Mahabaleshwar Condensed Matter School, December 5-12, 2009

Neel (AF) to valence-bond-solid (VBS) quantum phase transition in two dimensions

Anders W. Sandvik, Boston University

Extended Heisenberg models (“J-Q” models) with AF-VBS transitions

The “deconfined” quantum-criticality scenario

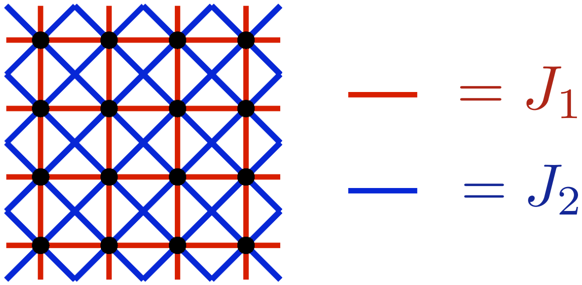
QMC simulations in the valence-bond basis; finite-size scaling results

Emergent U(1) symmetry and U(1)-Z_4 symmetry cross-over

Detection of spinon confinement/deconfinement

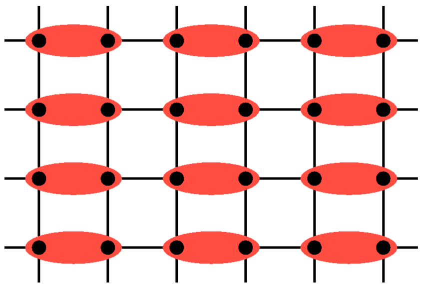
- triplet states in an extended valence-bond basis
- tests in 1D; ladders (2 coupled chains)
- preliminary results for J-Q model

A challenging problem: frustrated quantum spins



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

- ground state for $g=J_2/J_1 \approx 1/2$ is most likely a VBS [Read & Sachdev (1989)]

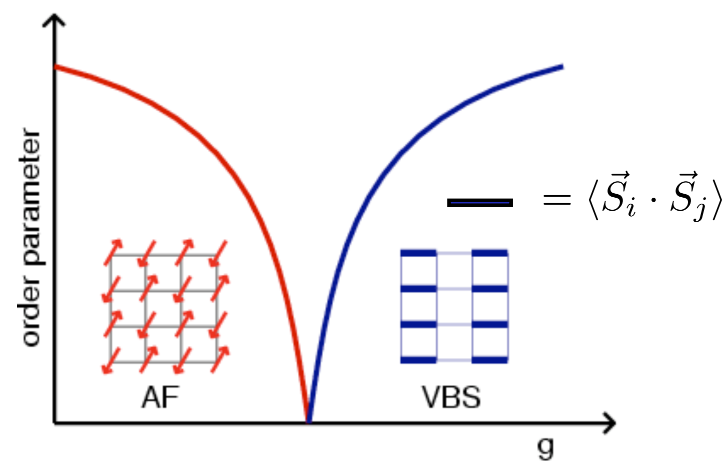


- No spin (magnetic) order
- Broken translational symmetry

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

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

- but difficult to study in this model
- exact diagonalization only up to 6×6
- sign problems for QMC

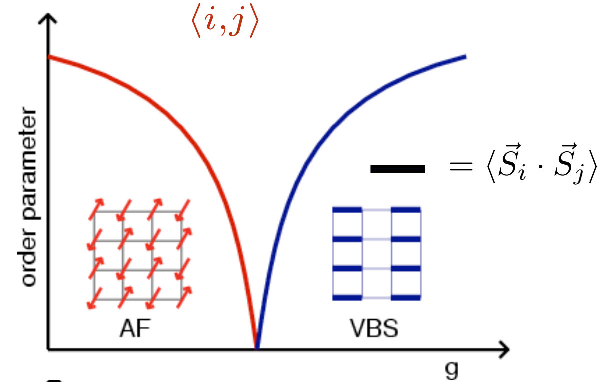


Are there models with AF-VBS transitions that do not have QMC sign problems?

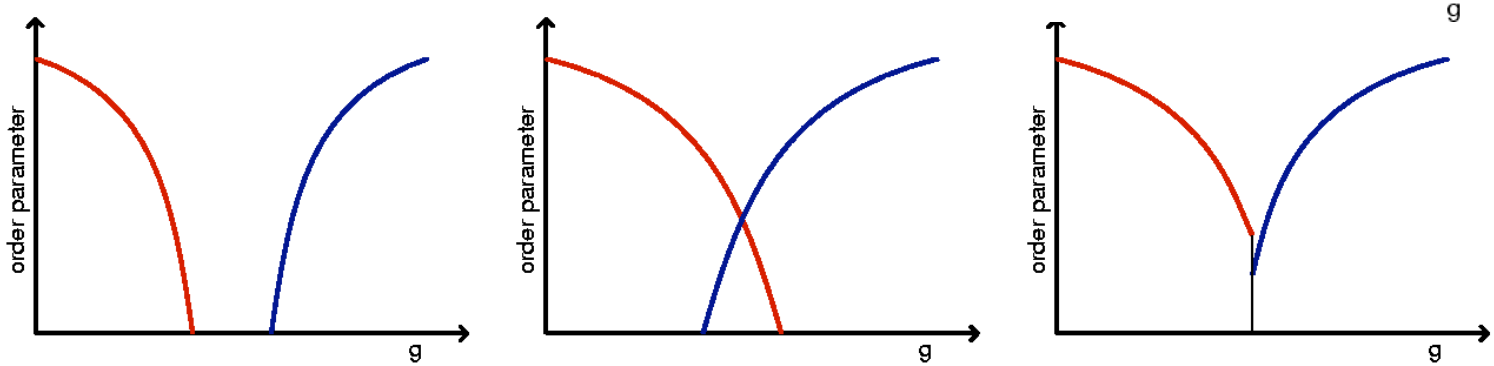
Deconfined quantum criticality

Senthil, Vishwanath, Balents, Sachdev, Fisher,
Science 303, 1490 (2004)

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \; g \; \ldots$$

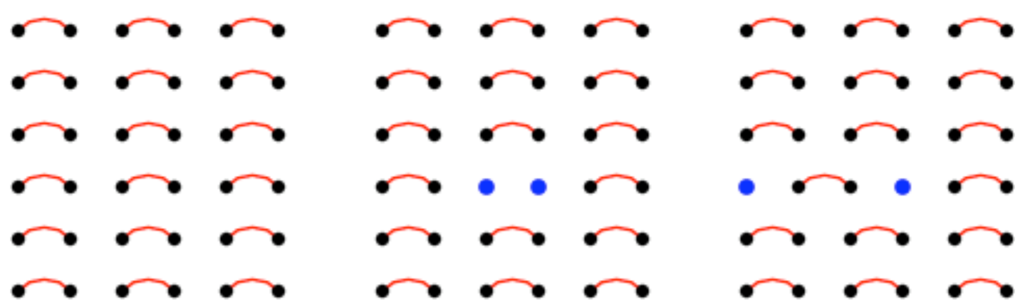


Generic continuous AF-VBS transition
- beyond the Landau-Ginzburg paradigm (generically continuous AF-VBS transition)



Spinon deconfinement at the critical point

Confinement inside VBS phase associated with new length scale and **emergent U(1) symmetry**
- how to study this numerically?
- in what models (hamiltonians)?

