Simple Models with Singular Free Energy (and more than one phase of matter)

Now we begin our study of phases and phase transitions in earnest.

One of the most useful model we will encounter to develop our understanding is the Ising model.

$$H = \sum_{i,j=1}^{N} J_{ij}\, s_i\, s_j + \sum_i h_i s_i$$

$$s_i = \pm 1 \qquad i,j \in \text{some graph.}$$

Total number of microstates $= 2^N$

We will first restrict ourselves to graphs which form a lattice. Even more, we will restrict ourselves to cubic lattice in various dimensions.

Ising Model on d-dimensional cubic lattice with nearest neighbour interactions.

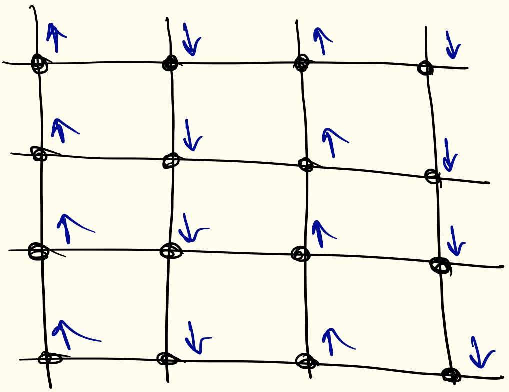
1d chain :

$$H = J\sum_i S_i \, S_{i+1} + h\sum_i S_i$$

$$\begin{array}{cccccc} \uparrow & \downarrow & \uparrow & \downarrow & \uparrow & \downarrow \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ 1 & 2 & 3 & & & N \end{array}$$

2d square lattice :

$$H = J\Big[\sum_{\vec r} S_{\vec r} \, S_{\vec r+\hat x} + \sum_{\vec r} S_{\vec r} \, S_{\vec r+\hat y}\Big] + h\sum_{\vec r} S_{\vec r}$$



d- dimensional hypercubic lattice:

$$H = J \sum_{\vec{r},\, i=1-d} S_{\vec{r}}\, S_{\vec{r}+\hat{e}_i}$$

$$+ \; h \sum_{\vec{r}} S_{\vec{r}}$$

What are the analog of parameters $\{K\}$?

$$Z = \sum_{\{S\}} e^{-\beta H}$$

$$= \sum_{\{S\}} e^{-\beta J \sum S_r S_{r+\hat{e}} - \beta h \sum_{\vec{r}} S_{\vec{r}}}$$

$K_1 = \beta J, \quad K_2 = \beta h.$

Two- dimensional space.

But this is slightly misleading.
Better to define a model solely using symmetries.

What are the symmetries of Ising model?

$$H = J \sum_{\vec{r},\, i=1-d} S_{\vec{r}}\, S_{\vec{r}+\hat{e}_i} + h \sum_{\vec{r}} S_{\vec{r}}$$

$$S_r \to -S_r \quad \forall\, r$$

$$h \to -h$$

Noting this, one can write down a general Ising model with symmetry $S \to -S$, $h \to -h$

$$H = \sum_{r_1 r_2} J_{r_1 r_2} S_{\vec{r}_1} S_{\vec{r}_2} + \sum h_{\vec{r}} S_{\vec{r}}$$

$$+ \sum_{r_1 r_2 r_3 r_4} J_{\vec{r}_1 \vec{r}_2 \vec{r}_3 \vec{r}_4} S_{\vec{r}_1} S_{\vec{r}_2} S_{\vec{r}_3} S_{\vec{r}_4}$$

$$+ \sum_{\vec{r}_1 \vec{r}_2 \vec{r}_3} h_{r_1 r_2 r_3} S_{\vec{r}_1} S_{\vec{r}_2} S_{\vec{r}_3}$$

Since magnetic field is generally fixed from the outset, the symmetry that requires $h \to -h$ is a bit unphysical.

when $h = 0$, $S \to -S$ a more physical symmetry is Hamiltonian restricted to terms that contains an even number of product of S's.

$$H = \sum J_1 S_i S_j + J_2 \sum S_i S_j S_k S_l + \cdots$$

Impossibility of Phase Transition in Ising Model ??

