ICTP School in Computational Condensed Matter Physics:
From Atomistic Simulations to Universal Model Hamiltonians
September 2015

Lecture 2
Ground-state projection of quantum spins in the valence bond basis

Anders W Sandvik, Boston University

Suggested reading: A. W. Sandvik, H. G. Evertz, Phys. Rev. B 82, 024407 (2010)

SIMONS FOUNDATION
Advancing Research in Basic Science and Mathematics

Lecture outline

- Basic principle of ground-state projection

- Properties of the valence-bond basis

- Projector QMC in the valence-bond basis

- Implementation for 2D S=1/2 Heisenberg antiferromagnet

- Valence-bond solids and spinons (1D system)

- Look at program if we have time

Projector QMC

Use an operator which "filters out" the ground state

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

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

"Trial state" (bad name) as expansion in eigenstates of H:

$$|\Psi_0\rangle = \sum_{n=0}^{M} c_n|n\rangle$$

assume c_0 not 0

- unless quantum numbers differ, hard for this not to be true
- can be a random state or in some way optimized state

$$H^m|\Psi_0\rangle = \sum_{n=0}^{M} c_n (E_n)^m |n\rangle$$

$$= a|0\rangle + b\sum_{n=1}^{M} c_n \left(\frac{E_n}{E_0}\right)^m |n\rangle \quad \to a|0\rangle \quad (m \to \infty)$$

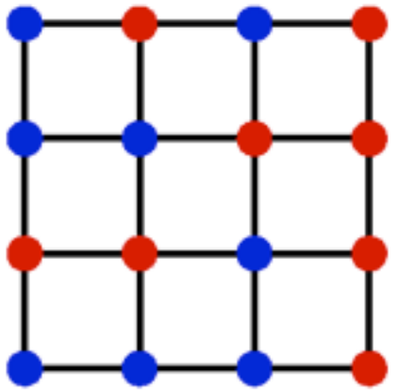
provided $|E_0| > |E_n|$ for all $n > 0$ (add constant if not true)

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

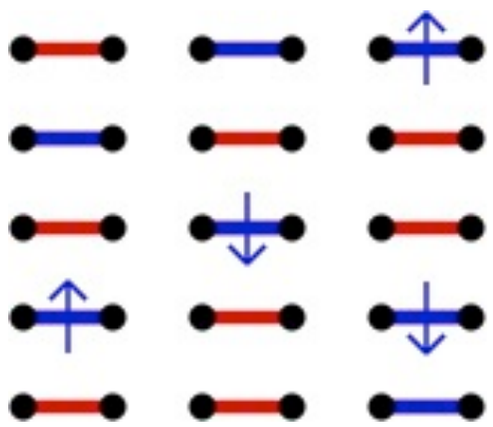


$$\bullet = |\uparrow\rangle = |S^z = +1/2\rangle$$

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

One can also use eigenstates of two or more spins

- dimer singlet-triplet basis



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

$$= |\uparrow\uparrow\rangle$$

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

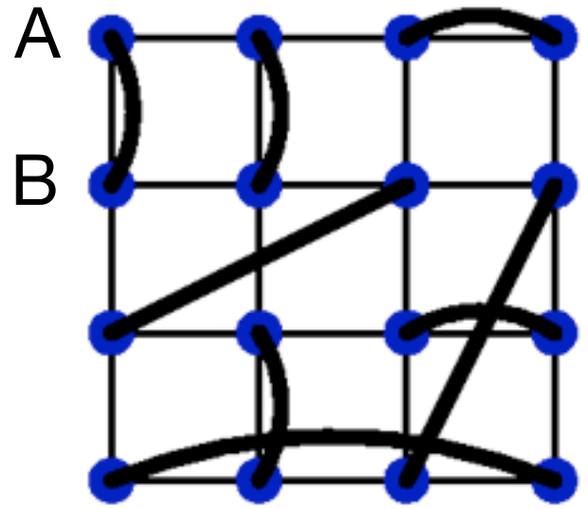
$$= |\downarrow\downarrow\rangle$$

The hamiltonian is more complicated in this basis

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

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

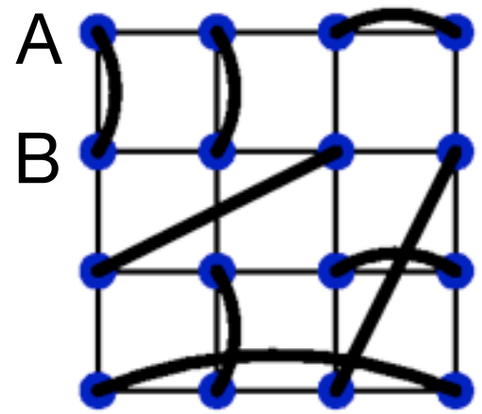
The valence bond basis is overcomplete and non-orthogonal

- expansion of arbitrary singlet state is not unique

$$|\Psi\rangle = \sum_r f_r |V_r\rangle$$

.... but in some cases, e.g., ground states of bipartite Heisenberg systems, f_r can be taken positive and is then unique

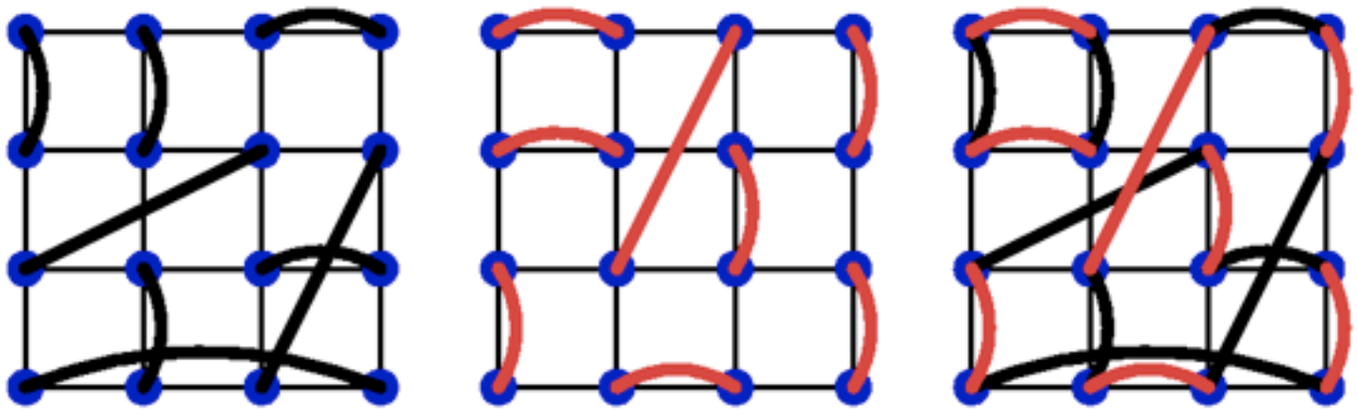
Properties of valence bond basis for S=1/2 spins



All valence bond states overlap with each other

$$\langle V_l | V_r \rangle = 2^{N_\circ - N/2}$$

$$N_\circ = \text{ number of loops in overlap graph}$$



overlap graph
or ***transition graph***

If we put spins back:
staggered spins on loops: ↓↑↓↑↓↑...
- 2 states per loop

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; Sorella et al. (1998); AWS, Phys. Rev. Lett 95, 207203 (2005)

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

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

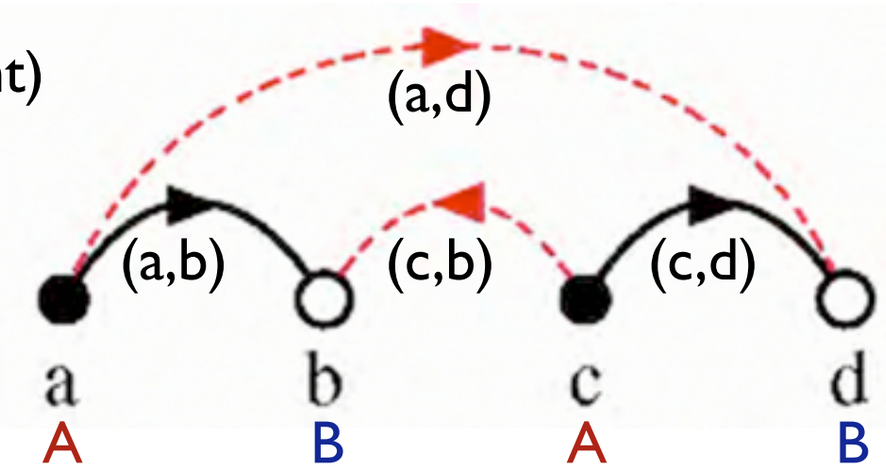
S=1/2 Heisenberg model

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

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

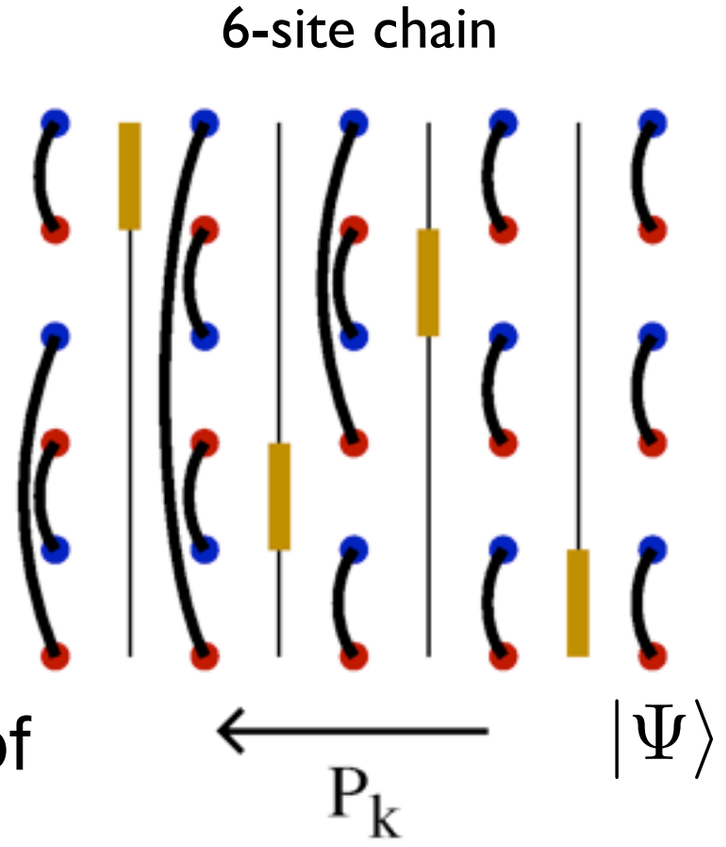
Sampling the wave function

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}

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

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

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

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....)

