Quantum Monte Carlo Simulations in the Valence Bond Basis

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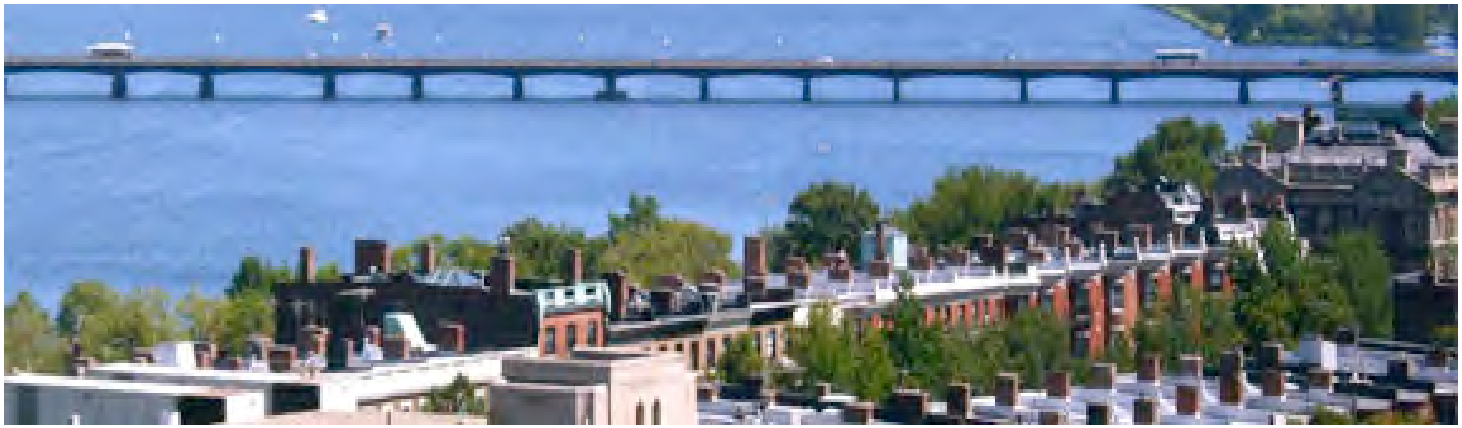

Outline

- The valence bond basis for S=1/2 spins
- Projector QMC in the valence bond basis
- Heisenberg model with 4-spin interactions
- The valence bond basis for frustrated systems

Papers

- A. S., Phys. Rev. Lett. 95, 207203 (2005)
- K. Beach and A. S., Nucl. Phys. B 750, 142 (2006)

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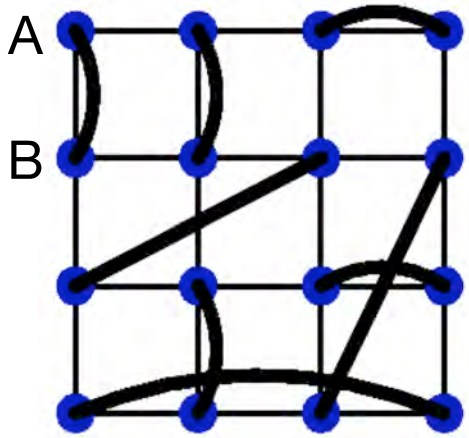
WHERE DISCOVERIES BEGIN

The valence bond basis for S=1/2 spins

- Dates back to the 1930s; Pauling, Romer, Hulthen...
- Spans the singlet space



Consider N (even) spins
- divide into 2 groups; A and B
- e.g., sublattices (not necessarily)
- bonds from A sites to B sites; singlets

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

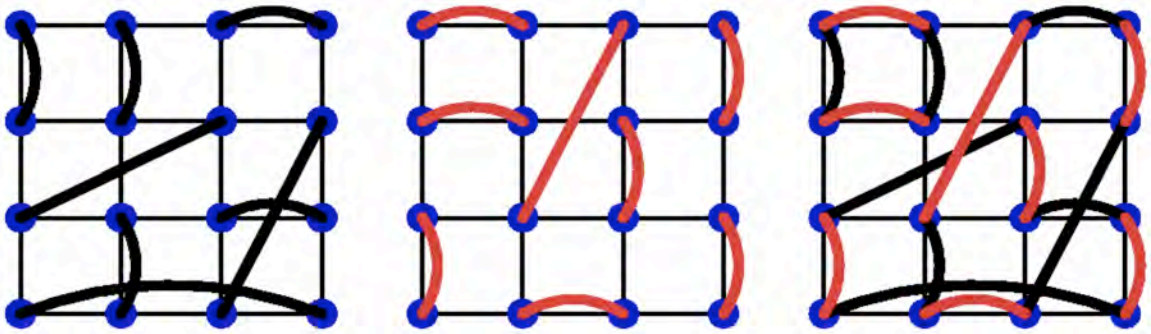
Basis states: $$|V_k\rangle = \prod_{b=1}^{N/2}(i_{k,b},j_{k,b}), \quad k = 1,\ldots,(N/2)!$$

The valence bond basis is **overcomplete**, **non-orthogonal**
- expansion of singlet sate not unique

$$|\Psi\rangle = \sum_k f_k |V_k\rangle$$

Overlap of VB states

- given by the number of loops N_l in superimposed graphs
- all basis states overlap with each other (useful...)



$|V_k\rangle$ $|V_p\rangle$ $\langle V_k|V_p\rangle = 2^{N_l - N/2}$

Matrix elements

- spin correlations related to loop structure

$$\frac{\langle V_k|\mathbf{S}_i \cdot \mathbf{S}_j|V_p\rangle}{\langle V_k|V_p\rangle} = \begin{cases} 0, & i,j \text{ in different loops} \\ \pm\frac{1}{4}, & i,j \text{ in the same loop} \end{cases}$$

More complicated matrix elements discussed in
K. Beach, A.S., Nucl. Phys. B 750, 142 (2006)

Projector Monte Carlo in the valence bond basis

$(-H)^n$, or $(C\text{-}H)^n$, projects out ground state from an arbitrary state

$$(-H)^n|\Psi\rangle \rightarrow c_0|E_0|^n|0\rangle$$

S=1/2 Heisenberg model

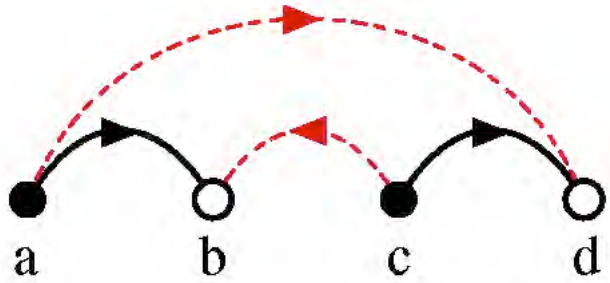
$$H = -\sum_{\langle i,j\rangle} H_{ij}, \quad H_{ij} = -(\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4})$$

Project with strings of bond operators

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

Arrow - "direction" of (i,j)

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



Action of bond operator on VB state

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

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

- No branching when acting on a VB basis state
- No minus signs for bipartite lattice if "direction" of singlet (i,j) is $A \rightarrow B$ (i on sublattice A, j on sublattice B)

Sampling the wave function

Simplest trial wave function; a single basis state $|V_k\rangle$

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

The weight of the path is given by # of off-diagonal operations

$$W(\{H_{ij}\}) = \left(\frac{1}{2}\right)^{n_{\text{off}}} \qquad n = n_{\text{dia}} + n_{\text{off}}$$

How to sample? Trivial way:

- **Randomly replace m operators at string positions $p_1,\ldots,p_m$**
- **Recalculate weight (n_{off}) by propagating $|V_k\rangle$**
- **Accept using Metropolis probability**

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

- Gives good acceptance probability for $m = 2 \sim 6$
- Works because of non-orthogonality of basis
- Faster way to calculate acceptance probability desired...

