

Content



0. Introduction

1. Differential equations

1.1 Classical equation of motion (classical mechanics, pendulum)

1.2 Partial differential equation relaxation methods (electromagnetism, diffusion)

1.3 Partial differential equation in space-time (traffic flow, tsunami)

2. Eigenvalue problem

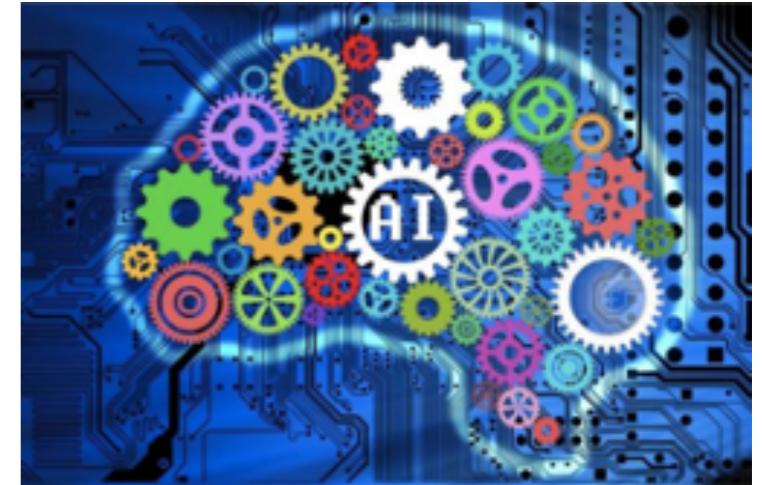
2.1 Schrödinger equation and Hamiltonian (Harmonic oscillator, wave package)

2.2 Quantum lattice model and Hibert space (Heisenberg model)

2.3 Exact diagonalization of spin chain (Spin wave, Haldane conjecture, topology)

2.4 Matrix product state and density matrix renormalization group (DMRG)

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)

Hamiltonian matrix

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

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

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

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

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

$$\begin{aligned}\langle \uparrow\uparrow | H | \uparrow\uparrow \rangle &= \frac{J}{4} \\ \langle \downarrow\downarrow | H | \downarrow\downarrow \rangle &= \frac{J}{4} \\ \langle \uparrow\downarrow | H | \uparrow\downarrow \rangle &= -\frac{J}{4} \\ \langle \downarrow\uparrow | H | \uparrow\downarrow \rangle &= \frac{J}{2} \\ \langle \uparrow\downarrow | H | \downarrow\uparrow \rangle &= \frac{J}{2} \\ \langle \downarrow\uparrow | H | \downarrow\uparrow \rangle &= -\frac{J}{4}\end{aligned}$$

$$H = J \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & -\frac{1}{4} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & -\frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix} \quad \text{in the basis} \quad \begin{pmatrix} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{pmatrix}$$

Hilbert space size

Dimensionality of the Hilbert space

$$d = \dim(H) = 2^N$$

Computation complexity for diagonalising

$$d \times d \text{ matrix } O(d^3) = O(2^{3N})$$

💡 Lead to the “exponential wall”

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

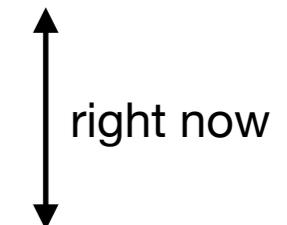
$$N = 20 \quad \dim = 1,048,576 \sim 10^6$$

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

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

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

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.



	a	b	c	d	e	f	g	h	
8	♕	♘	♗	♔	♕	♗	♘	♕	8
7	♙	♙	♙	♙	♙	♙	♙	♙	7
6									6
5									5
4									4
3									3
2	♙	♙	♙	♙	♙	♙	♙	♙	2
1	♕	♘	♗	♔	♕	♗	♘	♕	1
	a	b	c	d	e	f	g	h	

Solving exponentially complex problem in polynomial time

Quantum Monte Carlo (for spin systems)

