Lecture 16

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

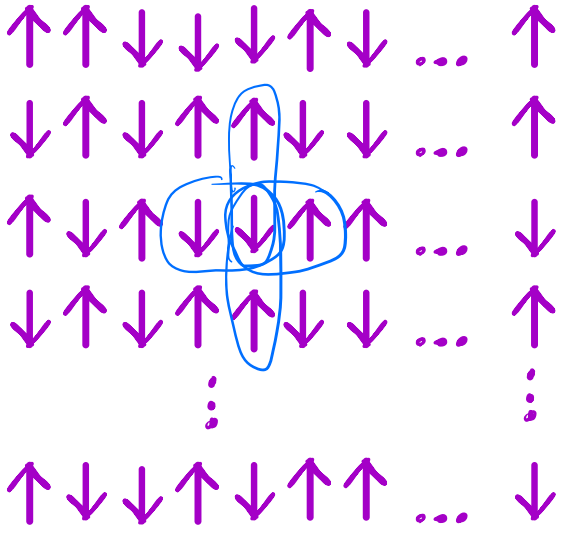
an interaction between spins

"Coupling constant"

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

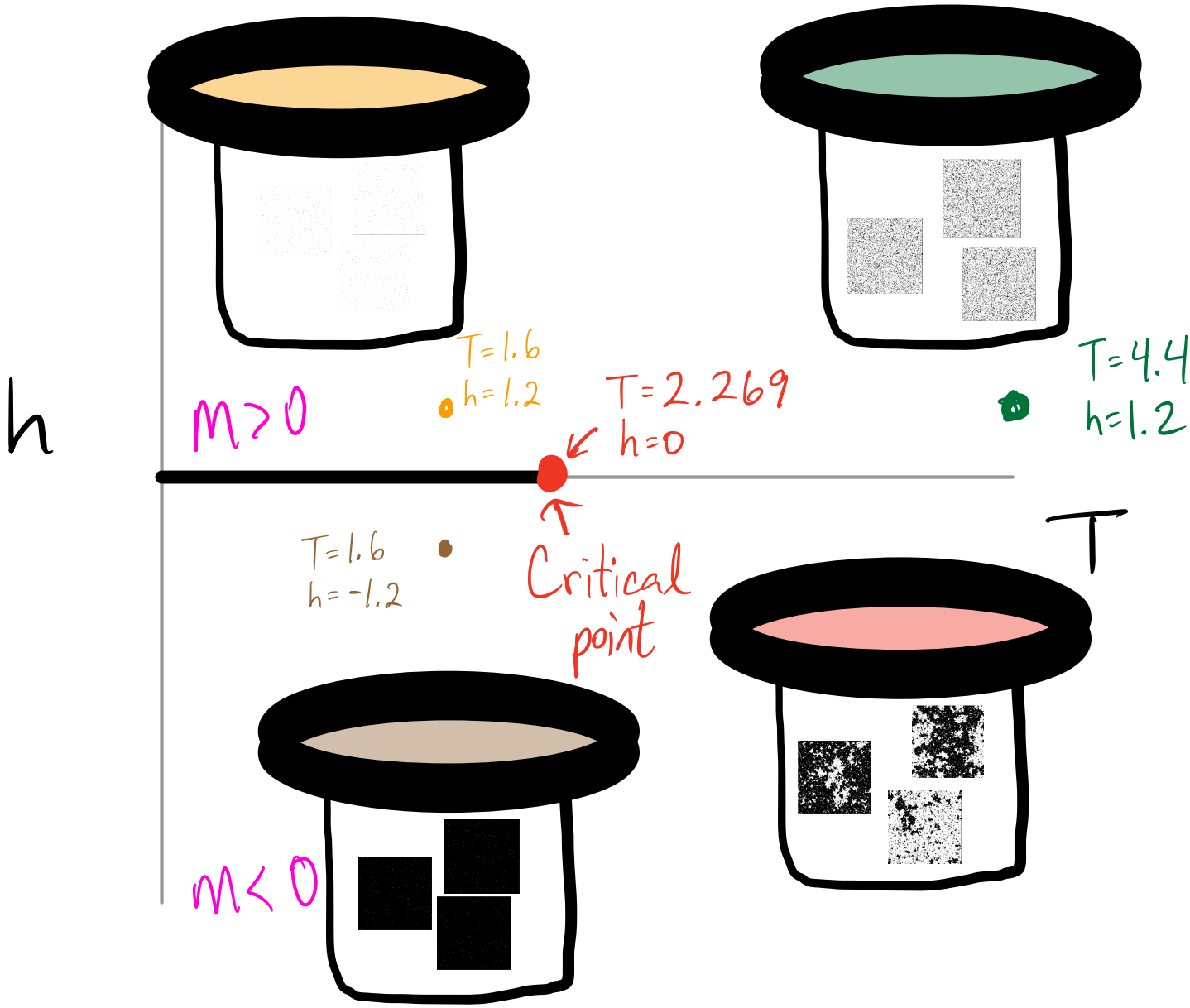
The $\frac{1}{2}$ allows us to include $i=1, j=2$ and $i=2, j=1$ terms in the sum — "double counting"

