

Classical spin models

$$U = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

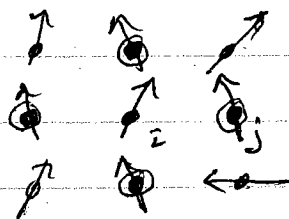
simple model of interacting magnetic

classical spins \vec{S}_i of unit magnitude $|\vec{S}_i| = 1$ on sites i of a periodic d -dimensional lattice.

\vec{S}_i interacts only with its neighbors \vec{S}_j

$\langle ij \rangle$ indicates nearest neighbor bonds of the lattice.

If coupling $J > 0$, then ferromagnetic interaction i.e. spins are in lower energy state when they are aligned.



\vec{S}_i interacts with spins on sites labeled by \odot .

Behavior of model depends significantly on dimensionality of lattice d , and number of components of the spin \vec{S} n .

Examples: $\vec{S} = (S_x, S_y, S_z)$ points in 3-dimensional space.
 $n=3$ called the Heisenberg model

$\vec{S} = (S_x, S_y)$ restricted to lie in a plane
 $n=2$ called the XY model

$S = S_z = \pm 1$ restricted to lie in one direction
 $n=1$ called the Ising model

less obvious possibilities $\left\{ \begin{array}{l} \underline{n=0} \\ \underline{n=\infty} \end{array} \right.$ called the polymer model
called the spherical model

We will focus on the Ising model (1925)

$$S = \pm 1$$

Ensembles

① fixed magnetization $M = \sum_i S_i$ M is total magnetization

partition function $\tilde{Z}(T, M) = \sum_{\{S_i\}} e^{-\beta \mathcal{H}[S_i]}$
s.t. $\sum_i S_i = M$

sum over all spin configurations

obeying the constraint $\sum_i S_i = M = N^+ - N^-$

\uparrow # up spins \quad # down spins

(similar to canonical ensemble with $\sum_i n_i = N$ total # particles)

Helmholtz free energy $F(T, M) = -k_B T \ln \tilde{Z}(T, M)$

② fixed magnetic field

to remove constraint of fixed M we can Legendre transform to a conjugate variable h , ~~the magnetic field~~. We will see that h is just the magnetic field.

Gibbs free energy $G(T, h) = F(T, M) - h M$

where ~~the~~ $\left(\frac{\partial F}{\partial M}\right)_T = h \quad \Rightarrow \quad \left(\frac{\partial G}{\partial h}\right)_T = -M$

$$dF = -SdT + h dM \quad \text{and} \quad dG = -SdT - Mdh$$

\uparrow entropy \uparrow entropy

To get partition function for G , take Laplace transform of \tilde{Z}

$$Z(T, h) = \sum_M e^{\beta h M} \tilde{Z}(T, M)$$

$$= \sum_M e^{\beta h M} \sum_{\{s_i\}} e^{-\beta H[s_i]} \quad \text{use } M = \sum_i s_i$$

st $\sum_i s_i = M$

$$Z(T, h) = \sum_{\{s_i\}} e^{-\beta [H[s_i] - h \sum_i s_i]}$$

← looks like interaction of magnetic field h with total magnetization $M = \sum_i s_i$

↳ unconstrained sum over all spin configs $\{s_i\}$
 (similar to grand canonical ensemble with $\sum_i n_i = N$ unconstrained)

$$G(T, h) = -k_B T \ln Z(T, h)$$

Check:

$$\frac{\partial G}{\partial h} = -k_B T \frac{\partial Z}{Z \partial h} = -k_B T \sum_{\{s_i\}} \frac{\partial}{\partial h} \left(e^{-\beta [H - h \sum_i s_i]} \right)$$

$$= -k_B T \sum_{\{s_i\}} e^{-\beta [H - h \sum_i s_i]} \left(\beta \sum_i s_i \right)$$

$$= - \frac{\sum_{\{s_i\}} e^{-\beta [H - h \sum_i s_i]} \left(\sum_i s_i \right)}{\sum_{\{s_i\}} e^{-\beta [H - h \sum_i s_i]}}$$

$$= - \left\langle \sum_i s_i \right\rangle = -M$$

so $\frac{\partial G}{\partial h} = -M$ as required

we can work in fixed magnetization or fixed magnetic field ensemble according to our convenience. Usually it is easiest to work with fixed magnetic field. In this case we usually write

$$H = -J \sum_{\langle ij \rangle} S_i S_j - h \sum_i S_i$$

including the magnetic field part in the definition of H .

$$Z = \sum_{\{S_i\}} e^{-\beta H} \quad \uparrow \text{ includes } h \text{ term}$$

define magnetization density

$$m = \frac{M}{N} = \frac{1}{N} \left\langle \sum_i S_i \right\rangle \quad N = \text{total number spins}$$

