Impossibility of phase transitions in systems with short-range interactions (Peierls) in one dimension.

Think of an ordered Ising model

```
++ + + + + + + + + + + + + + + + +
```

How stable is it to the opposite phase

```
++ + + + + + + + + + + + + + + + +
```

Clearly the extra energy $\Delta E$ is due to the boundary

$$\Delta E = + J$$

If $J$ is the interaction constant. But the system's state is determined by minimizing the free energy, at non-zero temperature.

$$\Delta F = \Delta E - T \Delta S$$

where

$$\Delta S = k_b \ln (\# \text{ of states})$$

Clearly the boundary can be anywhere in the 1-d chain of length $L$, so

$$\# \text{ of states} = O(L).$$
and
\[ \Delta F = +J - k_B T \ln L \]
so that the free energy decreases and is minimized as \( L \to \infty \) by adding boundaries in \( d = 1 \). No stable phases for \( d = 1 \) and short range forces. Special cases involve interactions \( J \) or \( \frac{1}{|x_i - x_j|} \) when \( \theta \leq 2 \), where "phases" can be stabilized. In higher dimensions, phases are stable.

Consider \( d = 2 \)

\[
\begin{array}{c}
+++
+ + +
\end{array}
\]

With boundary

\[
\begin{array}{c}
+++
+ + +
\end{array}
\]

\[
\begin{array}{c}
+++
+ + +
\end{array}
\]

\[
\begin{array}{c}
+++
+ + +
\end{array}
\]

As before, \( \Delta E = +J \times L \), where \( L \) is length of boundary, and
\[ \Delta S = k_B \ln L^2 \]
as the boundary can go anywhere.
So in two dimensions
\[ \Delta F = + JL - 2kqL \ln L \]
and the 1st term wins. F is minimized by minimizing boundaries, and stable phases arise. It is straightforward to do this for higher dimensions. Some subtleties in \( d = 2 \) with oriented "vector" order (Mermin-Wagner theorem, Kosterlitz-Thouless phase transition) which we will not cover.

Continuing in \( d = 2 \), we can get some idea of the nature of symmetry breaking for \( H = 0 \), where, in the partition function, \( \langle m \rangle = +1 \) as \( \langle m \rangle = -1 \) are equally likely. Consider the dynamical process of going from one stable \( \langle m \rangle = -1 \) state to the \( \langle m \rangle = +1 \) state by applying a small external field \( H \to 0^+ \).
Process involves nucleation of droplet of more stable phase when $H > 0$ is applied.

E_{droplet} = + J R_{d-1} - H R_d

Droplet must be bigger than critical size or else it shrinks and disappears. Get critical size of droplet from

$$\frac{\partial E_{droplet}}{\partial R} = 0 = J (d-1) R_c^{d-2} - dH R_c^{d-1}$$

So

$$R_c = \frac{J}{H}$$

as $H \to 0$.

Probability of droplet is $e^{-E_{droplet}}$. 

- E_{droplet}/tc
Rate of appearance of droplet is:

\[ \text{Rate} = \left( \text{attempt frequency} \right) \left( \frac{\text{phase volume}}{\text{space volume}} \right) e^{-\frac{E_{\text{PROPELLENT}}}{k_B T}} \]

\[ = \left( 10^{-10} \right) (N) \exp - \frac{1}{\left( \frac{J}{H k_B T} \right)} \]

\[ \text{Rate} \rightarrow 0 \quad \text{as} \quad H \rightarrow 0 \]

Let \( H = 0 \) above

\[ \text{Rate} \leq \exp - \frac{JR^{2-d}}{k_B T} \]

Time to happen \( \propto \exp \left( \frac{1}{d-1} \right) \)

Put in \( R \sim (10^{23})^{\frac{1}{d}} \)

Time to happen \( \propto \exp \left( 10^{23} \right)^{\frac{d-1}{d}} \)

Impossible crazy long time.

Same as Boltzmann calculation on direction of time.
Another example of mean-field theory.