Calculating the energy

Using a state which has equal overlap with all VB basis states

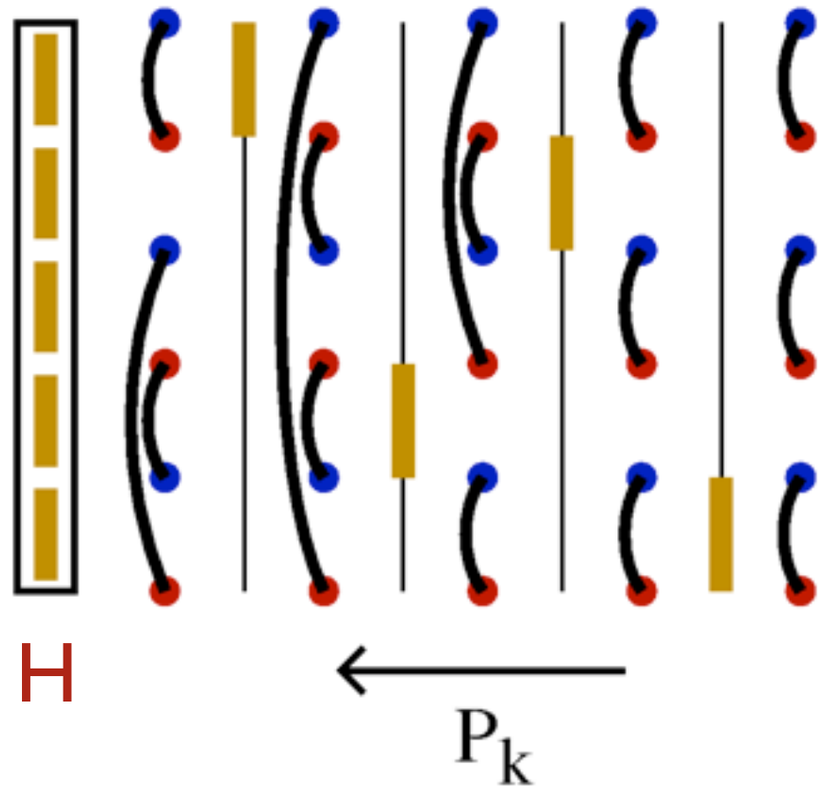
- e.g., the Neel state $|N\rangle$ $\quad\quad \langle N|V_r\rangle = (\sqrt{2})^{-N/2}$

$$E_0 = \frac{\langle N|H|0\rangle}{\langle N|0\rangle} = \frac{\sum_k \langle N|HP_k|V_r\rangle}{\sum_k \langle N|P_k|V_r\rangle}$$

H acts on the projected state

- n_f = number of bond flips
- n_d = number of diagonal operations

$$E_0 = -\langle n_d + n_f/2\rangle$$



General expectation values: $\langle A\rangle = \langle 0|A|0\rangle$

Strings of singlet projectors

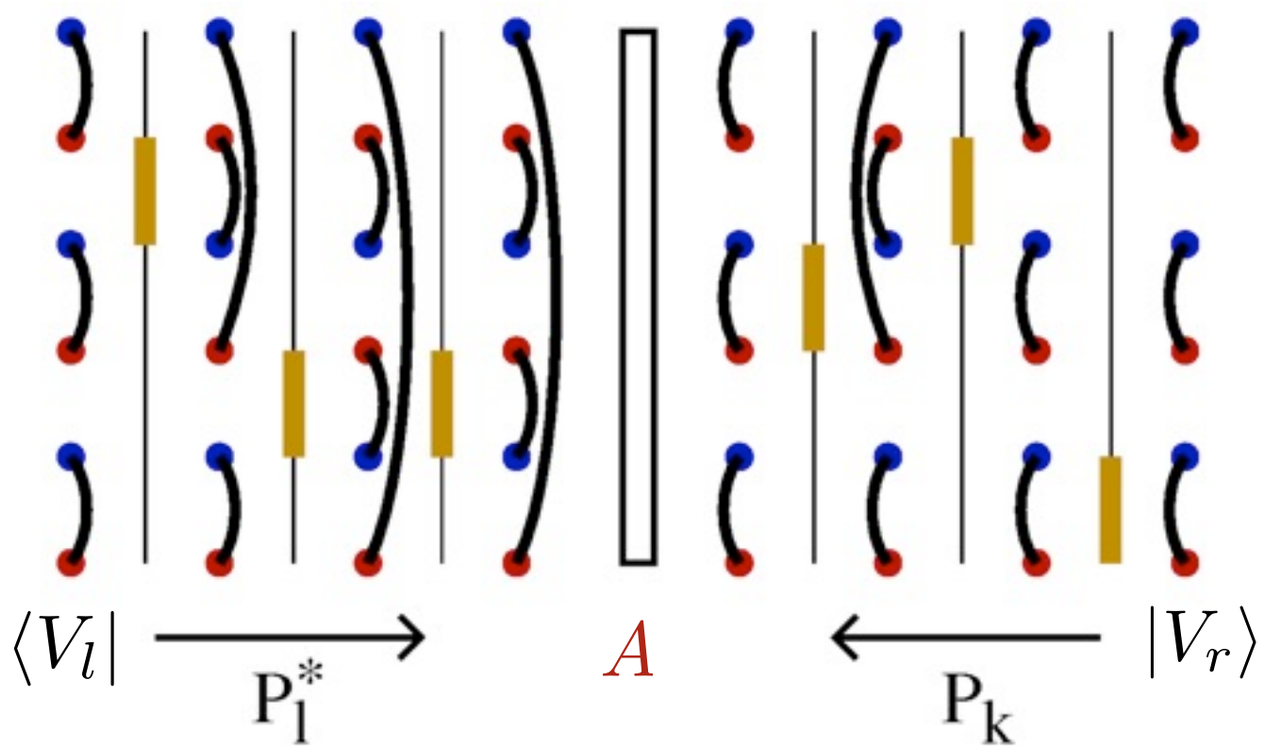
$$P_k = \prod_{p=1}^{n} H_{i_k(p)j_k(p)}, \quad k = 1, \ldots, N_b^n \quad (N_b = \text{number of interaction bonds})$$

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:



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

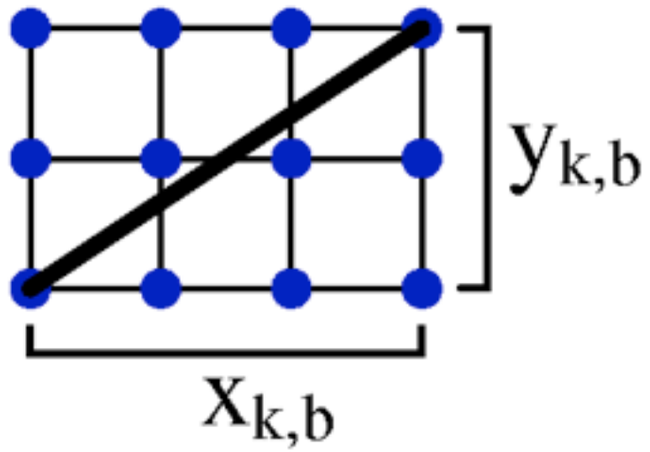
Monte Carlo sampling of operator strings

Sampling an amplitude-product state

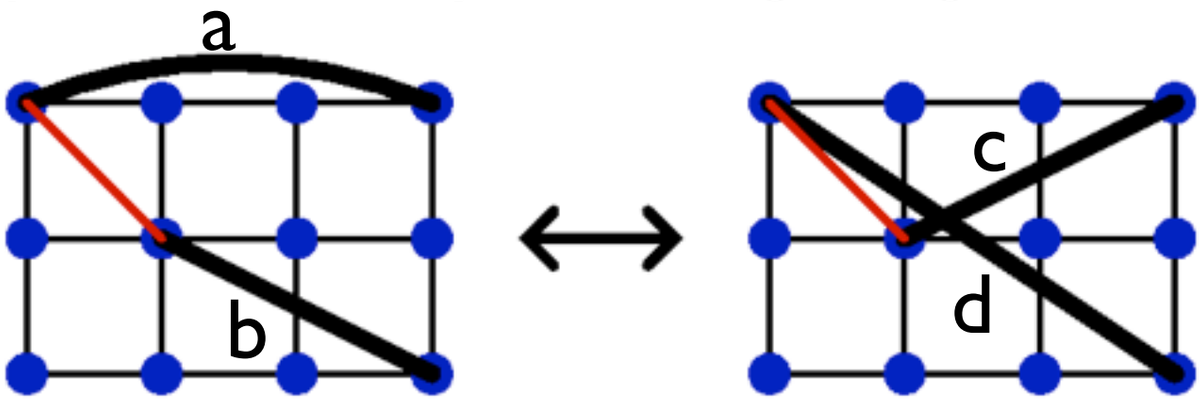
A better trial state leads to faster n convergence

