Lecture 17

Recall from last lecture...

Phase transitions arise due to interactions.

Ising Hamiltonian

$$E(\nu) = -h \sum_i S_i - \frac{J}{2} \sum_{i,j}{}' S_i S_j$$

non-interacting

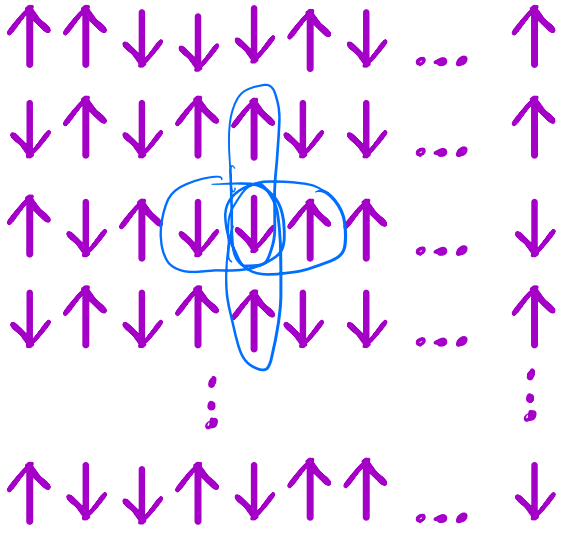
an interaction between spins

"Coupling constant"

If aligned, $S_i S_j = 1$
If not, $S_i S_j = -1$

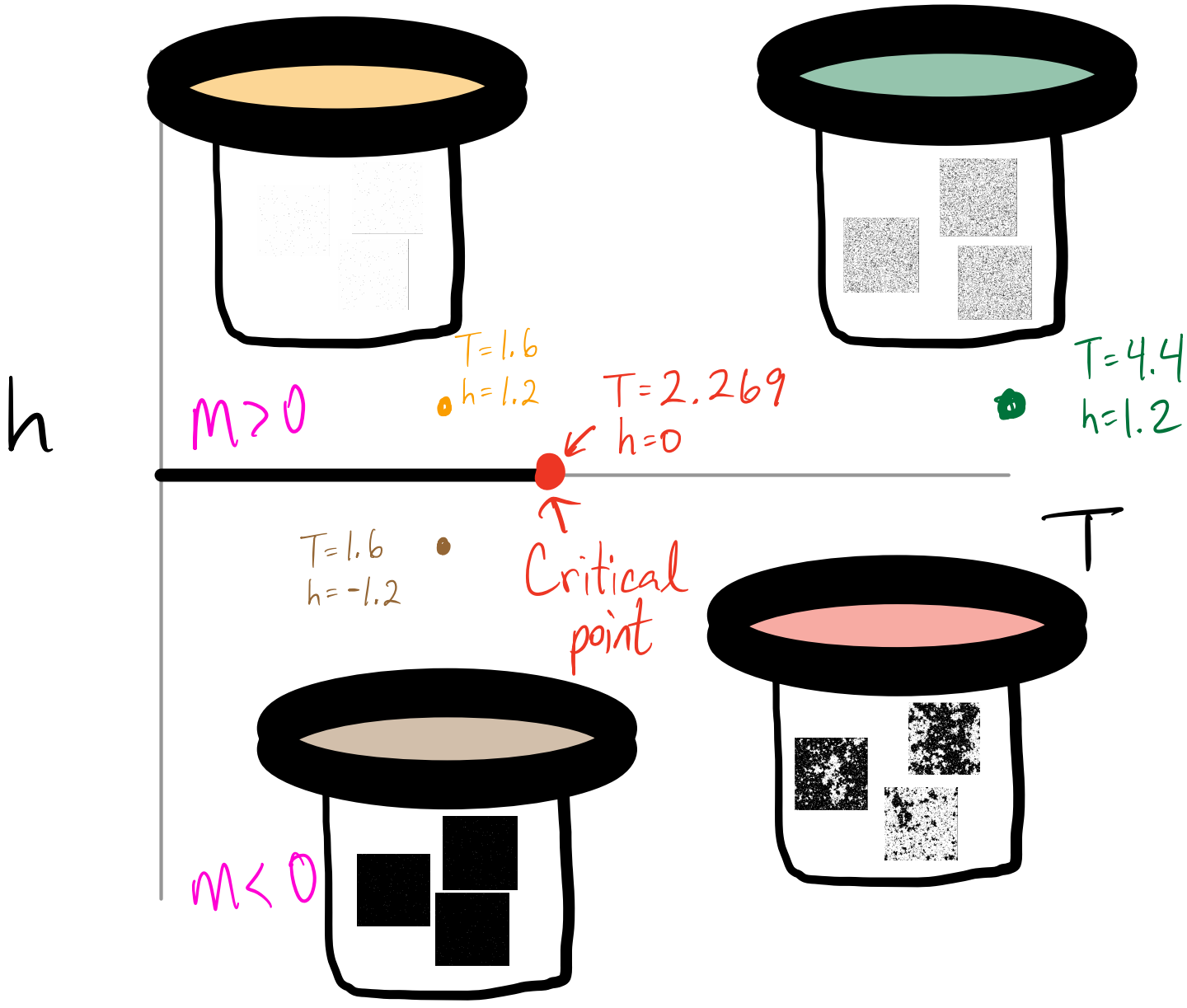
The $\frac{1}{2}$ allows us to include $i=1, j=2$ and $i=2, j=1$ terms in the sum — "double counting"

