# Lecture October 30

Detailed balance + Metropolis:

$$\frac{w_i}{w_j} = \frac{T(j \to i) A(j \to i)}{T(i \to j) A(i \to j)}$$

$$T(j \to i) = T(i \to j)$$

$$\frac{w_i}{w_j} = \frac{A(j \to i)}{A(i \to j)}$$

P4 : $w_i = P_i(\beta) = \frac{e^{-\beta E_i}}{Z}$

$$Z = \sum_{i=1}^{M} e^{-\beta E_i} \qquad \beta = 1/k_B T$$

$$\frac{w_i}{w_j} = e^{-\beta \Delta E} \qquad \Delta E = E_i - E_j$$

# microstates $= 2^N$ ← # objects (spins)

Metropolis algo = sampling rule for accepting move configurations (states)

$$A(j \to i) = \min\left(1, \frac{w_i}{w_j}\right)$$

suggest new $E_i$ (config)

Draw RN - $r \in [0, 1]$ using uniform PDF

Accept if $r \leq w_i / w_j$

For P4, only five possible values for $\Delta E$, can precalculate $e^{-\beta \Delta E}$ for each $\beta$.

<u>Example</u>

$$W = \begin{bmatrix} 3/4 & 1/2 \\ 1/4 & 1/2 \end{bmatrix} \quad \text{(known)}$$

$\lambda = \{1, 1/4\}$

guess $w_0 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

$w_\infty = ?$

$w_{17} = \begin{bmatrix} 2/3 \\ 1/3 \end{bmatrix}$

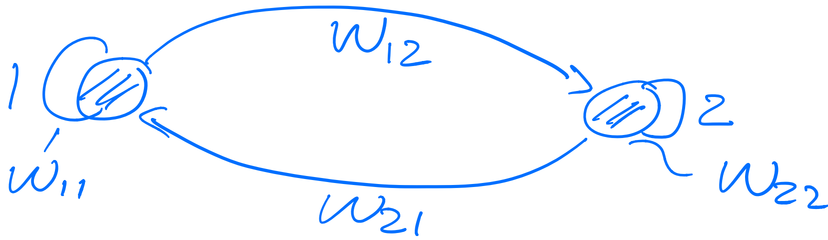
General case: have Model $w_i$

unknown $W$

Use Metropolis to make W

$$w = \begin{bmatrix} 1/3 \\ 2/3 \end{bmatrix} \quad \text{known}$$

$w_1 = 1/3$
$w_2 = 2/3$




$$W_{ij} = T_{ij} A_{ij} \qquad (A(i \to j))$$

$$T_{12} = T_{21} = 1/2$$

$$\frac{w_2}{w_1} = 2 = \frac{W_{12}}{W_{21}} = \frac{A_{12}}{A_{21}}$$

$w_2 > w_1 \Rightarrow$ $\qquad 0 \le A_{ij} \le \underline{1}$

$A_{12} = \underline{1}$

$$\frac{w_1}{w_2} = \frac{1}{2} \Rightarrow \begin{array}{l} A_{12} = \underline{1} \\ A_{21} = 1/2 \end{array}$$

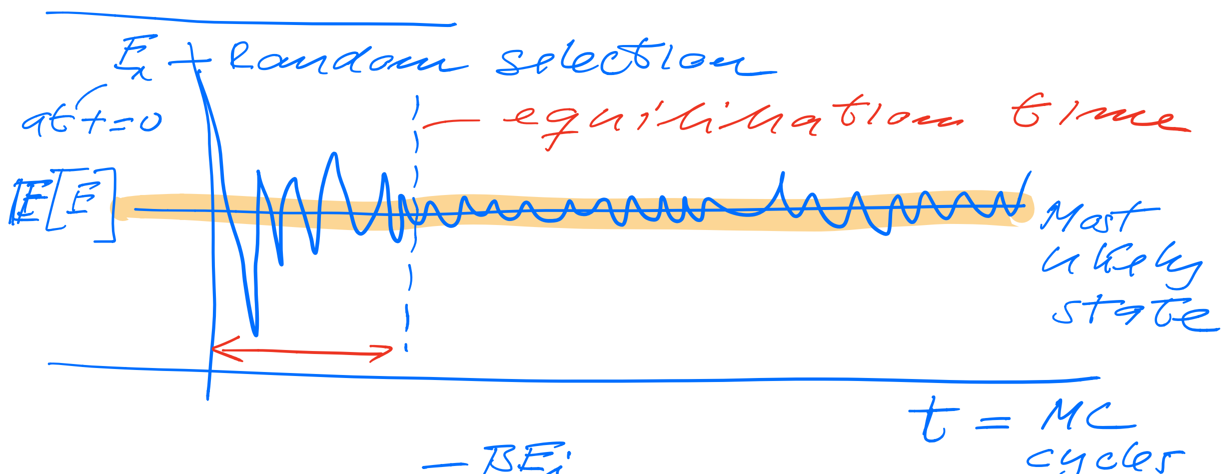
$$W = \begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix}$$