- 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



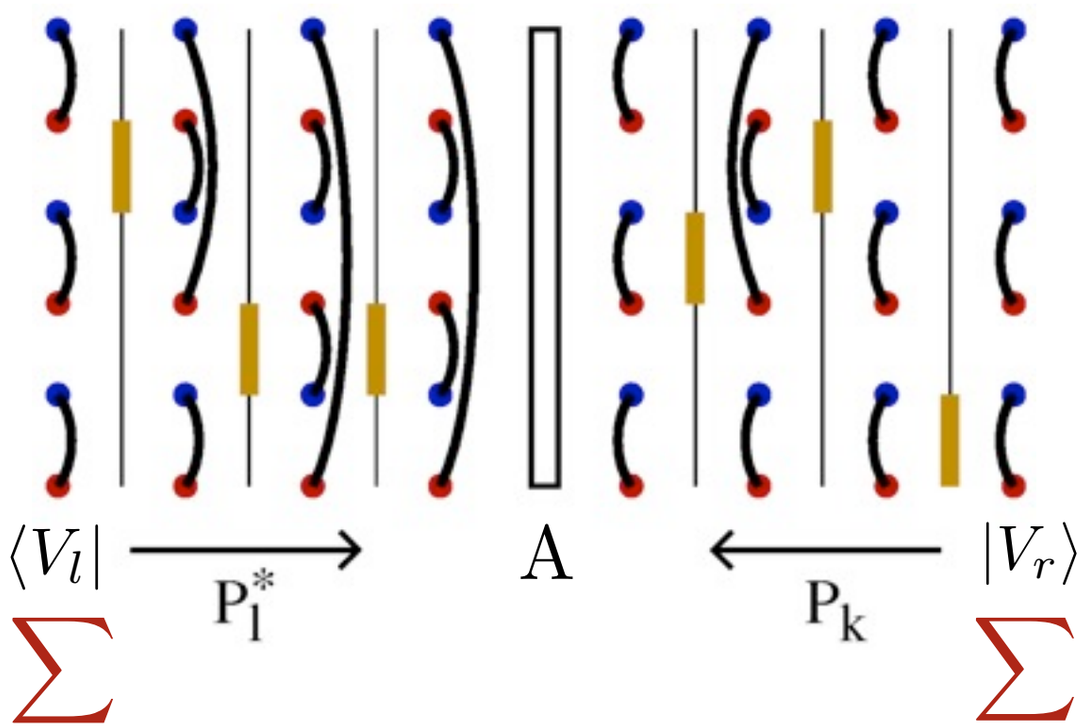
$$P_{\text{accept}} = \frac{h(x_c, y_c)h(x_d, y_d)}{h(x_a, y_a)h(x_b, y_b)}$$

If reconfiguration accepted

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

In principle we can:

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

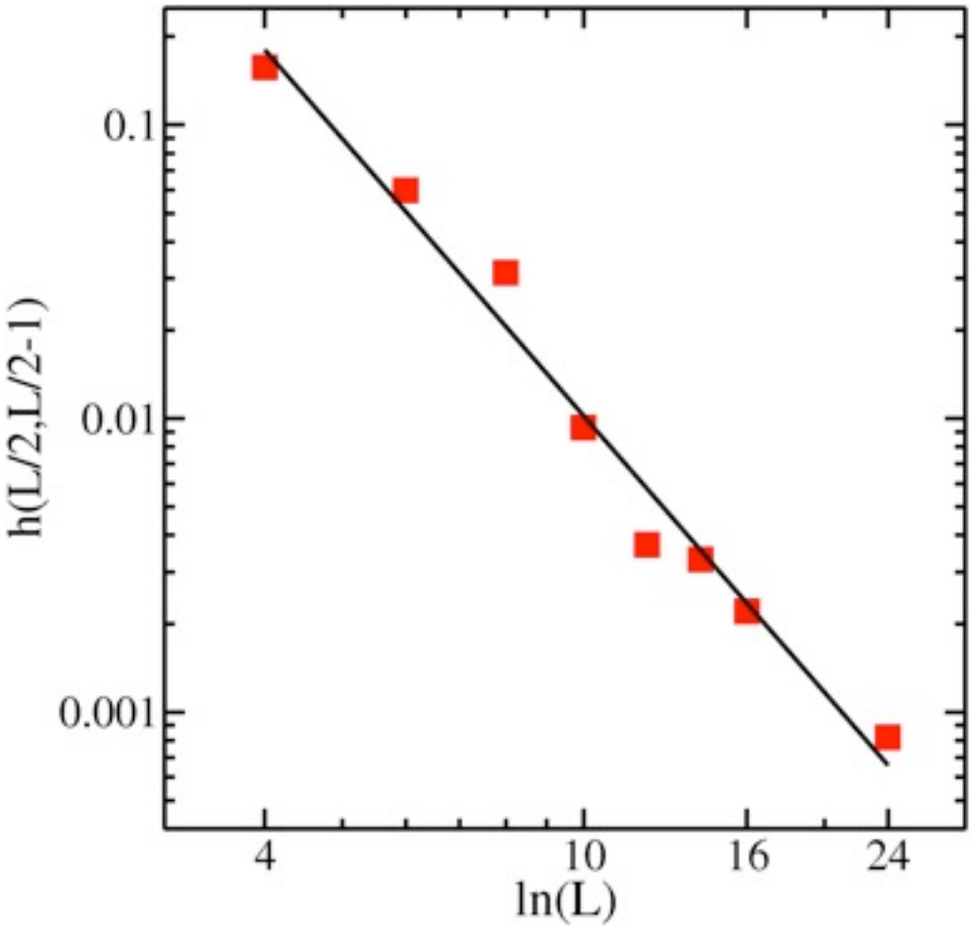


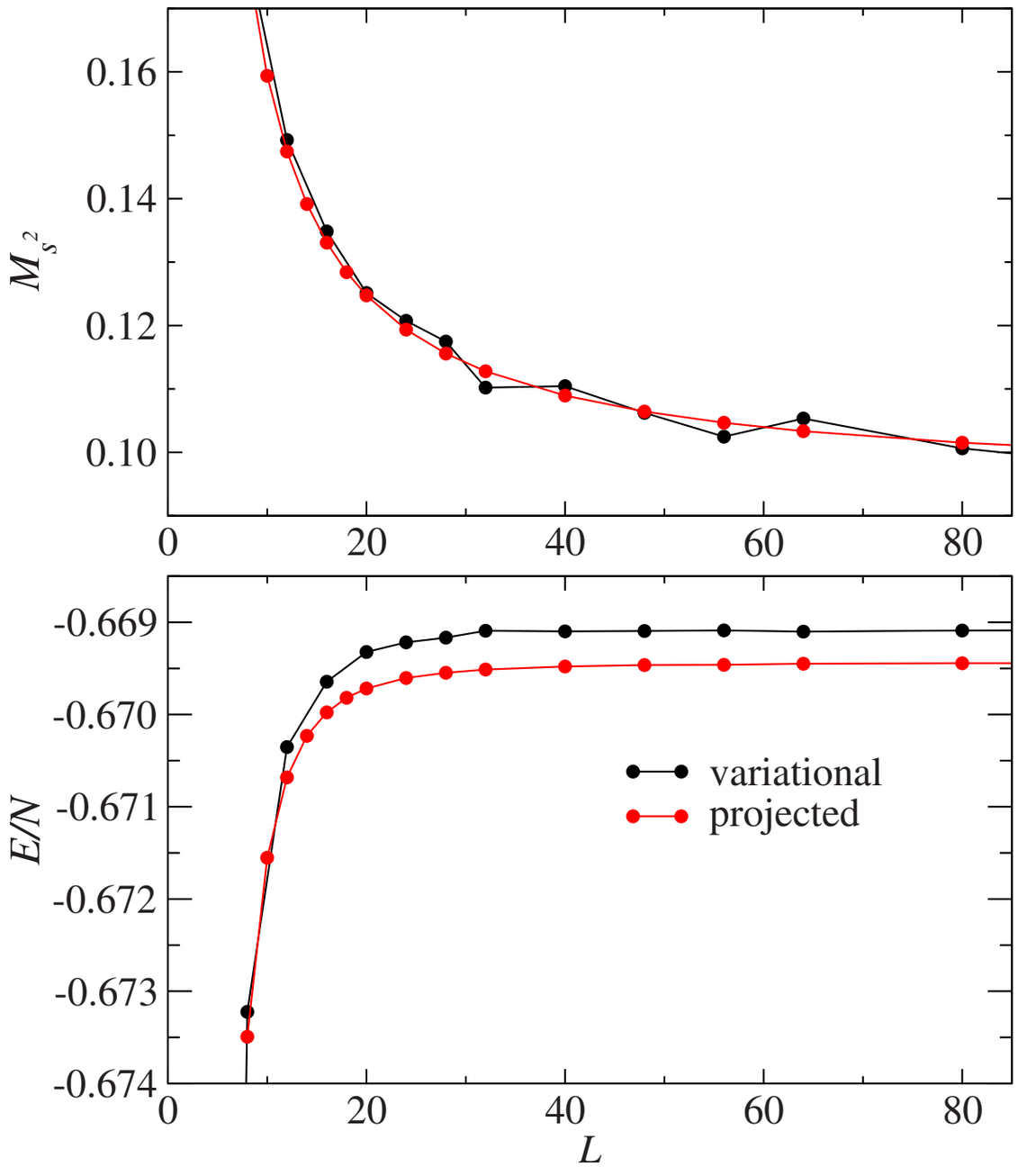
Variational wave function (2D Heisenberg)

