XIV Training Course on Strongly Correlated Systems
Vietri Sul Mare, Salerno, Italy, October 5-16, 2009

Valence-bond methods and valence-bond solid (VBS) states

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The valence-bond basis and resonating valence-bond states

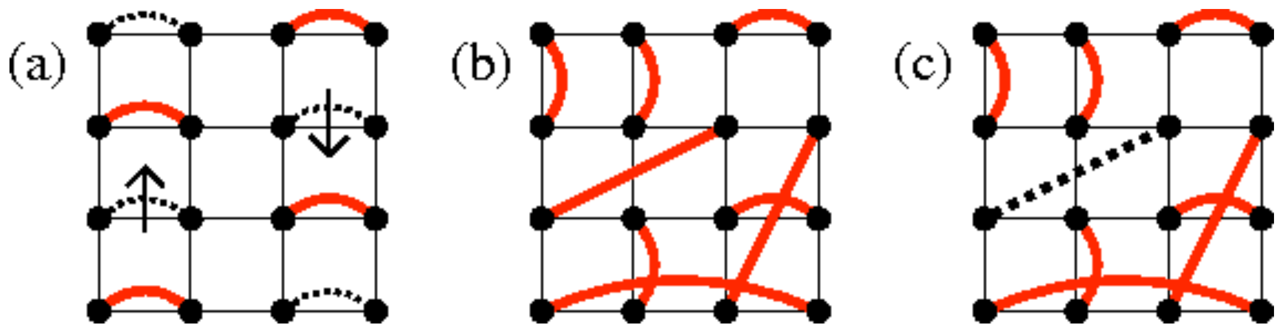
- Alternative to single-spin ↑,↓ basis
  - for qualitative insights and computational utility
- Exact solution of the frustrated chain at the “Majumdar-Ghosh” point
- Amplitude-product states

Neel to valence-bond solid transition (T=0)

- sign-problem free models exhibiting Neel and VBS phases
- evidence for “deconfined” quantum criticality
- method for direct detection of spinon confinement/deconfinement

Valence-bond basis and resonating valence-bond states

As an alternative to single-spin ↑ and ↓ states, we can use singlets and triplet pairs

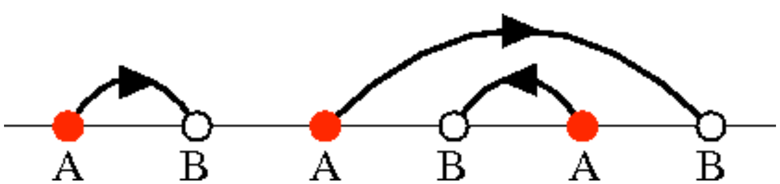


static dimers (complete basis)

arbitrary singlets (overcomplete in singlet subspace)

one triplet in the singlet soup (overcomplete in triplet subspace)

In the valence-bond basis (b,c) one normally includes pairs connecting two groups of spins - sublattices A and B (bipartite system, no frustration)



arrows indicate the order of the spins in the singlet definition

$$(a,b) = (\uparrow_a \downarrow_b - \downarrow_a \uparrow_b)/\sqrt{2} \qquad a \in A, b \in B$$

Superpositions, “resonating valence-bond” states

$$|\Psi_s\rangle = \sum_\alpha f_\alpha |(a_1^\alpha, b_1^\alpha) \cdots (a_{N/2}^\alpha, b_{N/2}^\alpha)\rangle = \sum_\alpha f_\alpha |V_\alpha\rangle$$

Marshall's sign rule for the ground-state wave function

The (a,b) singlet definition corresponds to a particular choice of ↑↓ wave-function signs

$$|\Psi\rangle = \sum_\sigma \Psi(\sigma)|\sigma\rangle \qquad |\sigma\rangle = |S_1^z, S_2^z, \ldots, S_N^z\rangle$$

Consider this as a variational state; we want to minimize the energy

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

Let us consider a bipartite Heisenberg model

$$H = J\sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} = J\sum_{i=1}^{N}[S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z],$$

$$= J\sum_{i=1}^{N}[S_i^z S_{i+1}^z + \tfrac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)] \qquad i \in A, \quad i+1 \in B$$

Diagonal and off-diagonal energy terms

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

To minimize E, the wave-function ratio should be negative →

$$\text{sign}[\Psi(S_1^z, \ldots, S_N^z)] = (-1)^{n_B}$$

This holds for the singlets $(a,b) = (\uparrow_a\downarrow_b - \downarrow_a\uparrow_b)/\sqrt{2}$ $\qquad a \in A, b \in B$

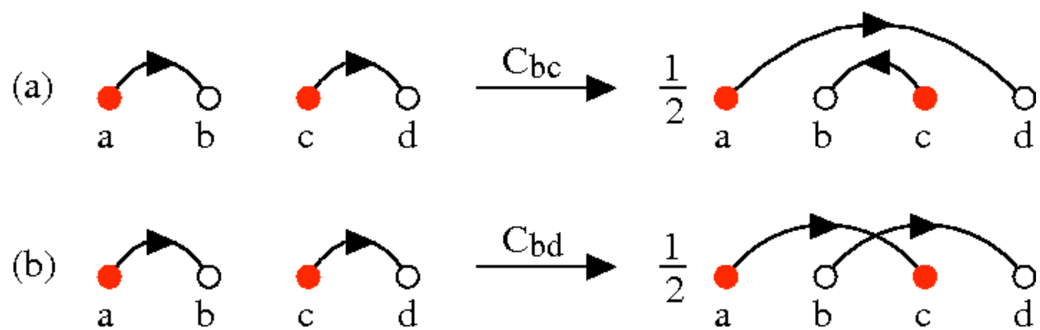
Useful operator: singlet projector operator

$$C_{ij} = -(\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4})$$

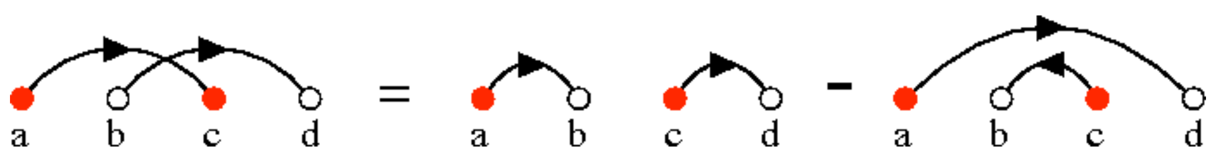
Creates a singlet (valence bond), if one is not present on (i,j);

$$C_{ab}(a,b) = (a,b)$$
$$C_{bc}(a,b)(c,d) = \frac{1}{2}(c,b)(a,d)$$

Graphical representation of the off-diagonal operation



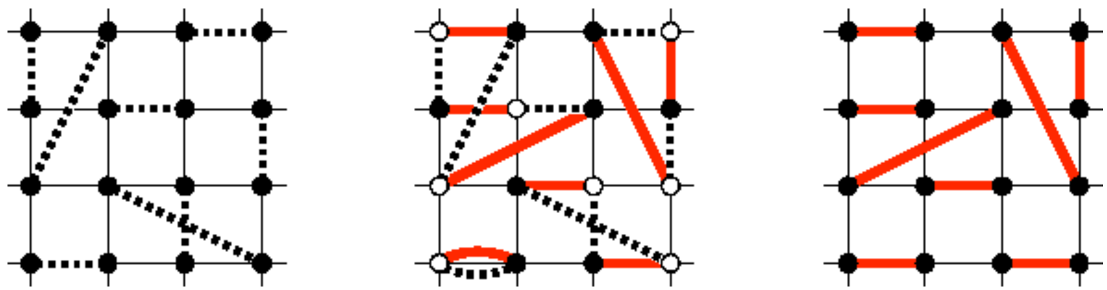
In (b) there are non-bipartite bonds; can be eliminated using



The Heisenberg hamiltonian is a sum of singlet projectors

Calculating with valence-bond states

All valence-bond basis states are non-orthogonal
- the overlaps are obtained using transposition graphs (loops)



Each loop has two compatible spin states → $\langle V_\beta|V_\alpha\rangle = 2^{N_{\rm loop}-N/2}$

This replaces the standard overlap for an orthogonal basis; $\langle\beta|\alpha\rangle = \delta_{\alpha\beta}$

Many matrix elements can also be expressed using the loops, e.g.,

$$\frac{\langle V_\beta|\mathbf{S}_i\cdot\mathbf{S}_j|V_\alpha\rangle}{\langle V_\beta|V_\alpha\rangle} = \begin{cases} 0, & \text{for } \lambda_i \neq \lambda_j \\ \frac{3}{4}\phi_{ij}, & \text{for } \lambda_i = \lambda_j \end{cases}$$

λ_i is the loop index (each loop has a label), staggered phase factor

$$\phi_{ij} = \begin{cases} -1, & \text{for } i,j \text{ on different sublattices} \\ +1, & \text{for } i,j \text{ on the same sublattice} \end{cases}$$

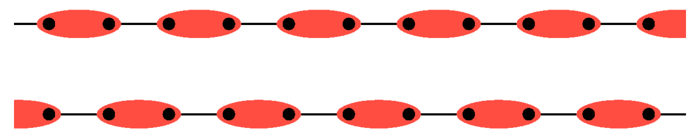
More complicated cases derived by K.S.D. Beach and A.W.S., Nucl. Phys. B 750, 142 (2006)

Solution of the frustrated chain at the Majumdar-Ghosh point

$$H = \sum_{i=1}^{N} \left[J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_i \cdot \mathbf{S}_{i+2} \right]$$

We will show that this state is an eigenstate when $J_2/J_1=1/2$

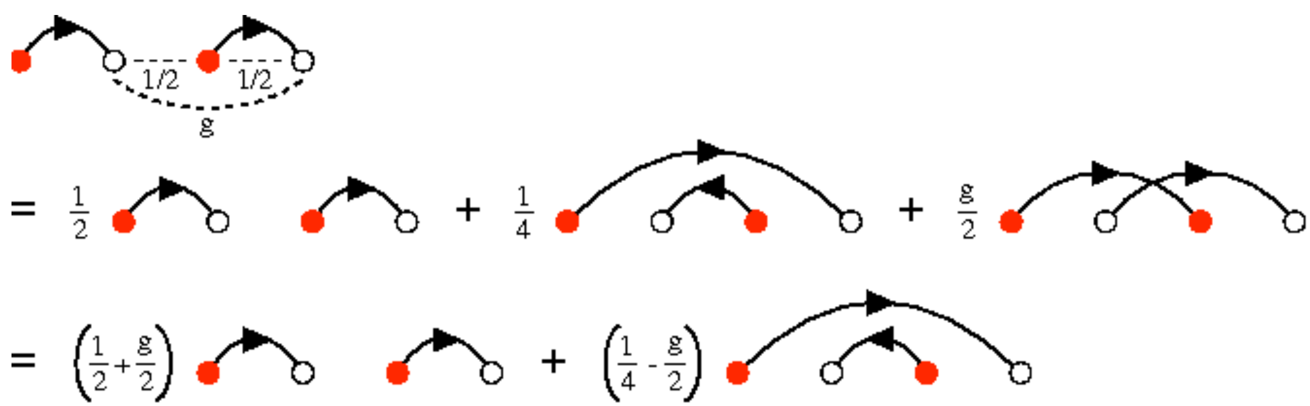
$$|\Psi_A\rangle = |(1,2)(3,4)(5,6)\cdots\rangle$$



Write H in terms of singlet projectors

$$H = -\sum_{i=1}^{N} (C_{i,i+1} + gC_{i,i+2}) + N\frac{1+g}{4}, \qquad C_{ij} = -(\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4})$$

Act with one “segment” of these terms on the state; graphically



Eigenstate for g=1/2; one can also show that it’s the lowest eigenstate

Amplitude-product states

Good variational ground state for bipartite models can be constructed

$$|\Psi_s\rangle = \sum_\alpha f_\alpha |(a_1^\alpha, b_1^\alpha)\cdots(a_{N/2}^\alpha, b_{N/2}^\alpha)\rangle = \sum_\alpha f_\alpha |V_\alpha\rangle$$

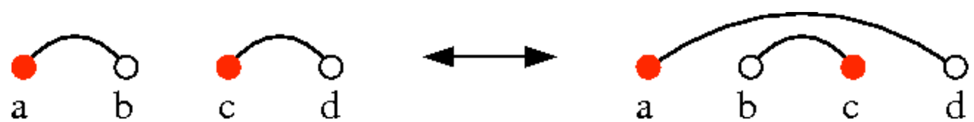
Let the wave-function coefficients be products of “amplitudes” (real positive numbers)

$$f_\alpha = \prod_{\mathbf{r}} h(\mathbf{r})^{n_\alpha(\mathbf{r})},$$

Liang, Doucot, Anderson (1990)

The amplitudes h(r), r=1,3,...,N/2 (in one dimension) are adjustable parameters

What are the properties of such states (independently of any model H)?
- given fixed h(r), one can study the state using Monte Carlo sampling of bonds
- elementary move by reconfiguring two bonds
- simple accept/reject probability (Metropolis algorithm)