Consider the model of $N$ vector spins in three dimensions. At every site $i = 1, 2, \ldots, N$ there is a three-dimensional vector $\vec{S}_i$ which can point in any direction on a unit circle. First let's solve the paramagnetic case.

$$E = -\vec{H} \cdot \sum_{i=1}^{N} \vec{S}_i = -H \sum_{i=1}^{N} S_i \cos \theta_i$$

and the sum over states is

$$\sum_{\text{states}} = \frac{1}{4\pi} \sum_{\text{orientations}} = \frac{N}{4\pi} \frac{2\pi}{4\pi} \int_{0}^{\pi} \sin \Theta \, d\Theta_i$$

so the partition function is

$$Z_N = (Z_1)^N$$

where

$$Z_1 = \frac{1}{2} \int_{0}^{\pi} \sin \Theta \, d\Theta \, e^{\frac{H}{k_B T} \cos \Theta}$$

Letting $x = \frac{H}{k_B T} \cos \Theta$, we can do this.
\[
\frac{1}{Z_1} = \frac{1}{N} \exp \left( \frac{1}{k_B T} \sinh \frac{H}{k_B T} \right)
\]

and
\[
F = -k_B T \ln N \sinh \frac{H}{k_B T}
\]

The magnetization is
\[
m = -\frac{1}{N} \frac{\partial F}{\partial H} = -\frac{1}{N k_B T} \frac{\partial F}{\partial H} = \frac{1}{N k_B T} \sinh \frac{H}{k_B T}
\]

Note this is the magnitude of the magnetization \( |m| \).

\[
m = -\frac{1}{h} \coth h + \frac{1}{3h^5} \coth h
\]

where \( h = \frac{H}{k_B T} \).

We need to investigate \( m \) small and \( h \) small so we use
\[
\coth h = \frac{1}{h} + \frac{h}{3} - \frac{h^3}{45} + \ldots
\]

\[
m = \frac{h}{3} - \frac{h^3}{45} + \ldots \quad \text{with} \quad h = \frac{H}{k_B T}
\]

For \( H = 0 \), \( m = 0 \) is the only solution.
Back to mean field. The interaction vector model is

$$E = -J \sum_{i,j \neq i} \mathbf{S}_i \cdot \mathbf{S}_j - H \sum_i \mathbf{S}_i$$

8 neighbours = 6 for cubic lattice with no double counting.

Let

$$E = -\sum_i H_i \cdot \mathbf{S}_i$$

as before, so

$$\frac{\Delta E}{\Delta \mathbf{S}_i} = H_i$$

and

$$\frac{\Delta E}{\Delta \mathbf{S}_i} = J \sum_{j \neq i} \left( \mathbf{S}_j \cdot \mathbf{S}_{k, \neq i} + \mathbf{S}_j \cdot \mathbf{S}_{k, \neq i} \right) + H$$

$$= J, z \times \sum_j \mathbf{S}_j + H$$

so

$$H_i = J \sum_{j \neq i} \mathbf{S}_j + H$$

mean field

$$H_i \approx \langle H_i \rangle = \beta J m + H$$
\[ m = \frac{4}{3} \left( \frac{gJ}{k_B T} \right)^3 (for \ T = 0) \]

\[ m = \frac{gJ}{3k_B T} m - \left( \frac{gJ}{45k_B T} \right)^3 m^3 \]

Solutions are \( m = 0 \) for \( T > T_c \)

\[ \frac{4gJ^2}{k_B T} m^2 = \left( \frac{gJ}{3k_B T} \right)^3 - 1 \]

Let \( T_c = \frac{gJ}{3k_B} \), then close to \( T_c \)

\[ m < \left( \frac{T_c - T}{T_c} \right)^{1/2} \]

Note \( T_c \) is lower than Ising estimate from mean field.

Can also do this in \( d = 2 \) for the \( xy \) model. Will involve Bessel functions, but straightforward to get magnetization alone.
Again, start by solving paramagnet
\[ E = -\mathbf{J} \mathbf{H} \cdot \sum_i \mathbf{S}_i \]

We will have
\[ Z_N = (Z_1)^N \quad \text{and} \]
\[ F = -kT N \ln Z_1 . \]

\[ Z_1 = \frac{1}{\pi} \int_0^{\pi} \sin e \]

where
\[ h = \frac{\mathbf{J}}{k_B T} . \]

As before,
\[ m = -\frac{d \ln Z_1}{dh} = 2 \left[ \frac{1}{\pi} \int_0^{\pi} \sin e \right] \]

so,
\[ m = -\frac{\int_0^{\pi} \sin(e \cos \theta) \, e \, d\cos \theta}{\int_0^{\pi} e \, d\cos \theta} \]