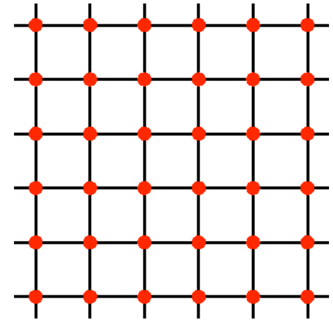


“angular” VBS fluctuations → new length scale
- U(1) - Z_4 cross-over length
- spinon confinement length

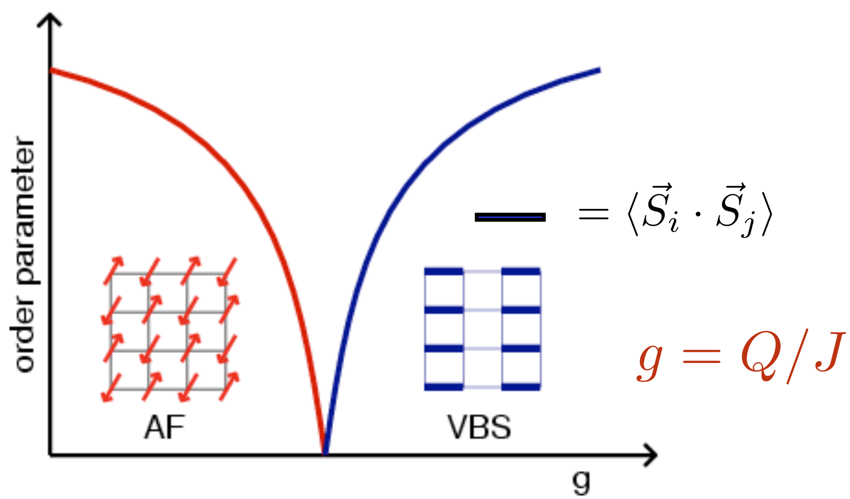
2D S=1/2 Heisenberg model with 4-spin interactions

AWS, Phys. Rev. Lett (2007)

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



- no sign problems in QMC simulations
- has an AF-VBS transition at J/Q≈0.04
- microscopic interaction not necessarily realistic for real materials
- macroscopic physics (AF-VBS transition) relevant for
  - testing and stimulating theories (e.g., quantum phase transitions)
  - there may already be an experimental realization of the critical point



In agreement with theory:

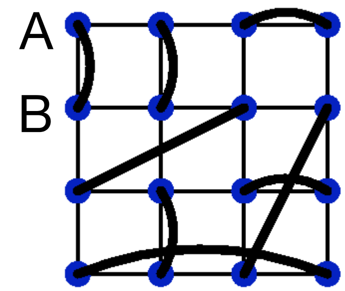
- dynamic exponent z=1
- “large” exponent η_{spin}
- emergent U(1) VBS symmetry

weakly 1st order argued by
Jiang et al., JSTAT, P02009 (2008)
Kuklov et al., PRL 101, 050405 (2008)

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

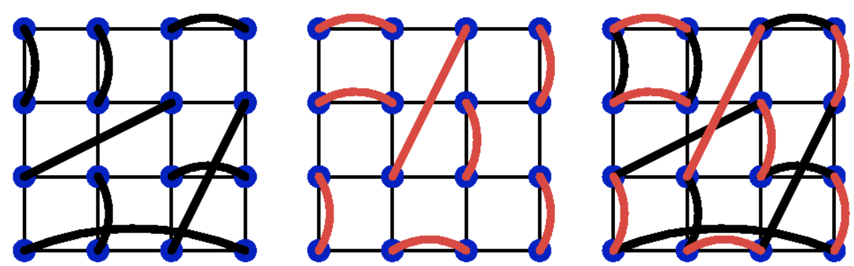
$$\langle V_l | V_r \rangle = 2^{N_\circ - N/2} \qquad N_\circ = \text{ number of loops in overlap graph}$$

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)



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

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

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

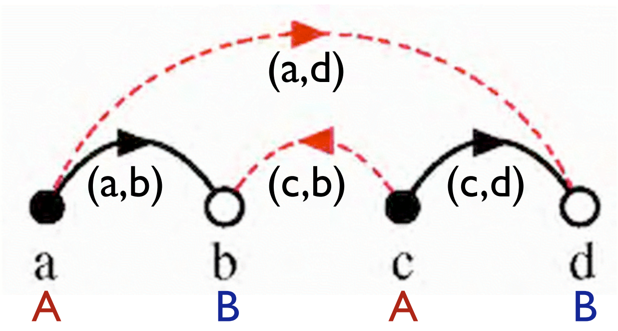
S=1/2 Heisenberg model

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

Project with string of bond operators

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

(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’ convetion
- sign problem does appear for frustrated systems

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

Strings of singlet projectors

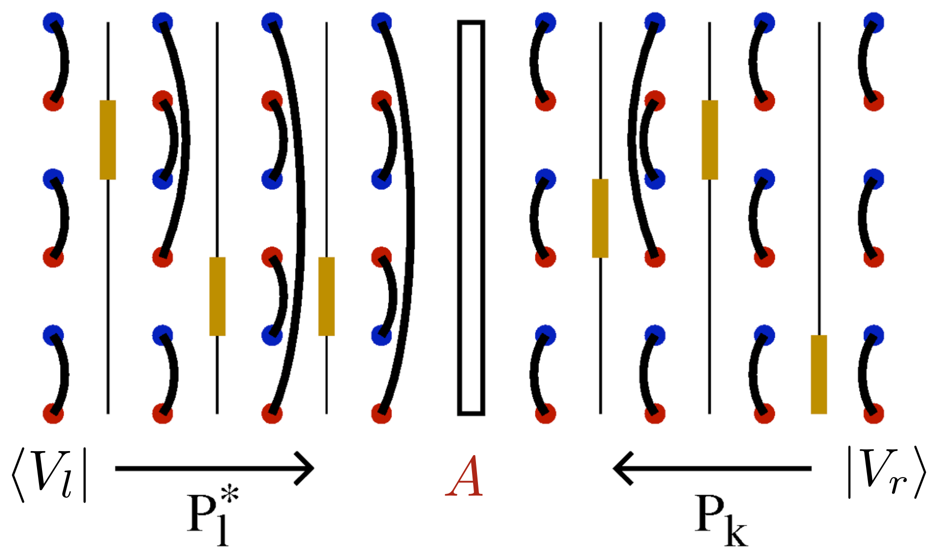
$$P_k = \prod_{p=1}^{n} H_{i_k(p)j_k(p)}, \quad k = 1, \ldots, N_b^n \quad (N_b = \text{number of interaction bonds})$$

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

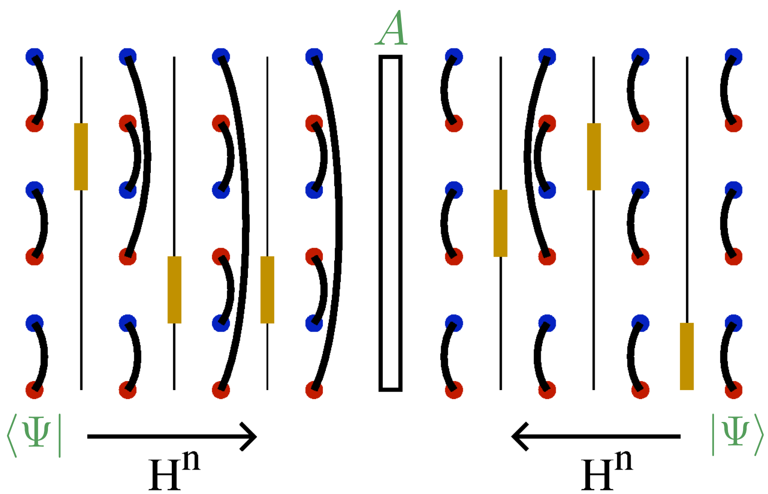
Loop updates in the valence-bond basis

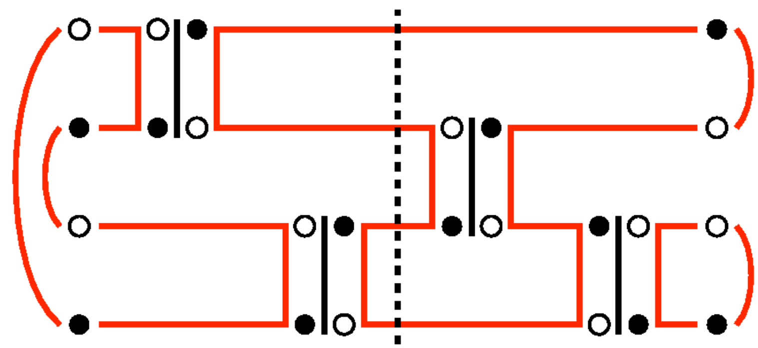
AWS and H. G. Evertz, ArXiv:0807.0682

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)

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

T=0 results with the improved valence-bond algorithm

J. Lou, A.W. Sandvik, N. Kawashima, PRB (2009)

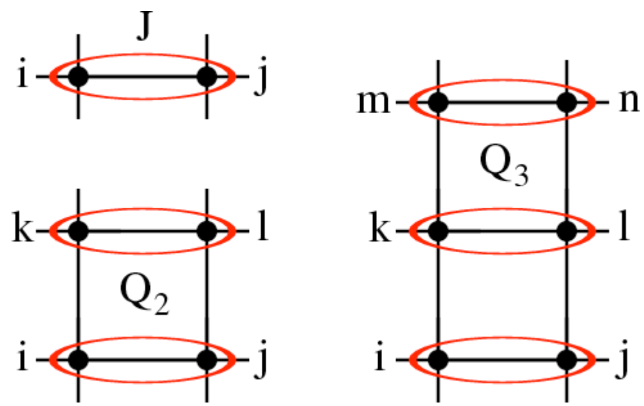
Universal exponents? Two different models: **J-Q_2 and J-Q_3**