Test of two cases for the amplitudes in 1D:

$$h(r) = \mathrm{e}^{-r/\kappa}$$

$$h(r) = r^{-\kappa}$$

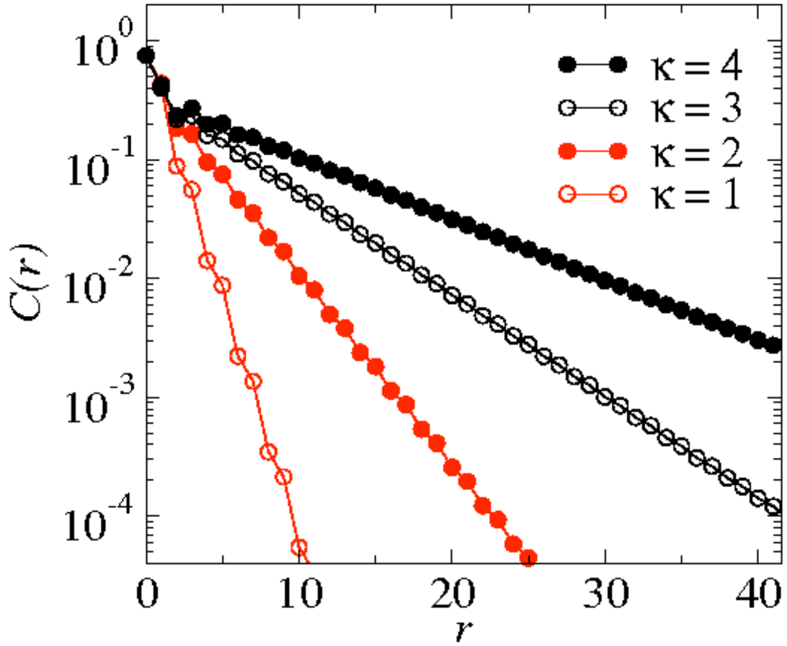
exponentially-decaying amplitudes

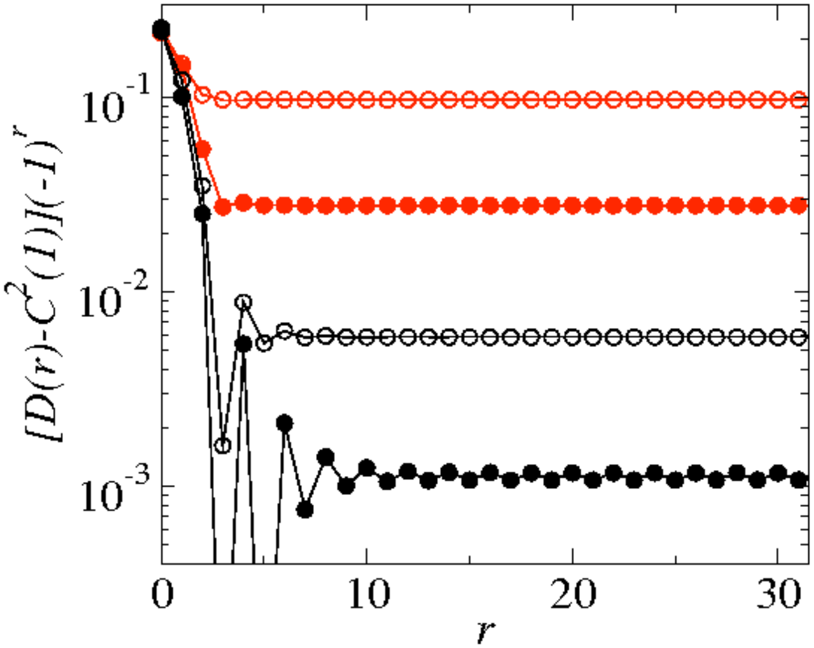
Spin and dimer correlations obtained with MC sampling (N=256)

dimer correlation: $D(r_{ij}) = \langle(\mathbf{s}_i \cdot \mathbf{s}_{i+\hat{x}})(\mathbf{s}_j \cdot \mathbf{s}_{j+\hat{x}})\rangle$

Used to defined VBS order parameter

- subtract average = $C^2(1)$, gives $(-1)^r$ sign oscillations in VBS state

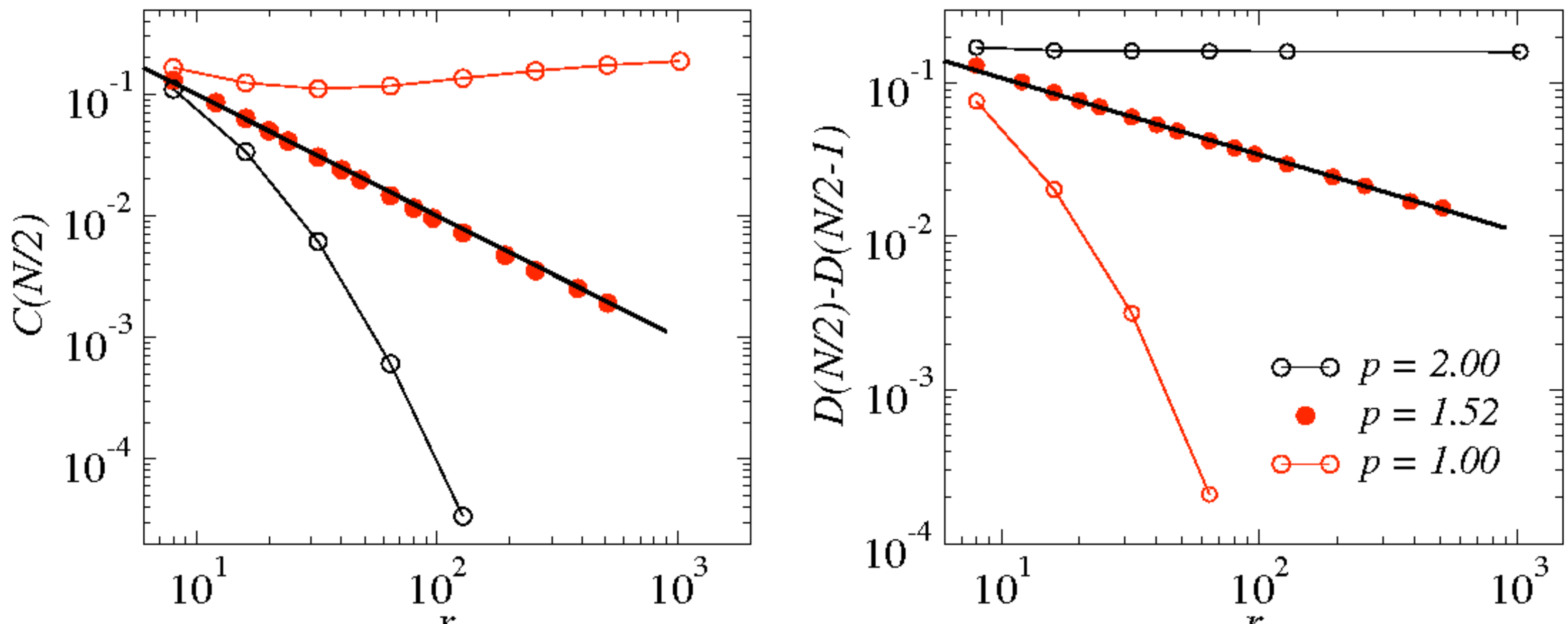




The state is always a valence-bond solid

power-law decaying amplitudes

Spin and dimer correlations obtained with MC sampling for different N at r=N/2



There is a “quantum phase transition” when κ≈1.52

- Long-range antiferromagnetic order for κ<1.52
- Valence-bond-solid order for κ>1.52

The critical state is similar to the ground state of the Heisenberg chain

- but not quite C(r)~1/r and D(r)~1/r for Heisenberg chain
  - C(r)~1/r and D(r)~$1/r^{1/2}$ for amplitude-product state
  - exponents depend on details of the amplitudes

Neel to VBS Quantum Phase transitions

Introduction to quantum phase transitions

Finite-size scaling at critical points

“J-Q” models exhibiting Neel - VBS transitions

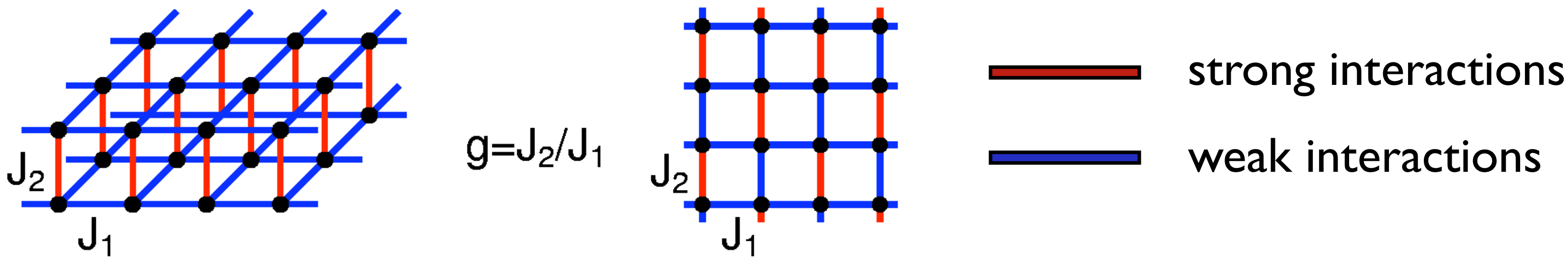
Simulation results
• exponents, emergent U(1) symmetry

Method for detecting spinon deconfinement

2D quantum-criticality (T=0 transition)

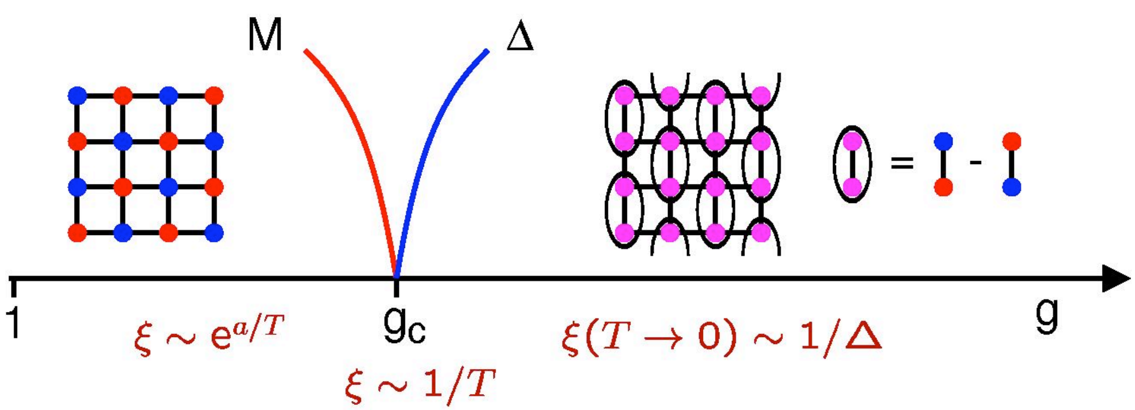
“Manually” dimerized S=1/2 Heisenberg models

Examples: bilayer, dimerized single layer



Singlet formation on strong bonds ➙ Neel - disordered transition

Ground state (T=0) phases



2D quantum spins map onto (2+1)D classical spins (Haldane)

