Institute of Physics, Chinese Academy of Sciences, Beijing, October 24, 2014

Introduction to quantum spin systems and quantum Monte Carlo simulations

Anders W Sandvik, Boston University

- Classical spins and classical Monte Carlo
- Path integrals in quantum statistical mechanics
- Stochastic Series expansion (incl technical details)
- Ground-state projection with valence bonds

Review article on quantum spin systems and numerical methods**: ArXiv:1101.3281**

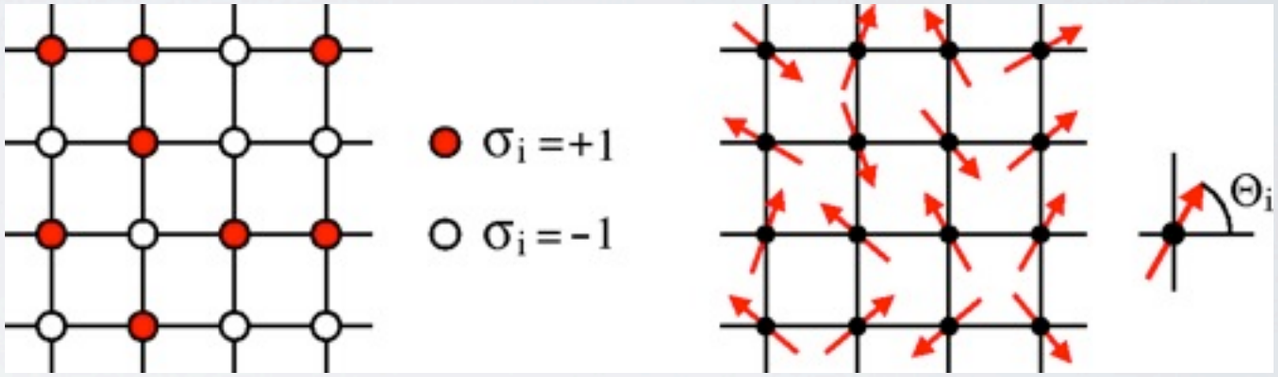
Classical spin systems and Monte Carlo simulations

Classical spin models

Lattice models with "spin" degrees of freedom at the vertices

Classified by type of spin:

- **Ising model: discrete spins, normally two-state $\sigma_i = -1, +1$**
- **XY model: planar vector spins (fixed length)**
- **Heisenberg model: 3-dimensional vector spins.**



Statistical mechanics

- **spin configurations C**
- **energy E(C)**
- **some quantity Q(C)**
- **temperature T (k_B=1)**

$$\langle Q \rangle = \frac{1}{Z} \sum_C Q(C) \mathrm{e}^{-E(C)/T}$$

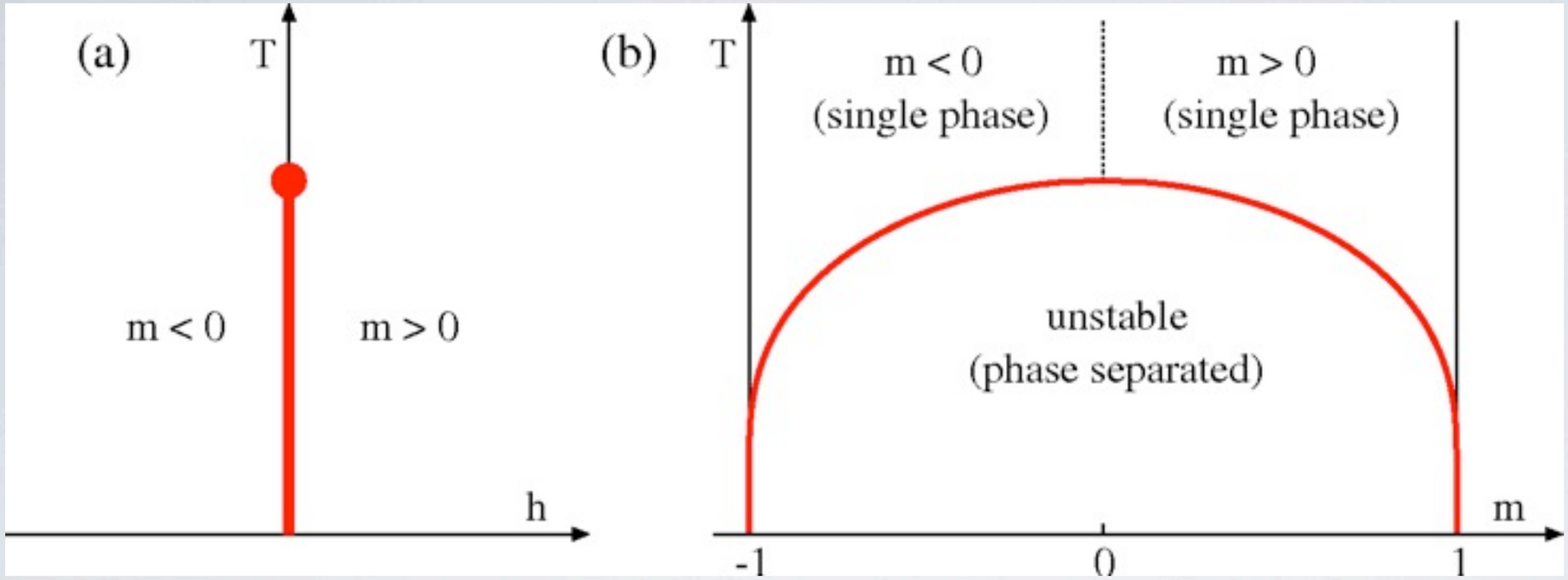
$$Z = \sum_C \mathrm{e}^{-E(C)/T}$$

$$E = \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j \qquad \textbf{(Ising)}$$

$$E = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_{\langle ij \rangle} J_{ij} \cos(\Theta_i - \Theta_j) \qquad \textbf{(XY)}$$

$$E = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j \qquad \textbf{(Heisenberg)}$$

Phase transition in the Ising model

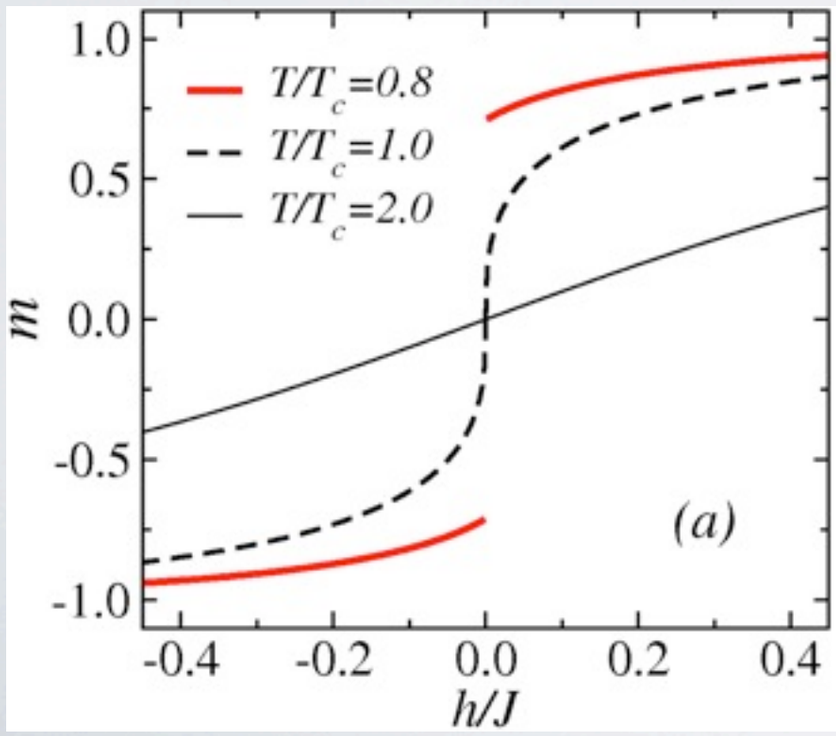


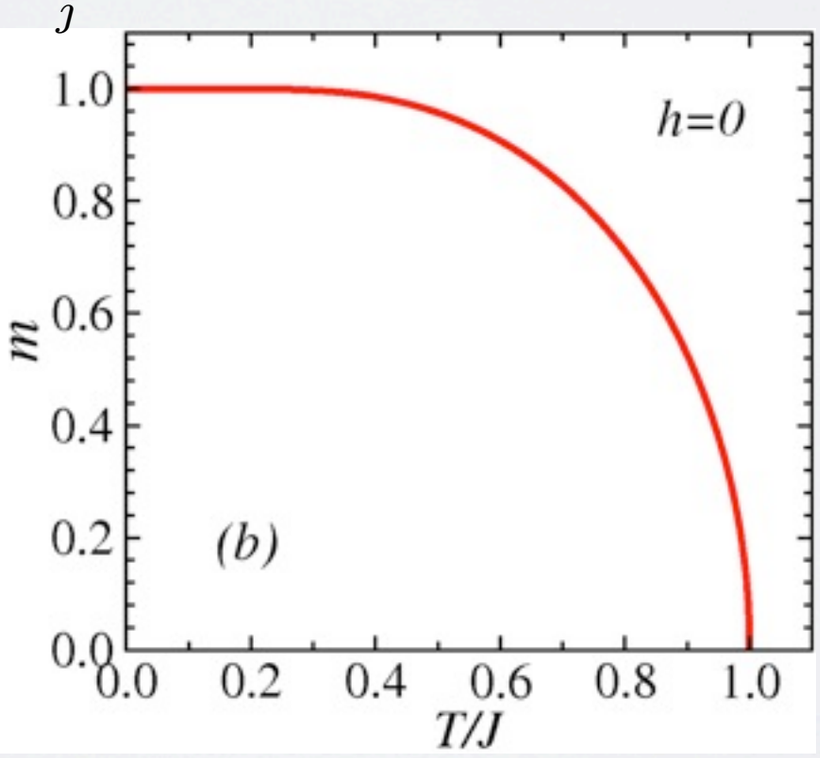
For 2D square lattice with nearest-neighbor couplings

$$\frac{T_c}{J} = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269$$

- first-order transition versus h (at h=0) for $T<T_c$
- continuous transition at h=0

Mean-field solution: $J = J_i = \sum_j J_{ij} \qquad m = \tanh[(Jm+h)/T], \qquad (m = \langle \sigma_i \rangle)$





- Here J is the sum of local couplings

$$J = \sum_j J_{ij}$$

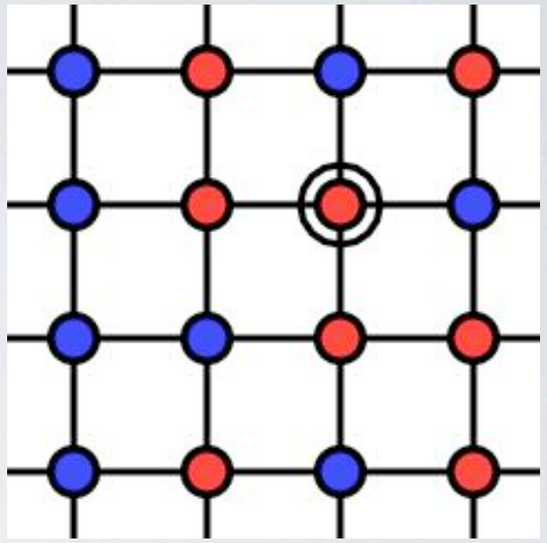
Monte Carlo simulation of the Ising model

The Metropolis algorithm

[Metropolis, Rusenbluth, Rosenbluth, Teller, and Teller, Phys. Rev. 1953]

Generate a series of configurations (Markov chain); $C_1 \rightarrow C_2 \rightarrow C_3 \rightarrow C_4 \rightarrow \ldots$

- C_{n+1} obtained by modifying (updating) C_n



- changes satisfy the **detailed-balance principle**

$$\frac{P_{\rm change}(A \to B)}{P_{\rm change}(B \to A)} = \frac{W(B)}{W(A)} \qquad W(A) = {\rm e}^{-E(A)/T}$$

$$P_{\rm change}(A \to B) = P_{\rm select}(B|A) P_{\rm accept}(B|A)$$

$$P_{\rm select} = 1/N, \quad P_{\rm accept} = \min[W(B)/W(A), 1]$$

$$\frac{W(B)}{W(A)} = e^{-\Delta_E/T} = e^{[E(A)-E(B)]/T}$$

is easy to calculate (only depends on spins interacting with lipped spin)

Starting from any configuration, such a repeated stochastic process leads to configurations distributed according to W

- the process has to be **ergodic**
  - any configuration reachable in principle
- it takes some time to reach equilibrium (typical configurations of the Boltzmann distribution)

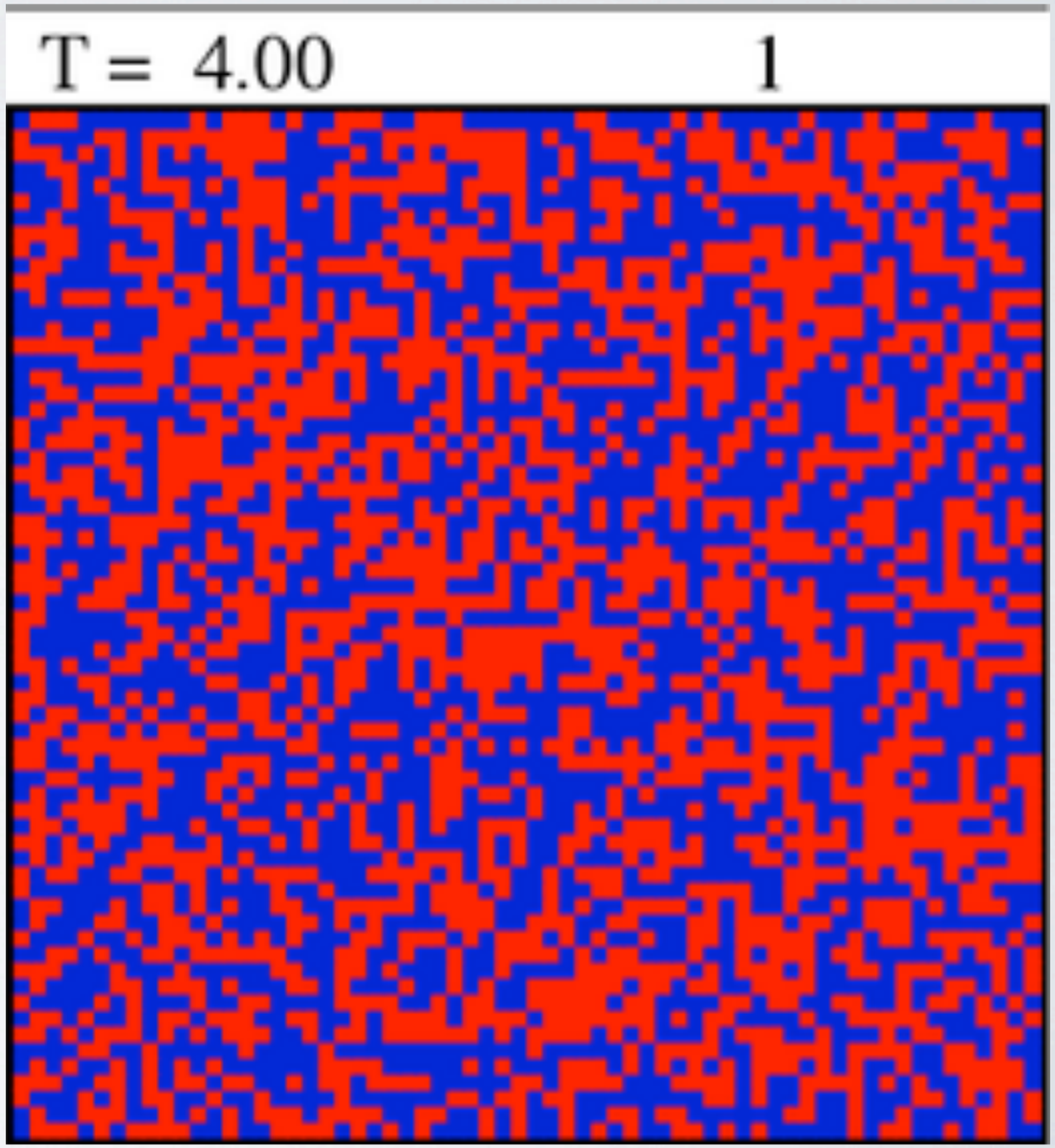
Metropolis algorithm for the Ising model. For each update perform:

- select a spin i at random; consider flipping it $\sigma_i \rightarrow -\sigma_i$
- compute the ratio $R=W(\sigma_1,...-\sigma_i,...,\sigma_N)/W(\sigma_1,...\sigma_i,...,\sigma_N)$
  - for this we need only the neighbor spins of i
- generate **random number $0<r\leq 1$; accept flip if $r<R$** (stay with old config else)
- repeat (many times...)

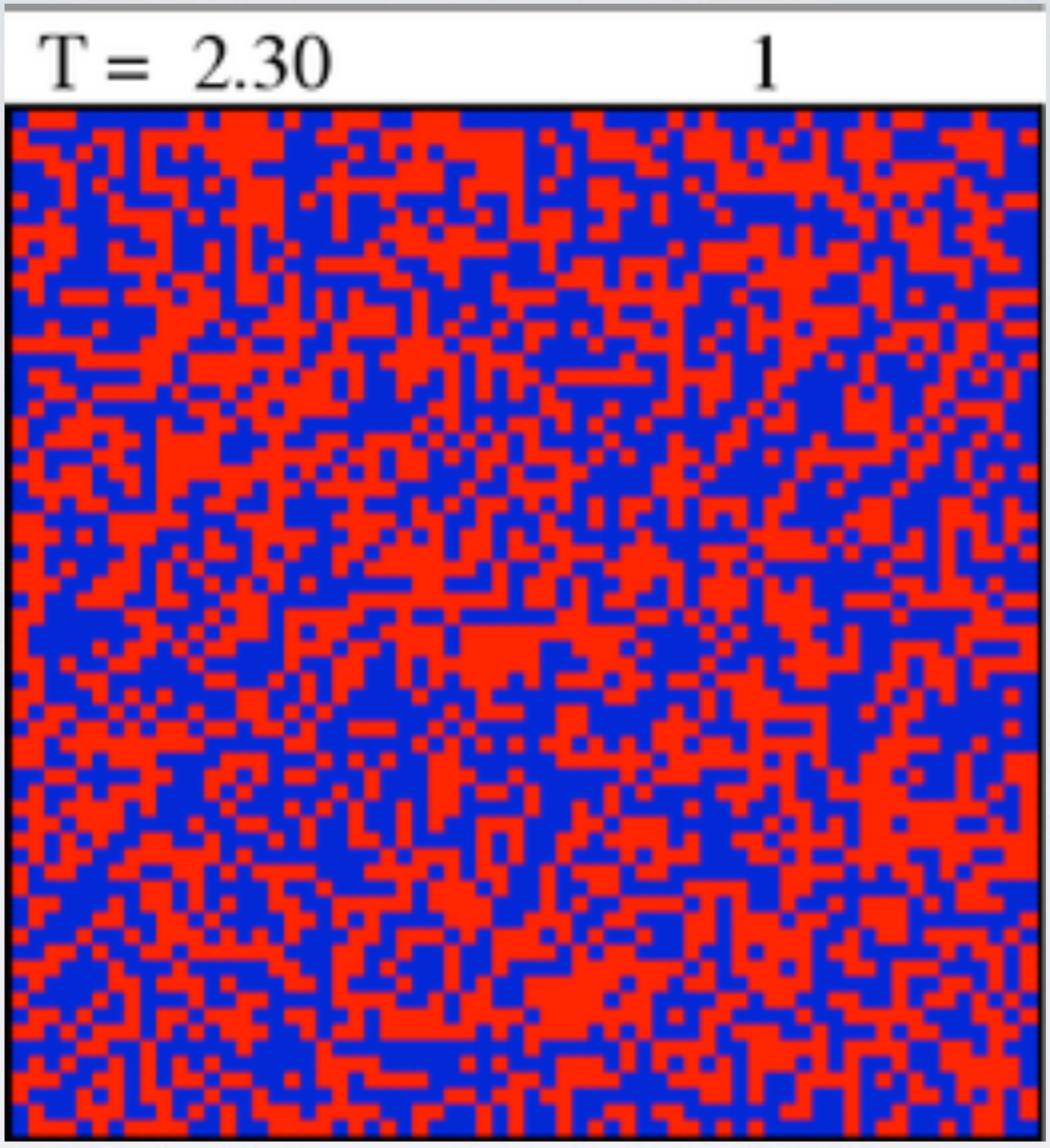
Simulation time unit
(Monte Carlo step or sweep)
- N spin flip attempts

"**Measure**" physical observables (averaged over time) on the generated configurations
- begin **after equilibration** (when configurations are typical representatives of the Boltzmann distribution)

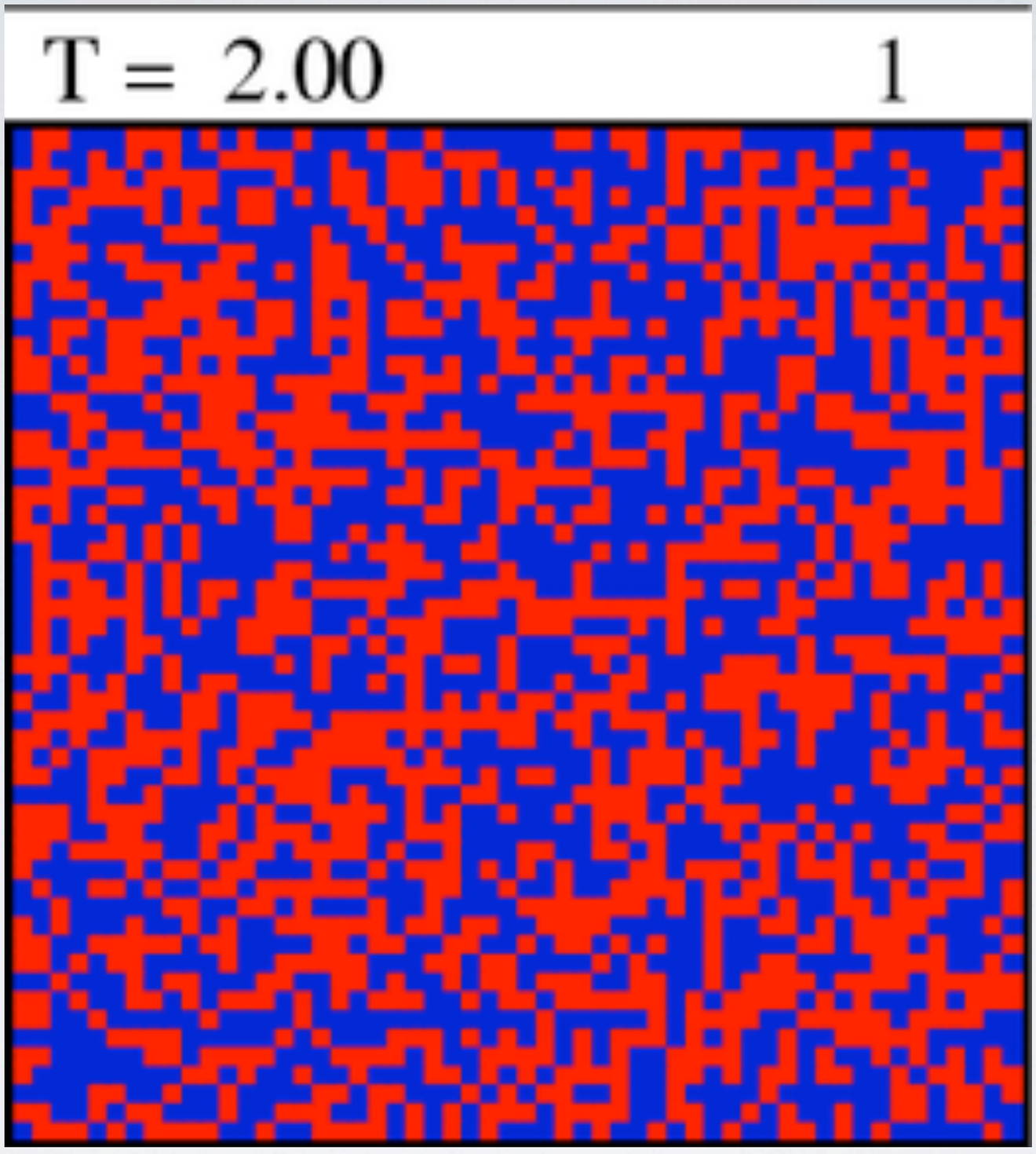
Example
- 128×128 lattice (N=16384) at T/J=4 ($> T_c/J \approx 2.27$)



