National High Magnetic Field Lab, Tallahassee, Florida
Theory Winter school, January 9-13, 2012

Anders W. Sandvik, Boston University

Lecture 1

Stochastic Series Expansion Algorithms
for Quantum Spin Systems

Lecture 2

Quantum Monte Carlo simulations of
"deconfined" quantum criticality

Tutorial

SSE code for 1D and 2D S=1/2 Heisenberg models

http://physics.bu.edu/~sandvik/maglab12/

Review article on quantum spin systems
ArXiv:1101.3281

Why study quantum spin systems?

Solid-state physics

- localized electronic spins in Mott insulators (e.g., high-Tc cuprates)
- large variety of lattices, interactions, physical properties
- search for “exotic” quantum states in such systems (e.g., spin liquid)

Ultracold atoms (in optical lattices)

- some spin hamiltonians can be engineered (ongoing efforts)
- some bosonic systems very similar to spins (e.g., “hard-core” bosons)

Quantum information theory / quantum computing

- possible physical realizations of quantum computers using interacting spins
- many concepts developed using spins (e.g., entanglement)

Generic quantum many-body physics

- testing grounds for collective quantum behavior, quantum phase transitions
- identify “Ising models” of quantum many-body physics

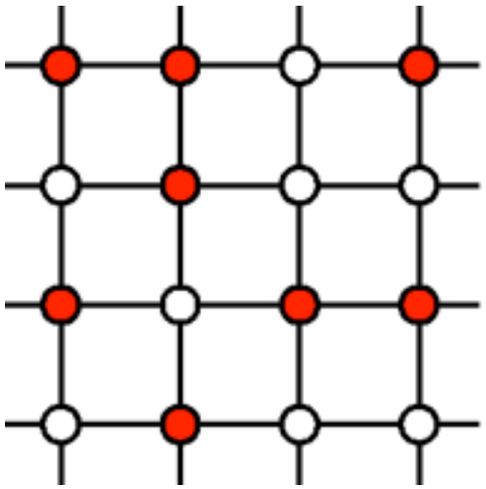
Particle physics / field theory / quantum gravity

- some quantum-spin phenomena have parallels in high-energy physics
  - e.g., spinon confinement-deconfinement transition
- spin foams, string nets: models to describe “emergence” of space-time and elementary particles

Mott insulators; origins of the Heisenberg antiferromagnet

Hubbard model (half-filling; one electron per site)

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} c^{+}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} = H_t + H_U$$



● $=\uparrow$ ○ $=\downarrow$

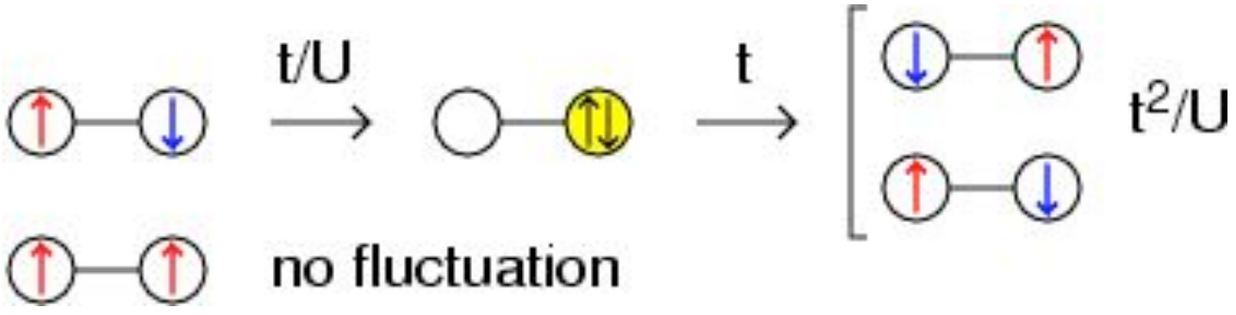
U>>t : use degenerate perturbation theory (e.g., Schiff)

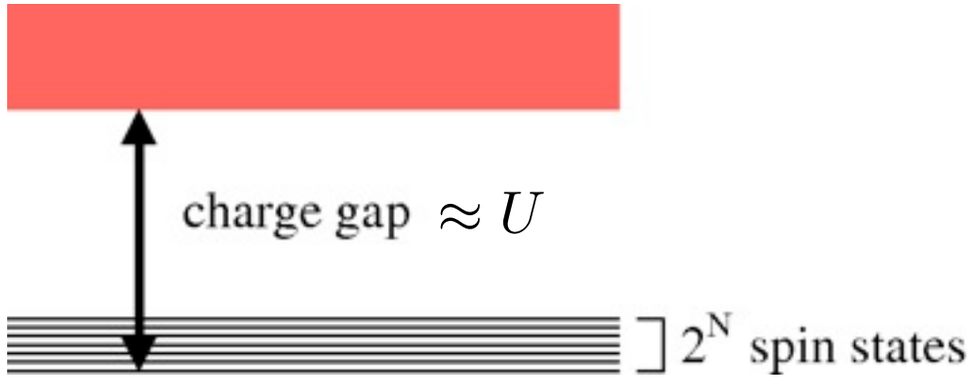
Treat H_t as a perturbation to the ground states of H_U

- **U=∞**, one particle on every site; 2^N degenerate spin states
- degeneracy lifted in order t^2/U - **1 doubly-occupied site, d=1**
- leads to the Heisenberg model

$$H^{\text{eff}}_{mn} = \sum_{i} \frac{\langle n|H_t|i\rangle\langle i|H_t|m\rangle}{E_0 - E_i} \qquad \begin{aligned} |i\rangle &: \ d = 1 \\ |m\rangle, |n\rangle &: \ d = 0 \end{aligned}$$

Exchange mechanism





$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j = J \sum_{\langle ij \rangle} [S^z_i S^z_j + \tfrac{1}{2}(S^+_i S^-_j + S^-_i S^+_j)] \qquad J = \frac{4t^2}{U}$$

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Stochastic Series Expansion Algorithms for Quantum Spin Systems

Anders W. Sandvik, Boston University

Outline

- Path integrals in quantum statistical mechanics
- The series-expansion representation
- Stochastic Series Expansion (SSE) algorithm for the Heisenberg model
- The valence-bond basis for S=1/2 systems
- Ground-state projector algorithm with valence bonds

