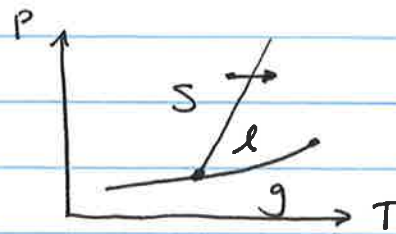
## Phase Transitions




$$G(P, T, N_A, N_B \cdots)$$

$$dG = \left(\frac{\partial G}{\partial P}\right) dP + \left(\frac{\partial G}{\partial T}\right) dT + \left(\frac{\partial G}{\partial N_A}\right) dN_A + \left(\frac{\partial G}{\partial N_B}\right) dN_B$$

$$dG = V\,dP - S\,dT \underbrace{+ \mu_A\,dN_A + \mu_B\,dN_B}_{+\sum_i \nu_i \mu_i\, d\lambda}$$

A phase transition happens when two phases are in equilibrium

$$A_{(s)} \rightleftharpoons A_{(l)}$$

We know the condition for equilibrium is that:

$$\sum_i \nu_i \mu_i = 0$$

chemical potential in phase $\alpha$

or:

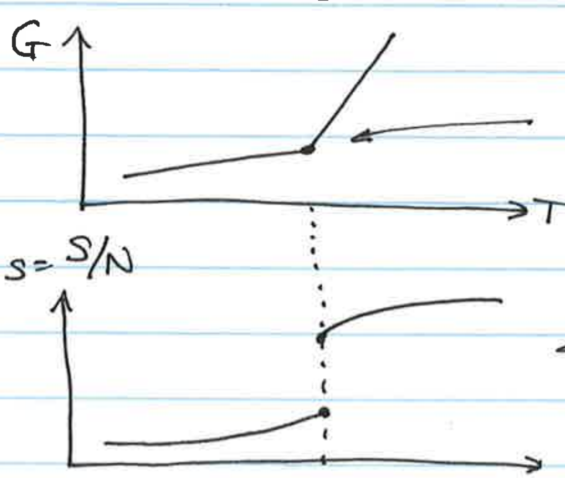
$$\mu_i^{(\alpha)}(T,P) = \mu_i^{(\beta)}(T,P)$$

chemical potential in phase $\beta$

$$\mu_A^{(s)}(T,P) = \mu_A^{(l)}(T,P)$$

We also know that $dG = 0$ at a phase boundary (e.g. G is continuous)

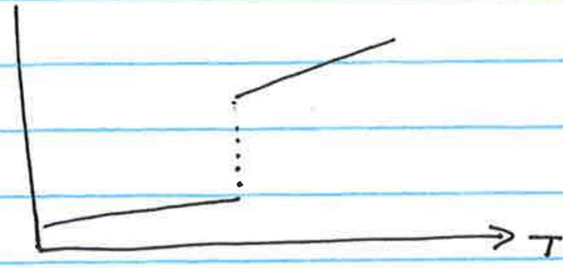
Suppose we come from solid to liquid:



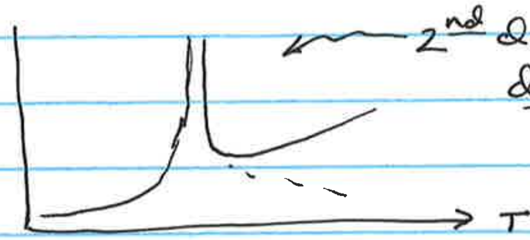

$dG = 0$, but has a different slope on either side of phase boundary

The "derivative" quantities are discontinuous

$v = \frac{V}{N}$




$C_p = \left(\frac{\partial S}{\partial T}\right)_p$




$2^{nd}$ derivative quantity diverges at phase boundary

$C_p \approx |T - T_c|^{-\alpha} + \text{constant}$

$\alpha$ = critical scaling exponent

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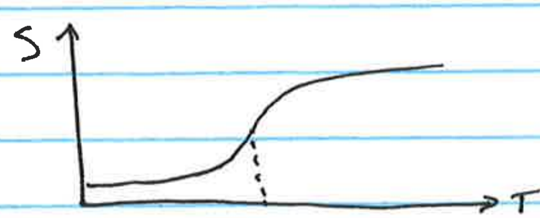
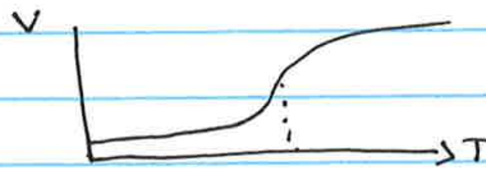
$2^{nd}$ order phase transitions: $1^{st}$ derivatives are continuous
$2^{nd}$ derivatives are discontinuous

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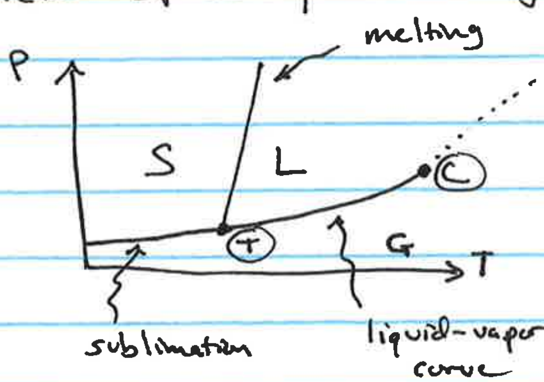
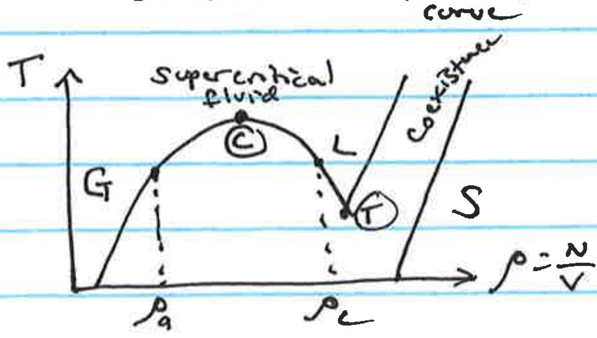
Field - space phase diagrams