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

$$H_1 = -J \sum_{\langle ij \rangle} C_{ij}$$

$$H_2 = -Q_2 \sum_{\langle ijkl \rangle} C_{kl} C_{ij}$$

$$H_3 = -Q_3 \sum_{\langle ijklmn \rangle} C_{mn} C_{kl} C_{ij}$$

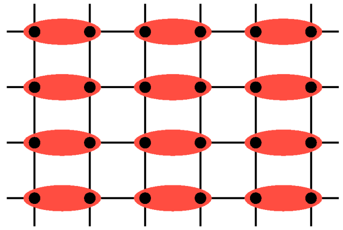


Studies of J-Q_2 model and J-Q_3 model on L×L lattices with L up to 64

Exponents η_s, η_d, and ν from the squared order parameters

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

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



coupling ratio

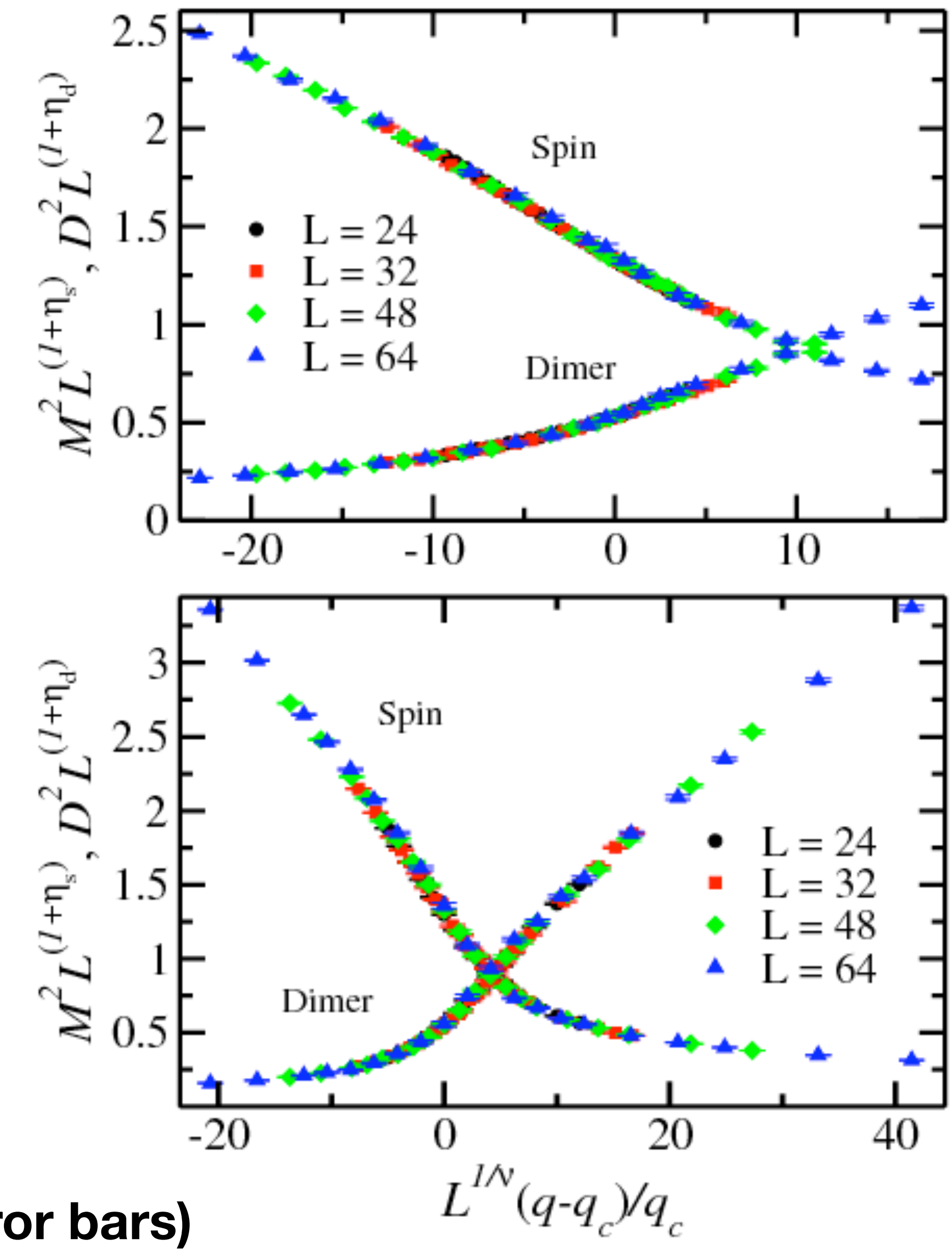
$$q = \frac{Q_p}{Q_p + J}, \qquad p = 2, 3$$

J-Q$_2$ model; q$_c$=0.961(1)

$$\eta_s = 0.35(2)$$
$$\eta_d = 0.20(2)$$
$$\nu = 0.67(1)$$

J-Q$_3$ model; q$_c$=0.600(3)

$$\eta_s = 0.33(2)$$
$$\eta_d = 0.20(2)$$
$$\nu = 0.69(2)$$



Exponents universal (within error bars)

- still higher accuracy desired (in progress)