Let \( x = \cos \theta \) to do top integral

and
\[ m = 2 \sinh h \]

\[ \frac{1}{\pi} \int_0^{\pi} \sinh e \cos \theta \, d\cos \theta \]

So,
\[ m (H=0) = 0 , \quad \text{as it should for a paramagnet} . \]

In mean-field theory, we again have in the sum over states,
\[ E = \langle \mathbf{H} \rangle \cdot \sum_i \mathbf{S}_i \]
where \( \langle H \rangle = g \langle \frac{1}{J} \rangle m + H \).

so, for \( H = 0 \), \( \langle H \rangle = g \langle \frac{1}{J} \rangle m \).

Go back to the expression for \( m \) and expand around small \( h \):

\[
m = \frac{-Z}{\beta} \frac{1}{\beta} \int_0^\beta \frac{d\beta}{1 + \frac{h^2}{4} + \frac{h^2}{6} + \ldots}
\]

\[
m = \frac{2h}{\beta} \left( 1 + \frac{h^2}{4} \right) \left( 1 - \frac{h^2}{12} \right) + \ldots
\]

\[
m = \frac{h}{\beta} \left( 1 + \frac{h^2}{4} + \frac{h^2}{6} + \ldots \right)
\]

so \( m = \frac{2h}{\beta} \left( 1 - \frac{h^2}{12} + \ldots \right) \)

Same form as before

\( m = aH - bH^3 \)

so we get solutions \( m = 0 \), \( T > T_c \)

and \( m \propto (T_c - T)^{2/3} \), \( \beta = \frac{1}{\delta}, \ T < T_c \)

where it turns out \( T_c = \frac{2gJ}{n} \)

a little less than mean-field for Ising.
Analyticity in phase transitions and in microscopic models

Microscopic models feature naturalness and locality, what we might call analyticity on small length scales.

Emergent behavior — the sum of \( N \to \infty \) of these microscopic entities — usually exhibits non-analytic behavior.

We have done one example in passing. The rate of nucleation in a first-order phase transition (involving discontinuities in the first derivatives of a free energy) was

\[
\text{Rate} \propto \exp \left( \frac{1}{4} \left( \frac{1}{4} - 1 \right) \right)
\]

so there is an essential singularity as \( H \to 0^+ \). First-order transitions are dynamical phenomena, and are fairly common place (water boiling, snowflake forming, ice melting). We will not discuss 1st-order transitions further.
Continuous phase transitions (historically called second-order phase transitions, because mean field theory give a discontinuity in the second-derivative of a free energy) occur in equilibrium. They exhibit power-law singularities which arise from non-analytic behavior. These transitions are uncommon, but their behavior is nevertheless very common in other emergent systems (power-laws, scaling).

\[ \text{Paramagnet} \quad \overset{H}{\rightarrow} \quad \overset{T}{\rightarrow} \quad \text{Paramagnet} \quad \overset{\text{Continuous phase transition}}{\rightarrow} \quad \text{Continuous phase transition} \]

\[ \text{Line of 1st order phase transitions} \]

\[ \text{H=0} \quad \overset{H\rightarrow0}{\rightarrow} \quad \overset{H\rightarrow\infty}{\rightarrow} \]

\[ T \quad M \rightarrow M \rightarrow \]

\[ \text{HCO} \]
The same things occur for a pure substance, though it is a little messier.

Compare this to

If we assume, for the magnet for simplicity, that the emergent
thermodynamic properties, like the shape of the $H$ vs. $m$ isotherm at $T = T_c$ are analytic

$$H = H(m=0) + \frac{\partial H}{\partial m} \bigg|_{T_c} m + \frac{1}{2} \frac{\partial^2 H}{\partial m^2} \bigg|_{T_c} m^2 + \cdots$$

But $\frac{\partial H}{\partial m} \bigg|_{T_c} = 0$, and $\frac{\partial^2 H}{\partial m^2} \bigg|_{T_c} = 0$

so, if the isothermic analytic, we always have

$$1 + \alpha m$$

critical exponent $\alpha = 3$. In fact wrong, $\alpha = 7/4$ in $d = 2$, $\alpha \geq 5$ in $d = 3$ and $\alpha = 3$ for $d \geq 4$.

One can show that all the mean-field values of the critical exponents follow if one assumes analyticity.