$'$ is shorthand that means we only include nearest neighbor $i \neq j$.

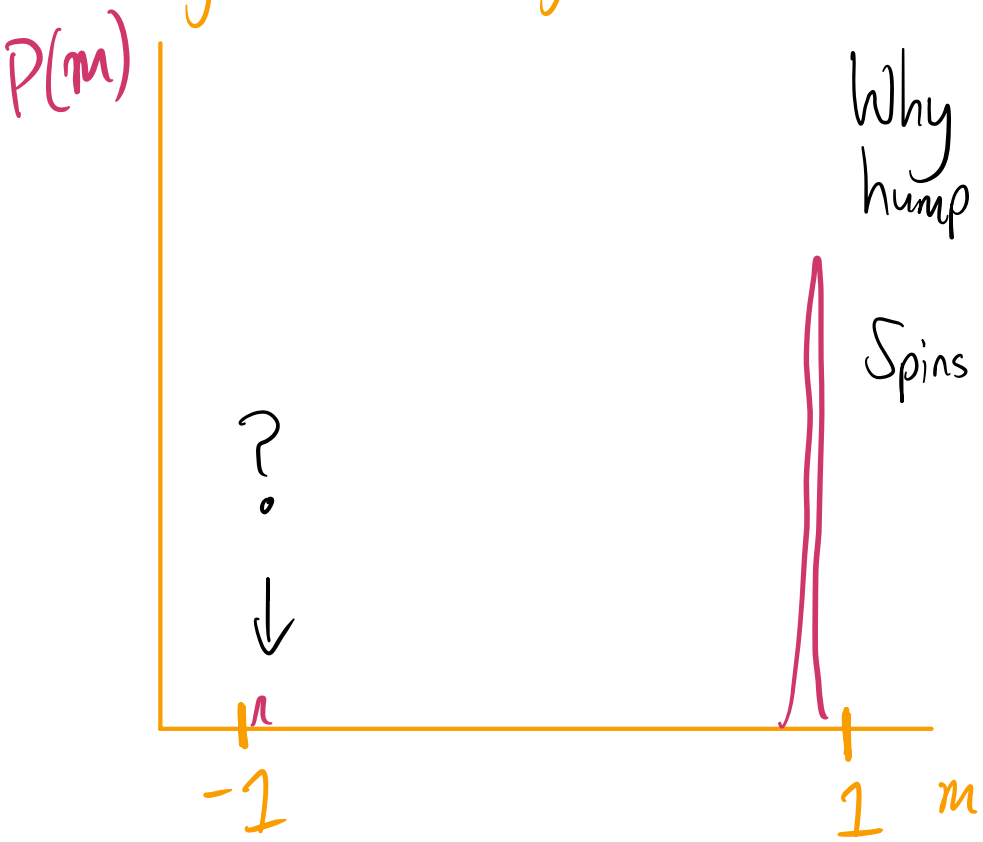


One can do it by hand. Perhaps not you or I. Lars Onsager did it.