Reference: AIP Conf. Proc. 1297, 135 (2010); arXiv:1101.3281

Detailed lecture notes on quantum spin models and methods

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

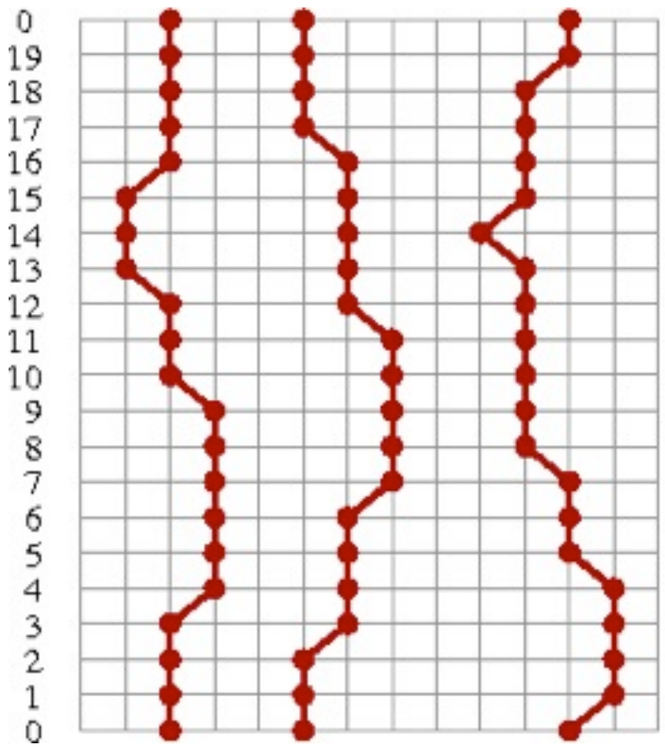
$$H = K = -\sum_{\langle i,j \rangle} K_{ij} = -\sum_{\langle i,j \rangle} (a_j^\dagger a_i + a_i^\dagger a_j) \qquad n_i = a_i^\dagger a_i \in \{0, 1\}$$

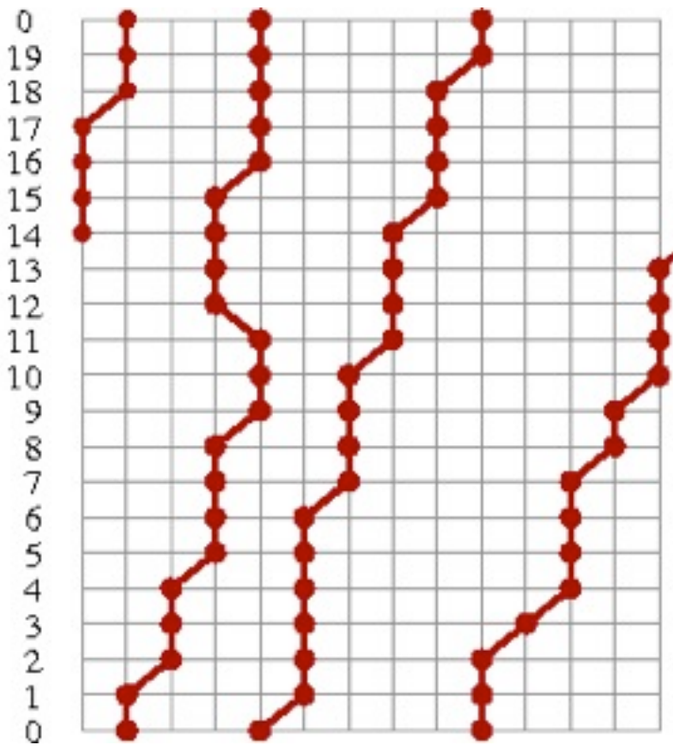
Equivalent to S=1/2 XY model

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

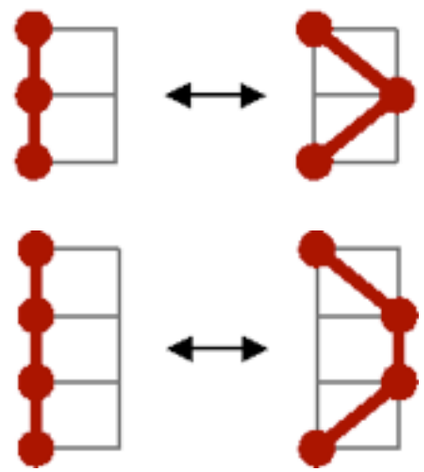
"World line" representation of

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





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

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

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

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

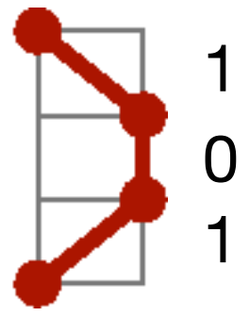
$$W(\{\alpha\}) = \text{weight}$$
$$A(\{\alpha\}) = \text{estimator}$$

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

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

Kinetic energy (here full energy). Use

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



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" (regardless of approximation used)

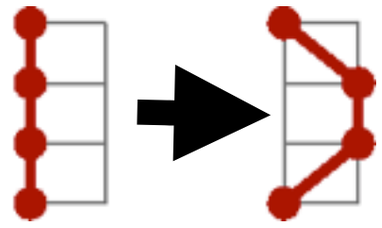
Including interactions

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 →

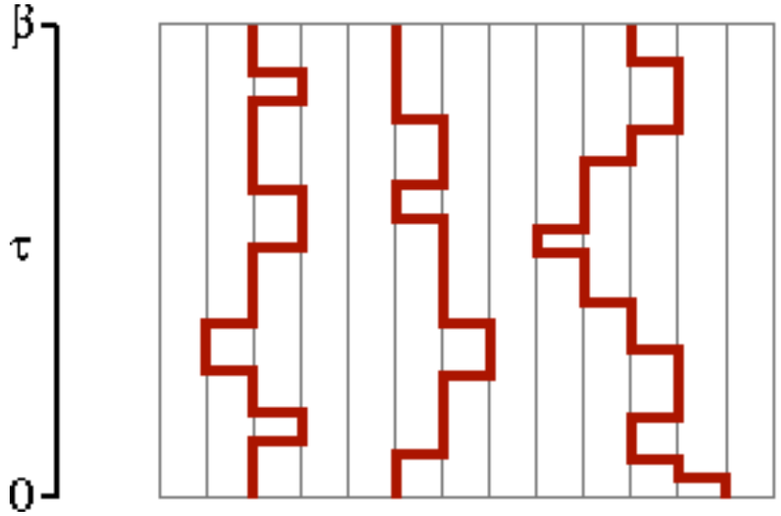
$$W(\{\alpha\}) = \Delta_\tau^{n_K}\exp\left(-\Delta_\tau\sum_{l=0}^{L-1}V_l\right)$$



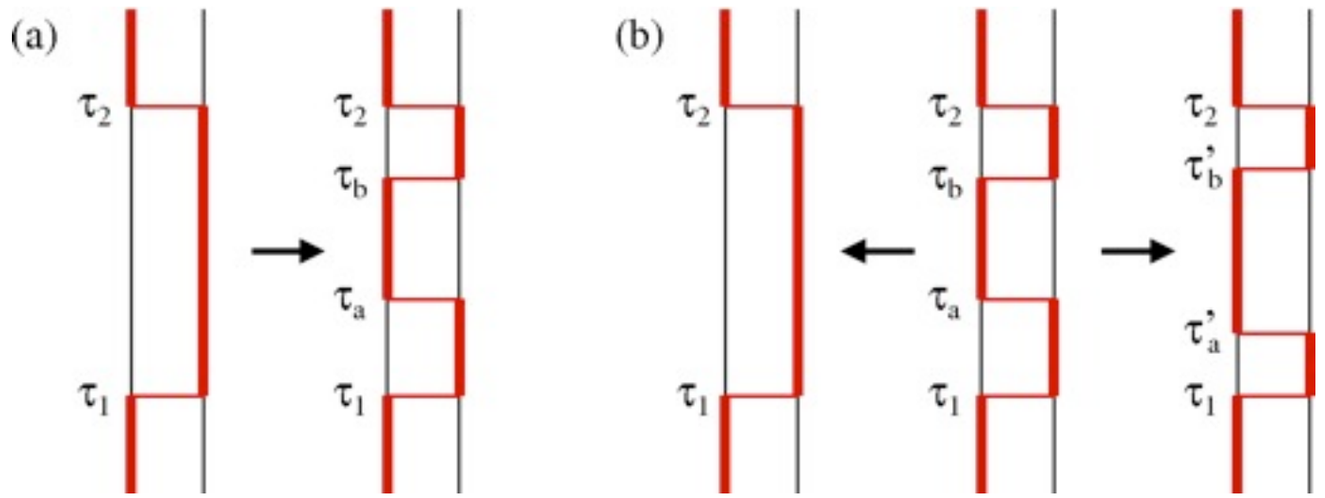
$$P_{\mathrm{acc}} = \min\left[\Delta_\tau^2\exp\left(-\frac{V_{\mathrm{new}}}{V_{\mathrm{old}}}\right),1\right]$$

