Content

Content

3. Statistical and many-body physics
   3.1 Classical Monte Carlo and phase transitions (Ising model and critical phenomena)
   3.2 Quantum Monte Carlo methods (Path-integral and cluster update)

4. Machine learning in physics and High performance computation
   4.1 AI in quantum physics
   4.2 HPC and parallelism
   4.3 …

Hamiltonian matrix

$$H = J\sum_{\langle i,j\rangle} \overrightarrow{S}_i \cdot \overrightarrow{S}_j = J\sum_{\langle i,j\rangle} (\frac{1}{2}(S_i^+S_j^- + S_i^-S_j^+) + S_i^zS_j^z)$$

$$H|\uparrow\uparrow\rangle = \frac{J}{4}|\uparrow\uparrow\rangle$$

$$H|\downarrow\downarrow\rangle = \frac{J}{4}|\downarrow\downarrow\rangle$$

$$H|\uparrow\downarrow\rangle = J(\frac{1}{2}(S_1^+S_2^- + S_1^-S_2^+) + S_1^zS_2^z)|\uparrow\downarrow\rangle = \frac{J}{2}|\downarrow\uparrow\rangle - \frac{J}{4}|\uparrow\downarrow\rangle$$

$$H|\downarrow\uparrow\rangle = J(\frac{1}{2}(S_1^+S_2^- + S_1^-S_2^+) + S_1^zS_2^z)|\downarrow\uparrow\rangle = \frac{J}{2}|\uparrow\downarrow\rangle - \frac{J}{4}|\downarrow\uparrow\rangle$$

$$\langle\uparrow\uparrow|H|\uparrow\uparrow\rangle = \frac{J}{4}$$

$$\langle\downarrow\downarrow|H|\downarrow\downarrow\rangle = \frac{J}{4}$$

$$\langle\uparrow\downarrow|H|\uparrow\downarrow\rangle = -\frac{J}{4}$$

$$\langle\downarrow\uparrow|H|\uparrow\downarrow\rangle = \frac{J}{2}$$

$$\langle\uparrow\downarrow|H|\downarrow\uparrow\rangle = \frac{J}{2}$$

$$\langle\downarrow\uparrow|H|\downarrow\uparrow\rangle = -\frac{J}{4}$$

$$H = J\begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix}$$

in the basis

$$\begin{pmatrix} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{pmatrix}$$

Hilbert space size

Dimensionality of the Hilbert space $d = dim(H) = 2^N$

Computation complexity for diagonalising $d \times d$ matrix $O(d^3) = O(2^{3N})$

Lead to the "exponential wall"

$N = 10 \quad dim = 1{,}024 \sim 10^3$

$N = 20 \quad dim = 1{,}048{,}576 \sim 10^6$

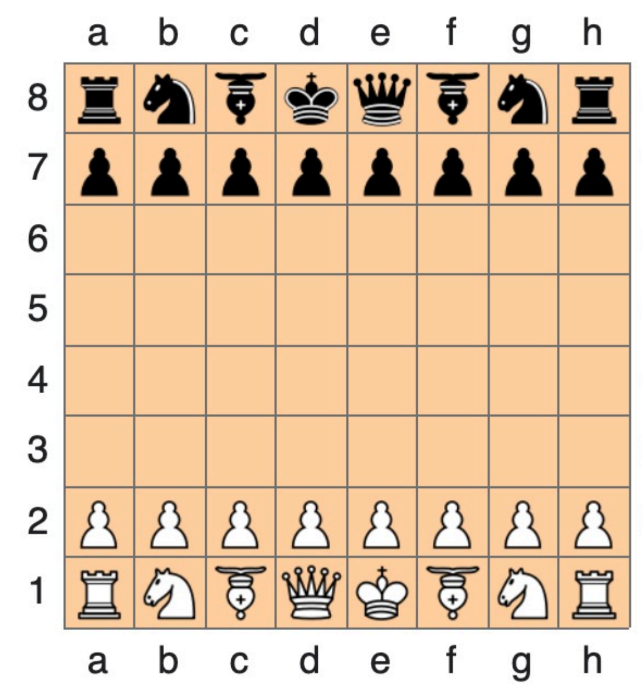
$N = 30 \quad dim = 1{,}073{,}741{,}824 \sim 10^9$