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

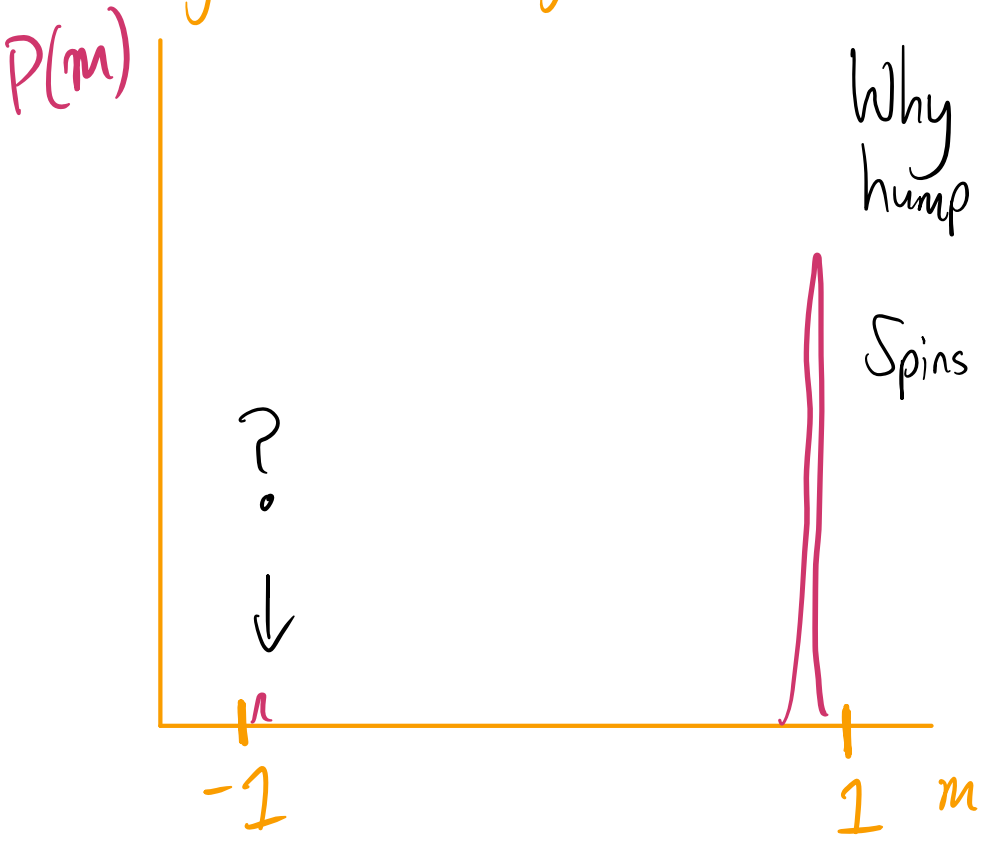


One can do it by hand. Perhaps not you or I. Lars Onsager did it.

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

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

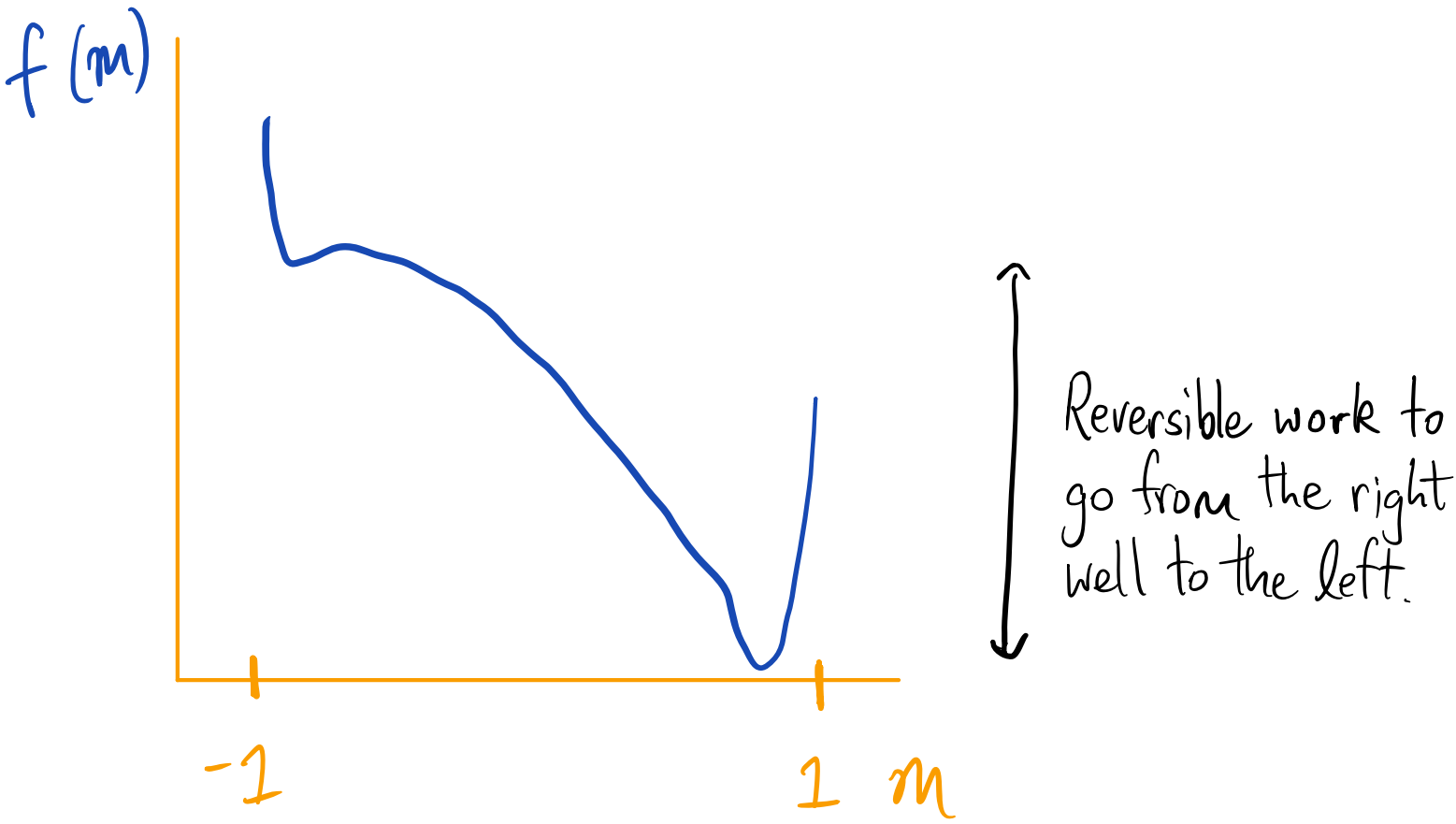
$f(m)$: free energy of magnetization (per spin)