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)

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

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

this is the operator we "measure"

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}=L (exponentially small error)
- cutt-off at n=L, fill in operator string with unit operators H_0=I

n=10 | H_4 | H_7 | H_1 | H_6 | H_2 | H_1 | H_8 | H_3 | H_3 | H_5 | $\Longrightarrow$

M=14 | H_4 | I | H_7 | I | H_1 | H_6 | I | H_2 | H_1 | H_8 | H_3 | H_3 | I | H_5 |

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

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

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

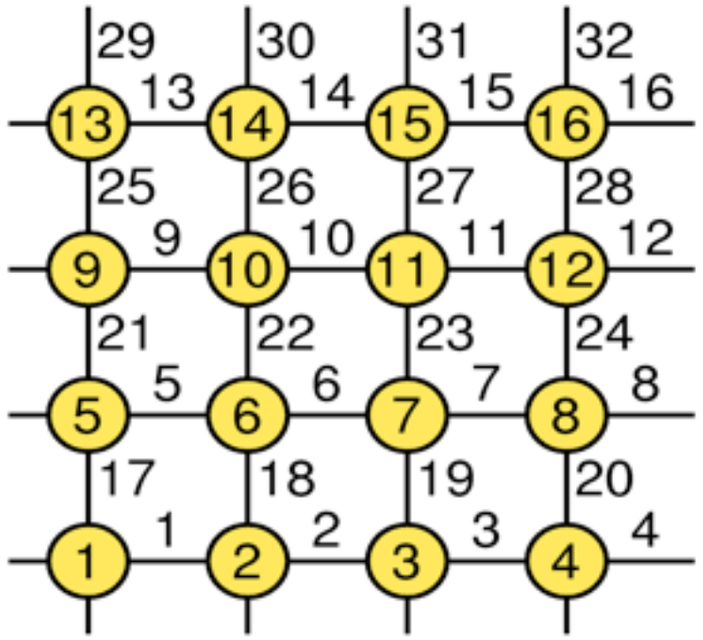
$$Z = \sum_{\{\alpha\}_L} \sum_{\{H_i\}} \frac{(-\beta)^n (L-n)!}{L!} \langle \alpha_0 | H_{i(L)} | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | H_{i(2)} | \alpha_1 \rangle \langle \alpha_1 | H_{i(1)} | \alpha_0 \rangle$$

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

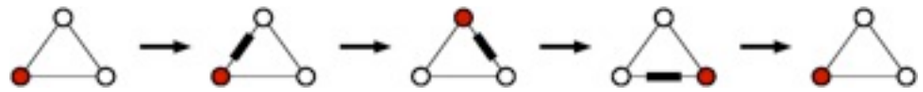
Index sequence: $S_n = [a(0), b(0)], [a(1), b(1)], \ldots, [a(n-1), b(n-1)]$

For fixed-length scheme

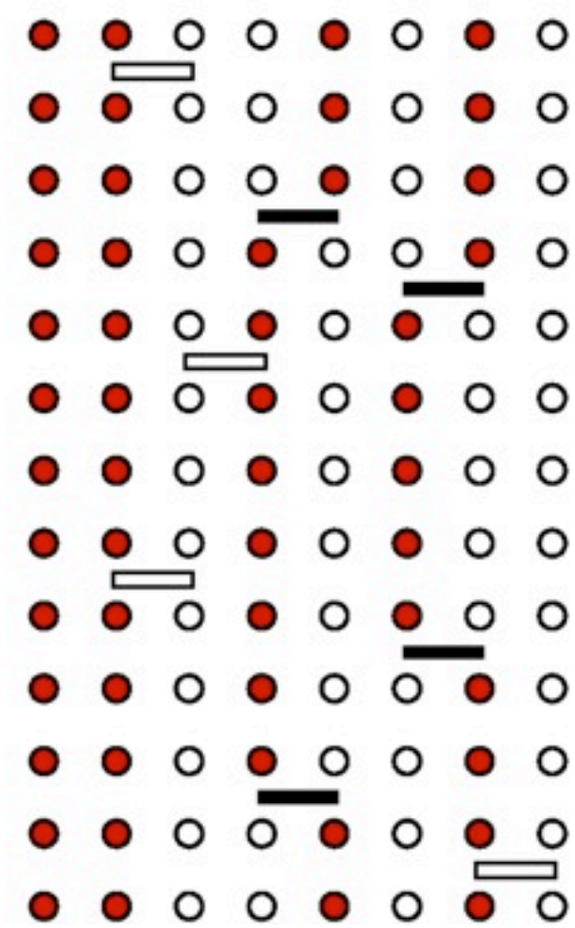
$$Z = \sum_{\alpha} \sum_{S_L} (-1)^{n_2} \frac{\beta^n (L-n)!}{L!} \left\langle \alpha \left| \prod_{p=0}^{L-1} H_{a(p),b(p)} \right| \alpha \right\rangle \qquad W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

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**



i =	1	2	3	4	5	6	7	8
$\sigma(i)$ =	-1	+1	-1	-1	+1	-1	+1	+1



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:

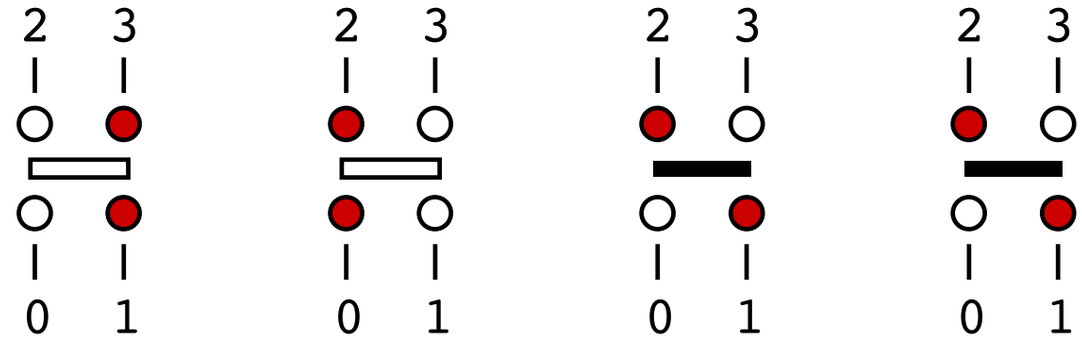
s(p) = operator-index string
- **s(p) = 2*b(p) + a(p)-1**
- diagonal; s(p) = even
- off-diagonal; s(p) = off