$N = 40 \quad dim = 1{,}099{,}511{,}627{,}776 \sim 10^{12}$

$N = 50 \quad dim = 1{,}125{,}899{,}906{,}842{,}624 \sim 10^{15}$

right now

Wheat grains on chessboard — Sissa ibn Dahir, inventor of Chaturanga

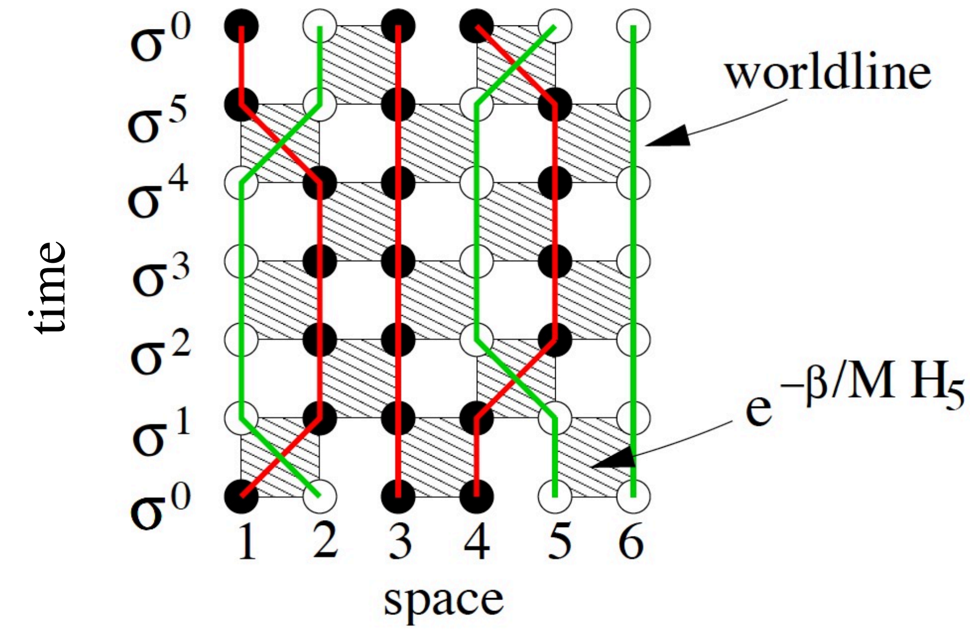


$2^{64} - 1$ = 18,446,744,073,709,551,615 grains of wheat,
weighing about 1,199,000,000,000 tons.
About 1,645 times the global production of wheat.

Solving exponentially complex problem in polynomial time

Quantum Monte Carlo （for spin systems）

$$H = J\sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j = J\sum_{\langle i,j\rangle} \left(\frac{1}{2}(S_i^+S_j^- + S_i^-S_j^+) + S_i^zS_j^z\right)$$



In statistical (classical) physics

$$\langle H\rangle = \frac{1}{Z}Tr[He^{-\beta H}] = \frac{1}{Z}\sum_n E_n e^{-\beta E_n}$$

$$Z = Tr[e^{-\beta H}] = \sum_n e^{-\beta E_n}$$

In quantum system, one doesn't know the full spectrum a priori (otherwise the problem is solved, such as exact diagonalization)

$$Z = Tr[e^{-\beta H}]$$

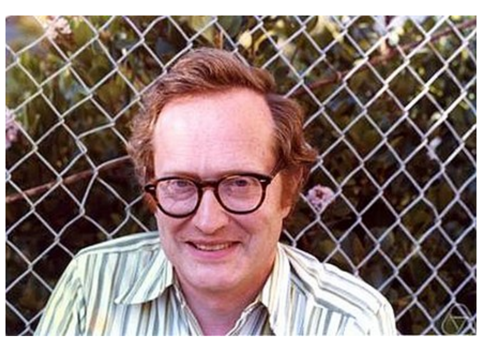
$$H = \sum_i H_i, \quad H_i = J\vec{S}_i \cdot \vec{S}_{i+1}$$

$$H = \underbrace{H_A}_{\sum_{i\in even} H_i} + \underbrace{H_B}_{\sum_{i\in odd} H_i}$$

$$[H_A, H_B] \neq 0$$

$[H_i, H_j] = 0 \quad i \neq j \quad i, j$ both in even or odd

Trotter - Suzuki Decomposition

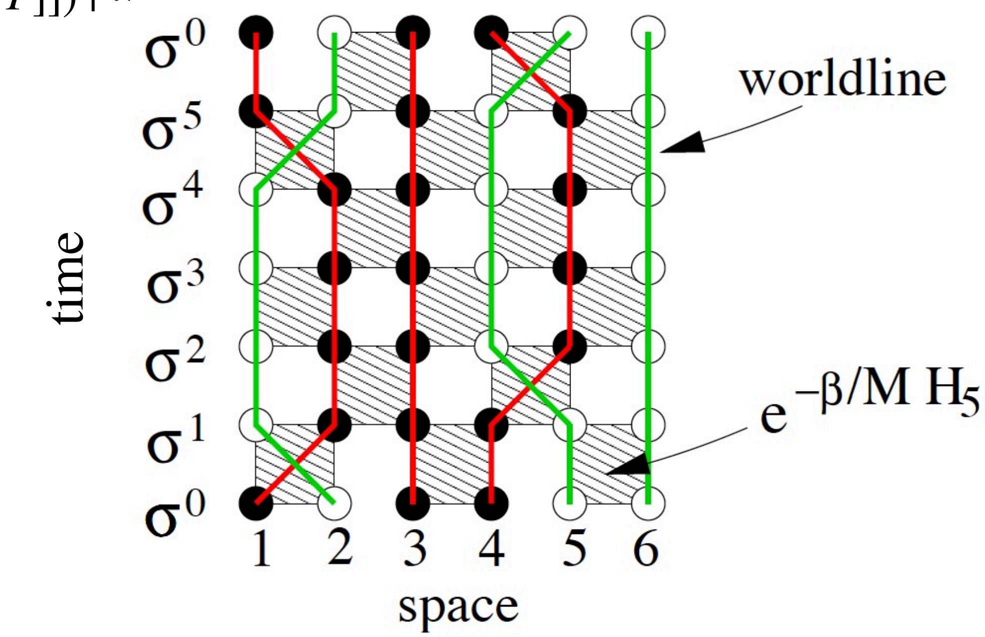


Hale Trotter (1931 -)
Canadian-American mathematician

Masuo Suzuki (1937 -)
Japanese physicist

Baker-Campbell-Hausdorff $e^X e^Y = e^{X+Y+\frac{1}{2}[X,Y]+\frac{1}{12}([X,[X,Y]]-[Y,[X,Y]])+\cdots}$