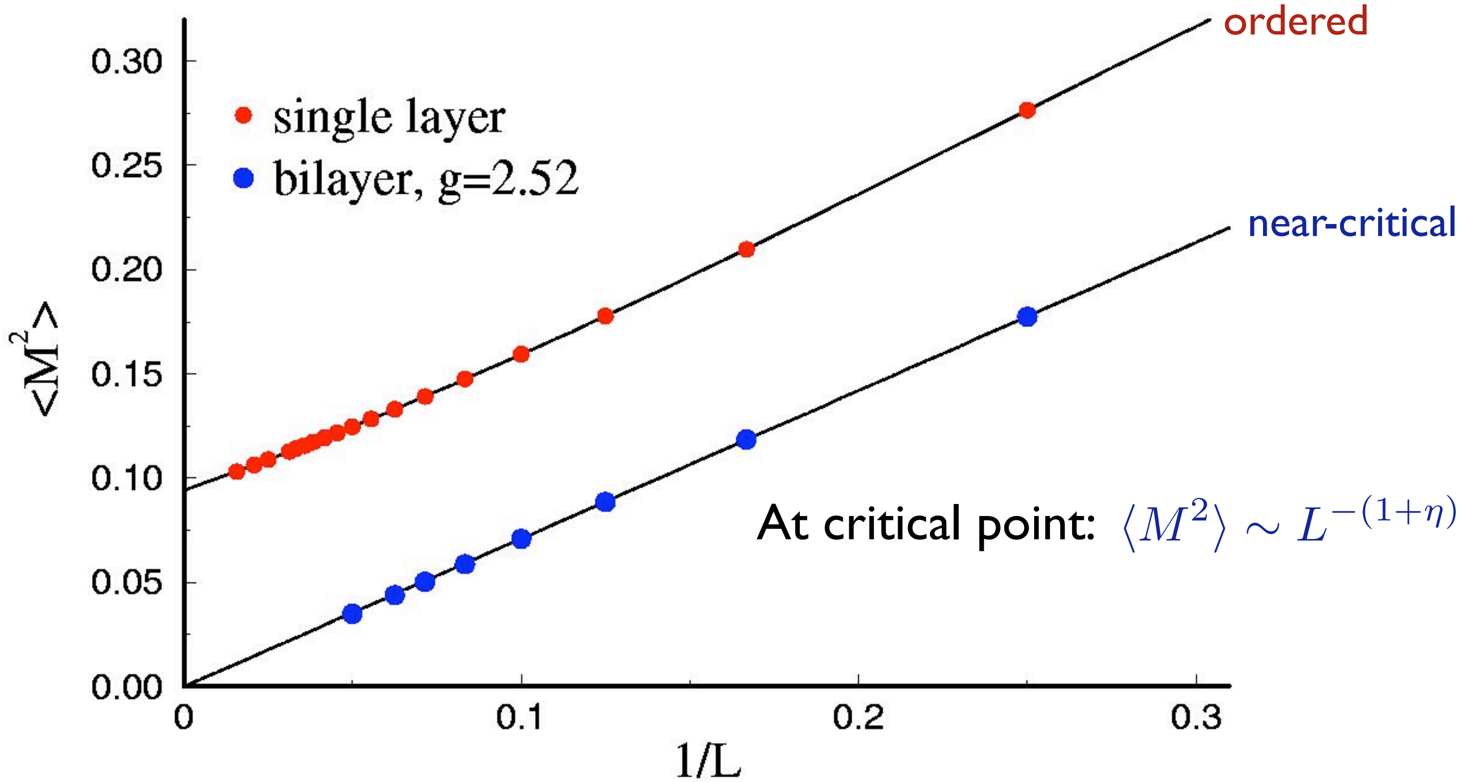
- Continuum field theory: nonlinear σ-model (Chakravarty, Halperin, Nelson)

⇒3D classical Heisenberg (O3) universality class expected

Example: 2D Heisenberg model (T→0) simulations
Finite-size scaling of the sublattice magnetization

$$\vec{M} = \frac{1}{N}\sum_i (-1)^{x_i+y_i}\vec{S}_i$$

In simulations we calculate <M^2>



At critical point: $\langle M^2 \rangle \sim L^{-(1+\eta)}$

Simulations & theory agree: O(3) universality class (e.g., $\eta \approx 0.03$) for bilayer

many papers, e.g., L. Wang and A.W.S., Phys. Rev. B 73, 014431 (2006)

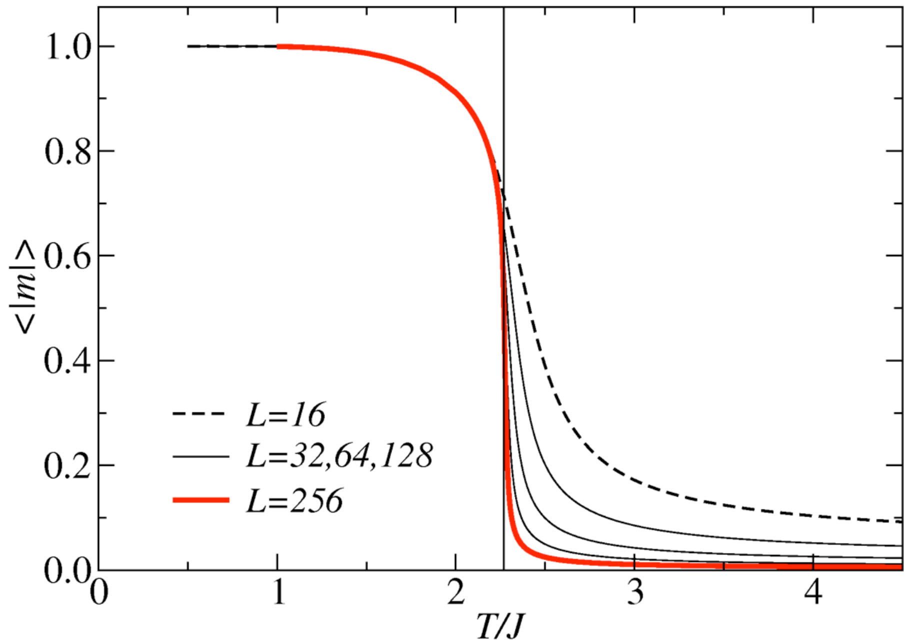
Finite-size scaling, critical exponents

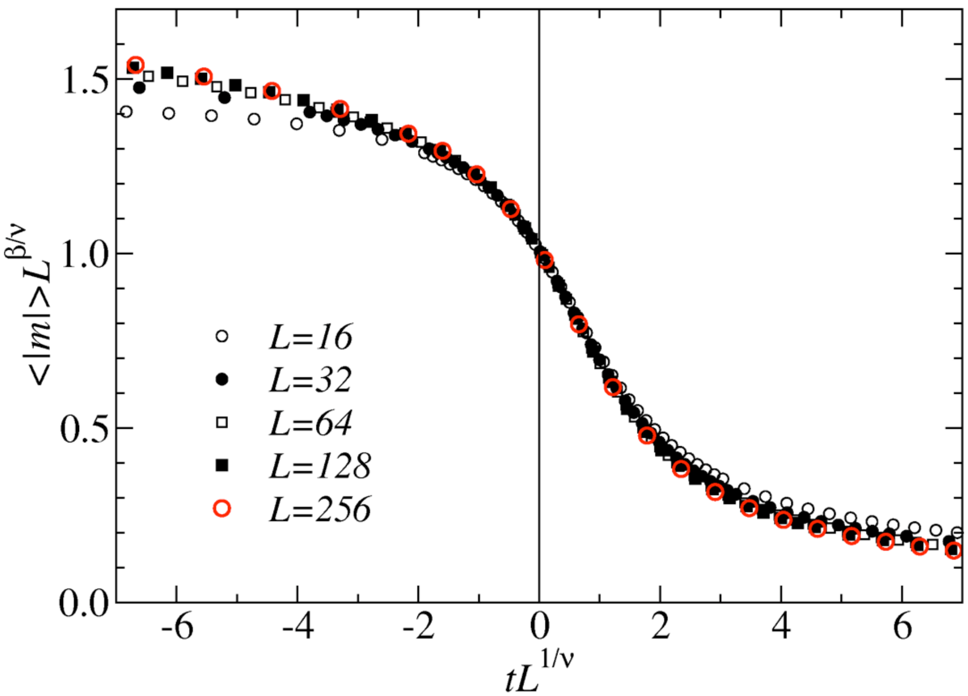
Order parameter close to T_c in a classical system or at critical coupling g_c at T=0 in a quantum system

$$m \sim \begin{cases} (T_c - T)^\beta \\ (g_c - g)^\beta \end{cases}$$

At T_c or g_c in finite system of length L:

$$m \sim L^{-\beta/\nu}$$





A quantity A in the neighborhood of the critical point scales as

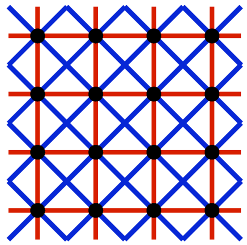
$$A(L,T) = L^{-\kappa/\nu} f(tL^\nu)$$

$$t = \frac{T - T_c}{T_c}$$

Data collapse: plot

$$AL^{\kappa/\nu} \text{ versus } tL^\nu$$

A challenging problem: frustrated quantum spins



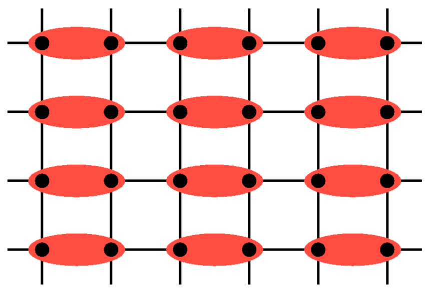
— $= J_1$

— $= J_2$

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

What is the nature of the non-magnetic ground state for $g=J_2/J_1 \approx 1/2$?

- most likely a **Valence-bond solid** (crystal) [Read & Sachdev (1989)]

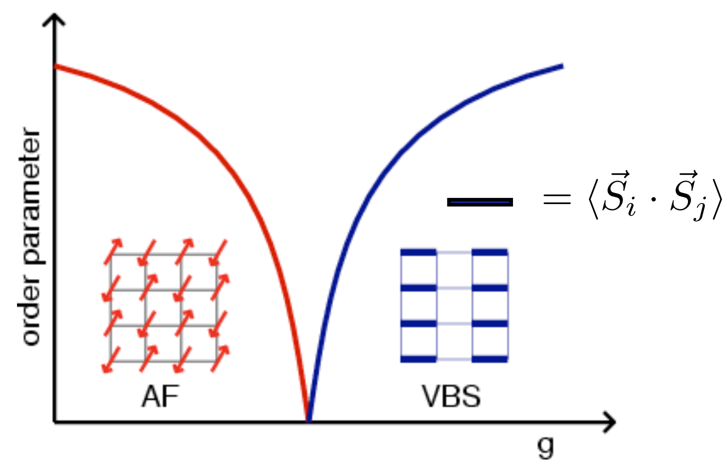


- No spin (magnetic) order
- Broken translational symmetry

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

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

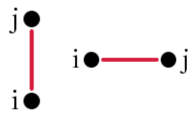


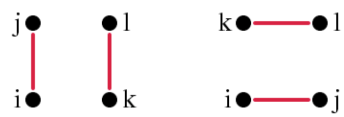
Are there models with AF-VBS transitions that do not have QMC sign problems?

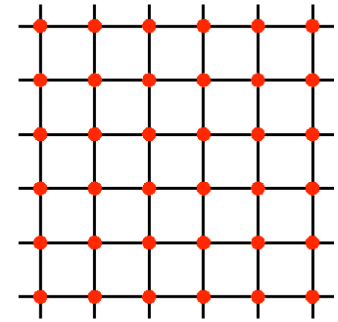
2D S=1/2 Heisenberg model with 4-spin interactions

A.W.S, Phys. Rev. Lett. 98, 227202 (2007)

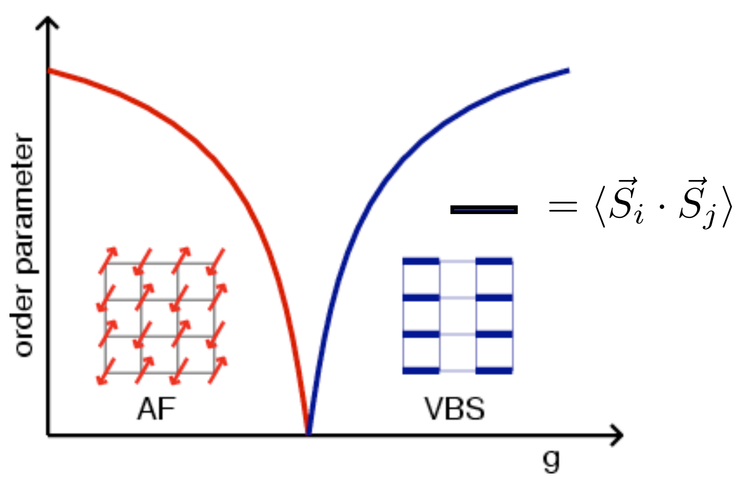
$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - Q \sum_{\langle ijkl \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4})(\mathbf{S}_k \cdot \mathbf{S}_l - \tfrac{1}{4})$$







- no sign problems in QMC simulations
- has an AF-VBS transition at J/Q≈0.04
- microscopic interaction not necessarily realistic for 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



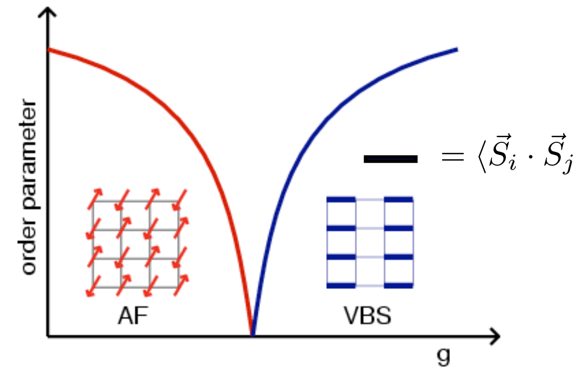
Questions

- is the transition continuous?
  - normally order-order transitions are first order (Landau-Ginzburg)
  - theory of "deconfined" quantum critical points has continuous transition
- nature of the VBS quantum fluctuations
  - emergent U(1) symmetry predicted