—— = $1^{st}$ order

- - - - = $2^{nd}$ order



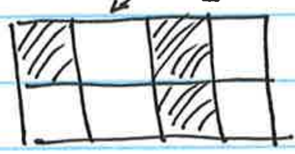

highly symmetric around critical point

$$\Delta\rho = \rho_l - \rho_g = \left(\frac{T - T_c}{T_c}\right)^{\beta}$$

$\beta = 0.326$

Can we model phase behavior

$s_2 = 0$

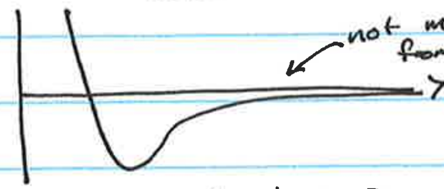


$s_1 = 1$

Lattice Gas

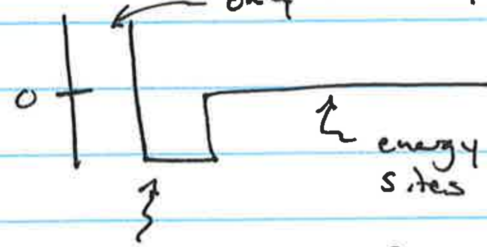
Squares are occupied or unoccupied

too close is forbidden




not much contribution from far away

only 1 or 0 particles / site

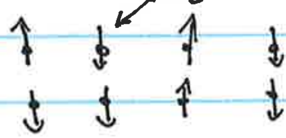



energy = 0 for sites far away

Energy = $-\epsilon$ for adjacent occupied sites

The lattice gas is an important model for L-G and L-S phase transitions. It maps exactly onto a model for magnetic phase transitions:

$\sigma_2 = -1$



$\sigma_1 = +1$

These are exactly the same model after a simple transformation

$$\mathcal{H} = \underbrace{-\sum_n h_n \sigma_n}_{\substack{\text{interactions}\\ \text{of spins with}\\ \text{external field}}} \underbrace{- \frac{1}{2} \sum_n \sum_{n'} J_{n,n'} \sigma_n \sigma_{n'}}_{\substack{\text{interactions of}\\ \text{spins with each}\\ \text{other}}} \underbrace{- \frac{1}{6} \sum_n \sum_{n'} \sum_{n''} L_{nn'n''} \sigma_n \sigma_{n'} \sigma_{n''}}_{\text{3-body interactions}}$$

$\sigma_n = \pm 1$

The Ising model is a simplification. We stop at pairwise interactions and only include contributions from nearest neighbors:

$$J_{n,n'} = \begin{cases} J & \text{if } n \,\&\, n' \text{ are nearest neighbors} \\ 0 & \text{otherwise} \end{cases}$$

$$h_n = H$$

$$\mathcal{H}_{ising} = -H\sum_n \sigma_n - \frac{J}{2}\sum_n \sum_{n'}^{NN} \sigma_n \sigma_{n'}$$

The ising model is <u>discrete</u> ($\sigma_n = \pm 1$) and short ranged.

<u>Basic properties</u>

What is configuration at $T=0$ & $H=0$ ?

With $J>0$ $\quad \mathcal{H} = -\frac{J}{2}\sum_n\sum_{n'} \sigma_n \sigma_{n'}$

Ferromagnetic $\begin{matrix}\uparrow\uparrow\uparrow\uparrow\\ \uparrow\uparrow\uparrow\uparrow\end{matrix}$ ← all spins point in same direction

$\begin{matrix}\downarrow\downarrow\downarrow\downarrow\\ \downarrow\downarrow\downarrow\downarrow\end{matrix}$ ← also a ferromagnetic low energy state

These two solutions are <u>symmetric</u>

With $J<0$: $\left.\begin{matrix}\uparrow\downarrow\uparrow\downarrow\uparrow\\ \downarrow\uparrow\downarrow\uparrow\downarrow\\ \uparrow\downarrow\uparrow\downarrow\uparrow\end{matrix}\right\}$ antiferromagnetic (all spins surrounded by spins going the other direction)

Is <u>this</u> state symmetric?

What happens if $H \neq 0$ $(J>0)$

we break the symmetry

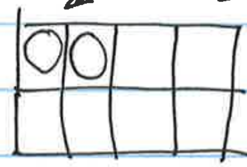
$\begin{matrix}\uparrow\uparrow\uparrow\uparrow\\ \uparrow\uparrow\uparrow\uparrow\end{matrix}$ $\quad$ $\begin{matrix}\downarrow\downarrow\downarrow\downarrow\\ \downarrow\downarrow\downarrow\downarrow\end{matrix}$ ← not the same with

$$\mathcal{H} = -H\sum_n \sigma_n - \frac{J}{2}\sum_n\sum_{n'} \sigma_n \sigma_{n'}$$

# Lattice Gase


$$\mathcal{H}_{LG} = -\frac{\epsilon}{2} \sum_{n,n'}^{NN} S_n S_{n'} \quad \leftarrow S_n = 0, 1$$

nearest neighbors



$$\mathcal{H}_{ising} = -\frac{J}{2} \sum_{n,n'}^{NN} \sigma_n \sigma_{n'} - H \sum_n \sigma_n \quad \leftarrow \sigma_n = \pm 1$$

$$Q_{ising} = \underbrace{\sum_{\{\sigma_n = \pm 1\}}}_{\text{sum over all possible states of the lattice}} e^{\overbrace{-\beta \mathcal{H}_{ising}}^{\text{energy of that lattice state}}} = \sum_{\{\sigma_n = \pm 1\}} e^{\beta\left(\frac{J}{2} \sum_{nn'} \sigma_n \sigma_{n'} + H \sum_n \sigma_n\right)}$$