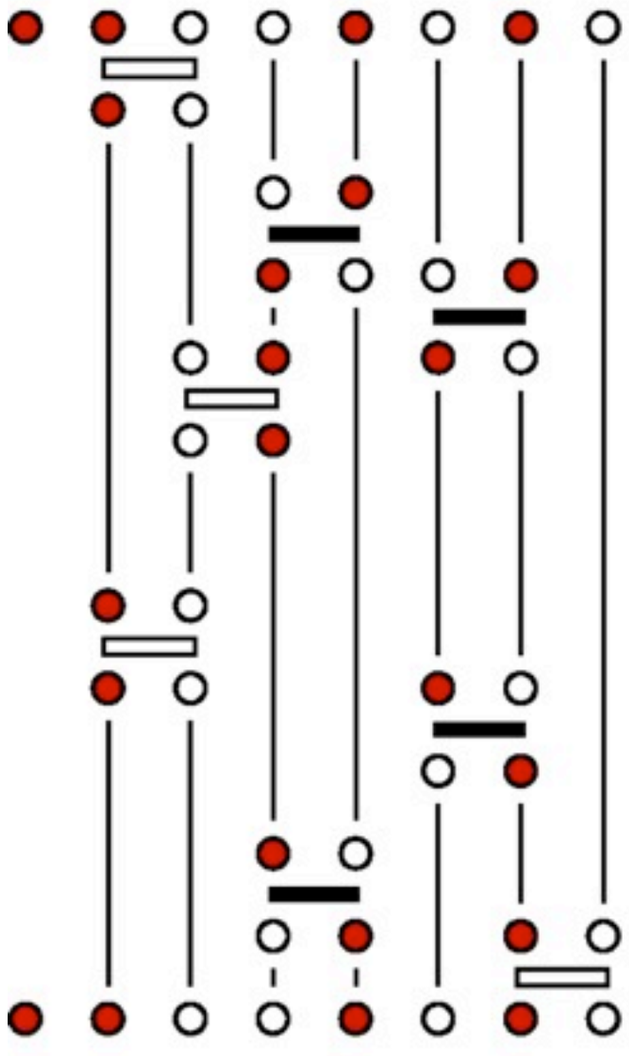
σ(i) = spin state, i=1,...,N
- only one has to be stored

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

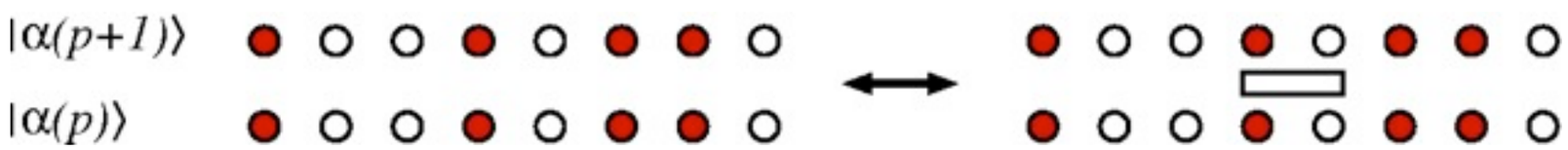
Monte Carlo sampling scheme

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



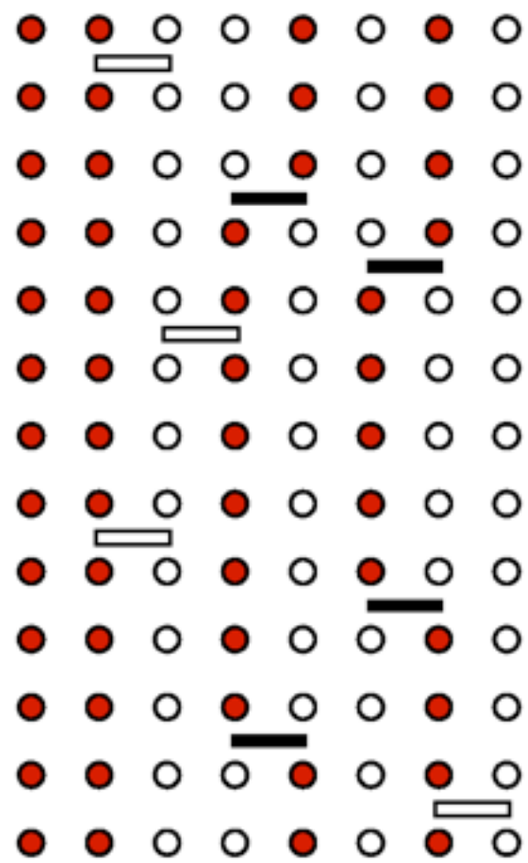
Attempt at p=0,...,L-1. Need to know |α(p)>

- 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

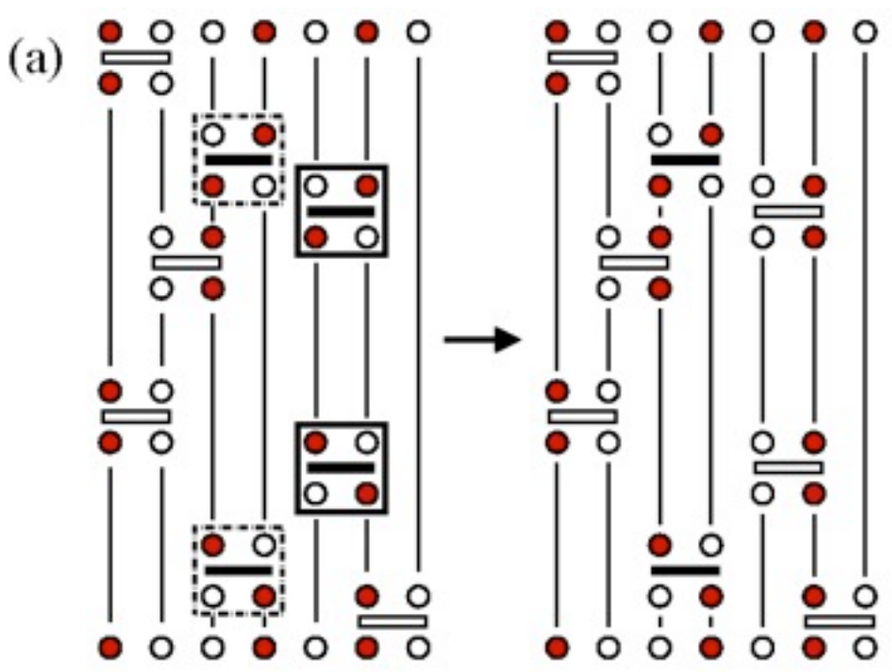
- n → n+1 (a=0 → a=1)
- n → n-1 (a=1 → a=0)