Deconfined quantum criticality

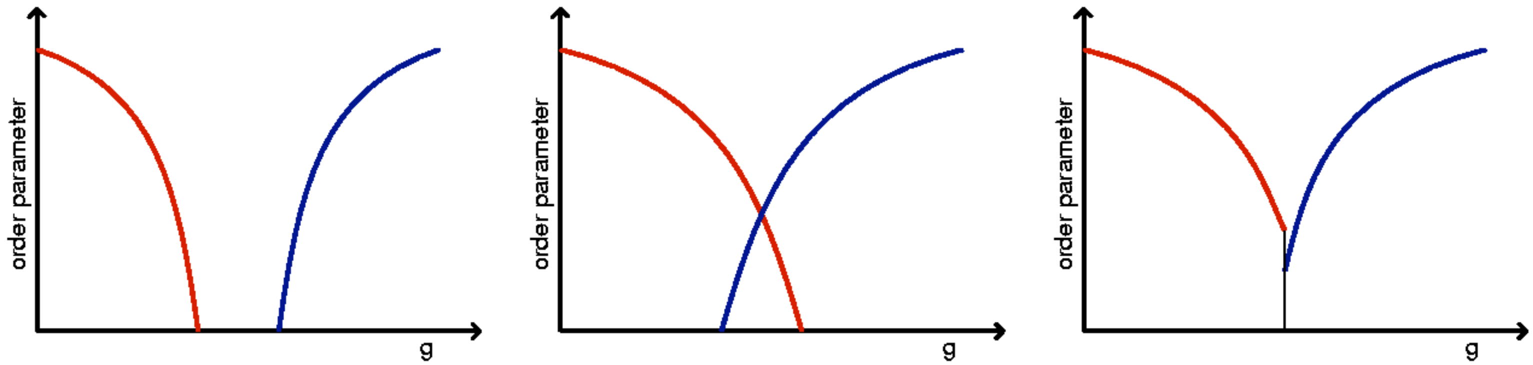
Senthil et al., Science 303, 1490 (2004)

[Read & Sachdev (1989)]



Generic continuous AF-VBS transition

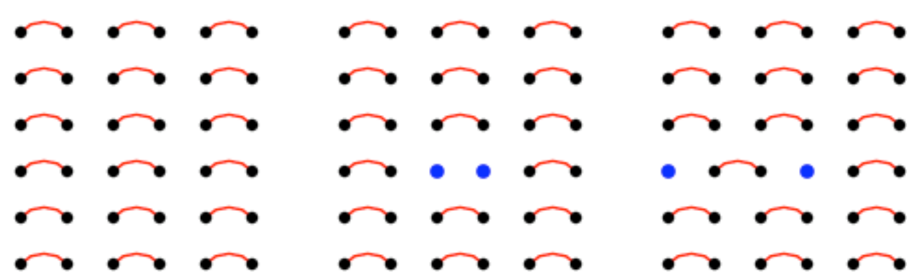
- beyond the Ginzburg-Landau paradigm (generically 1st order AF-VBS point)



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

Spinon deconfinement at the critical point

Confinement inside VBS phase associated with new length scale and emergent U(1) symmetry



Projector Monte Carlo in the valence-bond basis

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

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

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

S=1/2 Heisenberg model

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

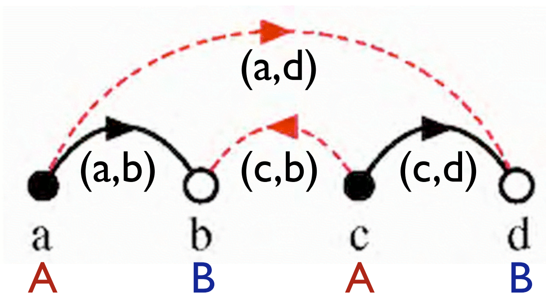
Project with string of bond operators

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

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

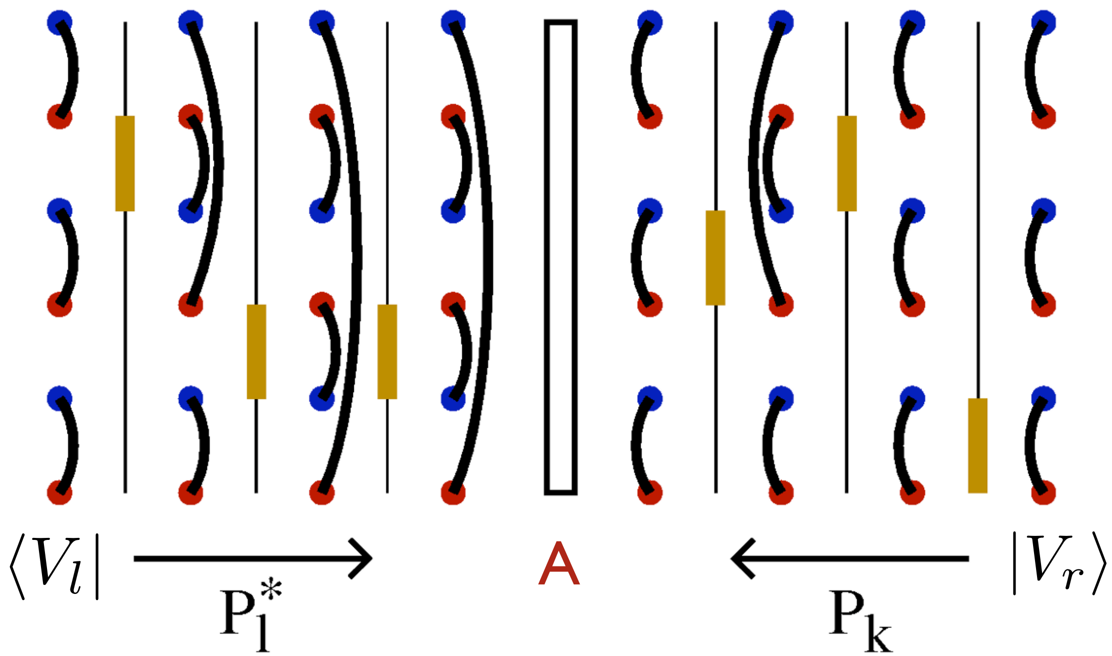
Expectation values

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

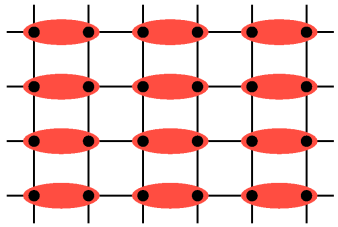
$$\sum_k P_k|V_r\rangle = \sum_k W_{kr}|V_r(k)\rangle \rightarrow (\tfrac{1}{4} - E_0)^n c_0|0\rangle$$

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

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



Results: VBS phase in the J-Q model

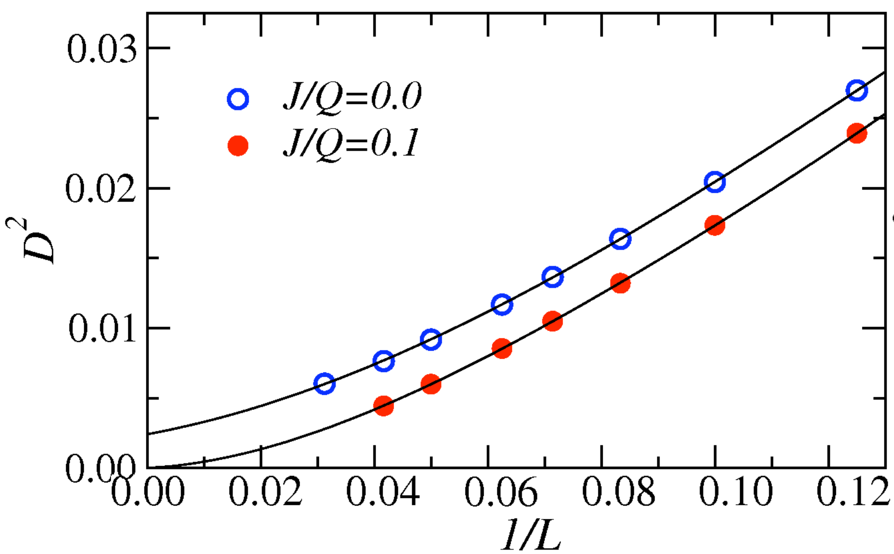


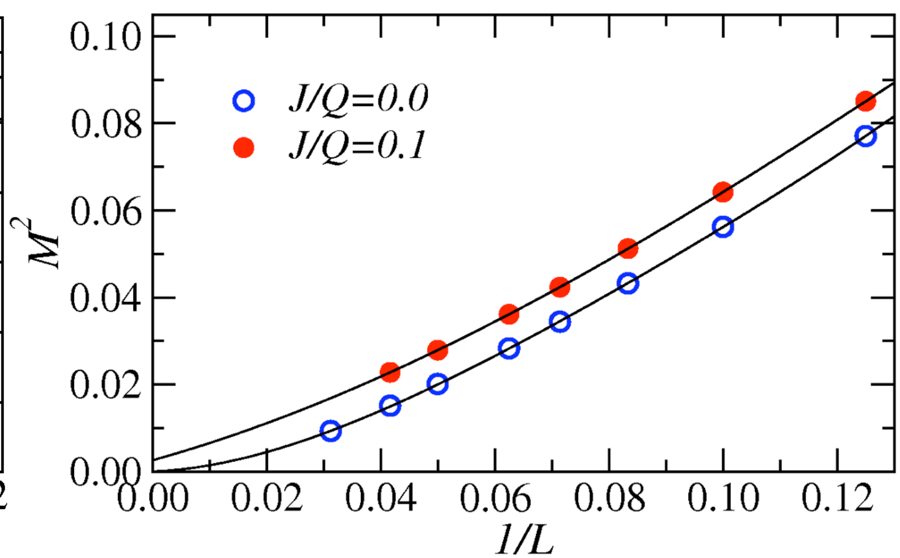
- **VBS order parameter**
  columnar dimer-dimer correlations

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

- **AF (Neel) order parameter**
  sublattice magnetization

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





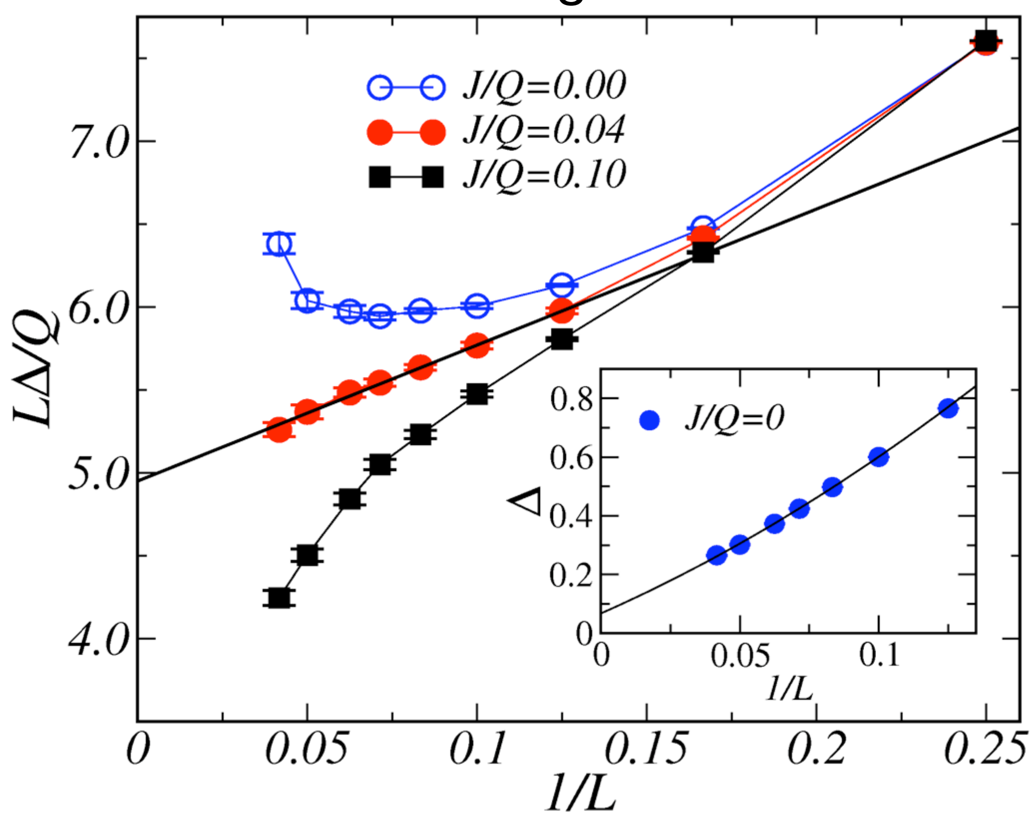
➤ J/Q=0.0 → VBS ➤ J/Q=0.1 → antiferromagnet

Singlet-triplet gap scaling → Dynamic exponent z

z relates length and time scales:
$\omega_q \sim |q|^z$ finite size → $\Delta \sim L^{-z}$