Recall that in the presence of a magnetic field, the free energy is given by

$$dF = -S\,dT - M\,dh$$

where M is the magnetization:

$$M = \left\langle \sum_i S_i \right\rangle = \frac{\sum_{\{S\}} e^{-\beta H} \left(\sum_i S_i\right)}{\sum_{\{S\}} e^{-\beta H}}$$

Due to the symmetry just discussed,

$$F(h, J, T) = F(-h, J, T)$$

$$\Rightarrow \quad -\frac{\partial F}{\partial h}(h, J, T) = -\frac{\partial F(-h, J, T)}{\partial h}$$

$$= \frac{\partial F(-h, J, T)}{\partial(-h)}$$

$$\Rightarrow \quad M(h, J, T) = -M(-h, J, T)$$

$$\Rightarrow \quad \boxed{M(0, J, T) = 0}$$

This seemingly implies that in zero magnetic field the Ising model can not have any magnetization.

This conclusion is manifestly wrong! We assumed that the free energy is not singular!

Spontaneous Symmetry Breaking & Singularity of free energy

"Spontaneous symmetry breaking" is the phenomena where the solution to a problem has lower symmetry than the problem itself.

In the context of phases of matter, it means that a phase of matter has lower symmetry than the underlying Hamiltonian. Singularity of free energy is a necessary condition for SSB.

e.g. in the Ising model at $h=0$, a non-zero magnetization M will imply SSB.

Ising Model in One Dimension

Consider 1d Ising model:

$$H = -J\sum_i S_i S_{i+1} - h\sum_i S_i$$

Chose Periodic boundary conditions for convenience (doesn't really matter for this discussion)

When $h=0$, ground state energy (= free energy at $T=0$) is minimized by <u>two</u> distinct configurations:

$$E = -NJ$$

a) $\uparrow \; \uparrow \; \uparrow \; - - - \; \uparrow \; \uparrow$ All up

b) $\downarrow \; \downarrow \; \downarrow \; — - - \downarrow \; \downarrow$ All down.

Therefore there are two ground states and neither of them have the symmetry $S \to -S$ of the Hamiltonian H.

Infact, under $S \to -S$, the two ground states interchange.

What happens at a non-zero h?

<u>When $h > 0$</u>, the ground state is

$$\uparrow \uparrow \uparrow \cdots \uparrow \uparrow \quad (\text{All up})$$

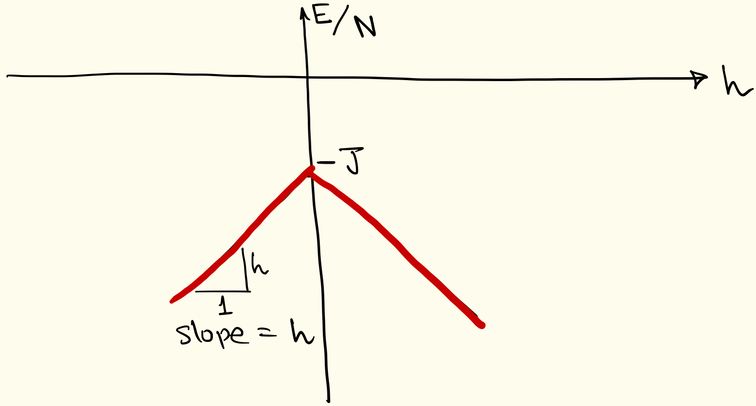
$$E_{g.s} = -NJ - Nh$$

<u>When $h < 0$</u>, the ground state is

$$\downarrow \downarrow \downarrow \cdots \downarrow \downarrow \quad (\text{All down})$$

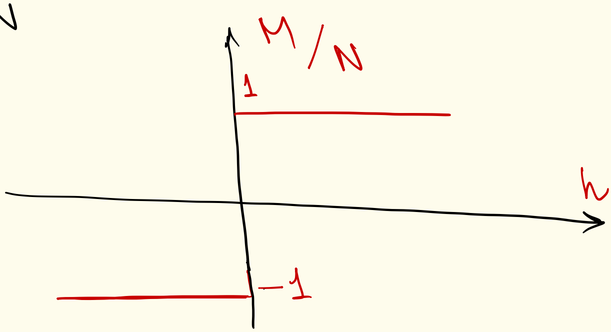
$$E_{g.s.} = -NJ + Nh = -NJ - N|h|$$

$\Rightarrow$



$\Rightarrow$ $E_{g.s.} = F(T=0)$ is a singular f^n of h, even for finite N.
Recall, this is allowed because $\beta \to \infty$, and $Z(\beta)$ is allowed to be singular.