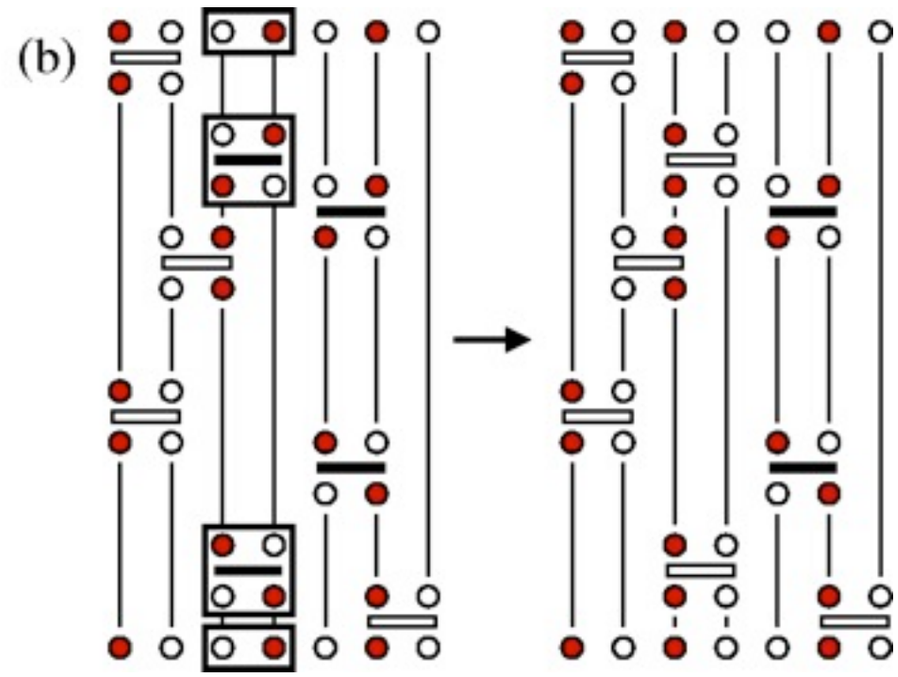
Acceptance probabilities

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

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

Off-diagonal updates

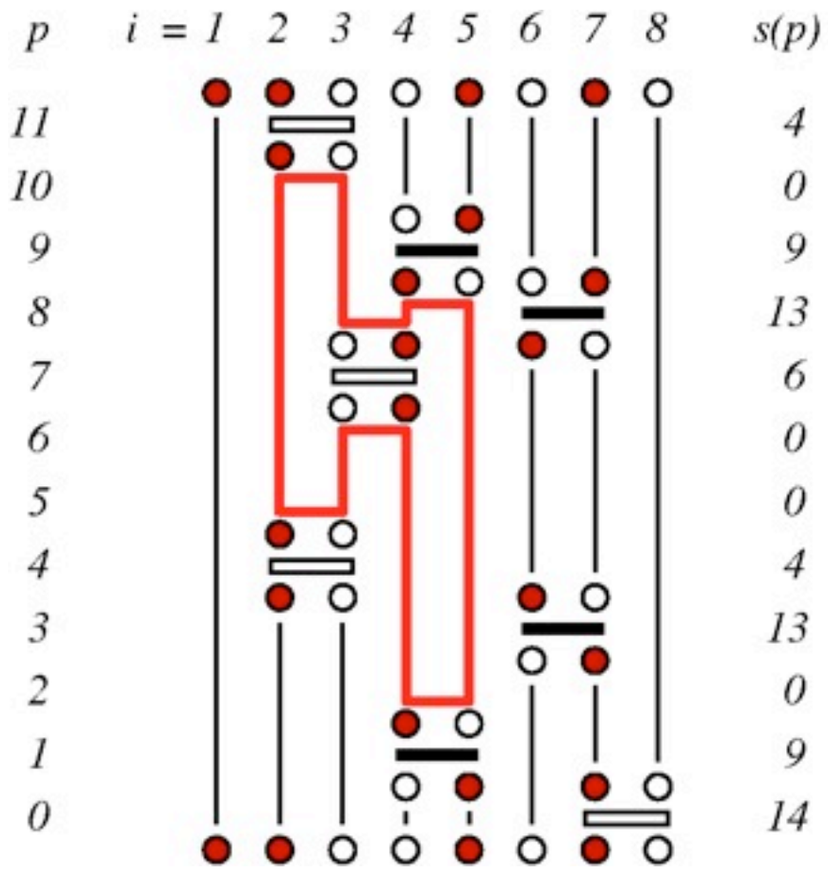