Consider the Grand canonical P.F. for the Lattice Gas

$$\Xi_{LG} = \sum_{\{S_n = 0,1\}} e^{-\beta \mathcal{H}_{LG}} e^{\beta \mu N} = \sum_{\{S_N = 0,1\}} e^{\beta\left(\frac{\epsilon}{2} \sum_{nn'} S_n S_{n'} + \mu \sum_n S_n\right)}$$

$$\therefore \quad Q_{ising} \equiv \Xi_{\substack{\text{Lattice} \\ \text{Gas}}}$$

with
$$\left.\begin{aligned} J &= 2\epsilon - 1 \\ H &= 2\mu - 1 \\ \sigma_n &= 2 S_n - 1 \end{aligned}\right\} \text{mapping from canonical ising to grand canonical Lattice Gas}$$

Solve one of these problems and you've solve the other!

## What do we want to know?

$$C_V \sim |T-T_c|^{-\alpha} + c \qquad \Delta\rho = \rho_l - \rho_g \sim \frac{(T-T_c)^\beta}{T_c}$$

To get $C_V$ we need $A(T)$

To get $A(T)$ we need $Q_{ising}$

$$\langle \rho \rangle = \frac{\langle N \rangle}{V} = \frac{1}{V}\frac{\partial \ln \Xi_{LG}}{\partial(\beta\mu)}$$

$$= \frac{1}{V}\frac{1}{\Xi}\sum_{\{s_n = 0,1\}} \left(\sum_n s_n\right) e^{\cdots}$$

what's the equivalent to $\rho$ for the ising model?

$$\langle m \rangle = \frac{1}{Q}\sum_{\text{states}} \left(\sum_n \sigma_n\right) e^{-\beta\cdots}$$

$$= \frac{\partial \ln Q_{ising}}{\partial(\beta H)} \leftarrow$$ net or bulk magnetization of the ising lattice!

$\langle m \rangle$ = magnetization

for ferromagnetic phases

↑↑↑↑↑
↑↑↑↑↑ $\langle m \rangle = +1$

↓↓↓↓↓↓
↓↓↓↓↓↓ $\langle m \rangle = -1$

anti-ferromagnetic : ↑↓↑↓↑
↓↑↓↑↓ $\langle m \rangle = 0$

random $\langle m \rangle = 0$

A quick note about Frustration: Assume $J<0$ ← favors antialigned

↑
↑ ↓

← A triangular lattice is frustrated when $J<0$

Types of Frustration:

<u>Complete</u>: situations like triangular lattice where it is <u>impossible</u> to satisfy microscopic preferences

<u>Partial</u>: involves higher order couplings:

next nearest neighbors

$$\mathcal{H} = -\frac{J_1}{2} \sum_{n,n'}^{NN} \sigma_n \sigma_{n'} \quad - \frac{J_2}{2} \sum_{n,n'}^{NNN} \sigma_n \sigma_{n'}$$

$$\text{If} \quad \underbrace{J_1 > 0}_{\text{prefers NN aligned}} \quad \text{and} \quad \underbrace{J_2 < 0}_{\text{prefers NNN anti-aligned}}$$

these are incommensurate desires

Depending on relative strengths of $J_1$ & $J_2$ one will always "win"

<u>Irregular</u> frustration: $\mathcal{H} = -\frac{1}{2} \sum_{n,n'} J_{n,n'} \sigma_n \sigma_{n'}$

Pick values of $J_{n,n'}$ <u>randomly</u> on $[-1, 1]$

<u>Locally</u> frustrated structures depend on random variables

This shows up in spin glasses & neural nets

# Ising model Partition Functions

$$\mathcal{H} = -\frac{J}{2} \sum_n \sum_{n'}{}' \sigma_n \sigma_{n'}$$ ← nearest neighbors

In 1-D: (no field, no periodic boundaries)

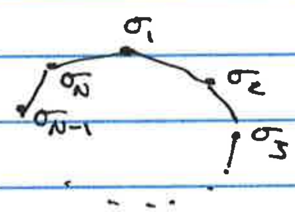
$$\mathcal{H} = -\frac{J}{2} \left( \underbrace{\sigma_1 \sigma_2 + (\sigma_2 \sigma_1}_{} + \underbrace{\sigma_2 \sigma_3) + (\sigma_3 \sigma_2}_{} + \underbrace{\sigma_3 \sigma_4)}_{} + \dots \right.$$

We can recombine these terms together

$$\mathcal{H} = -J \sum_{n=1}^{N-1} \sigma_n \sigma_{n+1}$$ ← written so each spin only couples to next one in line...

With periodic boundaries:

$$\mathcal{H} = -J \sum_{n=1}^{N} \sigma_n \sigma_{n+1}$$ ← one more term




← edge effects are gone because $\sigma_{N+1} = \sigma_1$

We can define a bond variable $b_i = \sigma_i \sigma_{i+1}$

It has values:

| $\sigma_i$ | $\sigma_{i+1}$ | $b_i$ |
|---|---|---|
| +1 | +1 | +1 |
| +1 | −1 | −1 |
| −1 | +1 | −1 |
| −1 | −1 | +1 |

We need an additional factor of 2 to distinguish degenerate states!