Trotter-Suzuki decomposition $e^{\tau(A+B)} = e^{\tau A} \cdot e^{\tau B} + O(\tau^2)$



$$e^{-\beta H} = (e^{-\frac{\beta}{M}H})^M, \quad M \to \infty$$

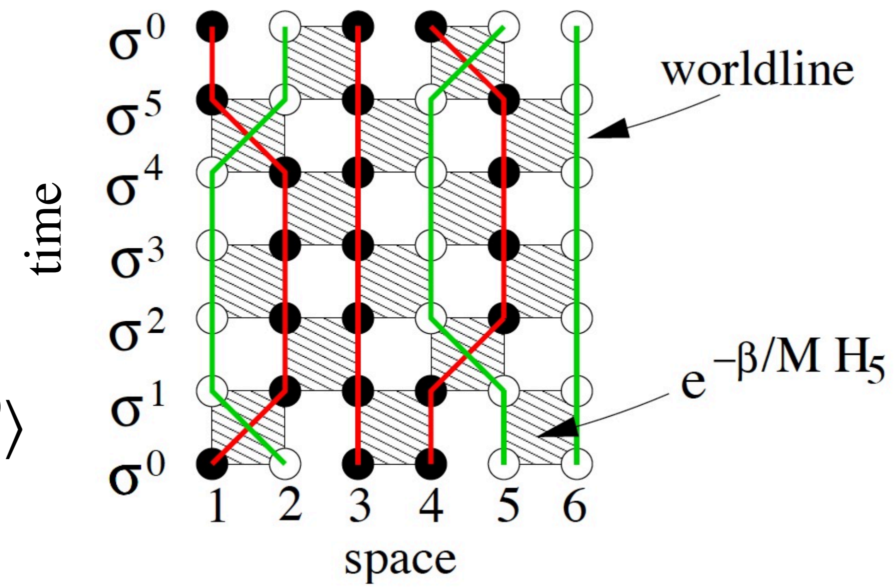
$$e^{-\frac{\beta}{M}H} = e^{-\frac{\beta}{M}(H_A+H_B)} = e^{-\frac{\beta}{M}H_A} \cdot e^{-\frac{\beta}{M}H_B} + O(1/M^2)$$

$$Z = Tr[e^{-\beta H}] \approx Tr[\underbrace{e^{-\frac{\beta}{M}H_A} \cdot e^{-\frac{\beta}{M}H_B}}_{M} \cdot \underbrace{e^{-\frac{\beta}{M}H_A} \cdot e^{-\frac{\beta}{M}H_B}}_{M-1} \cdot \cdots \cdot \underbrace{e^{-\frac{\beta}{M}H_A} \cdot e^{-\frac{\beta}{M}H_B}}_{1}]$$

$$\{\{\,|\sigma\rangle\}, |S_1^z, S_2^z, \cdots, S_N^z\rangle\} = \left\{ \begin{array}{c} |\sigma_1\rangle = |\uparrow, \uparrow, \cdots, \uparrow, \uparrow\rangle \\ |\sigma_2\rangle = |\uparrow, \uparrow, \cdots, \uparrow, \downarrow\rangle \\ |\sigma_3\rangle = |\uparrow, \uparrow, \cdots, \downarrow, \uparrow\rangle \\ \vdots \\ |\sigma_{2^N-1}\rangle = |\uparrow, \downarrow, \cdots, \downarrow, \downarrow\rangle \\ |\sigma_{2^N}\rangle = |\downarrow, \downarrow, \cdots, \downarrow, \downarrow\rangle \end{array} \right\}$$

Completeness relation $\sum_\sigma |\sigma\rangle\langle\sigma| = 1$

Write the partition function in the complete basis (Hilbert space)



$$Z = Tr[e^{-\beta H}] = \sum_{\sigma} \langle \sigma | e^{-\beta H} | \sigma \rangle$$

$$\approx \sum_{\sigma^0} \langle \sigma^0 | \underbrace{e^{-\frac{\beta}{M}H_A} \cdot e^{-\frac{\beta}{M}H_B}}_{M} \cdot \underbrace{e^{-\frac{\beta}{M}H_A} \cdot e^{-\frac{\beta}{M}H_B}}_{M-1} \cdot \cdots \cdot \underbrace{e^{-\frac{\beta}{M}H_A} \cdot e^{-\frac{\beta}{M}H_B}}_{1} | \sigma^0 \rangle$$

$$= \sum_{\sigma^0} \langle \sigma^0 | \underbrace{e^{-\frac{\beta}{M}H_A} \cdot e^{-\frac{\beta}{M}H_B}}_{M} \cdot \underbrace{e^{-\frac{\beta}{M}H_A} \cdot e^{-\frac{\beta}{M}H_B}}_{M-1} \cdot \cdots \cdot \underbrace{e^{-\frac{\beta}{M}H_A} (\sum_{\sigma^1} | \sigma^1 \rangle \langle \sigma^1 |) e^{-\frac{\beta}{M}H_B}}_{1} | \sigma^0 \rangle$$

$$= \sum_{\sigma^0,\sigma^1} \langle \sigma^0 | \underbrace{e^{-\frac{\beta}{M}H_A} \cdot e^{-\frac{\beta}{M}H_B}}_{M} \cdot \underbrace{e^{-\frac{\beta}{M}H_A} \cdot e^{-\frac{\beta}{M}H_B}}_{M-1} \cdot \cdots (\sum_{\sigma^2} | \sigma^2 \rangle \langle \sigma^2 |) e^{-\frac{\beta}{M}H_A} | \sigma^1 \rangle \langle \sigma^1 | e^{-\frac{\beta}{M}H_B} | \sigma^0 \rangle$$