Helmholtz free energy density: In limit $N \rightarrow \infty$, $F(T, M) = N f(T, m)$

$$\frac{F}{N} \equiv f(T, m) \quad \text{depends on magnetization density}$$

$$df = -s dT + h dm \quad s = \frac{S}{N} \text{ entropy per spin}$$

Gibbs free energy density: In limit $N \rightarrow \infty$, $G(T, h) = N g(T, h)$

$$\frac{G}{N} \equiv g(T, h)$$

$$dg = -s dT - m dh$$

$$\left(\frac{\partial f}{\partial m} \right)_T = h \quad , \quad \left(\frac{\partial g}{\partial h} \right)_T = -m$$

What behavior do we expect from Ising model?
For a given h , what is the resulting $m(T, h)$?

For $h > 0$, expect $m > 0$ as energetically favorable for spins to align parallel to h .
For $h < 0$, similarly expect $m < 0$.

In general, $m(T, -h) = -m(T, h)$, since Hamiltonian has the symmetry $\mathcal{H}[s_i, h] = \mathcal{H}[-s_i, -h]$

What if $h = 0$?

As $T \rightarrow \infty$ we expect each spin to be random so $m \rightarrow 0$.
But even at finite T we might expect $m = 0$ because of symmetry: $\mathcal{H}[s_i, 0] = \mathcal{H}[-s_i, 0]$ so a configuration $\{s_i\}$ in the partition function sum will enter with the same weight as the configuration $\{-s_i\}$ and so expect $\langle s_i \rangle = 0$.

But at $T = 0$, the system has two degenerate ground states: all up or all down, with $m = \pm 1$.
The ground state breaks the symmetry of the Hamiltonian.

More specifically:

limit $h \rightarrow 0$ from above $\rightarrow \lim_{h \rightarrow 0^+} \lim_{T \rightarrow 0} m(T, h) = +1$

limit $h \rightarrow 0$ from below $\rightarrow \lim_{h \rightarrow 0^-} \lim_{T \rightarrow 0} m(T, h) = -1$

Can one have such a broken symmetry state at finite T ?

$$\text{ie } \lim_{h \rightarrow 0^+} m(T, h) = m > 0$$

$$\lim_{h \rightarrow 0^-} m(T, h) = m < 0$$

For a finite size system, N finite, the answer is NO!

For a finite size system, the energy $H[s_i]$ is always finite. The statistical weight of $\{s_i\}$ will always be equal to that of $\{-s_i\}$ in a small h , as we take $h \rightarrow 0$

However, in the thermodynamic limit $N \rightarrow \infty$, the answer can be Yes! Now the energy of states with a finite $\sum_i s_i$ will grow infinitely large as N . The statistical weight of config $\{s_i\}$ can be infinitely different from that of $\{-s_i\}$ in a small h , even if take $h \rightarrow 0$. ($\infty \times 0 \neq 0$)

$H[s_i] - H[-s_i] \propto hN$ does not necessarily vanish as $h \rightarrow 0$, if $N \rightarrow \infty$ first

It is possible that at finite T

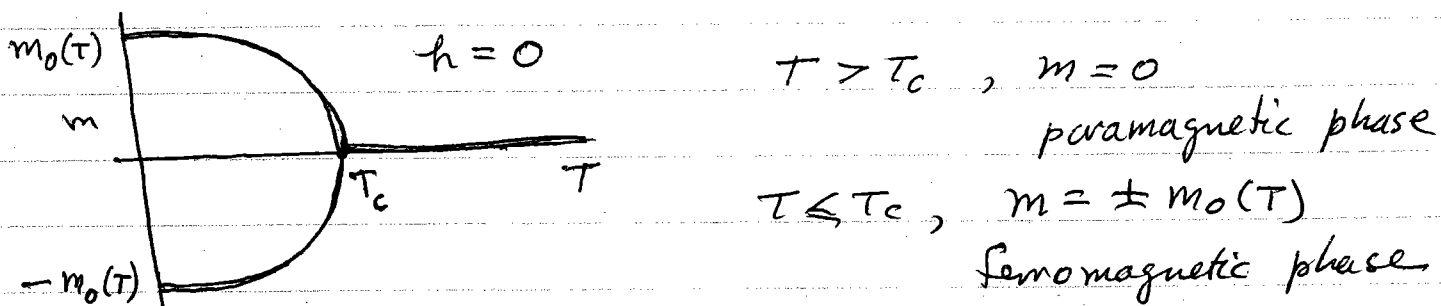
$$\lim_{h \rightarrow 0^+} \left[\lim_{N \rightarrow \infty} m(T, h) \right] = m > 0$$

$$\lim_{h \rightarrow 0^-} \left[\lim_{N \rightarrow \infty} m(T, h) \right] = m < 0$$

It is important to take the limits in the above order - ie first take $N \rightarrow \infty$ in a finite h , and then take $h \rightarrow 0$. Reversing the limits ($h \rightarrow 0$ first, then $N \rightarrow \infty$) gives $m=0$ by symmetry of H .