For N spins, we need N−1 bond variables (and a factor of 2) to visit all states

$$Q_N = \sum_{\{\sigma_i = \pm 1\}}^{N} e^{\beta J \sum_i \sigma_i \sigma_{i+1}} = 2 \sum_{\{b_i = \pm 1\}}^{N-1} e^{\beta J \sum_i b_i}$$

$$= 2 \sum_{\{b_i = \pm 1\}} e^{\beta J b_1} e^{\beta J b_2} \dots e^{\beta J b_{N-1}}$$

$$Q_N = 2\sum_{b_1=\pm 1} e^{\beta J b_1} \sum_{b_2=\pm 1} e^{\beta J b_2} \cdots \sum_{b_{N-1}=\pm} e^{\beta J b_{N-1}}$$

$$= 2\left(e^{\beta J} + e^{-\beta J}\right)^{N-1} \qquad = 2(2\cosh\beta J)^{N-1}$$

$$\boxed{Q_N = 2(2\cosh\beta J)^{N-1}}$$

Next, without periodic boundaries or dual-lattice bond variables: $\mathcal{H} = -J\sum_{n=1}^{N-1} \sigma_n \sigma_{n+1}$

$$Q_N = \sum_{\{\sigma_i=\pm 1\}} e^{\beta J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1}}$$

$$= \sum_{\{\sigma_i=\pm 1\}} e^{\beta J \sigma_1\sigma_2} e^{\beta J \sigma_2\sigma_3} \cdots e^{\beta J \sigma_{N-2}\sigma_{N-1}} e^{\beta J \sigma_{N-1}\sigma_N}$$

Do $\sigma_N = \pm 1$ first:

$$Q_N = \sum_{\{\sigma_i=\pm 1\}} e^{\beta J \sigma_1\sigma_2} e^{\beta J \sigma_2\sigma_3} \cdots e^{\beta J \sigma_{N-2}\sigma_{N-1}} \underbrace{\left(e^{\beta J \sigma_{N-1}} + e^{-\beta J \sigma_{N-1}}\right)}$$

If $\sigma_{N-1} = +1$ $\quad (e^{\beta J} + e^{-\beta J})$

If $\sigma_{N-1} = -1$ $\quad (e^{-\beta J} + e^{\beta J})$

$= 2\cosh\beta J$

$\therefore$

$$Q_N = 2\cosh\beta J \sum_{\{\sigma_i\}} e^{\beta J \sum_{n=1}^{N-2} \sigma_n \sigma_{n+1}}$$

$$Q_N = 2\cosh\beta J \; Q_{N-1}$$

We can continue the sequence all the way down to $Q_1$:

$$Q_N = (2\cosh\beta J)^{N-1}\, Q_1$$

$$= (2\cosh\beta J)^{N-1} \sum_{\sigma_1=\pm1}\sum_{\sigma_2=\pm1} e^{\beta J\sigma_1\sigma_2}$$

These last terms we can do explicitly:

$$Q_N = (2\cosh\beta J)^{N-1}\left(\underbrace{e^{\beta J}}_{\substack{\sigma_1=1\\ \sigma_2=1}} + \underbrace{e^{-\beta J}}_{\substack{\sigma_1=1\\ \sigma_2=-1}} + \underbrace{e^{-\beta J}}_{\substack{\sigma_1=-1\\ \sigma_2=1}} + \underbrace{e^{+\beta J}}_{\substack{\sigma_1=-1\\ \sigma_2=-1}}\right)$$

$$Q_N = (2\cosh\beta J)^{N-1}\, 2\left(e^{\beta J}+e^{-\beta J}\right)$$

$$\boxed{Q_N = 2\cdot(2\cosh\beta J)^N} \leftarrow \text{without periodic boundaries}$$

$$\boxed{Q_N = 2\cdot(2\cosh\beta J)^{N-1}} \leftarrow \text{with periodic boundaries}$$

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Free energies:

$$A(N,V,T) = -k_BT\ln Q_N = -k_BT\left[\ln 2 + N\ln 2\cosh\beta J\right]$$

$$A(N,V,T) = -kT\ln 2 - NkT\ln\left[2\cosh\beta J\right)$$

$$\langle E\rangle = -kT^2\frac{\partial \ln Q}{\partial T} = \frac{\partial \ln Q}{\partial \beta} = N\frac{1}{2\cosh\beta J}\cdot 2\sinh\beta J\cdot J$$

$$\langle E\rangle = NJ\tanh\beta J$$

$$C_V = \frac{\partial\langle E\rangle}{\partial T} = \frac{-J^2N}{kT^2}(\operatorname{sech}\beta J)^2$$

## With a field

$$\mathcal{H} = -H\sum_{i=1}^{N}\sigma_i - J\sum_{i=1}^{N-1}\sigma_i\sigma_{i+1} \xrightarrow{\text{PBC}} = -\frac{H}{2}\sum_{i=1}^{N}(\sigma_i+\sigma_{i+1}) - J\sum_{i=1}^{N}\sigma_i\sigma_{i+1}$$

$$Q = \sum_{\{\sigma_i=\pm1\}} e^{\beta J\sum_i \sigma_i\sigma_{i+1} + \frac{\beta H}{2}\sum_i(\sigma_i+\sigma_{i+1})}$$

Define a transfer matrix $\underline{P}$:

$$\langle\sigma|P|\sigma'\rangle = e^{\beta[J\sigma\sigma' + H(\sigma+\sigma')/2]}$$

$$\langle 1|P|1\rangle = e^{\beta(J+H)}$$
$$\langle 1|P|-1\rangle = e^{-\beta J}$$
$$\langle -1|P|1\rangle = e^{-\beta J}$$
$$\langle -1|P|-1\rangle = e^{\beta(J-H)}$$

$$\underline{P} = \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ +e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}$$

connects states of two adjacent spins

$$Q = \sum_{\{\sigma_i=\pm1\}} \langle\sigma_1|P|\sigma_2\rangle\langle\sigma_2|P|\sigma_3\rangle\langle\sigma_3|P|\sigma_4\rangle \cdots \langle\sigma_N|P|\sigma_1\rangle$$

using closure relation $\sum_{\sigma_i}|\sigma_i\rangle\langle\sigma_i| = 1$

$$Q = \sum_{\sigma_1=\pm1}\langle\sigma_1|P^N|\sigma_1\rangle = \mathrm{Tr}[\underline{P}^N]$$

To carry out the trace, we first diagonalize P:

A brief interlude on 2x2 matrices

$$\underline{\underline{A}} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \qquad \underline{\underline{B}} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$$

$$[A \cdot B]_{ij} = \sum_{k=1}^{2} A_{ik} B_{kj}$$

$$tr[\underline{\underline{A}}] = A_{11} + A_{22} = \sum_{k=1}^{2} A_{kk}$$

The Trace is conserved for cyclic permutations

$$tr[ABC] = tr[CAB] = tr[BCA]$$

but not for acyclic permutations:

$$tr[ABC] \neq tr[BAC]$$

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Diagonalization

$$\underline{\underline{M}} = \underline{\underline{U}}^T \cdot \underline{\underline{A}}\, \underline{\underline{U}}$$

for an arbitrary square matrix $\underline{\underline{A}}$, there is a Unitary transformation which results in a diagonal matrix $\underline{\underline{M}}$

$$\underline{\underline{M}} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

For $\lambda_1$ & $\lambda_2$ are the eigenvalues of $\underline{\underline{A}}$

$\underline{\underline{U}}$ = matrix of unit eigenvectors of $\underline{\underline{A}}$

columns of $\underline{\underline{U}}$ are eigenvectors of $\underline{\underline{A}}$

$$\left.\begin{aligned} \underline{\underline{A}} \cdot u_1 &= \lambda_1 u_1 = \lambda_1 \begin{pmatrix} u_{11} \\ u_{12} \end{pmatrix} \\ \underline{\underline{A}} \cdot u_2 &= \lambda_2 u_2 = \lambda_2 \begin{pmatrix} u_{21} \\ u_{22} \end{pmatrix} \end{aligned}\right\} \longrightarrow \underline{\underline{U}} = \begin{pmatrix} u_{11} & u_{21} \\ u_{12} & u_{22} \end{pmatrix}$$

The diagonalization transform is a <u>unitary</u> similarity transform

$$U^T = U^{-1}$$

$$U^T \cdot U = U^{-1} U = \underline{\underline{I}}$$

The identity matrix

Now, consider: $Tr\left[P^N\right] = \sum_k \left[P^N\right]_{kk}$

hard to determine

Suppose we diagonalize $\underline{\underline{P}}$ first,

$$\underline{M} = \underline{\underline{U}}^T \cdot \underline{\underline{P}} \cdot \underline{\underline{U}}$$

$$\underline{\underline{M}}^N = (\underline{\underline{U}}^T \cdot \underline{\underline{P}} \cdot \underline{\underline{U}})(\underline{\underline{U}}^T \cdot \underline{\underline{P}} \cdot \underline{\underline{U}})(\underline{\underline{U}}^T \cdot \underline{\underline{P}} \cdot \underline{\underline{U}}) \cdots$$

$$= \underline{\underline{U}}^T \cdot \underline{\underline{P}} \cdot (\underline{\underline{U}}\,\underline{\underline{U}}^T) \cdot \underline{\underline{P}} \cdot (\underline{\underline{U}}\,\underline{\underline{U}}^T) \cdot \underline{\underline{P}} \cdot (\underline{\underline{U}}\,\underline{\underline{U}}^T) \cdots$$

$$\underline{\underline{U}}^T = \underline{\underline{U}}^{-1}$$

$$= \underline{\underline{U}}^T \cdot \underline{\underline{P}} \cdot \underline{\underline{I}} \cdot \underline{\underline{P}} \cdot \underline{\underline{I}} \cdot \underline{\underline{P}} \cdot \underline{\underline{I}} \cdots$$

$$\underline{\underline{M}}^N = \underline{\underline{U}}^T \cdot \underline{\underline{P}}^N \cdot \underline{\underline{U}}$$

So: $tr\left[\underline{\underline{M}}^N\right] = tr\left[\underline{\underline{U}}^T \cdot \underline{\underline{P}}^N \cdot \underline{\underline{U}}\right]$

cyclic permutation

$$= tr\left[\underline{\underline{U}}\,\underline{\underline{U}}^T P^N\right]$$

$$tr\left[M^N\right] = tr\left[P^N\right]$$

$$\therefore \quad Q_N = tr\left[\begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}^N\right] = tr\left[\begin{pmatrix} \lambda_1^N & 0 \\ 0 & \lambda_2^N \end{pmatrix}\right] = \lambda_1^N + \lambda_2^N$$

Now, back to the problem at hand:

$$\mathcal{H} = \sum_n \left[ -J\sigma_n\sigma_{n+1} - \frac{H}{2}(\sigma_n + \sigma_{n+1}) \right]$$

$$Q_N = \sum_{\sigma_1=\pm 1} \cdots \sum_{\sigma_N=\pm 1} \langle \sigma_1 | \underbrace{\left[ e^{\beta J\sigma_1\sigma_2 + \frac{\beta H}{2}(\sigma_1+\sigma_2)} \right]}_{\underline{P}} | \sigma_2 \rangle \langle \sigma_2 | \ldots$$

$\underline{P}$ = transfer matrix connecting $\sigma_1$ to $\sigma_2$

$$\begin{pmatrix} e^{\beta J + \beta H} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J - \beta H} \end{pmatrix}$$

$$Q_N = Tr[\underline{P}^N] = Tr[\underline{U}^T \underline{M}^N \underline{U}] = Tr[\underline{M}^N]$$

$$= M_{11}^N + M_{22}^N = \lambda_1^N + \lambda_2^N \Leftarrow \lambda_1 \,\&\, \lambda_2 \text{ are eigen values of } P$$

$$\det[\underline{P} - \lambda \underline{I}] = 0 \implies \begin{vmatrix} e^{\beta J + \beta H} - \lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J - \beta H} - \lambda \end{vmatrix} = 0$$

$$(e^{\beta J + \beta H} - \lambda)(e^{\beta J - \beta H} - \lambda) - e^{-2\beta J} = 0$$