Calculating the energy

Consider the Neel state |N>

- All VB basis states have equal overlap with |N>

$$\langle N|V_i\rangle = \left(\frac{1}{\sqrt{2}}\right)^{N/2}$$

- The energy can be calculated using any equal-overlap state

$$E_0 = \frac{\langle N|H|0\rangle}{\langle N|0\rangle} = \frac{\sum_{\{H_{ij}\}}\langle N|H\prod_{p=1}^{n}H_{i(p)j(p)}|V_k\rangle}{\sum_{\{H_{ij}\}}\langle N|\prod_{p=1}^{n}H_{i(p)j(p)}|V_k\rangle}$$

Operation with $H = -\sum_{\langle i,j\rangle} H_{ij}$ gives sum of 1(diagonal) and 1/2 (off-diagonal)

$$E_0 = -\langle n_{\mathrm{d}} + \tfrac{1}{2}n_{\mathrm{o}}\rangle = -\tfrac{1}{2}\langle N_{\mathrm{b}} + n_{\mathrm{d}}\rangle$$

n_d = number of diagonal bond operations H_{ij}

n_o = number of off-diagonal operations H_{ij}

N_b = number of bonds on the lattice ($n_o+n_d=N_b$)

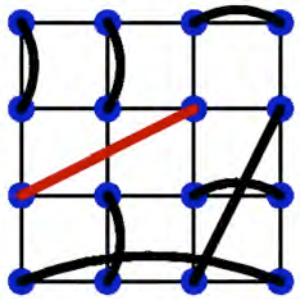
Direct improved estimator for the singlet-triplet gap

The valence bond basis spans the singlet sector

• with one **triplet bond**, one can study the lowest triplet state

$$(i,j) = \frac{1}{\sqrt{2}}(|\uparrow_i,\downarrow_j\rangle - |\downarrow_i,\uparrow_j\rangle)$$

$$[i,j] = \frac{1}{\sqrt{2}}(|\uparrow_i,\downarrow_j\rangle + |\downarrow_i,\uparrow_j\rangle)$$



H_{ij} propagates the triplet off-diagonally almost like a singlet

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

but a diagonal operation gives zero (kills the triplet state)

$$H_{ab}|\ldots[a,b]\ldots\rangle = 0$$

E_1 can be calculated by propagating a state with one triplet

• propagate for all initial triplet locations (N/2 different bonds)

• surviving paths contribute to the triplet energy

• subset of singlet and triplet configurations are the same

- **error cancellations** in $\Delta = E_1 - E_0$, improved gap estimator

General operator expectation values

We have to project both a bra and a ket state: $\langle A \rangle = \langle 0|A|0 \rangle$

Operator string notation: $S_n = [i(1), j(1)], \ldots, [i(n), j(n)]$

$$|0\rangle \sim \sum_{S_n} \prod_{p=1}^{n} H_{i(p)j(p)} |V_k\rangle = \sum_{S_n} W(S_n, k) |V_k(S_n)\rangle$$

Importance sampling of

$$\langle A \rangle = \frac{\sum_{S_n, T_n} W(S_n, k) W(T_n, k) \langle V_k(S_n)|V_k(T_n)\rangle A(S_n, T_n, k)}{\sum_{S_n, T_n} W(S_n, k) W(T_n, k) \langle V_k(S_n)|V_k(T_n)\rangle}$$

Estimator to be averaged

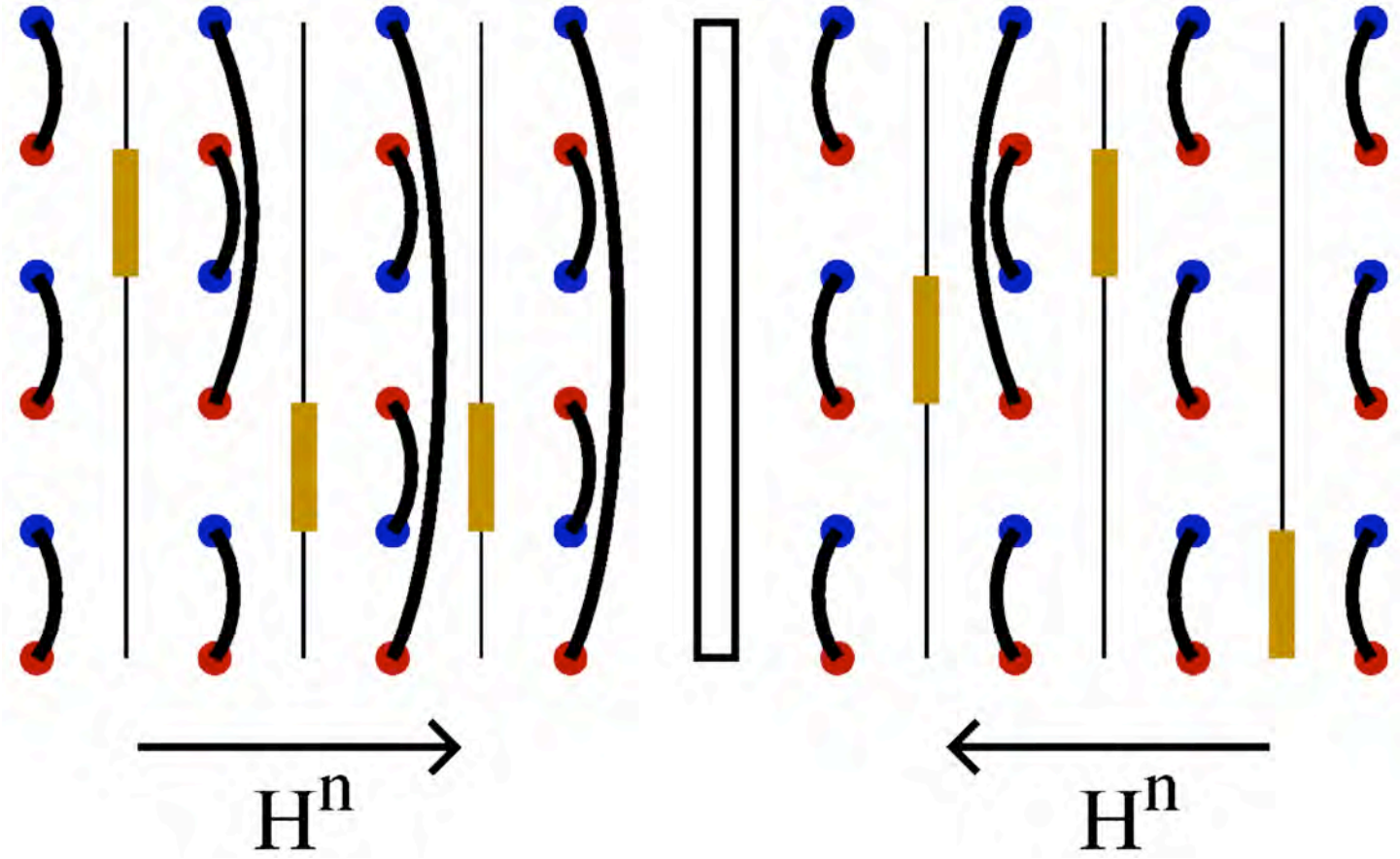
$$A(S_n, T_n, k) = \frac{\langle V_k(S_n)|A|V_k(T_n)\rangle}{\langle V_k(S_n)|V_k(T_n)\rangle}$$