Aside:

Rearranging...

An example of a large deviation function.

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



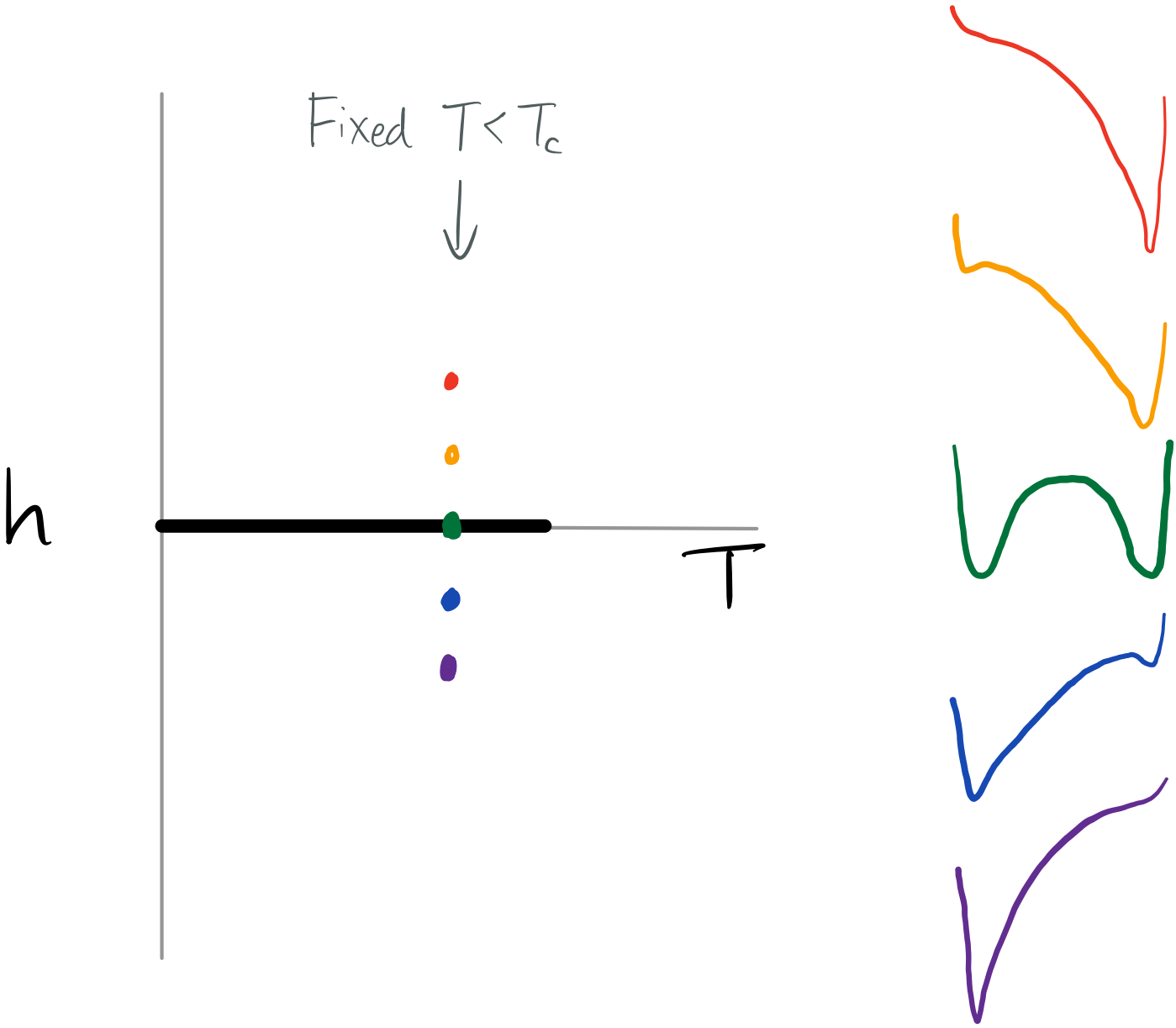
In what ways is $f(m)$ an effective energy?