$$e^{2\beta J} - \lambda(e^{\beta J + \beta H} + e^{\beta J - \beta H}) + \lambda^2 - e^{-2\beta J} = 0$$

$$(e^{2\beta J} - e^{-2\beta J}) - e^{\beta J}\lambda(e^{\beta H} + e^{-\beta H}) + \lambda^2 = 0$$

$$2\sinh 2\beta J - e^{\beta J}\lambda(2\cosh\beta H) + \lambda^2 = 0$$

$$\lambda = \frac{e^{\beta J}2\cosh\beta H \pm \sqrt{e^{2\beta J}4\cosh^2\beta H - 8\sinh 2\beta J}}{2}$$

$$\lambda = e^{\beta J}\cosh\beta H \pm \sqrt{e^{2\beta J}\cosh^2\beta H - 2\sinh(2\beta J)}$$

$$= e^{\beta J}\cosh\beta H \pm \sqrt{e^{2\beta J}\cosh^2\beta H - e^{2\beta J} + e^{-2\beta J}}$$

$$= e^{\beta J}\left(\cosh\beta H \pm \sqrt{\cosh^2\beta H - 1 + e^{-4\beta J}}\right)$$

$$\boxed{\lambda_\pm = e^{\beta J}\left(\cosh\beta H \pm \sqrt{\sinh^2\beta H + e^{-4\beta J}}\right)}$$

$$Q_N = \lambda_+^N + \lambda_-^N \longleftarrow$$ one will always be larger

$1.1^N + 0.9^N$

$\uparrow$ will dominate as $N \to \infty$

$$Q_N \approx \left(e^{\beta J}\left(\cosh\beta H + \sqrt{\sinh^2\beta H - e^{-4\beta J}}\right)\right)^N$$

$$A \approx -Nk_BT\ln\left[e^{\beta J}\cosh\beta H + \left(e^{2\beta J}\sinh^2\beta H + e^{-2\beta J}\right)^{1/2}\right]$$

$$m = \langle\sigma_n\rangle = \frac{-1}{N}\frac{\partial A}{\partial H} = \frac{1}{\beta\lambda_+}\frac{\partial\lambda_+}{\partial H}$$

$$m = \frac{\sinh(\beta H)}{\sqrt{\sinh^2 \beta H + e^{-4\beta J}}}$$

$\therefore$ when $H = 0$, there is no spontaneous magnetization at any temperature in 1 dimension

In 2D, there is!

Experimental tie: magnetic susceptibility $\chi = \frac{\partial \langle m \rangle}{\partial H}$

A review of what we know:

$$\mathcal{H} = -H\sum_{i=1}^{N}\sigma_i - \frac{J}{2}\sum_{i=1}^{N}\sum_{j\in NN_i}\sigma_i\sigma_j$$

nearest neighbor sum

$0^{\circ}K$ states with $H=0$:

$J>0 \longrightarrow$ degenerate ferroelectric states
all up, $\langle m\rangle = +1$
all down, $\langle m\rangle = -1$

$J<0 \longrightarrow$ degenerate anti-ferroelectric states
$+-+-$ and $-+-+$
both with $\langle m\rangle = 0$

At any temperature in 1D, we've shown that

no field

$$Q_N = 2\left(2\cosh\beta J\right)^N$$

field

$$Q_N \simeq \left(e^{\beta J}\left(\cosh\beta H + \sqrt{\sinh^2\beta H - e^{-4\beta J}}\right)\right)^N$$

we got here using a transfer matrix diagonalization & the cyclic invariance of the trace

More derivative tricks:

$$\langle m\rangle = \frac{1}{Q}\sum_{\{\sigma_i=\pm1\}}\left(\left(\sum_{i=1}^{N}\sigma_i\right)\frac{1}{N}\, e^{\beta\left(H\sum\sigma_i + \frac{J}{2}\sum\sum\sigma_i\sigma_j\right)}\right)$$

you should be able to look at this and see

$$\langle m\rangle = \frac{\partial \ln Q}{\partial(\beta H)}\cdot\frac{1}{N} = \frac{k_B T}{N}\frac{\partial \ln Q}{\partial H}$$

$$\langle m \rangle = \frac{\sinh(\beta H)}{\sqrt{\sinh^2 \beta H + e^{-4\beta J}}}$$ ← always 0 when $H = 0$

The <u>other</u> first derivative property of interest

$$\frac{\langle E \rangle}{N} = \frac{1}{N} \frac{-\partial \ln Q}{\partial \beta} = -J \tanh \beta J$$

has no discontinuities

The <u>second</u> derivative properties

<u>susceptibility</u>

$$\chi = \frac{\partial \langle m \rangle}{\partial H}$$

$$= \frac{\beta \cosh(\beta H)}{\left(1 + e^{4\beta J} \sinh^2(\beta H)\right)^{3/2}}$$

$$\lim_{H \to 0} \chi = \frac{\beta}{\sqrt{e^{-4\beta J}}}$$ ← only diverges at $T = 0$

<u>heat capacity</u>

$$C_V = \frac{\partial \langle E \rangle}{\partial T}$$

$$= \frac{+J^2}{kT^2} \operatorname{sech}^2(\beta J)$$

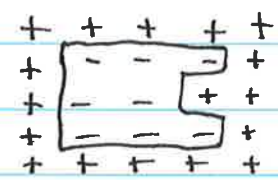
no divergences!

Conclusions: there are <u>no</u> phase transitions in the 1-D Ising model!!

