# Quantum Monte Carlo Simulations in the Valence Bond Basis

Anders W. Sandvik, Boston University

Collaborators

- Kevin Beach (U. of Alberta)
- Jie Lou (Boston U.)
- Hans-Gerd Evertz (U. Graz, Austria)
- Ribhu Kaul (Microsoft Station Q)
- Naoki Kawashima (ISSP, Tokyo)

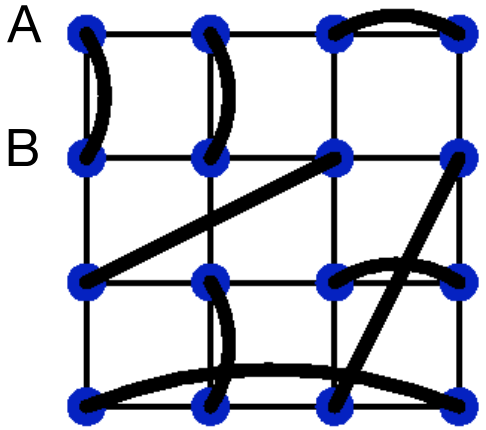
Outline

- The valence bond basis for S=1/2 spins
- Projector Monte Carlo
- Variational and self-optimized trial states
- Projecting triplet states at finite momentum
- Combining loop updates and valence bonds
- Application: Neel-VBS transition in "J-Q" model
  - new results for SU(N) generalization


# The valence bond basis for S=1/2 spins

- Dates back to the 1930s (Pauling, Romer, Hulthen...)
- Spans the singlet space (generalizations for triplets, etc)

- Consider N (even) spins
- Divide into two groups A,B
  - e.g., sublattices (but not necessarily)
- Bonds between A and B sites; singlets




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

Basis states; pair up all spins

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

The valence bond basis is overcomplete and non-orthogonal

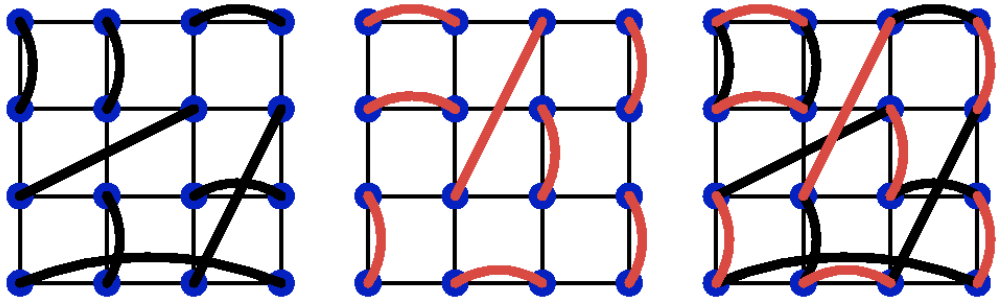
- expansion of arbitrary singlet is not unique

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

# Some useful properties

All valence bond states overlap with each other

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



$|V_l\rangle$ $|V_r\rangle$ $\langle V_l|V_r\rangle$

Spin correlations are related to the loop structure

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

More complicated matrix elements are also related to loops

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

# Projector Monte Carlo

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

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

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

## 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

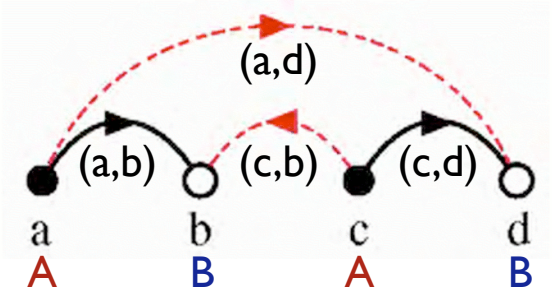
$$\sum_{\{H_{ij}\}} \prod_{p=1}^{n} H_{i(p)j(p)}|\Psi\rangle \rightarrow r|0\rangle$$

(r = unknown normalization)

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

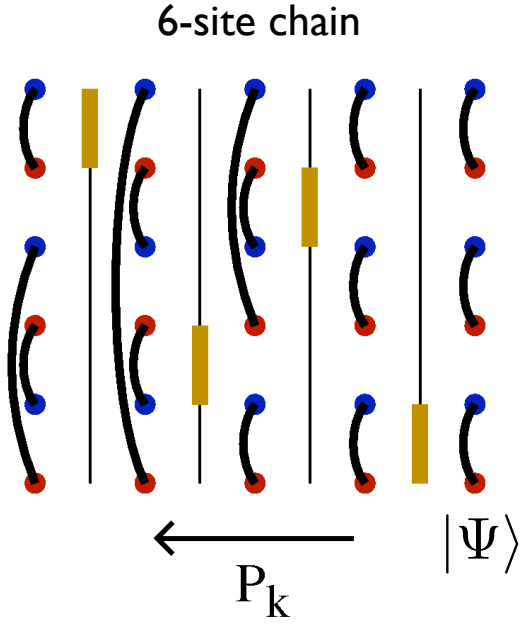
# Sampling the wave function

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

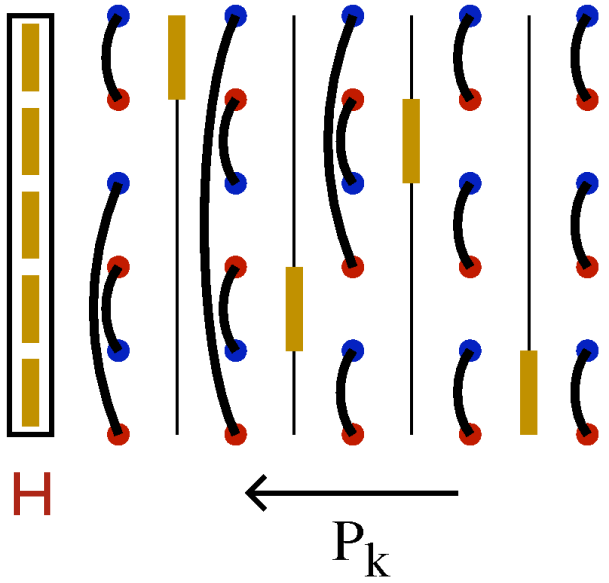
- Loop updates can also be used

# Calculating the energy

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

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

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




H acts on the projected state, giving

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

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

This energy estimator is not variational

- The energy can be below the true ground state energy
- But becomes exact in the limit of large n
- <0|H|0> can also be calculated and is variational

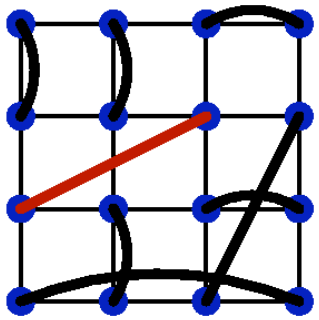
# Estimator for the singlet-triplet gap

The original VB basis spans the singlet space

- with one triplet bond, one can obtain the lowest triplet state

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

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

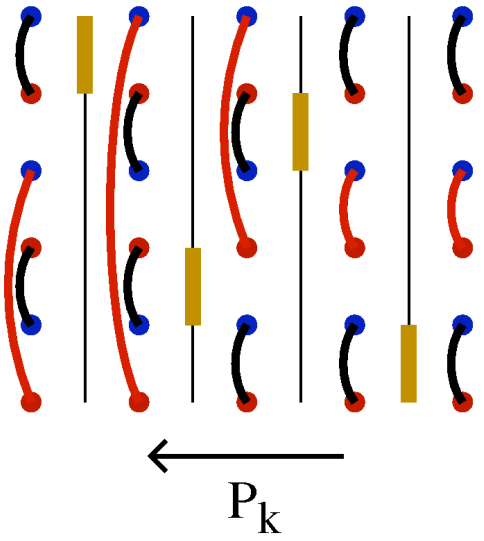


Under propagation, the triplet flips like a singlet

- but a diagonal operation on a triplet kills it

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

$$H_{ab}|...[a,b]...(c,d)...\rangle = 0$$




The initial triplet can be placed anywhere

- *N*/2 different triplet propagations
- Those that survive contribute to $E_1$
- Partial error cancellations in the gap