Sampling by operator replacements as before

- note that the **weight includes an overlap**

$$W(S_n, T_n, k) = W(S_n, k) W(T_n, k) \langle V_k(S_n)|V_k(T_n)\rangle$$

Illustration: 6-site chain, n=3



Note: in this basis the **propagation is non-hermitean**

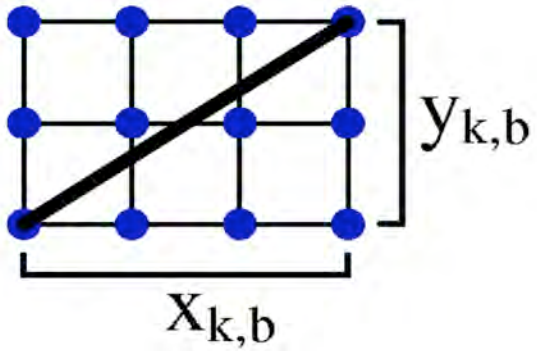
- the left state is propagated from the left
- the right state is propagated from the right
- the propagated states always have some overlap

Sampling a bond-amplitude product state

Instead of using a single basis state as the trial state, it is possible to sample a wave function

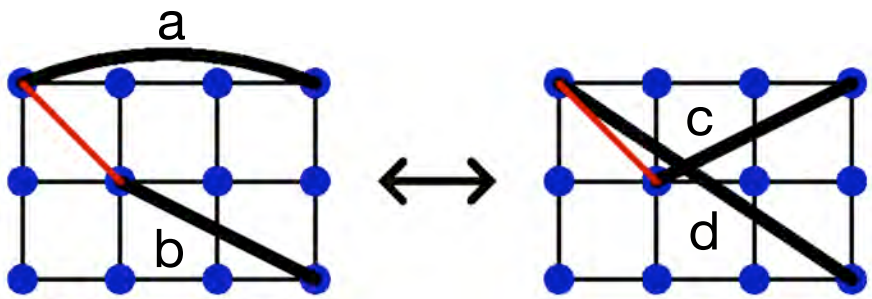
$$|\Psi_0\rangle = \sum_k \prod_{b=1}^{N/2} h(x_{k,b}, y_{k,b})|V_k\rangle$$

bond b of state k



Update by reconfiguring two bonds

[Liang, Doucot, Anderson, PRL 61, 365 (1988)]



Acceptance probability

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

If reconfiguration accepted

- calculate change in string-projection weight as before
- final accept/reject based on projection weight only

Liang [PRB 42, 6555 (1990)] used **parametrized h(x,y) for 2D Heisenberg**

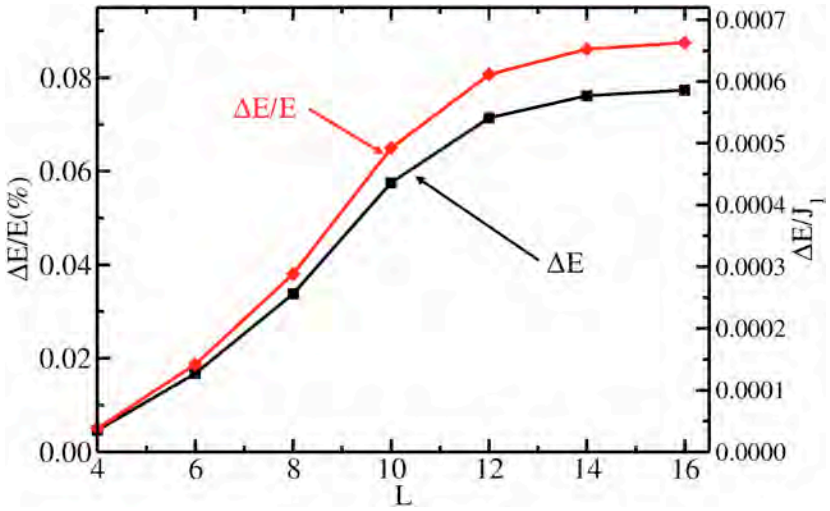
- determined parameters variationally
- improved the variational wave function by projection

Variational wave function

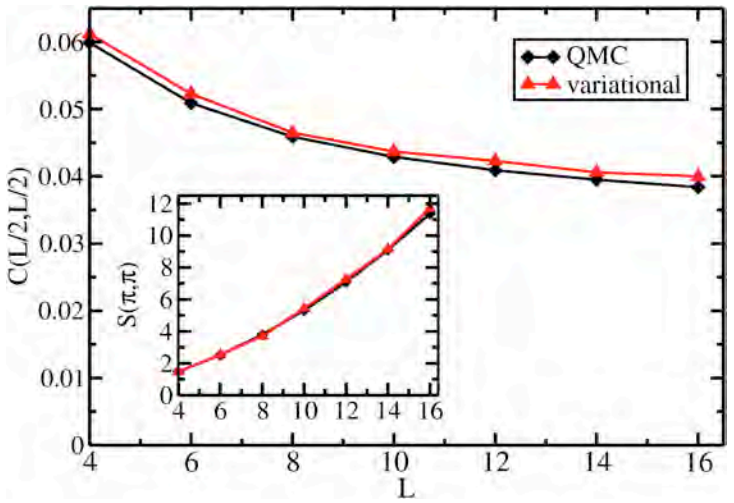
It is very time consuming to fully optimize all $h(x,y)$ variationally

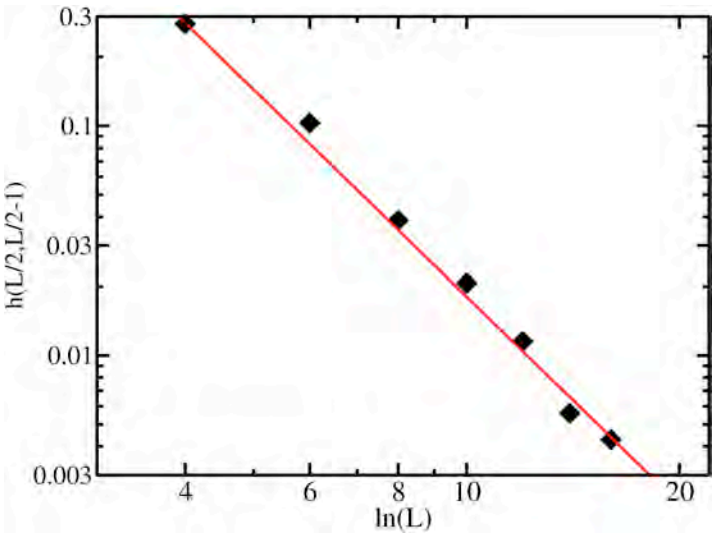
- Newton/conjugate-gradient method [J. Lou and A. S., cond-mat/0605034]

Energy



Spin correlations





Variational energy error

- 25% smaller than Liang et al.'s

Asymptotic form h(x,y)=h(r)

- **h(r) decays as $1/r^3$**
- previous work gave $1/r^p$, p = 2-5
- mean-field theory [K. Beach] explains $1/r^3$ form

Self-optimized trial wave function

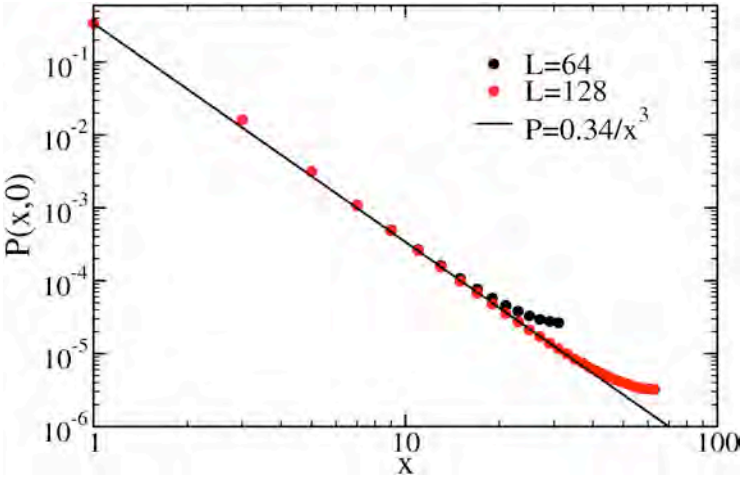
Projector method can access the **bond-length probability** $P(x,y)$