## Peierls Theorem

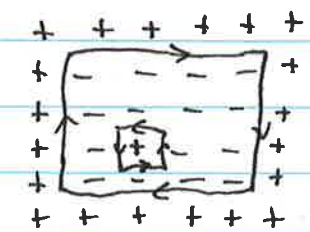
For 2D Ising model, $\exists$ a temperature $T_c$ at which the probability of "+" spins $\neq$ the probability of "−" spins. (i.e $\langle \sigma_n \rangle \neq 0$ below $T_c$)

Consider an array of spins:



energy = J × length of perimeter

N spins on an array, with all spins on outside set to "+"



a "contour" passes through the midpoint of every +− bond

a "closed" contour meets itsel

length

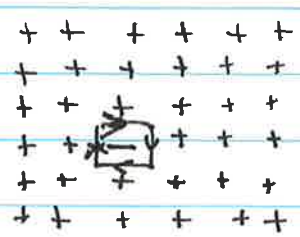
$C(l, i)$

label

Energy of closed contour = $E(C) = Jl$

Direction: RHS of path has "−" spins

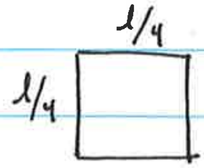
Conjugate: Reverse all spins to RHS of contour



$\tilde{C}(l, i)$

$E(\tilde{C}) = E(C) - lJ$

the contour with the maximal # of enclosed spins for a given length is a regular polygon:




$$A = N_{max} = \frac{l^2}{16}$$

$\mathcal{M}(l) =$ total # of contours of length $l$

$\mathcal{M}(l) \leq$ total # of contours we can draw

$$\mathcal{M}(l) \leq N \times 4 \times 3^{l-1} \times \frac{1}{2l}$$

$N$: places to start

$4$: choices of direction on step 1

$3^{l-1}$: choices of direction on following steps

$\frac{1}{2l}$: required to close loop

$$X(l,i) = \begin{cases} 1 & \text{if configuration contains contour } c(l,i) \\ 0 & \text{otherwise} \end{cases}$$

# of negative spins

$$N_- \leq \sum_l \left(\frac{l^2}{16}\right) \sum_{i=1}^{\mathcal{M}(l)} X(l,i) = \underline{\text{overestimate}} \text{ of } N_-$$

$\mathcal{M}(l)$: maximal # of contours of length $l$

$X(l,i)$: does configuration contain this contour

$\frac{l^2}{16}$: maximal enclosed spins

$$\langle X(l,i) \rangle = \frac{\sum_{\{\sigma_n\}} e^{-\beta \mathcal{H}(\{\sigma_n\})} X(l,i)}{\sum_{\{\sigma_n\}} e^{-\beta \mathcal{H}(\{\sigma_n\})}}$$

we can do this as a "constrained" sum over only those configurations containing $c(l,i)$

27-3

$$\langle X(\ell,i)\rangle = \frac{\sum\limits_{\substack{\text{constrained}\\ \text{configs}}} e^{-\beta E[C(\ell,i)]}}{\sum\limits_{\{\sigma_n\}} e^{-\beta \mathcal{H}}}$$

← we can underestimate the denominator using the same constrained configurations but without that contour

$$\langle X(\ell,i)\rangle \leq \frac{\sum\limits_{\text{configs}}' e^{-\beta E[C(\ell,i)]}}{\sum\limits_{\text{configs}}' e^{-\beta E[\tilde{C}(\ell,i)]}}$$

Since $E[\tilde{C}(\ell,i)] = E[C(\ell,i)] - J\ell$

$$\langle X(\ell,i)\rangle \leq e^{-\beta J \ell}$$

$$\frac{\langle N_-\rangle}{N} \leq \frac{1}{N}\sum_{\ell}\left(\frac{\ell^2}{16}\right)\sum_{i=1}^{m(\ell)}\langle X(\ell,i)\rangle$$

$$\leq \frac{1}{N}\sum_{\ell=4}^{\infty}\left(\frac{\ell^2}{16}\right) N\cdot 3^{\ell-1}\cdot e^{-\beta J\ell}\cdot\frac{4}{2\ell}$$

$$\leq \sum_{\ell=4}^{\infty}\frac{\ell}{24}\left(3\cdot e^{-\beta J}\right)^{\ell} = \frac{1}{24}\cdot\frac{(3e^{-\beta J})^4(9e^{-\beta J}-4)}{(3e^{-\beta J}-1)^2}$$

$$\frac{\langle N_-\rangle}{N} \leq \frac{e^{-3\alpha}(4e^{\alpha}-3)}{24(e^{\alpha}-1)} \quad \text{with} \quad \alpha = \frac{J}{k_B T} - \ln 3$$

$\frac{\langle N_-\rangle}{N} \ll \frac{1}{2}$ as $T\to 0$, and this was an overestimate

$\therefore$ There must be a $T_c$ below which

$$\frac{\langle N_-\rangle}{N} \leq \frac{1}{2}$$

27-4

2D exact solution:

Lars Onsager 1940's Phys. Rev. 65, 117-149 (1944)

$$Q(\beta, N) = \left[2\cosh(\beta J)\, e^{I}\right]^N$$

$$I = \frac{1}{2\pi}\int_0^{\pi} d\phi \, \ln\left\{\frac{1}{2}\left[1 + \left(1-\mathcal{K}^2\sin^2\phi\right)^{1/2}\right]\right\}$$

$$\mathcal{K} = \frac{2\sinh(2\beta J)}{\cosh^2(2\beta J)}$$

Critical Temperature: $T_c = \dfrac{2.269\,J}{k_B}$

$$\frac{C_v}{N} \approx \frac{8k_B}{\pi}(\beta J)^2 \ln\left|\frac{1}{T-T_c}\right| \qquad \alpha = 0$$

$$\frac{M}{N} \approx (\text{const})\,(T_c - T)^{1/8} \quad \leftarrow \quad T < T_c$$

$\beta = \frac{1}{8}$

3D : No exact solution yet!

Numerically :

$$\frac{C_v}{N} \propto |T-T_c|^{-0.125}$$

$$\frac{M}{N} \propto (T_c - T)^{0.313} \qquad T < T_c$$

$$T_c \sim \frac{4J}{k_B}$$

Next time : Approximate theories for 2 & 3D!