$$\Delta = E_1 - E_0$$

**The ability to generate singlet and triplet states in the same run is a unique feature of VB projector Monte Carlo**

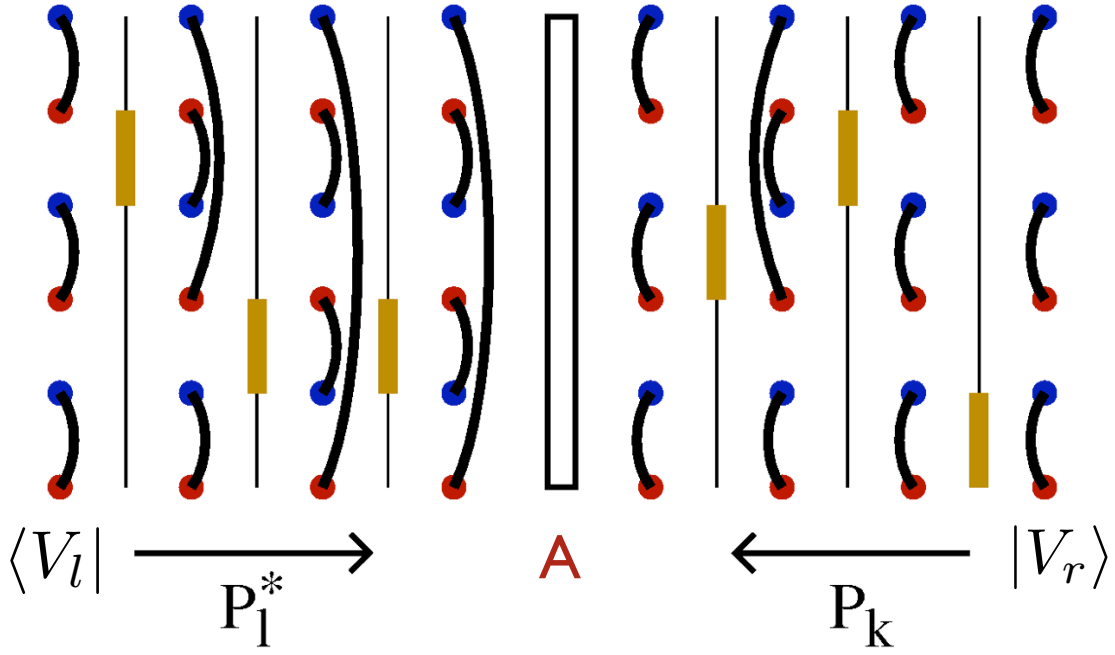
# General expectation values

We have to project bra and ket states $\langle A \rangle = \langle 0|A|0\rangle$

$$\sum_k P_k|V_r\rangle \rightarrow W_{kr}(\tfrac{1}{4} - E_0)^n c_0|0\rangle$$

$$\sum_g \langle V_l|P_g^* \rightarrow \langle 0|c_0 W_{gl}(\tfrac{1}{4} - E_0)^n$$

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

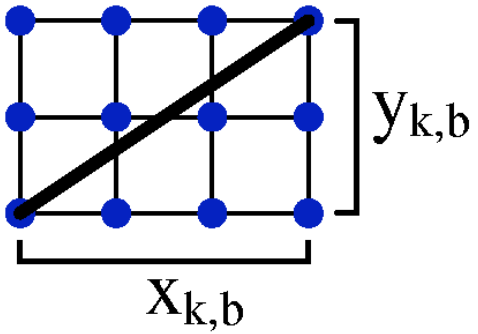


# Sampling a bond-amplitude product state

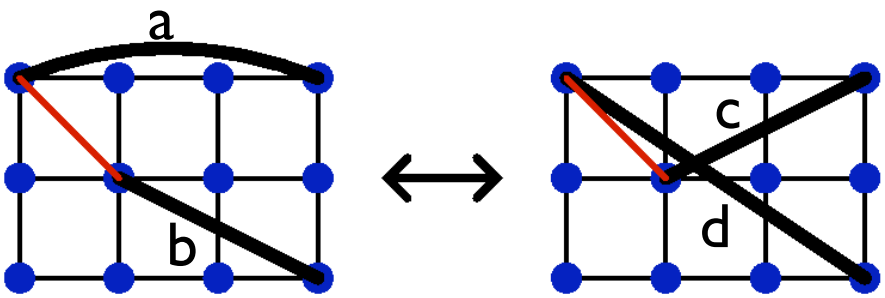
A better trial state leads to faster n convergence

- 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



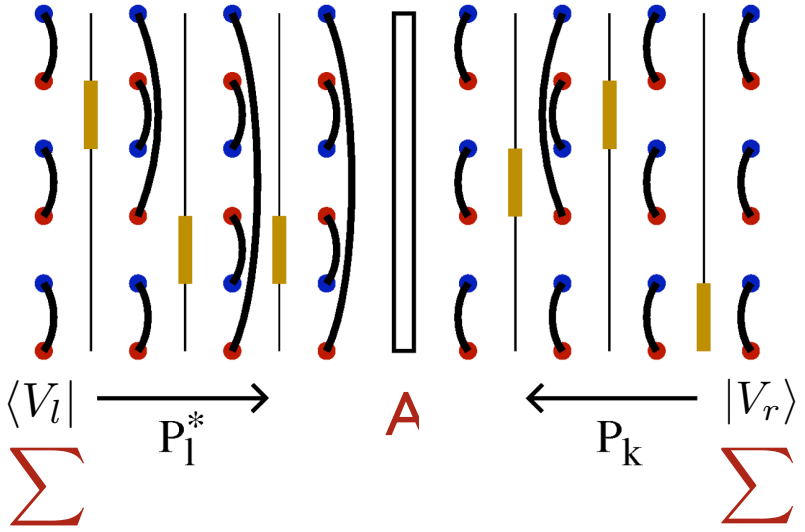

$$P_{\text{accept}} = \frac{h(x_c, y_c)h(x_d, y_d)}{h(x_a, y_a)h(x_b, y_b)}$$

If reconfiguration accepted

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

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

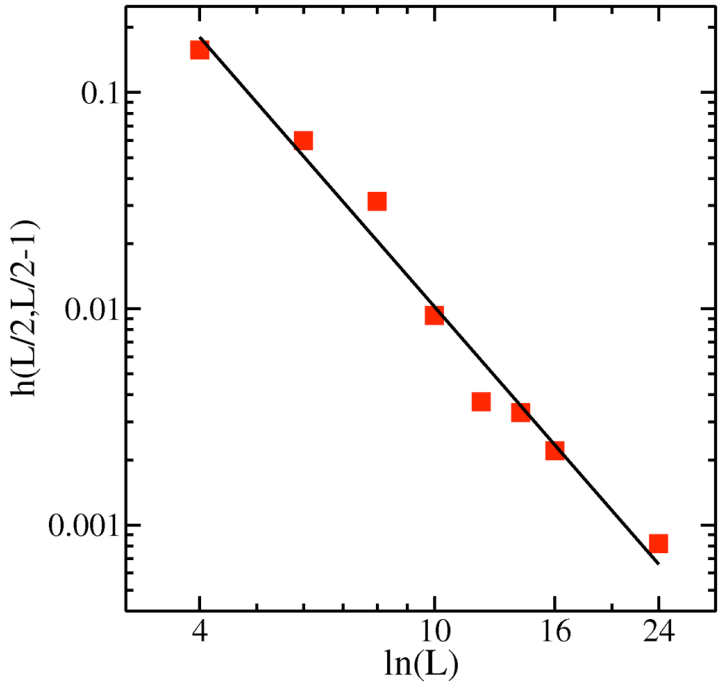
- used parametrized state amplitudes
- determined parameters variationally
- improved state by projection

