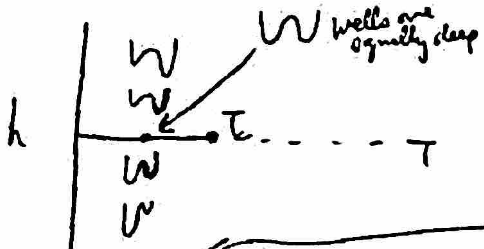
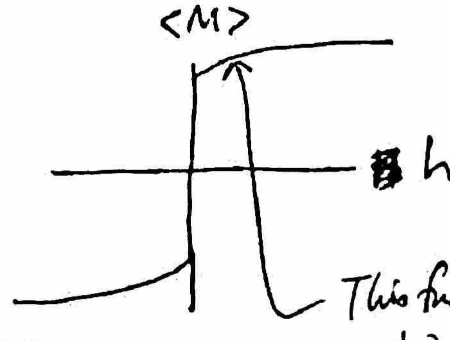
Recap: Ising model – A minimal model for phase transitions in ferromagnets and in liquid/vapor phase transitions of a "lattice gas"

$$E = -h\sum_i S_i - J\sum_{i,j}{}' S_i S_j$$



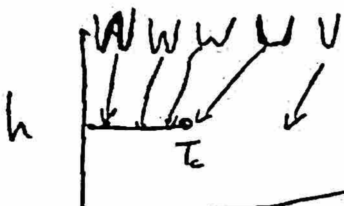


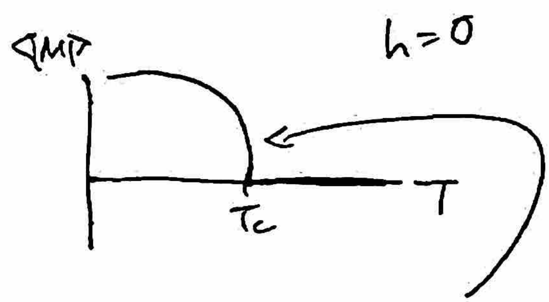
This function is not continuous at $h=0$

Whether the left or the right well is lower changes when $h>0$ vs $h<0$, so which minimum we see jumps discontinuously

A discontinuous phase transition like this is called first order.

Contrast this with...





The location of the minima are shifting around until they merge together at $T=T_c$

This function is continuous at $T=T_c$ but is not continuously differentiable

A continuous phase transition (whose derivative is discontinuous) is called second order

This is all a nice story, but how do we know it is right?

We must do calculations. There were two different (but related) calculations we considered.

(1) $\langle |M| \rangle = \sum_{\nu} P(\nu)\,|M(\nu)| = \sum_{\nu} \frac{e^{\beta E(\nu)}}{Q(\beta)}\,|M(\nu)|$

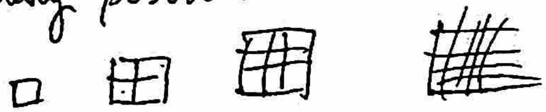
with $Q(\beta) = \sum_{\nu} e^{-\beta E(\nu)}$

(2) $P(M) = \sum_{\nu} P(\nu)\,\delta(M(\nu)-M) = \sum_{\nu} \frac{e^{-\beta E(\nu)}}{Q(\beta)}\,\underbrace{\delta(M(\nu)-M)}_{\text{count microstate iff it has magnetization } M.}$

 ← This is $\underbrace{A(M)}_{\text{free energy of magnetization}} = -\ln P(M)$

$\sum_{\nu}$ ← We can compute either if we just sum (average) over all possible microstates.

How many possible microstates are there?



grid	1x1	2x2	3x3	..	N×N
# of microstates	2	2^4	2^9		2^{N^2} ⟸ This is a BIG number. Uh oh.

When the spins did not interact, we got to split the sums

$\left(\sum_{\text{single spin}} \right)^{N}$ ← N independent copies.

Without that trick we have to either learn

A. To count w/ more complicated mathematical tools
- Mean field theory
- Variational Methods
- Renormalization Group (Not really a group)

$\boxed{\text{B. To count w/ computers by \underline{sampling}, not enumerating.}}$

Count by sampling? What's up with that?

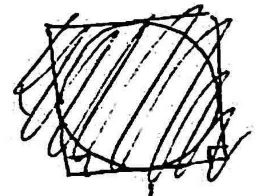
> In this discussion we will be very loose with distinctions between sums and integrals, discrete spaces and continuous spaces.

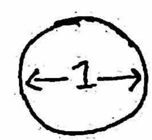
An average like $\langle |M| \rangle$ is effectively just an integral. But its a very high dimensional integral.

$$\langle |M| \rangle = \underbrace{\sum_{S_1=\pm1}}_{\text{Sum/integrate out 1st spin}} \sum_{S_2=\pm1} \cdots \sum_{S_N=\pm1} \frac{e^{-\beta E(S_1,S_2,\cdots S_N)}}{Q(\beta,h)} \cdot \left| \sum_{i=1}^{N} S_i \right|$$

Let's first think about a lower dimensional integral.

What is the area of a circle with diameter 1?





Area $= \dfrac{\pi}{4}$

Why is that an integral?

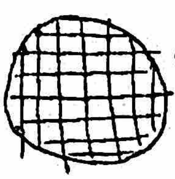
$$A = \underbrace{\int_{-\frac{1}{2}}^{\frac{1}{2}} dx \int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} dy}_{\text{These integrals are summing over all the possible points in the circle.}} \; 1$$

Hm. This is a lot like our microcanonical calculations in that every point (x,y) gets equal weight and then A is like a microcanonical partition function.