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

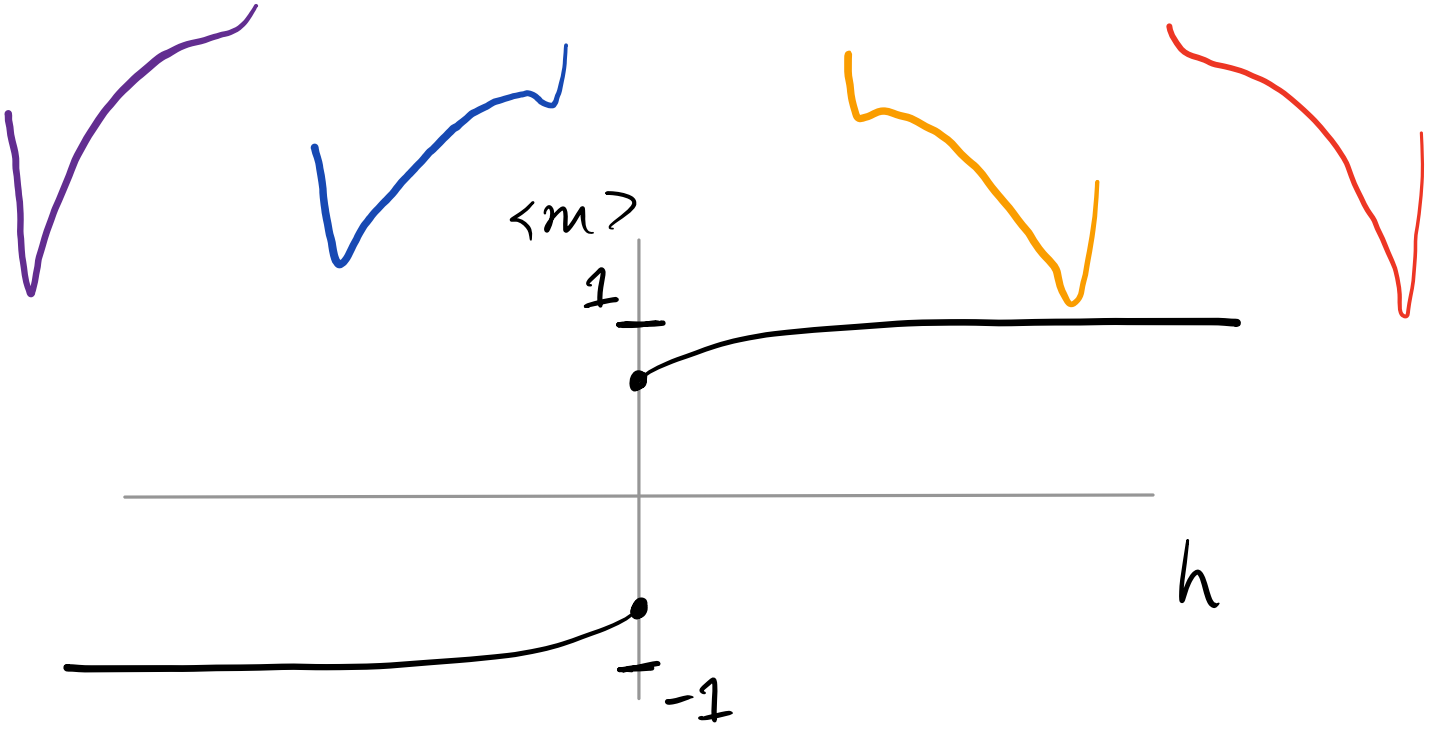
2. It is the reversible work to change the magnetization

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...