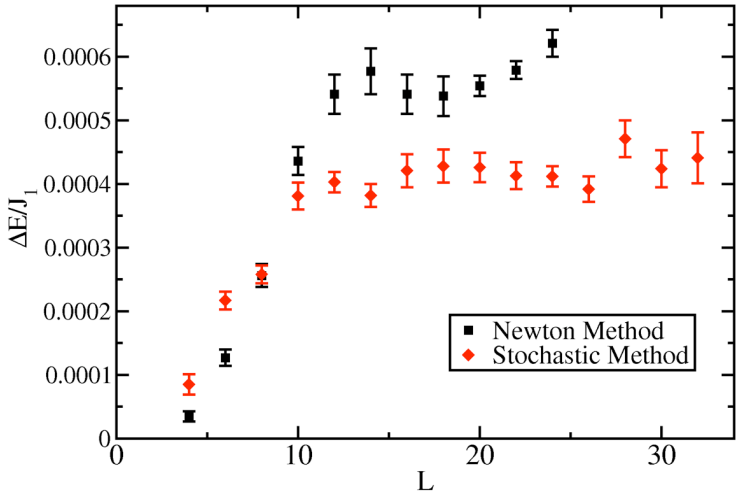


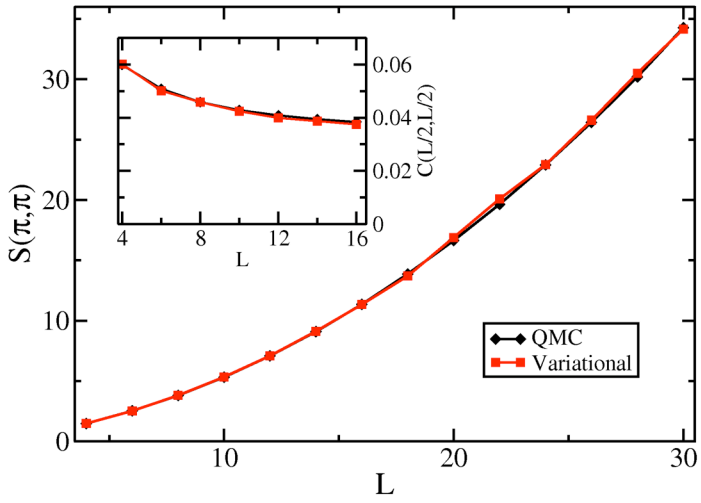
# Variational wave function (2D Heisenberg)

All amplitudes h(x,y) can be optimized [J. Lou and A.W.S., PRB 2007]

- variational energy error <0.1% (50% smaller than previously best)
- spin correlations deviate by less than 1% from exact values
- amplitudes $\sim r^{-3}$



# Self-optimized wave function

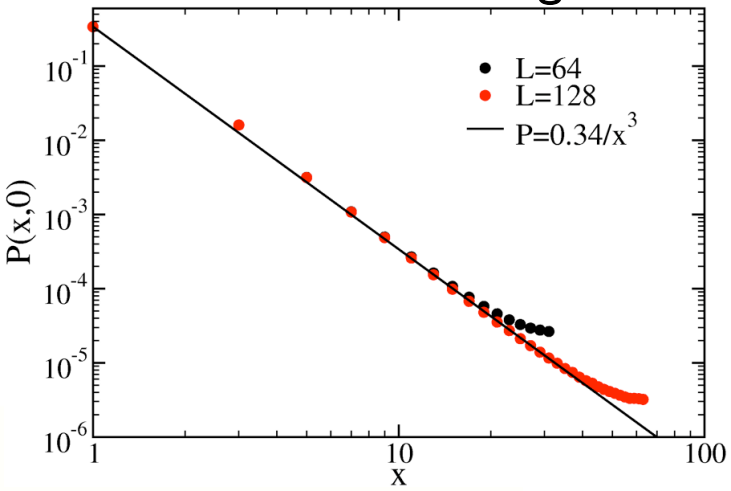
Projector method can access the
**bond-length probability P(x,y)**

