Valence bonds and Ground-State Projection in the valence-bond basis

PHYSICAL REVIEW B **82**, 024407 (2010)

Loop updates for variational and projector quantum Monte Carlo simulations in the valence-bond basis

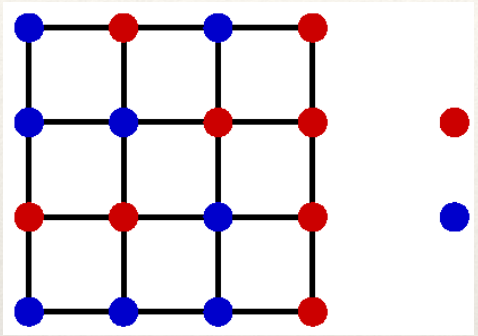
Anders W. Sandvik[1] and Hans Gerd Evertz[2]

Common bases for quantum spin systems

Lattice of S=1/2 spins, e.g., Heisenberg antiferromagnet

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

The most common basis is that of ‘up’ and ‘down’ spins

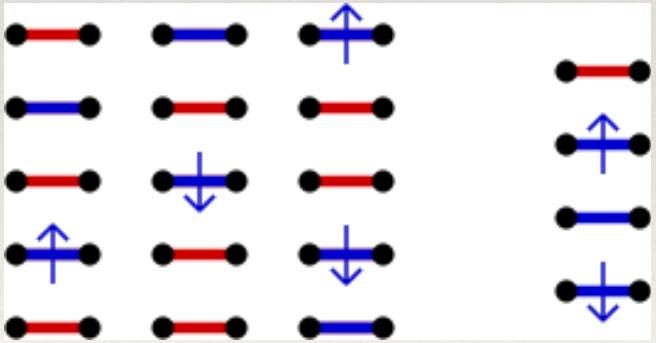


$= |\uparrow\rangle = |S^z = +1/2\rangle$

$= |\downarrow\rangle = |S^z = -1/2\rangle$

One can also use eigenstates of two or more spins

- dimer singlet-triplet basis



$= (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$

$= |\uparrow\uparrow\rangle$

$= (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$

$= |\downarrow\downarrow\rangle$

The hamiltonian is more complicated in this basis

- but some times can be used to solve sign problems
  [S. Wessel et al. Phys. Rev. B 98, 174432 (2018)]

Marshall's sign rule for bipartite antiferromagnets

Consider a bipartite S=1/2 Heisenberg model

$$H = J\sum_{\langle i,j\rangle}\vec{S}_i\cdot\vec{S}_j = J\sum_{\langle i,j\rangle}\left[S_i^z S_j^z + (S_i^+ S_j^- + S_i^- S_j^+)/2\right] \quad = H_{\rm dia} + H_{\rm off}$$

and a proposed wave function to describe its ground state

$$|\Psi\rangle = \sum_\sigma \Psi(\sigma)|\sigma\rangle \qquad \sigma = \{S_1^z,\ldots,S_N^z\}$$

In a variational calculation we minimize the energy wrt some parameters

$$E = \langle\Psi|H|\Psi\rangle = \sum_\sigma\sum_\tau \Psi^*(\tau)\Psi(\sigma)\langle\tau|H|\sigma\rangle$$

$$= \sum_\sigma |\Psi(\sigma)|^2\langle\sigma|H_{\rm dia}|\sigma\rangle + \sum_\sigma|\Psi(\sigma)|^2\sum_\tau\frac{\Psi^*(\tau)}{\Psi^*(\sigma)}\langle\tau|H_{\rm off}|\sigma\rangle$$

$$\langle\tau|S_i^-S_j^+|\sigma\rangle \quad \langle\tau|S_i^+S_j^-|\sigma\rangle \quad \geq 0$$

An extreme variational approach is to consider each wave function coefficient $\psi(\sigma)$ as an individually adjustable parameter

Let's focus on the signs (or phases) of the coefficients:

- diagonal energy contributions independent of the signs
- off-diagonal matrix elements positive; optimal E if wave-function signs change

$$\Psi^*(\tau)/\Psi^*(\sigma) = \mathrm{e}^{i\delta}|\Psi(\tau)|/|\Psi(\sigma)|$$

E must be real (ψ can also be real)

- minimum for all negative signs

$$\Psi(\tau)/\Psi(\sigma) \leq 0$$

Marshall's sign rule

$$\mathrm{sign}[\Psi(S_1^z,\ldots,S_N^z)] = (-1)^{n_{A\uparrow}}$$

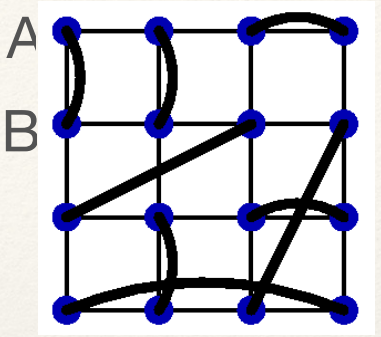
sign always changes when two spins flipped

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 (obey Marshall's sign rule)