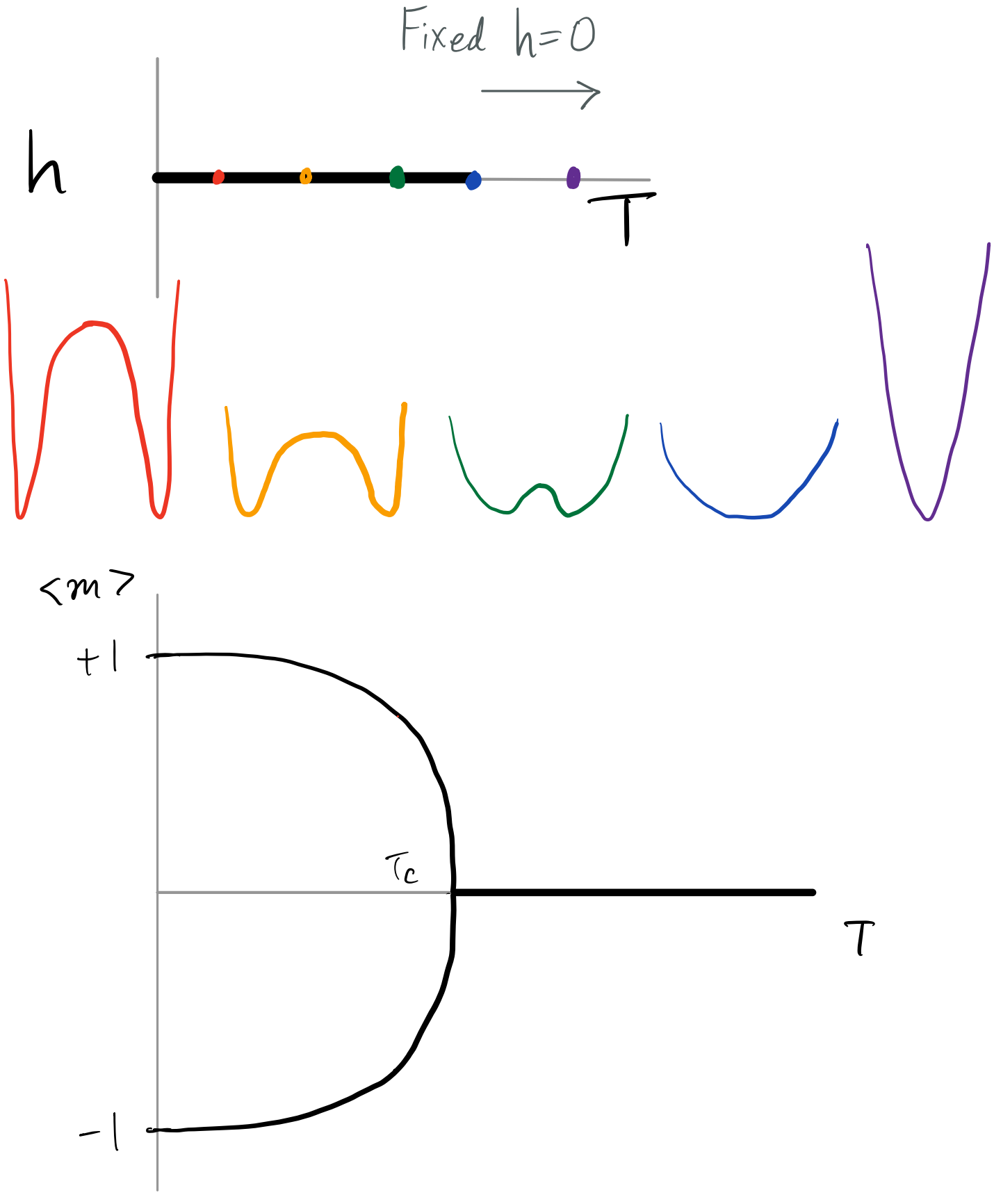


This is a "first order" phase transition —
a discontinuous jump in an order parameter (m)

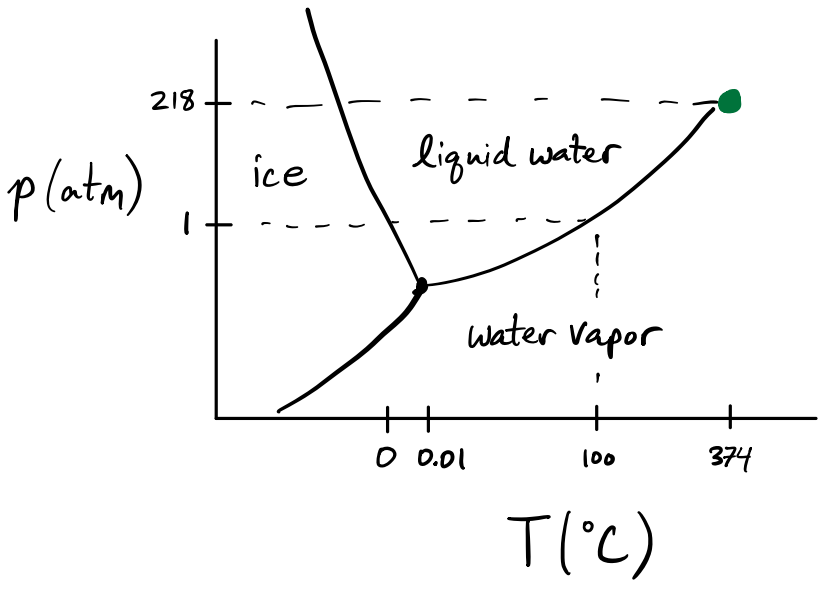
(Ex. liquid $H_2O \rightarrow$ ice)

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.

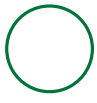
Counting by sampling?!

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?