- related to the amplitude $h(x,y)$
- for wave function with $h(x,y)$

$$P(x,y) \sim h(x,y)$$

$P(x,y)$ can be used to construct $h(x,y)$ almost as good as the variational h

Results for 2D Heisenberg



Definitions

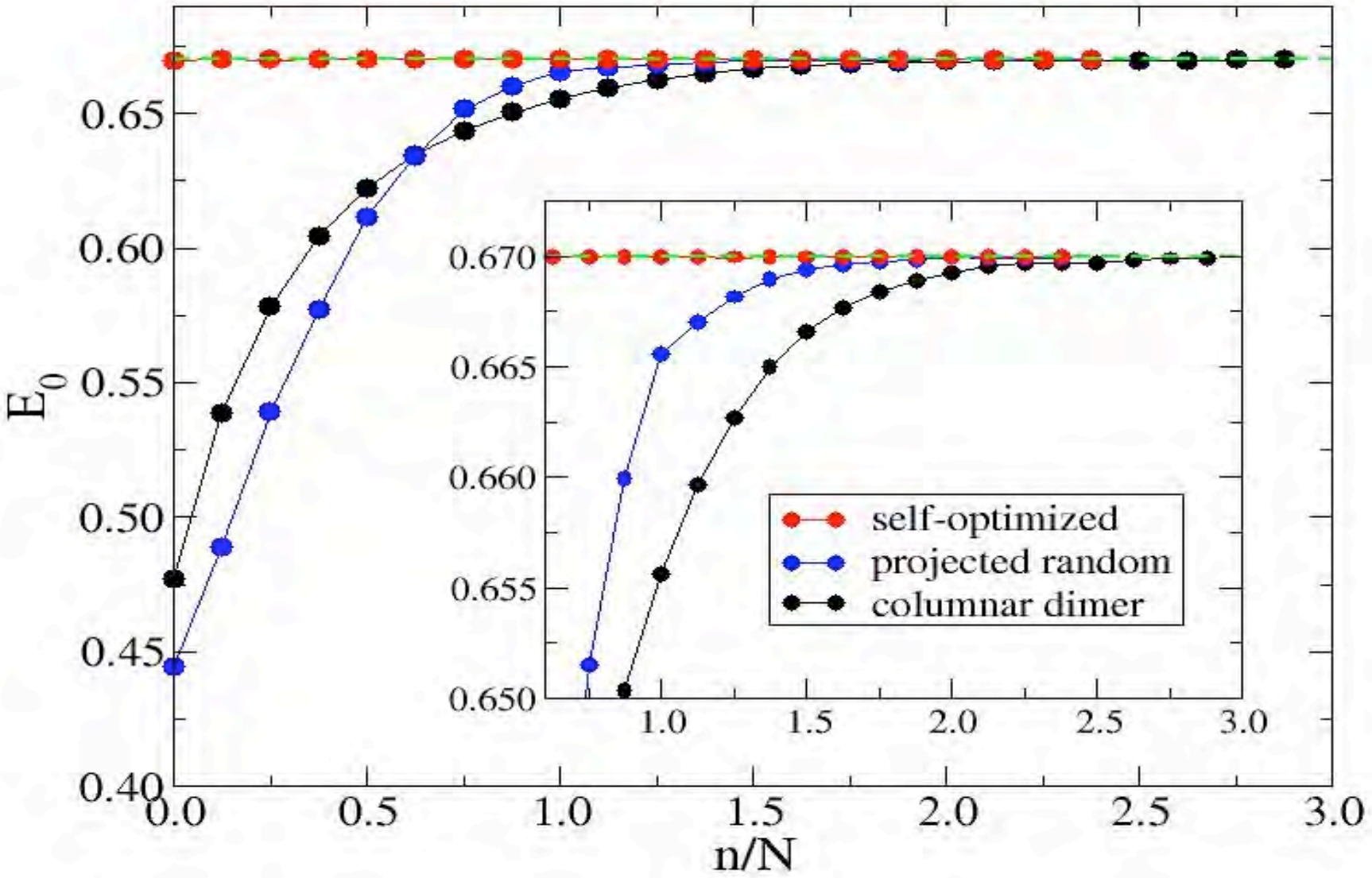
- $h(x,y)$ = bond amplitude of the trial state
- $P_0(x,y)$ = bond probability of the trial state
- $P_n(x,y)$ = bond probability of the H^n projected state

For large enough n, $P_n(x,y)$ is the exact ground-state distribution

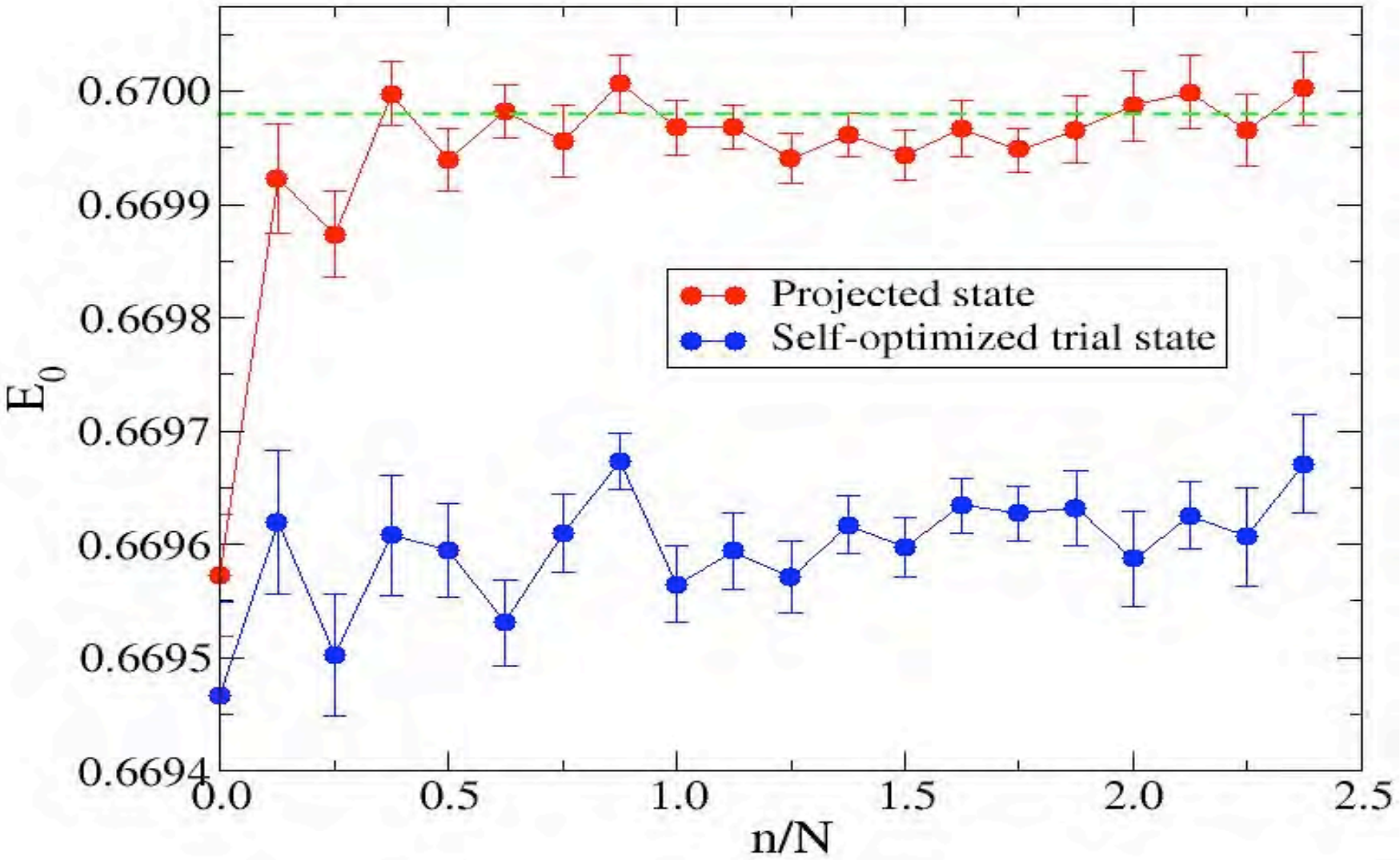
- if $P_0(x,y) > P_n(x,y)$, then **reduce $h(x,y)$**
- if $P_0(x,y) < P_n(x,y)$, then **increase $h(x,y)$**
- repeat until $P_0(x,y)=P_n(x,y)$ for all x,y
- fast method to obtain almost optimal $h(x,y)$
- **can be generalized to include bond correlations**