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

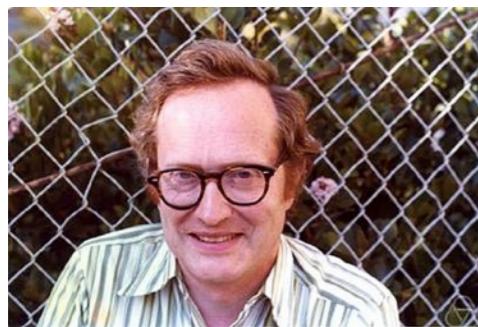
In statistical (classical) physics

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

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

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

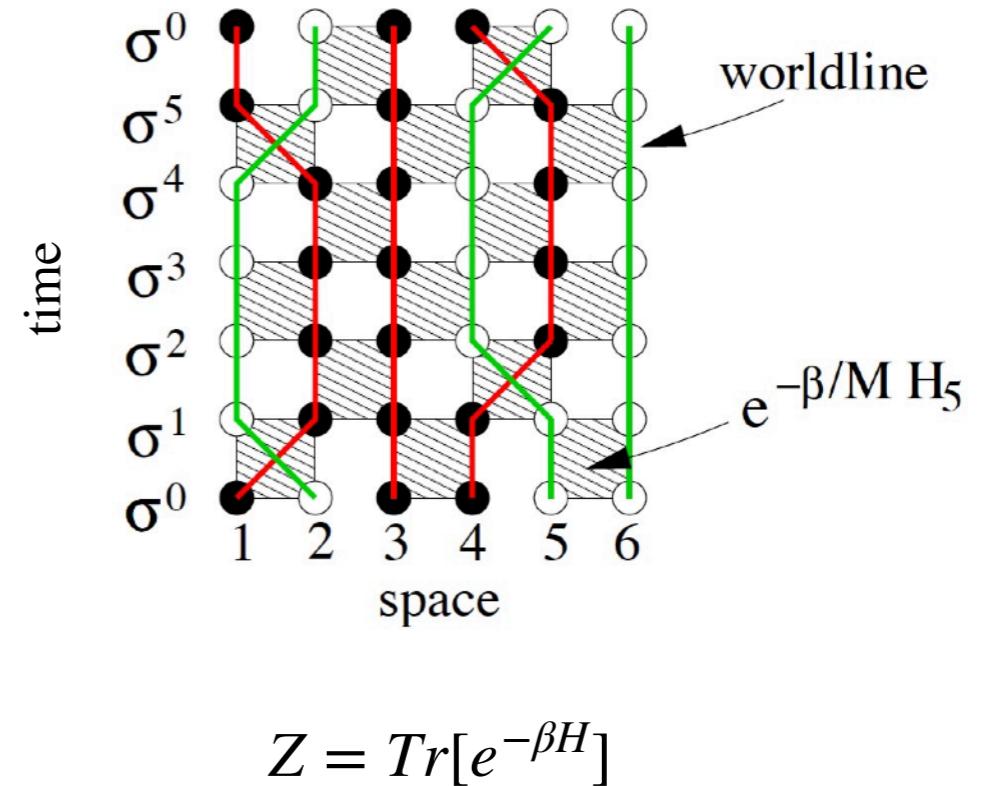
Trotter - Suzuki Decomposition



Hale Trotter (1931 -)
Canadian-American mathematician



Masuo Suzuki (1937 -)
Japanese physicist



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

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

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

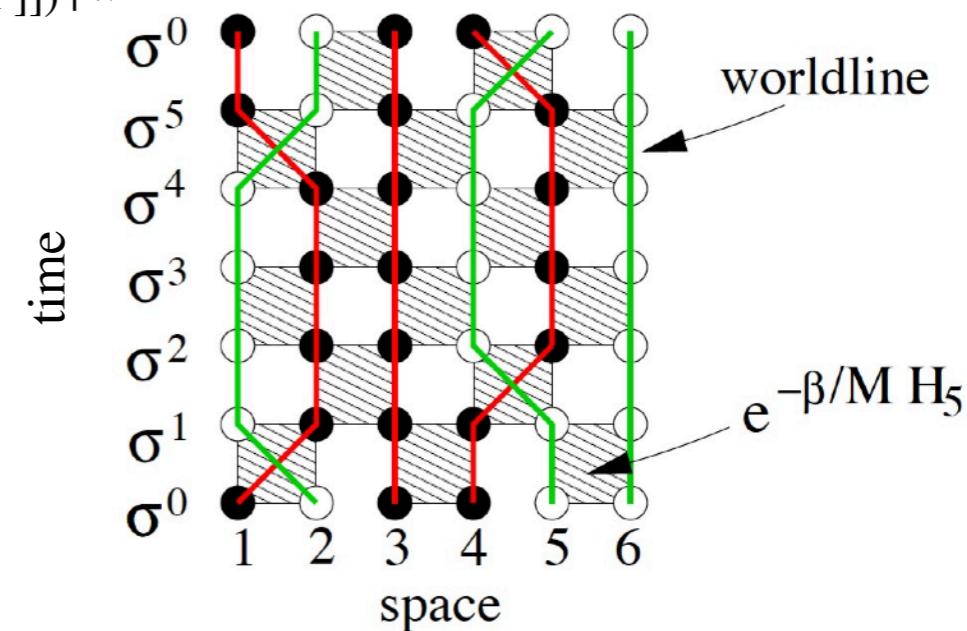
$$[H_i, H_j] = 0 \quad i \neq j \quad i, j \text{ both in even or odd}$$