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



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

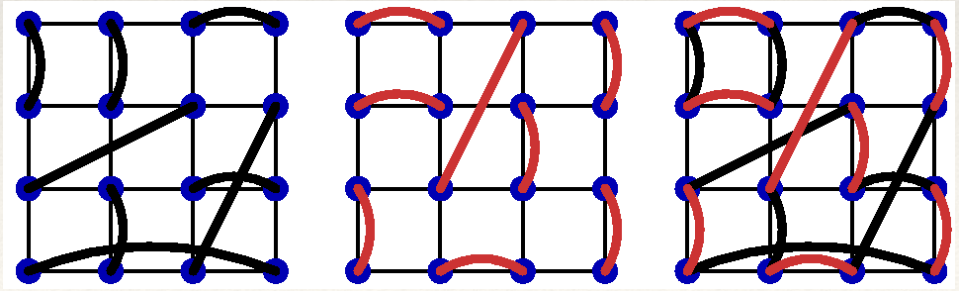
$$\langle V_l|V_r\rangle = 2^{N_\circ - N/2} \qquad N_\circ = \text{ number of loops in overlap graph}$$

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

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

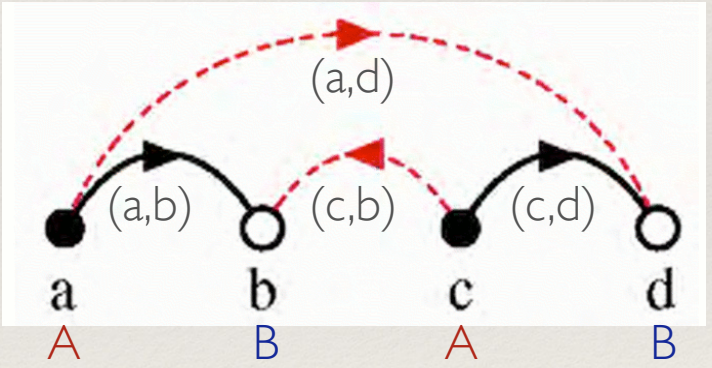
S=1/2 Heisenberg model

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

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)



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

Action of bond operators

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

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

Simple reconfiguration of bonds (or no change; diagonal)

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

Sampling the wave function

Simplified notation for operator strings

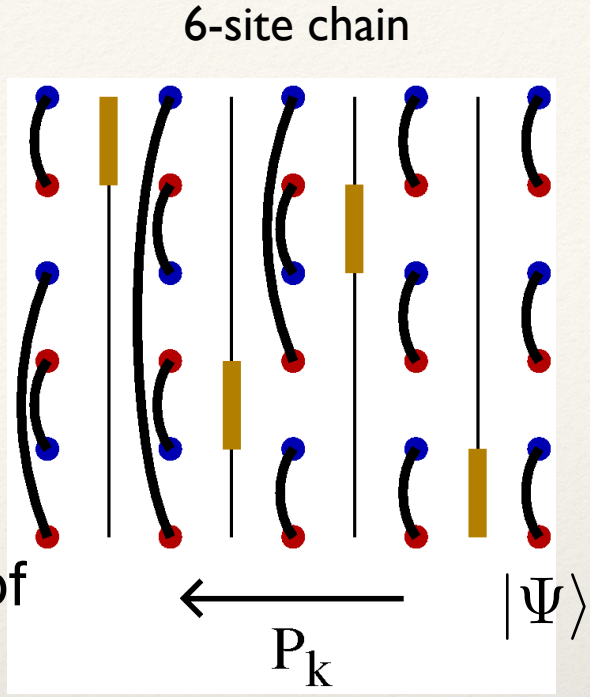
$$\sum_{\{H_{ij}\}} \prod_{p=1}^{n} H_{i(p)j(p)} = \sum_k P_k, \qquad k = 1, \ldots N_b^n$$

Simplest trial wave function: a basis state $|V_r\rangle$

$$P_k|V_r\rangle = W_{kr}|V_r(k)\rangle$$

The weight W_{kr} of a path is given by the number of off-diagonal operations ('bond flips') n_{flip}

$$W_{kr} = \left(\frac{1}{2}\right)^{n_{\rm flip}} \qquad n = n_{\rm dia} + n_{\rm flip}$$



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

Note: all paths contribute - no 'dead' (W=0) paths

Sampling: Trivial way: Replace m (m ≈ 2-4) operators at random

$$P_{\rm accept} = \left(\frac{1}{2}\right)^{n_{\rm flip}^{\rm new} - n_{\rm flip}^{\rm old}}$$

The state has to be re-propagated with the full operator string

- More efficient updating scheme exists (later....)