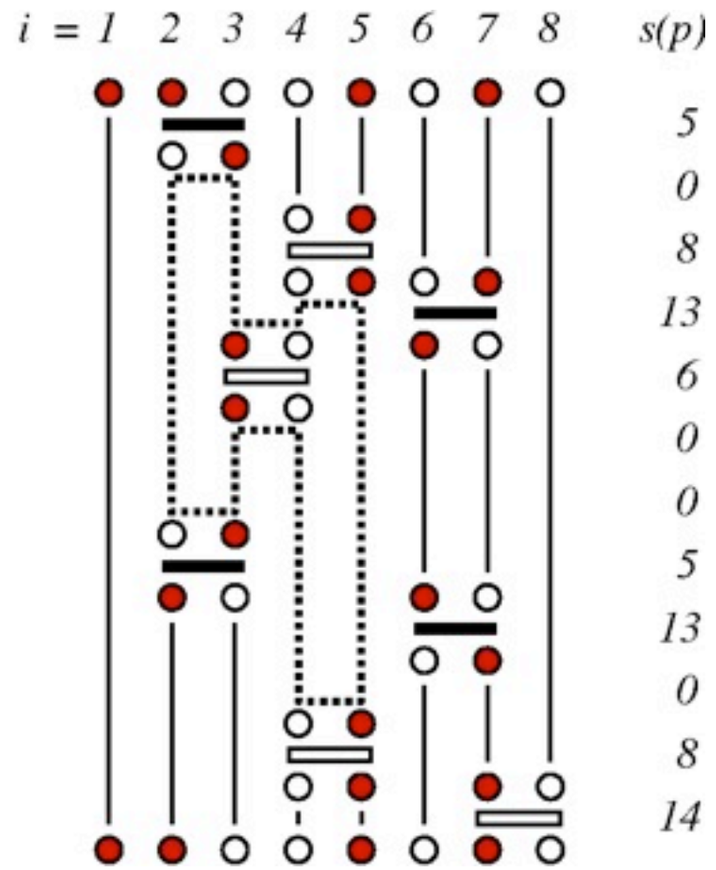


Local update

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

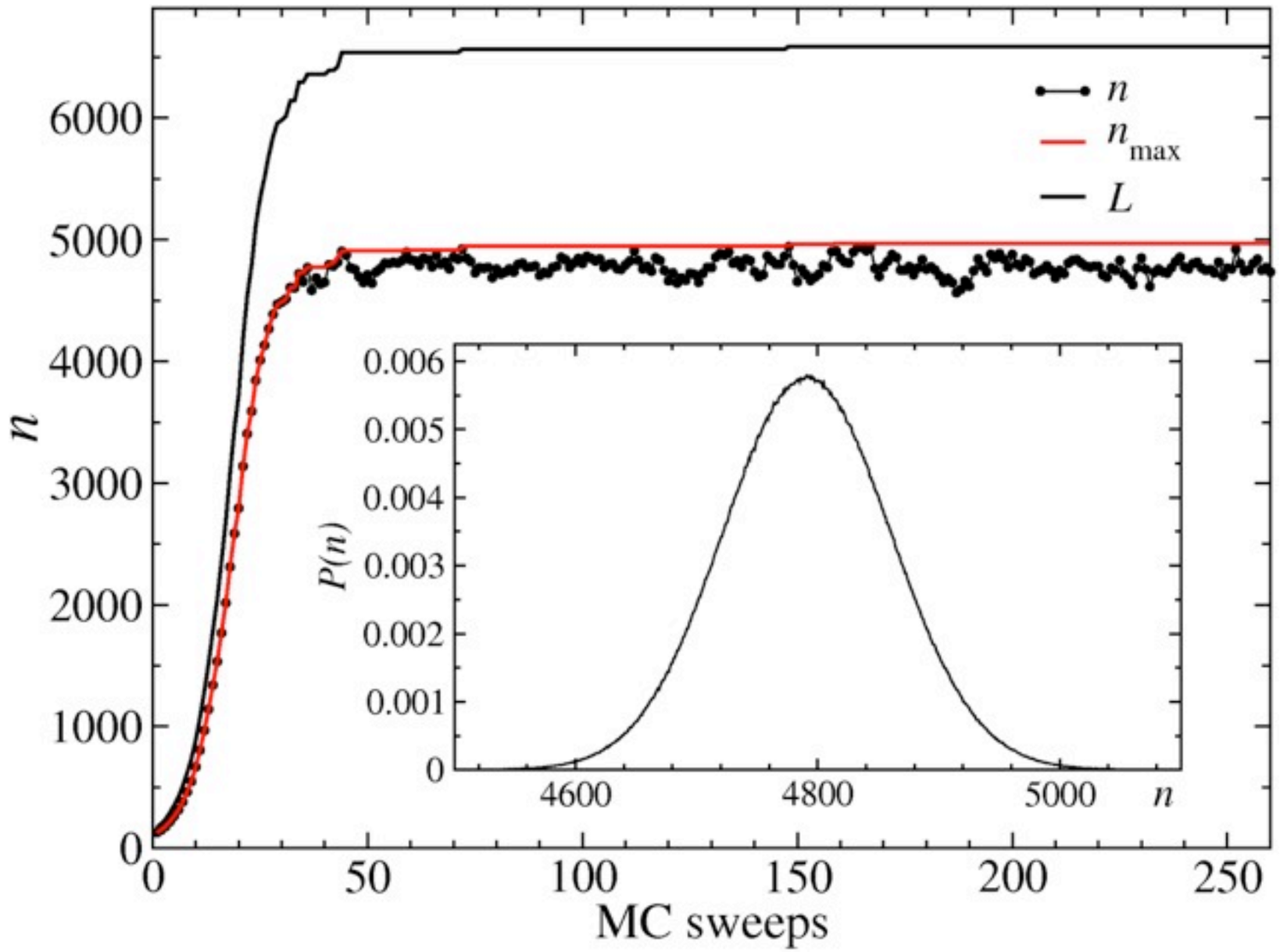
- adjust during equilibration
- start with arbitrary (small) n