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

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

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

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



$$Z = Tr[e^{-\beta H}] \approx Tr[\underbrace{e^{-\frac{\beta}{M}H_A} \cdot e^{-\frac{\beta}{M}H_B}}_M \cdot \underbrace{e^{-\frac{\beta}{M}H_A} \cdot e^{-\frac{\beta}{M}H_B}}_{M-1} \cdot \dots \cdot \underbrace{e^{-\frac{\beta}{M}H_A} \cdot e^{-\frac{\beta}{M}H_B}}_1]$$

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

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

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

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

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

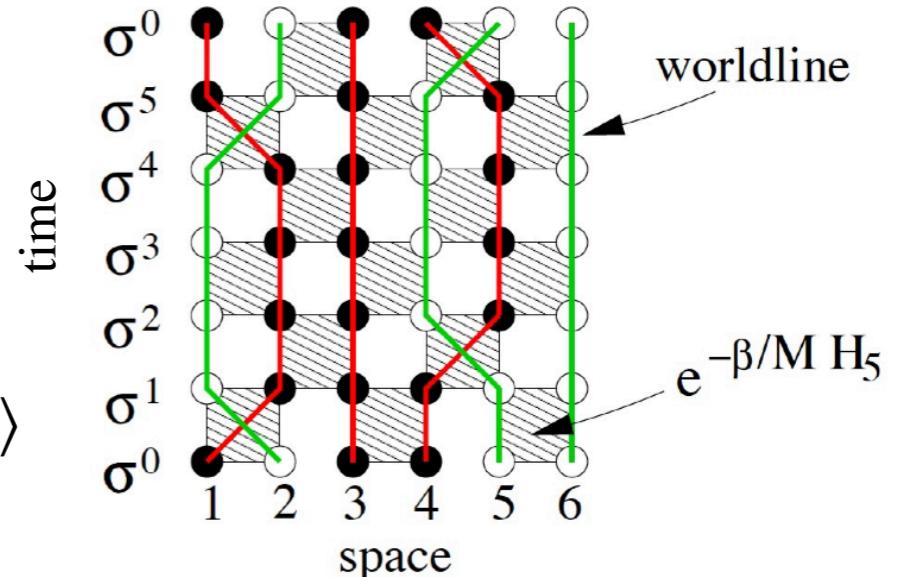
$$= \sum_{\sigma^0} \langle \sigma^0 | \underbrace{e^{-\frac{\beta}{M} H_A} \cdot e^{-\frac{\beta}{M} H_B} \cdot e^{-\frac{\beta}{M} H_A} \cdot e^{-\frac{\beta}{M} H_B} \cdot \dots \cdot e^{-\frac{\beta}{M} H_A}}_M \underbrace{\left(\sum_{\sigma^1} |\sigma^1\rangle\langle\sigma^1| \right)}_1 e^{-\frac{\beta}{M} H_B} | \sigma^0 \rangle$$