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 $\sim 1/r^3$





More efficient ground state QMC algorithm → larger lattices

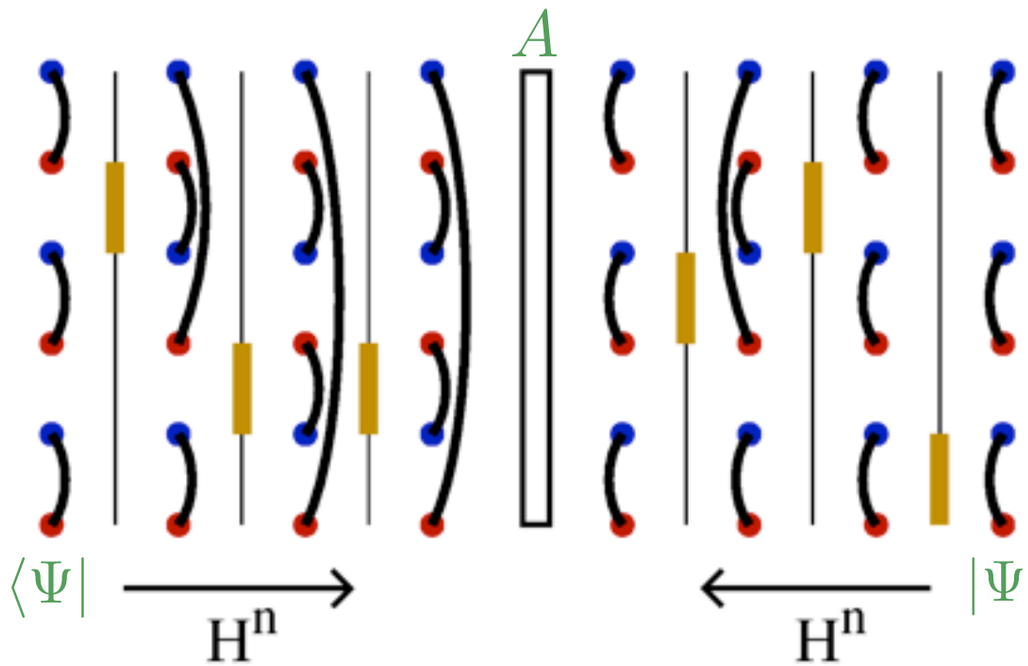
Loop updates in the valence-bond basis

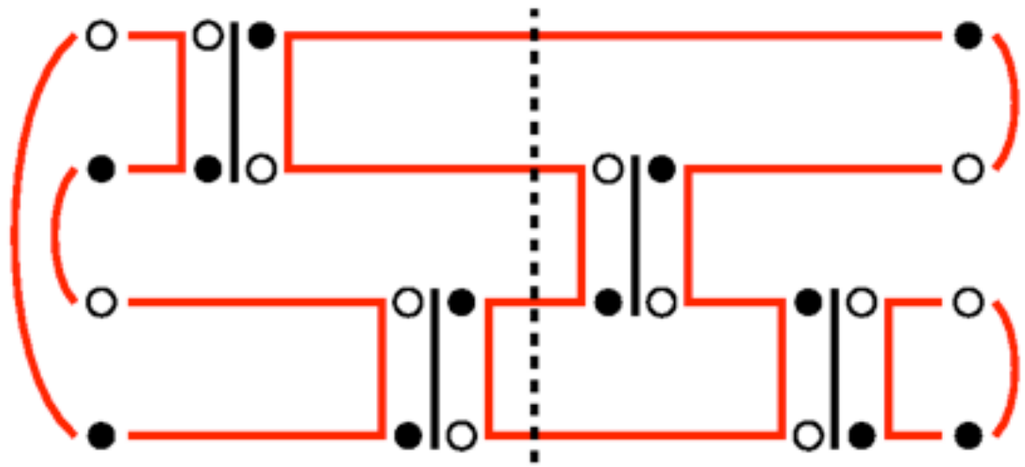
AWS and H. G. Evertz, PRB 2010

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 valence bonds (as before)

τ

$|V_\beta\rangle$

(graphs by Ying Tang)

$$\langle A\rangle = \frac{\langle\psi_1|(-H)^m A(-H)^m|\psi_2\rangle}{\langle\psi_1|(-H)^{2m}|\psi_2\rangle}$$

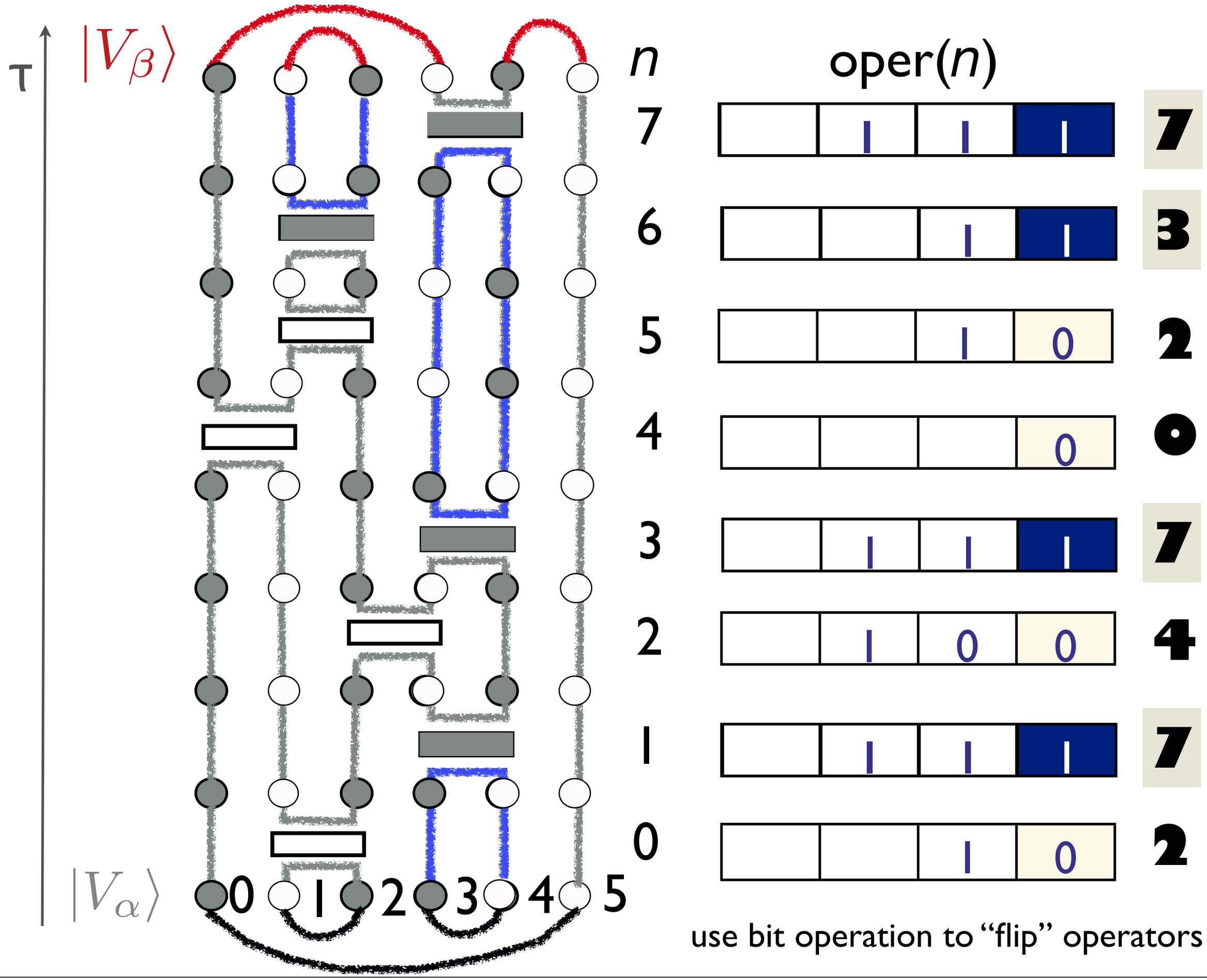
m

m

$\langle V'_\beta|V'_\alpha\rangle$

power m should be large enough to obtain ground state

$|V_\alpha\rangle$


τ
$|V_\beta\rangle$
$|V_\alpha\rangle$
0
1
2
3
4
5
n
oper(n)
7
I
I
I
7
6
I
I
3
5
I
0
2
4
0
0
3
I
I
I
7
2
I
0
0
4
1
I
I
I
7
0
I
0
2
use bit operation to “flip” operators

