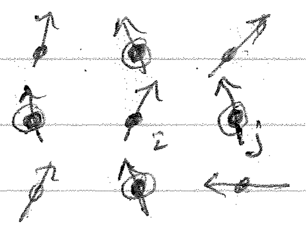
Classical spin models

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$ 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
$n = 3$ 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 $\left\{ \begin{array}{l} n = 0 \text{ called the polymer model} \\ n = \infty \text{ called the spherical model} \end{array} \right.$

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 $\sum_i s_i = M = \underbrace{N^+}_{\#\text{ up spins}} - \underbrace{N^-}_{\#\text{ down spins}}$

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

$dF = -\underbrace{S}_{\text{entropy}}dT + h\,dM$ and $dG = -\underbrace{S}_{\text{entropy}}dT - M\,dh$

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

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

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

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

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:

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

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

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

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

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 $N\to\infty$, $F(T,M) = N f(T,m)$

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

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

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

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

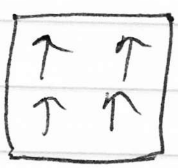
$$\lim_{h \to 0^-} \left[\lim_{N \to \infty} m(T, h) \right] = m < 0$$

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 $\mathcal{H}$.

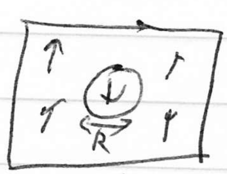
Physical reason why we can have $m \neq 0$ as $h \to 0$ but only when $N \to \infty$ and the system is infinite.

In principle, when $h=0$, the config $\{s_i\}$ has the same weight as $\{-s_i\}$ and so these cancel each other out when computing $\langle \sum_i s_i \rangle$. However, lets consider the physical process by which the system, originally in the config $\{s_i\}$, might wind up in the config $\{-s_i\}$

Consider $h=0$, at low T, when the config is mostly all spins up. As a fluctuation, there might appear a small domain of length R in which the spins have flipped sign. The energy of this fluctuation would be proportional to the perimeter of the domain, since that is where the spins are not aligned.



all spins up



domain of length R in which spins have flipped

energy of fluctuation is

$\Delta E \sim JR$

If the size of the spin flipped domain ever got large enough to be half the size of the system, then it would be equally likely for this domain to either shrink back down to zero, restoring the original config with all spins up, or to grow and fill the entire system, thereby transitioning the system to the config with all spins down.

such a critical domain fluctuation has a size $R \sim L/2$ where L is the length of the system

$\Rightarrow$ has an energy $\Delta E_c \sim JL$, so occurs with a probability $\sim e^{-\Delta E_c/k_BT} \sim e^{-JL/k_BT}$

when L is large, this is exceedingly small. But if L is finite, this probability is also finite, So if we wait long enough, even if we have to wait an exceeding long time, such a critical domain excitation will ultimately happen and cause the system to flip its spins. That will lead to a vanishing of $\langle \sum_i s_i \rangle$ when averaged over such domain crossing flips.

But if $L \to \infty$ (ie the system is infinite and $N \to \infty$) then the probability of having the critical sized domain $e^{-JL/k_BT} \to 0$ and so the system, if initially in a config with $m > 0$ will not necessarily flip even if we wait forever. So we can wind up with a situation where $\langle \sum_i s_i \rangle$ does not vanish.

The key thing is that we must have $\underline{N \to \infty}$ in order to have the possibility for $m \neq 0$ at finite T.