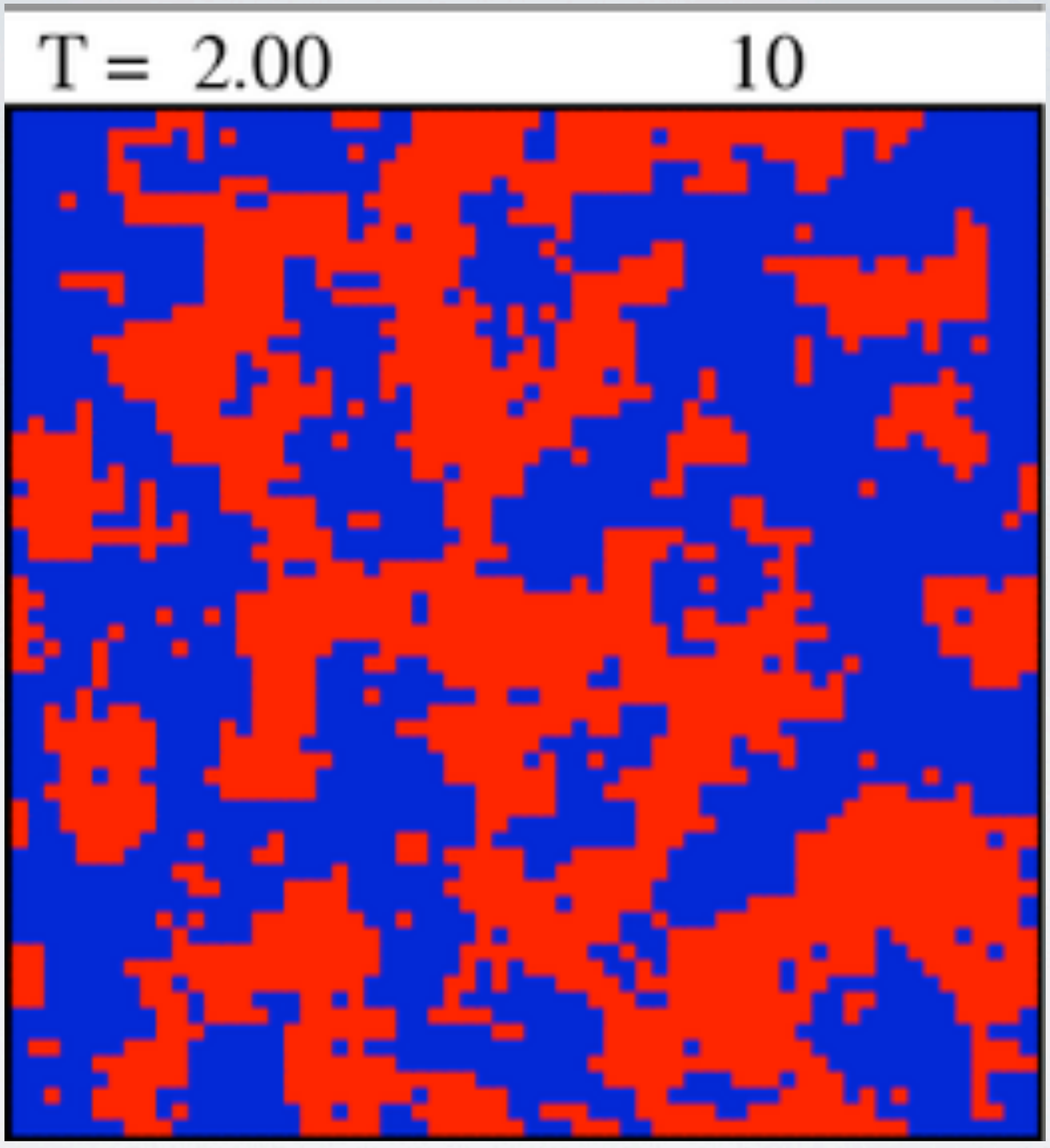
Going closer to Tc



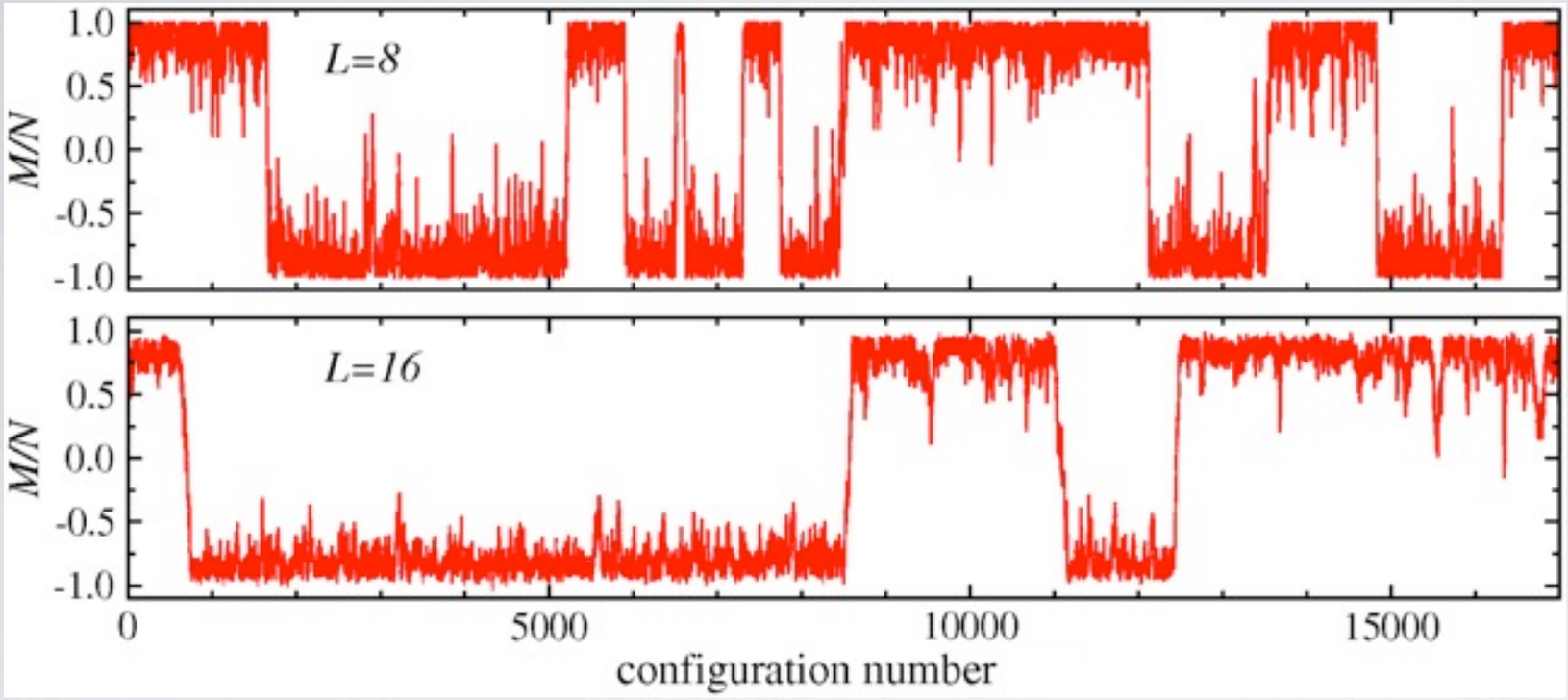
Going below Tc....



Staying at same T, speeding up time by factor 10



Time series of simulation data; **magnetization vs simulation time for $T<T_c$**



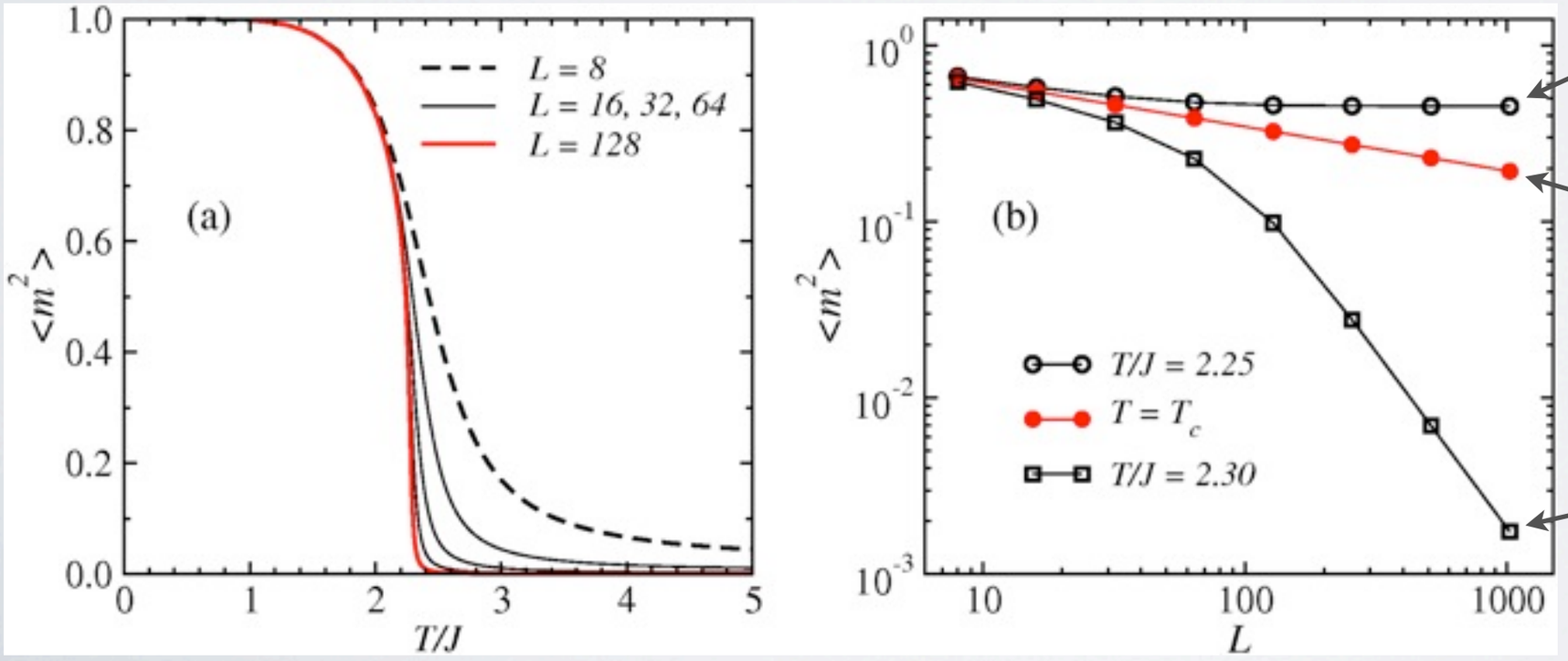
Order parameter (magnetization)

$$\frac{\mathbf{M}}{\mathbf{N}} = \mathbf{m} = \frac{\mathbf{1}}{\mathbf{N}} \sum_{\mathbf{i=1}}^{\mathbf{N}} \sigma_{\mathbf{i}}$$

Time-scale of m reversals diverges when $L \to \infty$
- symmetry breaking

Compute time-average of $\langle m^2 \rangle$ to carry out **finite-size scaling**

Squared magnetization for L×L Ising lattices



ordered
(size independent)

critical scaling
(non-trivial power-law)

disordered
(trivial power-law $1/N = 1/L^{-2}$)

Quantum spin systems, quantum antiferromagnets

Quantum spin models

- the spins have three (x,y,z) components, satisfy commutation relations
- interactions may contain 1 (Ising), 2 (XY), or 3 (Heisenberg) components

$$H = \sum_{\langle ij \rangle} J_{ij} S_i^z S_j^z = \frac{1}{4} \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j \qquad \textbf{(Ising)}$$

$$H = \sum_{\langle ij \rangle} J_{ij} [S_i^x S_j^x + S_i^y S_j^y] = \frac{1}{2} \sum_{\langle ij \rangle} J_{ij} [S_i^+ S_j^- + S_i^- S_j^+] \qquad \textbf{(XY)}$$

$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_{\langle ij \rangle} J_{ij} [S_i^z S_j^z + \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)] \qquad \textbf{(Heisenberg)}$$

+ many modifications and extensions... and local spin S=1/2,1,3/2,....

Quantum antiferromagnets

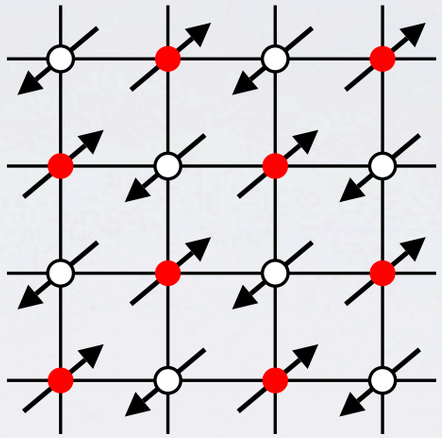
Nearest-neighbor <i,j> interactions (Heisenberg) on some lattice

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j, \qquad J > 0$$

Lattices can be classified as

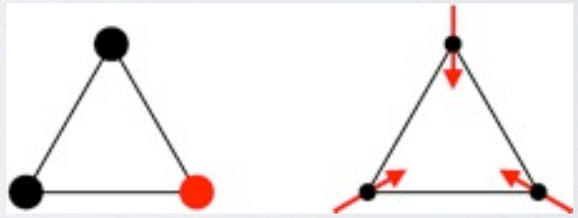
Bipartite

- nearest-neighbors i,j always on different sublattices
- compatible with Neel order
- but other states possible



Non-bipartite

- no bipartition is possible
- frustrated antiferromagnetic interactions
- different kinds of order or no long-range order (spin liquid)



Fully ordered Neel state (ground state of H for classical spins)
is not an eigenstate of H even on a bipartite lattice

- if there is order at T=0 it is reduced by quantum fluctuations

Mermin-Wagner theorem (on breaking a continuous symmetry) implies:

- No Neel order in 1D Heisenberg model
- Neel order possible only at T=0 in 2D system
- Order possible also at T>0 in 3D

Path Integrals in quantum statistical mechanics

Quantum statistical mechanics

$$\langle Q \rangle = \frac{1}{Z} \mathrm{Tr} \left\{ Q \mathrm{e}^{-H/T} \right\} \qquad Z = \mathrm{Tr} \left\{ \mathrm{e}^{-H/T} \right\} = \sum_{n=0}^{M-1} \mathrm{e}^{-E_n/T}$$

Large size M of the Hilbert space; $M=2^N$ for S=1/2

- difficult problem to find the eigenstates and energies
- we may be especially interested in the ground state (T→0)
  (for classical systems the ground state is often trivial)

Quantum Monte Carlo

Rewrite the quantum-mechanical expectation value into a classical form

$$\langle A \rangle = \frac{\mathrm{Tr}\{Ae^{-\beta H}\}}{\mathrm{Tr}\{e^{-\beta H}\}} \rightarrow \frac{\sum_c A_c W_c}{\sum W_c}$$

Monte Carlo sampling in the space **{c} with weights W_c** (if positive-definite...)

Different ways of doing it

- World-line methods for spins and bosons
- Stochastic series expansion for spins and bosons
- Fermion determinant methods

("sign problem" if not the case)

For ground state calculations we can also do projection from a "trial state"

$$|\Psi_m\rangle \sim H^m |\Psi_0\rangle \qquad |\Psi_m\rangle \rightarrow |0\rangle \quad \text{when} \quad m \rightarrow \infty$$

$$|\Psi_\beta\rangle \sim \mathrm{e}^{-\beta H} |\Psi_0\rangle \qquad |\Psi_\beta\rangle \rightarrow |0\rangle \quad \text{when} \quad \beta \rightarrow \infty$$

Particularly simple and efficient schemes exist for S=1/2 models

$$H = -J \sum_{b=1}^{N_b} \left(\frac{1}{4} - \mathbf{S}_{i(b)} \cdot \mathbf{S}_{j(b)} \right)$$

(+ certain multi-spin terms)

No sign problem on **bipartite lattices**

Path integrals in quantum statistical mechanics

We want to compute a thermal expectation value

$$\langle A \rangle = \frac{1}{Z} \mathrm{Tr}\{ A \mathrm{e}^{-\beta H} \}$$

where β=1/T (and possibly T→0). How to deal with the exponential operator?

"Time slicing" of the partition function

$$Z = \mathrm{Tr}\{\mathrm{e}^{-\beta H}\} = \mathrm{Tr}\left\{ \prod_{l=1}^{L} \mathrm{e}^{-\Delta_\tau H} \right\} \qquad \Delta_\tau = \beta / L$$

Choose a basis and insert complete sets of states;

$$Z = \sum_{\alpha_0} \sum_{\alpha_1} \cdots \sum_{\alpha_L - 1} \langle \alpha_0 | \mathrm{e}^{-\Delta_\tau H} | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | \mathrm{e}^{-\Delta_\tau H} | \alpha_1 \rangle \langle \alpha_1 | \mathrm{e}^{-\Delta_\tau H} | \alpha_0 \rangle$$

Use approximation for imaginary time evolution operator. Simplest way

$$Z \approx \sum_{\{\alpha\}} \langle \alpha_0 | 1 - \Delta_\tau H | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | 1 - \Delta_\tau H | \alpha_1 \rangle \langle \alpha_1 | 1 - \Delta_\tau H | \alpha_0 \rangle$$