There is another way to study the model even when it is not analytically tractable. Sampling



Collect lots of samples from the orange hat and get the marginal distribution for m.



Why is there a little hump near m=-1?

Spins are influenced by h

Marginal distributions $\Longleftrightarrow$ Effective energies

$$f(m) = -\frac{k_B T}{N} \ln P(m)$$

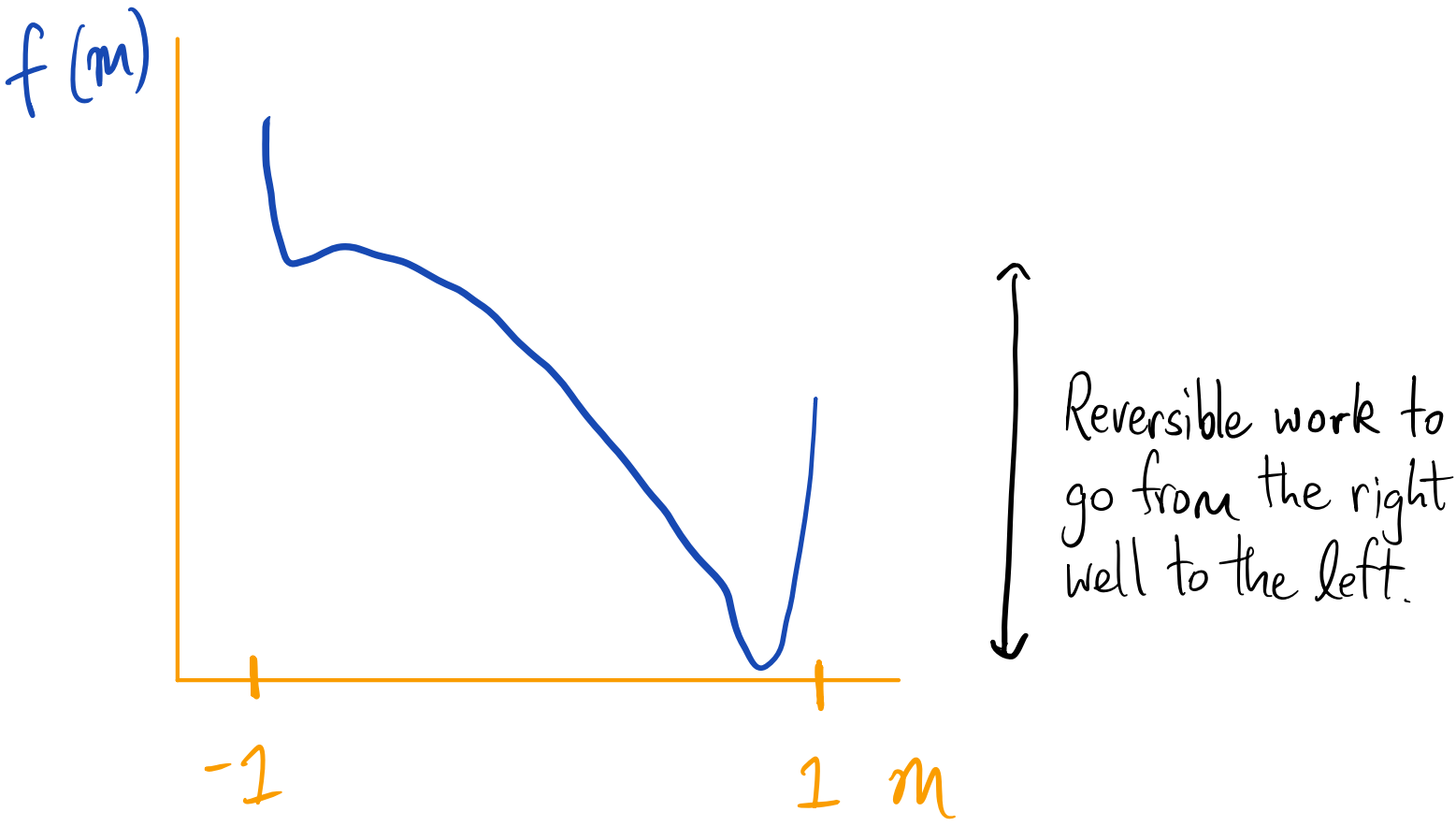
$f(m)$: free energy of magnetization (per spin)