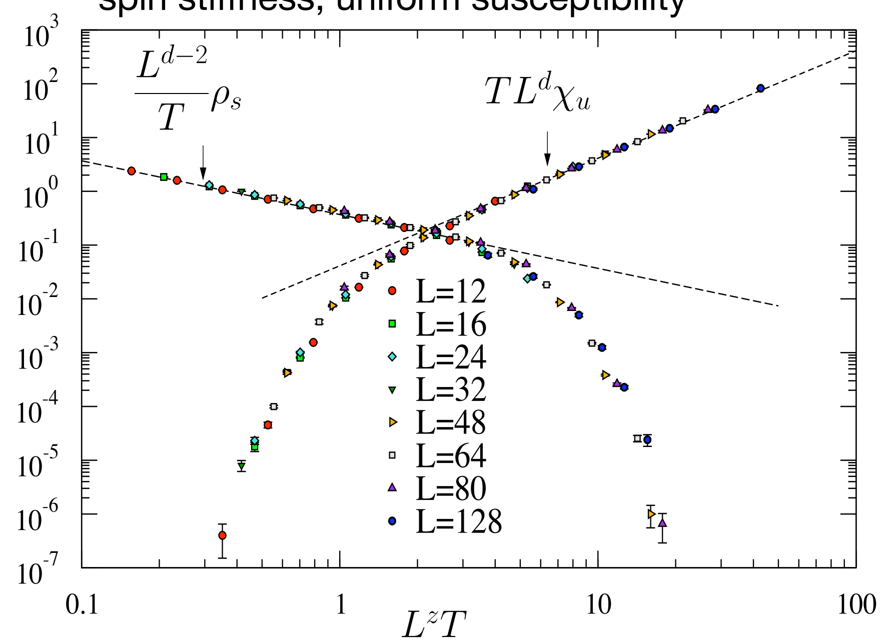
T,L scaling properties

R. G. Melko and R. Kaul, PRL 100, 017203 (2008)

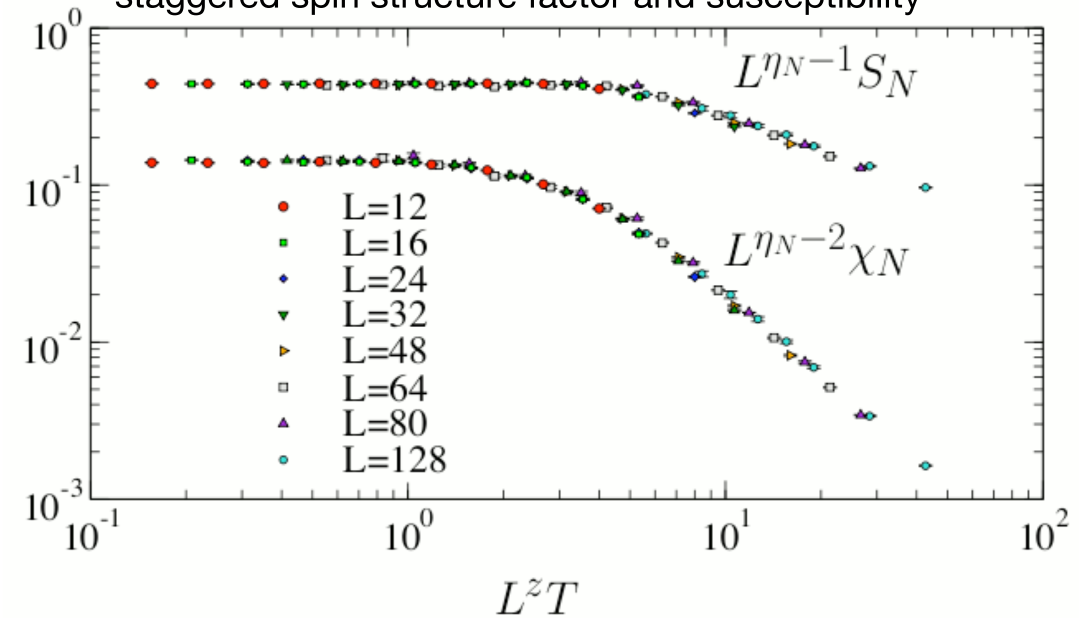
Additional confirmation of a critical point

- using finite-T SSE
- larger systems (because T>0)
- good agreement on critcal Q/J

spin stiffness, uniform susceptibility



staggered spin structure factor and susceptibility



$$z = 1, \eta \approx 0.35$$

Could the transition be first-order?

First-order transition argued for (vigorously) by

Jiang, Nyfeler, Chandrasekharan, Wiese, JSTAT, P02009 (2008)

Kuklov, Matsumoto, Prokof'ev, Svistunov, Troyer, PRL 101, 050405 (2008)

Let's look at a well known signal of first-order transition:

Binder ratio

$$Q_2 = \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2}$$

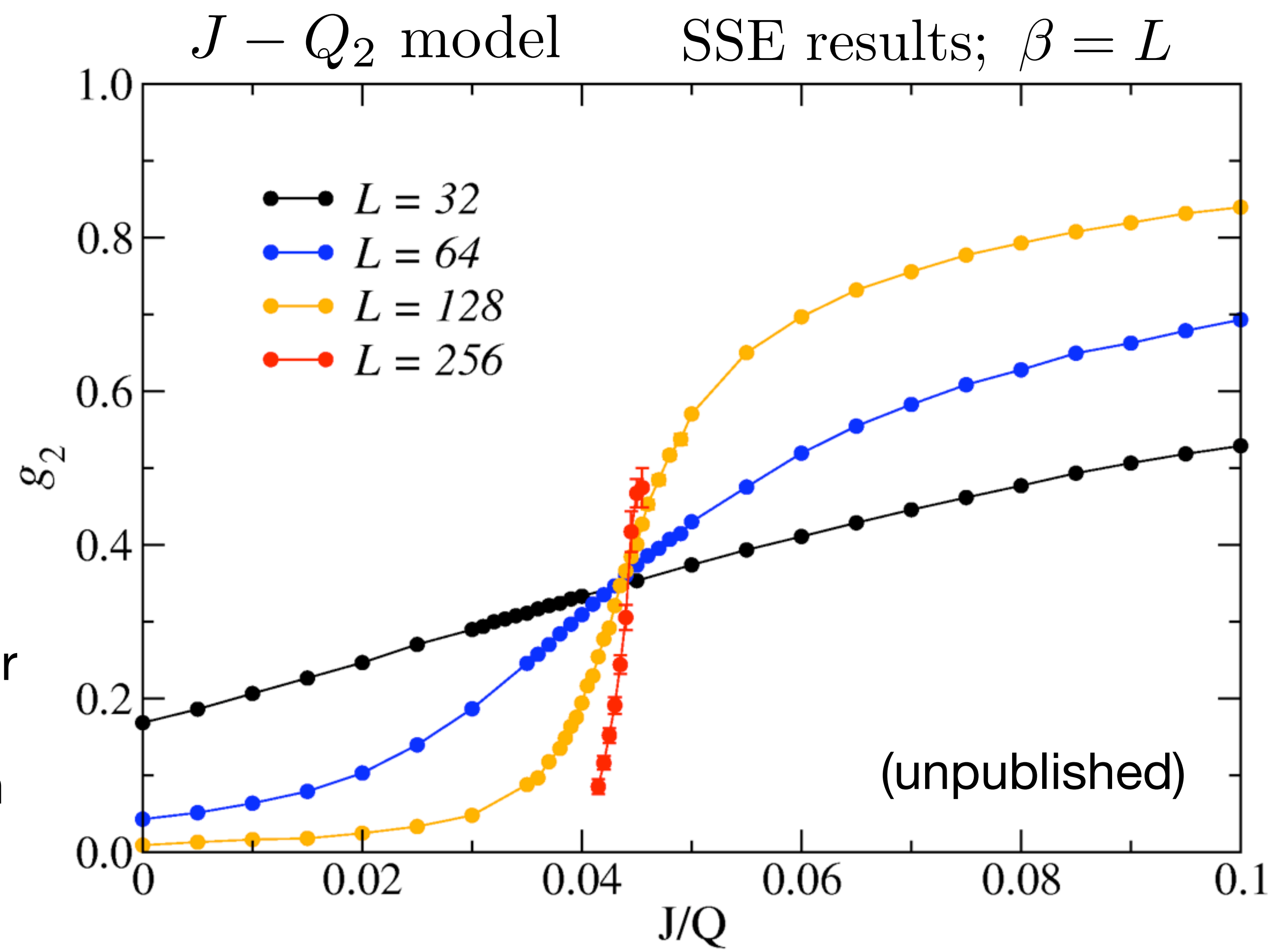
Binder cumulant

$$g_2 = (5 - 3Q_2)/2$$

Size independent (curve crossings) at criticality

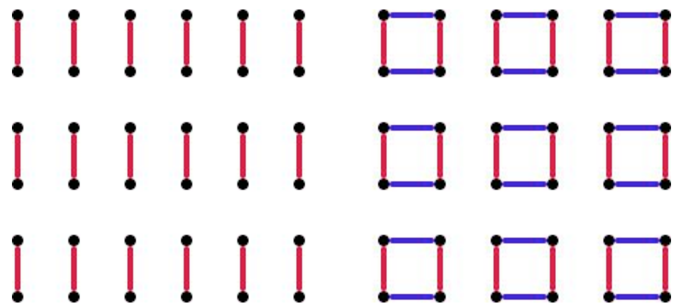
$g_2 < 0$ at a first-order transition

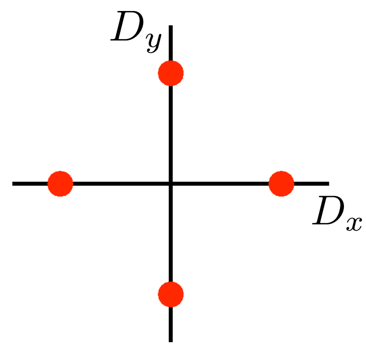
- no signs of $g_2<0$ in SSE results for L up to 256

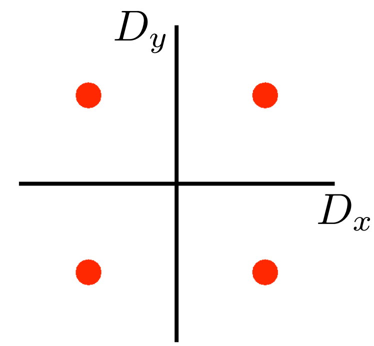


What kind of VBS; columnar or plaquette?