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

Why is that an integral?

$$\text{Area} = \int_{-\frac{1}{2}}^{\frac{1}{2}} dx \int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} dy \quad 1$$

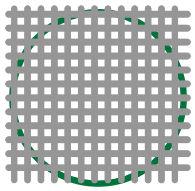
These integrals are summing over all the possible points in the circle

Hm... This is a lot like our microcanonical calculations in that every possible state (x,y) gets equal weight. Then Area is like a microcanonical partition function.

As continuous variables, you can never list out all of the possible values of x & y.
To get the value of the integral, we need either:

(A) to count with more complicated mathematical tools
calculus, geometry

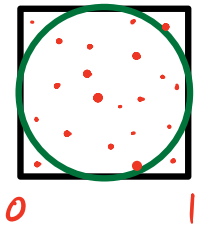
(B) to count by numerically approximating the integral



Break it up into boxes and count the boxes — a Reimann sum. Answer gets more correct as grid size $\to 0$.

But there is another way...

Throw darts. Monte Carlo



Throw darts in the square and count the fraction that land in the circle.

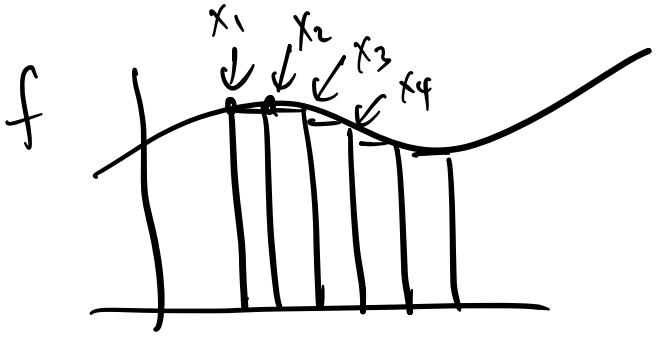
- Randomly draw x coordinate from $U[0,1)$
- Randomly draw y coordinate from $U[0,1)$
- Check if $x^2+y^2 \leq 1$.

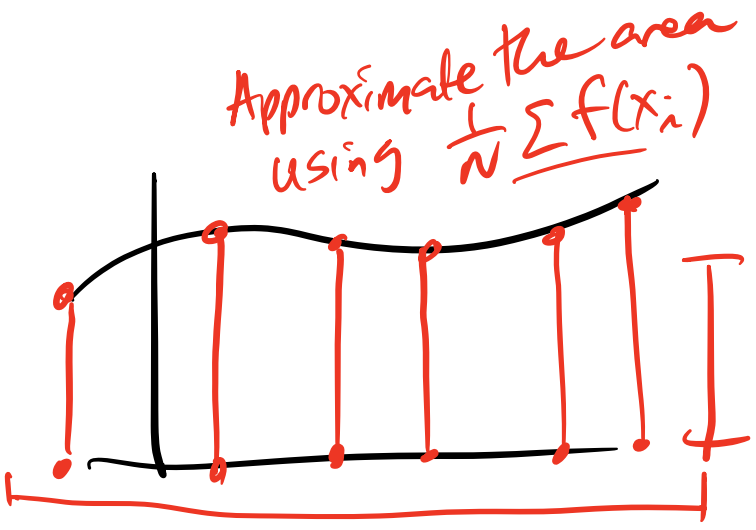
$$\lim_{\#\text{ of darts}\to\infty} (\text{fraction in circle}) = \frac{\pi}{4}$$

Reliance on random numbers ⇒ "Monte Carlo" (MC)

Why use MC in lieu of a grid?

Scaling with dimensionality.
Beyond 2 or 3 dimensions, grids get very expensive





MC is easily adaptable if we want to compute some other integral.

$$\text{Area} = \int_{-\frac{1}{2}}^{\frac{1}{2}} dx \int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} dy \; 1$$

$$\langle x^2 \rangle = \int_{-\frac{1}{2}}^{\frac{1}{2}} dx \int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} dy \; x^2 \Big/ \text{Area}$$

Throw darts

Weighted Average

- Randomly draw x coordinate from $U[0,1)$
- Randomly draw y coordinate from $U[0,1)$
- If $x^2+y^2 \leq 1$, add (x,y) to a list
- $\langle x^2 \rangle = \frac{1}{N} \sum x_i^2$ from that list

VERY SIMPLE! (That's why we like it)

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

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

Sum/integrate out 1st spin

Throw darts

Weighted Average

Randomly pick ± 1 for each S_i (uniformly)

Give the spin configuration a weight of

$$\frac{e^{-\beta E(S_1, S_2, \ldots, S_N)}}{Q(\beta, h)} \left| \frac{1}{N} \sum_i S_i \right|$$

Uh oh!