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

Strings of singlet projectors

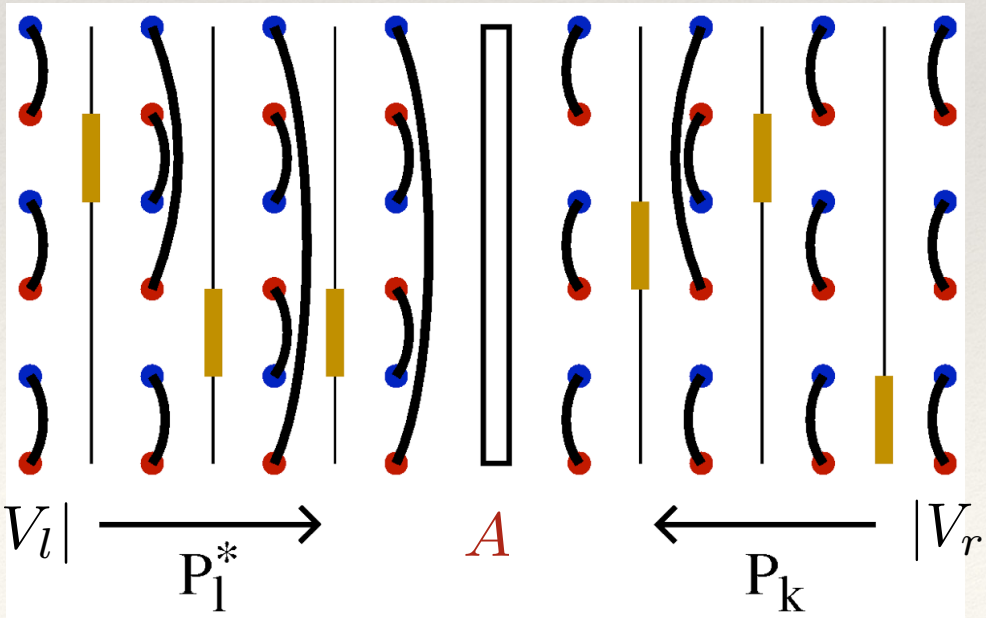
$$P_k = \prod_{p=1}^{n} H_{i_k(p) j_k(p)}, \quad k = 1, \ldots, N_b^n \quad (N_b = \text{number of interaction bonds})$$

We have to project bra and ket states

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

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

6-spin chain example:



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

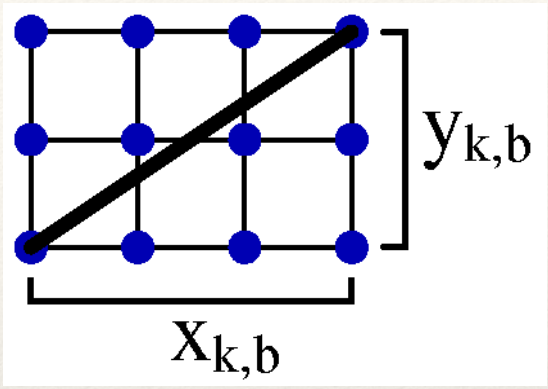
- Monte Carlo sampling of operator strings
- Estimators based on transition graphs

Sampling an amplitude-product state

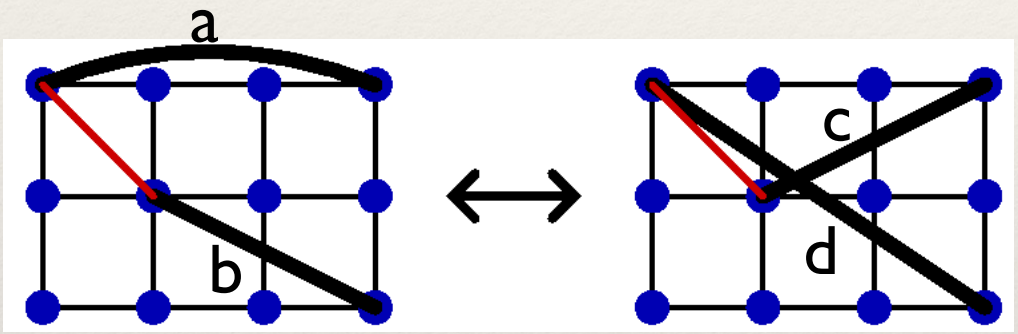
A better trial state leads to faster n convergence

- bond-amplitude product state [Liang, Doucot, Anderson, 1990]

$$|\Psi_0\rangle = \sum_k \prod_{b=1}^{N/2} h(x_{rb}, y_{rb})|V_k\rangle$$



Update state by reconfiguring two bonds



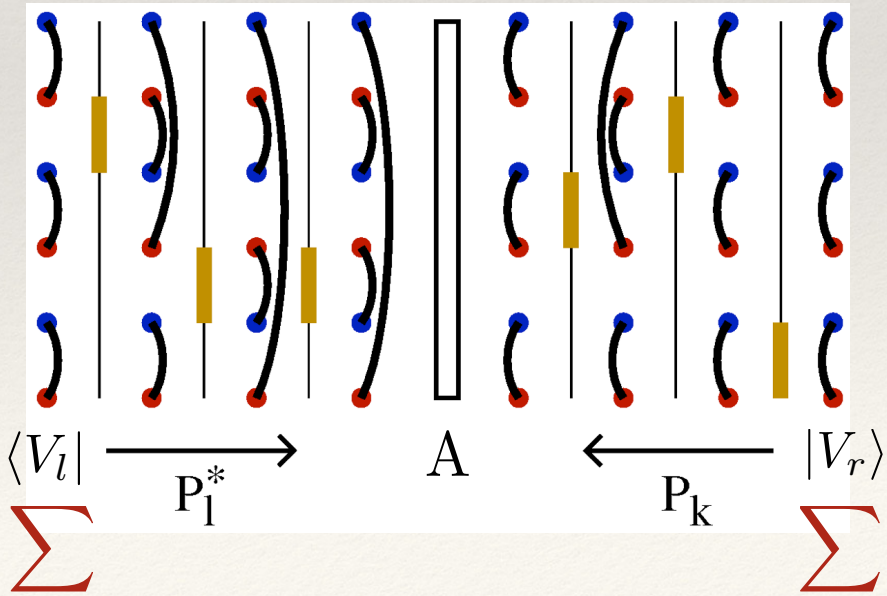
$$P_{\text{accept}} = \frac{h(x_c, y_c)h(x_d, y_d)}{h(x_a, y_a)h(x_b, y_b)}$$

If reconfiguration accepted

- calculate change in projection weight
- used for final accept/reject prob.

