Lecture November 5

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

$$= \sum_{i=1}^{M} P_i E_i \approx$$

$$\frac{1}{MCs} \sum_{i=1}^{MCs} E_i$$

$$\mathbb{E}[E^2] \simeq \frac{1}{MCs} \sum_i E_i^2$$

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

P4 a)

2x2 case:

$E = 0$	$E = -8J$	$E = 8J$
12 microstates	2 micro states	2 micro states

$$Z = 2e^{+8J\beta} + 2e^{-8J\beta} + 12e^{0}$$

$$= 4\cosh(8J\beta) + 12$$

$$\mathbb{E}[E] = \frac{1}{Z} \sum E_i' e^{-\beta E_i'}$$

$$= \frac{16J e^{-8\beta J} - 16J e^{+8\beta J}}{Z}$$

Writing our code for the Ising model.

$\beta \cdot J = J / k_B T$ $\qquad$ s_k are dimless

$[J]$ has dim energy

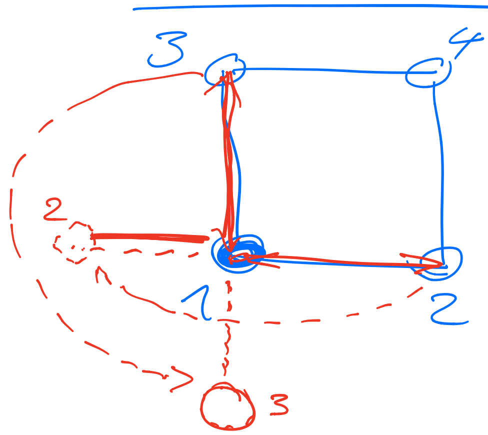
$[k_B T]$ — " —

$e^{-8\beta J}$ $\qquad$ $k_B = 1$

$\Downarrow$

T has dim energy

2x2 with PBC



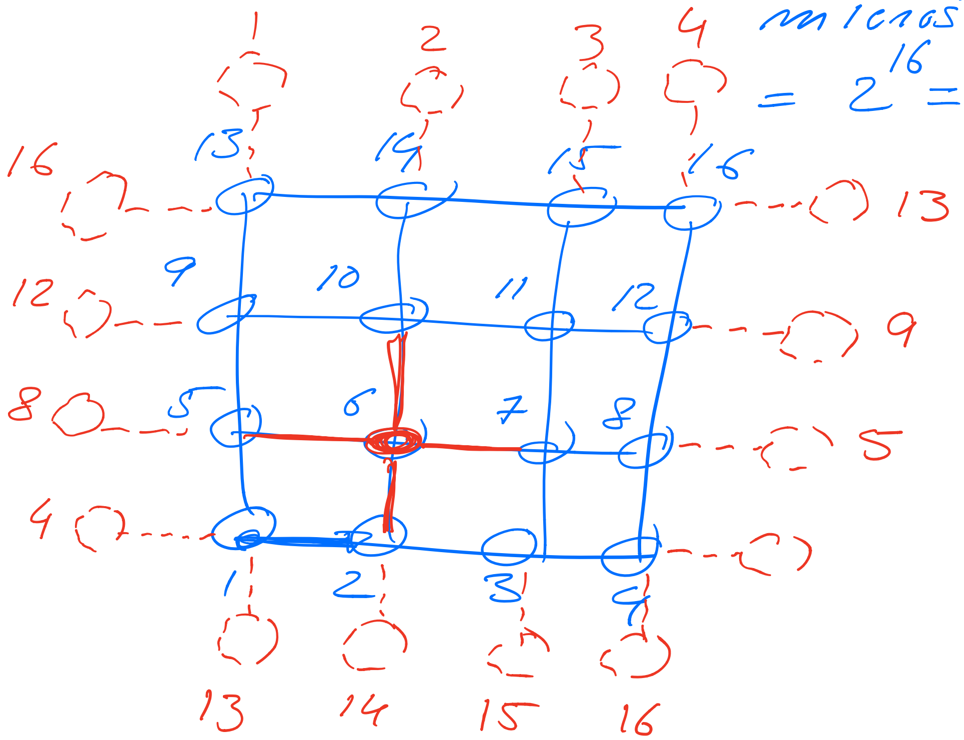
$$E_i' = -J\big(s_1 s_2 + s_2 s_1 + s_1 s_3 + s_3 s_1 + s_2 s_4 + s_4 s_2 + s_3 s_4 + s_4 s_3 \big)$$

$$M_i = \sum^{N} s_i'$$

$i=1$

4x4 PBC

Total # microstates $= 2^{16} = 65536$



$S_1 S_2 +$
$S_1 S_4 +$
$S_1 S_5 +$
$S_1 S_{13}$

How to compute boundary contributions most efficiently?