Convergence

Trial state expanded in H-eigenstates

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

Projected state after m-th power

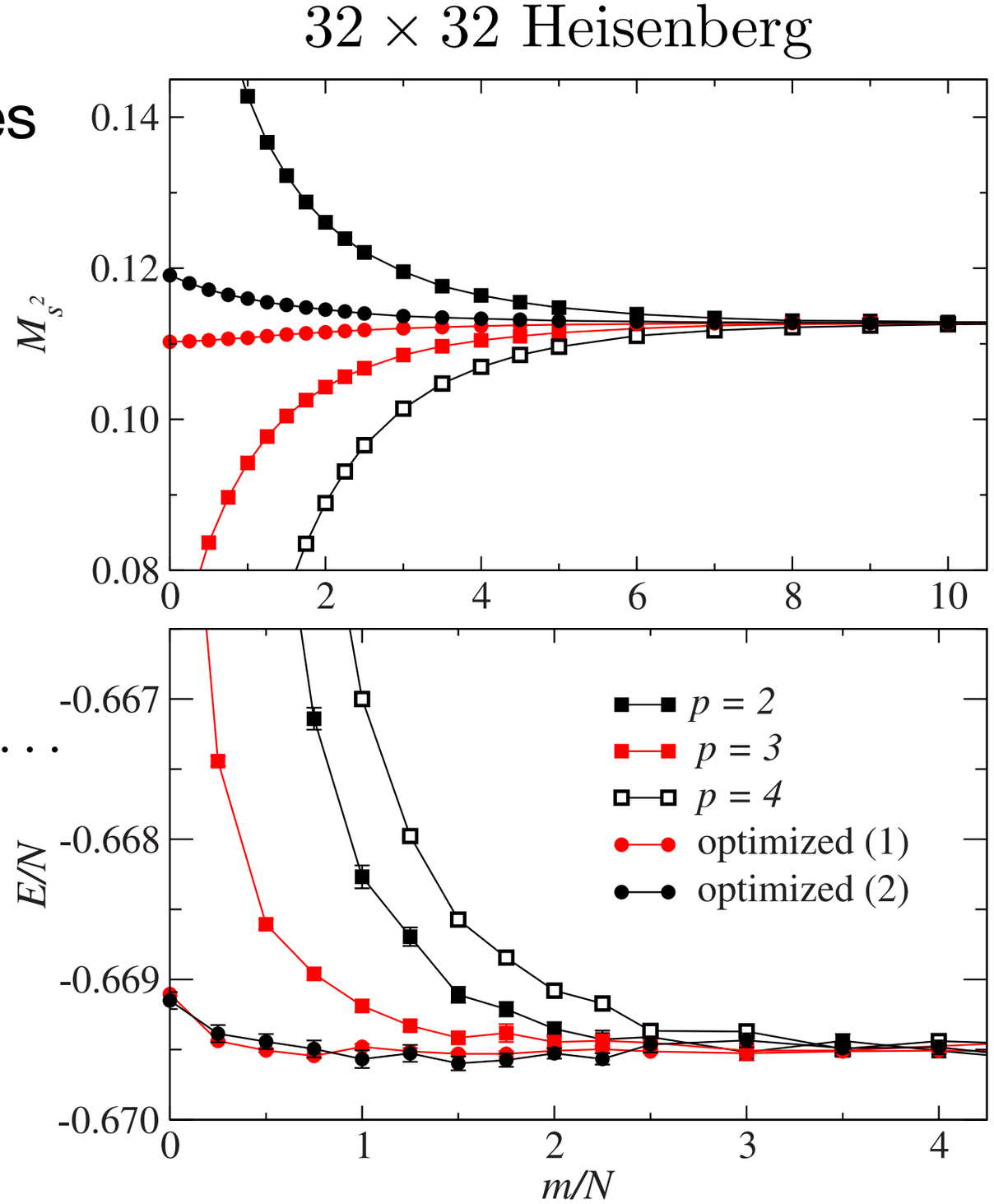
$$|\psi_m\rangle = H^m |\psi_0\rangle = \sum_n c_n E_n^m |n\rangle$$

Expectation value

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

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

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



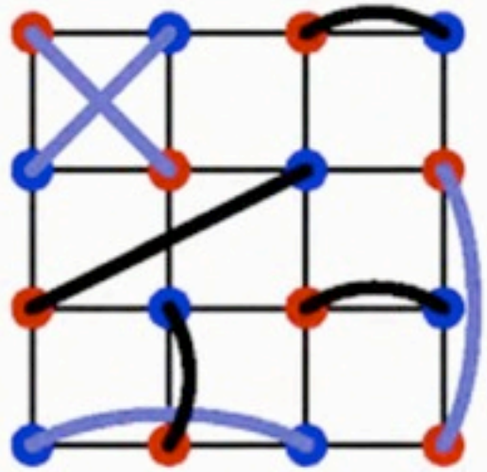
Conclusion:

- 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)

Frustrated systems

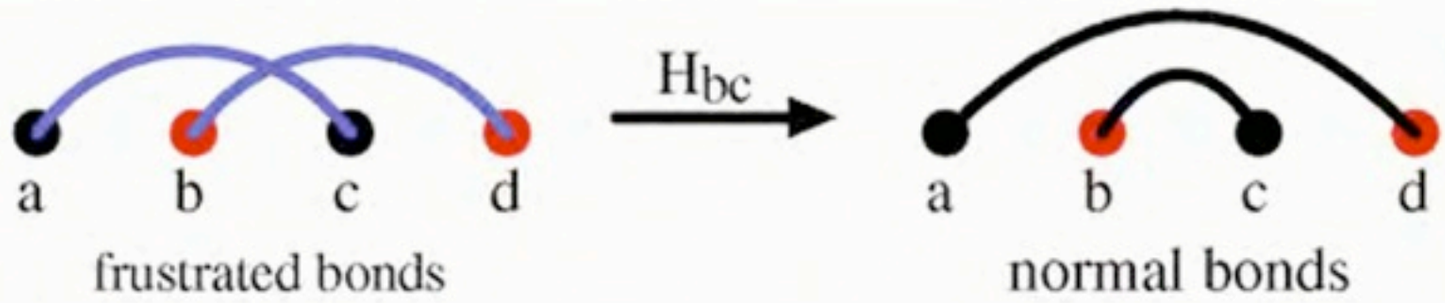
Consider the full valence-bond basis, including

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



For a non-frustrated system

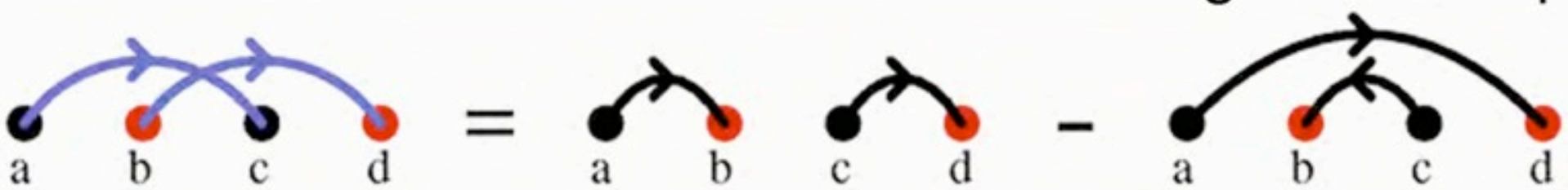
- projection eliminates frustarted bonds



frustrated bonds normal 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

VBS states from multi-spin interactions

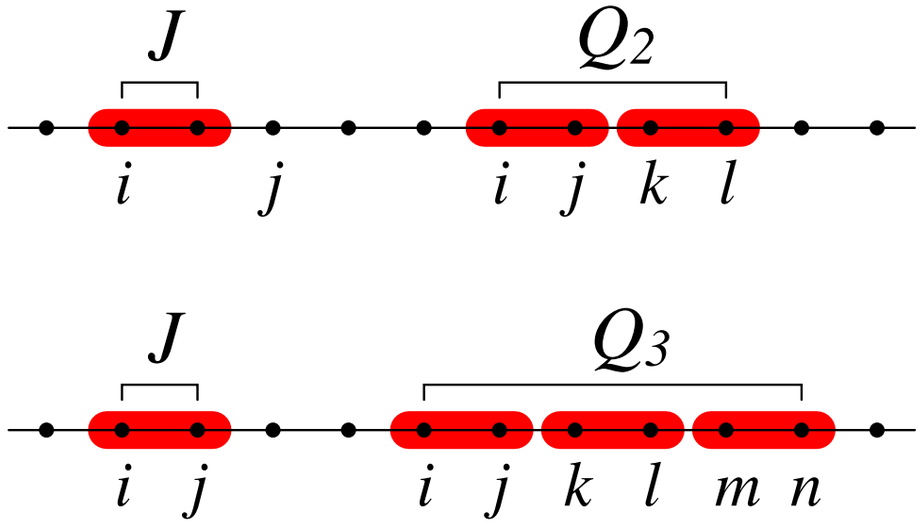
Sandvik, Phys. Rev. Lett. 98, 227202 (2007)

The Heisenberg interaction is equivalent to a singlet-projector

$$C_{ij} = \frac{1}{4} - \vec{S}_i \cdot \vec{S}_j$$

$$C_{ij}|\phi^s_{ij}\rangle = |\phi^s_{ij}\rangle, \qquad C_{ij}|\phi^{tm}_{ij}\rangle = 0 \quad (m = -1, 0, 1)$$

- we can construct models with products of singlet projectors
- no frustration in the conventional sense (QMC can be used)
- correlated singlet projection reduces antiferromagnetic order/correlations

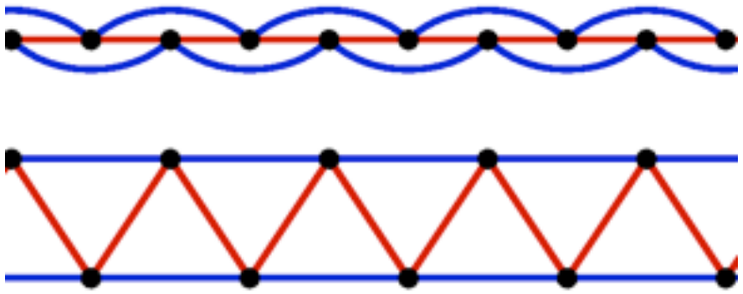


including all translations
- H is translationally invariant

$$H = -J \sum_{\langle ij \rangle} C_{ij} - Q_2 \sum_{\langle ijkl \rangle} C_{ij} C_{kl}$$

The J-Q chains have the same critical-VBS transition as the J_1-J_2 Heisenberg chain!
- Heisenberg SSE and projector codes can be easily adapted to Q-terms