$$= \begin{bmatrix} ? & \frac{1}{2} \cdot \underline{1} \\ \frac{1}{2} \cdot \frac{1}{2} & ? \end{bmatrix}$$

Norm as sum of column elements $\Rightarrow$

$$W = \begin{bmatrix} 3/4 & 1/2 \\ 1/4 & 1/2 \end{bmatrix}$$

where we started.




$$P_i = e^{-\beta E_i}/Z$$

P4: Expectation values

$$\mathbb{E}[E^i] = \sum_{j=1}^{M} P_j \cdot E_j^i$$

$$\boxed{\bar{\mu}_E \cong \frac{1}{N} \sum_{j=1}^{N} E_j}$$ sample mean.

$N \le M$

$$\mu_E = \sum_{j=1}^{M} P_j \cdot E_j = \left| \frac{1}{Z} \sum_{j=1}^{M} e^{-\beta E_j} E_j \right|$$

Helmholtz free energy

$F = -k_B T \ln Z$ (potential in the canonical ensemble)

$F = \mathbb{E}[E] - T \cdot S$

↑ entropy

$$\mu_E = -\frac{\partial \ln Z}{\partial \beta} = -\frac{1}{Z}\frac{\partial Z}{\partial \beta}$$

$$= \frac{\partial\, F/k_B T}{\partial \beta}$$

$$\rightarrow \sigma_E^2 = \sum_{i=1}^{M} p_i E_i^2 - \left[\sum_{i=1}^{M} p_i E_i\right]^2$$

$$C_V = \frac{\partial \mu_E}{\partial T} = \frac{1}{k_B T^2}\sigma_E^2$$

<u>P4</u> : $E_i = -J \sum_{\langle k\ell \rangle} S_k S_\ell$

$S_k = \pm 1$

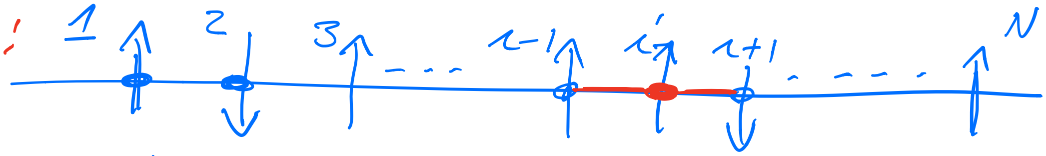
sum of nearest neighbors only

$S_k = +1 \Rightarrow \uparrow$

$S_k = -1 \Rightarrow \downarrow$

# 1-DIM

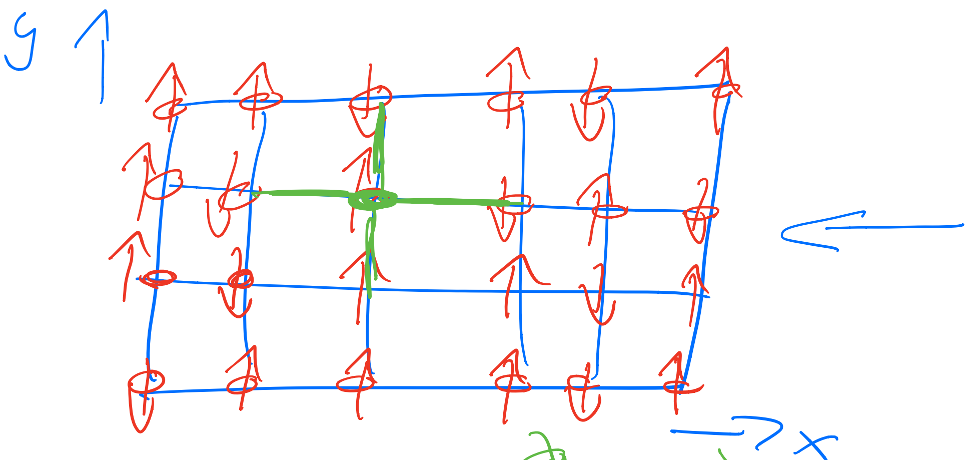
$E_i$:

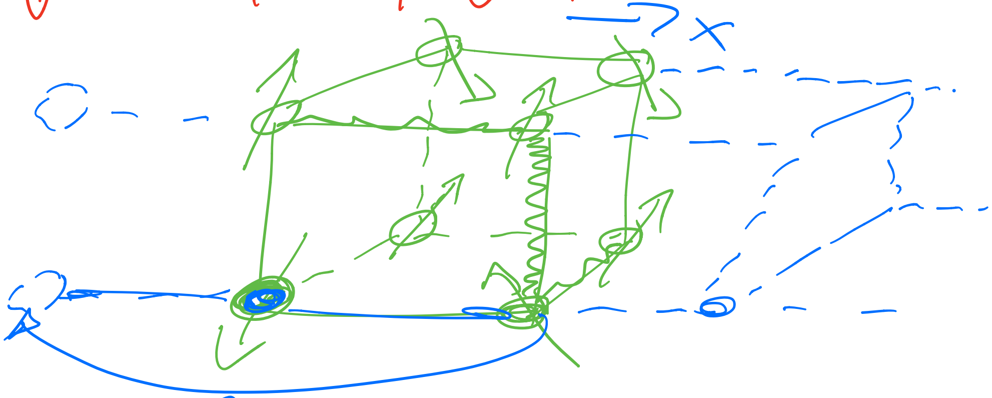


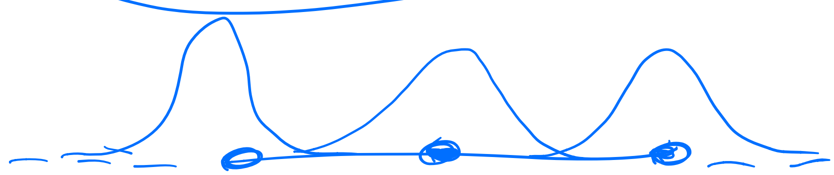

$2^N$ possible arrangements

$$\boxed{E_i = -J \sum_{\langle kl \rangle} S_k S_l}$$

## 2-DIM





Boundaries:

– Free ends

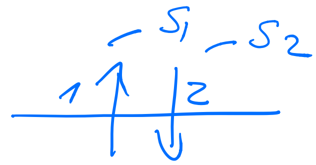
1-DIM case   2 spins

\# configs = $2^2$

$E_1 = \uparrow\uparrow$   $E_2 = \uparrow\downarrow$   $E_3 = \downarrow\uparrow$   $E_4 = \downarrow\downarrow$

$E_1 = -J s_1 s_2$

$= -J$

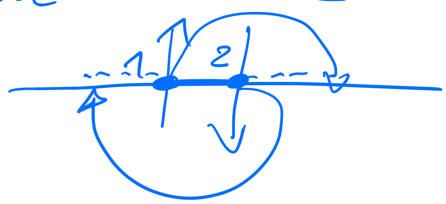


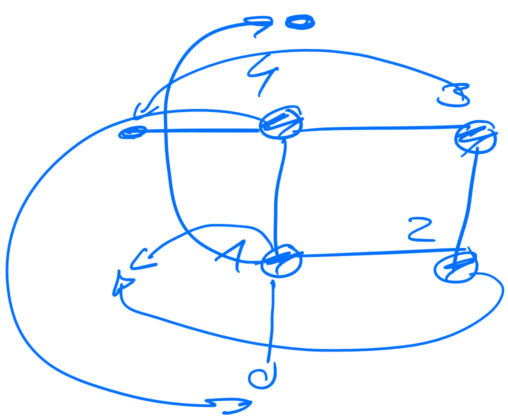

$E_2 = +J$   $E_3 = +J$   $E_4 = -J$

$$E_i = -J \sum_{i=1}^{N-1} s_i s_{i+1}$$

— Periodic Boundary conditions (PBC)

1dim   $s_1 s_2 + s_2 s_1$




$$E_i = -J \sum_{j=1}^{N} s_i s_{i+1}$$

1-DIM with PBC

$E_1 = -2J \qquad E_2 = +2J$

$E_3 = +2J \qquad E_4 = -2J$

## P4 part a+b

2DIM 2x2 spin system

$\# \text{ configs} = 2^4 = 16$

$E_1 = \underbrace{\begin{matrix}\uparrow & \uparrow \\ \uparrow & \uparrow\end{matrix}}_{} \qquad E_2 = \begin{matrix}\uparrow & \downarrow \\ \uparrow & \downarrow\end{matrix} \qquad \ldots \qquad E_{16} = \begin{matrix}\downarrow & \downarrow \\ \downarrow & \downarrow\end{matrix}$