$\dfrac{\text{Magnetization}}{N} = -\dfrac{1}{N}\dfrac{dF}{dh}$ jumps :



This is an example of first-order transition since $\dfrac{dF}{dh}$ is not continuous.

What happens at finite Temperature ?

Somewhat surprisingly, at finite T, the singular features of the free energy go away for 1d Ising model. This is because the thermal fluctuations are too strong in 1d. In Higher dimensions $(d>1)$, Ising model continues to have a singular behavior as a function of h (at $h=0$) even for $T>0$.

Simple argument for analytical free energy and absence of any phase transition at $T>0$ in the Ising model in $\underline{d=1}$:

The free energy is $F = E - TS$

At $T>0$, the E and S compete to minimize F.

Consider small T, so that the fluctuations around the ground state are expected to be small. Also define the ground state to be the zero of energy for convenience. The simplest fluctuation consist of a domain wall :

$$\begin{array}{ccccccccc} 1 & 2 & 3 & & & & & & N \\ \uparrow & \uparrow & \uparrow & \uparrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow \end{array} \quad \text{(open boundary condition)}$$

$$\begin{array}{cccccccccc} 1 & 2 & 3 & & & & & & N & 1 \\ \uparrow & \uparrow & \uparrow & \downarrow & \downarrow & \downarrow & \downarrow & \uparrow & \uparrow & \uparrow \end{array} \quad \text{(periodic b.c.)}$$

In either case $\Delta E_{\substack{\text{domain} \\ \text{wall}}} = \begin{cases} 2J & \text{(open)} \\ 4J & \text{(periodic)} \end{cases} \propto J$

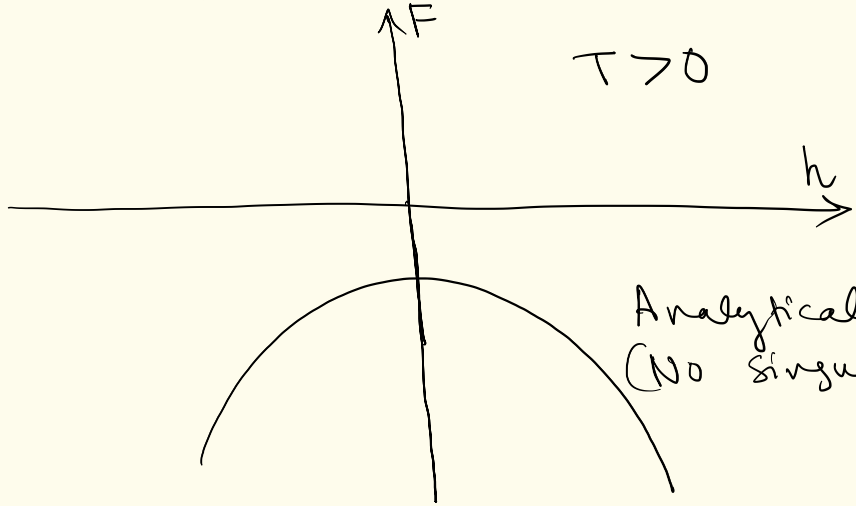
However, the entropy associated with the domain wall is huge :

$$S_{\substack{\text{Domain}\\ \text{wall}}} = \log(N)$$ since N places to put the domain wall.

$$\Rightarrow \quad F_{\substack{\text{domain}\\ \text{wall}}} = \alpha J - T\log(N)$$

as $N \to \infty$, entropy dominates over the energy and the system prefers to have proliferation of domain walls at <u>any</u> $T > 0$. $\Rightarrow$ No magnetization at $T > 0$

Thus, expect :