$$= \sum_{\sigma^0,\sigma^1,\sigma^2} \langle \sigma^0 | \underbrace{e^{-\frac{\beta}{M}H_A} \cdot e^{-\frac{\beta}{M}H_B}}_{M} \cdot \underbrace{e^{-\frac{\beta}{M}H_A} \cdot e^{-\frac{\beta}{M}H_B}}_{M-1} \cdot \cdots (\sum_{\sigma^3} | \sigma^3 \rangle \langle \sigma^3 |) e^{-\frac{\beta}{M}H_B} | \sigma^2 \rangle \langle \sigma^2 | e^{-\frac{\beta}{M}H_A} | \sigma^1 \rangle \langle \sigma^1 | e^{-\frac{\beta}{M}H_B} | \sigma^0 \rangle$$

$$= \sum_{\{\sigma^i\}} \underbrace{\langle \sigma^0 | e^{-\frac{\beta}{M}H_A} | \sigma^{2M-1} \rangle}_{2M} \underbrace{\langle \sigma^{2M-1} | e^{-\frac{\beta}{M}H_B} | \sigma^{2M-2} \rangle}_{2M-1} \underbrace{\langle \sigma^{2M-2} | e^{-\frac{\beta}{M}H_A} | \sigma^{2M-3} \rangle}_{2M-2} \cdots$$

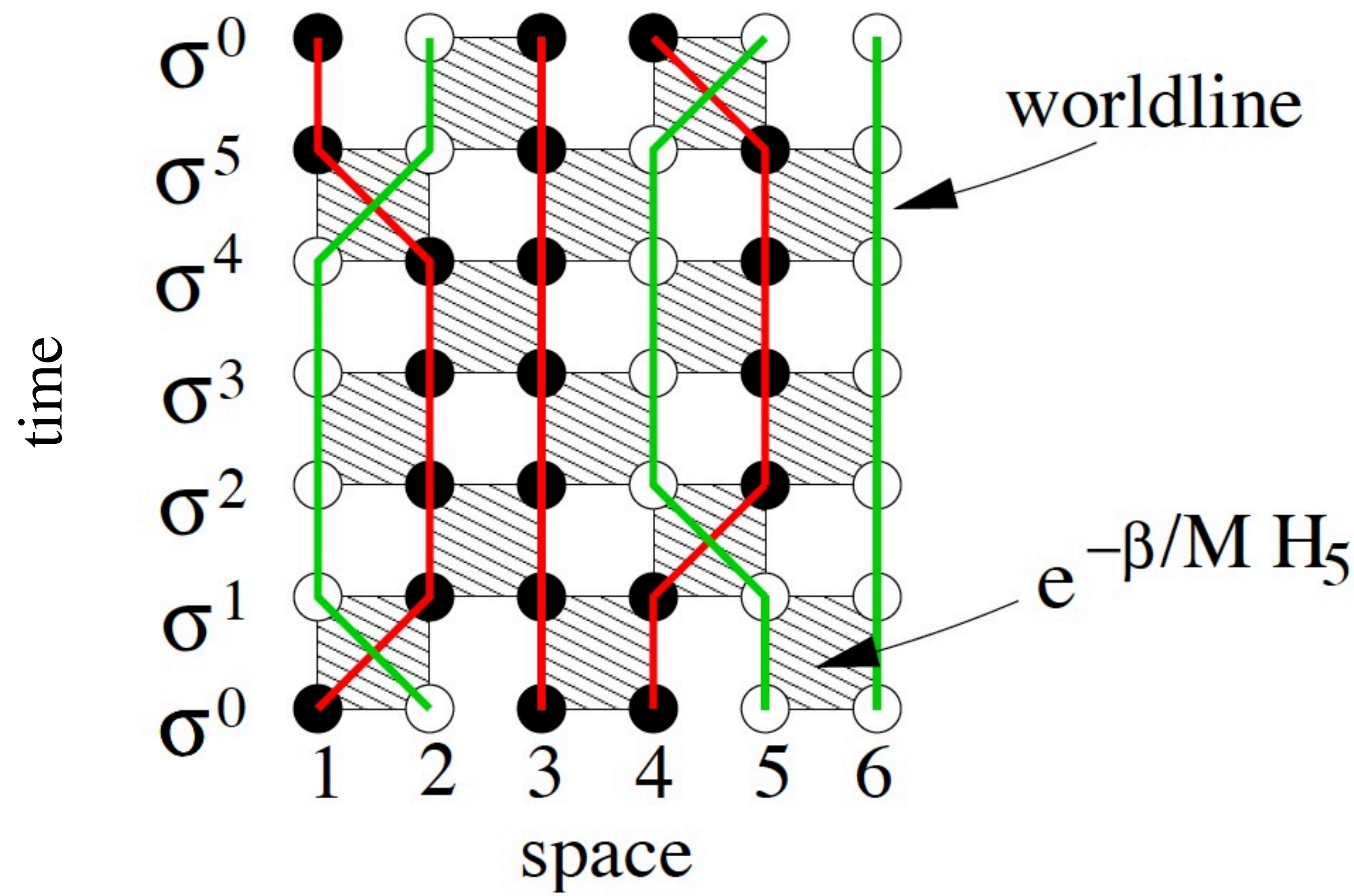
$$\cdots \underbrace{\langle \sigma^3 | e^{-\frac{\beta}{M}H_B} | \sigma^2 \rangle}_{3} \underbrace{\langle \sigma^2 | e^{-\frac{\beta}{M}H_A} | \sigma^1 \rangle}_{2} \underbrace{\langle \sigma^1 | e^{-\frac{\beta}{M}H_B} | \sigma^0 \rangle}_{1}$$