Leads to error $\propto \Delta_\tau$. Limit $\Delta_\tau \to 0$ can be taken

Example: hard-core bosons

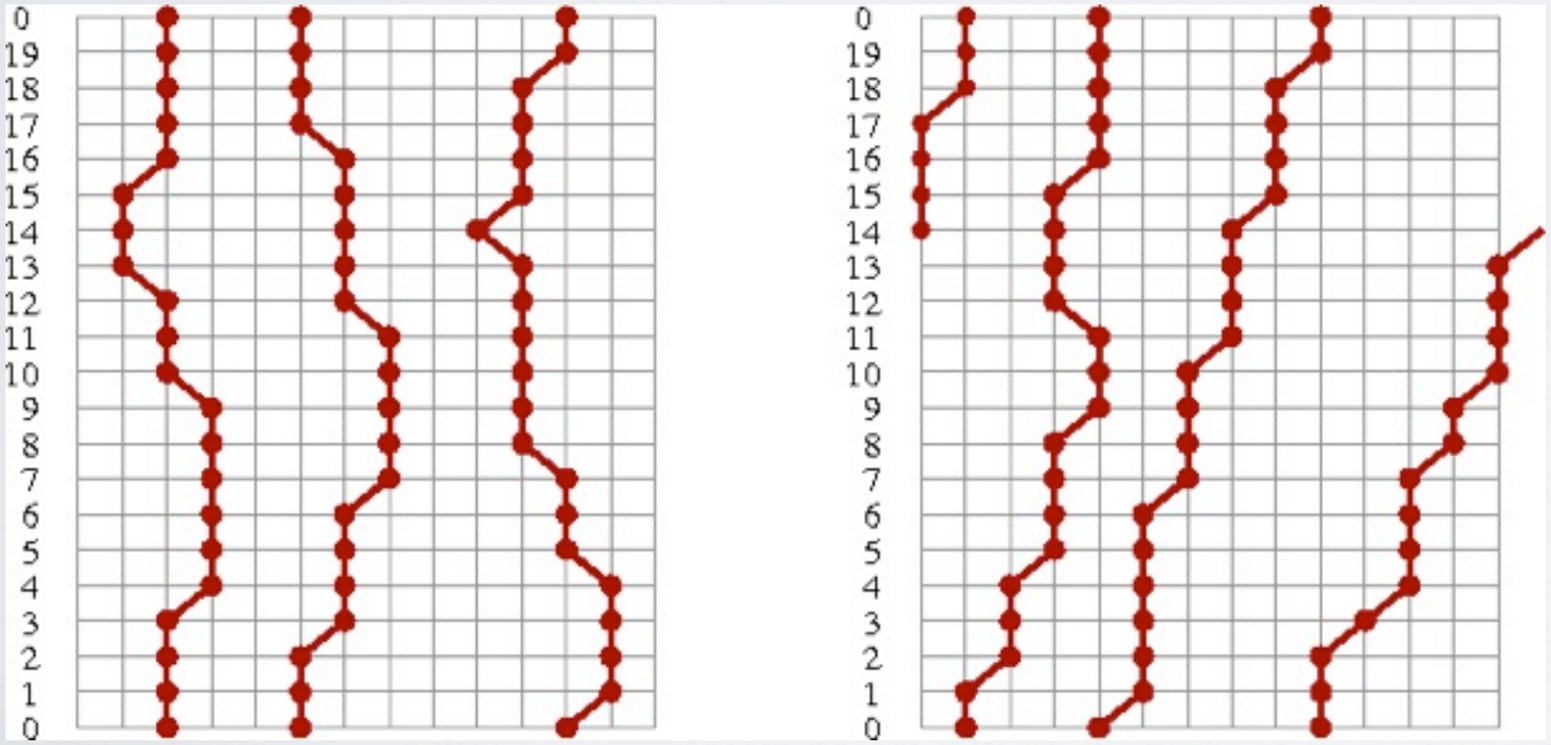
$$H = K = -\sum_{\langle i,j \rangle} K_{ij} = -\sum_{\langle i,j \rangle} (a_j^\dagger a_i + a_i^\dagger a_j) \qquad n_i = a_i^\dagger a_i \in \{0, 1\}$$

Equivalent to S=1/2 XY model

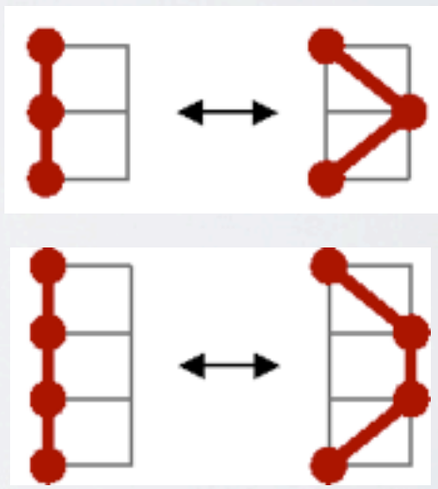
$$H = -2\sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y) = -\sum_{\langle i,j \rangle} (S_i^+ S_j^- + S_i^- S_j^+), \quad S^z = \pm\frac{1}{2} \sim n_i = 0, 1$$

"World line" representation of

$$Z \approx \sum_{\{\alpha\}} \langle \alpha_0 | 1 - \Delta_\tau H | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | 1 - \Delta_\tau H | \alpha_1 \rangle \langle \alpha_1 | 1 - \Delta_\tau H | \alpha_0 \rangle$$



world line moves for Monte Carlo sampling



$$Z = \sum_{\{\alpha\}} W(\{\alpha\}), \quad W(\{\alpha\}) = \Delta_\tau^{n_K}$$

n_K = number of "jumps"

Expectation values

$$\langle A\rangle = \frac{1}{Z}\sum_{\{\alpha\}}\langle\alpha_0|\mathrm{e}^{-\Delta_\tau}|\alpha_{L-1}\rangle\cdots\langle\alpha_2|\mathrm{e}^{-\Delta_\tau H}|\alpha_1\rangle\langle\alpha_1|\mathrm{e}^{-\Delta_\tau H}A|\alpha_0\rangle$$

$$Z = \frac{1}{Z}\sum_{\{\alpha\}}\langle\alpha_0|\mathrm{e}^{-\Delta_\tau}|\alpha_{L-1}\rangle\cdots\langle\alpha_2|\mathrm{e}^{-\Delta_\tau H}|\alpha_1\rangle\langle\alpha_1|\mathrm{e}^{-\Delta_\tau H}|\alpha_0\rangle$$

We want to write this in a form suitable for MC importance sampling

$$\langle A\rangle = \frac{\sum_{\{\alpha\}} A(\{\alpha\})W(\{\alpha\})}{\sum_{\{\alpha\}} W(\{\alpha\})} \quad\longrightarrow\quad \langle A\rangle = \langle A(\{\alpha\})\rangle_W$$

$$W(\{\alpha\}) = \text{weight}$$
$$A(\{\alpha\}) = \text{estimator}$$

For any quantity diagonal in the occupation numbers (spin z):

$$A(\{\alpha\}) = A(\alpha_n) \quad \text{or} \quad A(\{\alpha\}) = \frac{1}{L}\sum_{l=0}^{L-1} A(\alpha_l)$$

Measure quantities on all slices and average
- in practice full averaging may take too long and OK to do partial averages

Off-diagonal expectation values

$$\langle A\rangle = \frac{1}{Z}\sum_{\{\alpha\}}\langle\alpha_0|\mathrm{e}^{-\Delta_\tau}|\alpha_{L-1}\rangle\cdots\langle\alpha_2|\mathrm{e}^{-\Delta_\tau H}|\alpha_1\rangle\langle\alpha_1|\mathrm{e}^{-\Delta_\tau H}A|\alpha_0\rangle$$

In general the states $\alpha_1,\ldots,\alpha_n$ contributing to Z will not contribute to <A>
- more complicated measurements

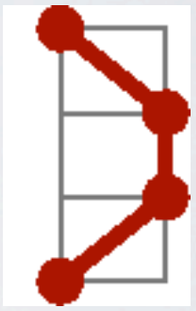
Special case: term K_{ij} in the kinetic energy

Multiply and divide by the weight

$$\langle A\rangle = \frac{1}{Z}\sum_{\{\alpha\}}\langle\alpha_0|\mathrm{e}^{-\Delta_\tau}|\alpha_{L-1}\rangle\cdots\langle\alpha_1|\mathrm{e}^{-\Delta_\tau H}|\alpha_0\rangle\frac{\langle\alpha_0|\mathrm{e}^{-\Delta_\tau}|\alpha_{L-1}\rangle\cdots\langle\alpha_1|\mathrm{e}^{-\Delta_\tau H}K_{ij}|\alpha_0\rangle}{\langle\alpha_0|\mathrm{e}^{-\Delta_\tau}|\alpha_{L-1}\rangle\cdots\langle\alpha_1|\mathrm{e}^{-\Delta_\tau H}|\alpha_0\rangle}$$

$$= \frac{1}{Z}\sum_{\{\alpha\}}W(\{\alpha\})\frac{\langle\alpha_0|\mathrm{e}^{-\Delta_\tau}|\alpha_{L-1}\rangle\cdots\langle\alpha_1|\mathrm{e}^{-\Delta_\tau H}K_{ij}|\alpha_0\rangle}{\langle\alpha_0|\mathrm{e}^{-\Delta_\tau}|\alpha_{L-1}\rangle\cdots\langle\alpha_1|\mathrm{e}^{-\Delta_\tau H}|\alpha_0\rangle}$$

$$\mathrm{e}^{-\Delta_\tau K}K_{ij}\approx K_{ij} \qquad K_{ij}(\{\alpha\}) = \frac{\langle\alpha_1|K_{ij}|\alpha_0\rangle}{\langle\alpha_1|1-\Delta_\tau K|\alpha_0\rangle}\in\{0,\frac{1}{\Delta_\tau}\}$$



Average over all slices → count number of kinetic jumps

$$\langle K_{ij}\rangle = \frac{\langle n_{ij}\rangle}{\beta}, \quad \langle K\rangle = -\frac{\langle n_K\rangle}{\beta} \qquad \langle K\rangle\propto N\rightarrow\langle n_K\rangle\propto\beta N$$

There should be of the order βN "jumps" of the worldlines

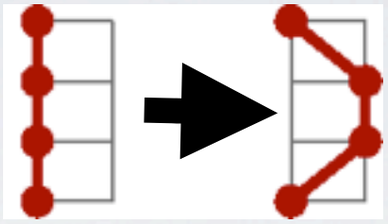
Including interactions

For any diagonal interaction V (Trotter, or split-operator, approximation)

$$\mathrm{e}^{-\Delta_\tau H} = \mathrm{e}^{-\Delta_\tau K}\mathrm{e}^{-\Delta_\tau V} + \mathcal{O}(\Delta_\tau^2) \rightarrow \langle\alpha_{l+1}|\mathrm{e}^{-\Delta_\tau H}|\alpha_l\rangle \approx \mathrm{e}^{-\Delta_\tau V_l}\langle\alpha_{l+1}|\mathrm{e}^{-\Delta_\tau K}|\alpha_l\rangle$$

Product over all times slices →

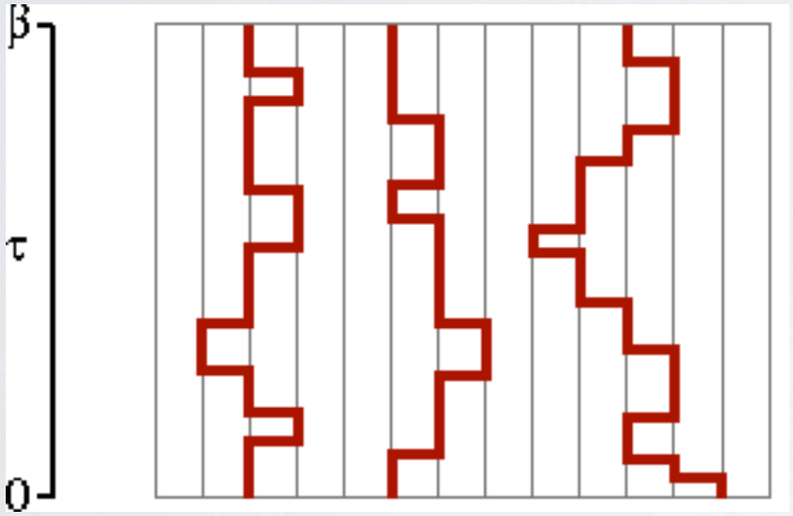
$$W(\{\alpha\}) = \Delta_\tau^{n_K}\exp\left(-\Delta_\tau\sum_{l=0}^{L-1}V_l\right)$$

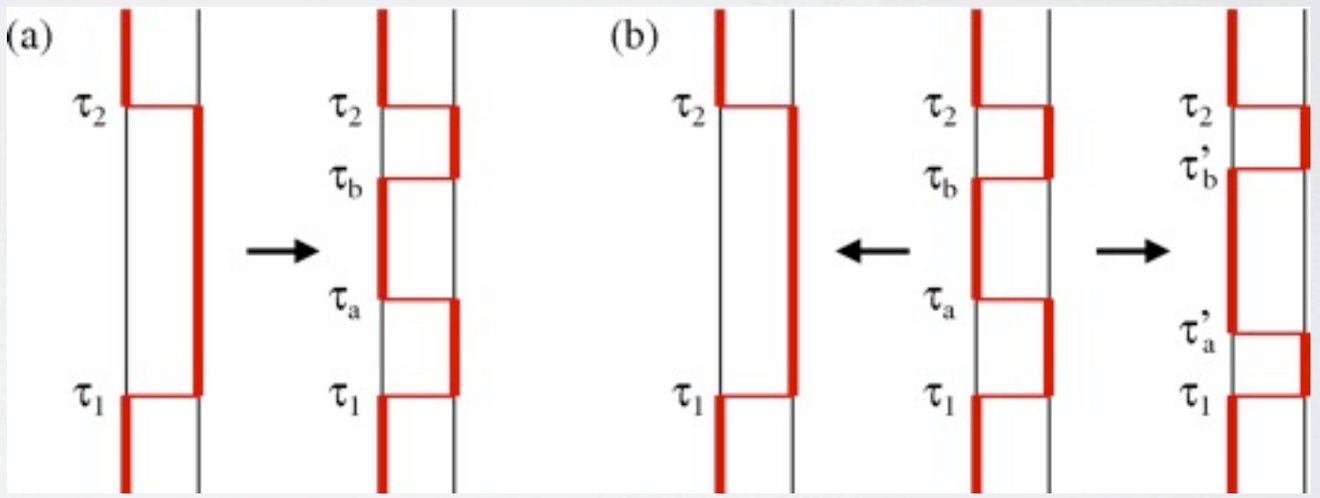


$$P_{\mathrm{acc}} = \min\left[\Delta_\tau^2\exp\left(-\frac{V_{\mathrm{new}}}{V_{\mathrm{old}}}\right),1\right]$$

The continuous time limit

Limit $\Delta_\tau \rightarrow 0$: number of kinetic jumps remains finite, store events only





Special methods (**loop and worm updates**) developed for efficient sampling of the paths in the continuum

local updates (problem when $\Delta_\tau \rightarrow 0$?)