- if tests (slow code)
- in lecture slides: function called Periodic.
- spin matrix S[x][y] with N spins $S \in \mathbb{R}^{N \times N}$ ← integers ?

↳ PBC: increase size of matrix to S of dim $(N+2) \times (N+2)$

— ?

Algorithm : MC calculation

- initialize S[x][y]
- Fix initial T
- Find initial E and M

$$P_i \sim e^{-\beta E_i}$$

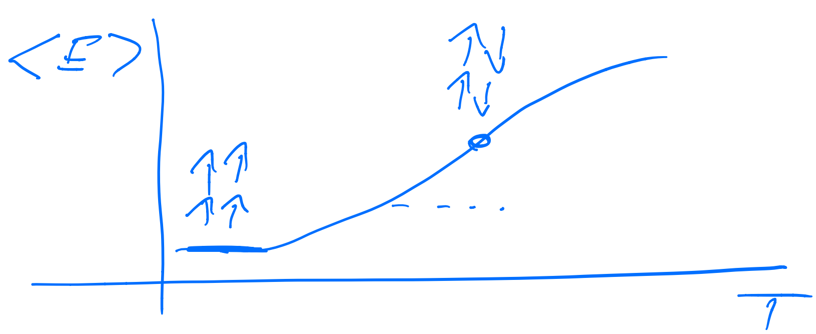
T is low : what is the most likely spin orientation?

2×2 : $E = -8J,\ 0,\ +8J$

$\uparrow\uparrow$ $\uparrow\uparrow$ $\quad$ $\uparrow\downarrow$ $\uparrow\downarrow$ ...

$\downarrow\downarrow$ $\downarrow\downarrow$

Low T : fix all spins up or down.



High T : randomly
$\uparrow$ or $\downarrow$

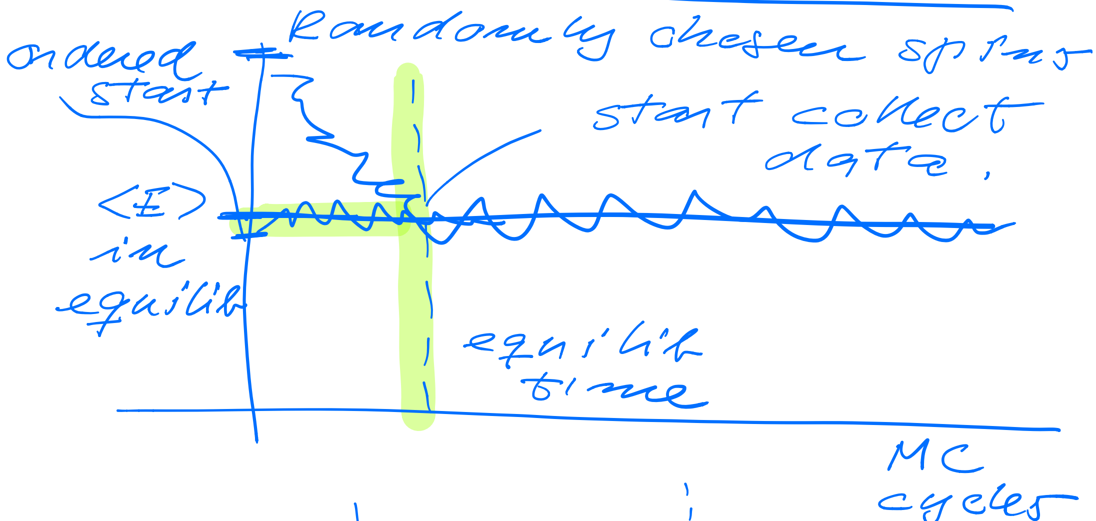
Loop over all spins :