PBC $E_1 = -8J$ $\qquad E_{16} = -8J$

$M = \sum_{i=1}^{2^4} M_i \qquad M_1 = +4 \qquad M_{16} = -4$

| # spin up | Deg | E | M | |
|---|---|---|---|---|
| 4 | 1 | $-8J$ | 4 | |
| 3 | 4 | 0 | 2 | $1 \to 0$ |
| 2 | 4 | 0 | 0 | $e^{-8\beta J}$ |
| 2 | 2 | $+8J$ | 0 | 1 |
| 1 | 4 | 0 | $-2$ | $e^{+\beta 8J}$ |
| 0 | 1 | $-8J$ | $-4$ | |

$2^4$

$$\mathbb{E}[E] = \frac{1}{Z} \sum_{i=1}^{16} E_i e^{-\beta E_i}$$

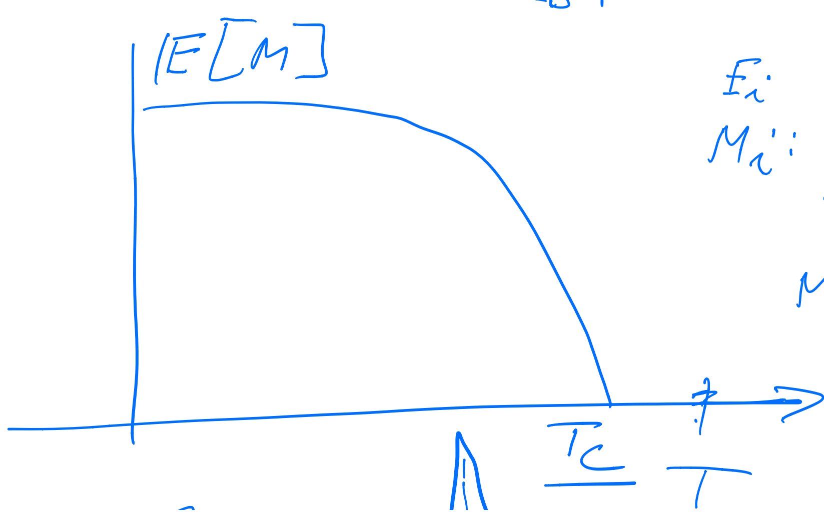
$$Z = \sum_{i=1}^{16} e^{-\beta E_i}$$

$$\frac{\sigma_E^2}{k_B T^2} = C_V = \frac{1}{k_B T^2}\left[\frac{1}{Z} \sum_{i=1}^{16} E_i^2 e^{-\beta E_i} - \mathbb{E}[E]^2\right]$$

$$\mathbb{E}[M] = \frac{1}{Z} \sum_{i=1}^{16} M_i e^{-\beta E_i}$$

$$\sigma_M^2 = \frac{1}{Z} \sum_{i=1}^{16} M_i^2 e^{-\beta E_i} - \mathbb{E}[M]^2 \implies$$

$$\chi = \frac{\sigma_M^2}{k_B T}$$

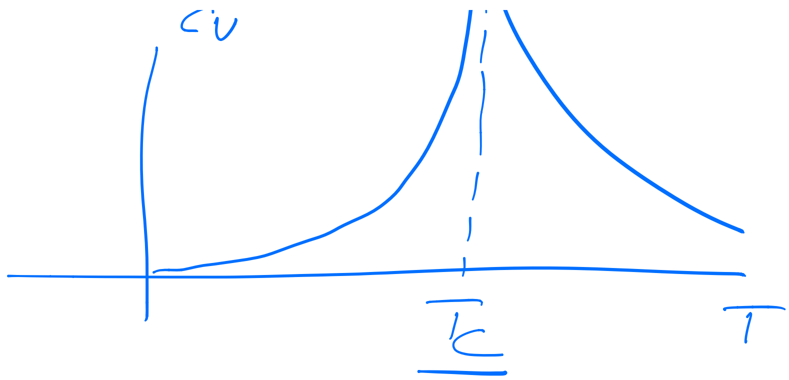



$E_i$: $\uparrow\uparrow$

$M_i$: $\uparrow\uparrow$

$\uparrow\uparrow$

$$M_i = \sum_{k=1}^{4} s_k$$



cv
$T_c$
T