There is an improved estimator for the gap in the VB basis QMC

Finite-size scaling of $L\Delta$



The gap at J=0 is small;
$\Delta/Q=0.07$
The VBS is near-critical

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

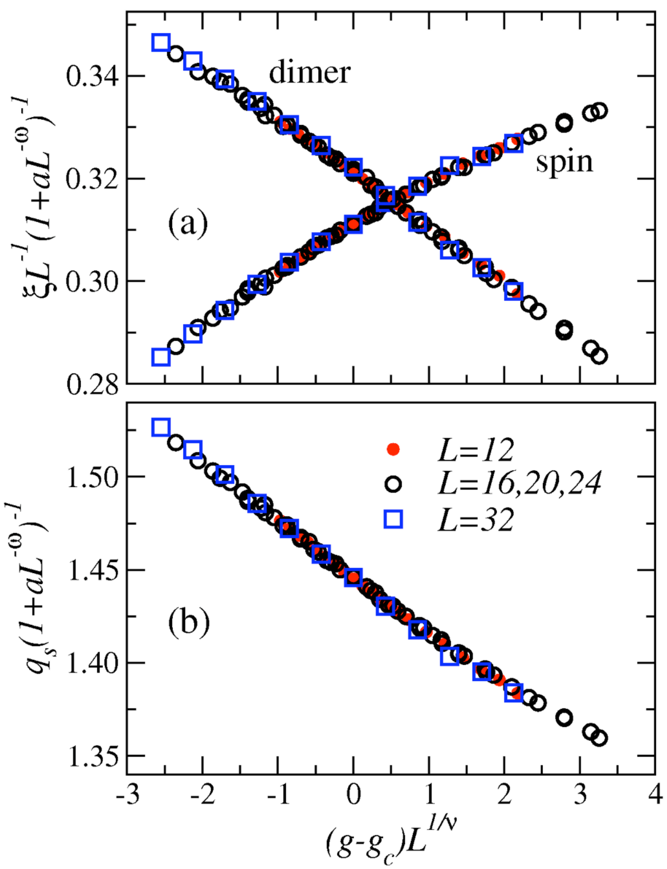
Exponents; finite-size scaling

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

$$g = \frac{J}{Q}$$

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

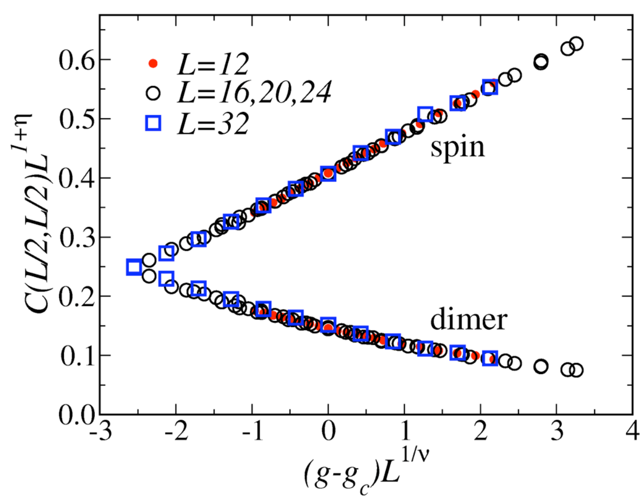
long-distance spin and dimer correlations: $C_{s,d}(L/2, L/2)$



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

(with subleading corrections)

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



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

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

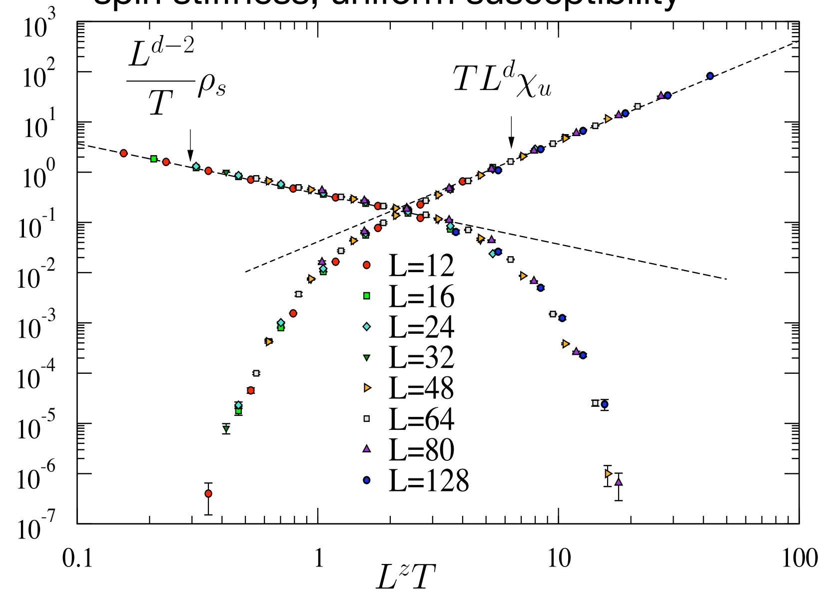
T,L scaling properties

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

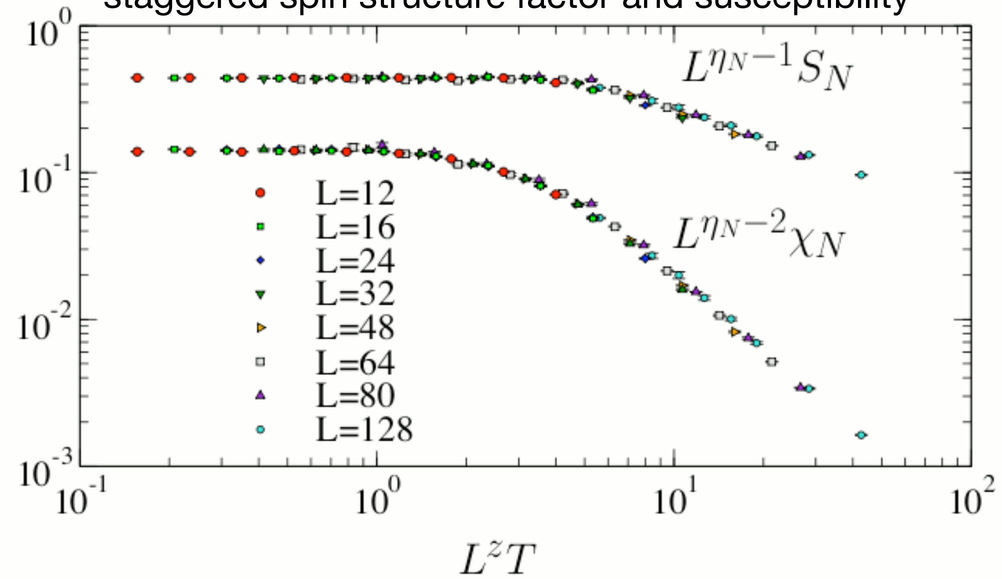
Additional confirmation
of a critical point

- finite-T stochastic series expansion
- larger systems (because T>0)
- good agreement on critcal Q/J

spin stiffness, uniform susceptibility



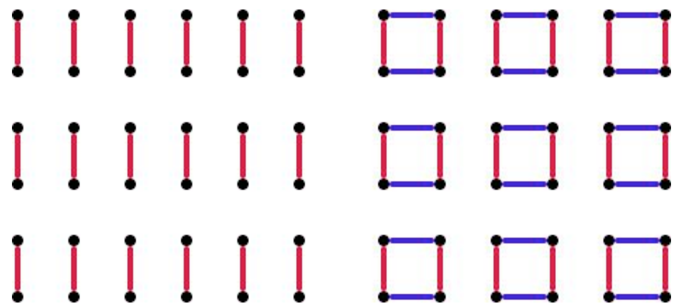
staggered spin structure factor and susceptibility

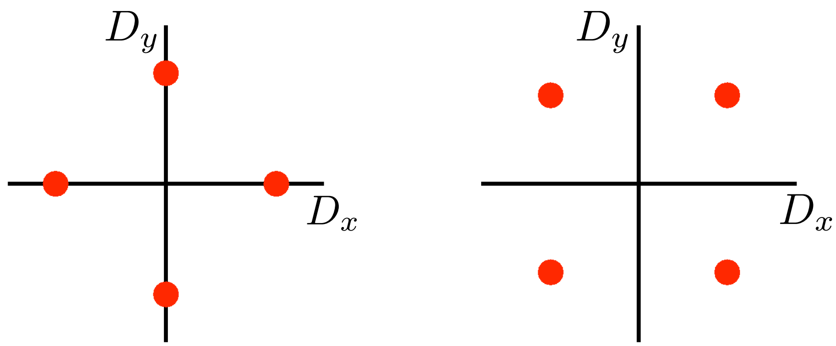


$$z = 1, \eta \approx 0.35$$

What kind of VBS; columnar or plaquette?

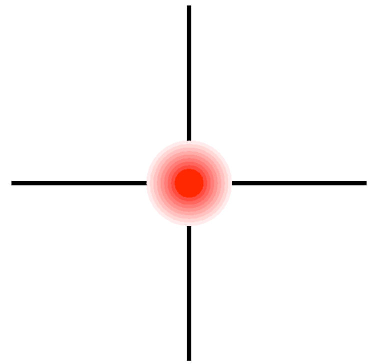
➪ look at joint probability distribution $P(D_x, D_y)$





The simulations sample the ground state;

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



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

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

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

➪ 4 peaks expected; Z_4-symmetry unbroken in finite system

VBS fluctuations in the theory of deconfined quantum-critical points

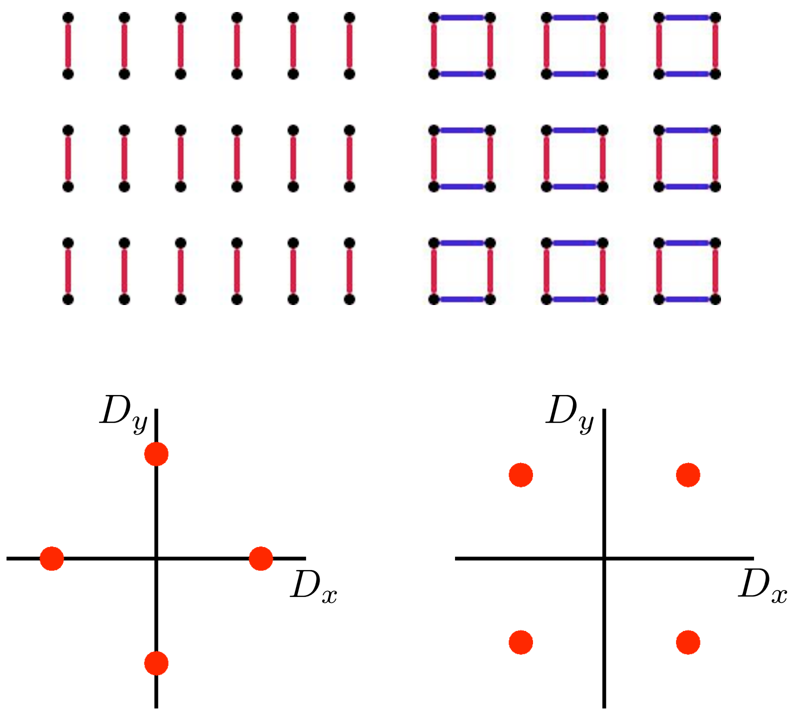
➣ plaquette and columnar VBS "degenerate" at criticality

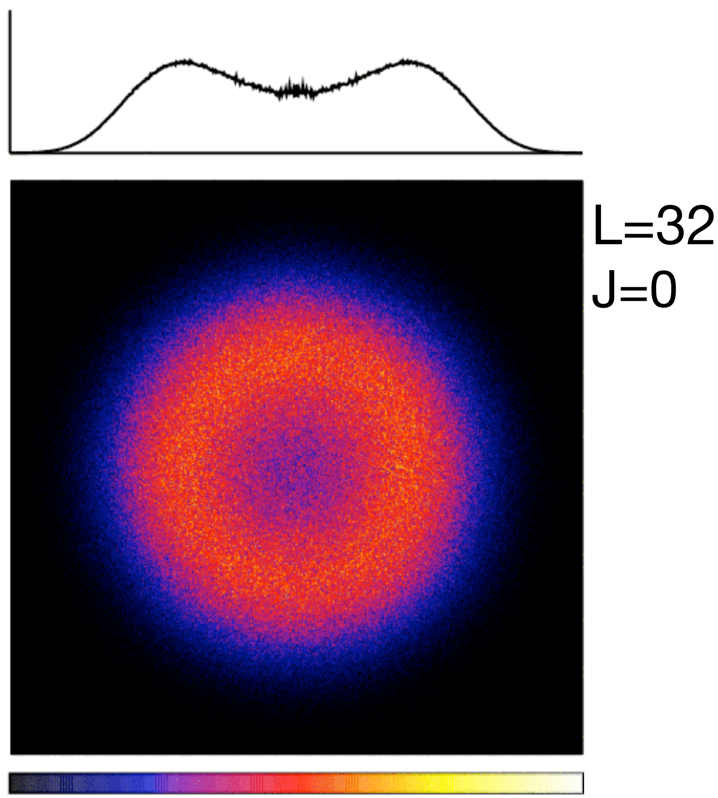
➣ Z_4 "lattice perturbation" irrelevant at critical point

– and in the VBS phase for L<Λ~ξ^a, a>1 (spinon confinement length)