- consider probability of inserting/removing events within a time window

⇐ Evertz, Lana, Marcu (1993), Prokofev et al (1996)
Beard & Wiese (1996)

Stochastic series expansion (SSE)

Alternative to path integral: Series expansion representation

Start from the Taylor expansion $\mathrm{e}^{-\beta H} = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} H^n$ (approximation-free method from the outset)

$$Z = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\{\alpha\}_n} \langle\alpha_0|H|\alpha_{n-1}\rangle \cdots \langle\alpha_2|H|\alpha_1\rangle\langle\alpha_1|H|\alpha_0\rangle$$

Similar to the path integral; $1 - \Delta\tau H \to H$ and weight factor outside

For hard-core bosons the (allowed) path weight is $W(\{\alpha\}_n) = \beta^n/n!$

For any model, the energy is

this is the operator we "measure"

$$E = \frac{1}{Z} \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\{\alpha\}_{n+1}} \langle\alpha_0|H|\alpha_n\rangle \cdots \langle\alpha_2|H|\alpha_1\rangle\langle\alpha_1|H|\alpha_0\rangle$$

one more "slice" to sum over here

$$= -\frac{1}{Z} \sum_{n=1}^{\infty} \frac{(-\beta)^n}{n!} \frac{n}{\beta} \sum_{\{\alpha\}_n} \langle\alpha_0|H|\alpha_{n-1}\rangle \cdots \langle\alpha_2|H|\alpha_1\rangle\langle\alpha_1|H|\alpha_0\rangle = \frac{-\langle n\rangle}{\beta}$$

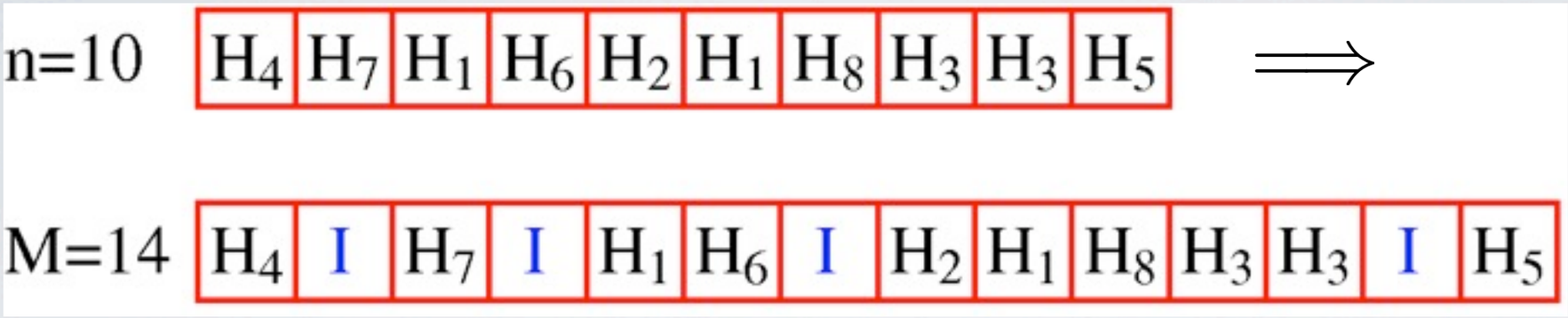
relabel terms to "get rid of" extra slice

$$C = \langle n^2\rangle - \langle n\rangle^2 - \langle n\rangle$$

From this follows: narrow n-distribution with $\langle n\rangle \propto N\beta, \quad \sigma_n \propto \sqrt{N\beta}$

Fixed-length scheme

- n fluctuating → varying size of the configurations
- the expansion can be truncated at some n_{max}=M (exponentially small error)
- cutt-off at n=M, fill in operator string with unit operators H_0=I



- conisider all possible locations in the sequence
- overcounting of actual (original) strings, correct by combinatorial factor:

$$\binom{M}{n}^{-1} = \frac{n!(M-n)!}{M!}$$

Here n is the number of H_i, i>0 instances in the sequence of M operators

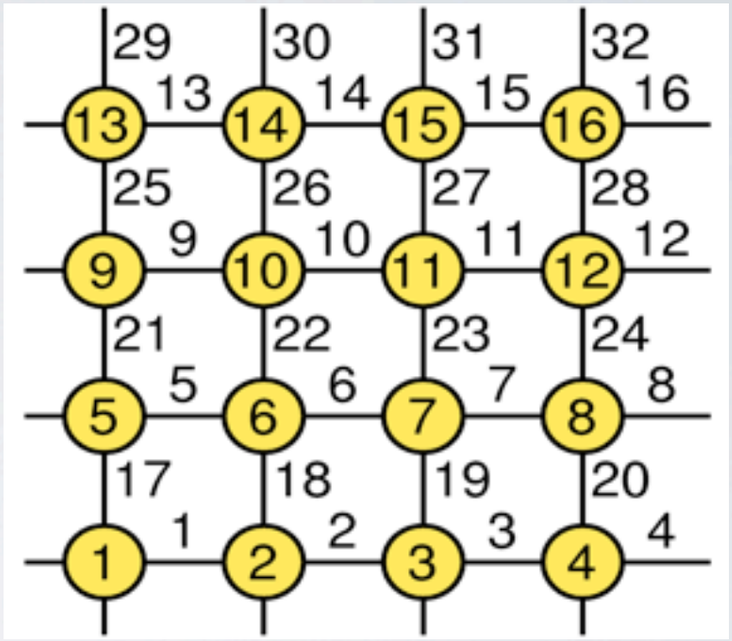
$$Z = \sum_{\{\alpha\}_M} \sum_{\{H_i\}} \frac{(-\beta)^n (M-n)!}{M!} \langle \alpha_0 | H_{i(M)} | \alpha_{M-1} \rangle \cdots \langle \alpha_1 | H_{i(1)} | \alpha_0 \rangle$$

Stochastic Series expansion (SSE): S=1/2 Heisenberg model

Write H as a bond sum for arbitrary lattice

$$H = J \sum_{b=1}^{N_b} \mathbf{S}_{i(b)} \cdot \mathbf{S}_{j(b)},$$

2D square lattice
bond and site labels



Diagonal (1) and off-diagonal (2) bond operators

$$H_{1,b} = \frac{1}{4} - S^z_{i(b)} S^z_{j(b)},$$

$$H_{2,b} = \frac{1}{2}(S^+_{i(b)} S^-_{j(b)} + S^-_{i(b)} S^+_{j(b)}).$$

$$H = -J \sum_{b=1}^{N_b} (H_{1,b} - H_{2,b}) + \frac{J N_b}{4}$$

Four non-zero matrix elements

$$\langle \uparrow_{i(b)} \downarrow_{j(b)} | H_{1,b} | \uparrow_{i(b)} \downarrow_{j(b)} \rangle = \frac{1}{2} \qquad \langle \downarrow_{i(b)} \uparrow_{j(b)} | H_{2,b} | \uparrow_{i(b)} \downarrow_{j(b)} \rangle = \frac{1}{2}$$

$$\langle \downarrow_{i(b)} \uparrow_{j(b)} | H_{1,b} | \downarrow_{i(b)} \uparrow_{j(b)} \rangle = \frac{1}{2} \qquad \langle \uparrow_{i(b)} \downarrow_{j(b)} | H_{2,b} | \downarrow_{i(b)} \uparrow_{j(b)} \rangle = \frac{1}{2}$$

Partition function

$$Z = \sum_{\alpha} \sum_{n=0}^{\infty} (-1)^{n_2} \frac{\beta^n}{n!} \sum_{S_n} \left\langle \alpha \left| \prod_{p=0}^{n-1} H_{a(p),b(p)} \right| \alpha \right\rangle$$

n_2 = number of a(i)=2
(off-diagonal operators)
in the sequence

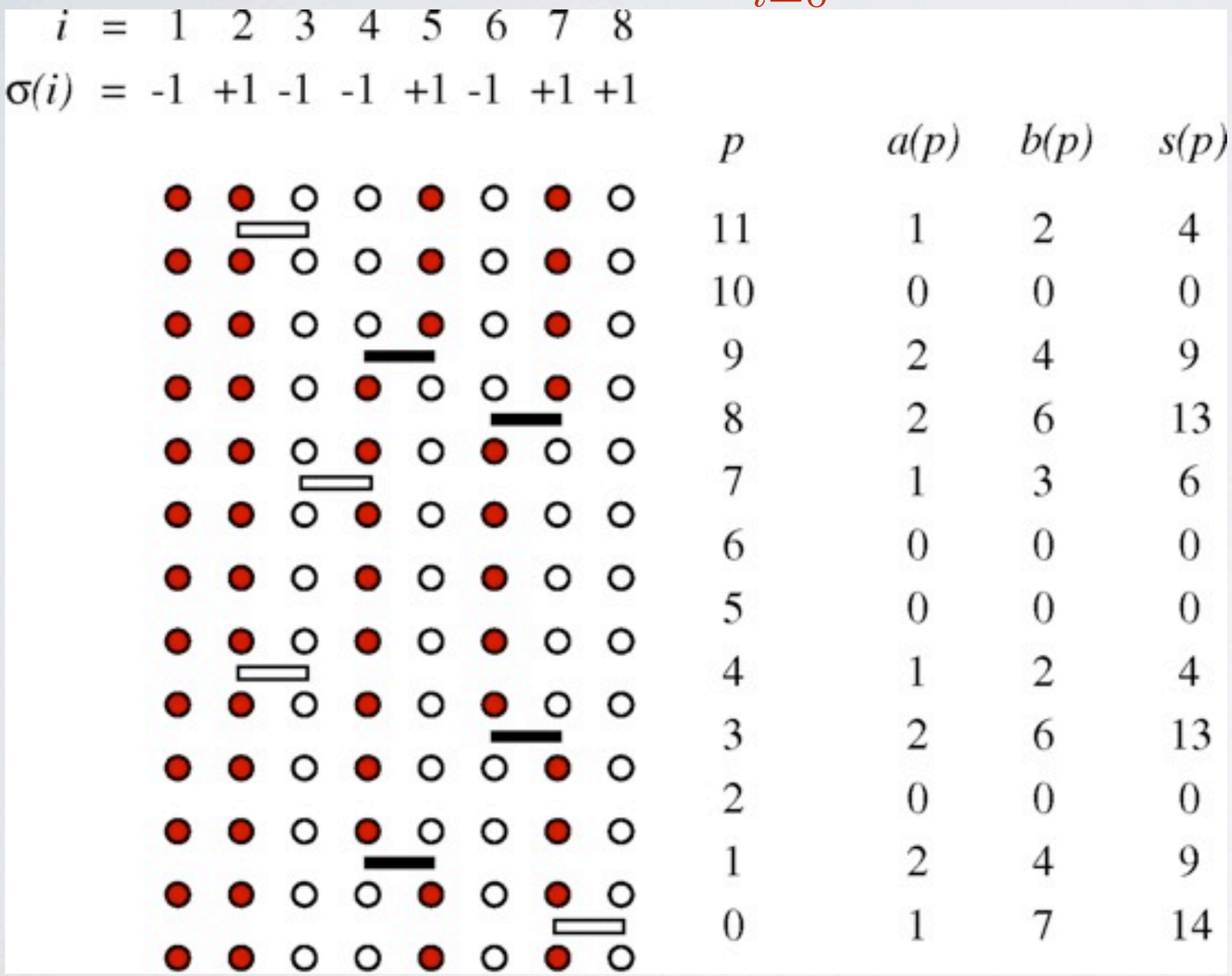
Index sequence: $S_n = [a(0), b(0)], [a(1), b(1)], \ldots, [a(n-1), b(n-1)]$

For fixed-length scheme (string length = L now)

$$Z = \sum_{\alpha} \sum_{S_L} (-1)^{n_2} \frac{\beta^n (L-n)!}{L!} \left\langle \alpha \left| \prod_{p=0}^{L-1} H_{a(p),b(p)} \right| \alpha \right\rangle \qquad W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

Propagated states: $|\alpha(p)\rangle \propto \prod_{i=0}^{p-1} H_{a(i),b(i)} |\alpha\rangle$

W>0 (n_2 even) for bipartite lattice
Frustration leads to **sign problem**



p	a(p)	b(p)	s(p)
11	1	2	4
10	0	0	0
9	2	4	9
8	2	6	13
7	1	3	6
6	0	0	0
5	0	0	0
4	1	2	4
3	2	6	13
2	0	0	0
1	2	4	9
0	1	7	14

In a program:

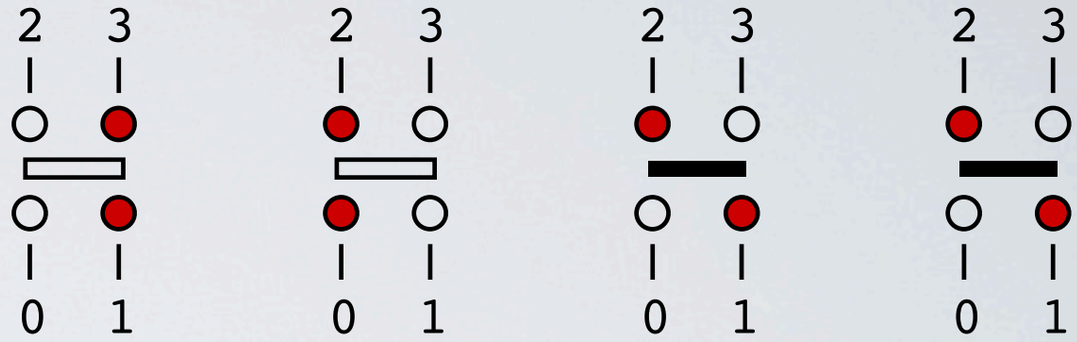
s(p) = operator-index string
- **s(p) = 2*b(p) + a(p)-1**
- diagonal; s(p) = even
- off-diagonal; s(p) = off

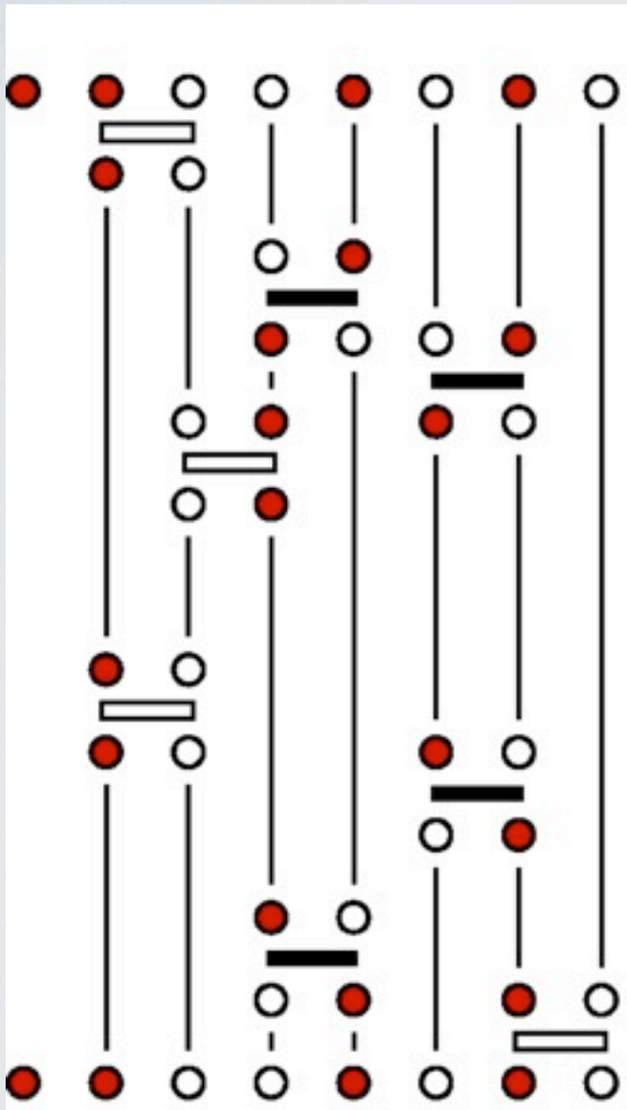
σ(i) = spin state, i=1,...,N
- only one has to be stored