Energy convergence; 2D Heisenberg, 16^2 spins

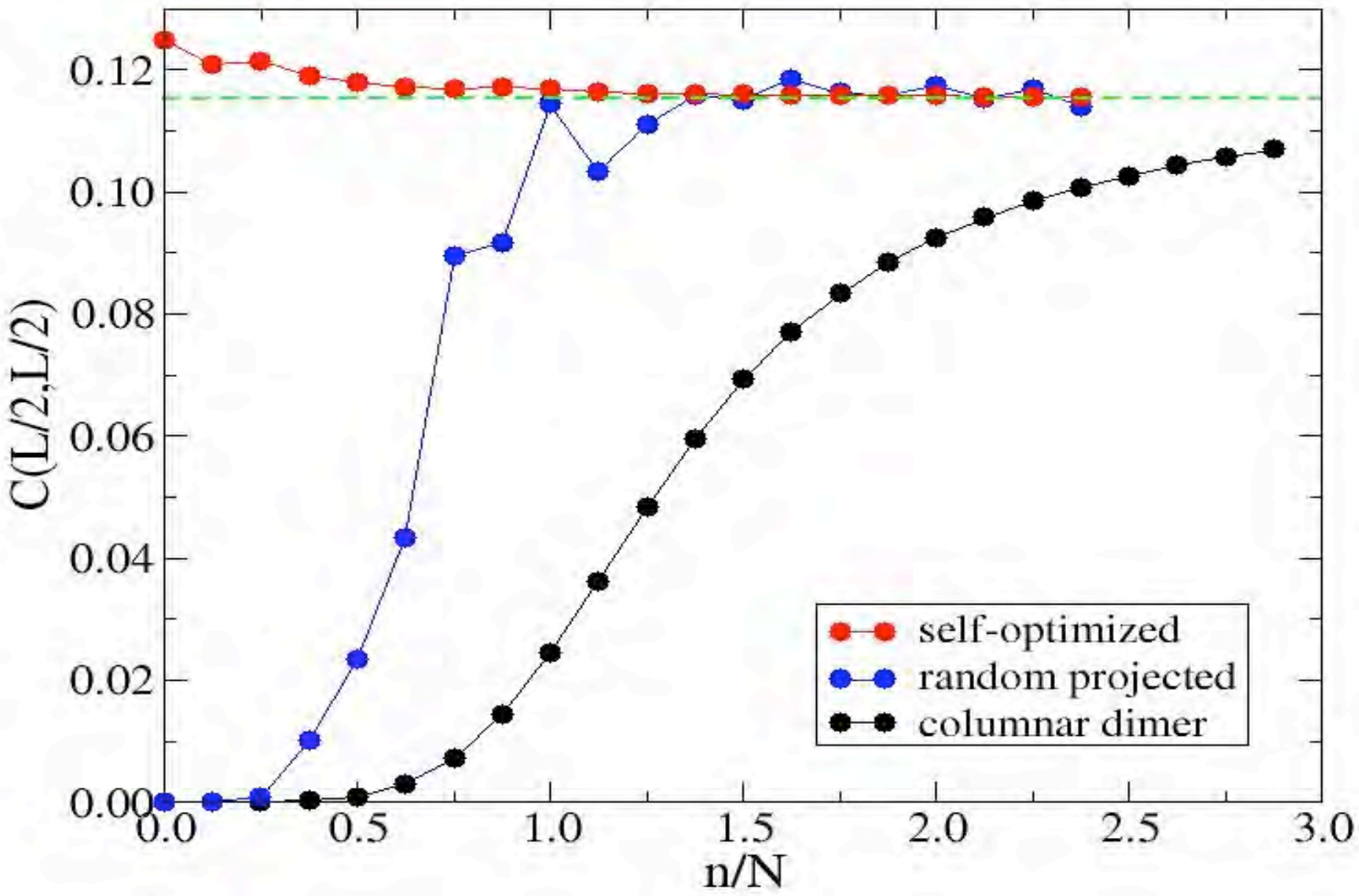
- comparison of different trial wave functions