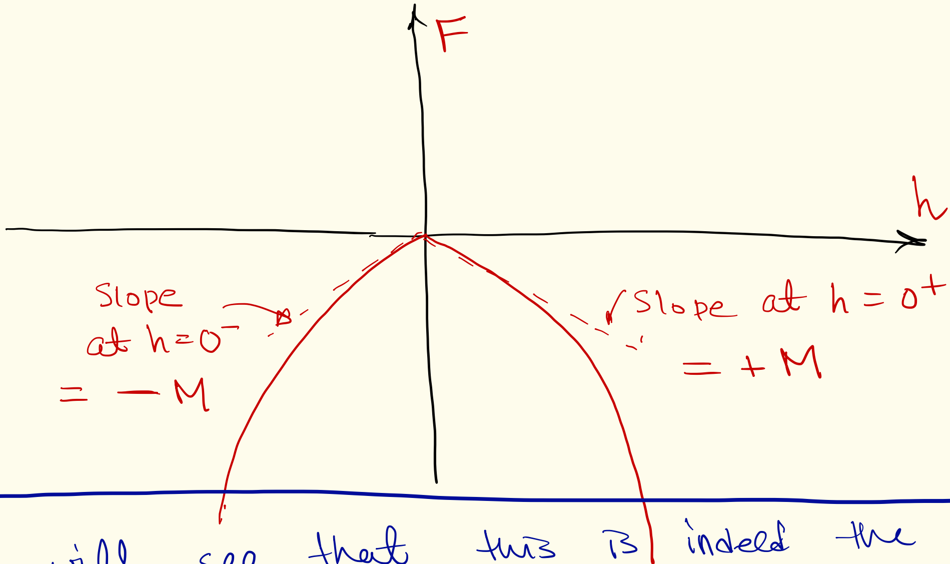
Analytical fn.
(No singularity)

What would take for Ising model to have SSB?

We want $\dot{M} = -\left.\frac{\partial F}{\partial h}\right|_{h=0}$ to be non-zero.

We also know that $F(h)$ is an even f^n of h.

So the only way for SSB to take place is:



We will see that this is indeed the case in all d at $T=0$ and $d>1$ at $T\neq 0$

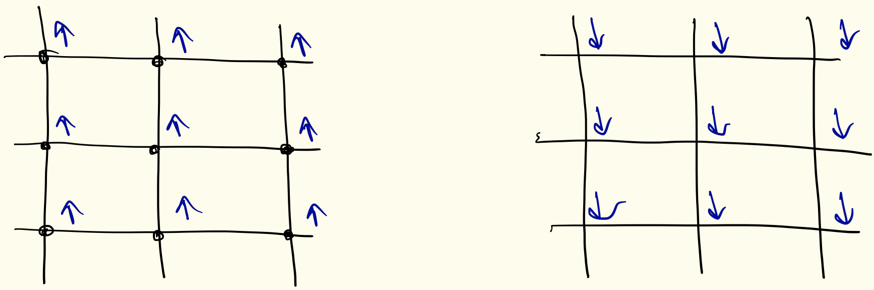
Ising Model in Two Dimensions

In two dimensions the counting of energy and especially entropy is quite different.

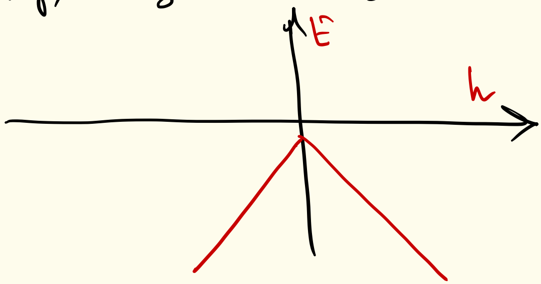
For concreteness, consider $d=2$ Ising model on square lattice <u>without</u> magnetic field.

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

At zero temperature, there are again two ground states,



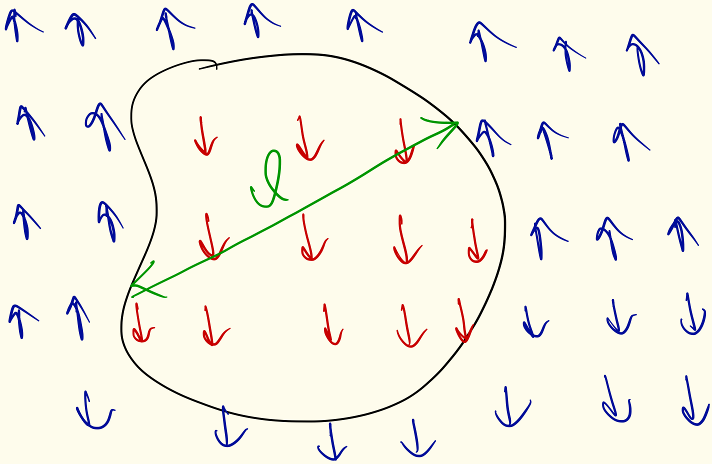
In the presence of magnetic field (i.e. the term $-h\sum_i s_i$ in the Hamiltonian) the $T=0$ free energy (= ground state energy) again looks like



The main difference between 1d and 2d is at $T \neq 0$.