SSE effectively provides a discrete representation of the time continuum
- computational advantage; only integer operations in sampling

Linked vertex storage

The “legs” of a vertex represents the spin states before (below) and after (above) an operator has acted





p	v X(v)		v X(v)		v X(v)		v X(v)	
11	44	18	45	30	46	16	47	17
10	40	-	41	-	42	-	43	-
9	36	31	37	7	38	4	39	5
8	32	14	33	15	34	12	35	0
7	28	19	29	6	30	45	31	36
6	24	-	25	-	26	-	27	-
5	20	-	21	-	22	-	23	-
4	16	46	17	47	18	44	19	28
3	12	34	13	2	14	32	15	33
2	8	-	9	-	10	-	11	-
1	4	38	5	39	6	29	7	37
0	0	35	1	3	2	13	3	1
	l=0		l=1		l=2		l=3	

X( ) = vertex list

- operator at p→X(v)
  v=4p+l, l=0,1,2,3
- links to next and previous leg

Spin states between operations are redundant; represented by links

- network of linked vertices will be used for loop updates of vertices/operators

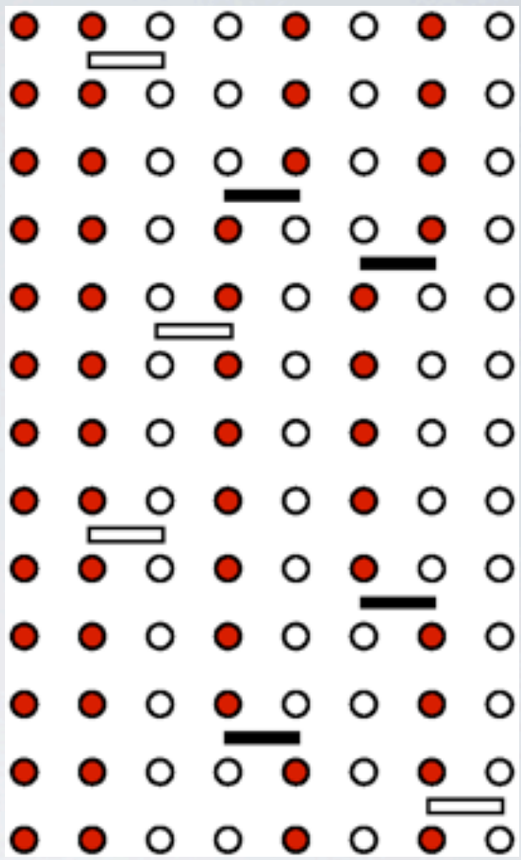
Monte Carlo sampling scheme

Change the configuration; $(\alpha, S_L) \to (\alpha', S'_L)$

$$W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

$$P_{\text{accept}} = \min\left[\frac{W(\alpha', S_L)}{W(\alpha, S_L)} \frac{P_{\text{select}}(\alpha', S'_L \to \alpha, S_L)}{P_{\text{select}}(\alpha, S_L \to \alpha', S'_L)}, 1\right]$$

Diagonal update: $[0,0]_p \leftrightarrow [1,b]_p$



Attempt at p=0,...,L-1. Need to know |α(p)>

- generate by flipping spins when off-diagonal operator

$$P_{\text{select}}(a = 0 \to a = 1) = 1/N_b, \quad (b \in \{1, \ldots, N_b\})$$

$$P_{\text{select}}(a = 1 \to a = 0) = 1$$

$$\frac{W(a=1)}{W(a=0)} = \frac{\beta/2}{L-n} \qquad \frac{W(a=0)}{W(a=1)} = \frac{L-n+1}{\beta/2}$$

n is the current power

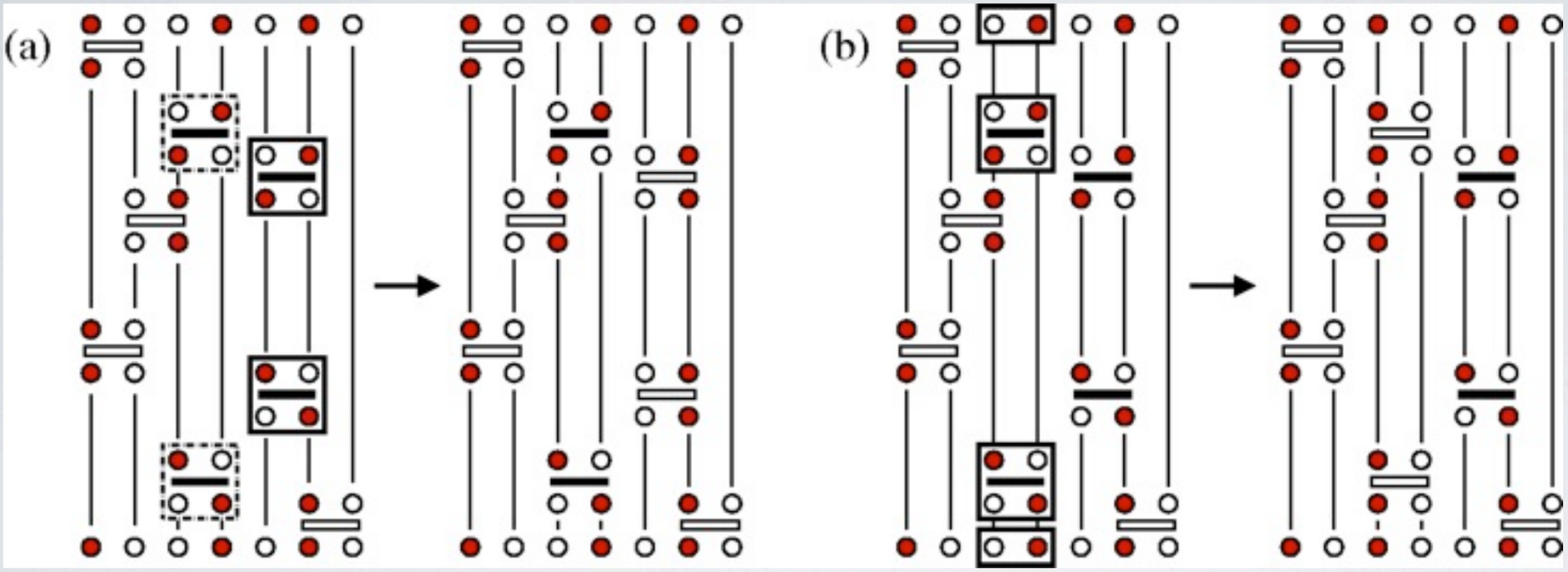
- n → n+1 (a=0 → a=1)
- n → n-1 (a=1 → a=0)

Acceptance probabilities

$$P_{\text{accept}}([0,0] \to [1,b]) = \min\left[\frac{\beta N_b}{2(L-n)}, 1\right]$$

$$P_{\text{accept}}([1,b] \to [0,0]) = \min\left[\frac{2(L-n+1)}{\beta N_b}, 1\right]$$

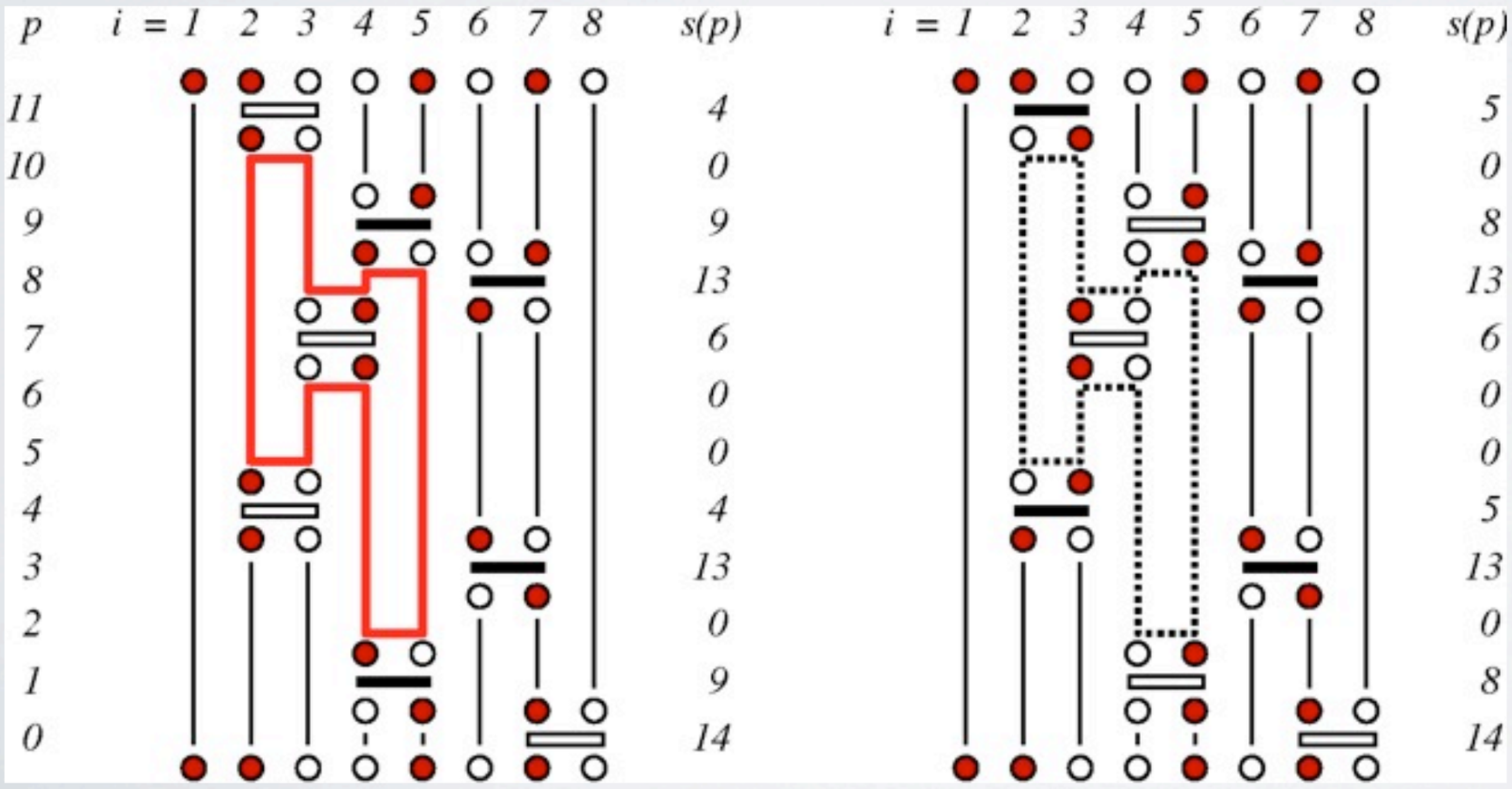
Off-diagonal updates



Local update

Change the type of two operators

- constraints
- inefficient
- cannot change winding numbers



Operator-loop update

- Many spins and operators can be changed simultaneously
- can change winding numbers

Determination of the cut-off L

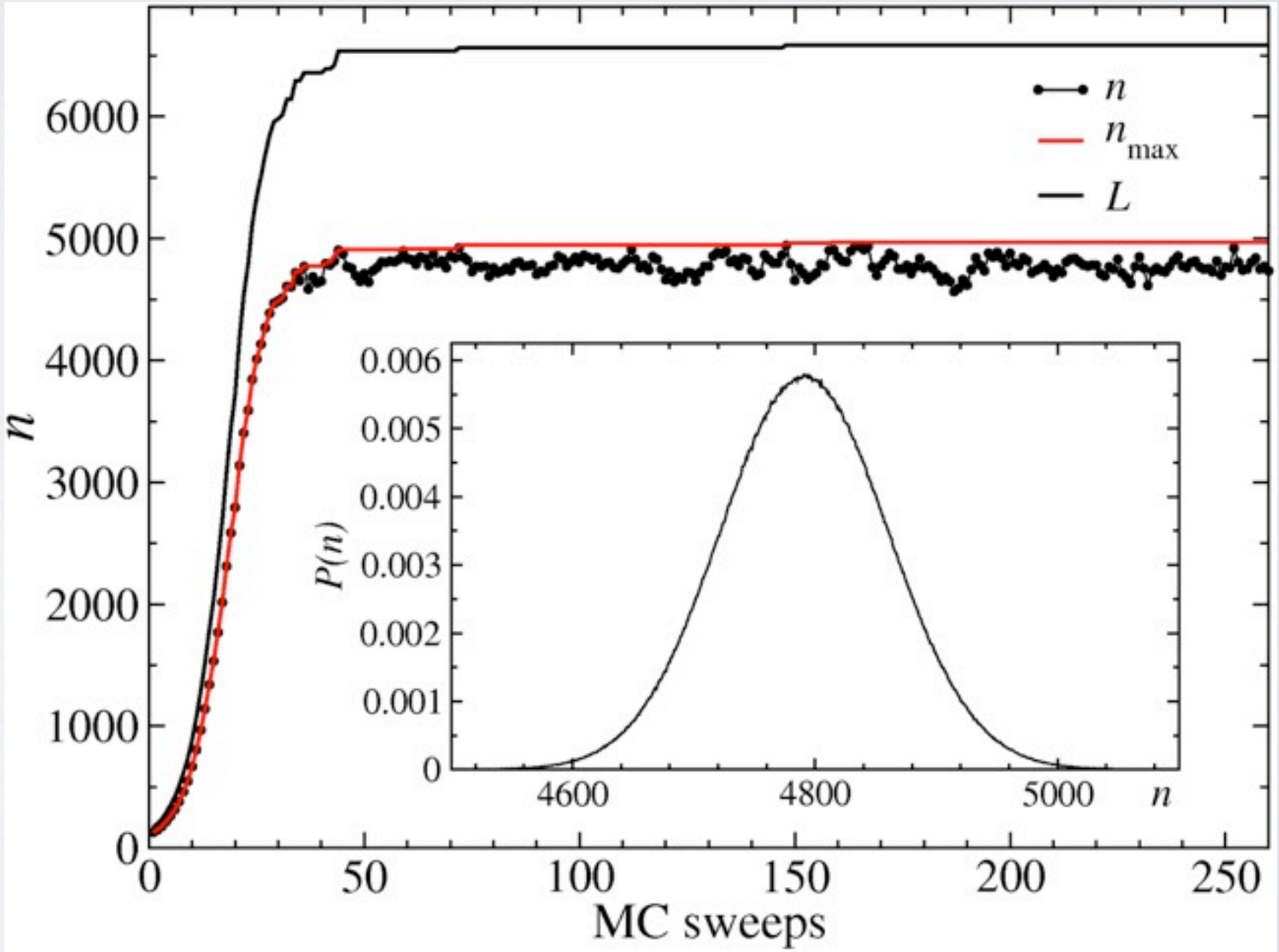
- adjust during equilibration
- start with arbitrary (small) n