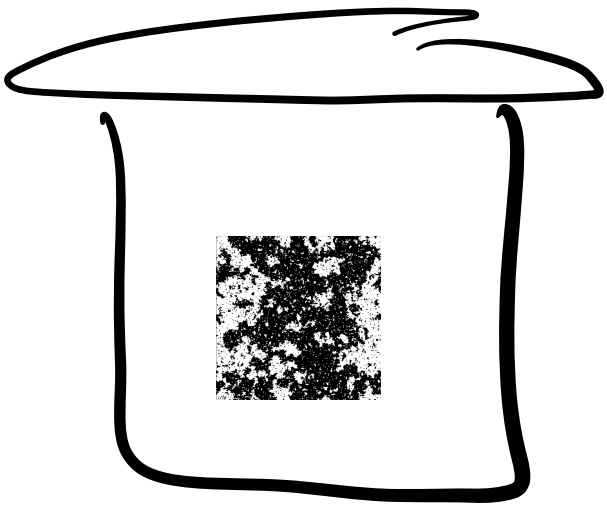
That weight requires that we know $Q(\beta, h)$

(If we already knew that we could have found $\langle m \rangle$ by differentiating!)

Let's inspect the weighted average

$$\underbrace{\frac{e^{-\beta E(S_1, S_2, \ldots, S_N)}}{Q(\beta, h)}}_{\text{Probability (in the canonical ensemble) of the particular spin configuration } S_1, S_2, \ldots, S_N} \underbrace{\left\langle \left| \frac{1}{N} \sum_i S_i \right| \right\rangle}_{\text{Weight that the configuration contributes}}$$

If I could write a computer program which behaves like the magic hat...



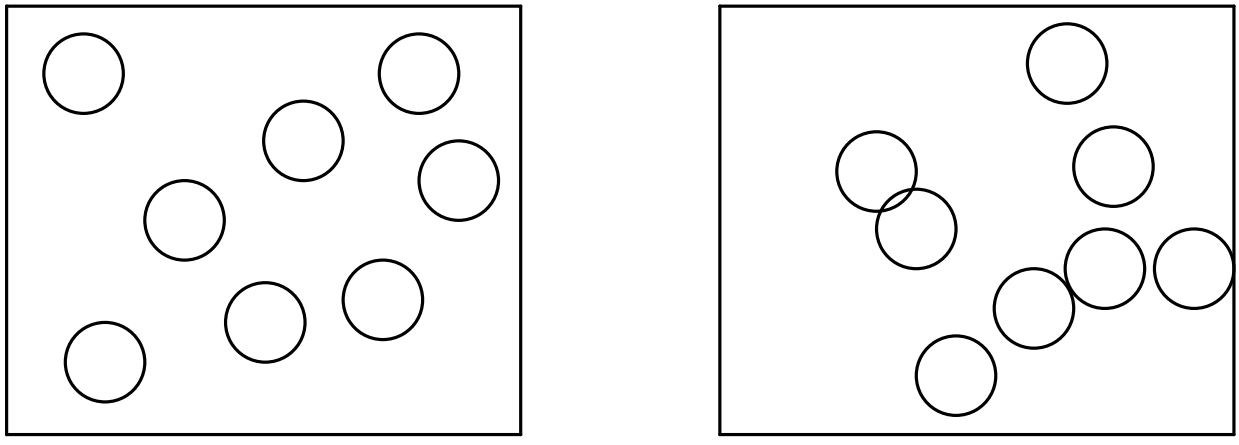
Hat contains every ν with the right probability $e^{-\beta E}/Q$

1. Draw a configuration
2. Compute $|m|$ for that configuration
3. Average these $|m|$ values over many randomly chosen configs.

How do I generate spin configurations with this correct probability?

Use Dynamics!

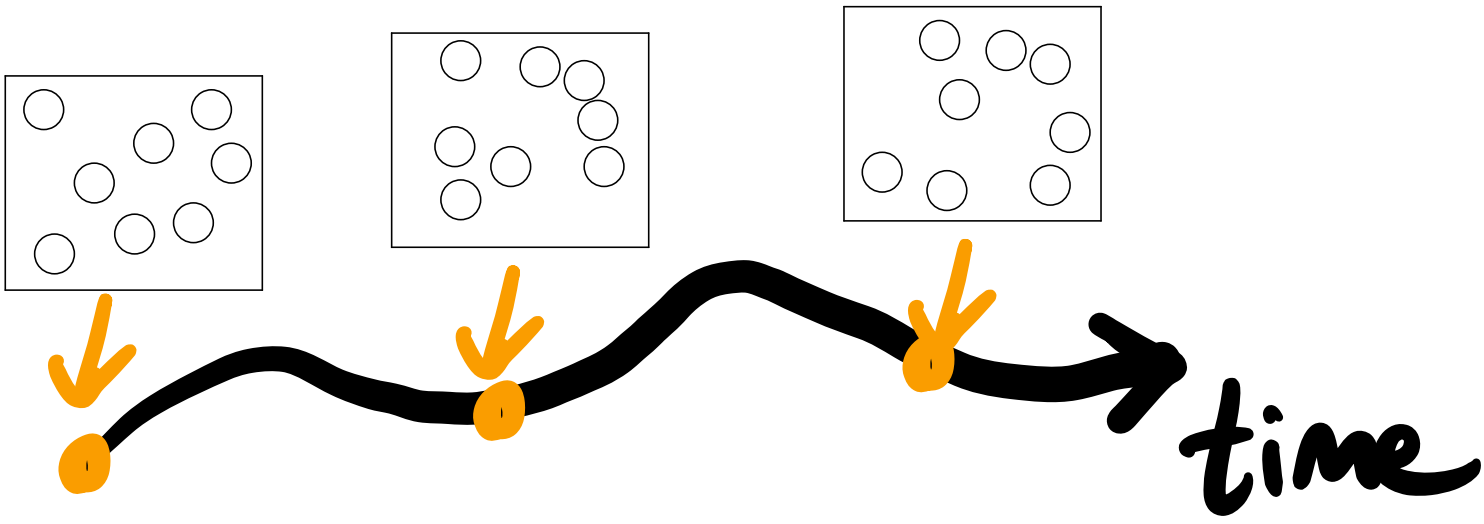
Suppose I had a bunch of hard spheres as a model of a gas. Hard means they can't overlap, so this is more complicated than an ideal gas.



