Ising model: represents alignment of spins in a material - magnetization w/ or w/o magnetic field

Suppose spins like to align

Observe behavior

\[ M = \frac{\sum \mu_i \hat{z}}{N} \]

max is \( N\mu \) all up

min is \( -N\mu \) all down

\[ B \text{ field along } \hat{z} \]

\[ m = \frac{M}{N\mu} \text{ tan } t + 1 \text{ to } y \]
But what about a field 

"spontaneous magnetization" 

@ high $T < \langle \vec{\mu} \rangle = 0$ random

So $M=0$

What about at low $T$'s if spins like to align

\[ m \]

\[ T \]

phase transition
First studied statistical therm by using using simplified model

can also be A/B (chem reaction or HC helix coil)

\[ S_i = \pm \frac{1}{2} \]

like to align with field.

\[ E_{\text{field}} = -hS_i \]

good to face up
like to align (feromagnetic)

\[ E_{\text{neighbor}} = -J S_i S_{i-1} - J S_i S_{i+1} \]

\[ E_{ik}^{Si} = -hS_i - J S_i (S_{i-1} + S_{i+1}) \]

\[ E_{\text{total}} = \sum_{i=1}^{N} -S_i \left[ h + \frac{J}{2} (S_{i-1} + S_{i+1}) \right] + \text{end terms} \]
$E$ is a function of $N$

can make pseudo infinite by saying $S_{\text{net}} = S_i$ and $S_0 = S_N$

then

$$E = \sum_{i}^{N} -J S_i S_{i+1} - h S_i$$

question is, what is $<S_i>$ may persis

have to consider partition function

what is partition func? Sum over all states

$$Q = \sum_{\text{States}} e^{-\beta E(S,kT)}$$

but what is a state?

particular set $S_1 = -\frac{1}{2}$ $S_2 = +\frac{1}{2}$ etc
\[ Q = \sum_{\{s_i\}} \sum_{j=1}^{s_1} \sum_{s_2} \ldots \sum_{s_n} e^{-\beta E(s_1, s_2, \ldots, s_n)} \]

Suppose \( \beta \gg h \) or \( s \) (energy units)

Then \( Q = 2 \sum_{j=1}^{s_1} \sum_{s_2} \ldots \sum_{s_n} = \text{counting states} = 2^n \)

\[ \text{What is } \langle s \rangle \]

\[ Q = \sum_{\{s_i\}} \sum_{j=1}^{s_1} \sum_{s_2} \ldots \sum_{s_n} e^{-\beta E(-\sum s_i + H)} \]

\[ \langle s \rangle = \langle \frac{\sum s_i}{N} \rangle = \frac{1}{N} \sum \sum \ldots \sum_{\{s_i\}} \sum_{j=1}^{s_1} \sum_{s_2} \ldots \sum_{s_n} e^{-\beta E(s_1, s_2, \ldots, s_n)} = \frac{1}{N} \cdot \langle s \rangle e^{-\beta E(s)} \]

\[ \frac{\partial \ln \theta}{\partial n} = \frac{1}{Q} \frac{\partial Q}{\partial n} = \sum_{\{s_i\}} \frac{\sum_{j=1}^{s_1} \sum_{s_2} \ldots \sum_{s_n} e^{-\beta E(s_1, s_2, \ldots, s_n)}}{Q} = \frac{N}{k_B T} \cdot \langle s \rangle \]
$\langle s \rangle = \frac{\partial \ln Q}{\partial n}$

$\langle s \rangle_{n=0} = \frac{k_B T}{N} \frac{\partial \ln Q}{\partial n}$

Another solvable case

$J=0$, this means $\mathcal{E} = -\frac{3}{2} h s_i$

$Q = \prod_{s_i=\pm 1} e^{\beta h s_i}$

$= \left( \prod_{s_i=\pm 1} e^{\beta h s_i} \right)^n = q^n$ (sites distinct)

$q = e^{\beta h/2} + e^{-\beta h/2}$
\[
\langle s \rangle = \frac{k_B T}{N} \frac{\partial \ln Q}{\partial \mathcal{H}} = k_B T \frac{\partial \ln Q}{\partial \mathcal{H}} = \left( \frac{3}{2} e^{\beta \lambda/2} - \frac{3}{2} e^{-\beta \lambda/2} \right) k_B T
\]

\[
= \frac{1}{2} \left[ \frac{e^{\beta \lambda/2} - e^{-\beta \lambda/2}}{e^{\beta \lambda/2} + e^{-\beta \lambda/2}} \right] = \frac{1}{2} \tanh (\beta \lambda/2)
\]

\[
\sinh (x) = \frac{1}{2} \left[ e^x - e^{-x} \right]
\]
\[
\cosh (x) = \frac{1}{2} \left[ e^x + e^{-x} \right]
\]

\[
\mathcal{E} = \sum_{i=1}^{N} \mathcal{H} s_i \quad \Rightarrow \quad \langle \mathcal{E} \rangle = \sum_{i=1}^{N} \mathcal{H} \langle s_i \rangle
\]

\[
= -N \mathcal{H} \langle s \rangle
\]

Question now is what happens if

\[ J \neq 0 \]
Turns out problem is solvable in 1d & 2d. \{3d or more no exact solution!

In 2d and higher, spontaneous magnetization even at zero field in thermodynamic limit will talk about how to solve 1d in context of helix-coil model.

What is H-C model?

\(\alpha\)-Helix is a common SS-element in proteins.

\(\rightarrow\) consider each residue as H or C conformation.