Keep track of number of operators n

- increase L if n is close to current L
- e.g., ***L=n+n/3***

Example

- 16×16 system, β=16 ⇒
- evolution of L
- n distribution after equilibration
- truncation is no approximation

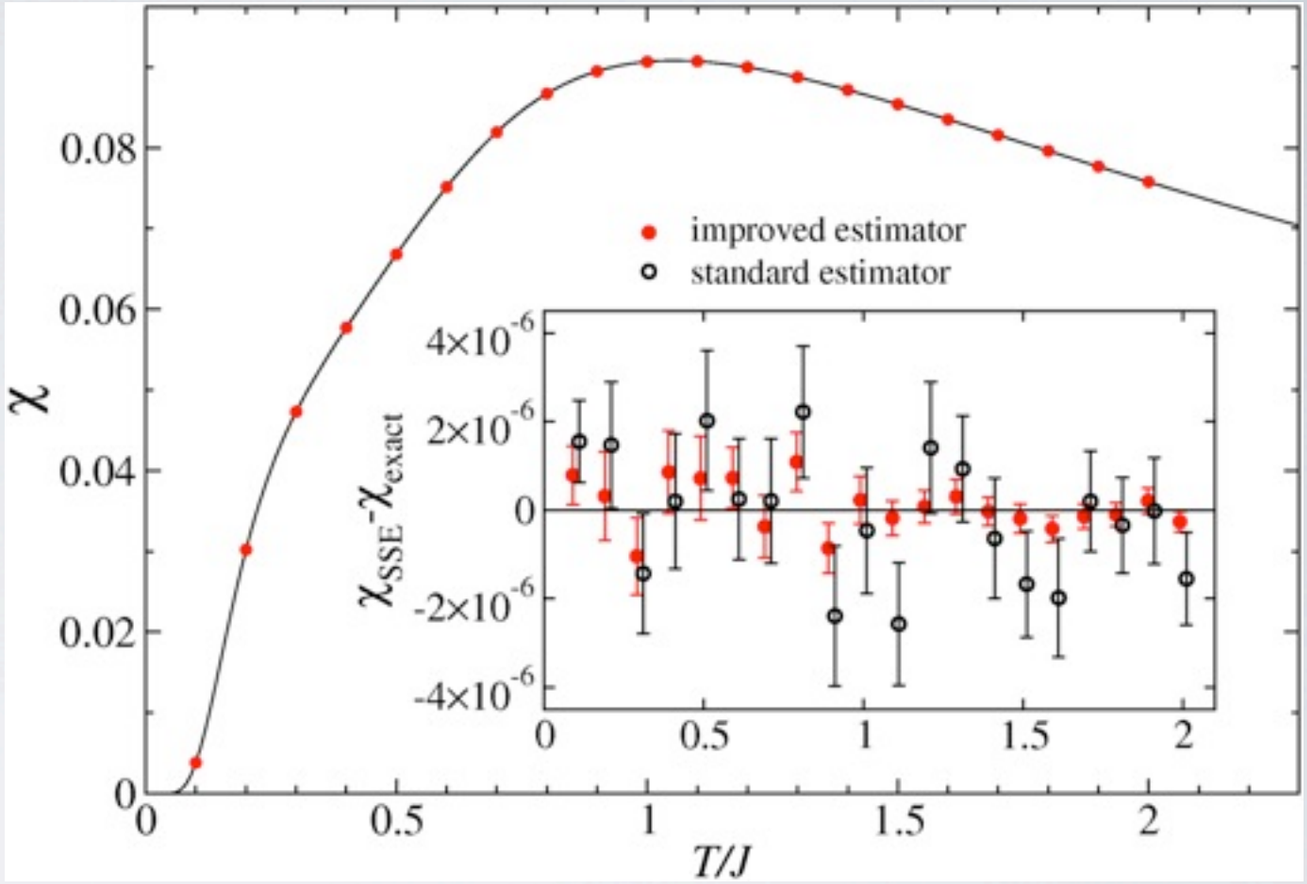


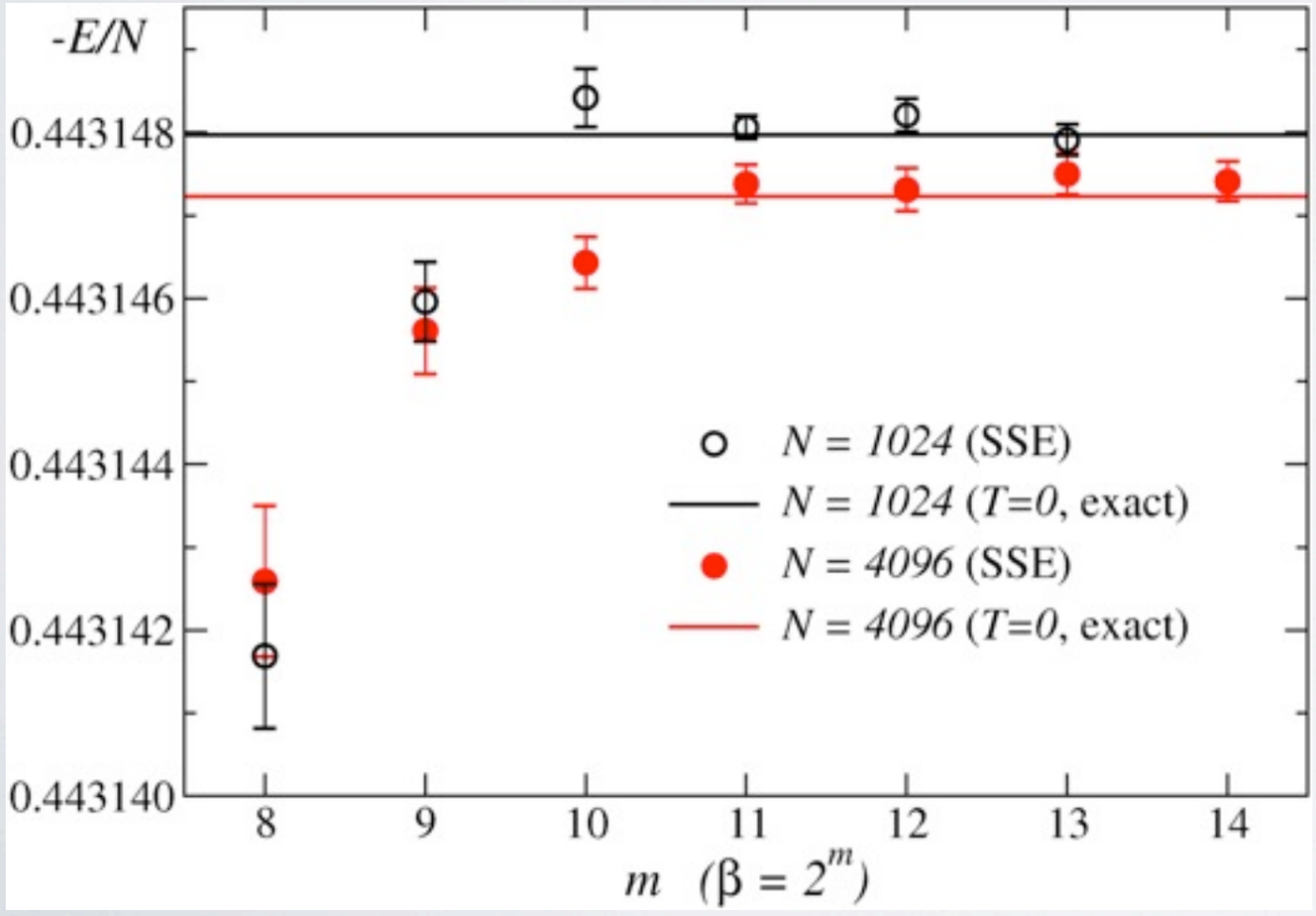
Does it work?
Compare with exact results

- 4×4 exact diagonalization
- Bethe Ansatz; long chains

Susceptibility of the 4×4 lattice ⇒

- SSE results from 10^{10} sweeps
- improved estimator gives smaller error bars at high T (where the number of loops is larger)





⇐ Energy for long 1D chains

- SSE results for 10^6 sweeps
- Bethe Ansatz ground state E/N
- SSE can achieve the ground state limit (T→0)

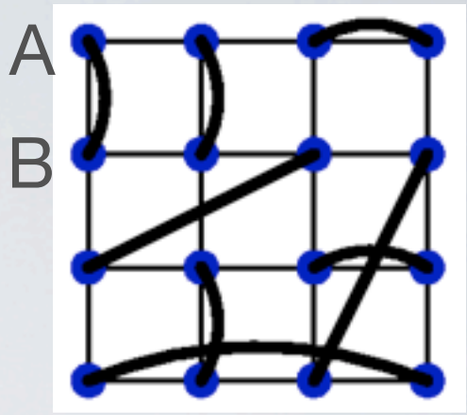
Valence bonds and Ground State Projection

The valence bond basis for S=1/2 spins

Valence-bonds between sublattice A, B sites $(i,j) = (|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle)/\sqrt{2}$

Basis states; singlet products

$$|V_r\rangle = \prod_{b=1}^{N/2}(i_{rb}, j_{rb}), \quad r = 1, \ldots (N/2)!$$



The valence bond basis is overcomplete and non-orthogonal

- expansion of arbitrary singlet state is not unique

$$|\Psi\rangle = \sum_r f_r |V_r\rangle$$ (all f_r positive for non-frustrated system)

All valence bond states overlap with each other

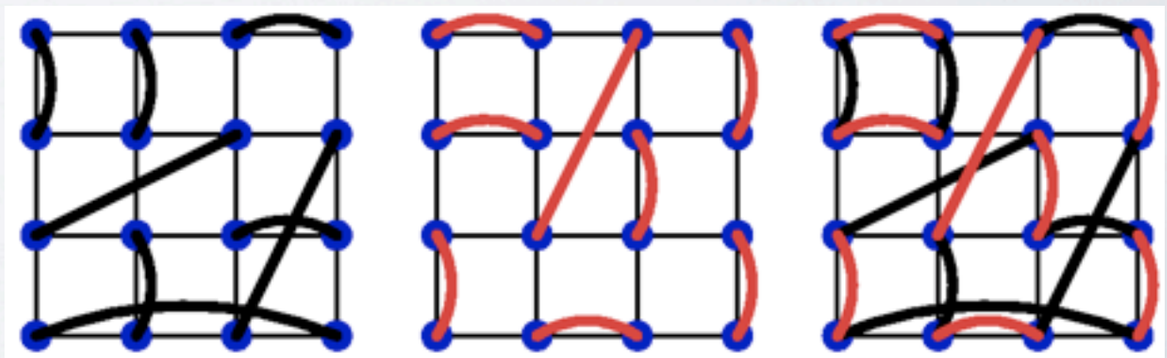
$$\langle V_l|V_r\rangle = 2^{N_\circ - N/2} \qquad N_\circ = \text{ number of loops in overlap graph}$$

Spin correlations from loop structure

$$\frac{\langle V_l|\vec{S}_i\cdot\vec{S}_j|V_r\rangle}{\langle V_l|V_r\rangle} = \begin{cases} \frac{3}{4}(-1)^{x_i - x_j + y_i - y_j} & \textit{(i,j in same loop)} \\ 0 & \textit{(i,j in different loops)} \end{cases}$$

More complicated matrix elements (e.g., dimer correlations) are also related to the loop structure

K.S.D. Beach and A.W.S.,
Nucl. Phys. B 750, 142 (2006)



Projector Monte Carlo in the valence-bond basis

Liang, 1991; AWS, Phys. Rev. Lett 95, 207203 (2005)

(-H)^n projects out the ground state from an arbitrary state

$$(-H)^n|\Psi\rangle = (-H)^n \sum_i c_i|i\rangle \rightarrow c_0(-E_0)^n|0\rangle$$

S=1/2 Heisenberg model

$$H = \sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j = -\sum_{\langle i,j\rangle} H_{ij}, \qquad H_{ij} = (\tfrac{1}{4} - \vec{S}_i \cdot \vec{S}_j)$$

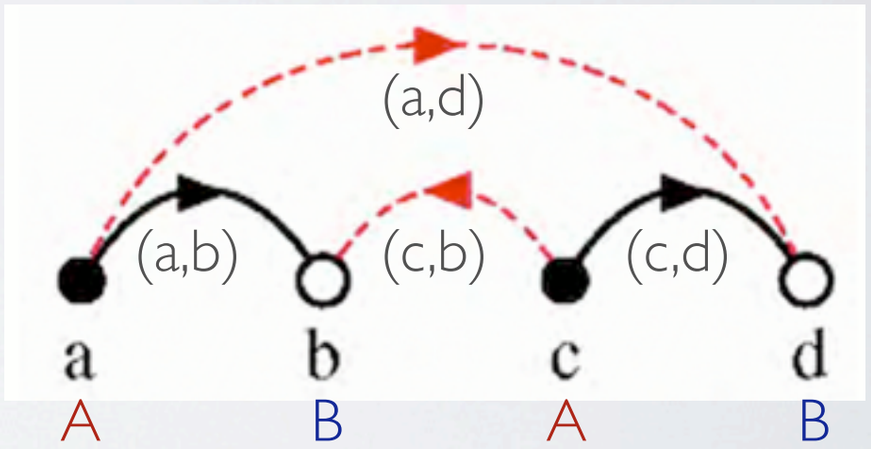
Project with string of bond operators

$$\sum_{\{H_{ij}\}} \prod_{p=1}^{n} H_{i(p)j(p)}|\Psi\rangle \rightarrow r|0\rangle \qquad \text{(r = irrelevant)}$$

Action of bond operators

$$H_{ab}|...(a,b)...(c,d)...\rangle = |...(a,b)...(c,d)...\rangle$$

$$H_{bc}|...(a,b)...(c,d)...\rangle = \frac{1}{2}|...(c,b)...(a,d)...\rangle$$



$$(i,j) = (|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle)/\sqrt{2}$$

Simple reconfiguration of bonds (or no change; diagonal)

- no minus signs for A→B bond 'direction' convetion
- sign problem does appear for frustrated systems