➣ **emergent U(1) symmetry**

➣ **ring-shaped distribution expected for L<Λ**





More efficient ground state QMC algorithm → larger lattices

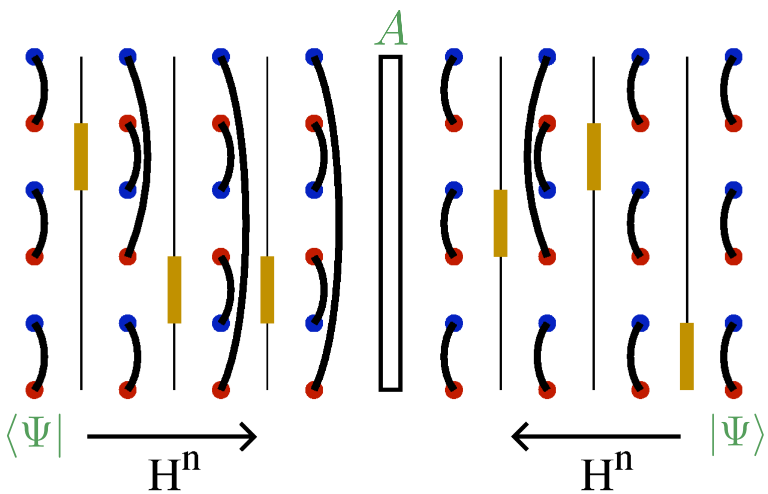
Loop updates in the valence-bond basis

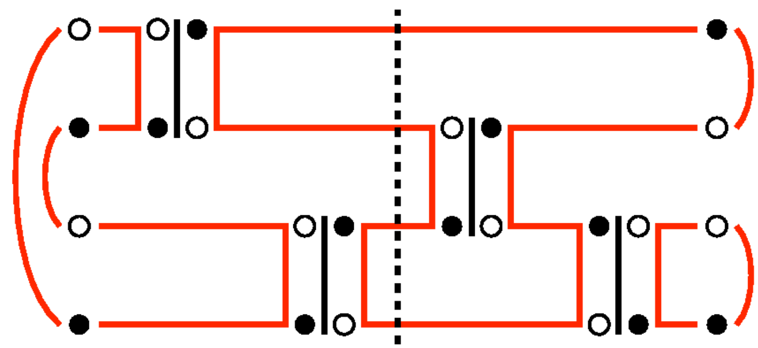
AWS and H. G. Evertz, ArXiv:0807.0682

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)

- 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, arXiv:0908.0740

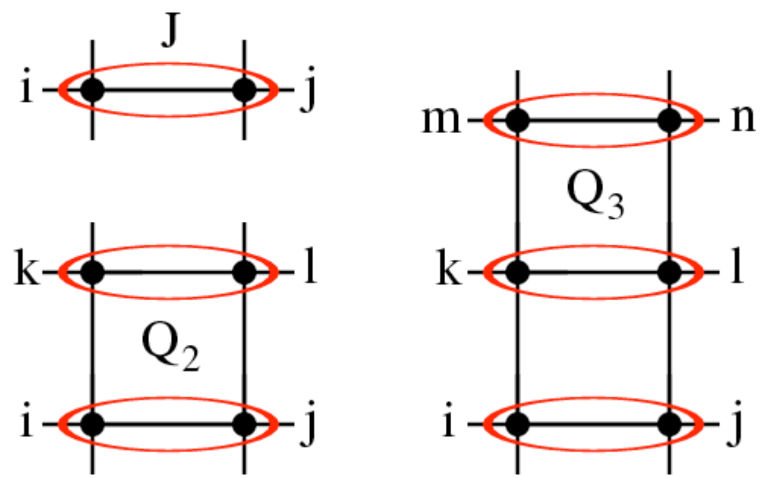
Universal exponents? Two different models:

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

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

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

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



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

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

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

Now using coupling ratio

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

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

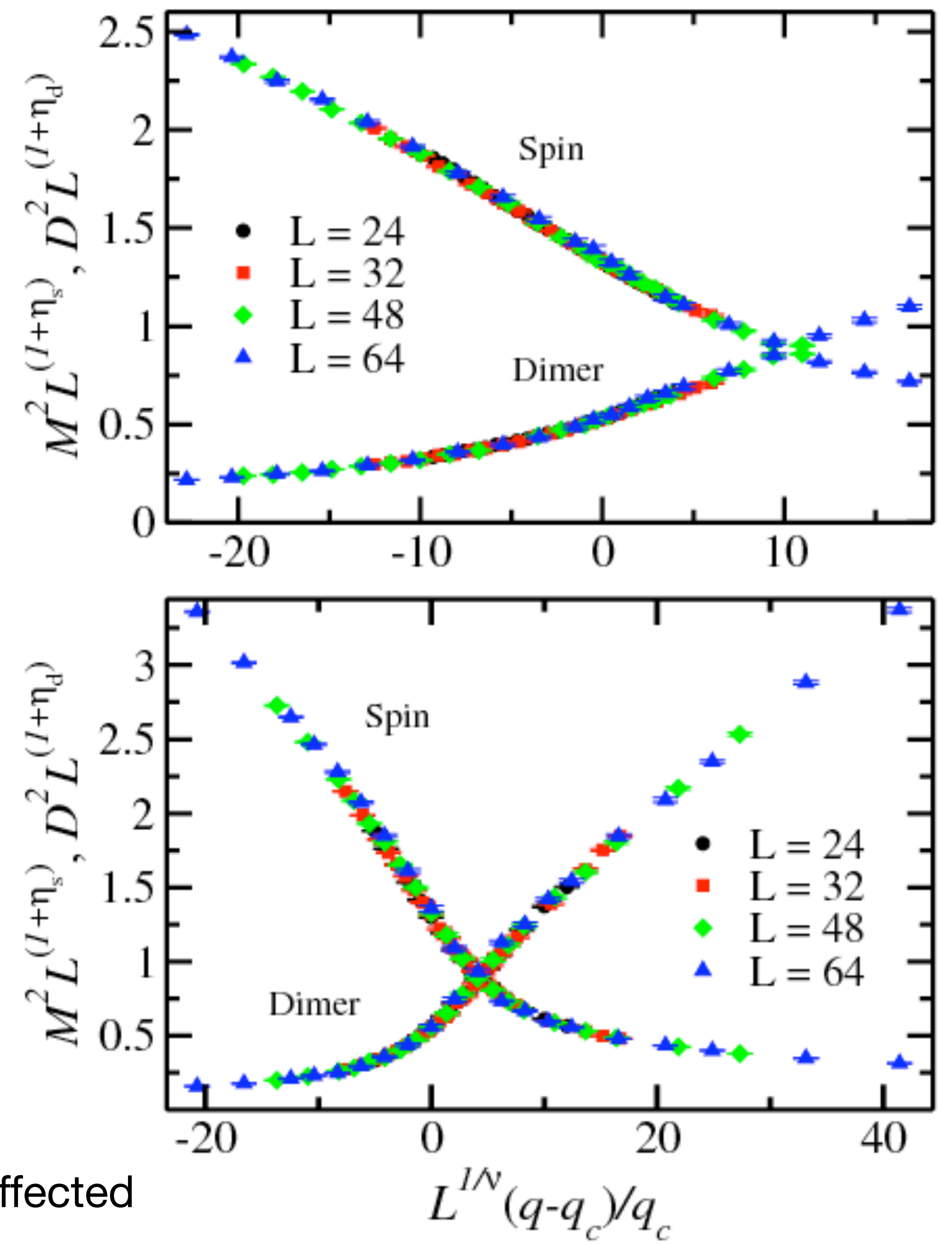
$$\eta_s = 0.35(2)$$
$$\eta_d = 0.20(2)$$
$$\nu = 0.67(1)$$

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

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

η_s, ν in perfect agreement with the finite-T results by Kaul and Melko

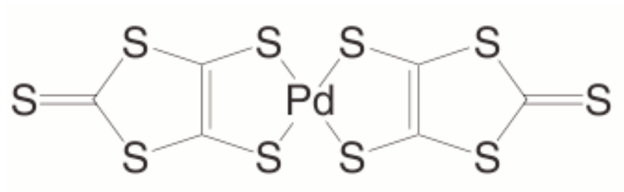
- previous T=0 results may have been affected by scaling corrections in small latticed

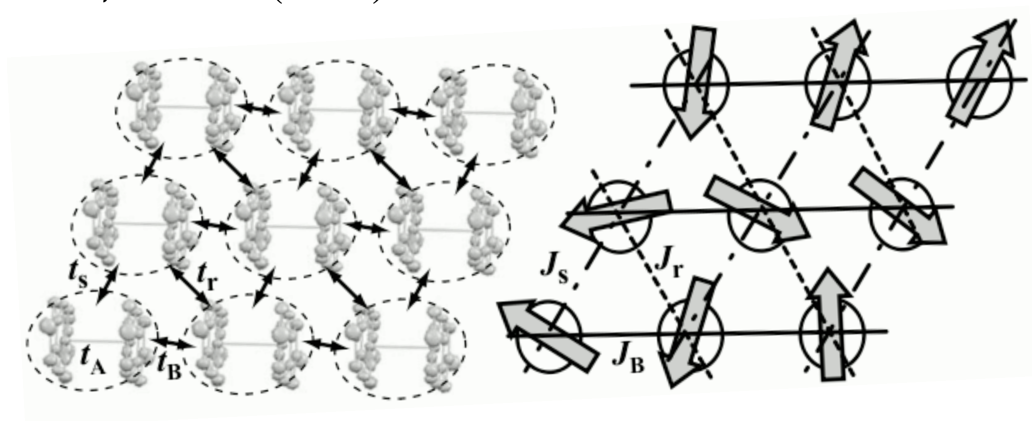


Experimental realizations of deconfined quantum-criticality?

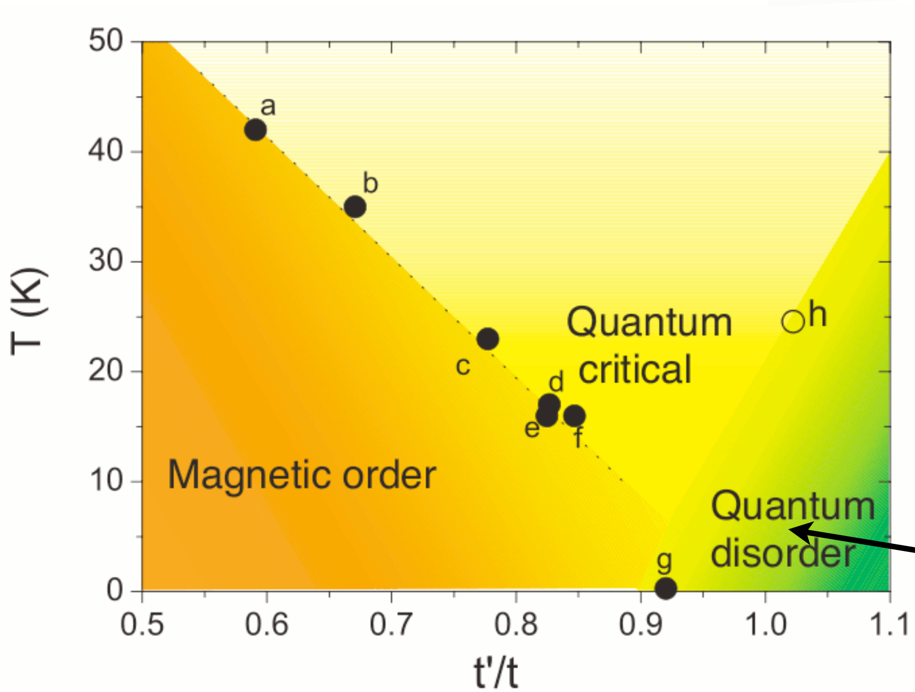
Layered triangular-lattice systems based on $[Pd(dmit)_2]_2$ dimers

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





J = 200-250 K



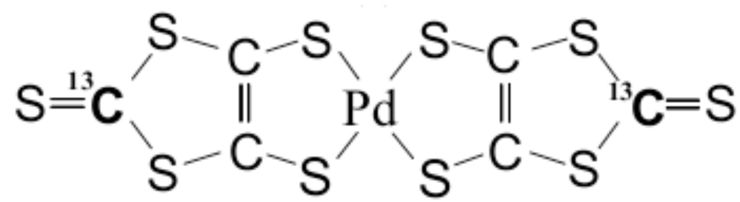
$EtMe_3Sb[Pd(dmit)_2]_2$ shows no magnetic order