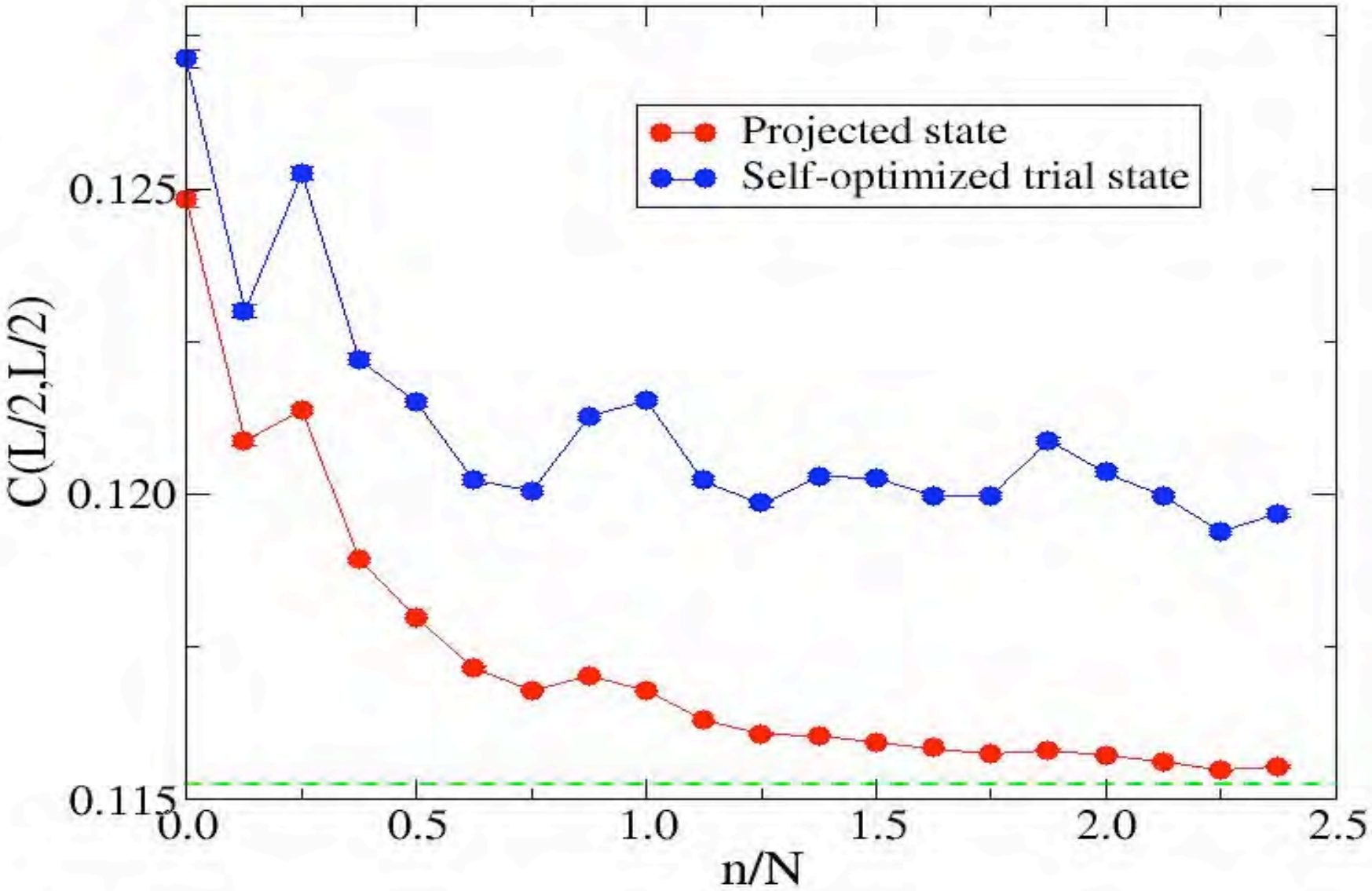
Energy of self-optimized state



Convergence of long-distance correlation function



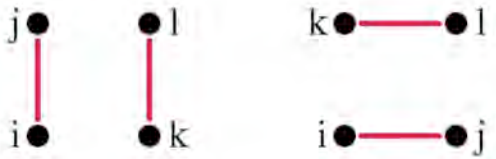
Correlation function of self-optimized state



2D Heisenberg model with 4-site interactions

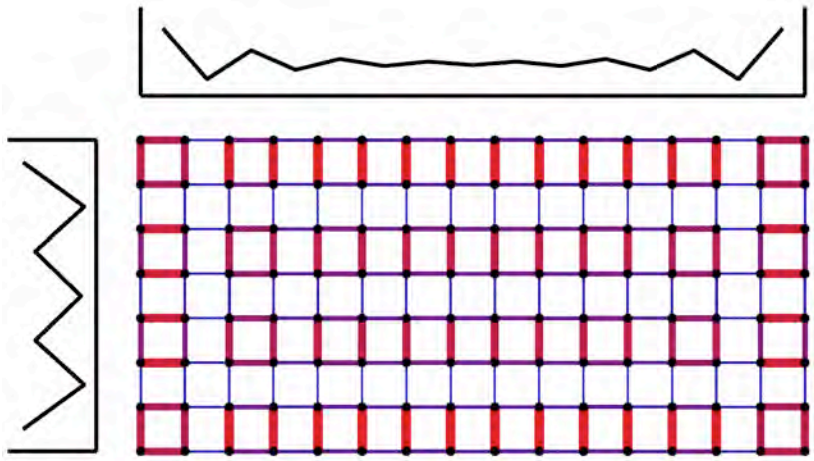
- Neel to VBS quantum phase transition
- **Candidate for "deconfined" quantum-criticality**
  - contunuous transition; "Landau rules" say 1st order

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - Q \sum_{\langle ijkl \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4})(\mathbf{S}_k \cdot \mathbf{S}_l - \tfrac{1}{4})$$

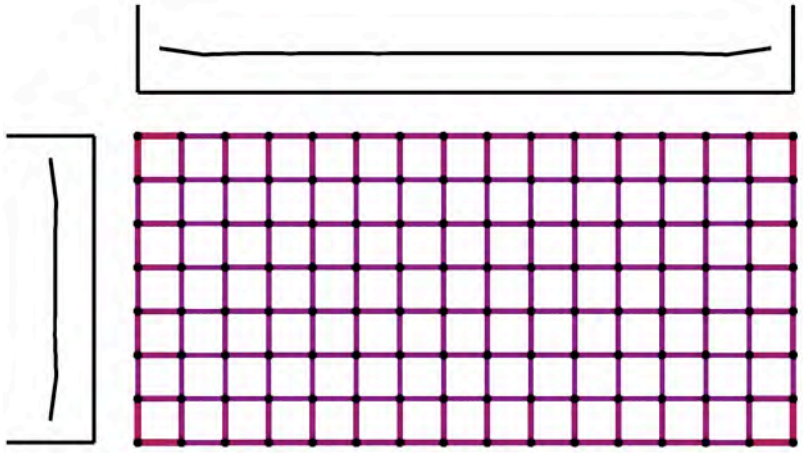


VBS order; open boundaries break symmetry - unique VBS

- order parameter; bond correlation $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$