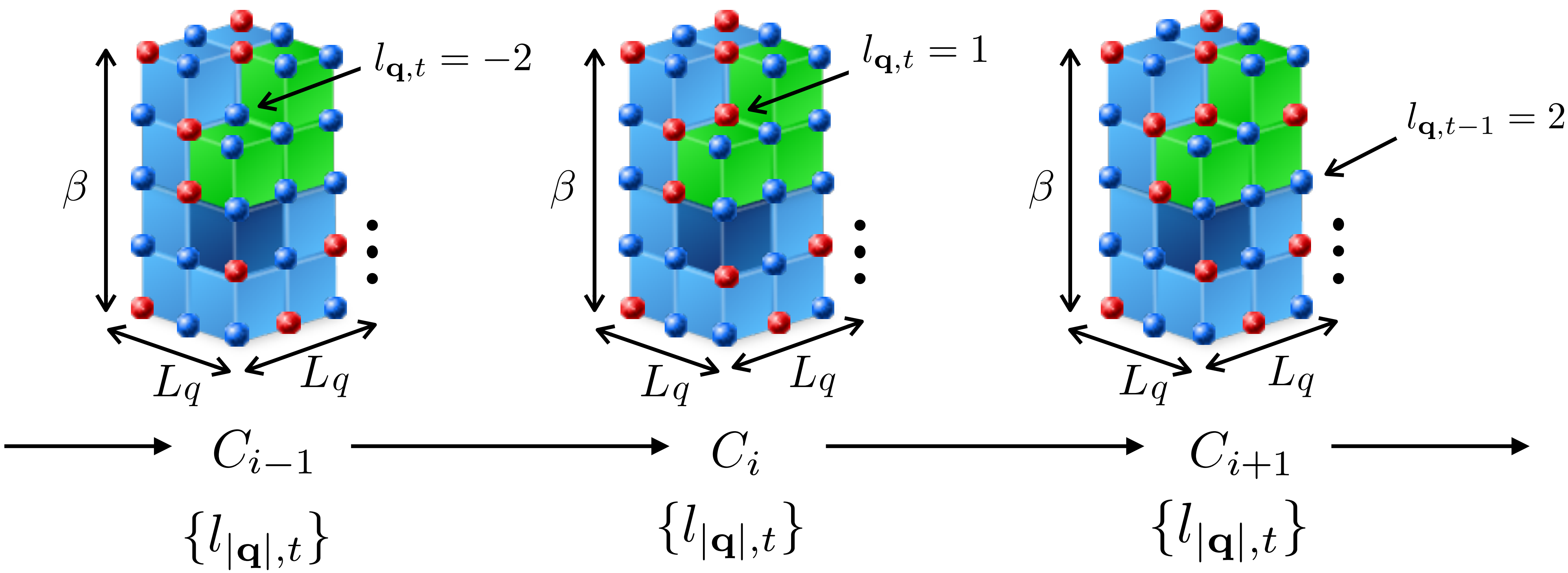
$$e^{-\frac{\beta}{M}H_A} = \prod_{i \in even} e^{-\frac{\beta}{M}H_i} = e^{-\frac{\beta}{M}H_2}\, e^{-\frac{\beta}{M}H_4}\, e^{-\frac{\beta}{M}H_6}\, \ldots$$

$$e^{-\frac{\beta}{M}H_B} = \prod_{i \in odd} e^{-\frac{\beta}{M}H_i} = e^{-\frac{\beta}{M}H_1}\, e^{-\frac{\beta}{M}H_3}\, e^{-\frac{\beta}{M}H_5}\, \ldots$$

$$Z = Tr[e^{-\beta H}] = \sum_{\sigma} \langle \sigma | e^{-\beta H} | \sigma \rangle$$ for $N = 6, \quad M = 3$ $\quad \Delta\tau = \beta / M$

Checkerboard decomposition





$$H_i = J\begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix}$$

in the basis of a bond

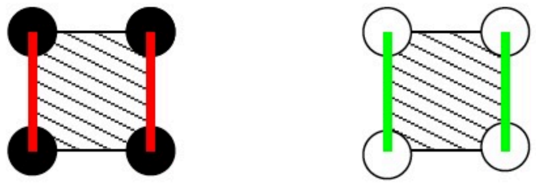
$$\begin{pmatrix} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{pmatrix}_{i,i+1}$$

$$\cosh(x) = \frac{1}{2}(e^x + e^{-x})$$

$$\sinh(x) = \frac{1}{2}(e^x - e^{-x})$$

$$e^{-\Delta\tau H_i} = \begin{pmatrix} e^{-\Delta\tau\frac{J}{4}} & 0 & 0 & 0 \\ 0 & e^{\Delta\tau\frac{J}{4}}\cosh(\Delta\tau\frac{J}{2}) & e^{\Delta\tau\frac{J}{4}}\sinh(-\Delta\tau\frac{J}{2}) & 0 \\ 0 & e^{\Delta\tau\frac{J}{4}}\sinh(-\Delta\tau\frac{J}{2}) & e^{\Delta\tau\frac{J}{4}}\cosh(\Delta\tau\frac{J}{2}) & 0 \\ 0 & 0 & 0 & e^{-\Delta\tau\frac{J}{4}} \end{pmatrix}$$