Aside:

Rearranging...

$$P(m) = e^{-\beta N f(m)}$$

An example of a large deviation function.



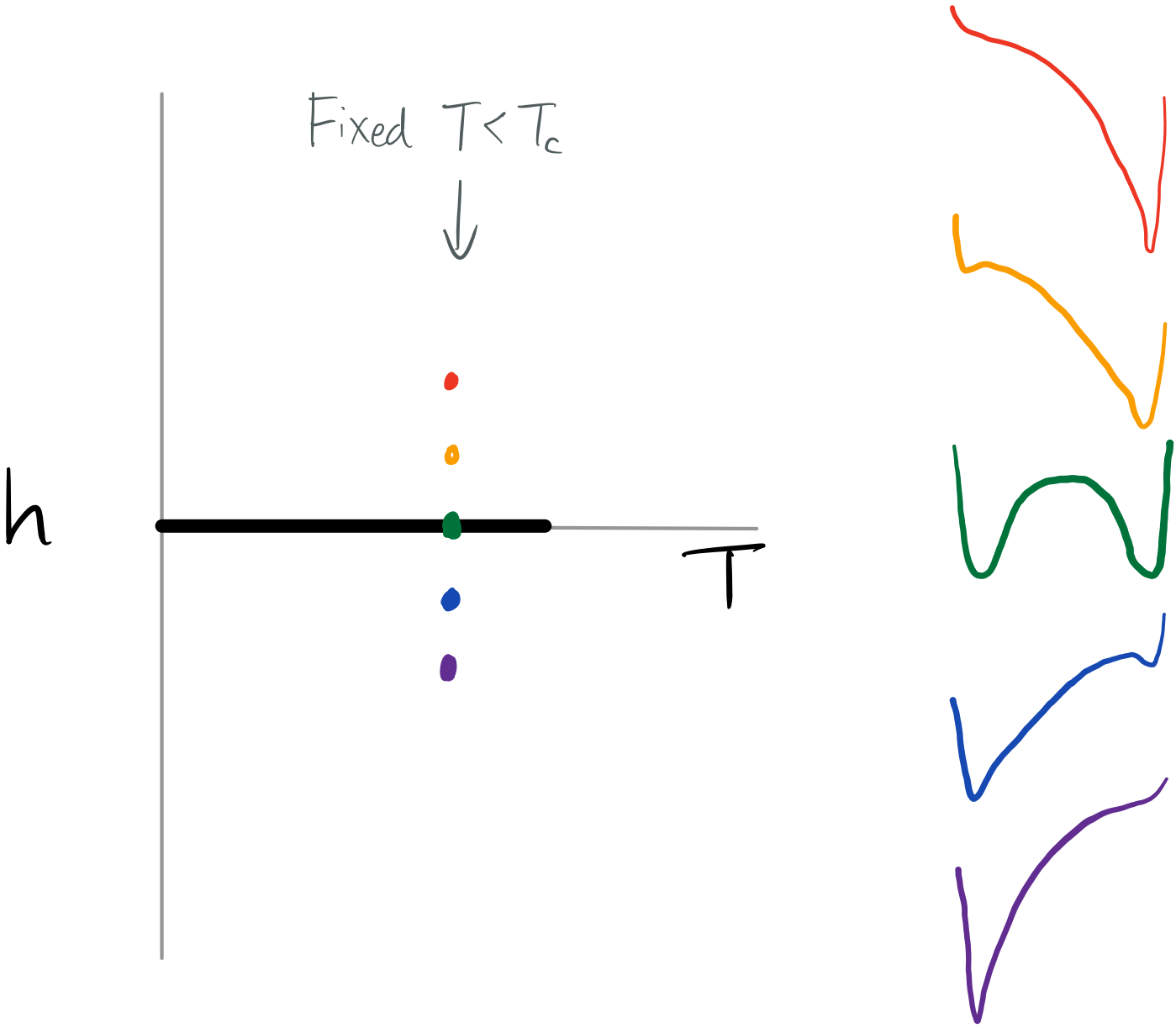
In what ways is $f(m)$ an effective energy?