S. Liang [PRB 42, 6555 (1990)]

- used parametrized state amplitudes
- determined parameters variationally
- improved state by projection

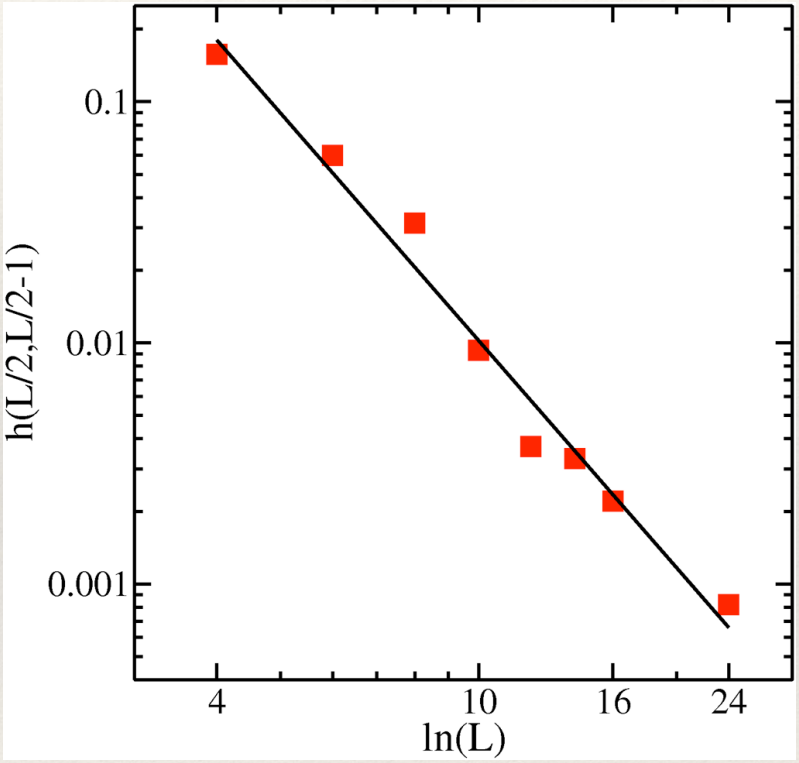


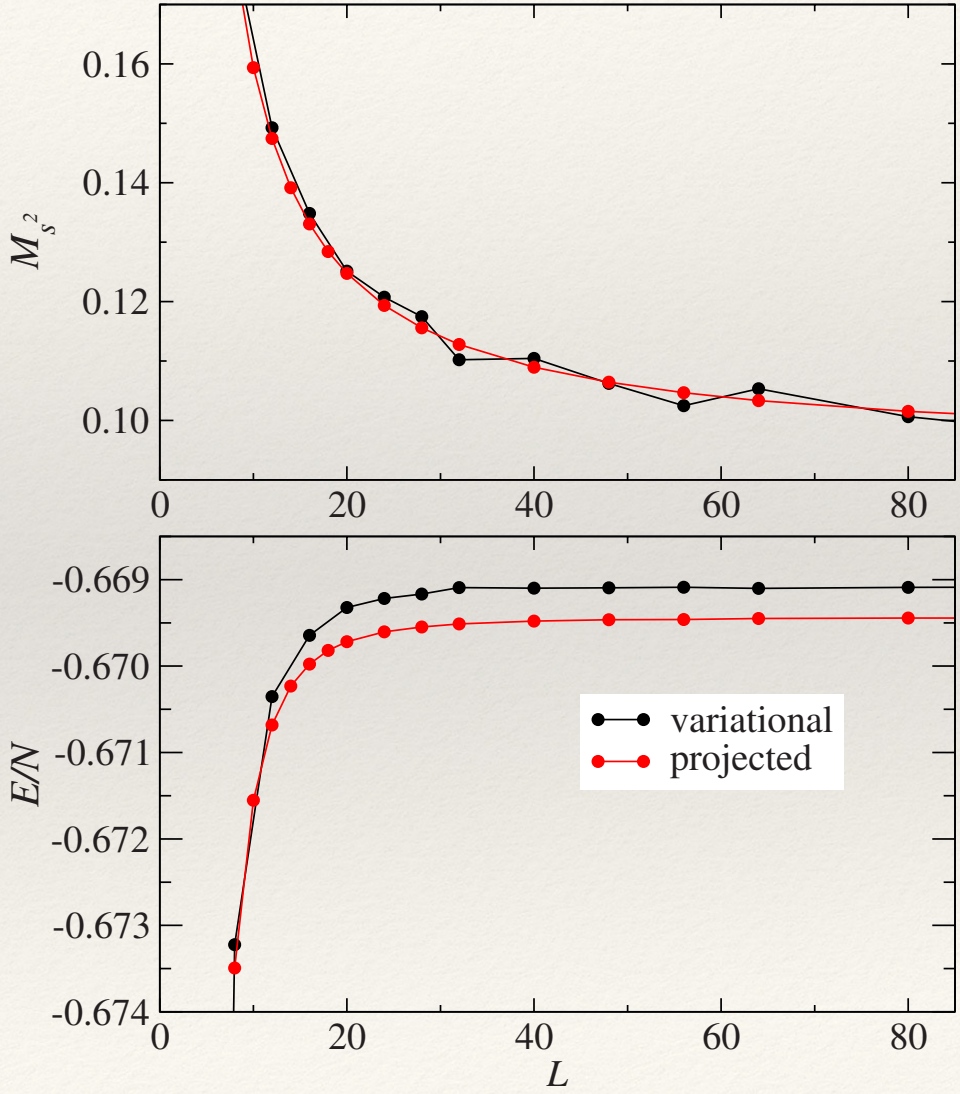
Variational wave function (2D Heisenberg)