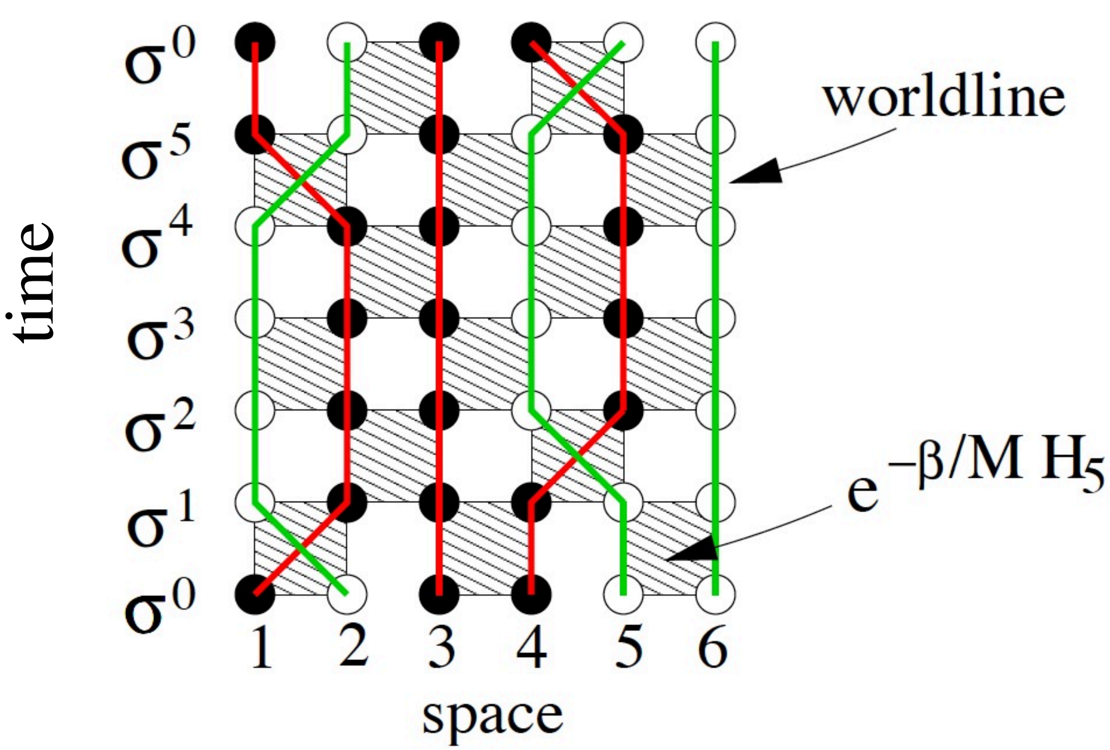
in the same basis



$$\langle \uparrow, \uparrow | e^{-\Delta\tau H_i} | \uparrow, \uparrow \rangle = \langle \downarrow, \downarrow | e^{-\Delta\tau H_i} | \downarrow, \downarrow \rangle = e^{-\Delta\tau \frac{J}{4}}$$

$$\langle \uparrow, \downarrow | e^{-\Delta\tau H_i} | \uparrow, \downarrow \rangle = \langle \downarrow, \uparrow | e^{-\Delta\tau H_i} | \downarrow, \uparrow \rangle = e^{\Delta\tau \frac{J}{4}} \cosh(\Delta\tau \frac{J}{2})$$

$$\langle \downarrow, \uparrow | e^{-\Delta\tau H_i} | \uparrow, \downarrow \rangle = \langle \uparrow, \downarrow | e^{-\Delta\tau H_i} | \downarrow, \uparrow \rangle = e^{\Delta\tau \frac{J}{4}} \sinh(-\Delta\tau \frac{J}{2})$$



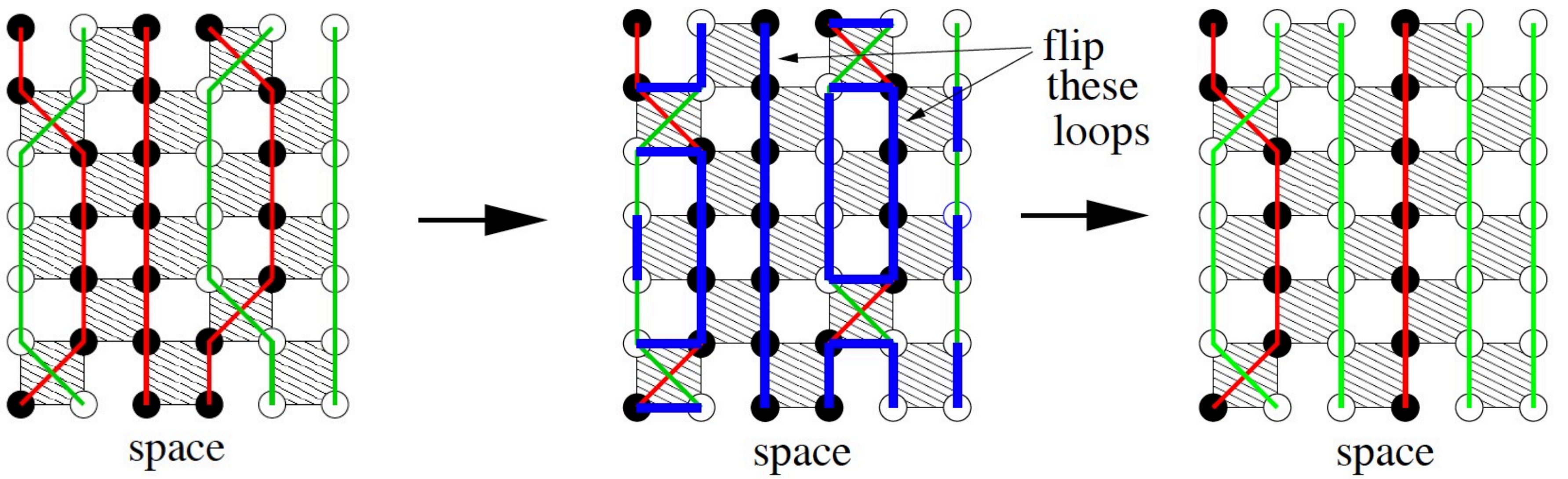
$$Z = Tr[e^{-\beta H}] = \sum_{\sigma} \langle \sigma | e^{-\beta H} | \sigma \rangle = \sum_{\{C\}} W(C)$$