1. If you start with m away from a minimum, you expect the system to "fall downhill" into a minimum.

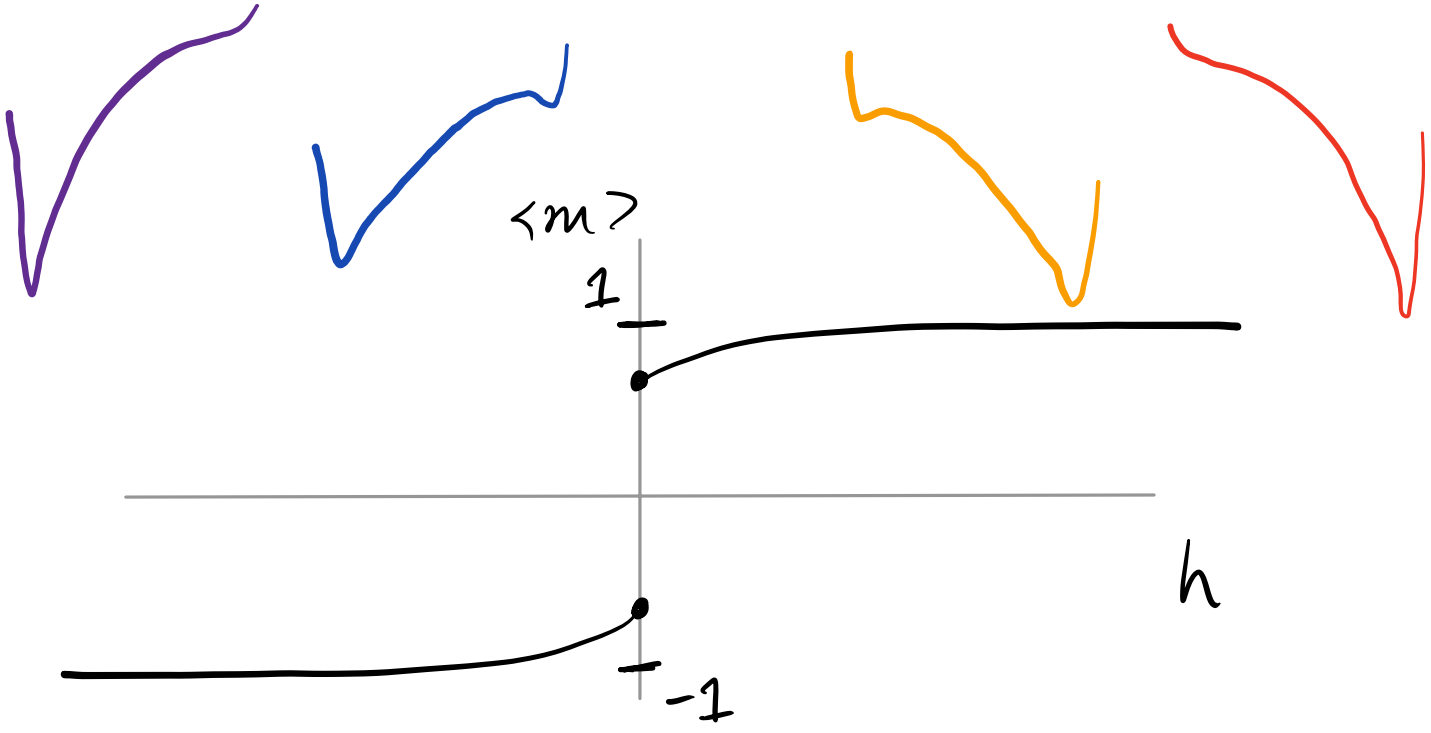
2. It is the reversible work to change the magnetization

3. Changing the "zero of energy" is not meaningful so we might as well set the minimum to zero.

There are different types of phase transitions



The typical <m> settles into the free energy minimum, so...