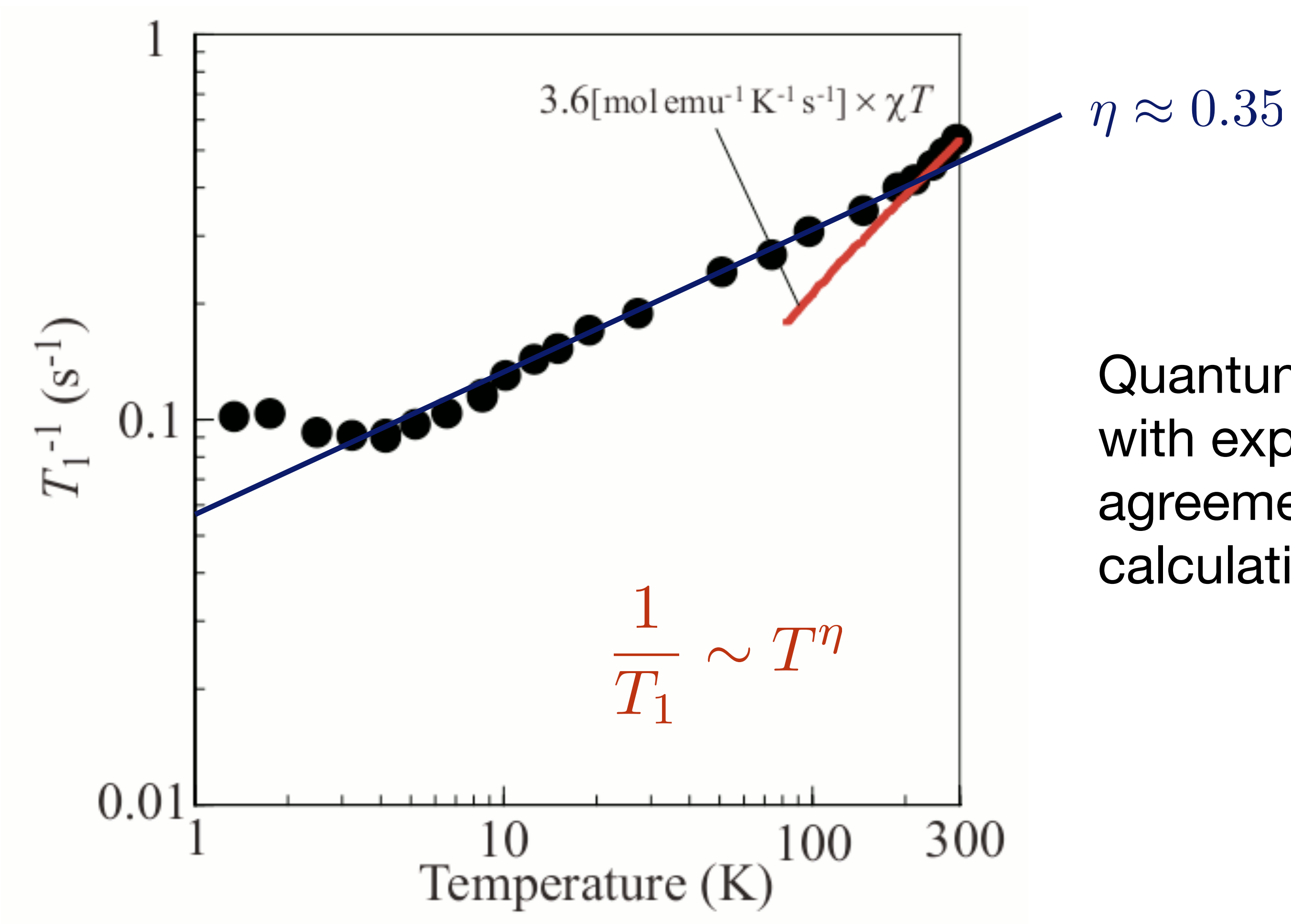
- May be a realization of the deconfined quantum-critical point [Xu and Sachdev, PRB 79, 064405 (2009)]

VBS state

NMR spin-lattice relaxation rate is sensitive to η

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





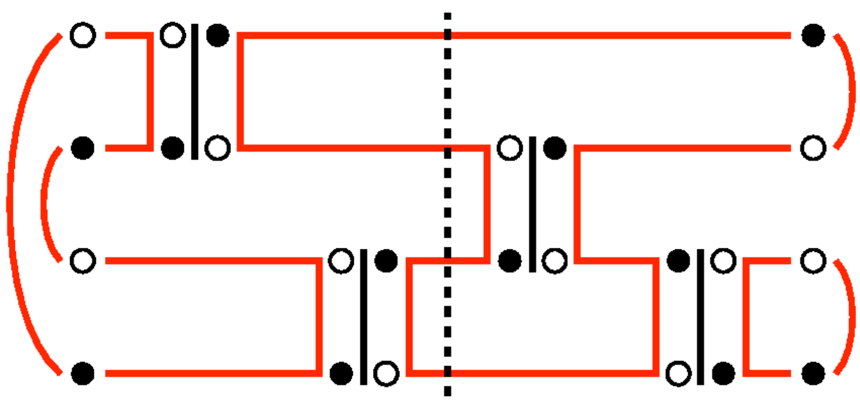
Quantum-critical scaling with exponent η in good agreement with the QMC calculations

SU(N) generalization of the J-Q model

J. Lou, A.W. Sandvik, N. Kawashima, arXiv:0908.0740

Heisenberg model with SU(N) spins has VBS state for large N
- Hamiltonian consisting of SU(N) singlet projectors
- In large-N mean-field theory Nc≈5.5 (Read & Sachdev, PRL 1988)
- QMC gives Nc≈4.5 (Tanabe & Kawashima, 2007; K. Beach et al. 2008)

The valence-bond loop projector QMC has a simple generalization
- N “colors” instead of 2 spin states
- Each loop has N “orientations”
- Stronger VBS order expected in SU(N) J-Q model



SU(N) J-Q_2 criticality

SU(2); q_c=0.961(1)

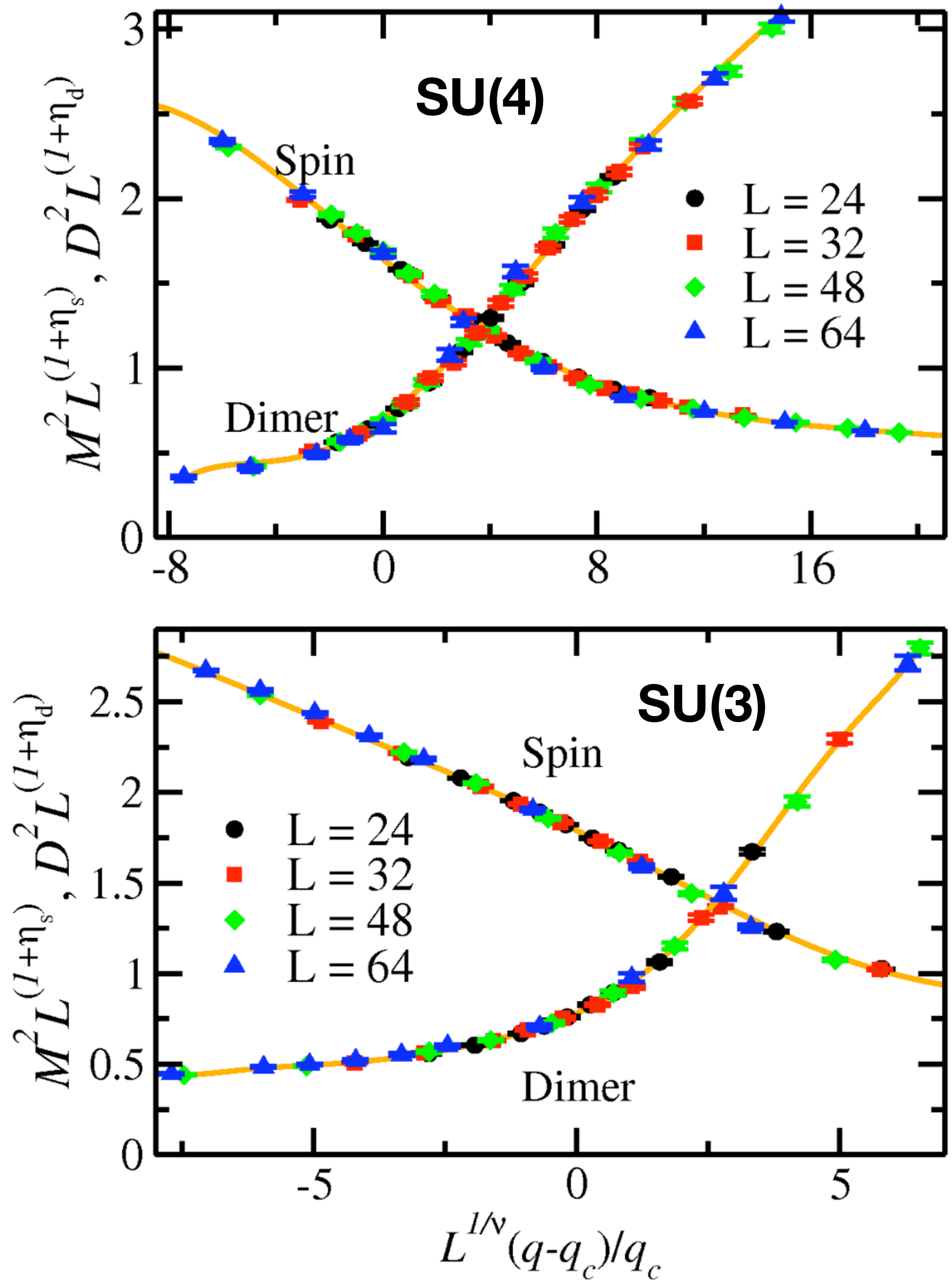
$$\eta_s = 0.35(2)$$
$$\eta_d = 0.20(2)$$
$$\nu = 0.67(1)$$

SU(3); q_c=0.335(2)

$$\eta_s = 0.38(3)$$
$$\eta_d = 0.42(3)$$
$$\nu = 0.65(3)$$

SU(4); q_c=0.082(2)