- 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**

2D Heisenberg



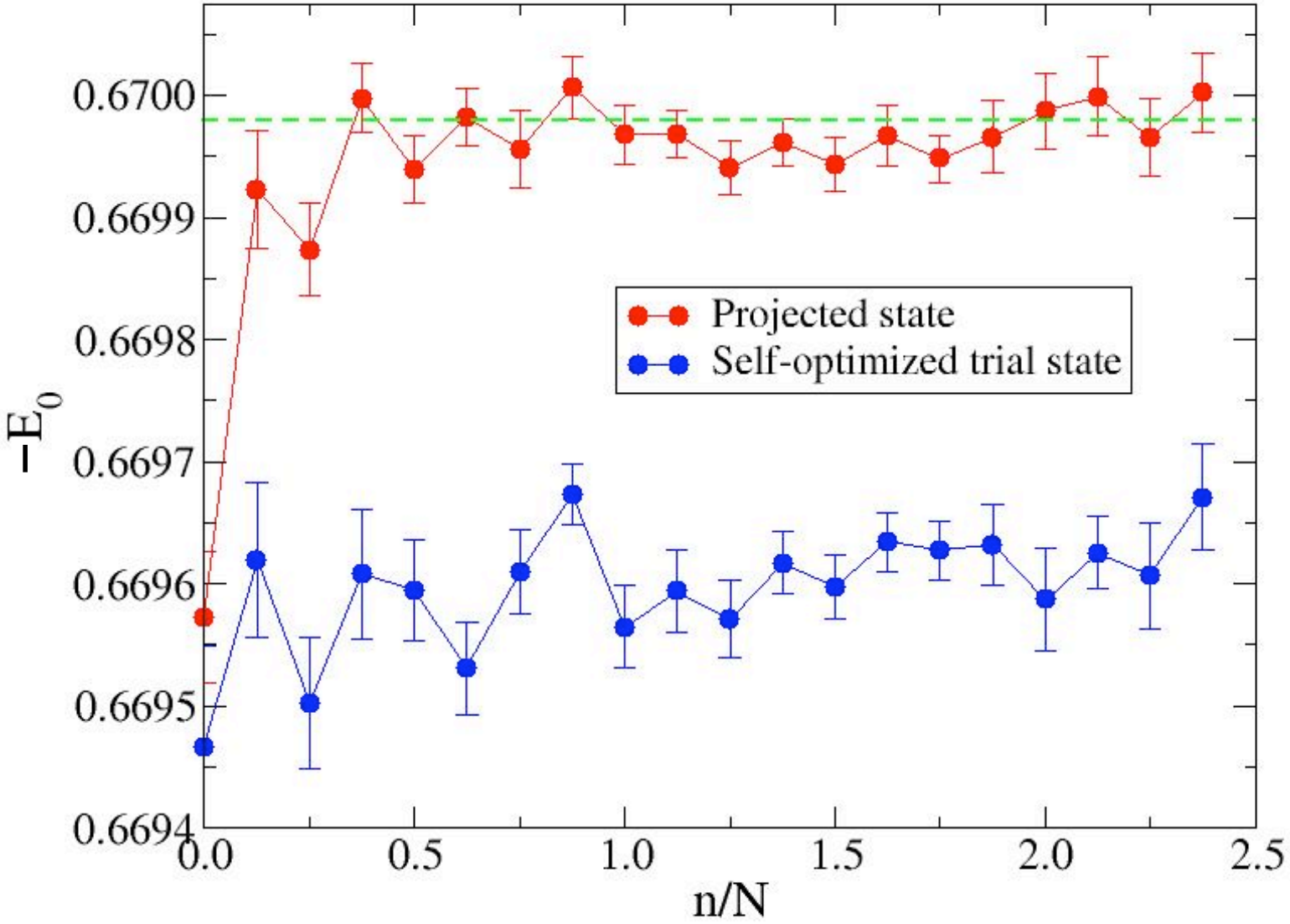

## Definitions

- $h(x,y)$ = 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

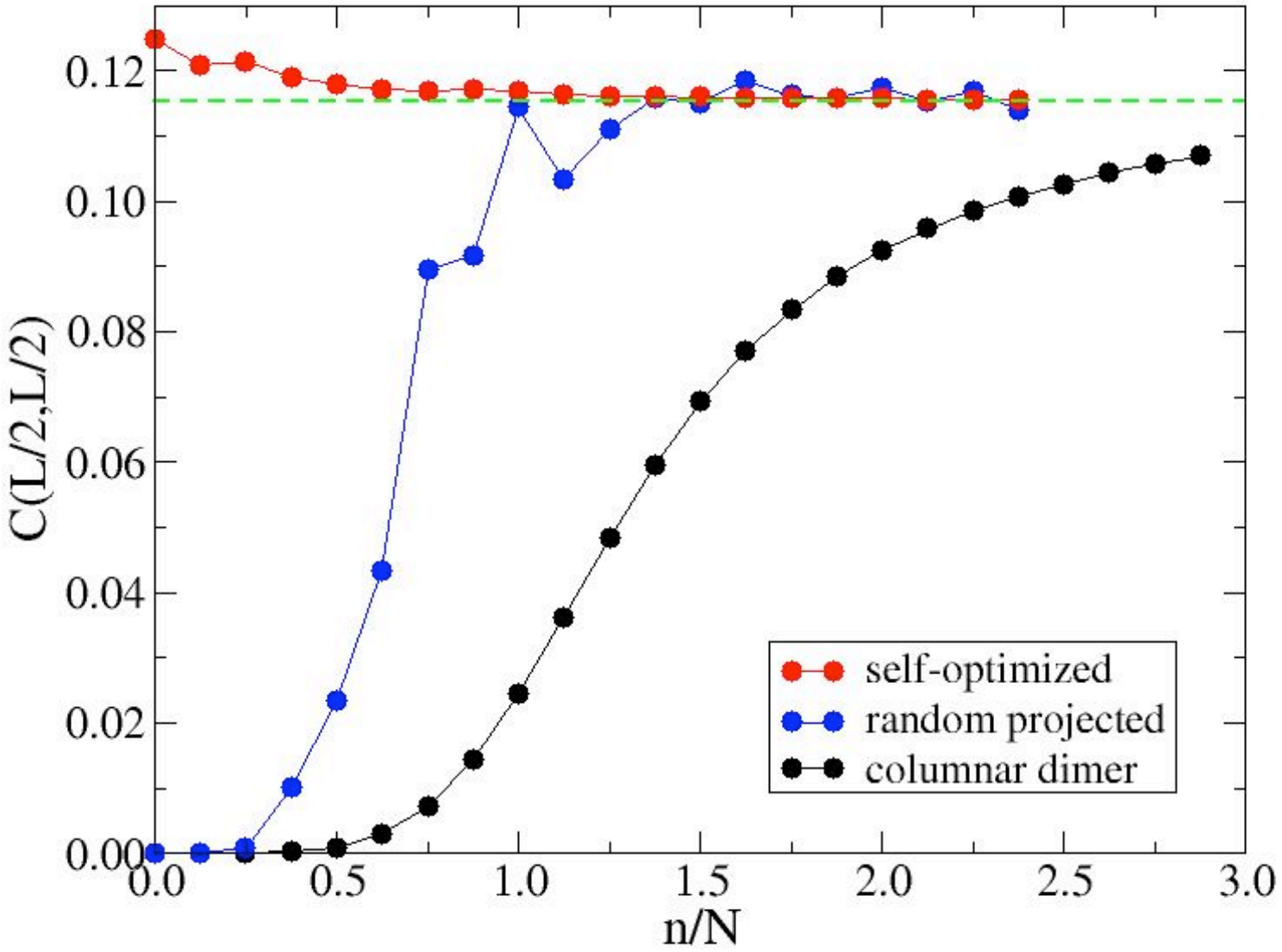
**For large enough n, $P_n(x,y)$ is the exact ground-state distribution**

- 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**

# Convergence: 16×16 lattice (Heisenberg model)



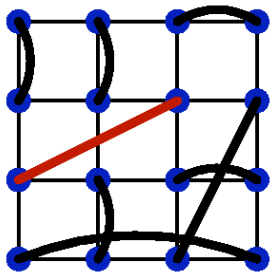
# Long-distance spin correlations



# Momentum dependence of triplet excitations

**Creating a triplet corresponds to acting with $S^z$ operators**

$$S^z(\mathbf{q})|\Psi_S(0)\rangle = |\Psi_T(\mathbf{q})\rangle \qquad S^z(\mathbf{q}) = \sum_r e^{i\mathbf{q}\cdot\mathbf{r}} S^z(\mathbf{r})$$



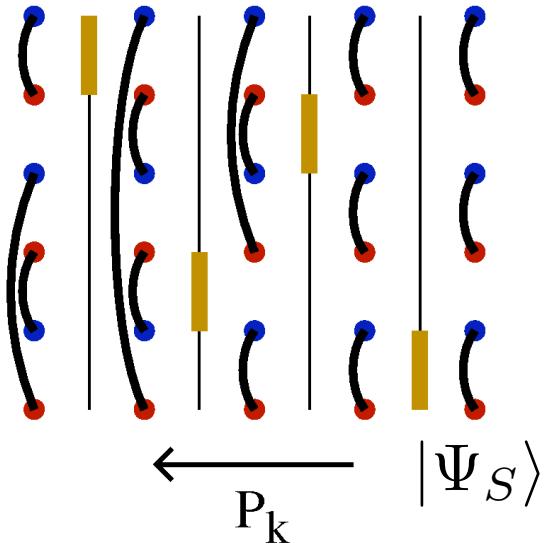
Triplets with arbitrary momentum can be created

- but phases cause problems in sampling
- in practice $\mathbf{q}$ close to $(0,0)$ and $(\pi,\pi)$ are accessible
- no phases factors corresponds to $(\pi,\pi)$

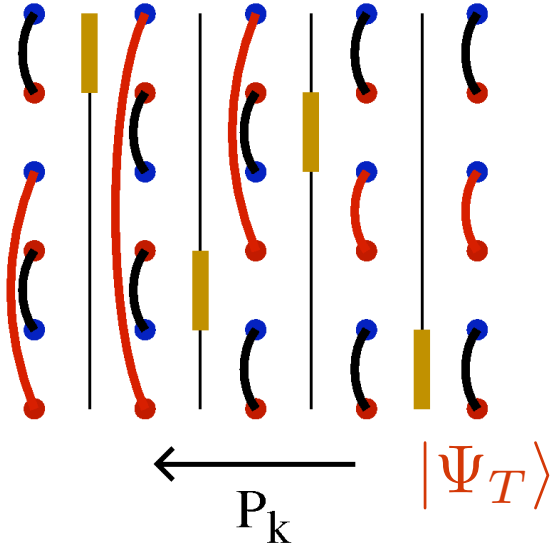
$$= (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$$

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

Singlet propagation




Triplet propagation

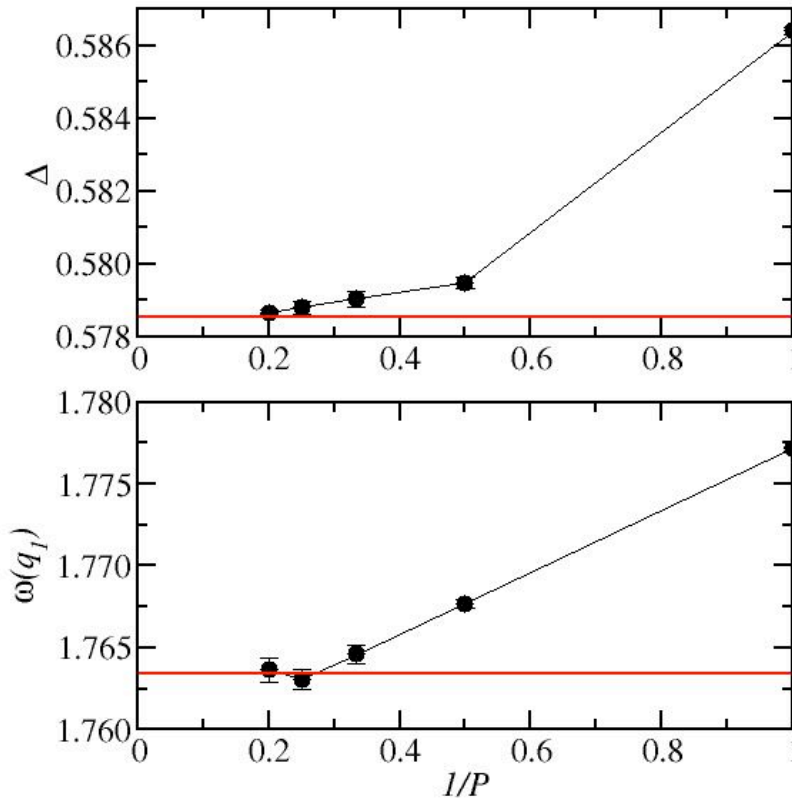


## **TEST:** Dispersion ω(q) for 2D Heisenberg antiferromagnet

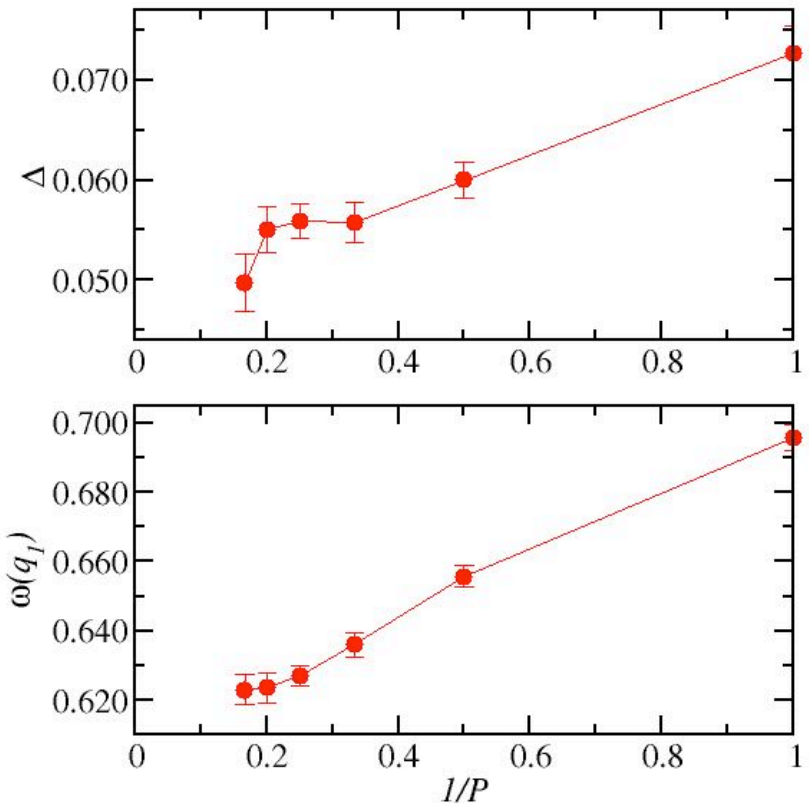
- Singlet-triplet gap: $\Delta = E_T(\pi,\pi) - E_S(0,0)$
- Dispersion close to q=(π,π): $\omega(q) = E_T(q) - \Delta$