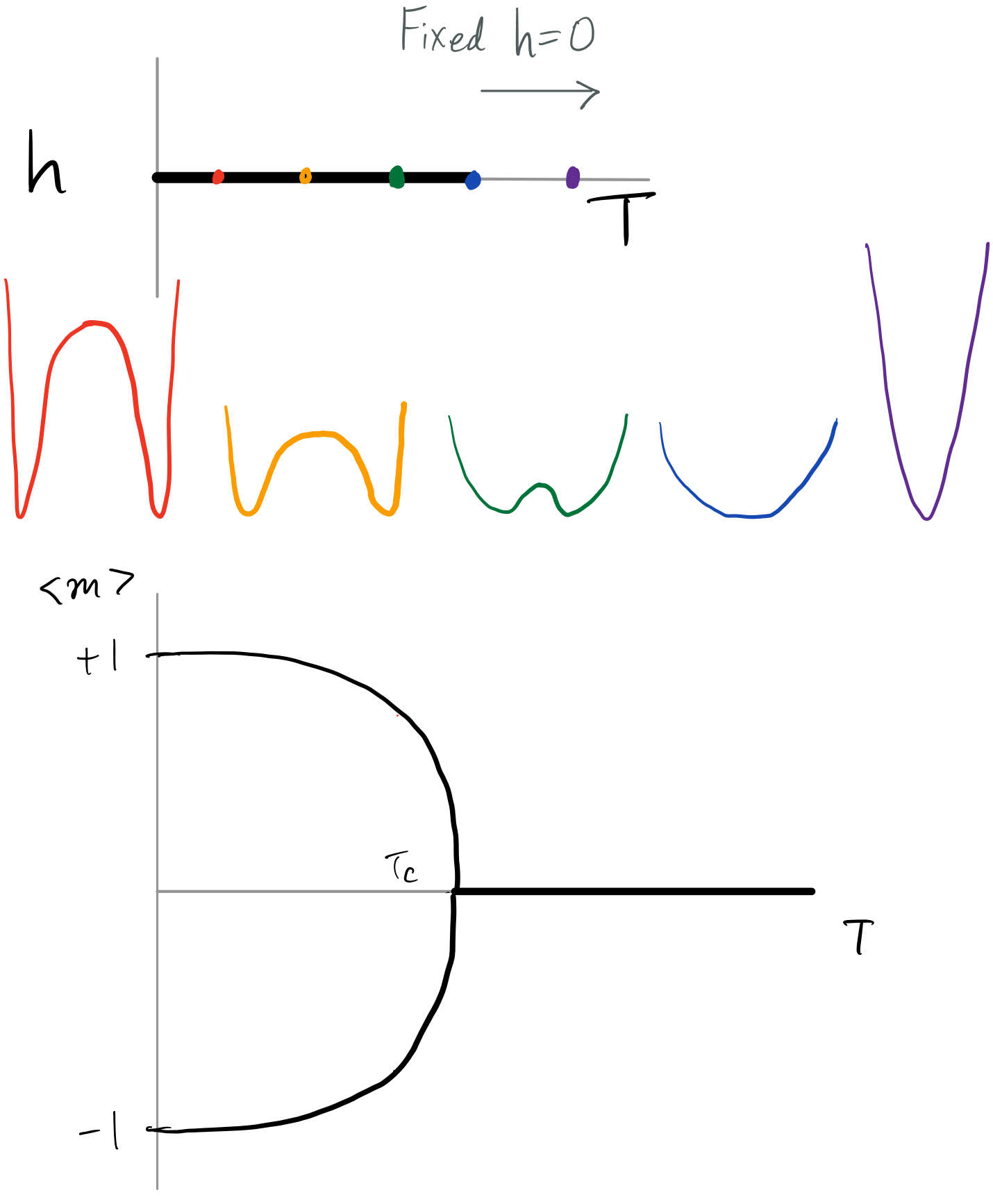


This is a "first order" phase transition —
a discontinuous jump in an order parameter (m)