But here x + y are continuous variables, so we can never hope to enumerate every possible point. To get the value of the integral we needed:

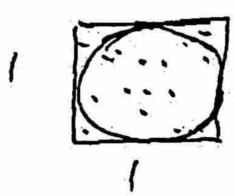
A. Fancy mathematical tools for counting
   • Calculus • Geometry

or B. Numerical ways to approximate the integral.



Break it up into boxes and count the boxes. - A numerical integral (Riemann sum)
This works very well,

But there is another way to numerically approximate the area.
You can throw darts.

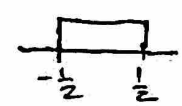


1. The area of the square is trivial, so we already know that integral.
2. Let's get the ratio of the circle's area to the square's area (like a ratio of partition functions)

What fraction of the darts land in the circle?

This is easy to compute! (Uniform dist. from $-\frac{1}{2}$ to $\frac{1}{2}$)

- Draw a random x coordinate from $U[-\frac{1}{2}, \frac{1}{2})$



- Draw a random y coordinate from $U[-\frac{1}{2}, \frac{1}{2})$
- Check if $\sqrt{x^2+y^2} \leq 1$, in which case your dart fell in the circle
- Repeat N times

$$\boxed{\text{Fraction of darts in the circle} \xrightarrow[N\to\infty]{} \frac{\pi}{4}}$$

Reliance on random numbers gave this the name Monte Carlo.

Why use Monte Carlo in lieu of a grid?

- Scaling w/ dimensionality.

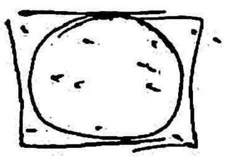
  Beyond 2 or 3 dimensions, grids get <u>very</u> expensive.

Note that the MC (Monte Carlo) scheme is easily adaptable when we want to integrate some other integrand.

For example

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

Now every point (x,y) does not get equal weight. Some pts. count for more than others.



1. Throw your darts
2. Of the darts that landed in the circle, compute x^2 for each pt. (x,y) and average.

VERY SIMPLE! That's why we like it.

Equivalent for

$$\langle |M| \rangle = \sum_{S_1=\pm1} \sum_{S_2=\pm1} \cdots \sum_{S_N=\pm1} \frac{e^{-\beta E(S_1,S_2,\dots,S_N)}}{Q(\beta, h)} \left| \sum_{i=1} S_i \right|$$

1. Throw your darts $\Rightarrow$ Randomly pick ±1 for each S_i
2. Weight the point by x^2 $\Rightarrow$ Weight the random spin configuration by

$$\frac{e^{-\beta E(S_1,S_2,\dots S_N)}}{Q(\beta)} \left| \sum_{i=1} S_i \right|$$

UH OH! That weight requires that we know $Q(\beta)$!
(If we already knew that we could have gotten $\langle M \rangle$ by differentiating!)

$$\underbrace{\frac{e^{-\beta E(s_1,\dots s_N)}}{Q(\beta,h)}}\quad \underbrace{\left|\sum_i s_i\right|}$$

We have a weighted average

Weight that the configuration contributes

Probability (in the canonical ensemble) of the particular spin configuration $s_1, s_2, \dots, s_N$

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

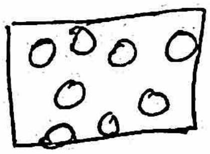
hat contains every spin configuration with the right probability $\frac{e^{-\beta E}}{Q}$

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

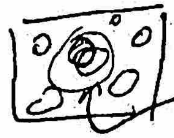
How do I generate spin configurations w/ this correct probability?

Answer: Utilize 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.

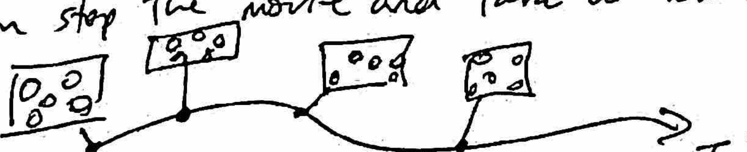


I'd love my magic hat to just randomly produce a new configuration from the microcanonical ensemble, but if I randomly pick a position for each particle, I'm likely to produce



overlap. (Invalid configuration)

But Hamiltonian dynamics conserves energy, so you could give every particle a momentum + carry out Newton's laws. Every so often you stop the movie and take a new configuration out.



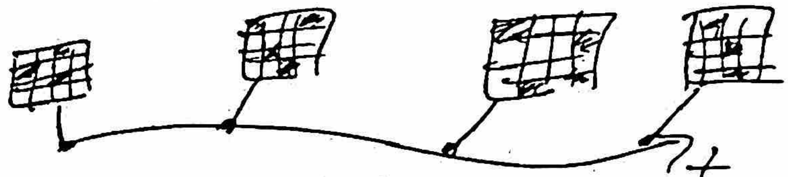
Time

The magic here is that we know what ensemble is generated by the Hamiltonian dynamics, so the stats. of a config. is baked in.

This strategy is not limited to sampling a microcanonical ensemble.

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

Then the game will become...



$\Rightarrow$ Run the dynamics $\leftarrow$ Markov chain Monte Carlo Dynamics

Collect samples occasionally

Average $|M|$ for each collected sample, but the $\frac{e^{-\beta E}}{Q}$ is not part of the average. It is already baked into the likelihood of generating each sample.