All amplitudes h(x,y) can be optimized

[J. Lou and A.W.S., PRB 2007, AWS and H.-G. Evertz, PRB 2010]

- variational energy error 50% smaller than previously best (<0.1%)
- spin correlations deviate by less than 1% from exact values
- amplitudes decay as ~$1/r^3$





Variational energy can be further improved by including optimized bond correlations; Lin et al. PRB 2012 (posted on course web site)

More efficient ground state QMC algorithm → larger lattices

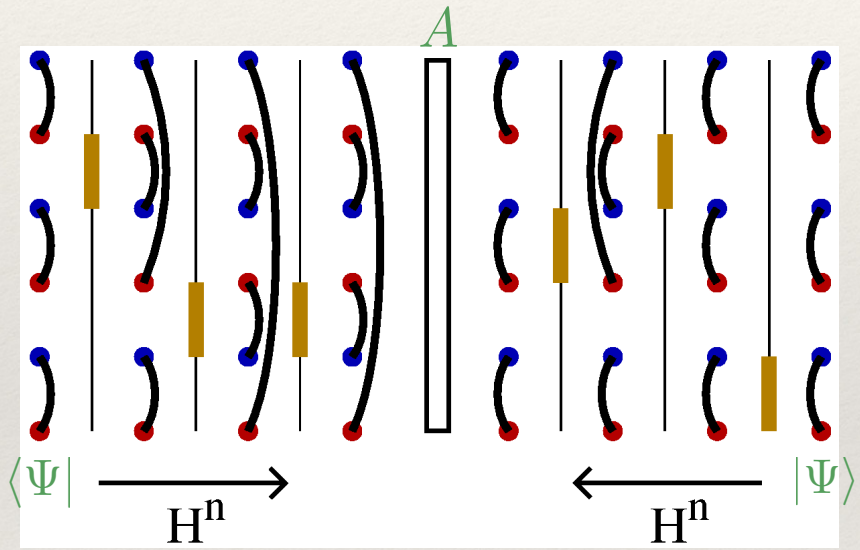
Loop updates in the valence-bond basis

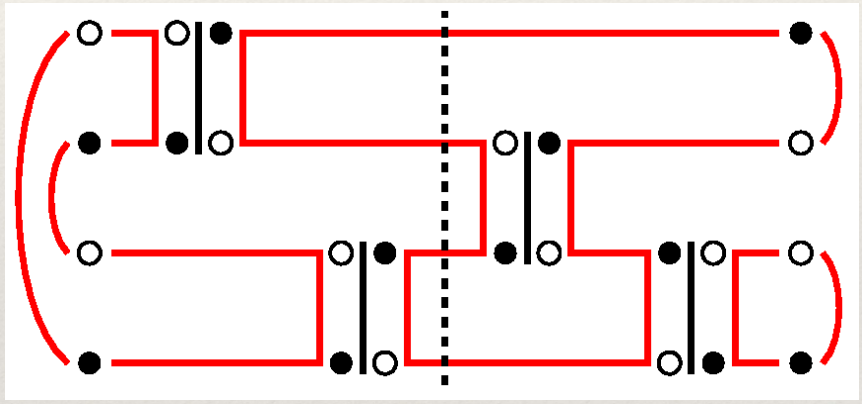
AWS and H. G. Evertz, PRB 2010

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



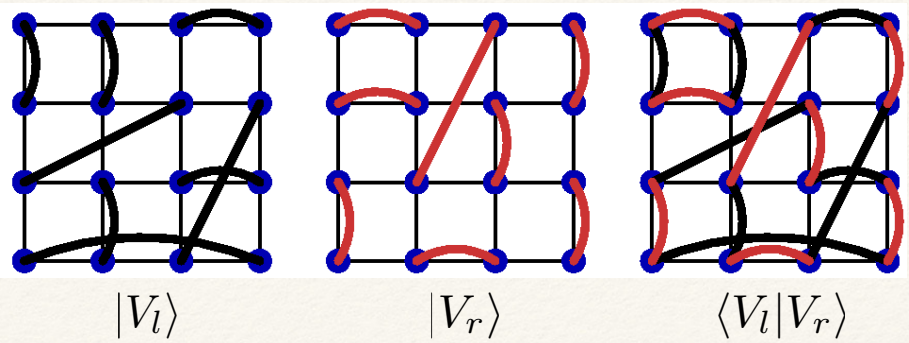


Loop updates similar to those in finite-T methods
(world-line and stochastic series expansion methods)