  $q_1 = (\pi,\pi) - (2\pi/L, 0)$

$4 \times 4$ lattice




$16 \times 16$ lattice




P=2n/L$^2$
projecting with H$^n$

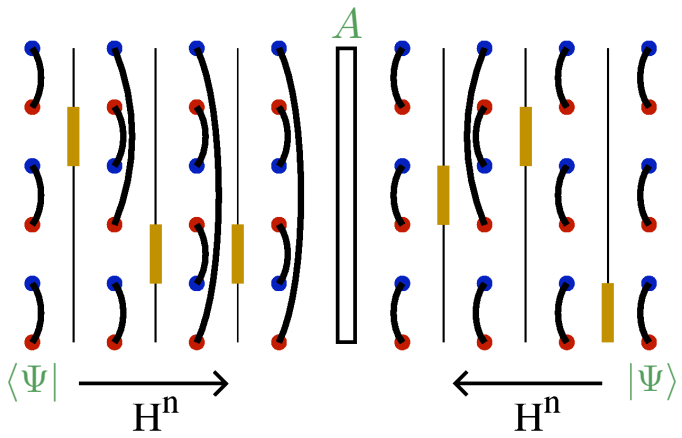
# Loop updates in the valence-bond basis

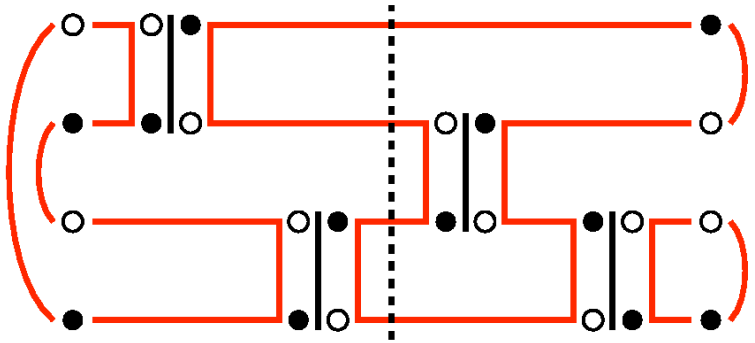
AWS and H. G. Evertz, ArXiv:0807.0682

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



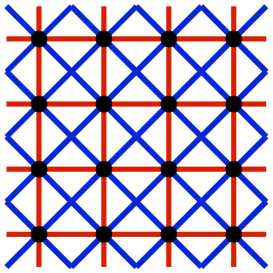



Loop updates similar to those in finite-T methods
(world-line and stochastic series expansion methods)

Larger systems accessible

# A challenging problem: frustrated quantum spins

$$H = \sum_{\langle i,j \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

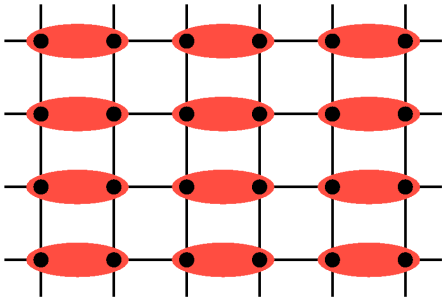


$$= J_1$$

$$= J_2$$

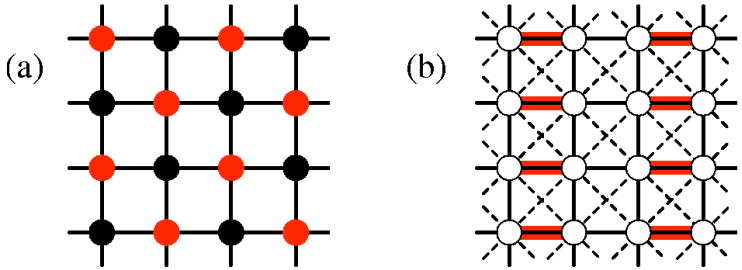
What is the ground state for $J_2/J_1 \approx 1/2$?

- Most likely a **Valence-bond-solid** (crystal)



- No spin (magnetic) order
- Broken translational symmetry

$$= (|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle)/\sqrt{2}$$



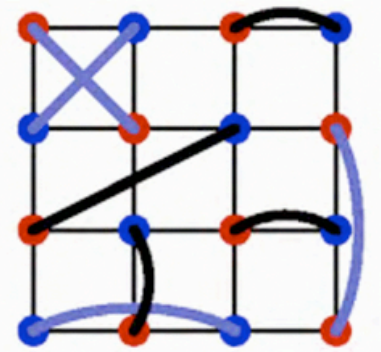

Quantum phase transition between Neel and VBS state expected at $J_2/J_1 \approx 0.45$

- but difficult to study in this model
- exact diagonalization only up to 40 spins
- QMC sign problems
- tensor-network methods promising

# Frustrated systems

Consider the full valence-bond basis, including

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

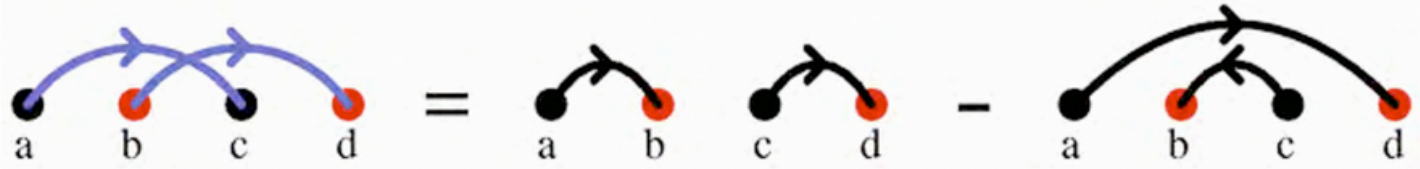


## For a non-frustrated system

- 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

**The over-completeness allows for a reduction of the sign problem**

[Kevin Beach; next talk]

# Is there a sign-free model with similar physics?

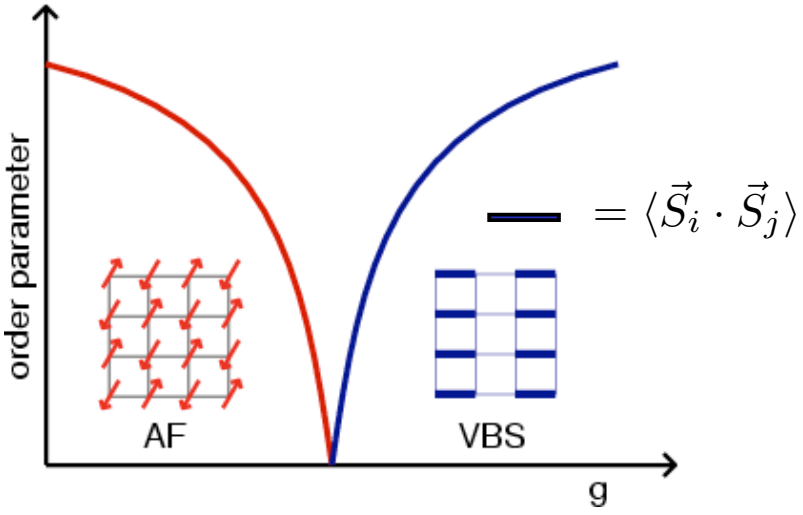
## 2D Heisenberg model with 4-spin term

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


➢ No sign problems in QMC simulations

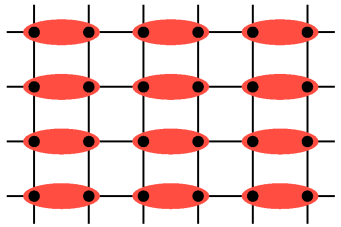
➢ Turns out to have a Neel-VBS transition for J/Q≈0.04

AWS, PRL 98, 227202 (2007)




- **Is the transition continuous?**
  - deconfined quantum-criticality?
    Senthil et al., Science 303, 1490 (2004)
  - good scaling seen in QMC
    AWS, PRL 07, Melko & Kaul, PRL 08
  - weakly 1st order argued by
    Jiang et al., JSTAT 08
    Kuklov et al., PRL 08
- **What is the nature of the VBS state?**
  - plaquette or columnar?
  - emergent U(1) symmetry?