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

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

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

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

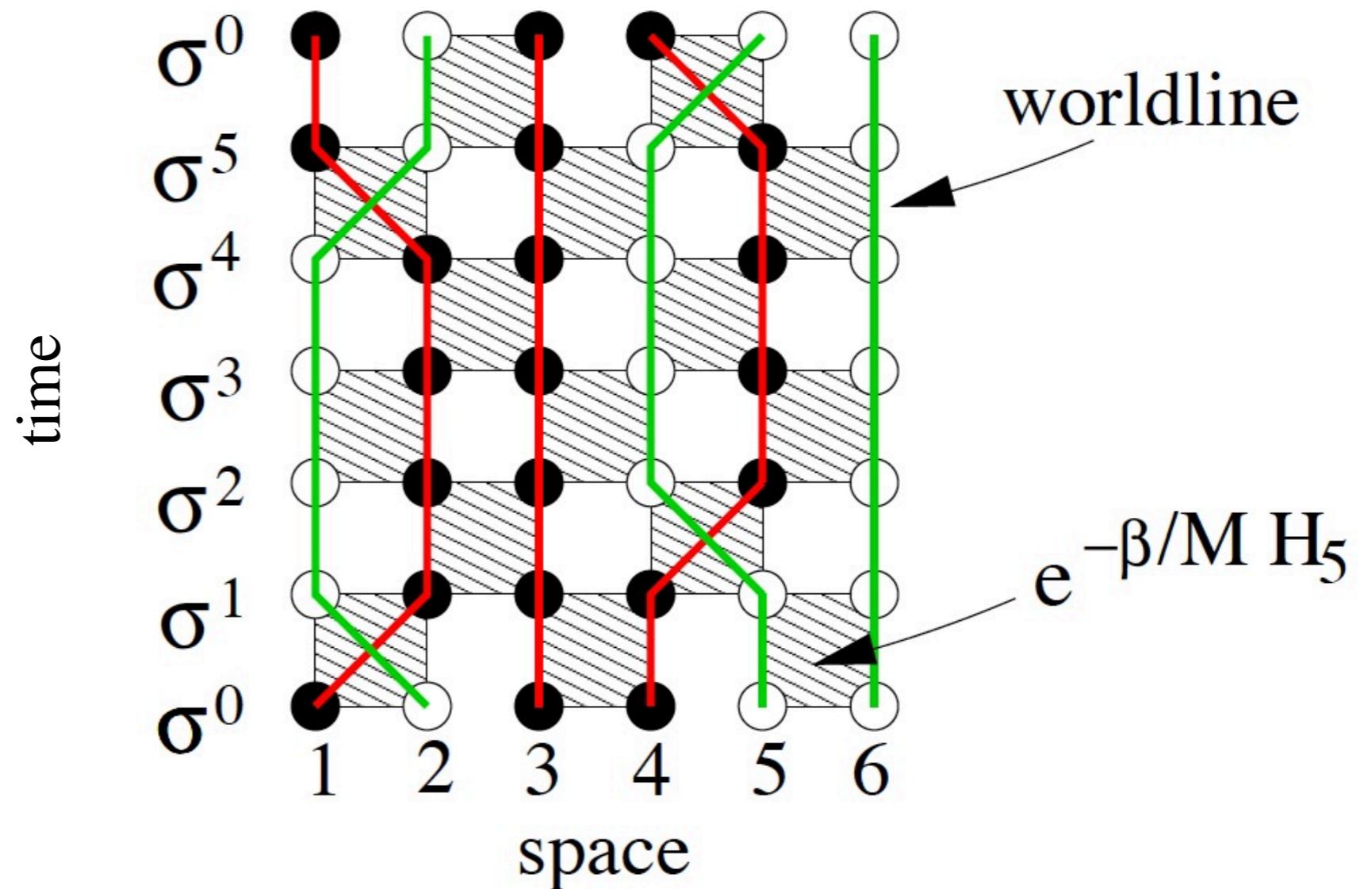


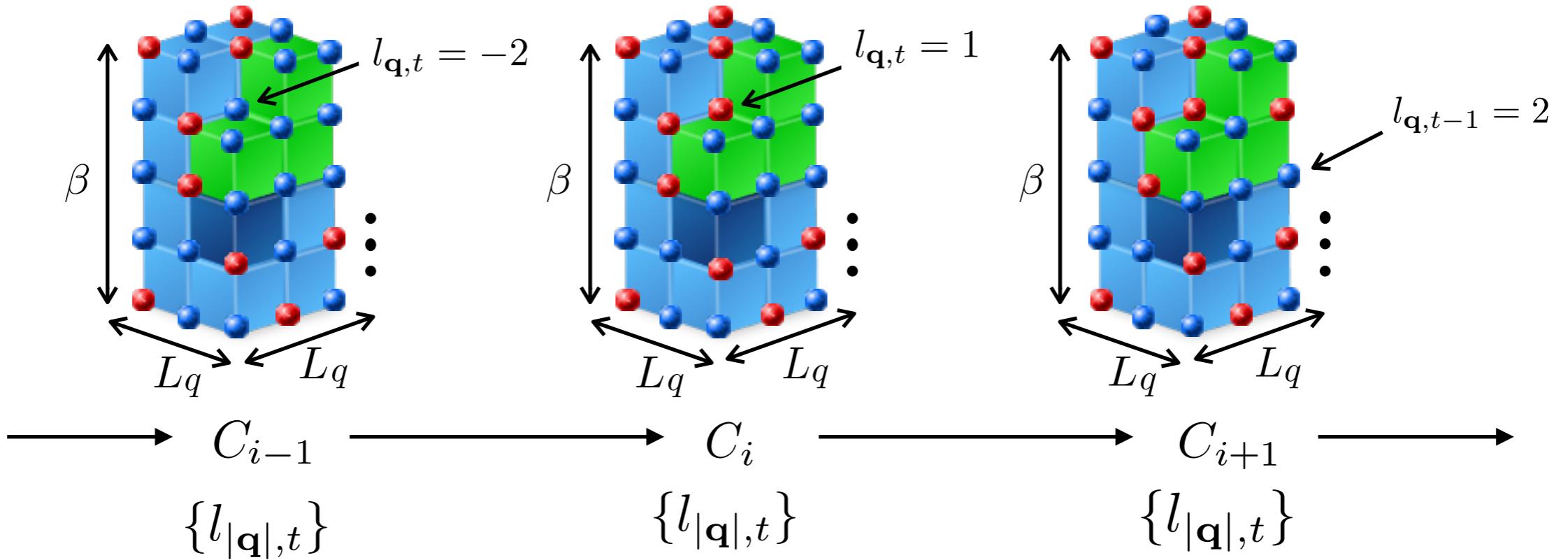
$$e^{-\frac{\beta}{M}H_A} = \prod_{i \in even} e^{-\frac{\beta}{M}H_i} = e^{-\frac{\beta}{M}H_2} e^{-\frac{\beta}{M}H_4} e^{-\frac{\beta}{M}H_6} \dots$$