S=1/2 Heisenberg chain with frustrated interactions (J_1-J_2 chain)



$= J_1$

$= J_2$

Different types of ground states, depending on the ratio **$g=J_2/J_1$** (both >0)

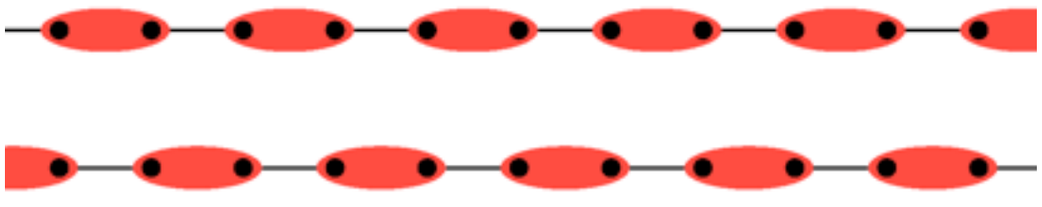
- **Antiferromagnetic "quasi order" (critical state) for g<0.2411...**
  - exact solution - Bethe Ansatz - for $J_2=0$
  - bosonization (continuum field theory) approach gives further insights
  - spin-spin correlations decay as 1/r

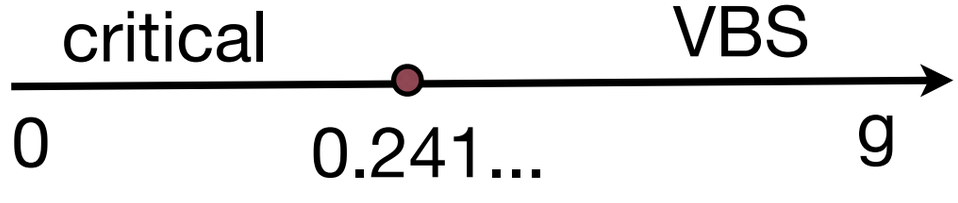
$$C(r) = \langle \vec{S}_i \cdot \vec{S}_{i+r} \rangle \sim (-1)^r \frac{\ln^{1/2}(r/r_0)}{r}$$

  - gapless spin excitations ("spinons", not spin waves!)
- **VBS order for g>0.2411... the ground state is doubly-degenerate state**
  - gap to spin excitations; exponentially decaying spin correlations

$$C(r) = \langle \vec{S}_i \cdot \vec{S}_{i+r} \rangle \sim (-1)^r \mathrm{e}^{-r/\xi}$$

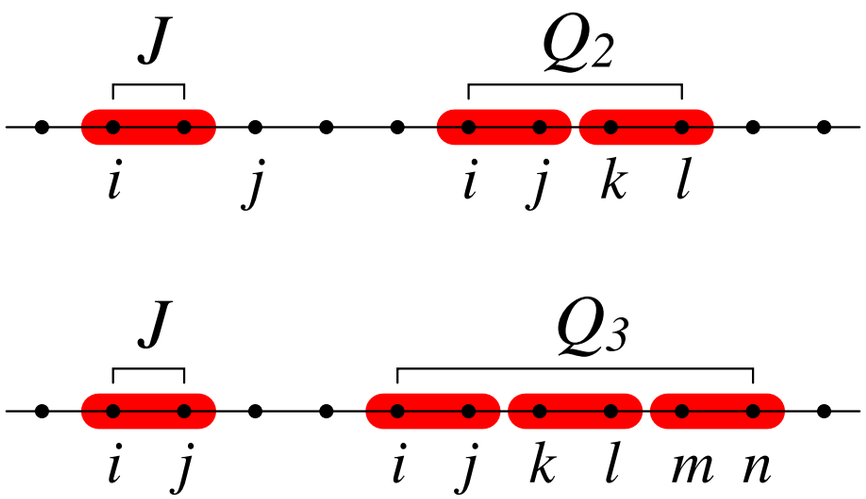
  - singlet-product state is exact for g=1/2 (Majumdar-Gosh point)

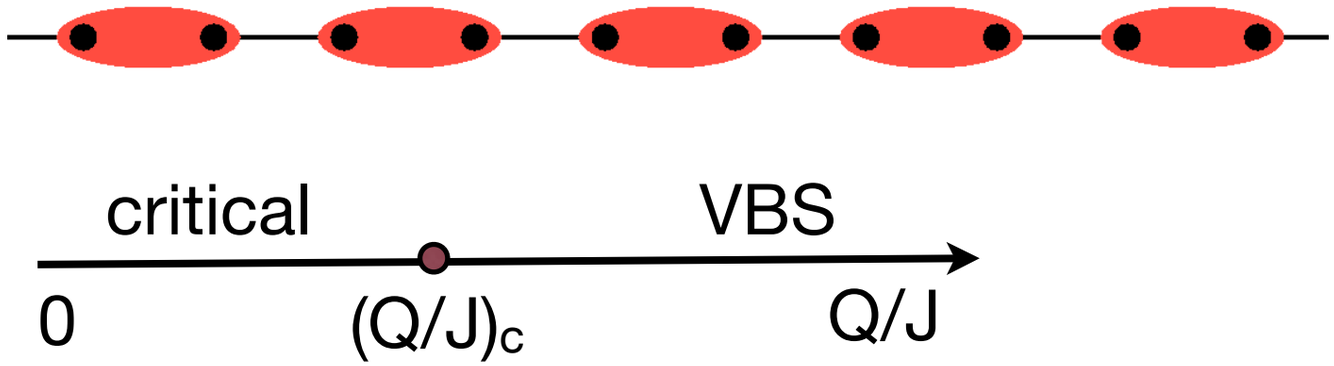




VBS state in J-Q chains

Y. Tang and AWS, PRL (2011)
S. Sanyal, A. Banerjee, and K. Damle, PRB (2011)





"dimer" operator: $B_i = \vec{S}_i \cdot \vec{S}_{i+1}$

In a symmetry-broken VBS: $\langle B_i \rangle = a + \delta(-1)^i$

In a finite system in which the symmetry is not broken: $\langle B_i \rangle = 0$

- detect VBS with dimer correlation function

$$D(r) = \frac{1}{N} \sum_{i=1}^{N} \langle B_i B_{i+r} \rangle$$

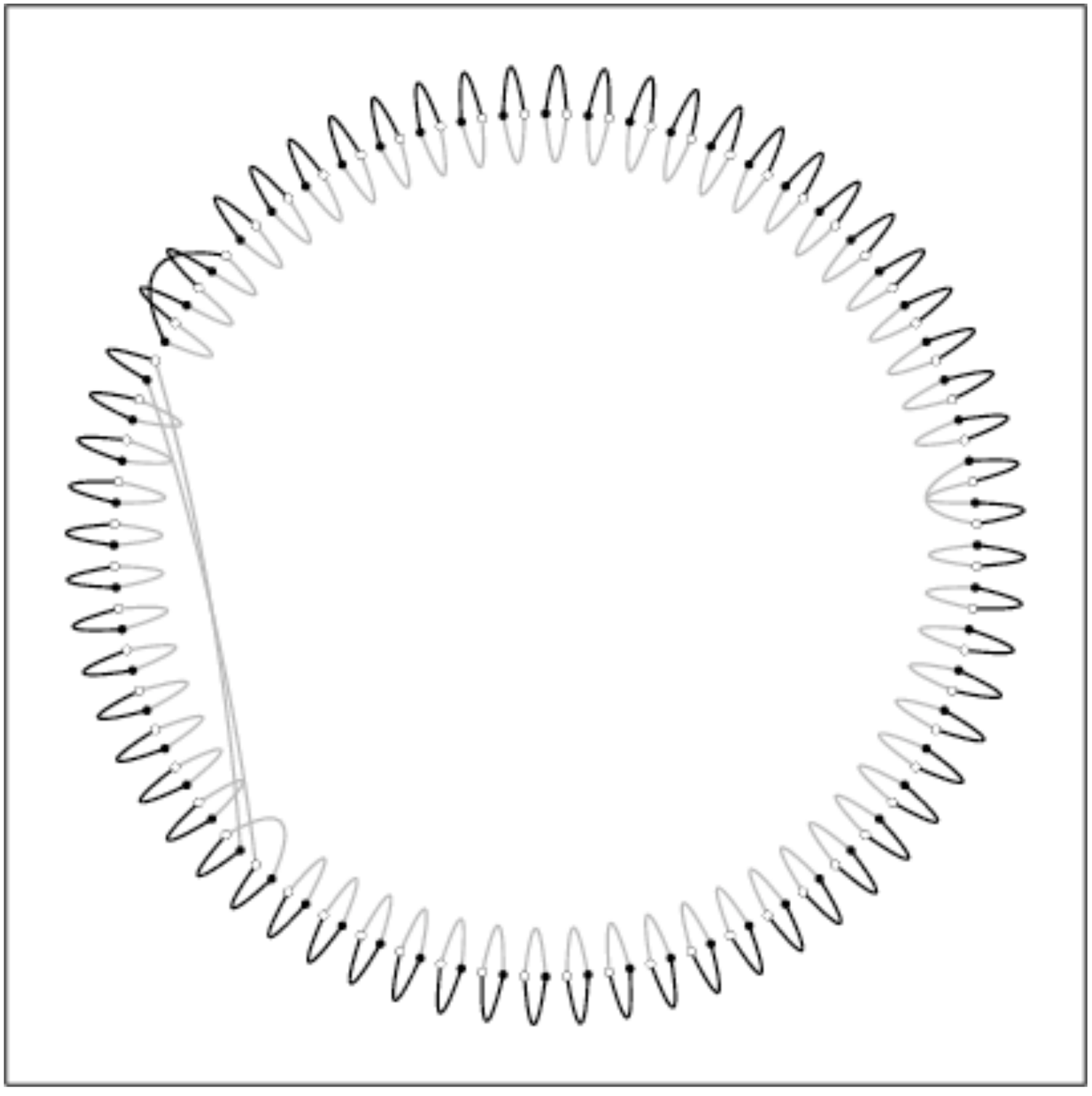
This is a 4-spin correlation function

- can be evaluated using the transition graphs (1- and 2-loop contributions)