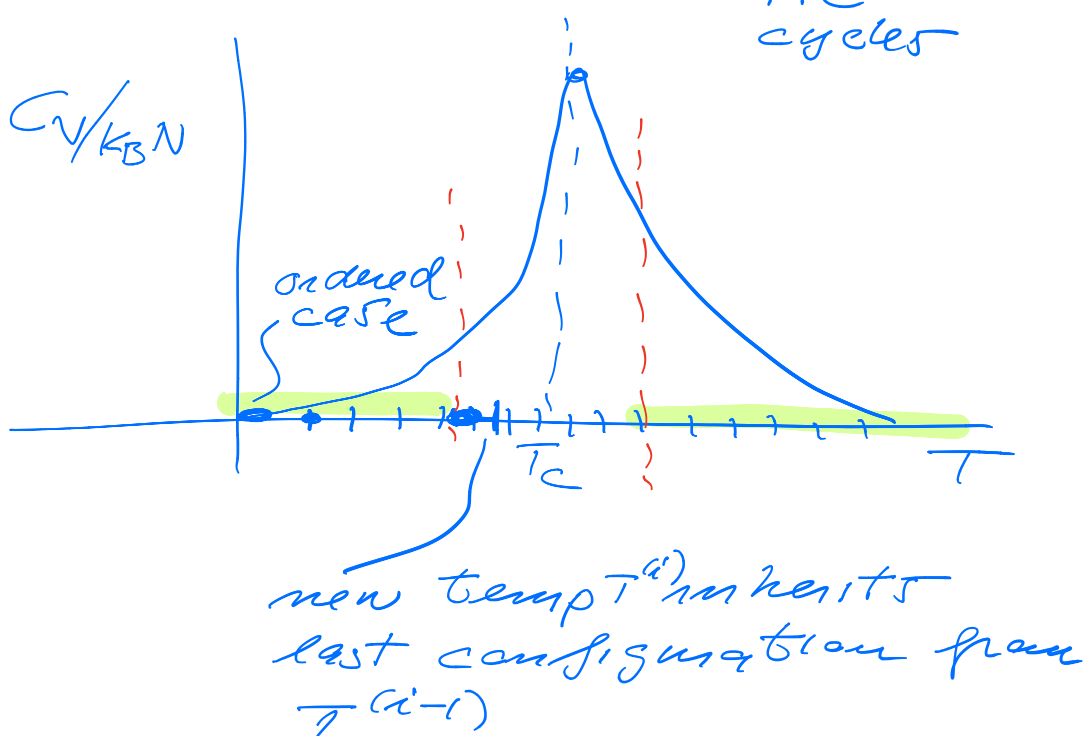
$r \in [0,1]$

if $r \leq 0.5$ $\quad s_i = \uparrow$

else $r > 0.5$ $\quad s_i = \downarrow$

Typical calculation





Set up a loop over T

For every T

FOR MCS = 1 : Final cycle

— pick new microstate and find E_i'

— Metropolis Test   previous state

$r \in [0,1]$ $r \leq e^{-\beta(E_i' - E_j')}$

— update $E = E + \Delta E$

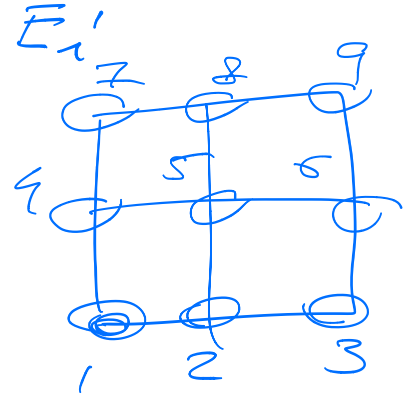
$M = M + \Delta M$

END FOR MCS

FINAL averages $E = E/MCS$

How to do this?

$E_j' \Rightarrow E_i'$

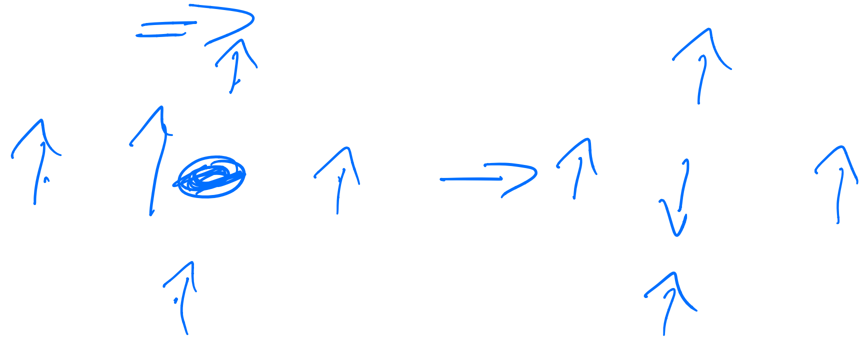


$$E_i' = -J \sum_{\langle kl \rangle} s_k s_l$$

(i) loop over all spins and compute E_i' eq flipping randomly all spins. Very inefficient

(ii) Flip one spin at the time and compute E_i' and Perform Metropolis

$\Rightarrow$



$E = -J \cdot 4$ $\qquad$ $E = +4 \cdot J$

$\Rightarrow \quad \Delta E = +8J$,

-1

$+3$

$\Rightarrow -2J$

$\underline{E = -2J}$ $\qquad$ $E = +2J$

$\Delta E = +4J$

$$\Delta E = \{-8J, -4J, 0, +4J, +8J\}$$

can precalculate

$e^{-\beta\Delta E}$ for given T

and store $e^{-\beta\Delta E}$

Find ΔE with E_j'.