The problem of overlap...

the computer will waste most of its time proposing impossible microstates that have overlapping particles.

But Hamiltonian dynamics conserves energy, so you could give every particle a momentum & carry out Newton's laws.

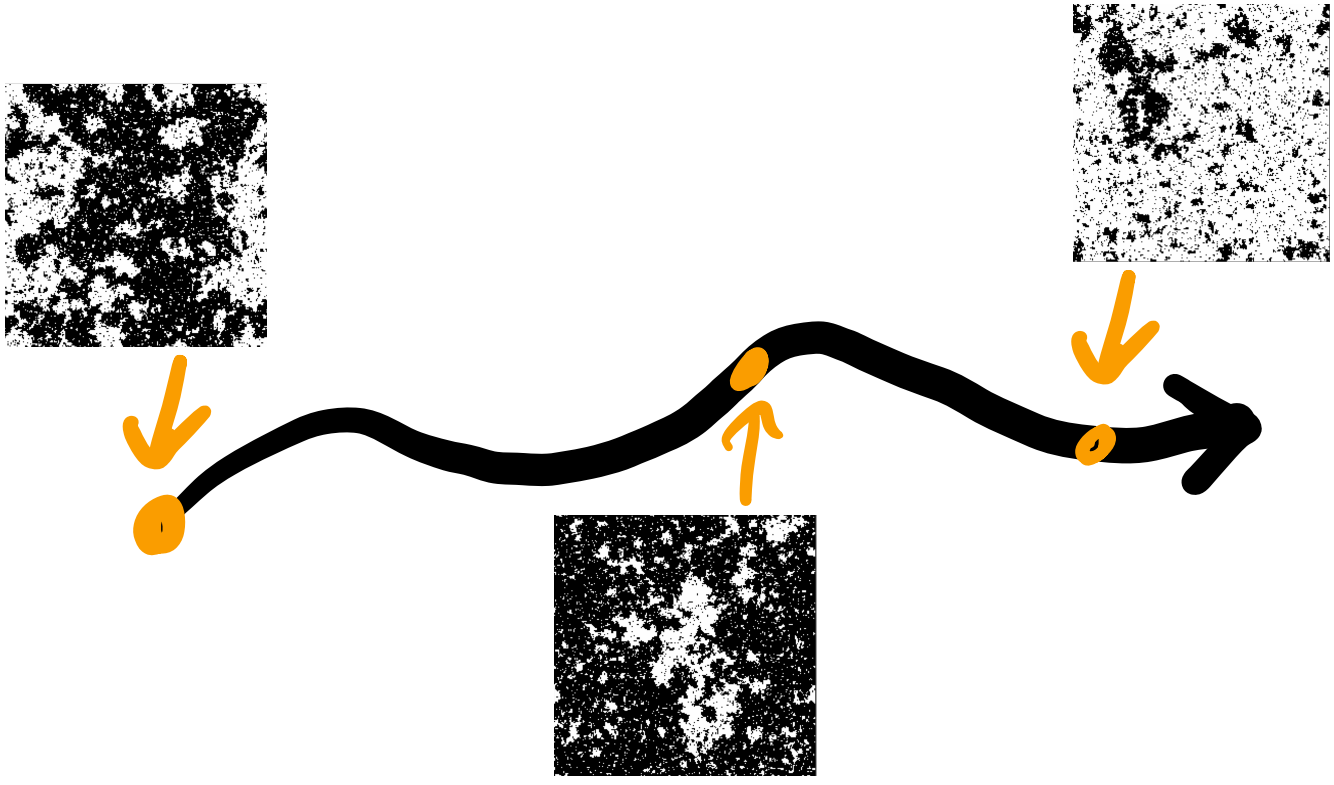


Every so often, stop the movie and take a new configuration out.

The magic here is that we know what ensemble (microcanonical) is generated by the Hamiltonian dynamics, so the probability of the configuration is automatically baked into the procedure for generating new configurations.

This strategy is <u>not</u> limited to sampling a microcanonical ensemble.

How should we sample spin configurations from the canonical ensemble?



?!

We will make up a dynamics (a set of rules for how to transition from one configuration to another), constructed for the sole purpose of visiting the various microstates with probability $e^{-\beta E}/Q$