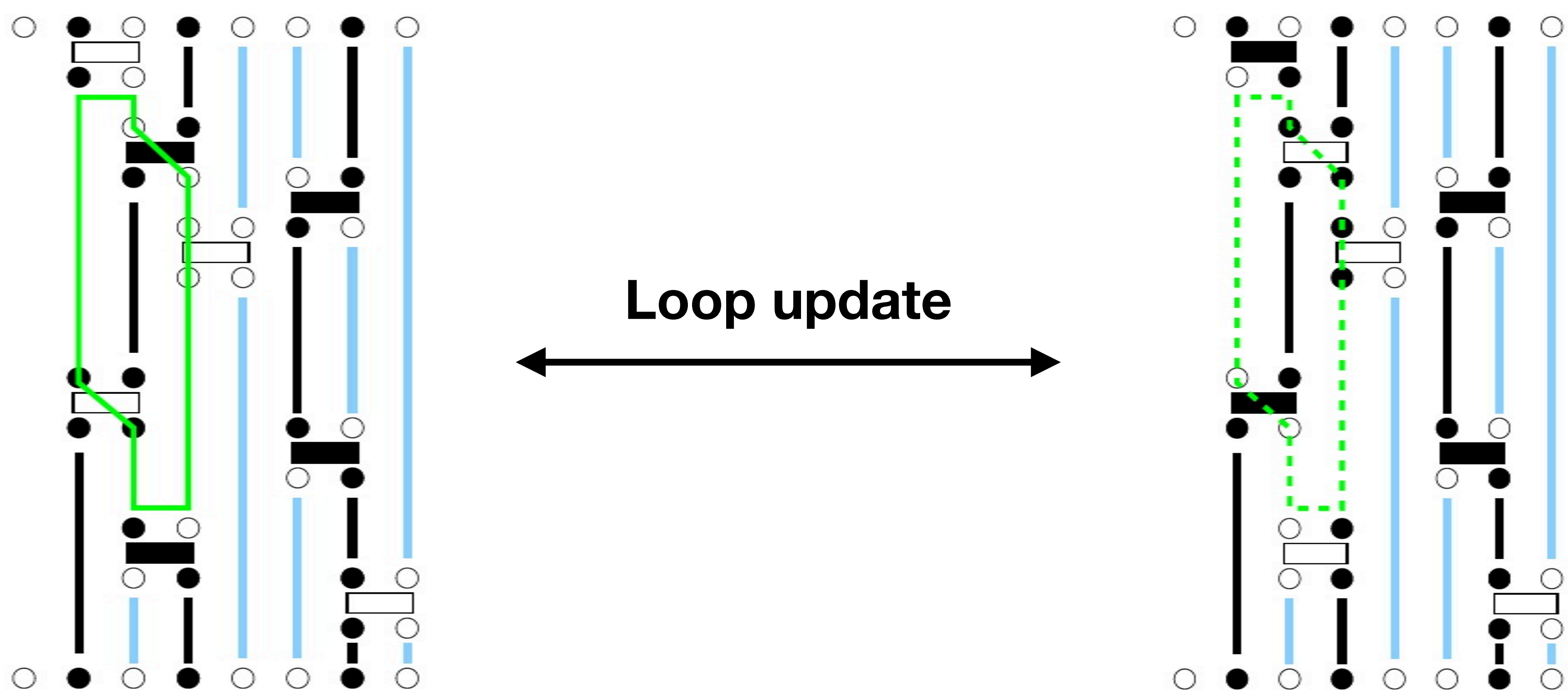
$$W(C) = \prod_{plaquettes\ P} W_P(C|_P)$$

Concepts of space-time configuration, path integral and world-line (worm)