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

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

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

$$\left(\begin{array}{c} | \uparrow \uparrow \rangle \\ | \uparrow \downarrow \rangle \\ | \downarrow \uparrow \rangle \\ | \downarrow \downarrow \rangle \end{array} \right)_{i,i+1}$$

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

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

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

in the same basis



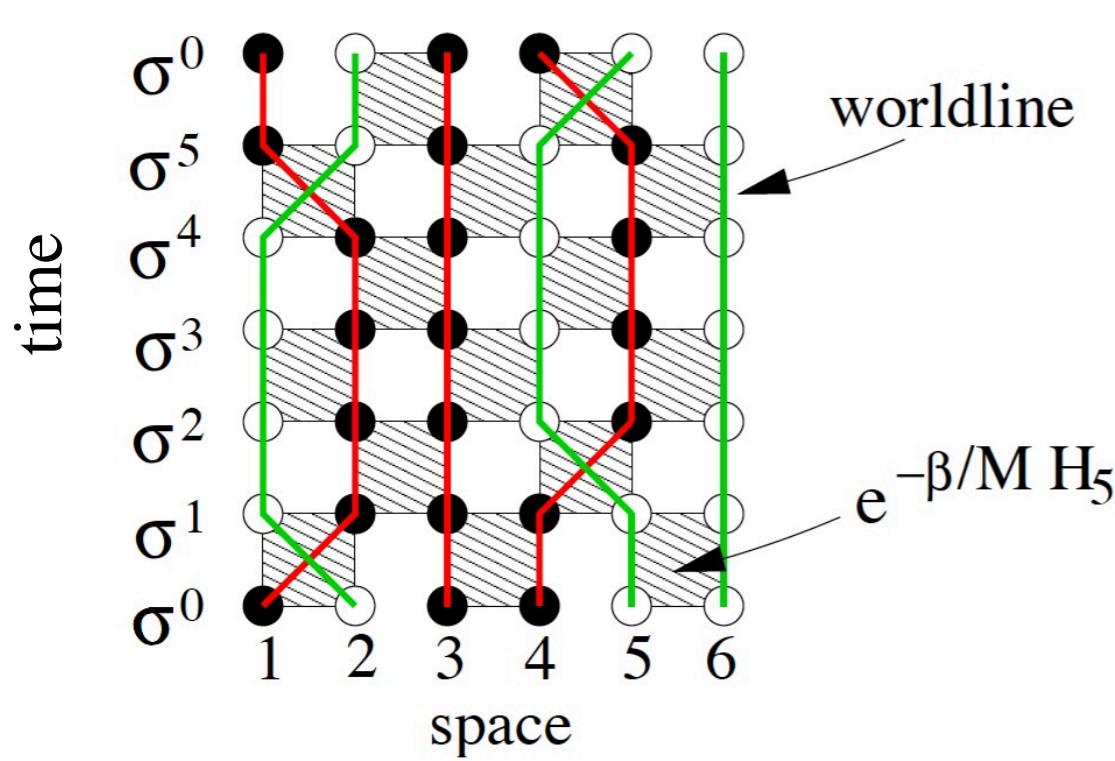
$$\langle \uparrow, \uparrow | e^{-\Delta\tau H_i} | \uparrow, \uparrow \rangle = \langle \downarrow, \downarrow | e^{-\Delta\tau H_i} | \downarrow, \downarrow \rangle = e^{-\Delta\tau \frac{J}{4}}$$