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

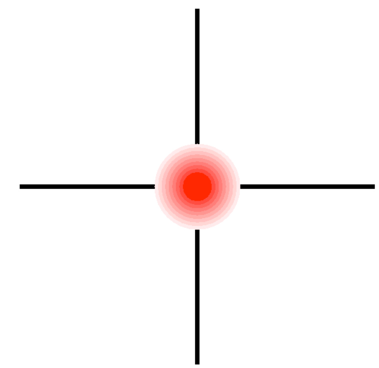






The simulations sample the ground state;

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



critical

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

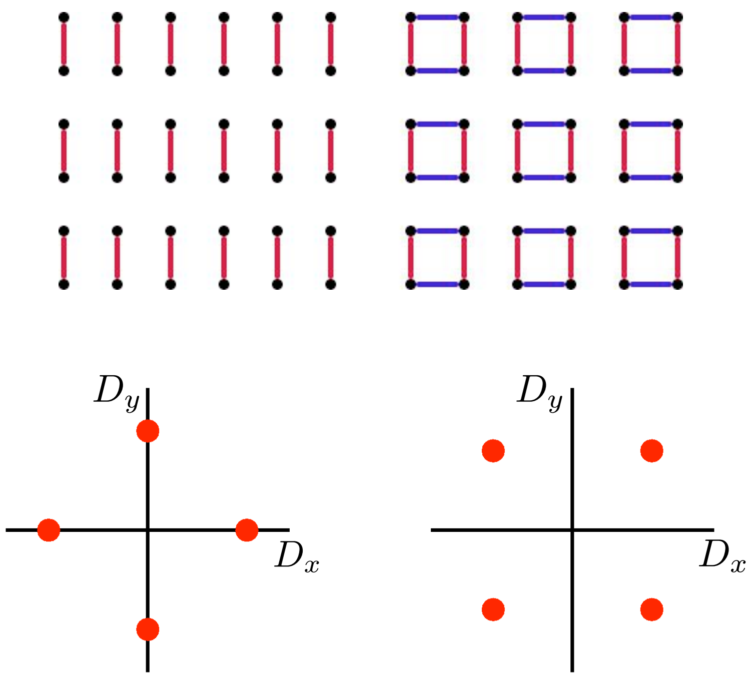
$$D_x = \frac{\langle V_k | \frac{1}{N} \sum_{i=1}^{N} (-1)^{x_i} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}} | V_p \rangle}{\langle V_k | V_p \rangle}$$

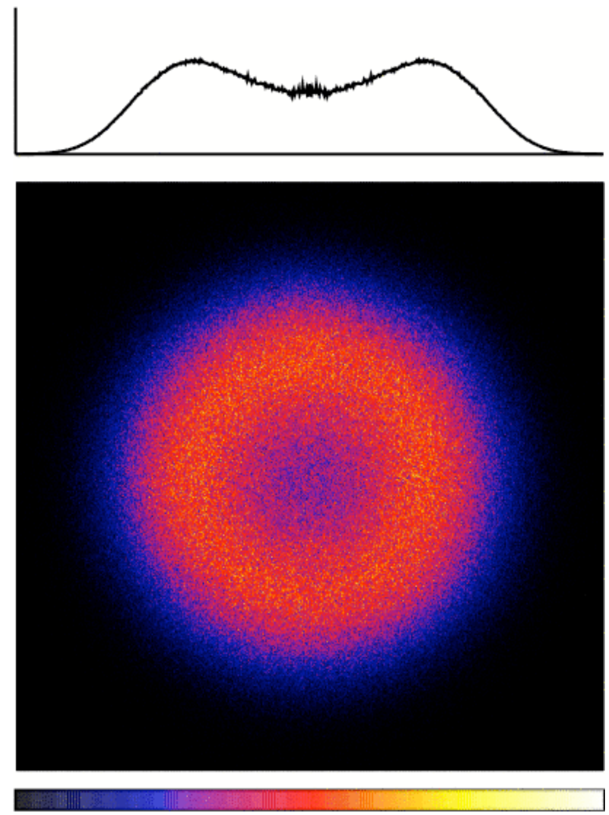
$$D_y = \frac{\langle V_k | \frac{1}{N} \sum_{i=1}^{N} (-1)^{y_i} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{y}} | V_p \rangle}{\langle V_k | V_p \rangle}$$

➪ 4 peaks expected; Z_4-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 $L<\Lambda\sim\xi^a$, $a>1$ (spinon confinement length)
- ➢ **emergent U(1) symmetry**
- ➢ **ring-shaped distribution expected for $L<\Lambda$**





L=32
J=0

No sign of cross-over to Z_4 symmetric order parameter seen in the J-Q_2 model

- length $\Lambda > 32$

AWS, Phys. Rev. Lett (2007)

Order parameter histograms $P(D_x,D_y)$, J-Q_3 model

J. Lou, A.W. Sandvik, N. Kawashima, PRB (2009)

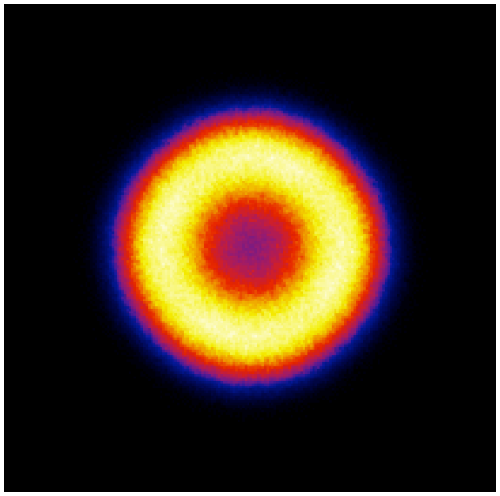
This model has a more robust VBS phase

- can the symmetry cross-over be detected?

$q = 0.635$

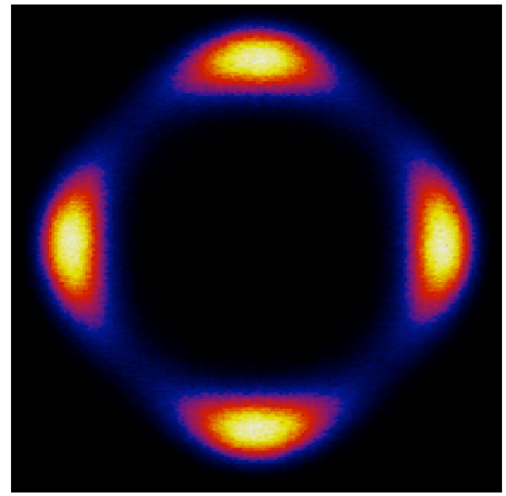
$(q_c \approx 0.60)$

$L = 32$



$q = 0.85$

$L = 32$



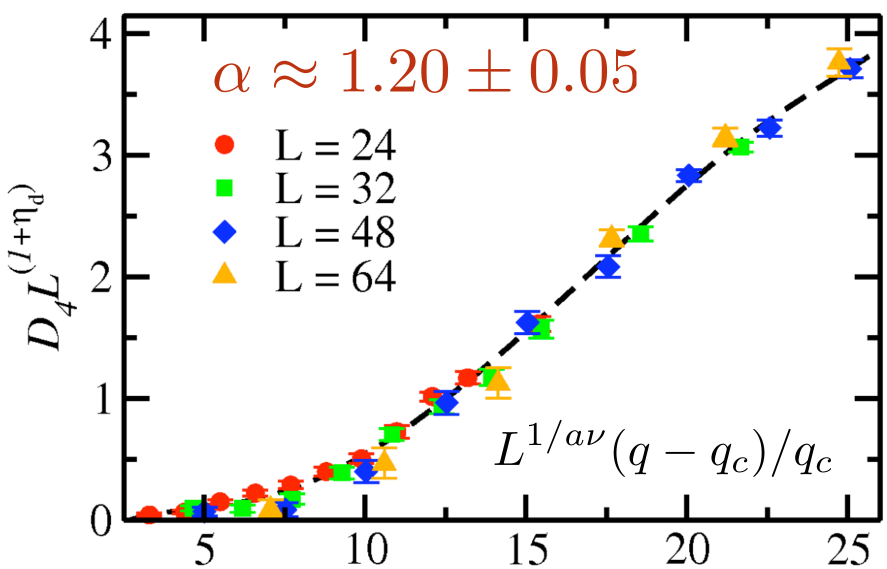
VBS symmetry cross-over

- Z_4-sensitive order parameter

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

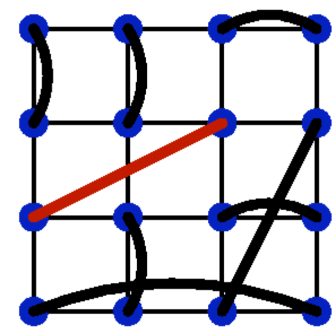
Finite-size scaling gives U(1) (deconfinement) length-scale

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

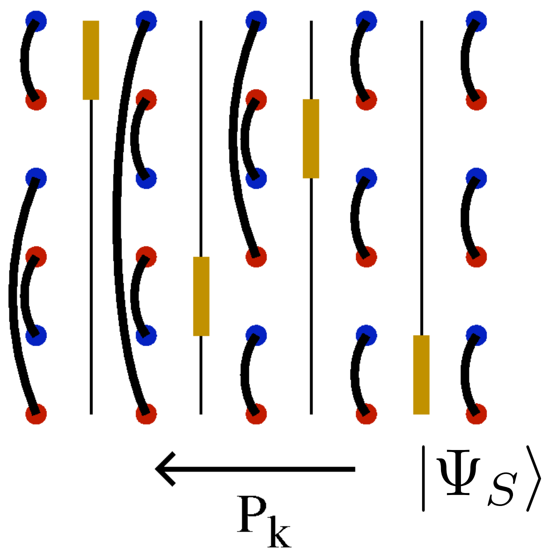


Is it possible to directly observe deconfinement of spinons?