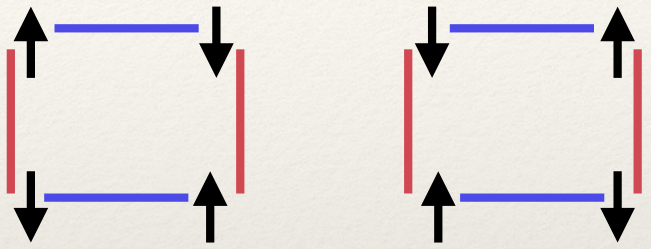
- good valence-bond trial wave functions can be used
- larger systems accessible
- sample spins, but measure using the valence bonds

Improved Valence-bond Estimators

The transition graphs give us improved estimators automatically



Put the spins back in:
- staggered spin configurations on each loop
- two 'orientations' (loop flips)



Average over all the two orientations of all the loops
- 2^{N_o} configurations -> determines overlap $\langle V_l|V_r\rangle = 2^{N_\circ - N/2}$

$$\langle M^2_{z,\mathrm{stagg}}\rangle = \frac{1}{4}\sum_{C=1}^{N_{\mathrm{clus}}}\langle n_C^2\rangle$$

Some off-diagonal operators can also be considered

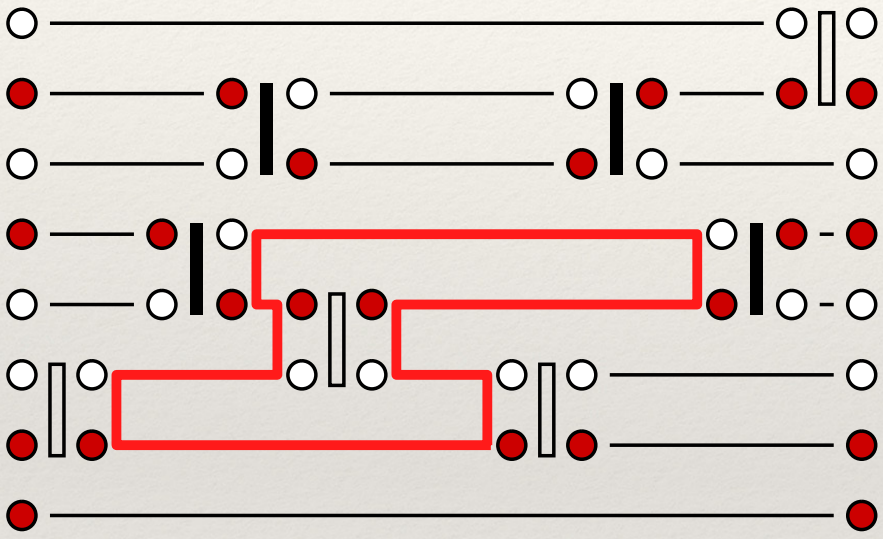
$$\frac{\langle V_l|\vec{S}_i\cdot\vec{S}_j|V_r\rangle}{\langle V_l|V_r\rangle} = \begin{cases} \frac{3}{4}(-1)^{x_i-x_j+y_i-y_j} & \text{(i,j in same loop)} \\ 0 & \text{(i,j in different loops)} \end{cases}$$

4-spin correlations depend on 2 loops, etc

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

Finite-temperature QMC
(world lines, SSE,...)

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

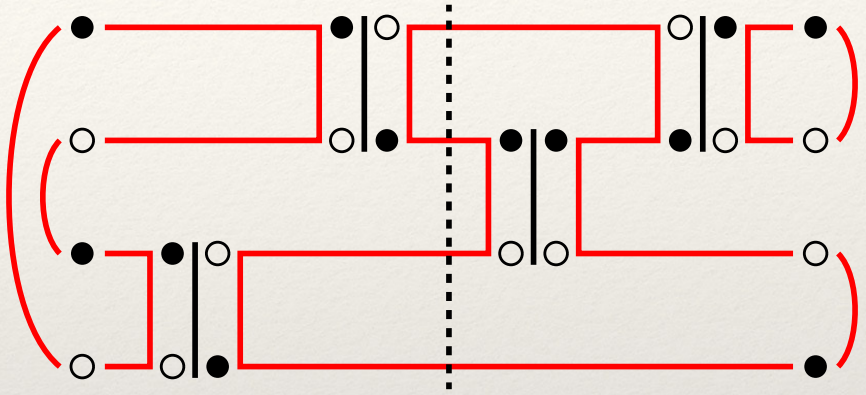


periodic time boundary conditions

- 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,...)