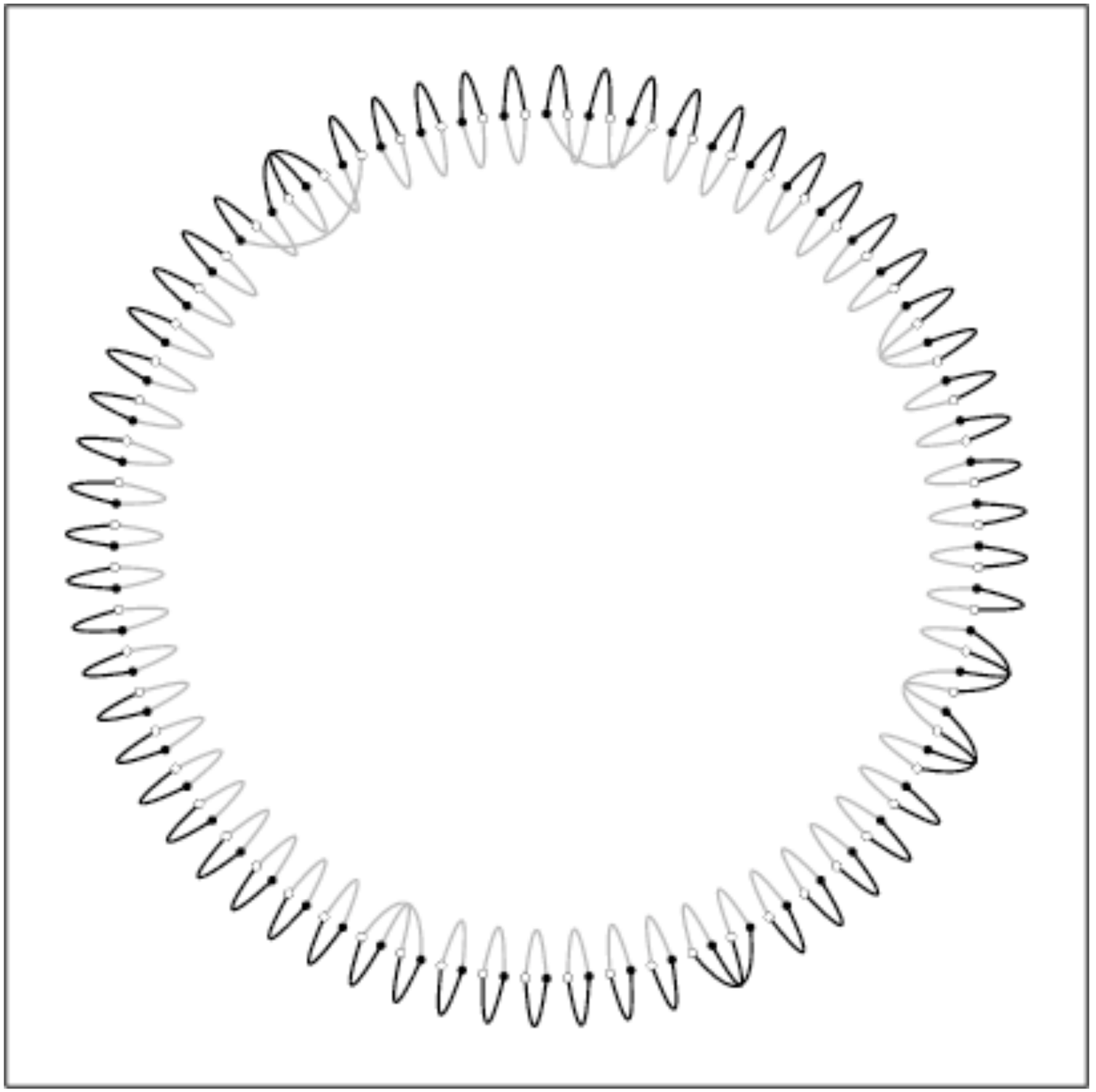
Animation of the projected states - transition graph

Animations by Ying Tang

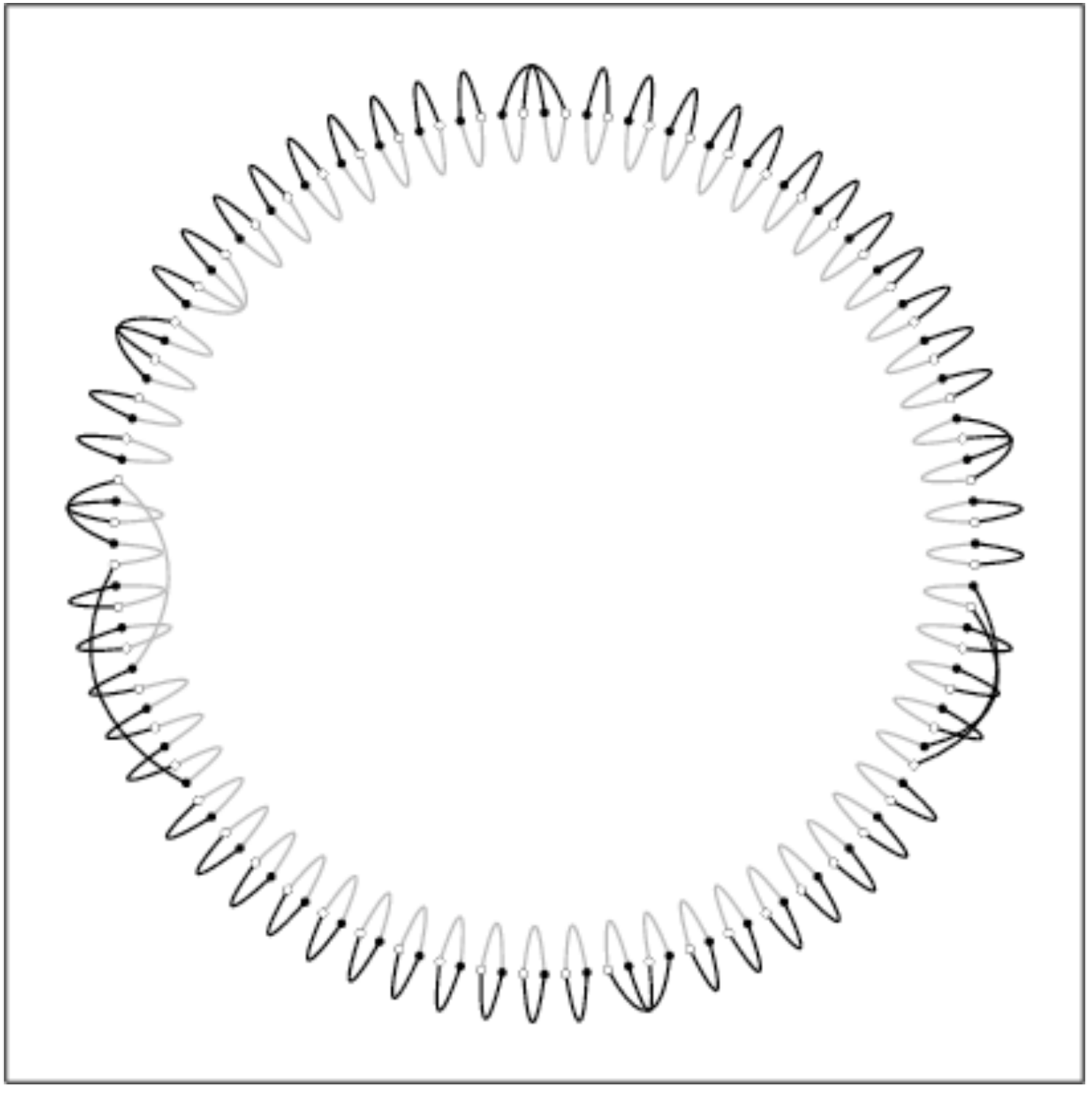
$J = 0$



$J/Q = 0.5$



$$J/Q = (J/Q)_c \approx 6$$

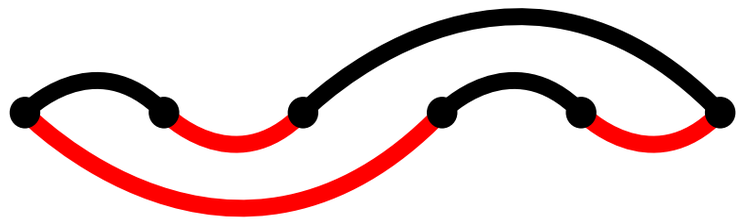


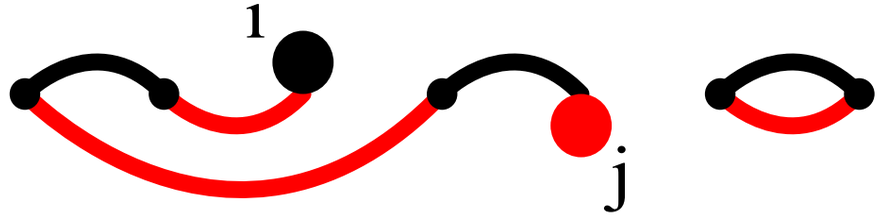
Extended valence-bond basis for S>0 states