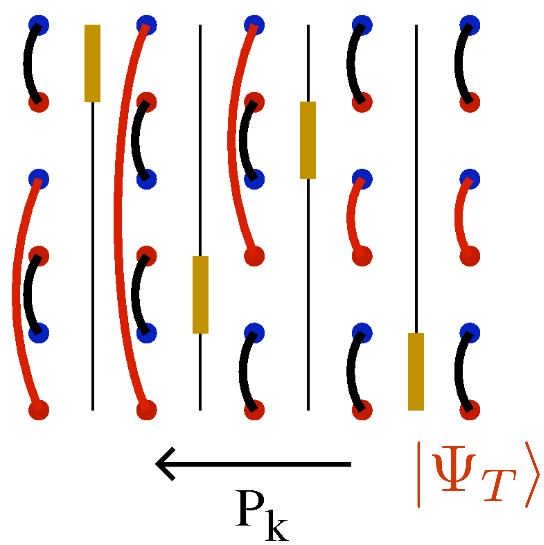
Valence bond projector method: direct access to the distribution of the triplet in an excited state



Singlet propagation



Triplet propagation



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

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

Creating a triplet corresponds to acting with S^z operators

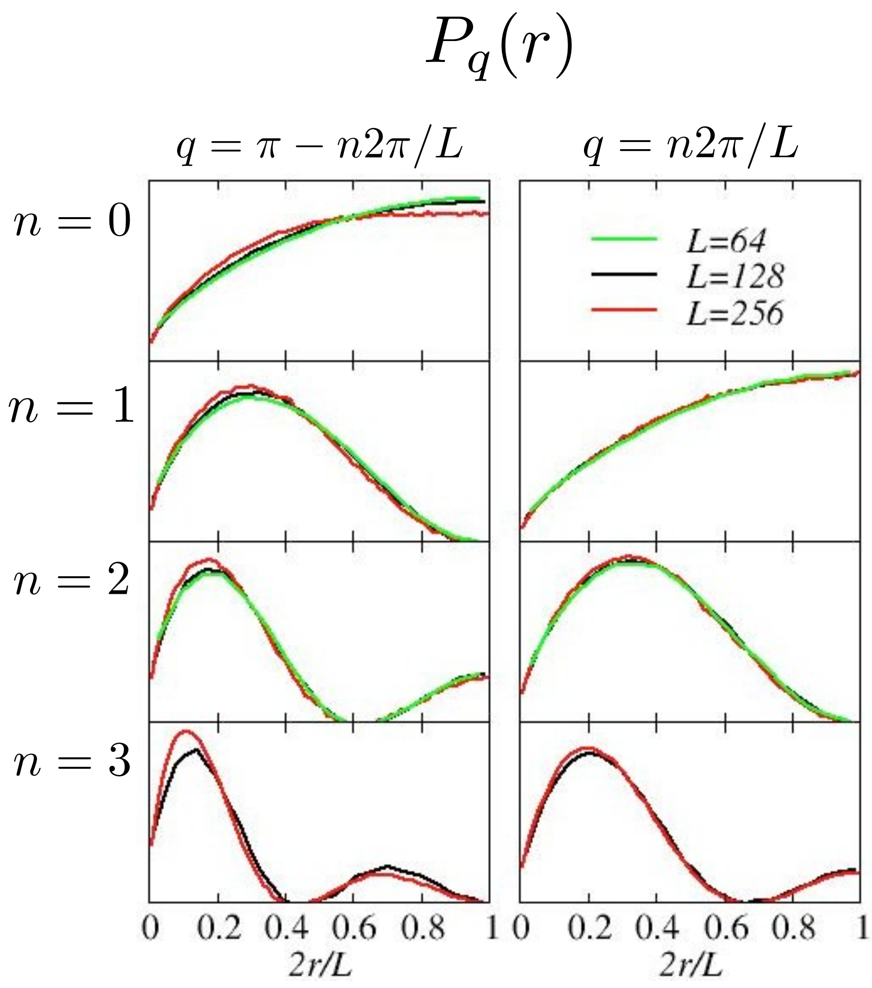
$$S^z(\mathbf{q})|\Psi_S(0)\rangle = |\Psi_T(\mathbf{q})\rangle \qquad S^z(\mathbf{q}) = \sum_r e^{i\mathbf{q}\cdot\mathbf{r}} S^z(\mathbf{r})$$

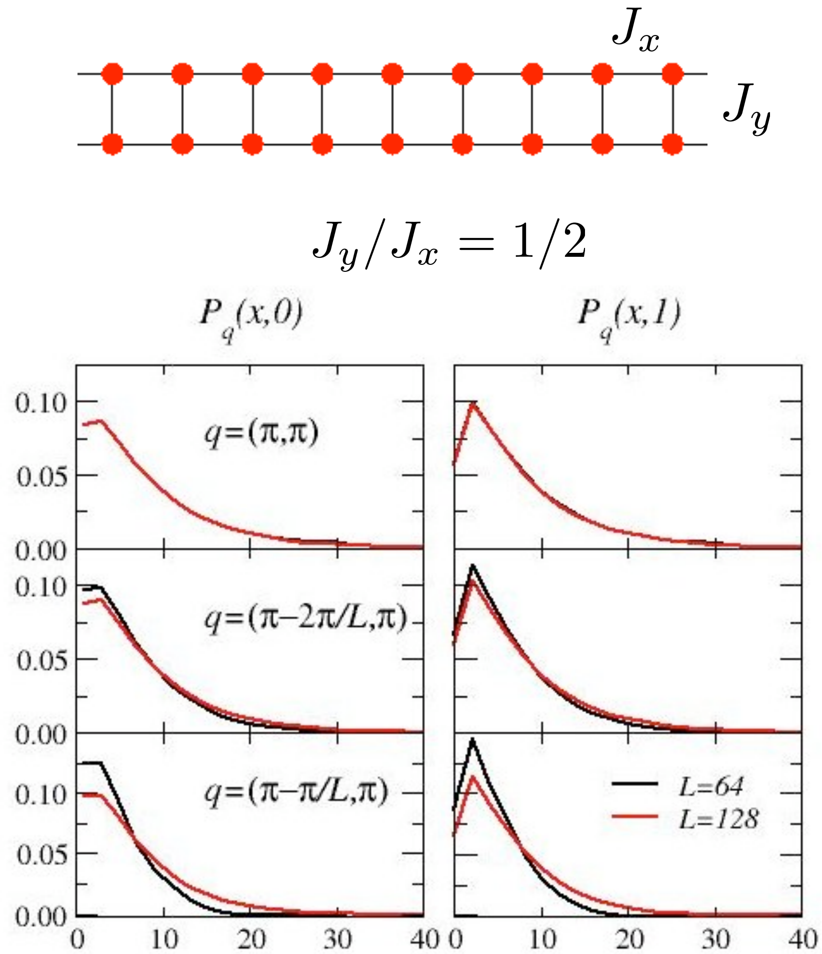
In principle triplets with arbitrary momentum can be studied

- but phases cause problems in sampling
- in practice q close to $(0,0)$ and (π,π) are accessible

Deconfinement of spinons in the 1D Heisenberg model

Probability distribution of the triplet bond length
- a triplet bond corresponds to two spinons; are they bound?