# VBS phase in the J-Q model

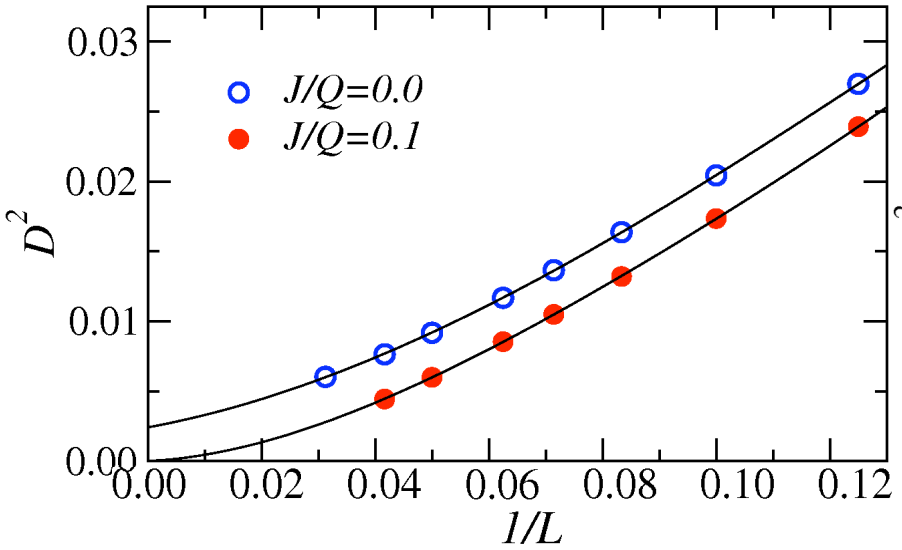


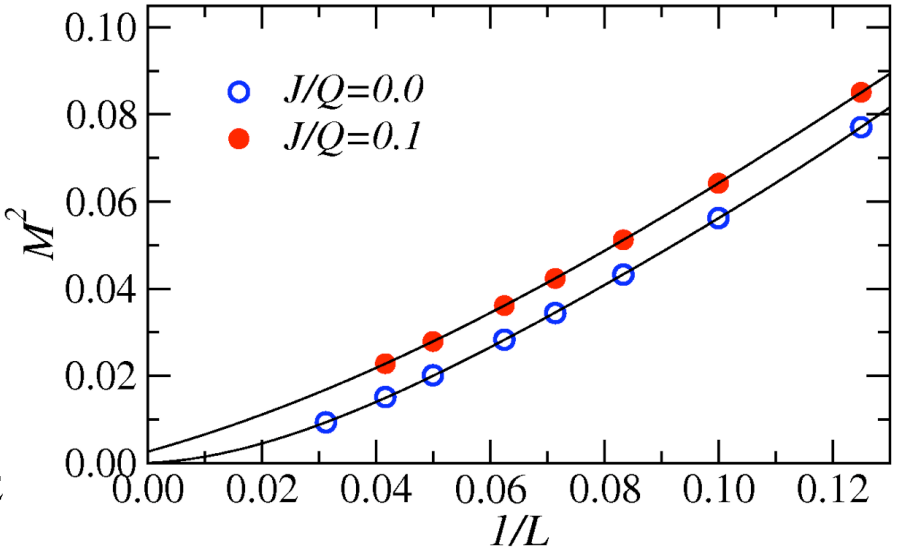
- VBS order parameter
  columnar dimer-dimer correlations

$$D^2 = \langle D_x^2 + D_y^2 \rangle, \quad D_x = \frac{1}{N}\sum_{i=1}^{N}(-1)^{x_i}\mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}}, \quad D_y = \frac{1}{N}\sum_{i=1}^{N}(-1)^{y_i}\mathbf{S}_i \cdot \mathbf{S}_{i+\hat{y}}$$

- AF (Nèel) order parameter
  sublattice magnetization

$$M^2 = \langle \vec{M} \cdot \vec{M} \rangle \qquad \vec{M} = \frac{1}{N}\sum_{i}(-1)^{x_i+y_i}\vec{S}_i$$



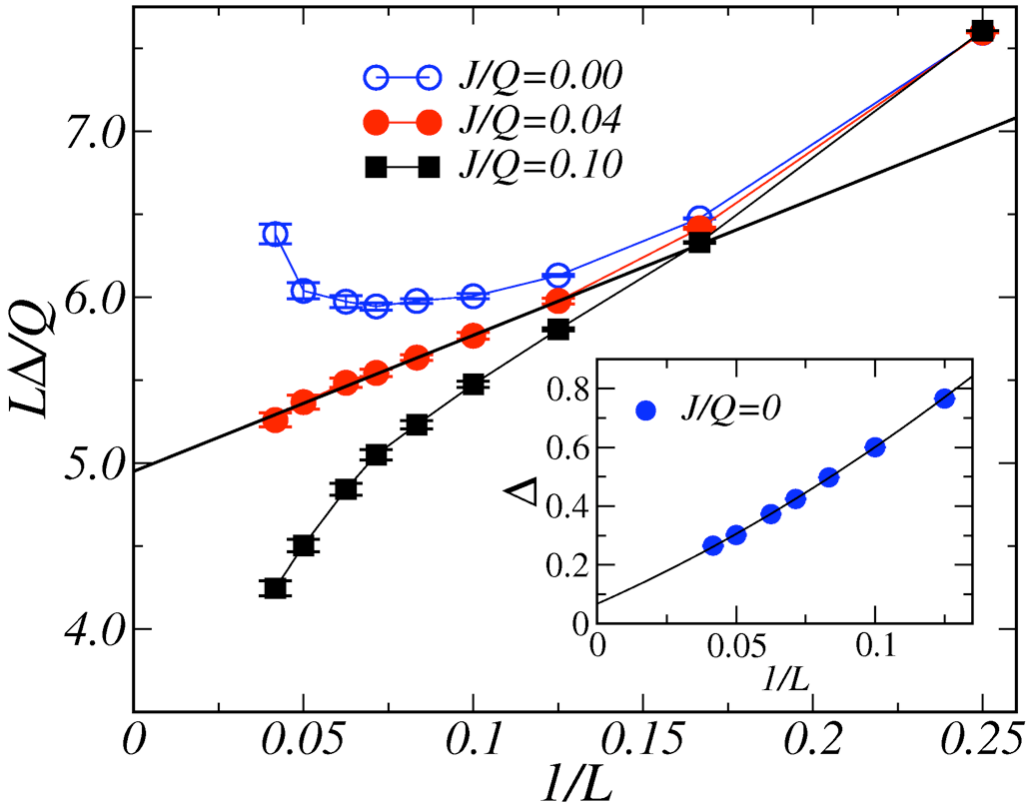

➤ J/Q=0.0 → VBS ➤ J/Q=0.1 → antiferromagnet

# Singlet-triplet gap scaling → Dynamic exponent z

z relates length and time scales:

$\omega_q \sim |q|^z$ finite size → $\Delta \sim L^{-z}$

Finite-size scaling of $L\Delta$




The gap at J=0 is small;