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



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



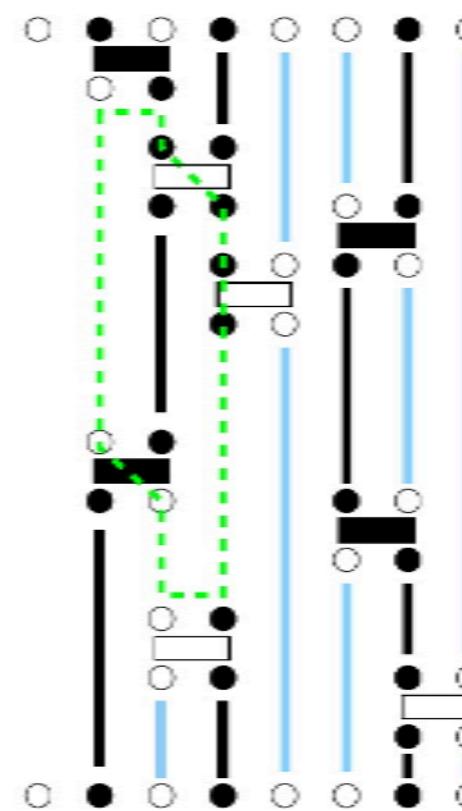
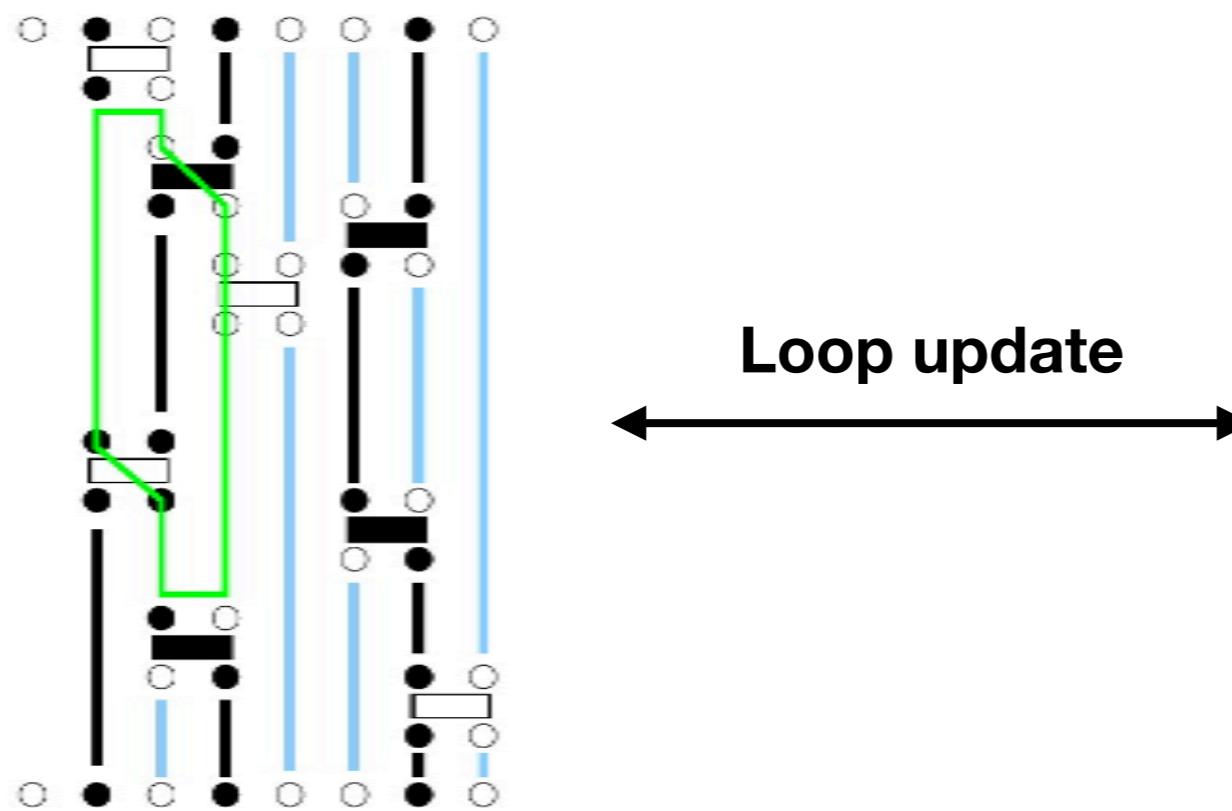