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

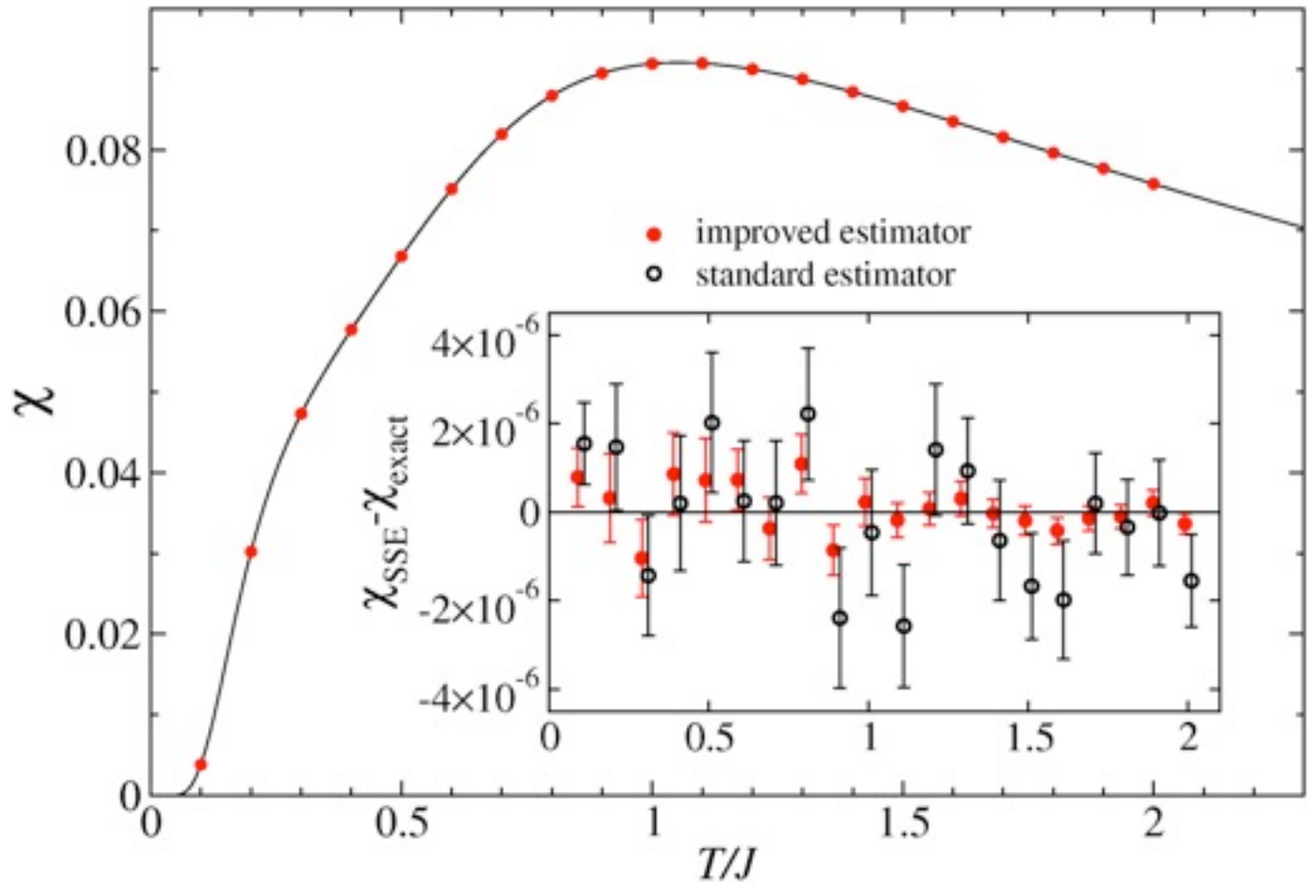


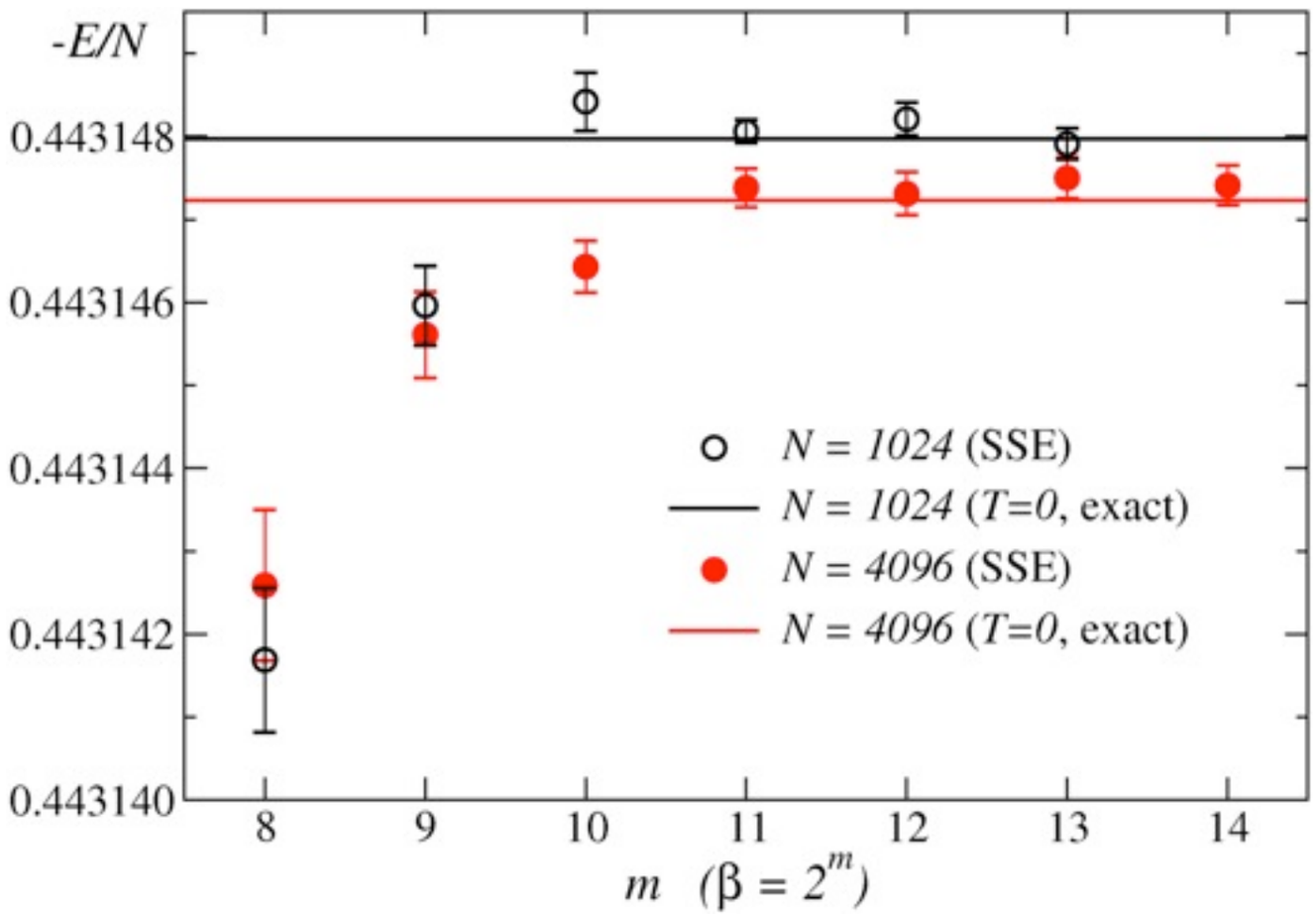
Does it work?
Compare with exact results

- 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

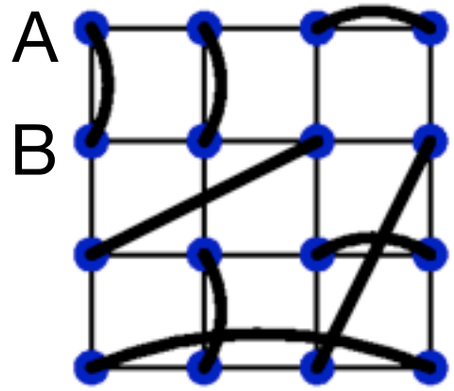
- SSE results for 10^6 sweeps
- Bethe Ansatz ground state E/N
- SSE can achieve the ground state limit (T→0)

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

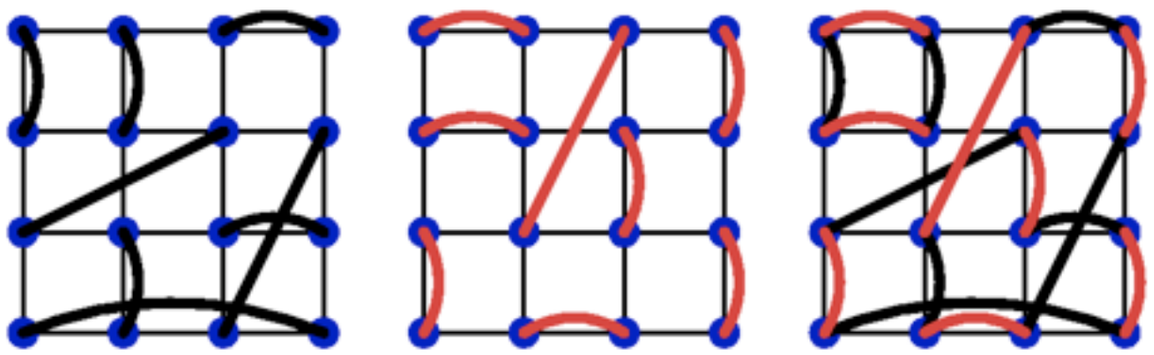
$$\langle V_l|V_r\rangle = 2^{N_\circ - N/2} \qquad N_\circ = \text{ number of loops in overlap graph}$$

