Classical spin models

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$ simple model of interacting magnetic moments

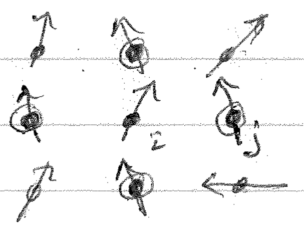
classical spins $\vec{S}_i$ of unit magnitude $|\vec{S}_i| = 1$ on sites i of a periodic d-dimensional lattice.

$\vec{S}_i$ 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

ie spins are in lower energy state when they are alligned.



$\vec{S}_i$ 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

$\underline{n = 3}$ called the Heisenberg model

$\vec{S} = (S_x, S_y)$ restricted to lie in a plane

$\underline{n = 2}$ called the XY model

$S = S_z = \pm 1$ restricted to lie in one direction

$\underline{n = 1}$ called the Ising model

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

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

sum over all spin configurations obeying the constraint $\sum_i s_i = M = N^+ - N^-$

N^+: # up spins, N^-: # 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.
We will see that h is just the magnetic field

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

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

$dF = -S\,dT + h\,dM$ and $dG = -S\,dT - M\,dh$

(S: entropy)

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

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

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

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

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:

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

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

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

$$= -\left\langle \sum_i s_i \right\rangle = -M \qquad \text{so } \frac{\partial G}{\partial h} = -M \text{ as required}$$

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

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

including the magnetic field part in the definition of $\mathcal{H}$.

$$Z = \sum_{\{S_i\}} e^{-\beta\mathcal{H}}$$ ← includes h term

define magnetization density

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

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

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

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

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

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

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

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

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 allign parallel to h.
For $h < 0$, similarly expect $m < 0$.

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

<u>What if $h = 0$?</u>

As $T \to \infty$ we expect each spin to be random so $m \to 0$.
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 <u>degenerate</u> ground states: <u>all up</u> or <u>all down</u>, with $m = \pm 1$.
The ground state <u>breaks</u> the symmetry of the Hamiltonian.

<u>More specifically</u>: $\lim_{h \to 0^+} \lim_{T \to 0} m(T, h) = +1$

limit $h \to 0$ from above

$\lim_{h \to 0^-} \lim_{T \to 0} m(T, h) = -1$

limit $h \to 0$ from below

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

i.e. $\lim_{h \to 0^+} m(T, h) = m > 0$

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

For a <u>finite size system</u>, N finite, the answer is <u>NO</u>!
For a finite size system, the energy $\mathcal{H}[s_i]$ 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 $h \to 0$

However, in the <u>thermodynamic limit</u> $N \to \infty$, the answer can be <u>Yes</u>! 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 $h \to 0$. $(\infty \times 0 \neq 0)$
$\mathcal{H}[s_i] - \mathcal{H}[-s_i] \propto hN$ does not necessarily vanish as $h \to 0$ if $N \to \infty$ first
It is possible that at finite T

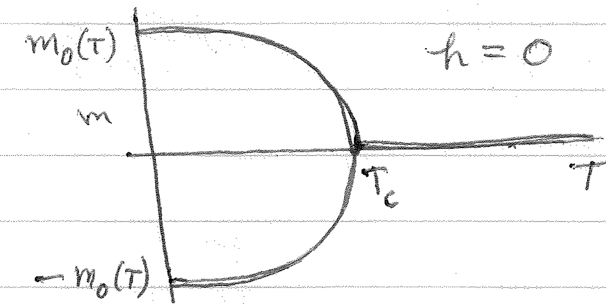
$$\lim_{h \to 0^+} \left[\lim_{N \to \infty} m(T, h) \right] = m > 0$$

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

It is important to take the limits in the above order — i.e. first take $N \to \infty$ in a finite h, and then take $h \to 0$. Reversing the limits ($h \to 0$ first, then $N \to \infty$) gives $m = 0$ by symmetry of $\mathcal{H}$.

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

Possibility of a phase transition



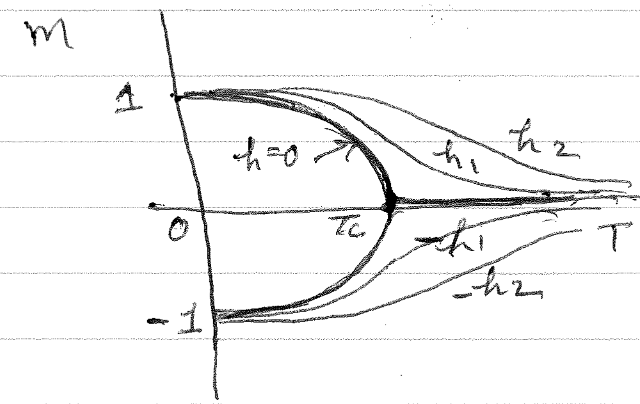
$T > T_c$, $m = 0$
paramagnetic phase

$T \leq T_c$, $m = \pm m_0(T)$
ferromagnetic phase

$m(T, 0)$ 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.

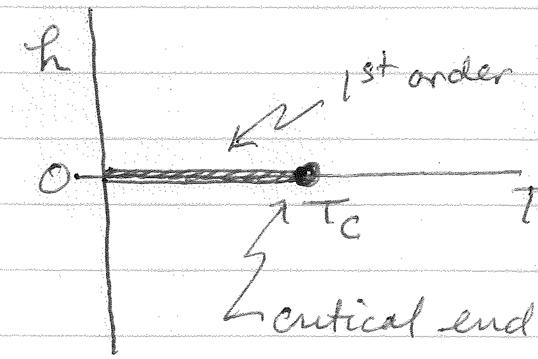
At finite h, expect $m(T,h)$ to behave like



$h_1 < h_2$

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

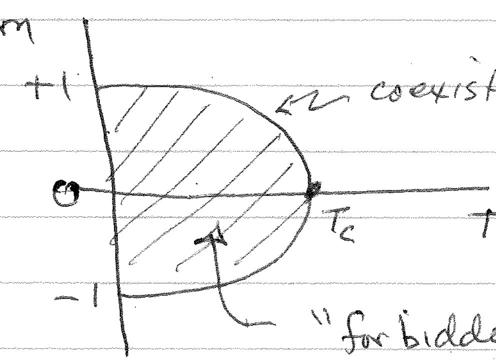
Phase diagram in $h-T$ plane



1st order phase transition. As cross this line decreasing h, $m(T,h)$ 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