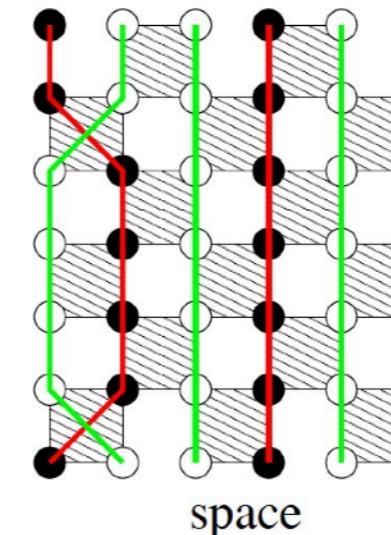
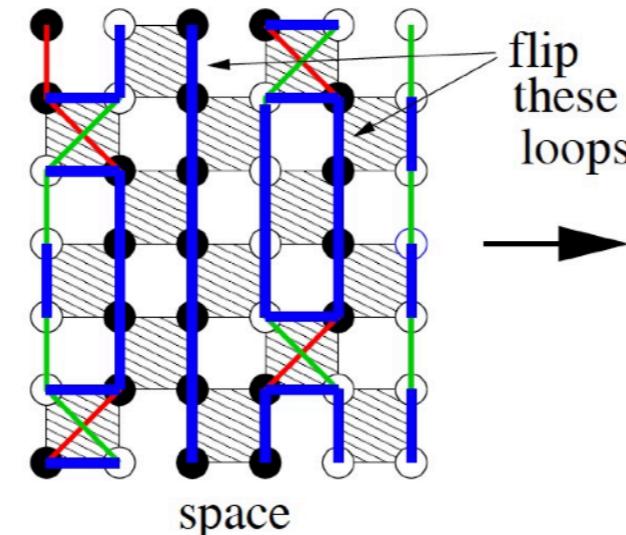
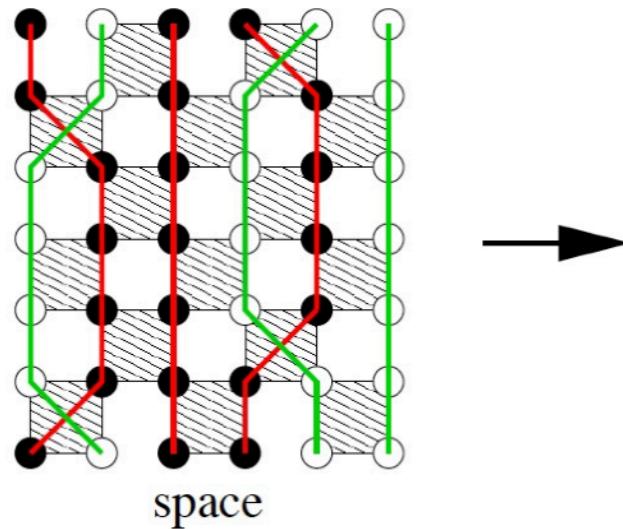
$$Z = Tr[e^{-\beta H}] = \sum_{\sigma} \langle \sigma | e^{-\beta H} | \sigma \rangle = \sum_{\{C\}} W(C)$$