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

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

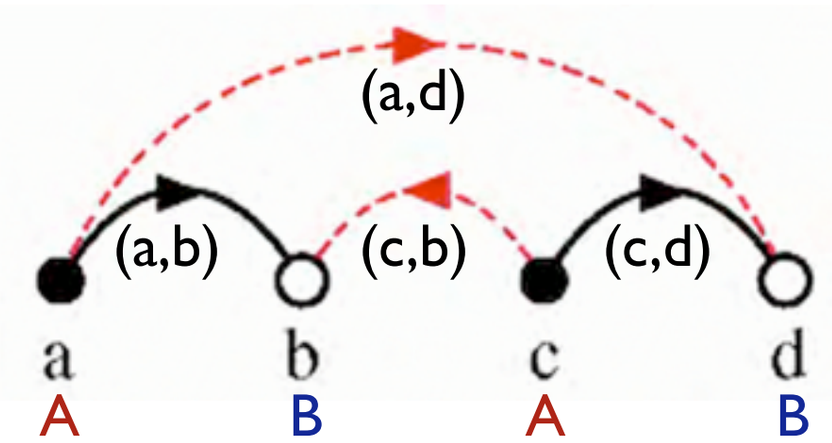
Project with string of bond operators

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

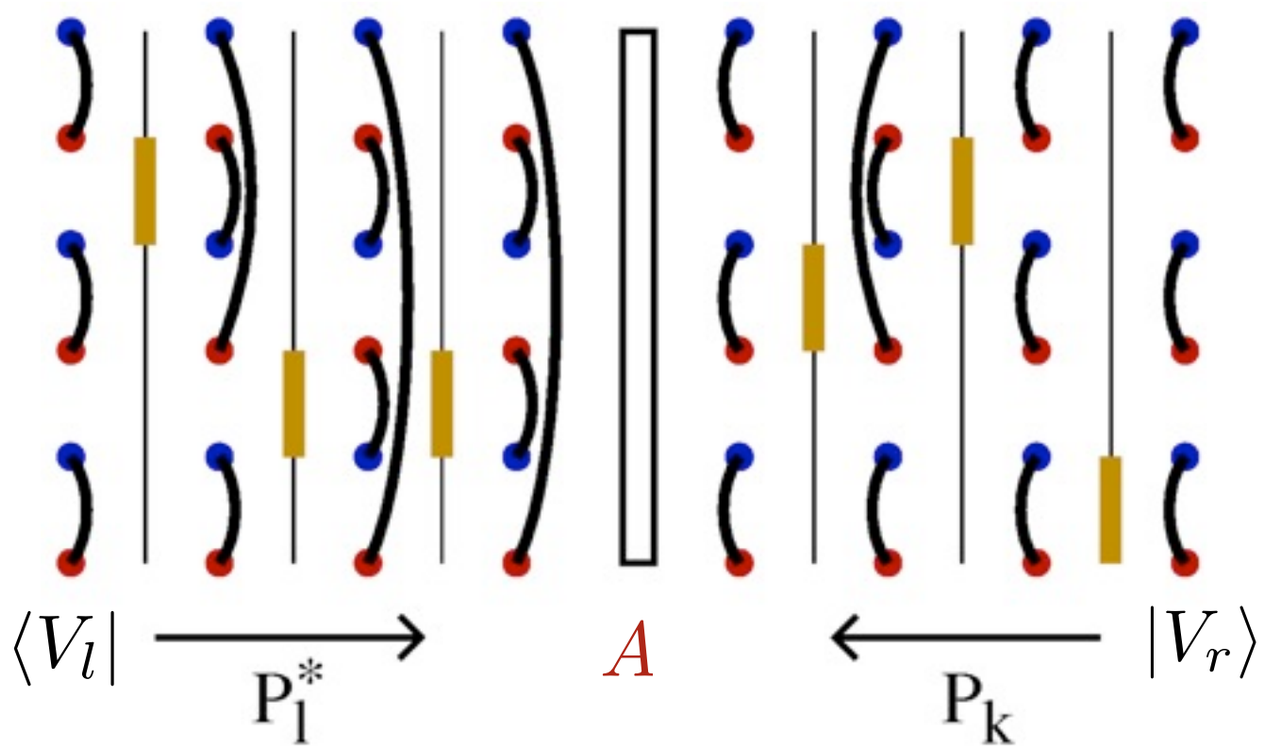
$$P_k = \prod_{p=1}^{n} H_{i_k(p)j_k(p)}, \quad k = 1, \ldots, N_b^n \quad (N_b = \text{number of interaction bonds})$$

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

More efficient ground state QMC algorithm → larger lattices

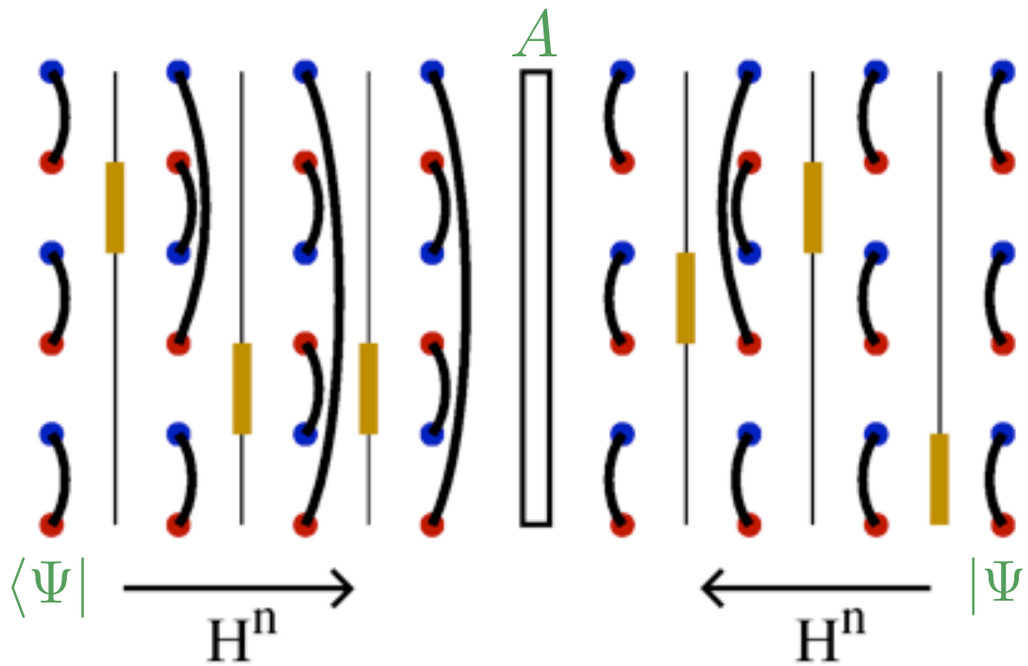
Loop updates in the valence-bond basis

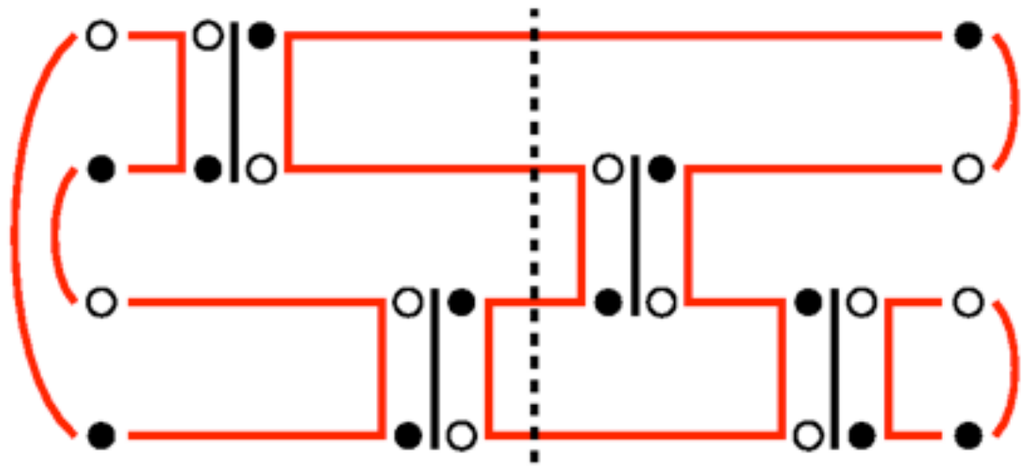
AWS and H. G. Evertz, PRB 2010

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