Δ/Q=0.07

The VBS is near-critical

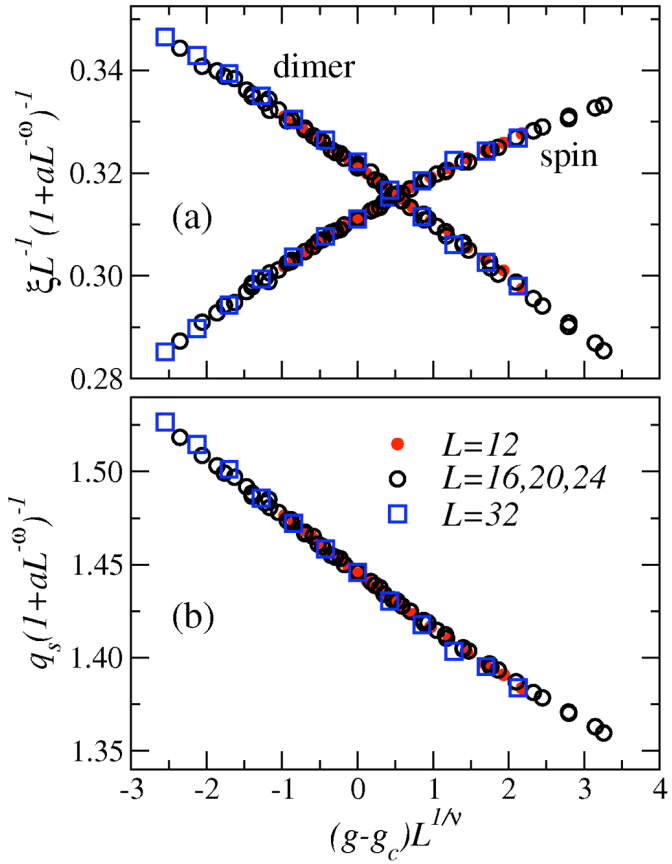
Critical gap scaling: $\Delta(L) = \frac{a_1}{L} + \frac{a_2}{L^2} + \cdots \quad \Rightarrow z = 1$

# Exponents; finite-size scaling

Correlation lengths (spin, dimer): $\xi_{s,d}$

Binder ratio (for spins): $q_s = \langle M^4 \rangle / \langle M^2 \rangle^2$

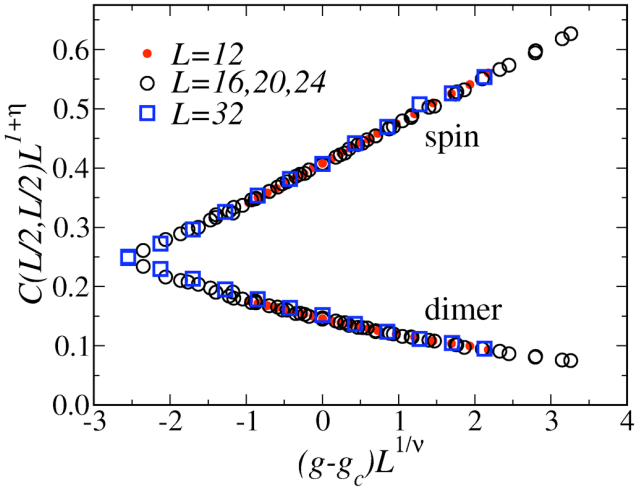
long-distance spin and dimer correlations: $C_{s,d}(L/2, L/2)$




All scale with a single set of critical exponents at $g_c \approx 0.04$

(with subleading corrections)

$$\nu = 0.78(3), \quad \eta = 0.26(3)$$

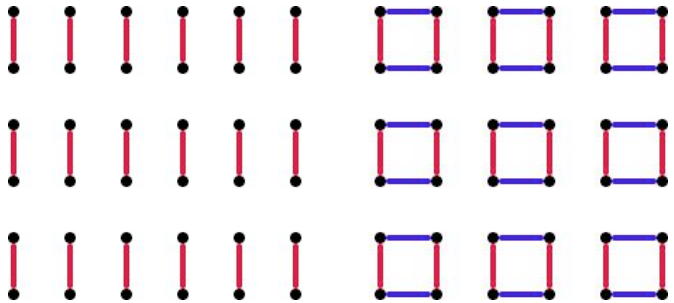


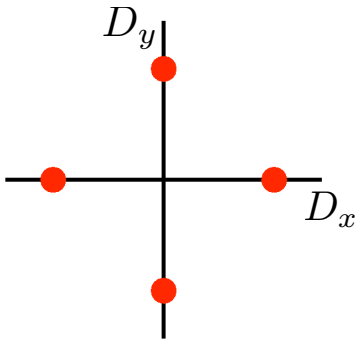

z=1, $\eta \approx 0.3$: consistent with deconfined quantum-criticality

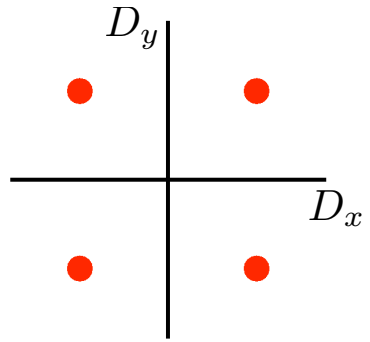
- z=1 field theory and "large" $\eta$ predicted (Senthil et al.)

**What kind of VBS; columnar or plaquette?**

➪ look at joint probability distribution P(Dx,Dy)





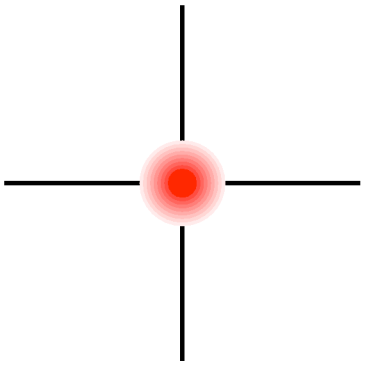

The simulations sample the ground state;

$$|0\rangle = \sum_k c_k |V_k\rangle$$

Graph joint probability distribution $P(D_x, D_y)$

$$D_x = \frac{\langle V_k | \frac{1}{N} \sum_{i=1}^{N} (-1)^{x_i} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}} | V_p \rangle}{\langle V_k | V_p \rangle}$$

$$D_y = \frac{\langle V_k | \frac{1}{N} \sum_{i=1}^{N} (-1)^{y_i} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{y}} | V_p \rangle}{\langle V_k | V_p \rangle}$$

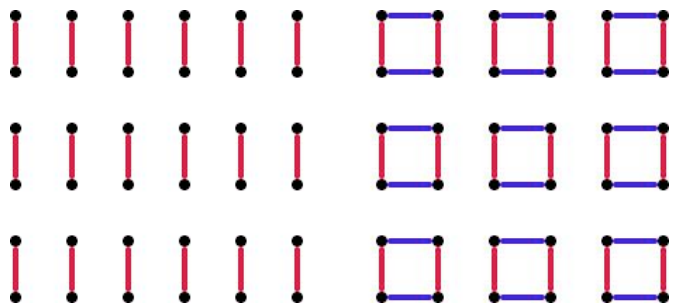


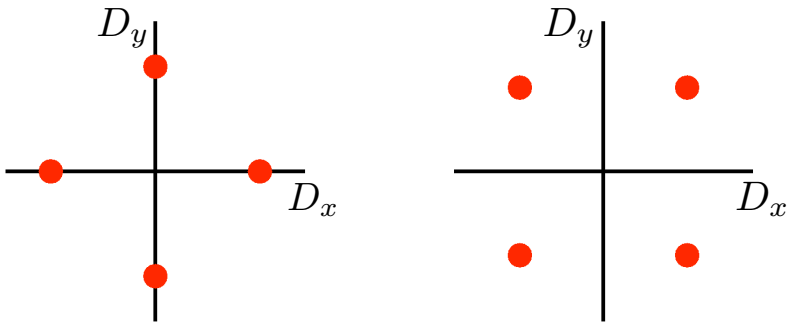
critical

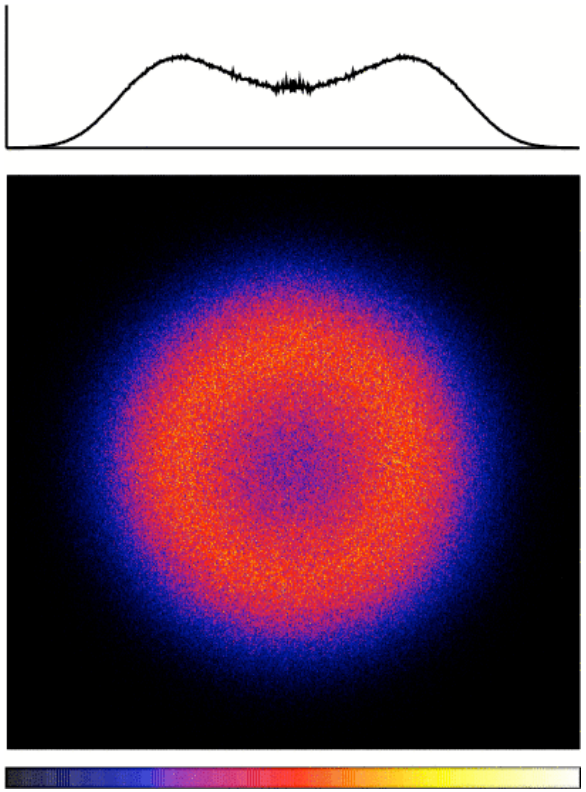
➪ 4 peaks expected; Z4-symmetry unbroken in finite system