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

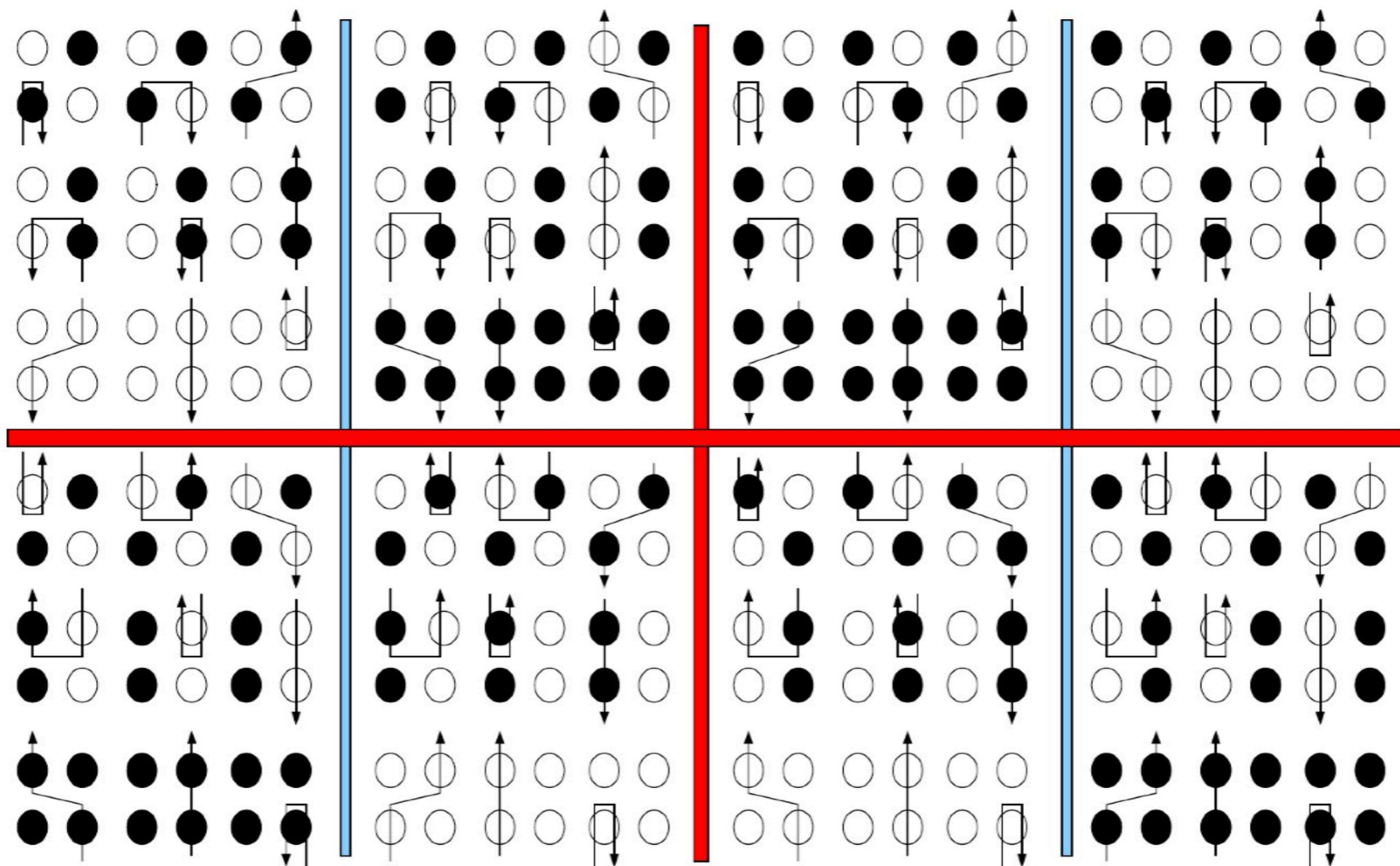
Concepts of space-time configuration, path integral and world-line (worm)

Sample the beginning point
Sample the history

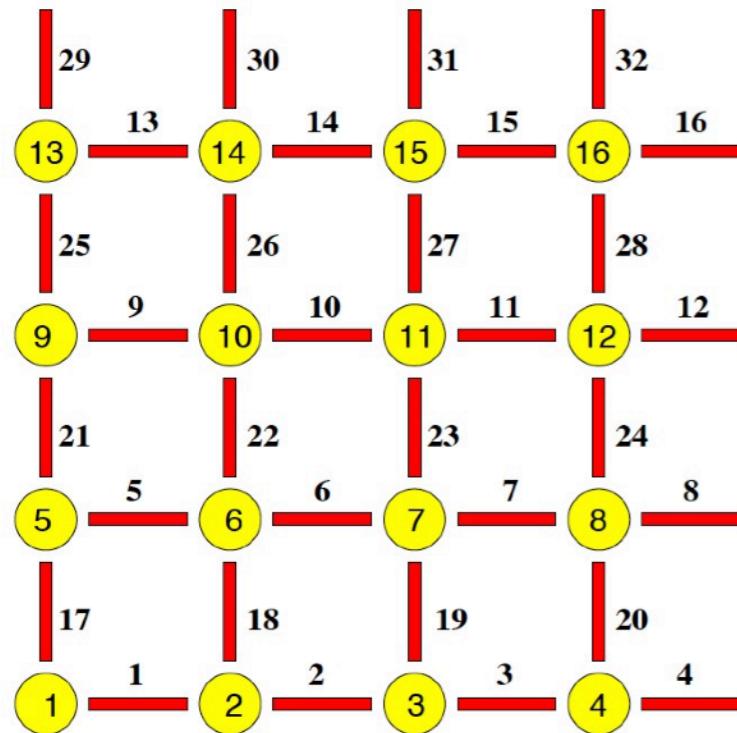
$$Z = \text{Tr}[e^{-\beta H}] = \sum_{\sigma} \langle \sigma | e^{-\beta H} | \sigma \rangle = \sum_{\{C\}} W(C)$$



Gate way to cure your OCD (obsessive compulsive disorder)



Square lattice



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

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

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

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

👤 Zi Yang Meng, Master Thesis, Stuttgart 2007