Convergence

Trial state expanded in H-eigenstates

$$|\psi_0\rangle = \sum_n c_n |n\rangle$$

Projected state after m-th power

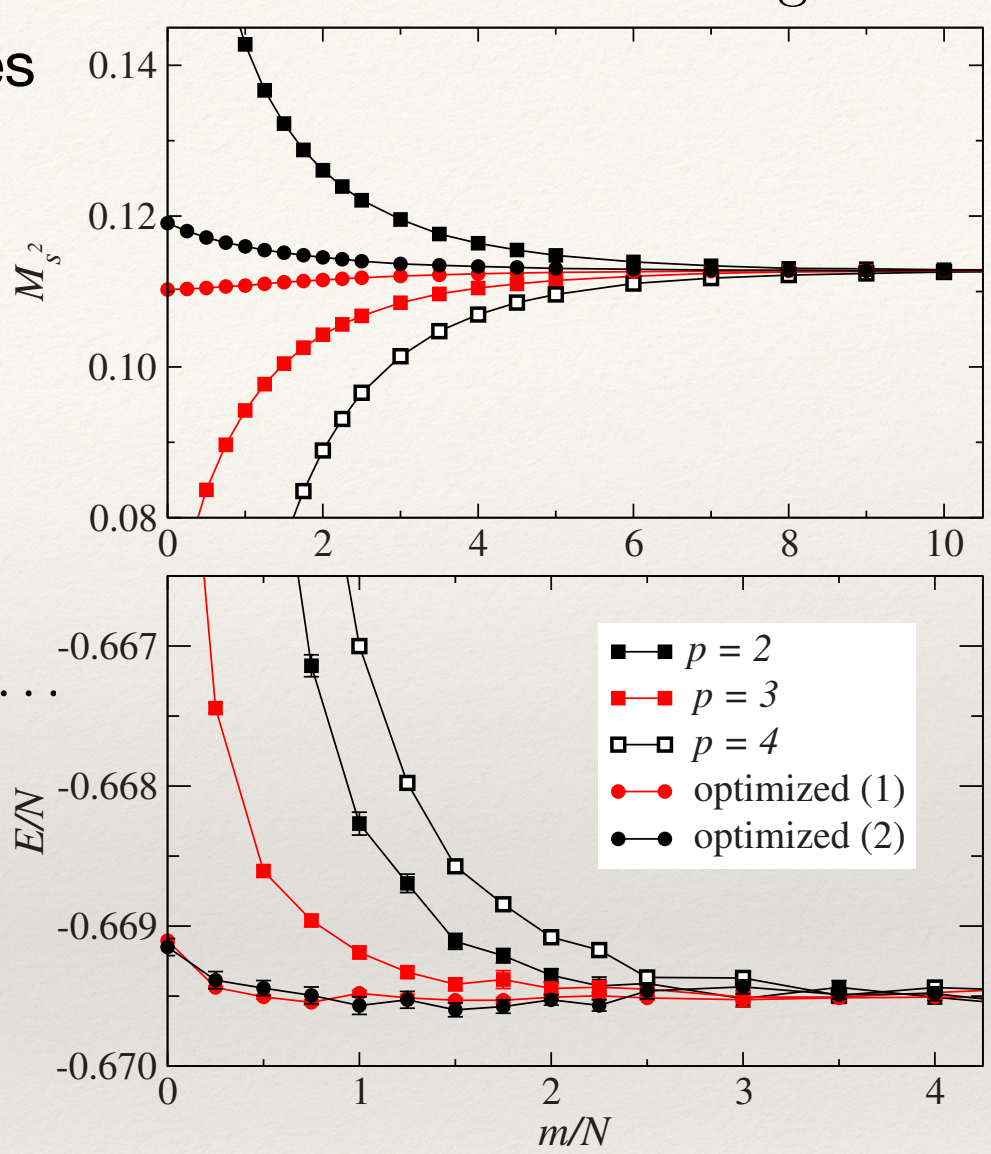
$$|\psi_m\rangle = H^m |\psi_0\rangle = \sum_n c_n E_n^m |n\rangle$$

Expectation value

$$\langle A\rangle_m = \langle 0|A|0\rangle + 2\langle 1|A|0\rangle \frac{c_1}{c_0}\left(\frac{E_1}{E_0}\right)^m + \dots$$

$$\langle A\rangle_m = \langle 0|A|0\rangle + c \times \exp\left(-\frac{m}{N}\frac{\Delta}{|e_0|}\right)$$

$$e_0 = E_0/M, \quad \Delta = E_1 - E_0$$

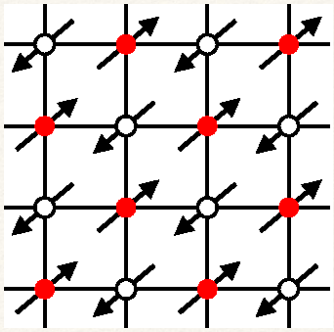


Conclusion:

- m/N >> e_0/Δ
- in valence-bond basis Δ is the singlet-singlet gap
- trial state also can have fixed momentum k=0 (e.g., ampl. product state)
  - only k=0 excited states (gap)