Consider $S^z=S$

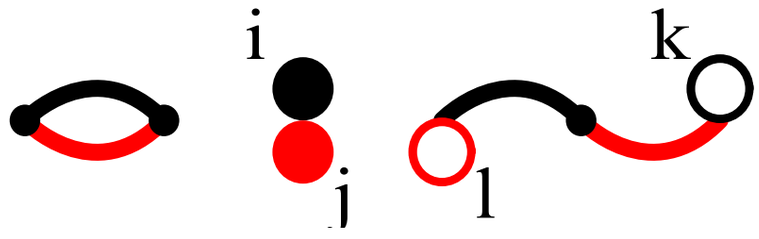
- for even N spins: N/2-S bonds, 2S unpaired “up” spins
- for odd: (N-2S)/2 bonds, 2S upnpaired spins

- transition graph has 2S open strings

$S = 0$  $<V_\beta|V_\alpha>$

$S = 1/2$ 

$<V_\beta(j)|V_\alpha(i)>$

$S = 1$ 

$<V_\beta(j,l)|V_\alpha(i,k)>$

Overlaps and matrix elements involve loops and strings

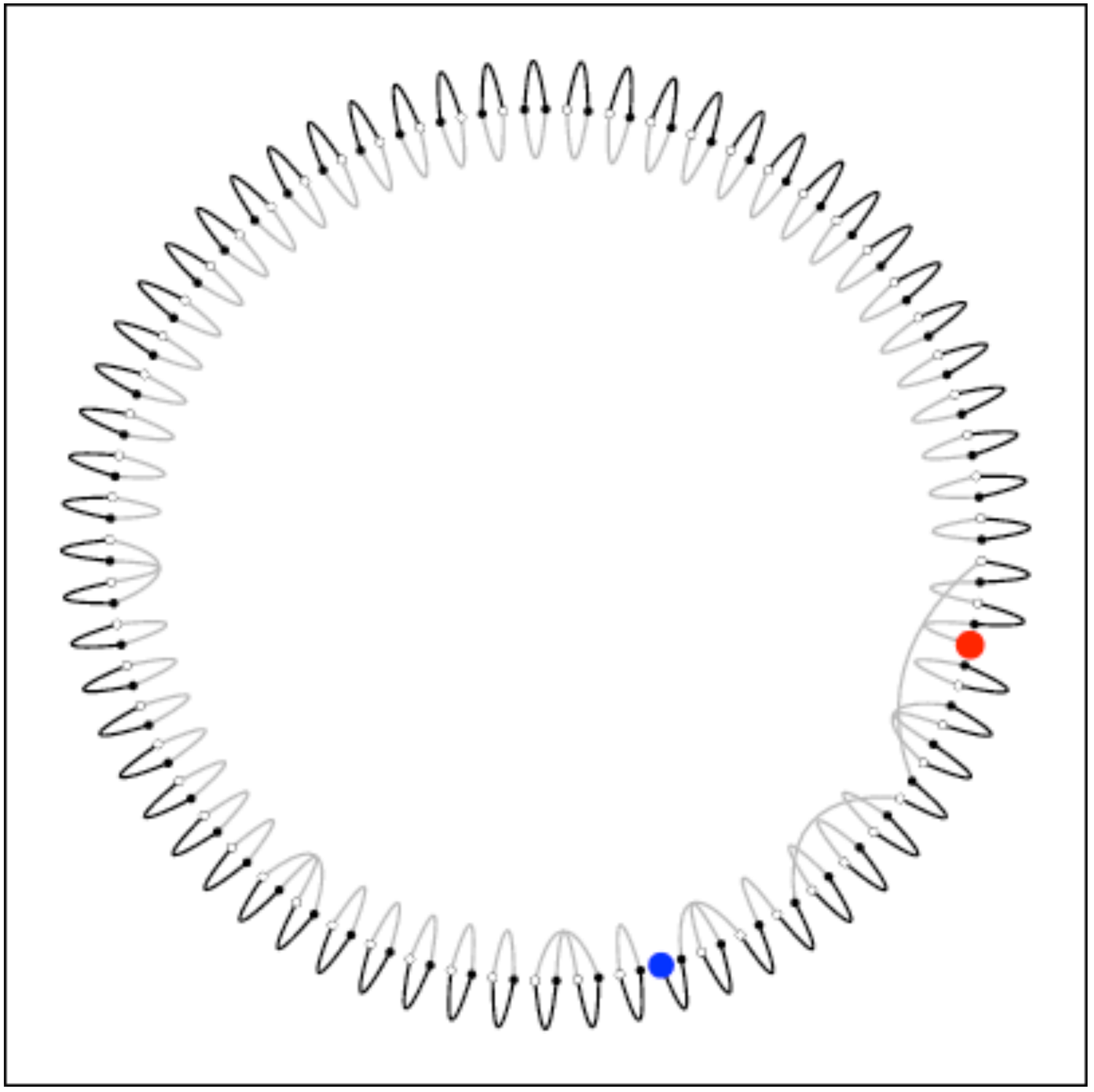
- very simple generalizations of the S=0 case
- loops have 2 states, strings have 1 state

Spinons in 1D: a single spinon in odd-N J-Q_3 model

- one spin (spinon) doesn't belong to any bond
- bra and ket spinons at different locations; non-orthogonality

The distance between the bra and ket spins can be used to define the size of a spinon

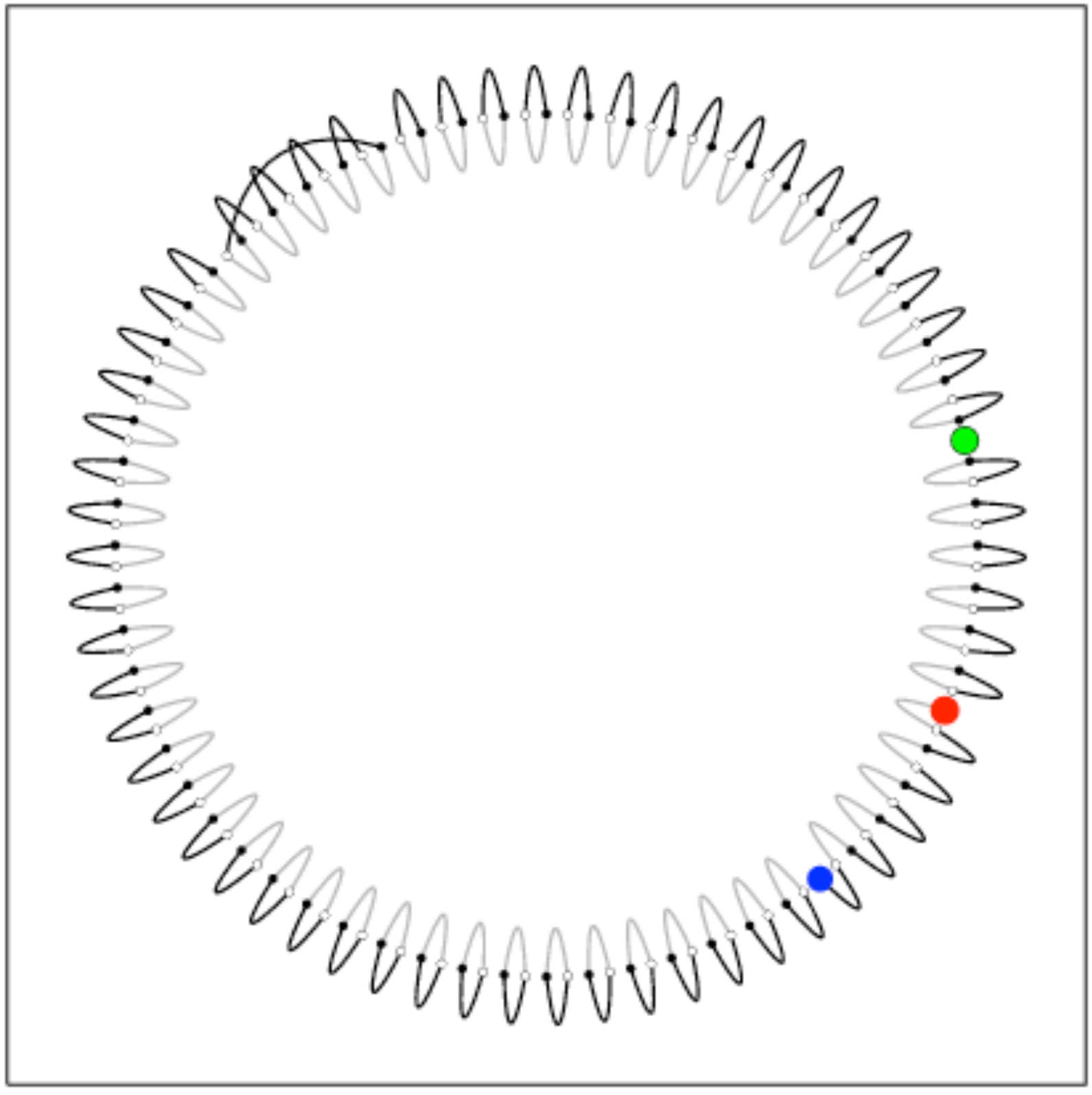
- the spinon is not just the unpaired spin



Y. Tang and AWS, Phys. Rev. Lett. 107, 157201 (2011)

Two spinons in 1D VBS are deconfined (no confining potential)

- 2 separated (deconfined) sets of bra/ket spinons



Basic projector code (Fortran90) available on-line:

https://physics.bu.edu/~sandvik/trieste15/

Simulation of the 2D Heisenberg model with N=Lx*Ly spins
- periodic boundary conditions
- Ly=1 for a chain (only x-periodic)
- Ly=2 for a 2-leg ladder (only x-periodic)

Calculates:
- spin correlation function along x direction