J=0 - columnar VBS

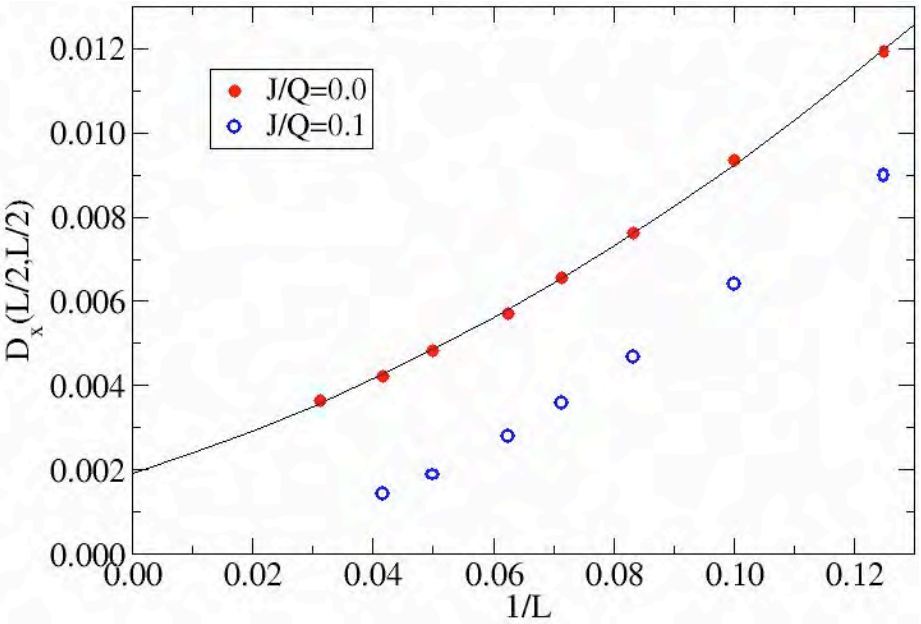


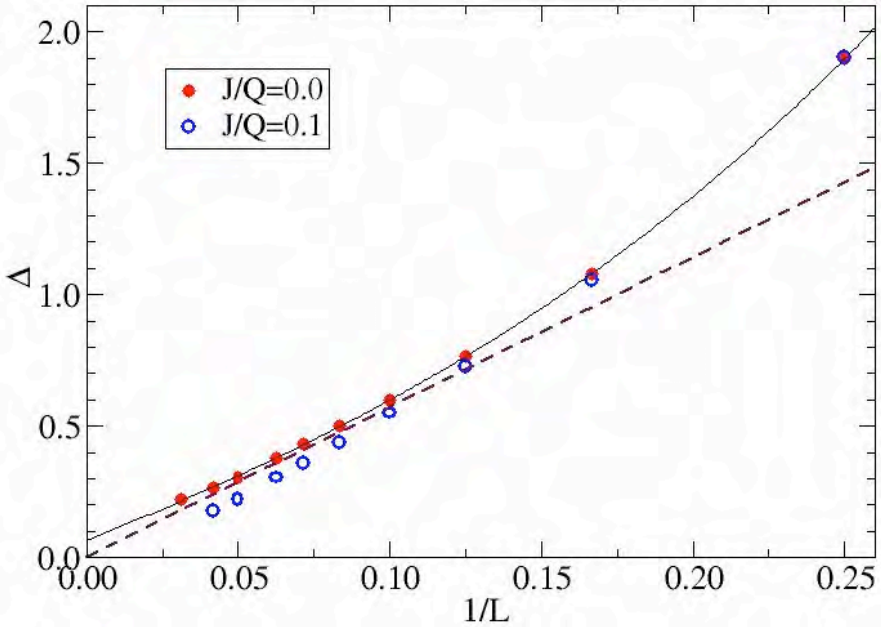
Q=0 - no VBS order

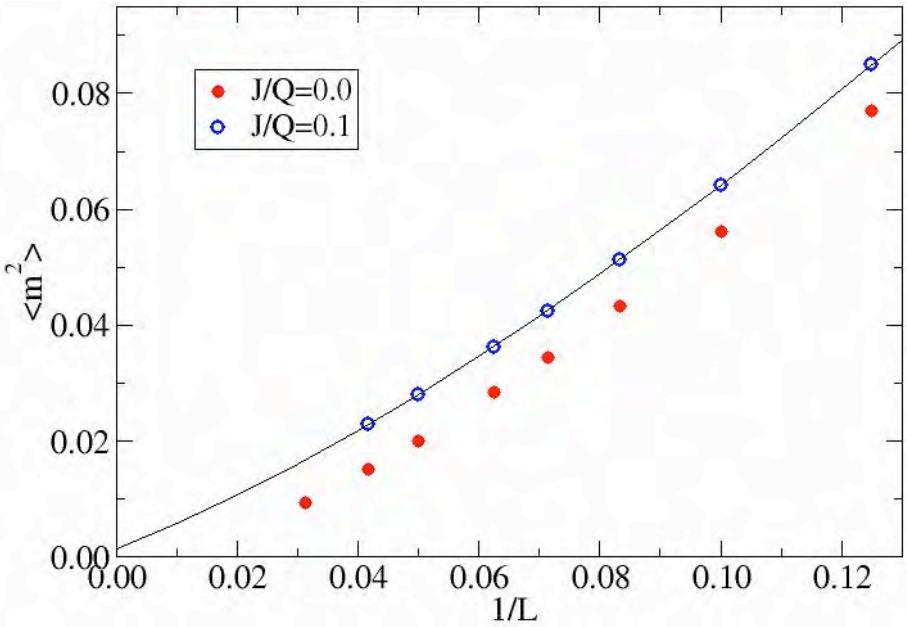
Finite-size scaling

periodic boundaries

- dimer correlations
- submattice magnetization
- singlet-triplet gap
- **J/Q=0.0**; VBS
- **J/Q=0.1**; antiferromagnet