Results for 2D Heisenberg model

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



Sublattice magnetization

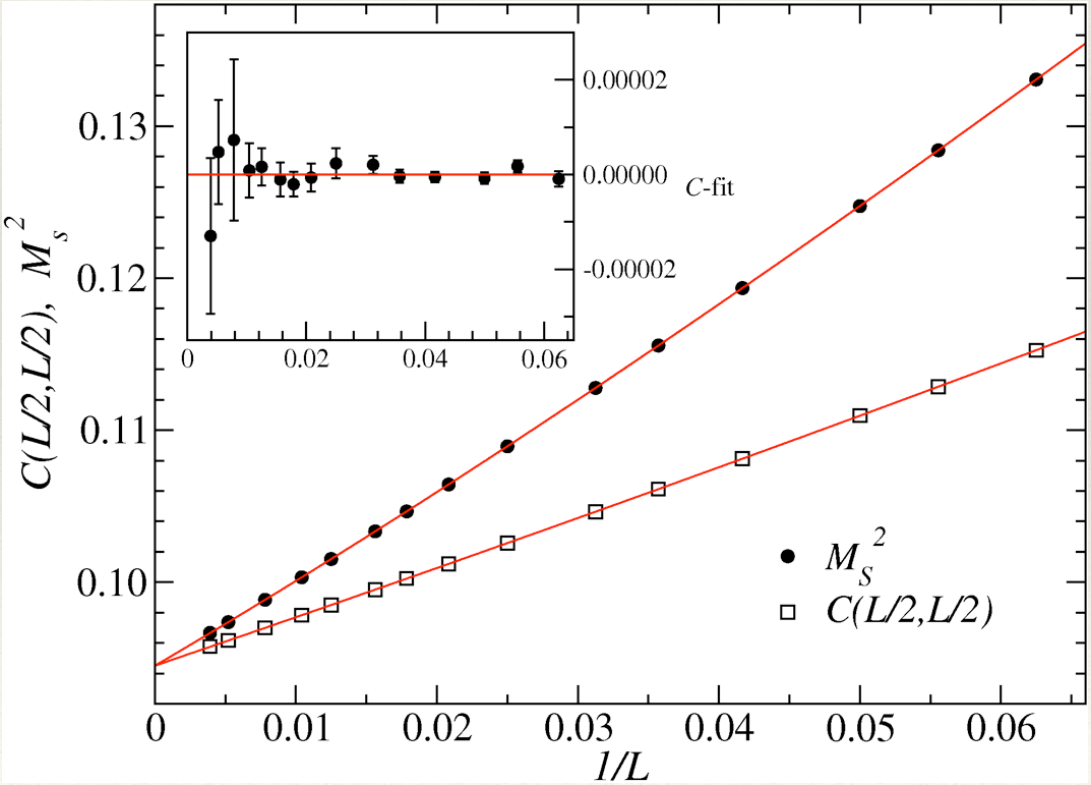
$$\vec{m}_s = \frac{1}{N} \sum_{i=1}^{N} \phi_i \vec{S}_i, \qquad \phi_i = (-1)^{x_i + y_i}$$

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

L×L lattices up to 256×256, T→0



Reger & Young (world-line) 1988

$$m_s = 0.30(2)$$

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

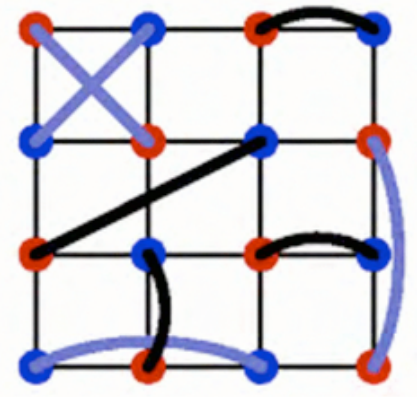
AWS & HG Evertz 2010

$$m_s = 0.30743(1)$$

Frustrated systems

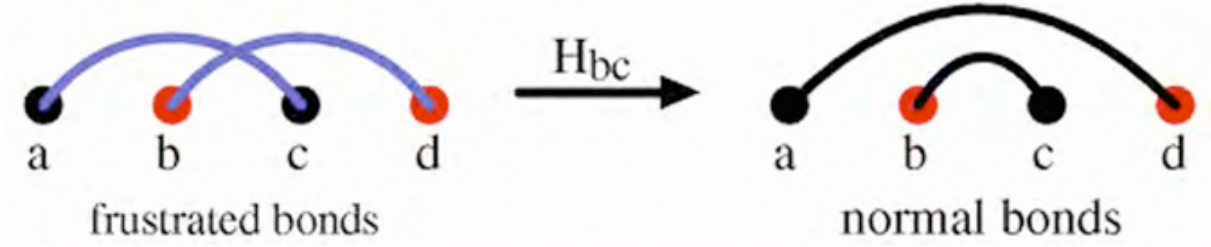
Consider the full valence-bond basis, including

- **normal bonds**, connecting A,B spins (sublattices)
- frustrated bonds, connecting A,A or B,B



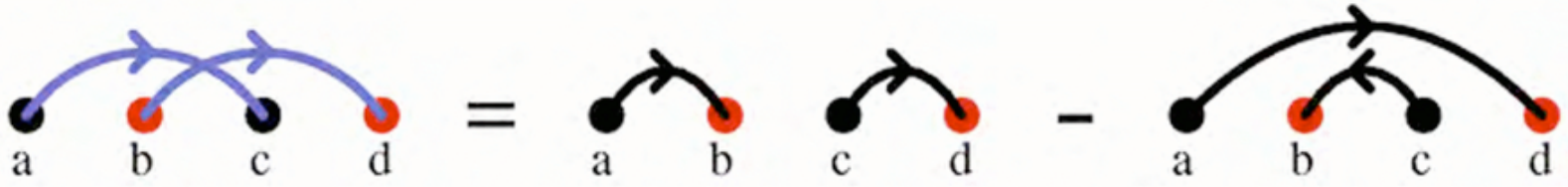
For a non-frustrated system

- projection eliminates frustarted bonds



For a frustrated system

- frustrated bonds remain and cause a sign problem
- frustrated bonds can be eliminated using over-completeness



In a simulation, one of the branches can be randomly chosen

- but there is a sign problem