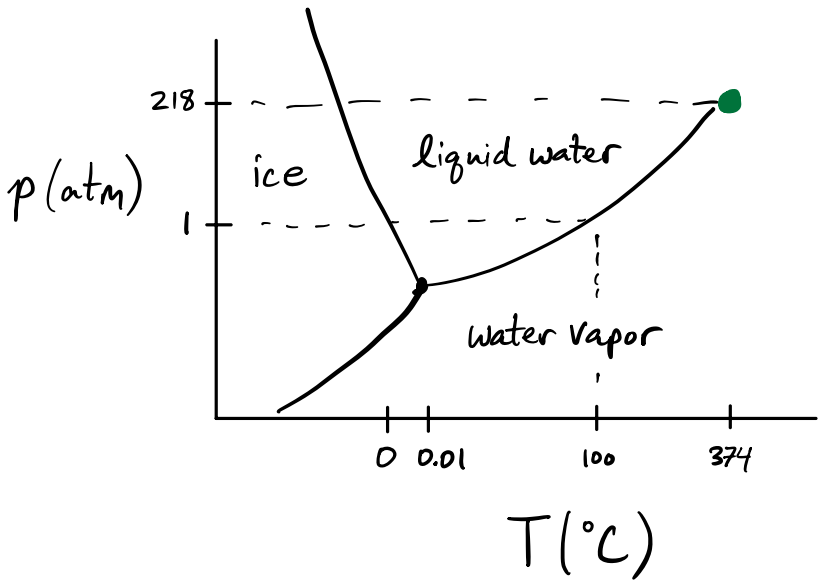
(Ex. liquid $H_2O \rightarrow$ ice)

The position of the minima shift smoothly, but which minimum dominates jumps as a function of h.

By contrast, a "second order" phase transition involves a critical point. Spontaneously broken symmetry on one side; the minima have merged together on the other.


Fixed h=0
h
T
<m>
+1
-1
T_c
T

Example:



Am I a liquid or a vapor?

Ok. This has all been a nice story, but how do we know it's right?

We must perform calculations.

We consider two different (but related) calculations

(1)

$$\langle |m| \rangle = \sum_\nu p(\nu)\,|m(\nu)|$$

$$= \sum_\nu \frac{e^{-\beta E(\nu)}}{Q}\,|m(\nu)|$$

(2)

$$P(m) = \sum_\nu P(\nu)\,\delta(m(\nu) - m) = \sum_\nu \frac{e^{-\beta E(\nu)}}{Q}\,\delta(m(\nu) - m)$$

We could compute both if we could handle $\sum_\nu$.

How many possible microstates are there?

2D Ising...

grid	1x1	2x2	3x3	...	nxn
# of microstates:	2	2^{2^2}	2^{3^2}		2^{n^2}

huge

When spins did not interact we got to split up sums over microstates...

$$\left(\sum_{\text{states of a single spin}} \right)^N$$

N independent copies

Without that trick, we must learn either

(A) to count with more complicated mathematical tools

Mean field theory, Variational Methods, Renormalization Group

(B) to count with computers by sampling rather than enumerating.

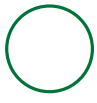
Counting by sampling?!

Claim: $\langle |m| \rangle$ is really a high-dimensional sum/integral

$$\langle |m| \rangle = \sum_{S_1=\pm 1} \sum_{S_2=\pm 1} \cdots \sum_{S_N=\pm 1} \frac{e^{-\beta E(S_1, S_2, \ldots, S_N)}}{Q(\beta, h)} \left\langle \left| \frac{1}{N} \sum_i S_i \right| \right\rangle$$

Sum/integrate out 1st spin

Let's first think about a lower dimensional integral. What is the area of a circle with diameter one?



$$\text{Area} = \frac{\pi}{4}$$