**VBS fluctuations** in the theory of deconfined quantum-critical points

- ➢ plaquette and columnar VBS "degenerate" at criticality
- ➢ $Z_4$ "lattice perturbation" irrelevant at critical point
  - and in the VBS phase for $L<\Lambda\sim\xi^a$, $a>1$
- ➢ **emergent U(1) symmetry**
- ➢ **ring-shaped distribution expected for $L<\Lambda$**





**J=0, L=32**

# SU(N) generalization of the J-Q model

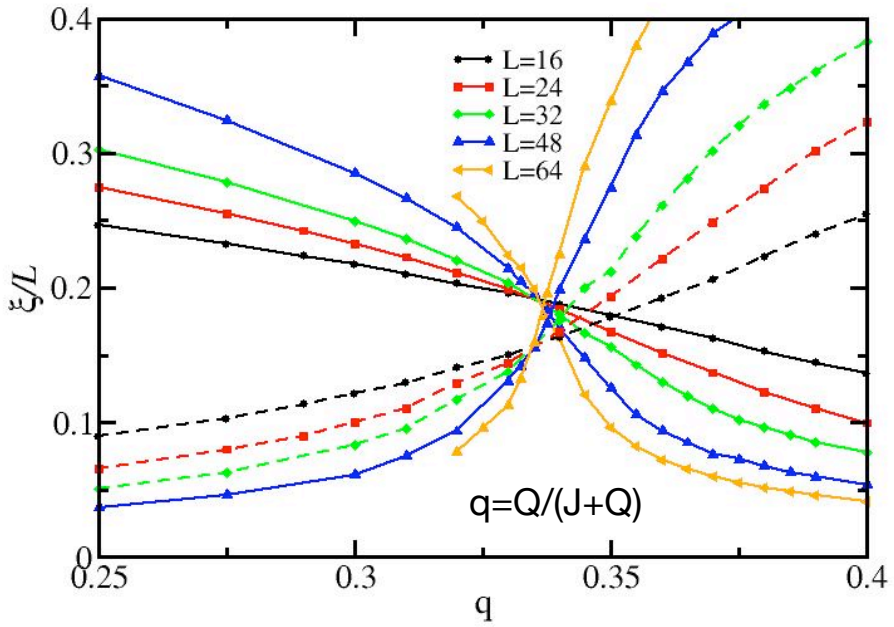
Heisenberg model with SU(N) spins has VBS state for large N

- Hamiltonian projecting on SU(N) singlets
- In large-N mean-field theory Nc≈5.5 (Read & Sachdev, PRL 1988)
- QMC gives Nc≈4.5 (Tanabe & Kawashima, PRL 2007)

The valence-bond loop projector QMC has a simple generalization

- Each loop has N “orientations”
- Stronger VBS order expected in SU(N) J-Q model

SU(3), spin and dimer correlation lengths



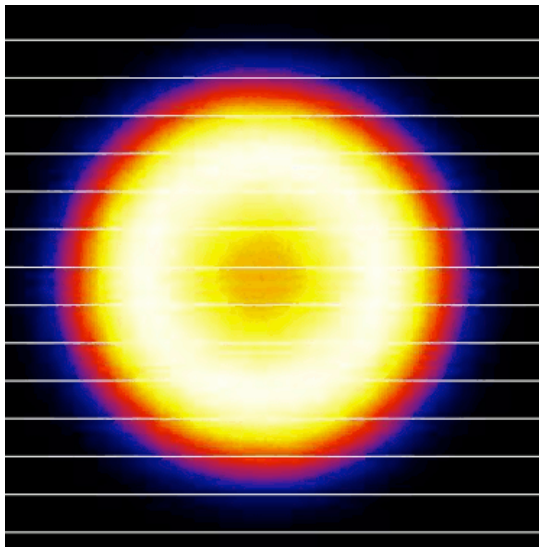

$$\nu \approx 0.65$$

$$\eta_{\mathrm{spin}} \approx \eta_{\mathrm{dimer}} \approx 0.40$$

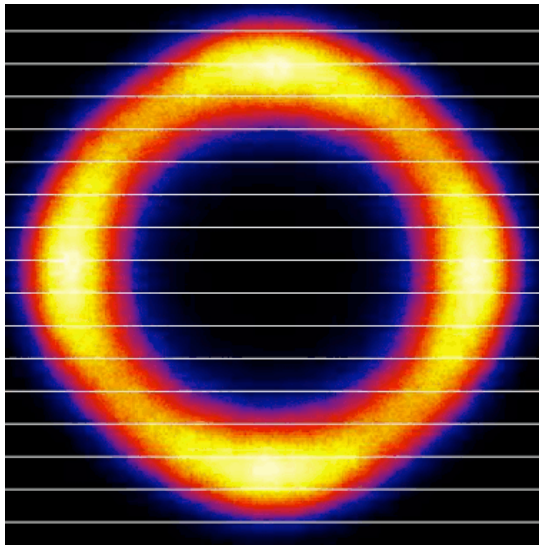
J. Lou, R. Kaul, N. Kawashima, AWS
(manuscript in preparation)

## Order parameter histograms

$L = 16, q = 0.4$



$L = 16, q = 0.6$

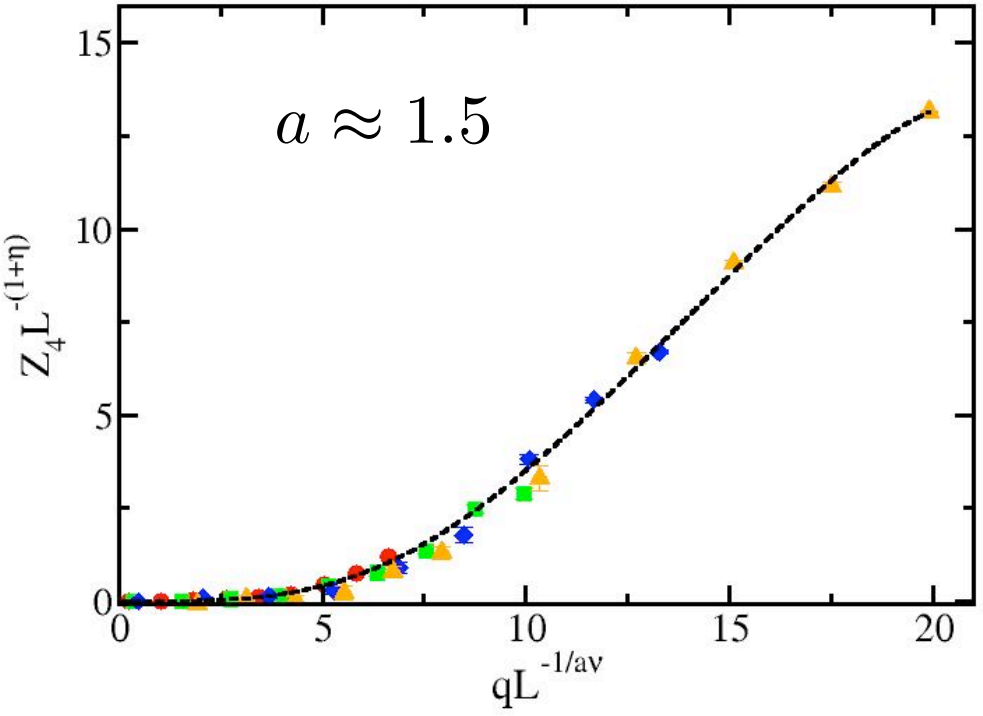


Symmetry cross-over

$$D_4 = \int r dr \int d\phi P(r,\phi)\cos(4\phi)$$

Finite-size scaling gives length-scale

$$\Lambda \sim \xi^a \sim q^{-a\nu}$$



## Summary & Conclusions

Simulation methods in the valence bond basis

- May be the most efficient tools for studying ground state of many unfrustrated quantum spin models

Unfrustrated multi-spin interactions

- J-Q model and wide range of generalizations
- Give unprecedented access to VBS states and transitions