At $T>0$, thermal fluctuations allow the existence of domain walls. As in 1d, the question is: do the domain walls completely kill the ordering at any $T>0$?

Domain wall looks like:



Energy cost of domain wall

$\propto$ length of the domain wall

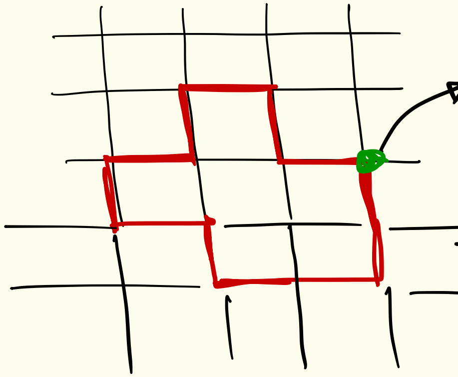
$\sim J l$

Entropy of a domain wall

$\sim \log(\#$ of ways of drawing a domain wall$)$

If the coordination # of the lattice is z, # of ways of drawing a domain wall $\sim (z-1)^{l}$ N

origin of D.W.



$$\Rightarrow \quad S_{D.W.} = \log (z-1)^l N \sim l \log(z-1) + \log N$$

$$\Rightarrow f_{D.W.} = E_{D.W.} - T S_{D.W.}$$
$$= Jl - Tl \log(z-1) - T \log N$$

If Domain wall can become arbitrarily large i.e $l \sim L (= \sqrt{N})$, then the system can't sustain ordering $\Rightarrow$

when $T > \dfrac{J}{\log(z-1)}$, entropy dominates and system wants to form domain walls.

On the other hand, for $T < \dfrac{J}{\log(z-1)}$, system will Spontaneously order (SSB).

$\Rightarrow$ Phase transition at $T_c \sim \dfrac{J}{\log(z-1)}$.

(Note this argument requires $L \to \infty$)

This argument works in any dimension,

$$E \sim J z L^{d-1}$$

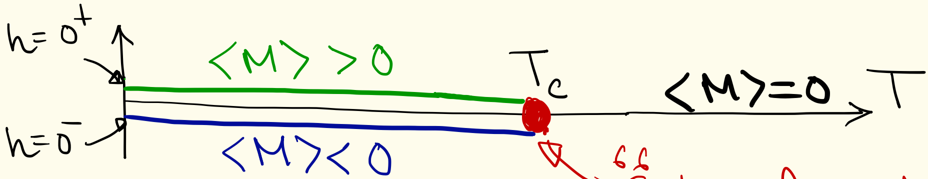
$$S \sim L^{d-1} \log(z-1)$$

$$\Rightarrow \quad T_c \sim \frac{Jz}{\log(z-1)}$$

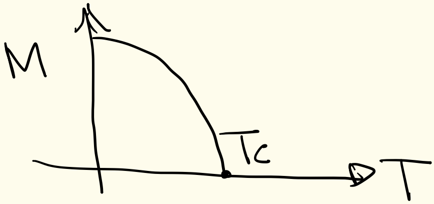
for a cubic lattice in d dimension,

$$z = 2d$$

$$\Rightarrow \quad T_c \sim \frac{Jd}{\log(2d-1)}$$

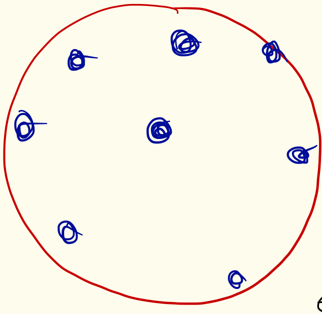


"Critical point" $\equiv$ 2nd order phase transition



Side Remarks:

There are several interesting examples of symmetry breaking in finite systems at $T=0$. These are all energy minimization problems like the Ising model at $T=0$.

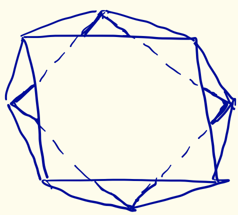


Eight particles on the surface of a sphere. Minimize Coulomb energy $E = \frac{1}{2}\sum_{i,j}\frac{1}{|\vec{r}_i - \vec{r}_j|}$

Naive guess : Highest symmetry solution = A cube ?

Correct answer : Square Antiprism.

Top view:



16 edges