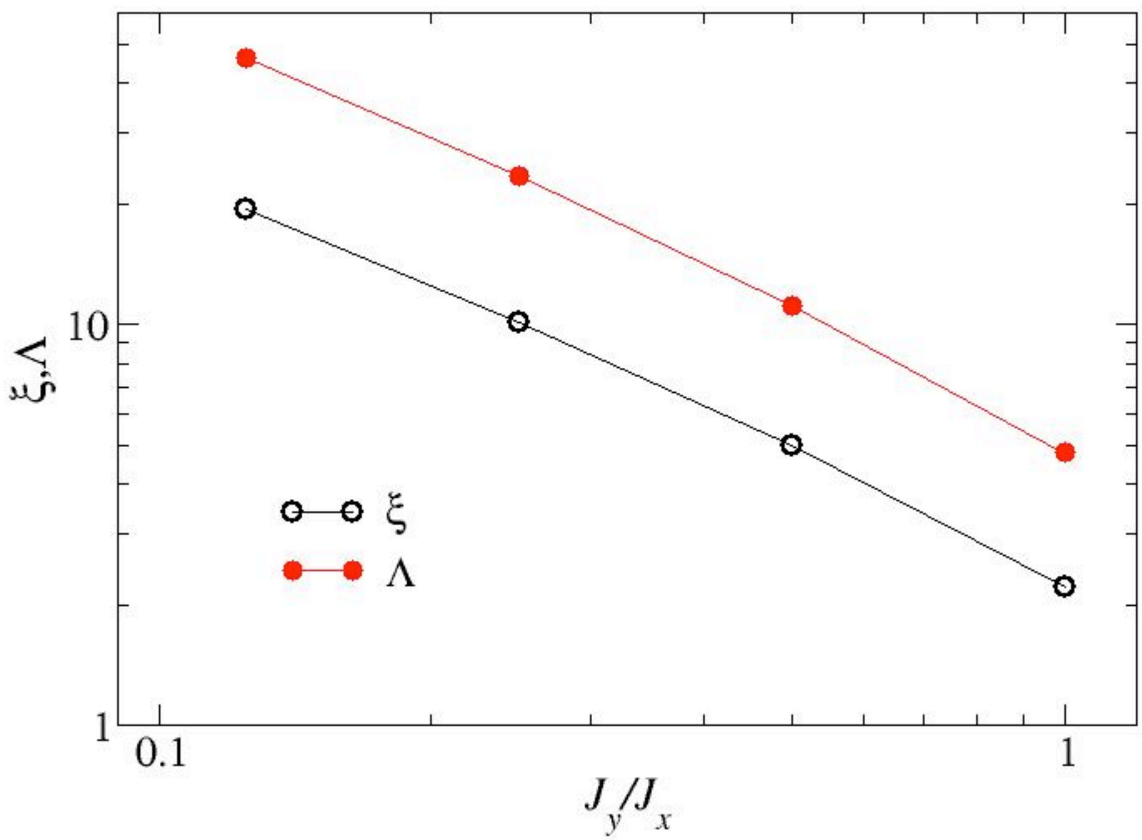




Spinon deconfinement for $J_y/J_x \to 0$

ξ = spin correlation length

Λ = confinement length (average triplet size)



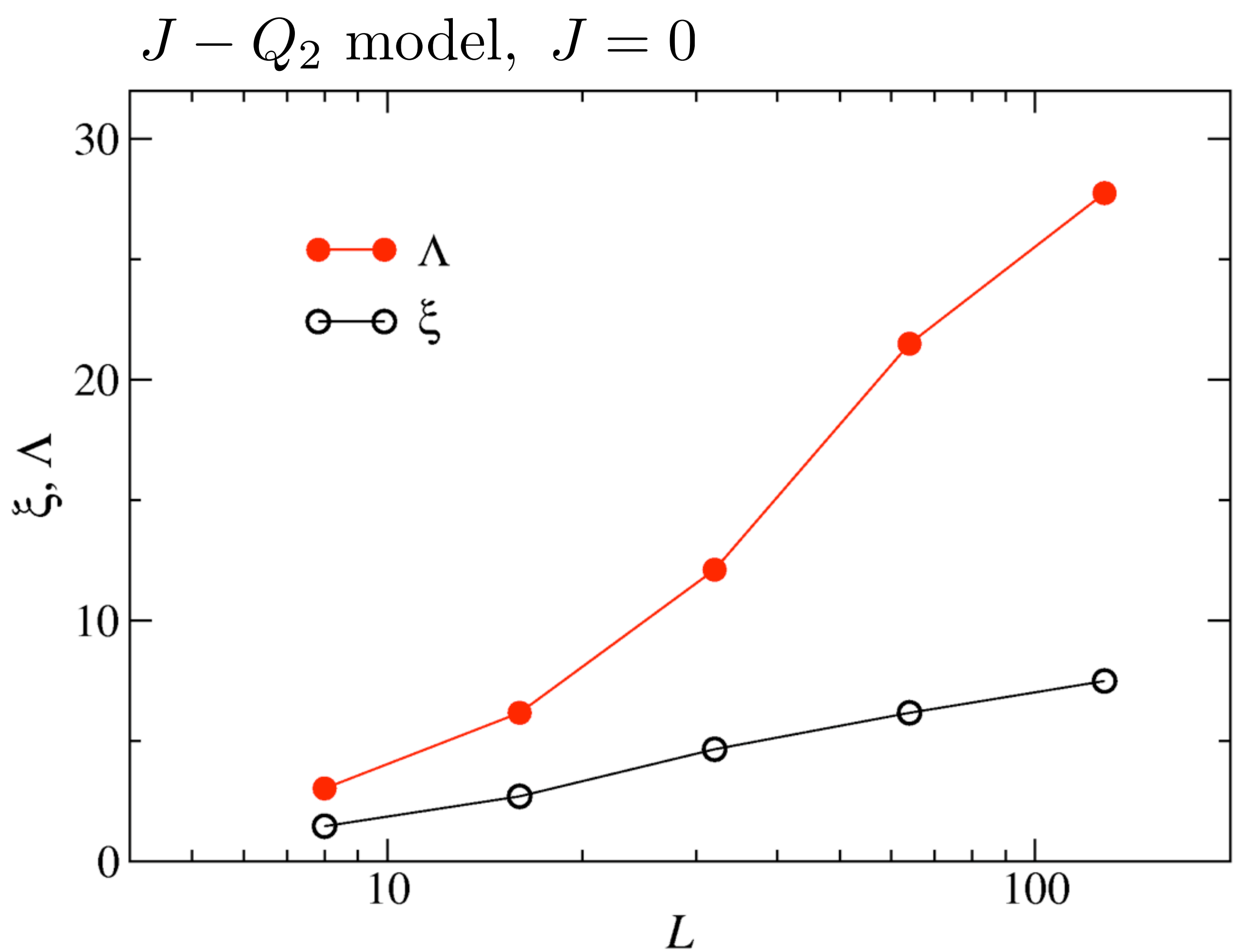
In this case

$\Lambda \propto \xi$

At a deconfined quantum-critical point

$\Lambda \sim \xi^a, \quad a > 1$

Confinement length in the VBS phase of the J-Q_2 model



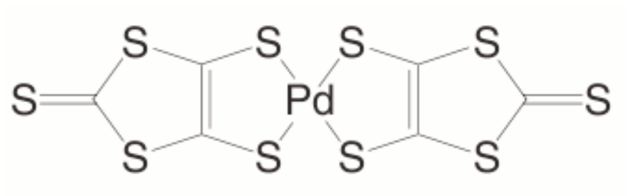
preliminary results show $\Lambda > \xi$ at J=0

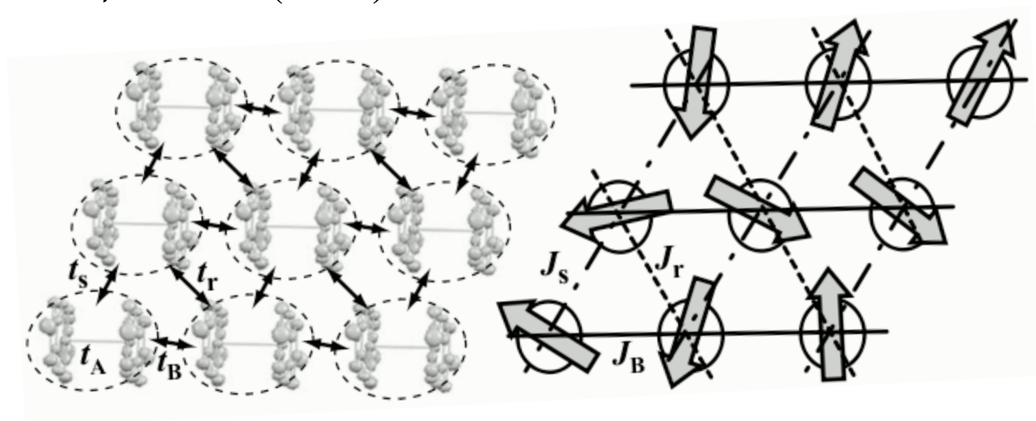
- does this Λ scale as the U(1) length?
- more calculations to be done (J-Q_3 model will be better)

Experimental realizations of deconfined quantum-criticality?

