h)$$

The density matrix is

$$\hat{\rho}_{M.F.} = \frac{e^{-\beta\left[\frac{1}{2} N \mathcal{J} m^2 - \sum_i \hat{\sigma}_{zi} (\mathcal{J}m + h)\right]}}{Z_N}$$

where

$$Z_N = \mathrm{Tr}\left(\exp\left[-\beta\left(\tfrac{1}{2} m^2 \mathcal{J} N - \sum_i \hat{\sigma}_{zi} (\mathcal{J}m + h)\right)\right]\right)$$

$$= e^{-\frac{1}{2}\beta m^2 \mathcal{J} N} \prod_{i=1}^{N} \left(e^{-\beta(\mathcal{J}m+h)} + e^{\beta(\mathcal{J}m+h)}\right)$$

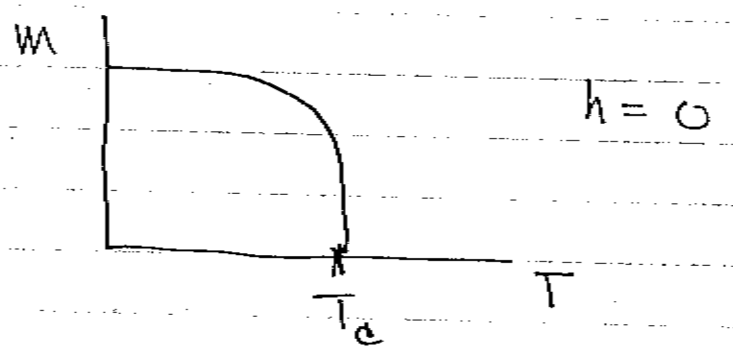
$$= \left[e^{-\frac{1}{2}\beta m^2 \mathcal{J}}\; 2 \cosh\left[\beta(\mathcal{J}m + h)\right]\right]^N$$

The free energy is then

$$F = -\frac{1}{\beta}\ln Z_N$$

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

Insight into the nature of the thermodynamic phase can be had by examining the region near the transition where m is small.



This temperature region is well defined if $h=0$. Setting h to zero, and supposing T is near T_c, we can expand F for small m. The cosh term can be expanded using

$$\ln\cosh x \simeq \frac{1}{2}x^2 - \frac{1}{12}x^4 + O(x^5)$$

Then

$$F \simeq -\frac{N}{\beta}\left\{-\frac{1}{2}m^2\beta J + \ln 2 + \frac{1}{2}m^2 J^2\beta^2 - \frac{1}{12}m^4 J^4\beta^4\right\}$$

or

$$F \simeq -NJ\left\{ -\frac{1}{2} m^2 + \frac{1}{2} m^2 J\beta - \frac{1}{12} m^4 (J\beta)^3 + \frac{\ln 2}{J\beta} \right\}$$

To see the structure, we note that J/k_B has units of temperature, and define

$$k_B T_c = J$$

Then

$$F \simeq -NJ\left\{ + m^2 \frac{1}{2}\left(1 - T_c/T\right) - m^4 \frac{1}{12}\left(\frac{T_c}{T}\right)^3 + \frac{T}{T_c} \ln 2 \right\}$$

Since this is only valid for $T_c - T = \delta \ll T_c$, we expand in terms of δ:

$$\frac{T_c}{T} \simeq 1 + \frac{\delta}{T_c}$$

Neglecting smallest terms (like $m^4 \delta$), then

$$F \simeq -N k_B T_c \left\{ m^2 \frac{1}{2} \frac{\delta}{T_c} - m^4 \frac{1}{12} + \frac{T}{T_c} \ln 2 \right\}$$

$$= -k_B N \left\{ m^2 \frac{1}{2}(T_c - T) - m^4 \frac{T_c}{12} + T \ln 2 \right\}$$

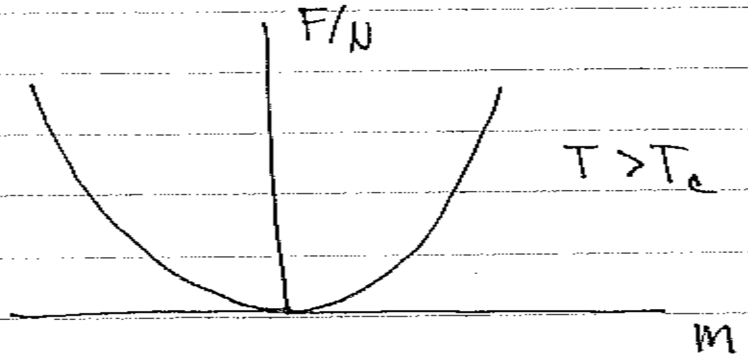
where we've used $\delta = T_c - T$.

The significance of this result is its generality. Near a critical point T_c, the free energy is a polynomial function of the average order parameter (m in our case). The form is (for our case):

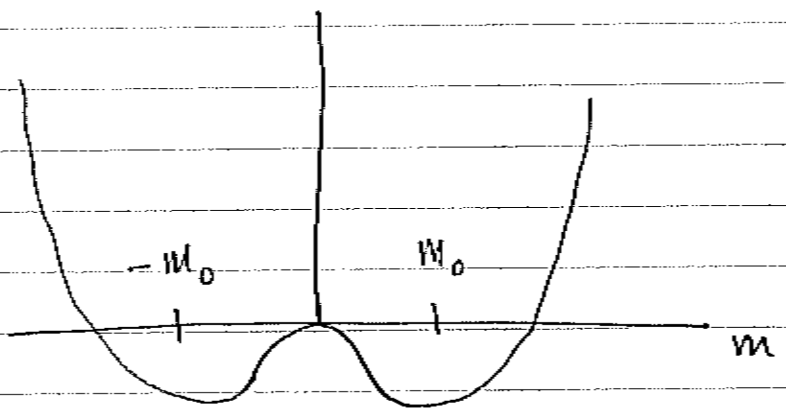
$$\frac{F}{N} = F_0 + \frac{1}{2} A\, m^2 + \frac{1}{4} B\, m^4$$

(where $A = k_B\,(T - T_c)$, $B = \frac{1}{3} k_B T_c$)

For $T > T_c$, F/N looks like



But for $T < T_c$, A becomes negative and



where $m_0 = \sqrt{\frac{-A}{B}}$. Note: m_0 can be determined from $\frac{\partial}{\partial m}\left(\frac{F}{N}\right) = 0$

The $m \neq 0$ phase corresponds to a minimum of the free energy with either $+m_0$ or $-m_0$, but not <u>both</u>. By this I mean that the system is in either one phase or the other at any given position, but not both simultaneously for $T < T_c$.

This is expressed as a "broken symmetry". The symmetry of the hamiltonian allows for the spins along either the + or − directions. In the ordered phase, the ground state is found along only one direction. In this sense, a preferred orientation of each spin is set by the system of N spins. Above T_c this does not exist and the spins can point in either direction with equal energy on average. The symmetry of orientation is broken for $T < T_c$.