## Mean-field theory

$$E = \mathcal{H} = -\frac{1}{2}\sum_{i,j} J_{i,j}\,\sigma_i\sigma_j - H\sum_i \sigma_i$$

$$J_{i,j} = \begin{cases} J & \text{if } i,j = NN \\ 0 & \text{otherwise} \end{cases}$$

A force ~~is~~ exerted on a particular spin $\sigma_i$ due to everything else

$$-\left(\frac{\partial E}{\partial \sigma_i}\right) = H + \sum_j J_{i,j}\,\sigma_j$$

where's the ½? ($\sigma_i\sigma_j$ appears twice)

We'll call this the instantaneous ~~[illegible]~~ field for spin $i$

$$H_i' = H + \sum_j J_{i,j}\,\sigma_j$$

$$\therefore \quad E = -\sum_i H_i'\,\sigma_i$$

energy is a single sum over instantaneous fields

$H_i'$ has an average value as the rest of the spins fluctuate:

$$\langle H_i' \rangle = \bar{H}_i' = H + \sum_j J_{i,j}\langle \sigma_j \rangle$$

Now, suppose all the spins are fluctuating in exactly the same way. That is, they all have the same average:

$$\langle \sigma_j \rangle = \langle \sigma_1 \rangle = \langle \sigma_i \rangle$$

$$\langle H_i' \rangle = H + \sum_j J_{i,j}\langle \sigma_i \rangle$$

$$\langle H_i' \rangle = H + 2d\,J\,\langle \sigma_i \rangle$$

# of nearest neighbors

28-2

We can now write an approximate Hamiltonian:

$$\mathcal{H} = -\sum_i' H_i' \sigma_i$$

exact ← ; ← instantaneous field

mean field ←

$$\mathcal{H}_0 = -\sum_i' \langle H_i' \rangle \sigma_i$$

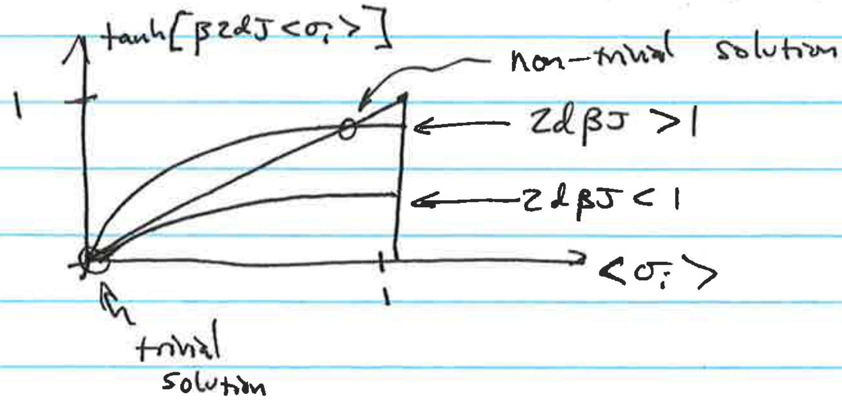
But how do we know what $\langle H_i' \rangle$ is? We need $\langle \sigma_i \rangle$

$$\langle \sigma_i \rangle \cong \left[ \frac{\sum'_{\{\sigma_i = \pm 1\}} e^{-\beta \mathcal{H}_0} \sigma_i}{\sum'_{\{\sigma_i = \pm 1\}} e^{-\beta \mathcal{H}_0}} \right]$$

All spins are identical, so:

$$\langle \sigma_i \rangle \approx \left[ \frac{\sum_{\sigma_i = \pm 1} e^{-\beta \langle H_i' \rangle \sigma_i} \sigma_i}{\sum_{\sigma_i = \pm 1} e^{-\beta \langle H_i' \rangle \sigma_i}} \right] = \frac{e^{\beta \langle H_i' \rangle} - e^{-\beta \langle H_i' \rangle}}{e^{\beta \langle H_i' \rangle} + e^{-\beta \langle H_i' \rangle}}$$

$$\langle \sigma_i \rangle = \tanh \beta \langle H_i' \rangle = \tanh \left( 2d \beta J \langle \sigma_i \rangle \right)$$




What is the magnetization of the lattice?

$$\langle M \rangle = \sum_i \langle \sigma_i \rangle = N \langle \sigma_i \rangle ; \quad m = \frac{\langle M \rangle}{N} = \langle \sigma_i \rangle$$

28-3

$$m = \frac{e^{\beta 2Jdm} - e^{-\beta 2Jdm}}{e^{\beta 2Jdm} + e^{-\beta 2Jdm}}$$

$$m = \frac{e^{4\beta Jdm} - 1}{e^{4\beta Jdm} + 1}$$

$$m\left(e^{4\beta Jdm} + 1\right) = e^{4\beta Jdm} - 1$$

$$e^{4\beta Jdm}(m-1) = -1 - m$$

$$e^{4\beta Jdm} = \frac{-1-m}{m-1} = \frac{m+1}{1-m}$$

$$4\beta Jdm = \ln \frac{m+1}{1-m}$$

$$\beta = \frac{1}{4dJm} \ln\left(\frac{1+m}{1-m}\right) \approx \frac{1}{4dJ}\frac{1}{m}\left(2m + \frac{2m^3}{3}\right)$$

Near $T_c$, $m$ is very small, so we can taylor expand in small $m$ to get $\beta$

$$\beta_c \approx \frac{1}{2dJ}$$

$$\frac{1}{k_B T_c} = \frac{1}{2dJ}$$

$$\boxed{T_c = \frac{2dJ}{k_B}}$$

So there is a critical $T_c$ in Mean Field Theory

| d | MFT | real |
|---|---|---|
| 1d | $2J/k_B$ | 0 |
| 2d | $4J/k_B$ | $2.269\ J/k_B$ |
| 3d | $6J/k_B$ | $4\ J/k_B$ |

MFT over estimates $T_c$, predicting one for 1-D where there is none

MFT neglects correlations!