Expectation values: $\langle A\rangle = \langle 0|A|0\rangle$

Strings of singlet projectors

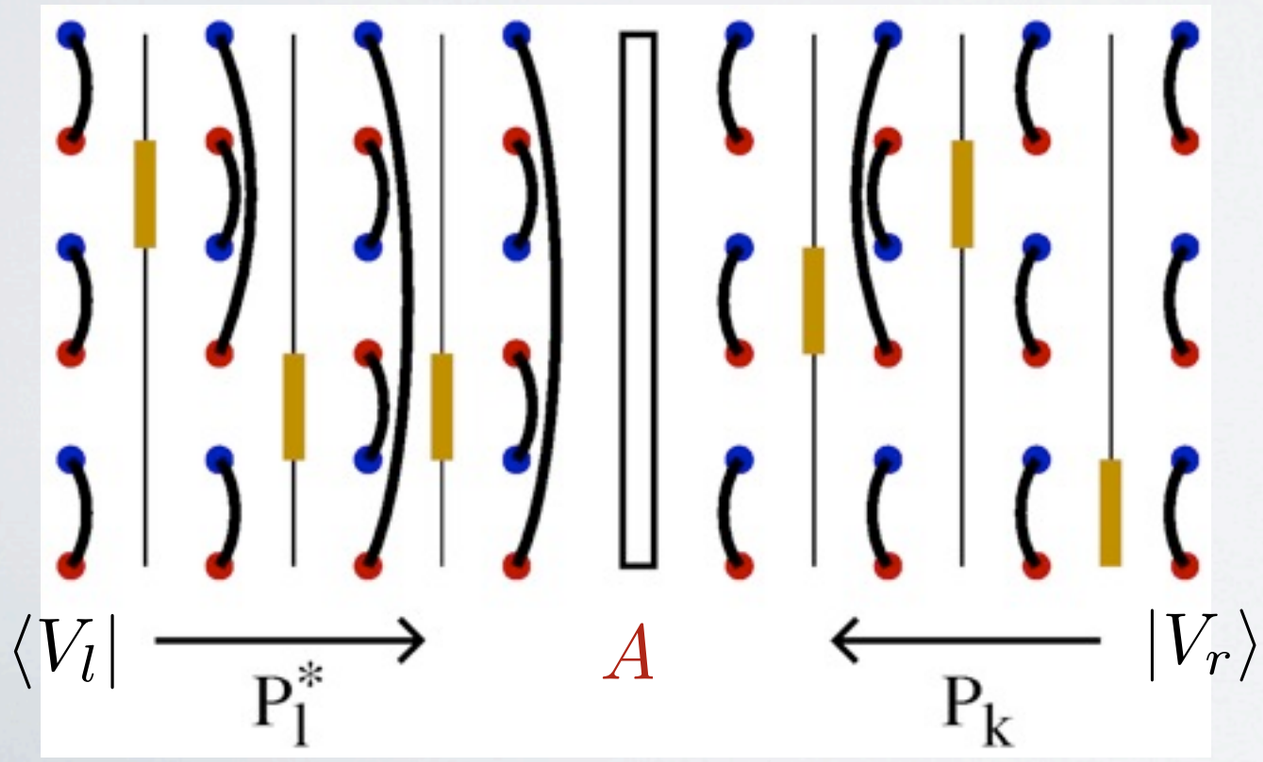
$$P_k = \prod_{p=1}^{n} H_{i_k(p)j_k(p)}, \quad k = 1, \ldots, N_b^n \quad (N_b = \text{number of interaction bonds})$$

We have to project bra and ket states

$$\sum_k P_k|V_r\rangle = \sum_k W_{kr}|V_r(k)\rangle \rightarrow (-E_0)^n c_0|0\rangle$$

$$\sum_g \langle V_l|P_g^* = \sum_g \langle V_l(g)|W_{gl} \rightarrow \langle 0|c_0(-E_0)^n$$

6-spin chain example:



$$\langle A\rangle = \frac{\sum_{g,k}\langle V_l|P_g^* A P_k|V_r\rangle}{\sum_{g,k}\langle V_l|P_g^* P_k|V_r\rangle} = \frac{\sum_{g,k} W_{gl}W_{kr}\langle V_l(g)|A|V_r(k)\rangle}{\sum_{g,k} W_{gl}W_{kr}\langle V_l(g)|V_r(k)\rangle}$$

- Monte Carlo sampling of operator strings
- Estimators based on transition graphs

More efficient ground state QMC algorithm → larger lattices

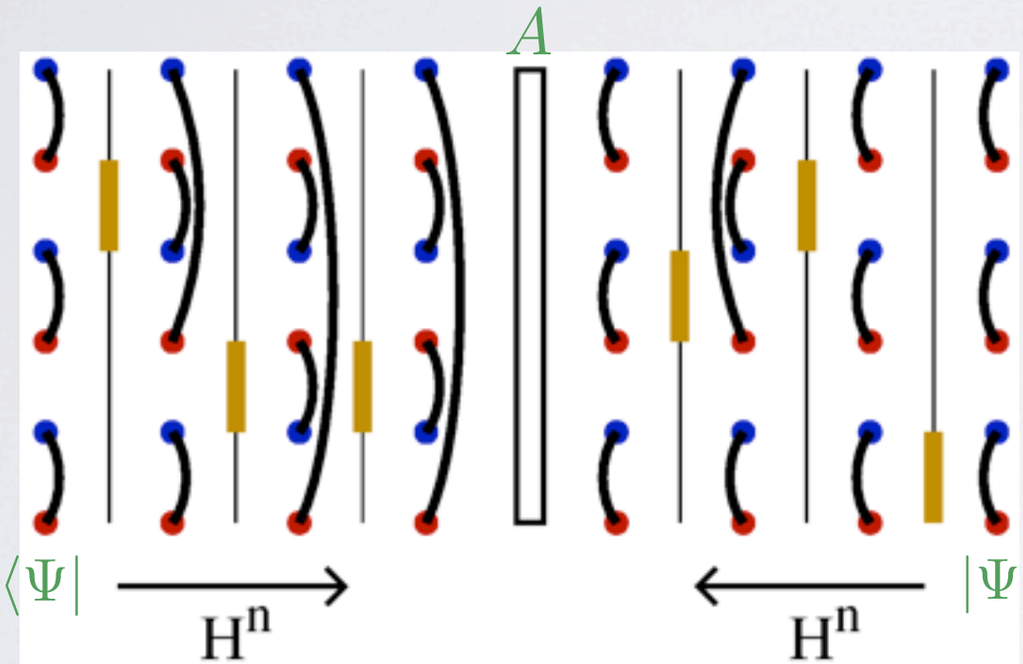
Loop updates in the valence-bond basis

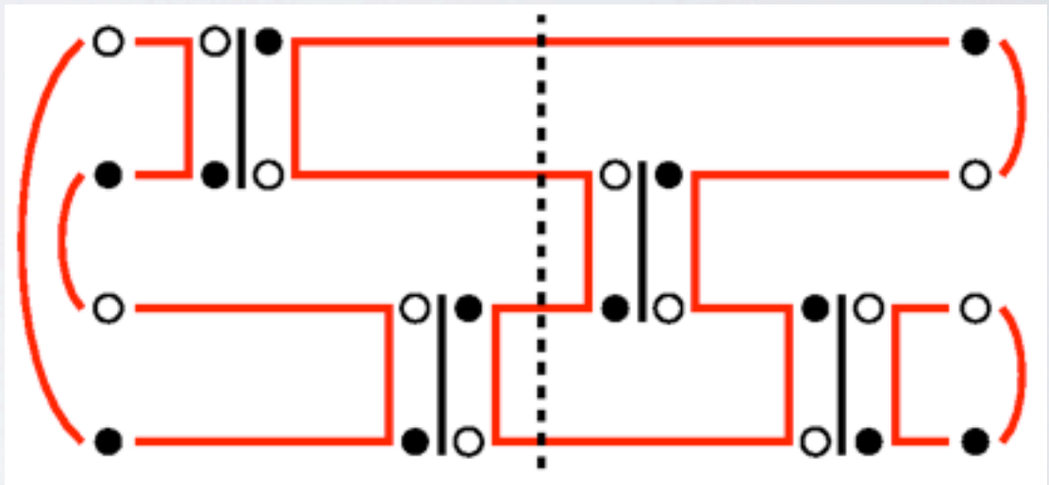
AWS and H. G. Evertz, PRB 2010

Put the spins back in a way compatible with the valence bonds

$$(a_i, b_i) = (\uparrow_i \downarrow_j - \downarrow_i \uparrow_j)/\sqrt{2}$$

and sample in a combined space of spins and bonds





Loop updates similar to those in finite-T methods
(world-line and stochastic series expansion methods)

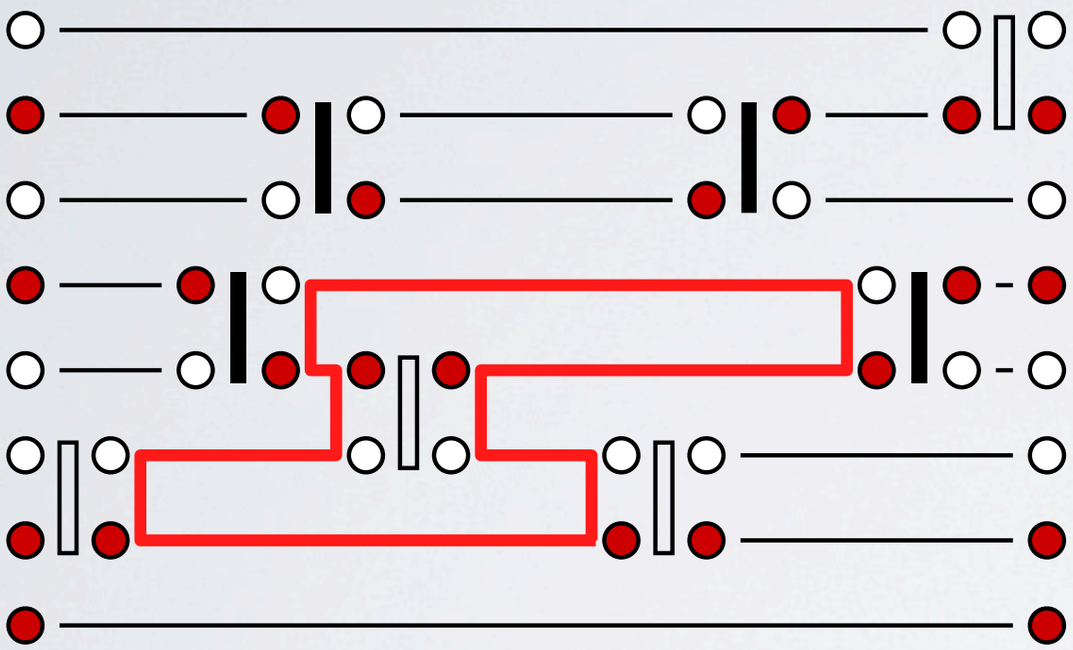
- good valence-bond trial wave functions can be used
- larger systems accessible
- sample spins, but measure using the valence bonds

T>0 and T=0 algorithms side-by-side

Finite-temperature QMC

(world lines, SSE,...)

$$\mathrm{tr}\{\mathrm{e}^{-\beta H}\} = \sum_n \frac{\beta^n}{n!}\langle\alpha|(-H)^n|\alpha\rangle$$

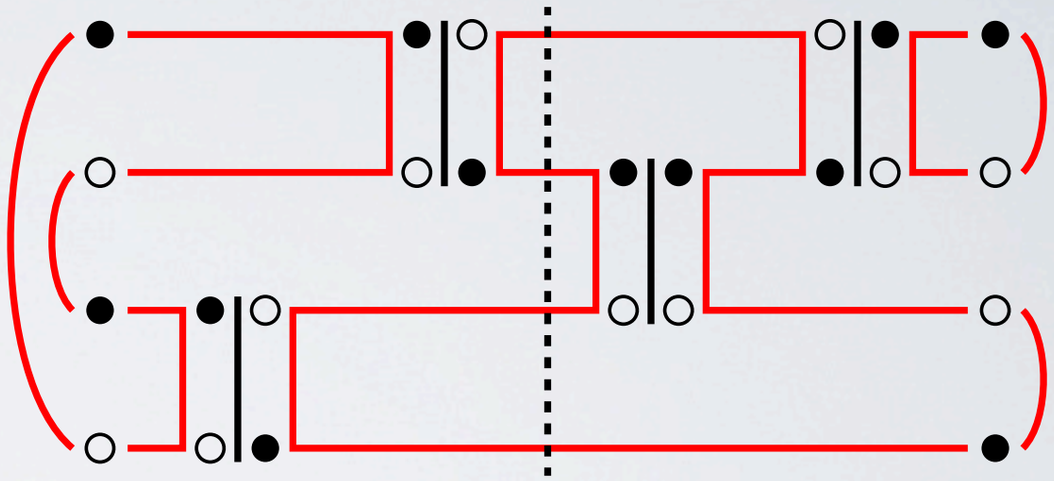


periodic time boundary conditions

- Computer implementations similar

Ground state projection

$$\sum_{\alpha\beta} f_\beta f_\alpha \langle\beta|(-H)^m|\alpha\rangle$$

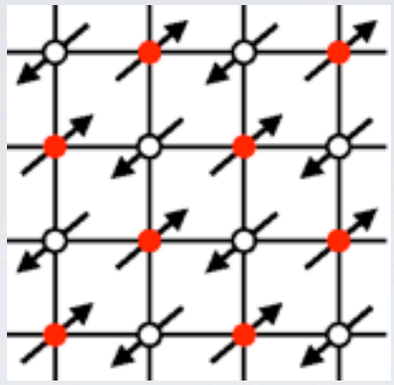


open boundaries capped by valence bonds (2-spin singlets) [AWS, HG Evertz, 2010]

Trial state can conserve relevant ground state quantum numbers (S=0, k=0,...)

Starting point: S=1/2 antiferromagnetic Heisenberg model

$$H = J \sum_{\langle i,j \rangle} S_i \cdot S_j$$



Sublattice magnetization

$$\vec{m}_s = \frac{1}{N} \sum_{i=1}^{N} \phi_i \vec{S}_i, \qquad \phi_i = (-1)^{x_i + y_i} \quad \text{(2D square lattice)}$$

Long-range order: **$\langle m_s^2 \rangle > 0$ for $N \to \infty$**

Quantum Monte Carlo

- finite-size calculations
- no approximations
- extrapolation to infinite size

Reger & Young 1988

$$m_s = 0.30(2)$$

$$\approx 60\ \%\ \text{of classical value}$$

AWS & HG Evertz 2010

$$m_s = 0.30743(1)$$

L×L lattices up to 256×256, T=0