Sample the beginning point
Sample the history

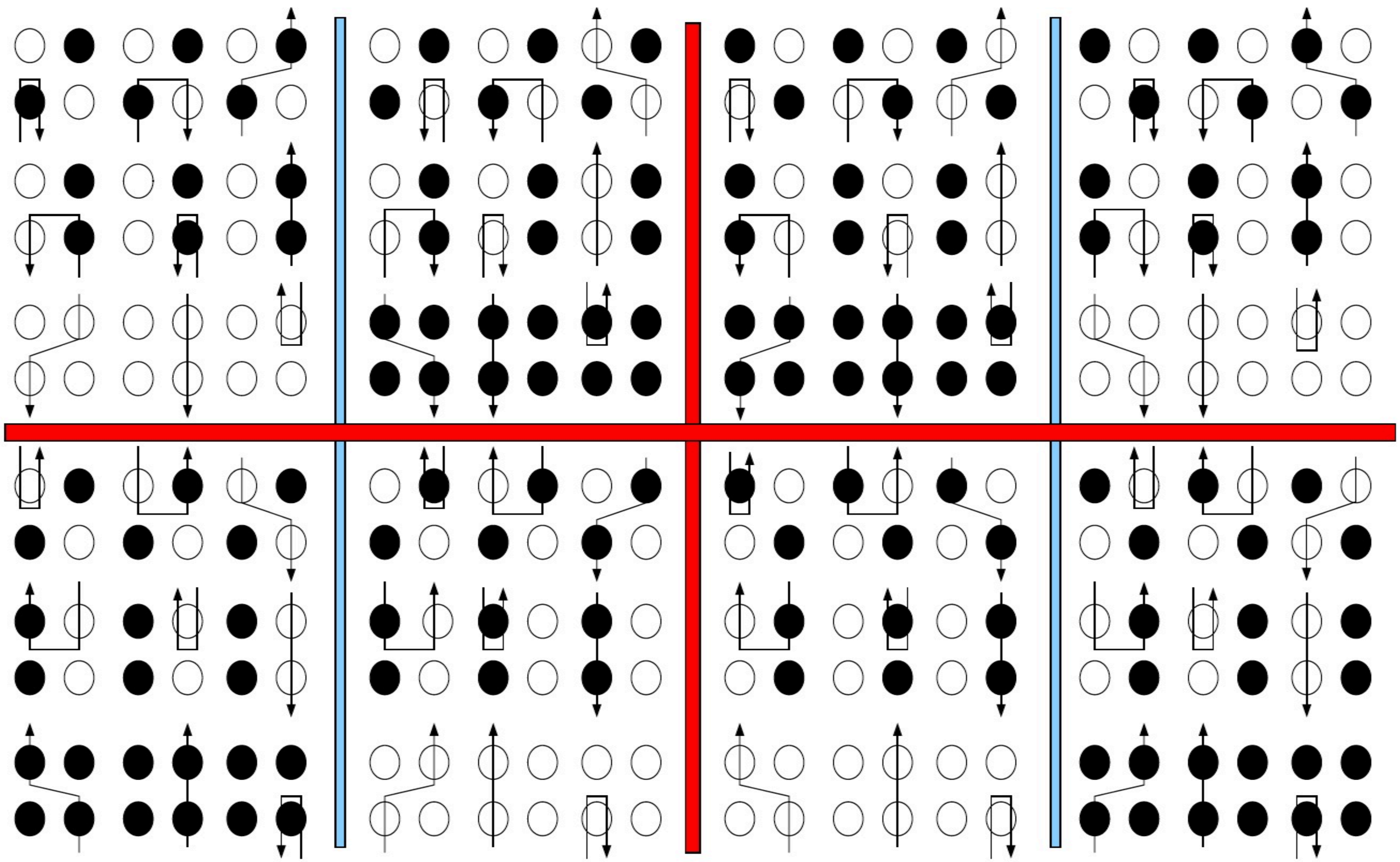
$$Z = Tr[e^{-\beta H}] = \sum_{\sigma} \langle \sigma | e^{-\beta H} | \sigma \rangle = \sum_{\{C\}} W(C)$$





Zi Yang Meng, Master Thesis, Stuttgart 2007

Gate way to cure your OCD (obsessive compulsive disorder)

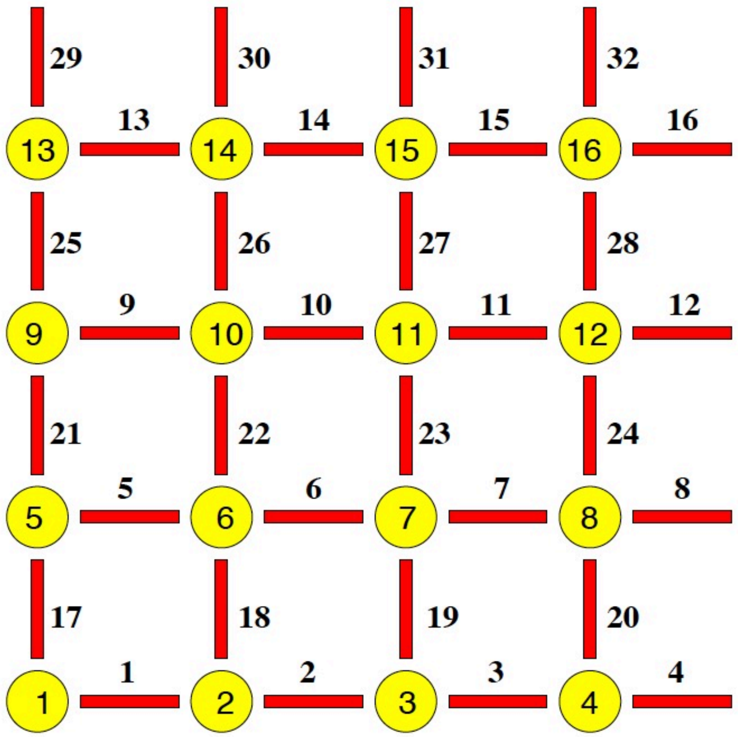


Zi Yang Meng, Master Thesis, Stuttgart 2007

Square lattice

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

$$m_s^z = \frac{1}{N} \langle | \sum_{i=1}^{N} (-1)^i S_i^z | \rangle$$



L_x	T/J	E/J	$S(\pi,\pi)$	ρ_s	m_s	MC steps
4	0.0312500	-0.70183(2)	1.47499(9)	0.18507(4)	0.25871(0)	10^6
6	0.0208333	-0.67873(6)	2.51806(6)	0.15816(3)	0.22627(2)	10^6
8	0.0156250	-0.67342(3)	3.79475(6)	0.14706(9)	0.20872(0)	10^6
10	0.0125000	-0.67155(7)	5.31278(9)	0.14082(9)	0.19786(2)	10×10^6
12	0.0104167	-0.67068(9)	7.07702(8)	0.13686(2)	0.19053(8)	5×10^6
14	0.0089290	-0.67022(9)	9.09229(9)	0.13438(7)	0.18531(1)	6×10^6
16	0.0078125	-0.66997(4)	11.35103(6)	0.13232(8)	0.18131(1)	6×10^6
20	0.0062500	-0.66971(3)	16.63246(9)	0.12982(3)	0.17580(3)	10×10^6

$$m_s = \sqrt{(m_s^x)^2 + (m_s^y)^2 + (m_s^z)^2} = \sqrt{3} m_s^z = 1.732 \times 0.176 = 0.304$$

Zi Yang Meng, Master Thesis, Stuttgart 2007