If such broken symmetry states exist at finite T , then do they persist at all T ? or do they disappear at a well defined T_c ?

Possibility of a phase transition

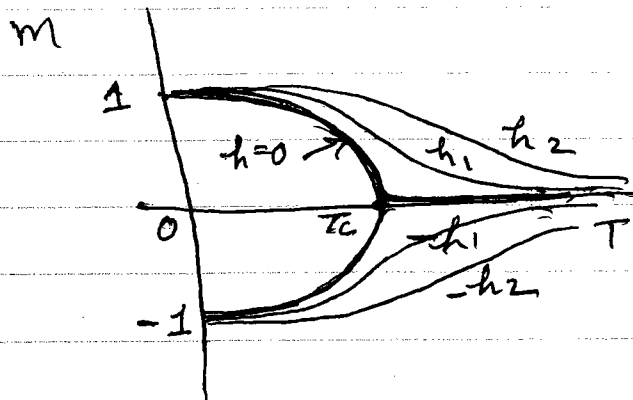


$m(T, 0)$ is singular at $T = T_c$

T_c is ferromagnetic phase transition

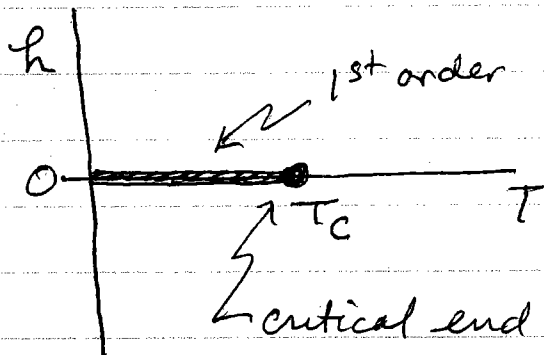
The ordered state at $T \leq T_c$ is a state of spontaneously broken symmetry. In $h=0$ the system will pick either the up or the down state to order in, breaking the symmetry of the Hamiltonian.

At finite h , expect $m(T, h)$ to behave like



$m(T, h)$ is smooth function of T for $h \neq 0$

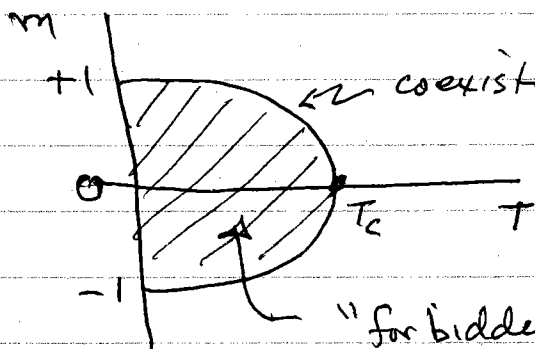
Phase diagram in $h-T$ plane



1st order phase transition. As cross this line $m(T, h)$ has a discontinuous jump from $m_0(T)$ to $-m_0(T)$

critical end point. $m(T, h)$ is continuous if cross $h=0$ line above T_c . We will see that T_c corresponds to a 2nd order phase transition - jump in $m(T, h)$ vanishes continuously as approach T_c from below.

Phase diagram in $m-T$ plane



coexistence curve. "up" and "down" states at $h=0$ can coexist in equilib along this line

"forbidden region" - there is no homogeneous phase with T and m in this region

"phase separation region" - if cool a system with fixed M into this region it will phase separate into domains of "up" and "down" with average magnetization M .

Many similarities to liquid-gas phase diagram

We said that to have a state of spontaneously broken symmetry at finite T ~~requires~~ one needs to be in thermodynamic limit $N \rightarrow \infty$.

Similarly, true singular phase transitions can only occur in this $N \rightarrow \infty$ limit. Proof as follows:
partition function sum:

$$Z(T, h) = \sum_{\{s_i\}} e^{-\beta H[s_i]}$$

For finite system (N finite) the number of configurations to sum over is 2^N is finite.

Z is therefore the sum of a finite number of analytic functions ("analytic" here in the sense of complex function theory - has no singularities as vary T, h). As such, Z must itself be an analytic function of T at h .

$\Rightarrow Z$ can have no singularities

\Rightarrow no singularities in any thermodynamic quantities

\Rightarrow no phase transitions.

Only in thermodynamic limit of $N \rightarrow \infty$ is Z now the sum of an infinite ~~real~~ number of analytic functions. Such an infinite sum need NOT be analytic, so phase transitions can exist.