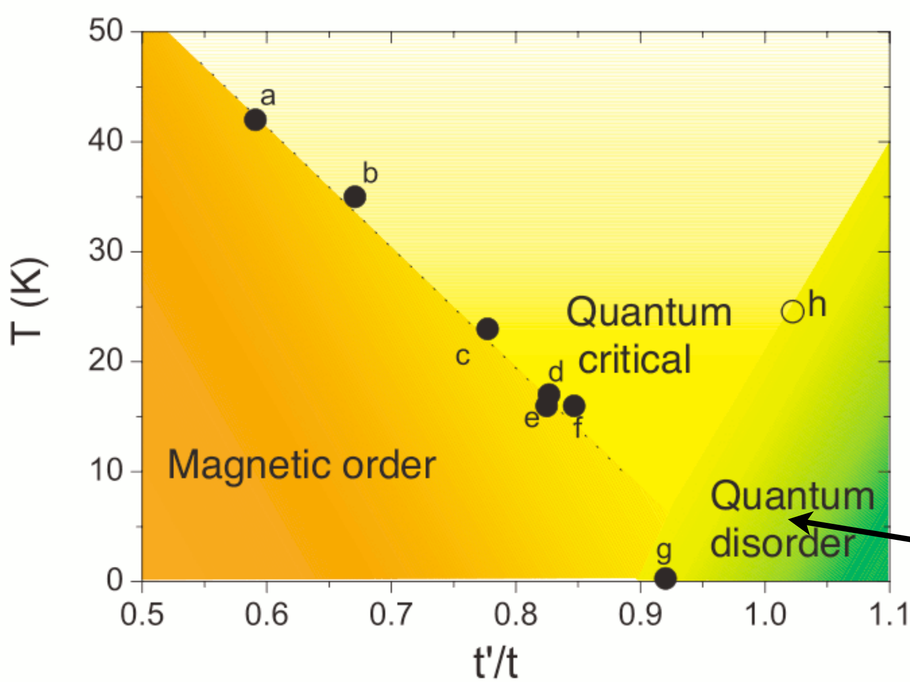
Layered triangular-lattice systems based on $[Pd(dmit)_2]_2$ dimers

Y. Shimizu et al, J. Phys.: Condens. Matter **19**, 145240 (2007)





J = 200-250 K



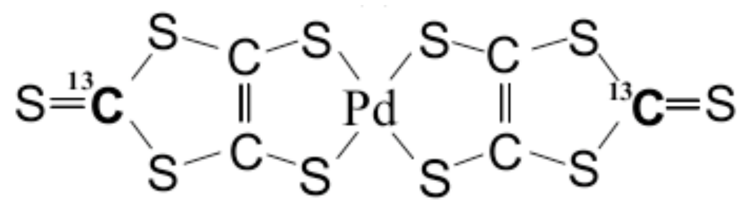
$EtMe_3Sb[Pd(dmit)_2]_2$ shows no magnetic order

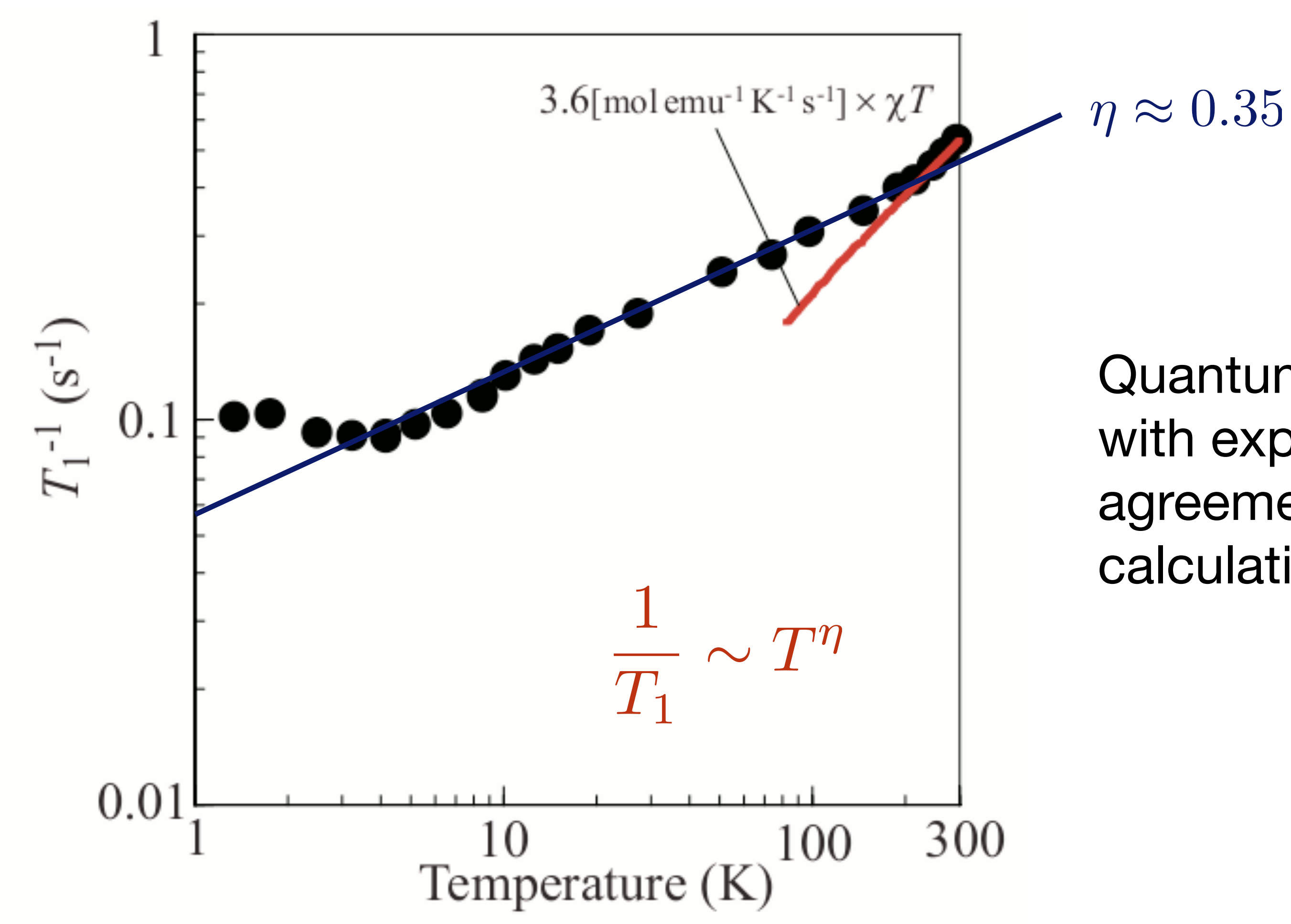
- May be a realization of the deconfined quantum-critical point [Xu and Sachdev, PRB 79, 064405 (2009)]

VBS state

NMR spin-lattice relaxation rate is sensitive to η

T. Itou et al, Phys. Rev. B **77**, 104413 (2008)





Quantum-critical scaling with exponent η in good agreement with the QMC calculations

Summary and Conclusions

Unfrustrated multi-spin interactions

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

Simulation methods in the valence bond basis

- May be the most efficient tools for studying ground state of many unfrustrated quantum spin models
- Direct way to investigate spinon confinement/deconfinement

Neel-VBS transition in square-lattice J-Q models

- Finite-size behavior indicated deconfined quantum-critical point
- Same exponents for two models; strengthens the case
- Emergent U(1) symmetry; cross-over quantified
- No signs of first-order transition (Binder cumulant is > 0)

Experimental realizations of deconfined quantum-criticality?

- $EtMe_3Sb[Pd(dmit)_2]_2$ is the most promising candidate so far
- NMR $1/T_1$ shows scaling with the QMC value for η_s