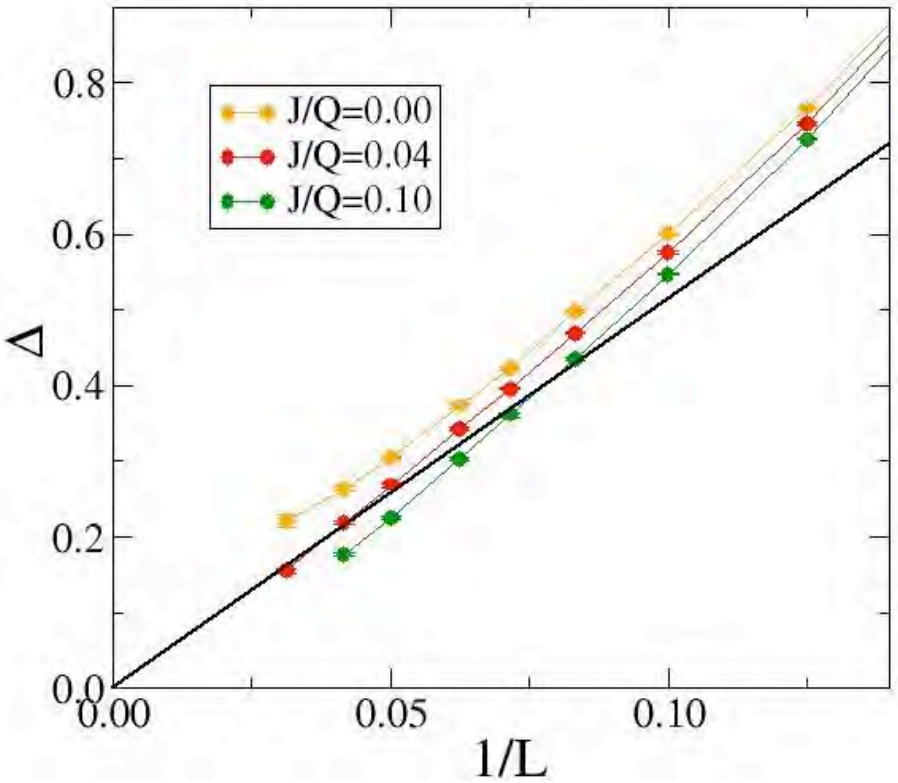


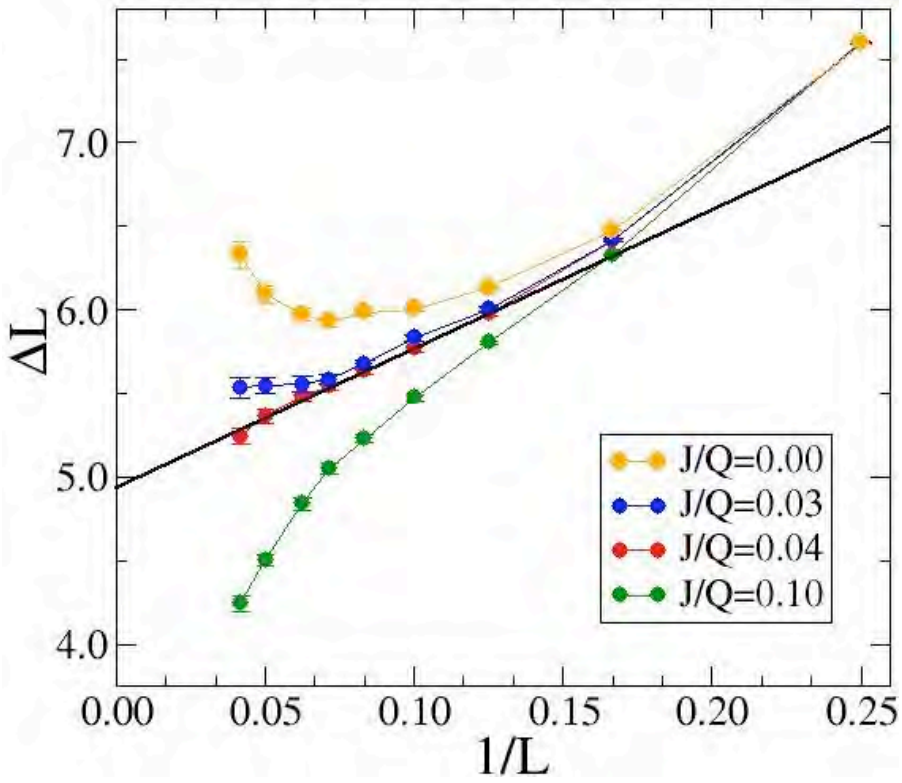


Singlet-triplet gap scaling; dynamic exponent z

z relates length and time scales

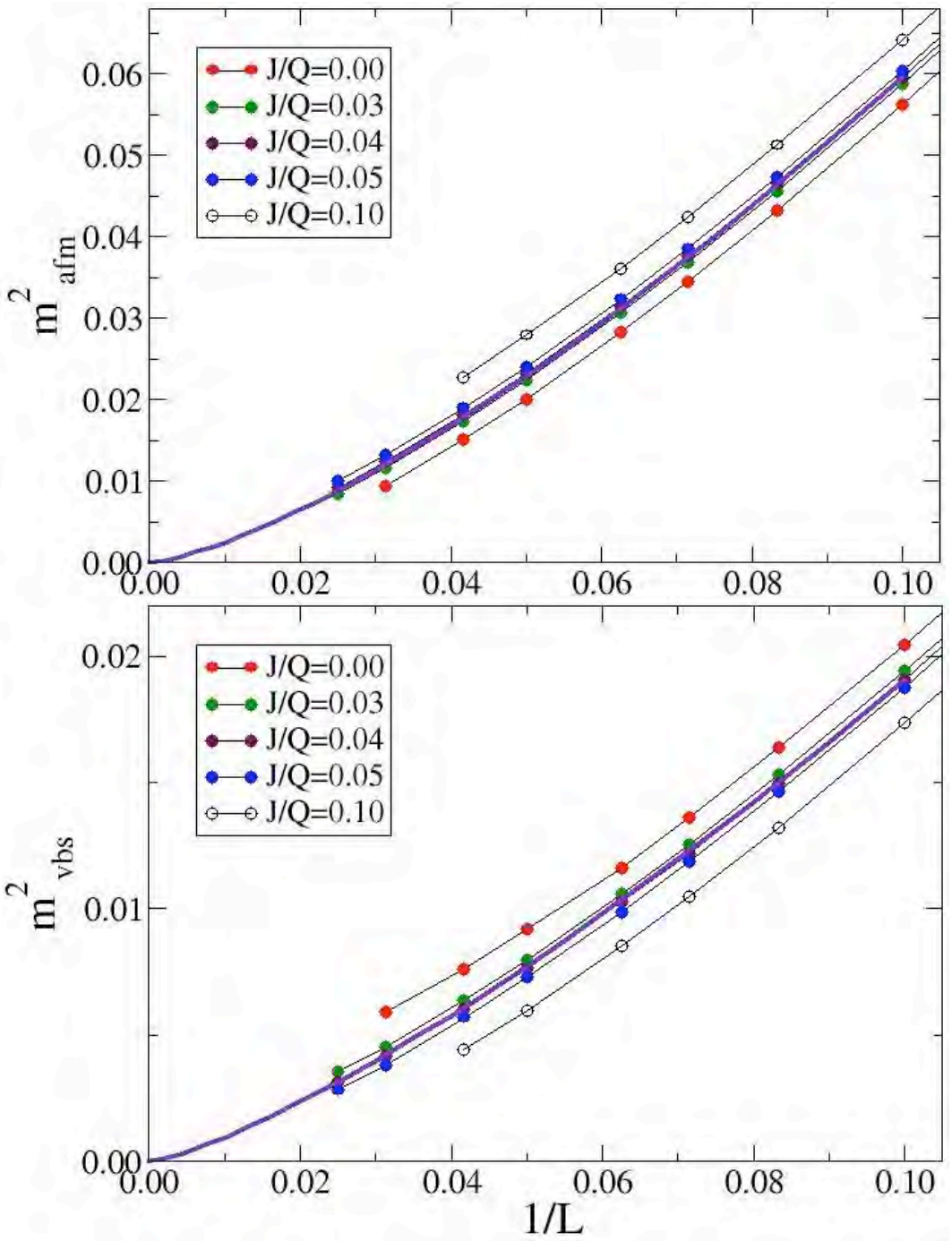
$$\omega_q \sim |q|^z, \quad \text{finite size} \rightarrow \Delta \sim \frac{1}{L^z}$$





Critical gap: $\Delta(L) \sim \frac{a_1}{L} + \frac{a_2}{L^2} + \cdots$ at J/Q≈0.04

Consistent with deconfined quantum-criticality (**z=1** theory)



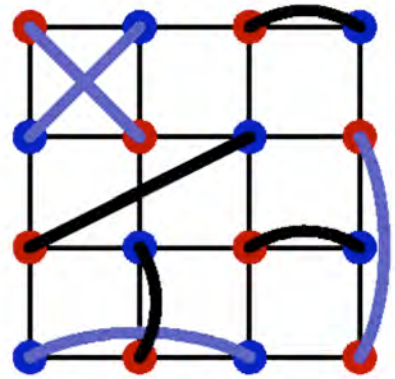
Neel and VBS orders

- finite-size scaling
- order parameters vanish at the same coupling; $(J/Q)_c \approx 0.035$
- correlation function exponent η is large; $\eta \approx 0.4$ for spin
- smaller for dimers
- more careful analysis in progress

Frustrated systems

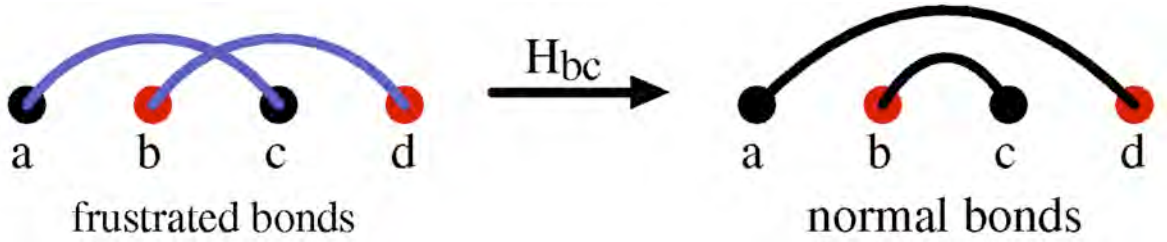
Consider the full valence-bond basis, including

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



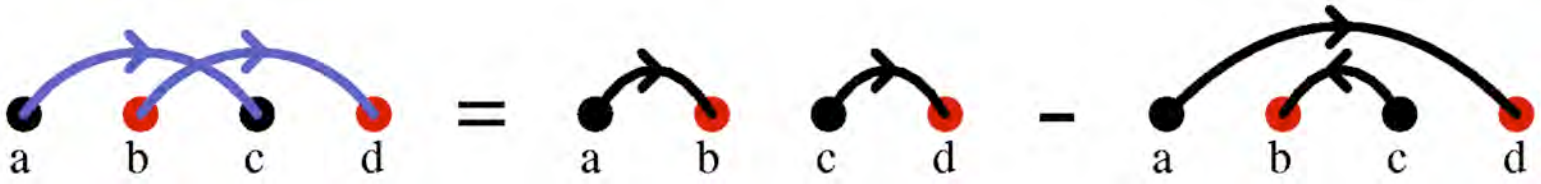
For a non-frustrated system

- 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

Summary

The valence bond basis can be used in projector QMC

- some observables easier to calculated than in z-basis
- easy to study certain types of multi-spin interactions
  - interesting phases/transitions; Neel-VBS
- self-optimized trial wave functions
  - including bond-correlations; explored currently

Sign problems for frustrated systems

- but freedom offered by overcompleteness should be explored; potentially there are sign-problem-free frustrated systems

More details for 2D J-Q model in symposium talk

- evidence for deconfined quantum-criticality, including emergent U(1) symmetry