Phase transitions:
Part 1
We are all very familiar w/ phase transitions in our day to day life, but we don't always think about many interesting aspects:

1) What is happening microscopically?
2) What is happening macroscopically?
3) How many phase transitions have "universal" properties that don't depend on the specific system. This is what has fascinated people from way back far ~100 years.

4 major modern areas of work:

1) How to sample/observe/predict phases in smalgtim
2) What happens in unusual environments, e.g. w/ confinement (water in a nanotube, protein...)
3) What is phase diagram for many components (lipids...)
4) What happens out of equilibrium?

We have to start w/ the basics to understand the more complex phenomena.
Cross a line, discontinuity in some quantity: e.g., density
Ehrenfest: discontinuity in deriv. of free energy (Density ~ \( n/p \))
Modern definition: has to be latent heat at crossing
C For right, can go between phases w/o latent heat or weird behavior.

C Critical point: 2nd order phase transition
Ehrenfest: Continuous in first deriv, but discontinuous change in second deriv.
Modern: "Continuous" phase transition, diverging susceptibility, power-law divergence of correlation length
(Discuss more later)

Typically, break symmetry in 1 direction

Liquid \rightarrow solid, translational symmetry
Liquid \rightarrow gas, \( \sigma \) correlation length \( \rightarrow \) finite correlation length
Need model systems to analyze to illustrate the important concepts and which can be "solved" on the computer or on paper.

Magnetization Phenomenon:

Spins on lattice, like being in same direction but entropy prevents ordering. Lower $T$ or increasing $B$ field has ordering transition.

Need "order parameter" to describe a phase transition, a quantity that distinguishes the phases. $P$, $P_r$ works for liquid-gas or liquid solid, 0 when a liquid, nonzero otherwise.

Here, $M = \left| \sum_{i=1}^{N} \sigma_i \right|$; $m = M/N$ is magnetization.

$M$ vs. $T$:

no field, "spontaneous magnetization"

$T_c$ is curie temp, Pierre Currie studied this transition.

Can we "derive" this result. Have to start w/ Hamiltonian in canonical ensemble and get $Z(N, V, T)$ to compute $M$. 

...
"Real" Hamiltonian: \( \mathcal{H} \) coupling tensor

\[
\mathcal{H} = -\frac{1}{2} \sum \mathbf{J}_{ij} \cdot \mathbf{S}_i \cdot \mathbf{S}_j - \mathbf{h} \cdot \mathbf{S}, \quad \mathbf{h} = \frac{\mathbf{h}_0 \mathbf{S}}{2}
\]

where \( \mathbf{S}_i = \frac{1}{2} \mathbf{\sigma}_i \leq \mathbf{1} \) matrix

**Approximation**, consider only \( z \) direction & field in \( z \)-direction, then

\[
\mathcal{H} = -\frac{1}{2} \sum \mathbf{J}_{ij} \cdot \mathbf{\sigma}_i \mathbf{\sigma}_j - \mathbf{h} \mathbf{\sigma}_i, \quad \mathbf{\sigma}_i = \mathbf{\sigma} \pm \frac{1}{2} \mathbf{\sigma}
\]

If we make the further approx that coupling is short ranged \( \mathbf{J}_{ij} = \mathbf{\sigma} \mathbf{\sigma}_i \mathbf{\sigma}_j \) & \( i \neq j \) neighboring sites

\[
\mathcal{H} = -\frac{1}{2} \sum \mathbf{J}_{ij} \mathbf{\sigma}_i \mathbf{\sigma}_j - \mathbf{h} \mathbf{\sigma}_i, \quad \mathbf{\sigma}_i \in \{\mathbf{\sigma}, \mathbf{\sigma} \pm \frac{1}{2} \mathbf{\sigma}\}
\]

\( \mathbf{\sigma} \) Ising Model

\( \mathbf{\sigma} \) (Invented by Lenz, given to good student \( \mathbf{\sigma} \) to study in 1924)

2 for free double We can solve in 1d, approx & exact, Onsager (1944) solved 2d exactly, no one has done 3d yet...

If \( J > 0 \), like to align, and \( h > 0 \), like to align facing up, \( h < 0 \), down

w/ \( h = 0 \), \( \mathcal{H} \) is min when all up or all down

So configuration \( \ldots \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \ldots \) has \( M = 0 \), and \( \mathcal{E} = -N J + \frac{1}{2} h \), so interface has constant \( \mathcal{E} \) at

\( \mathcal{E}_{\text{min}} \)

1 in \( N \), hence only at \( T = 0 \) do you expect full phases.
in 2d: interface typically of size $N^{1/2}$ and this is big enough cost to stabilize ordered state ("surface tension")

Still can learn a lot from 1d ising model, including mapping all sorts of physical problems to it, like adsorption to / surfen or folding of peptides. So what is $Z(N,V,T)$?

Let's rewrite $H = -J \sum_{i=1}^{N-1} s_i s_{i+1} - h \sum_{i=1}^{N} s_i$

we can add periodic boundary conditions, $s_N = s_1$ and write in a more symmetric way

$$H = -\frac{J}{2} \sum_{i=1}^{N} s_i s_{i+1} - h \sum_{i=1}^{N} \frac{1}{2} (s_i s_{i+1} + 1)$$

$$Z = \sum_{\{s_i\}} e^{-\beta E}$$

$$= \sum_{s_1} \sum_{s_2} \cdots \sum_{s_N} \prod_{i=1}^{N} \left( e^{\beta (s_i s_{i+1} + \frac{1}{2} (s_i + s_{i+1}))} \right)$$

for $h=0$

$$= \sum_{s_1,s_2,\cdots,s_N} e^{\beta s_1 s_2} \cdots e^{\beta s_{N-1} s_N} e^{\beta s_N s_1}$$

Let $s_0 = s_1 s_N$, can only be $\pm 1$, but 2 ways
\[
\sum_{\sigma_1, \sigma_2} e^{\beta J \sigma_1 \sigma_2} = 2 \left( \frac{\beta}{2} \right)^N \left( e^{\beta J} + e^{-\beta J} \right)^N = 2 \left( 2 \cosh (\beta J) \right)^N
\]

\[
f = \frac{F}{N} \approx k_B T / N \log 2 = - \frac{1}{\beta} \log \left[ 2 \cosh (\beta J) \right] + \text{const}
\]