$$\eta_s = 0.42(5)$$
$$\eta_d = 0.64(5)$$
$$\nu = 0.70(2)$$

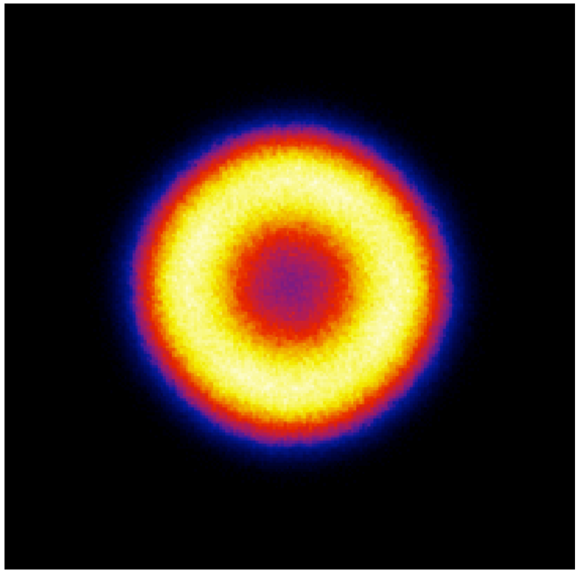


Order parameter histograms $P(D_x,D_y)$, L=32

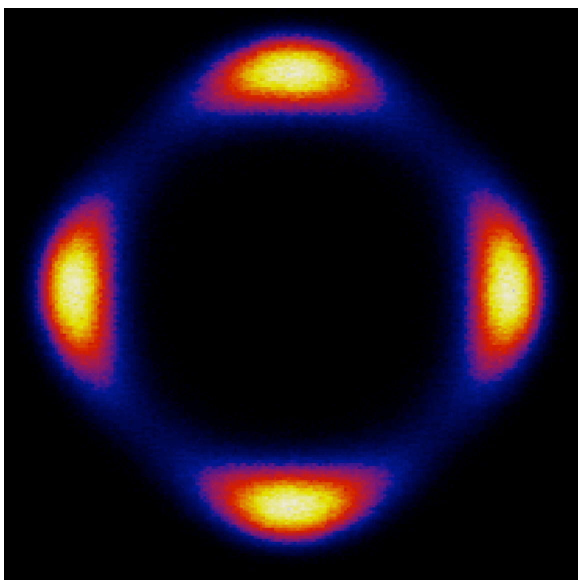
J-Q_3 model

$q = 0.635$

$(q_c \approx 0.60)$



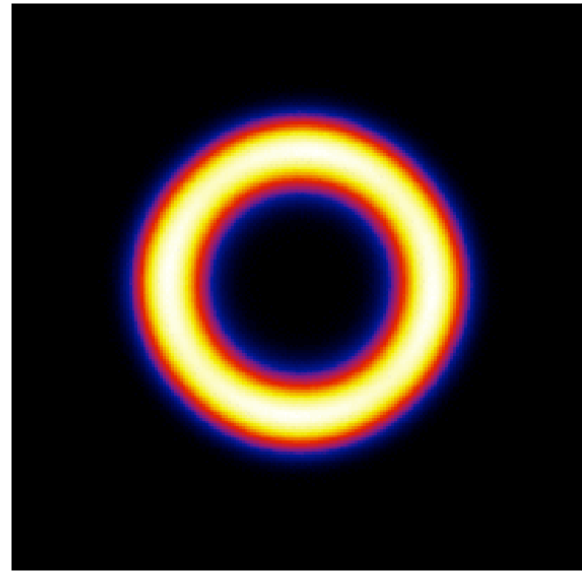
$q = 0.85$



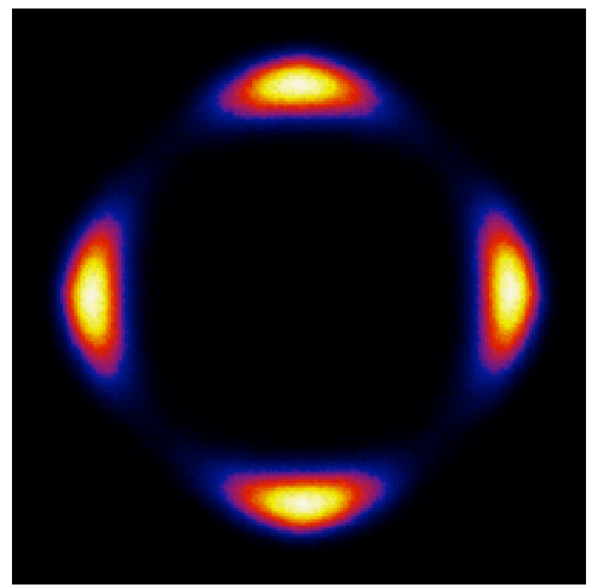
SU(3) J-Q_2 model

$q = 0.45$

$(q_c \approx 0.33)$



$q = 0.65$



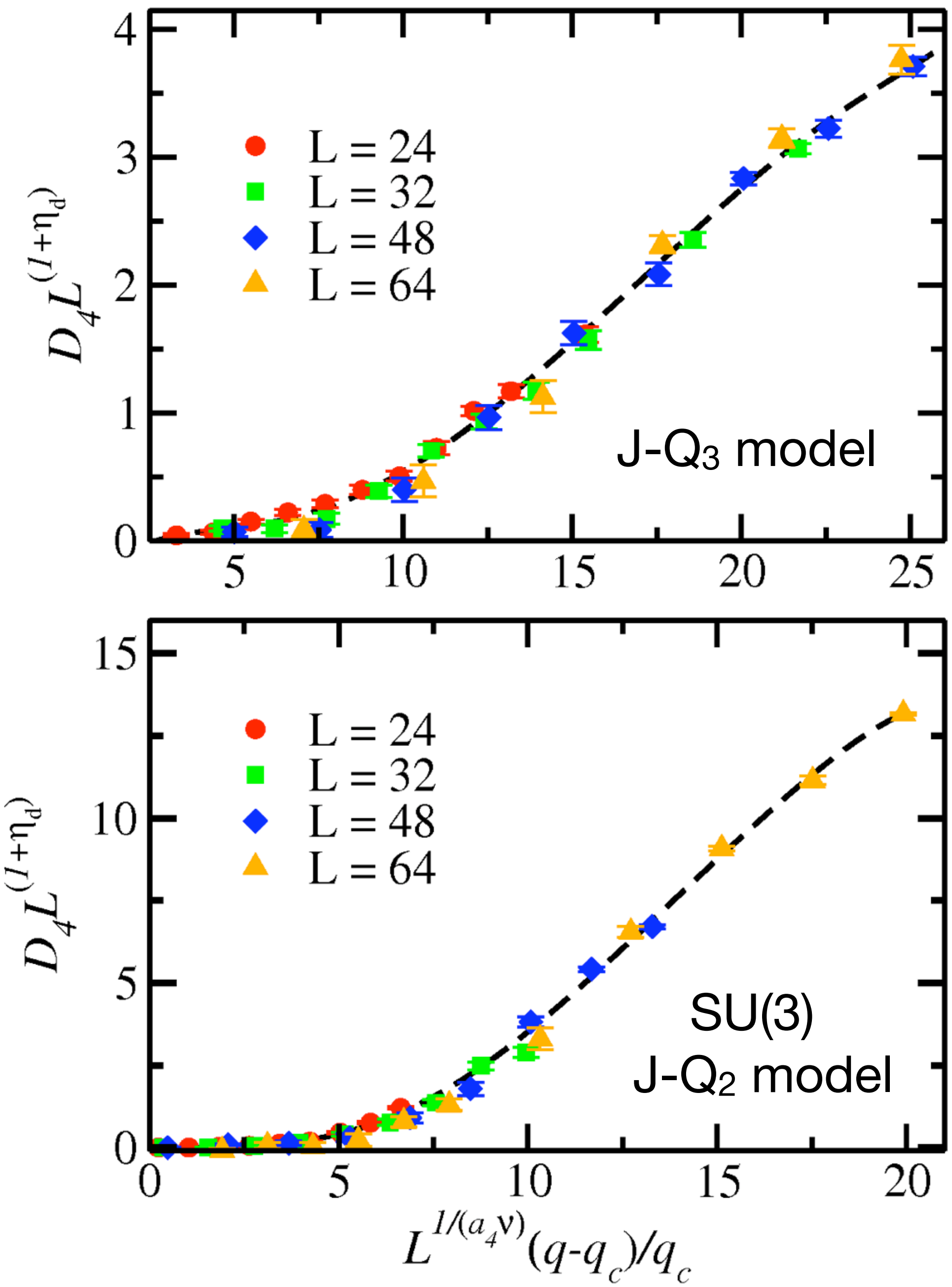
VBS symmetry cross-over

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

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

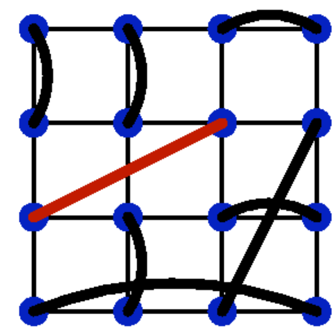
$$\Lambda \sim \xi^a \sim q^{-a\nu}$$

$$\alpha \approx 1.3$$

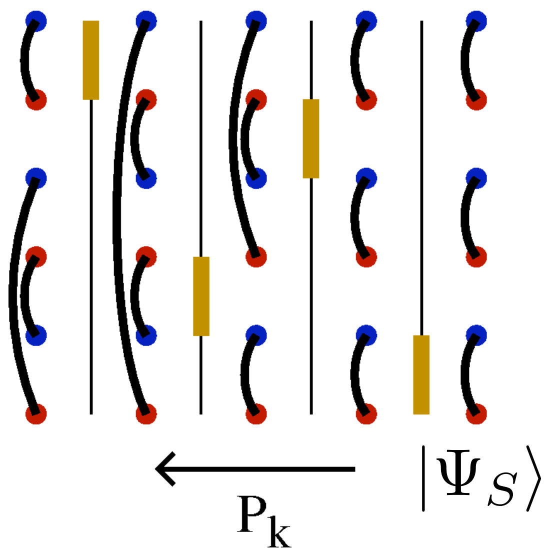


Is it possible to directly observe deconfinement of spinons?

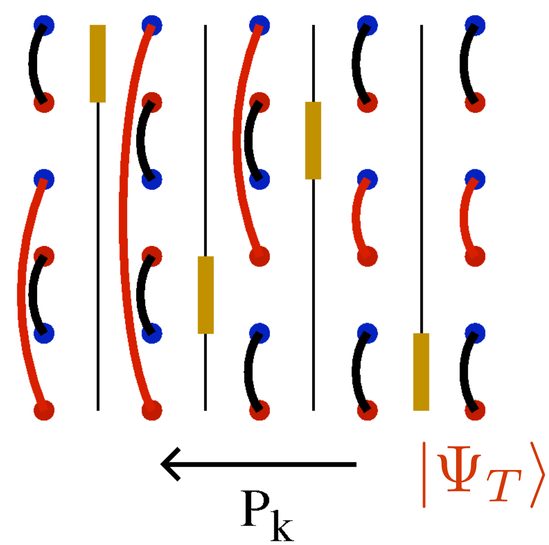
Valence bond projector method: direct access to the distribution of the triplet in an excited state



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

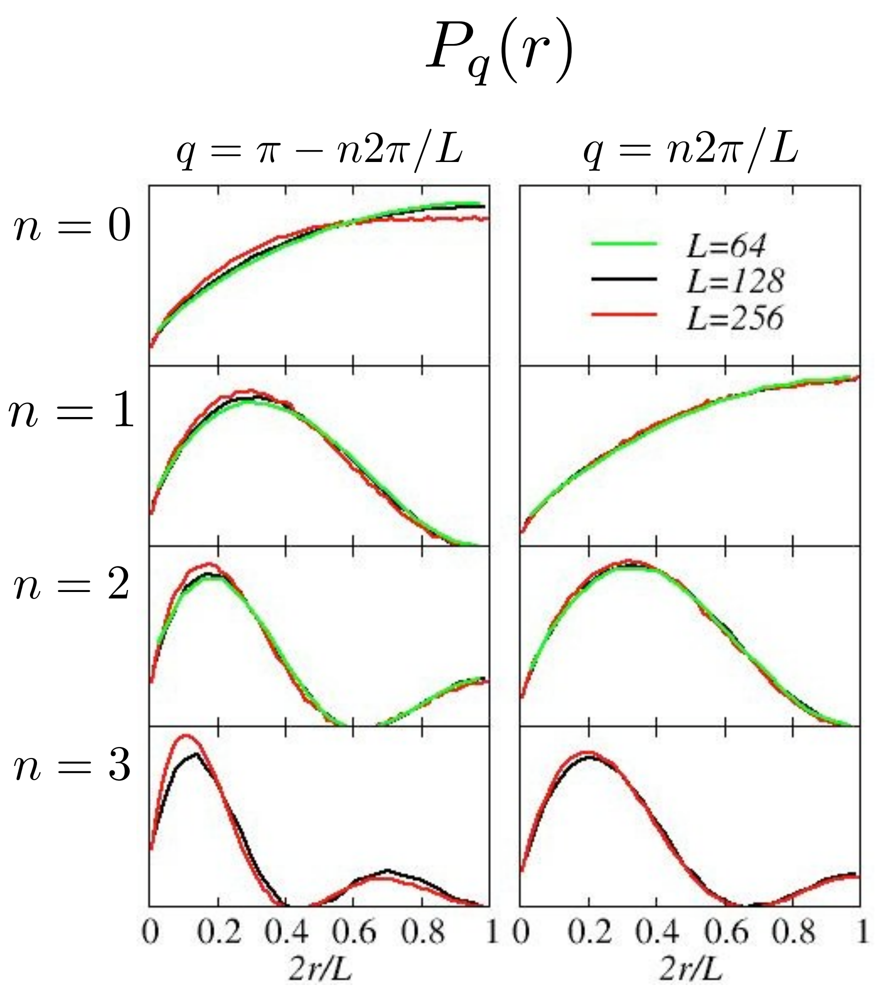
$$S^z(\mathbf{q})|\Psi_S(0)\rangle = |\Psi_T(\mathbf{q})\rangle \qquad S^z(\mathbf{q}) = \sum_r e^{i\mathbf{q}\cdot\mathbf{r}} S^z(\mathbf{r})$$

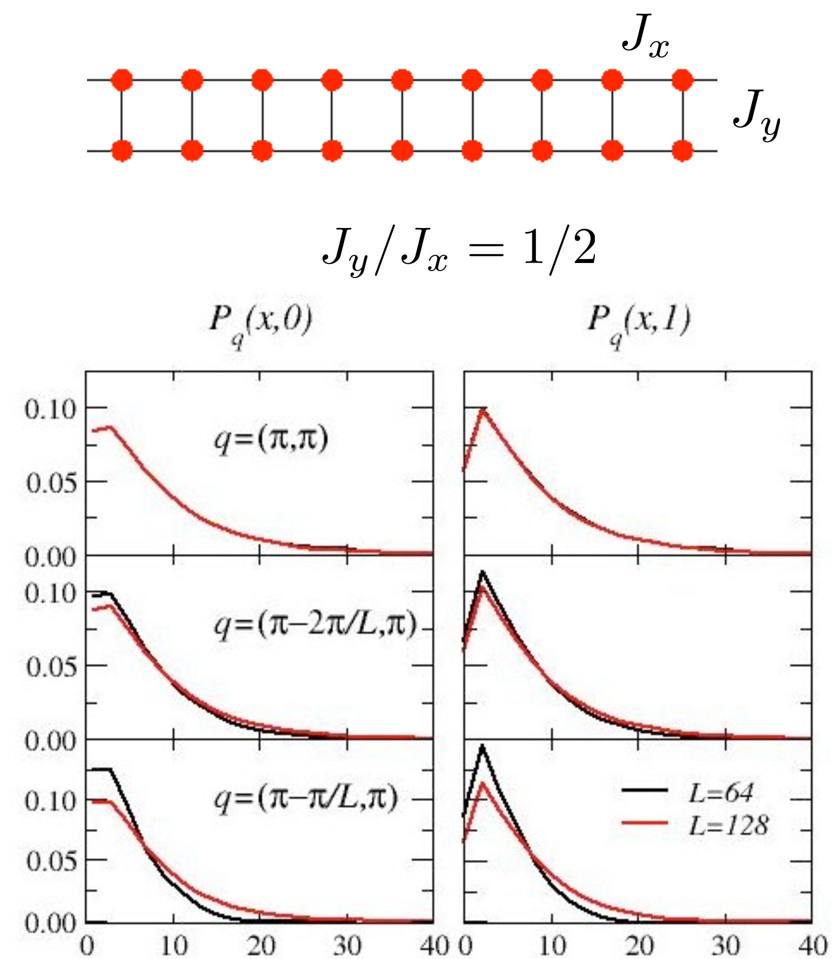
In principle triplets with arbitrary momentum can be studied

- 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?



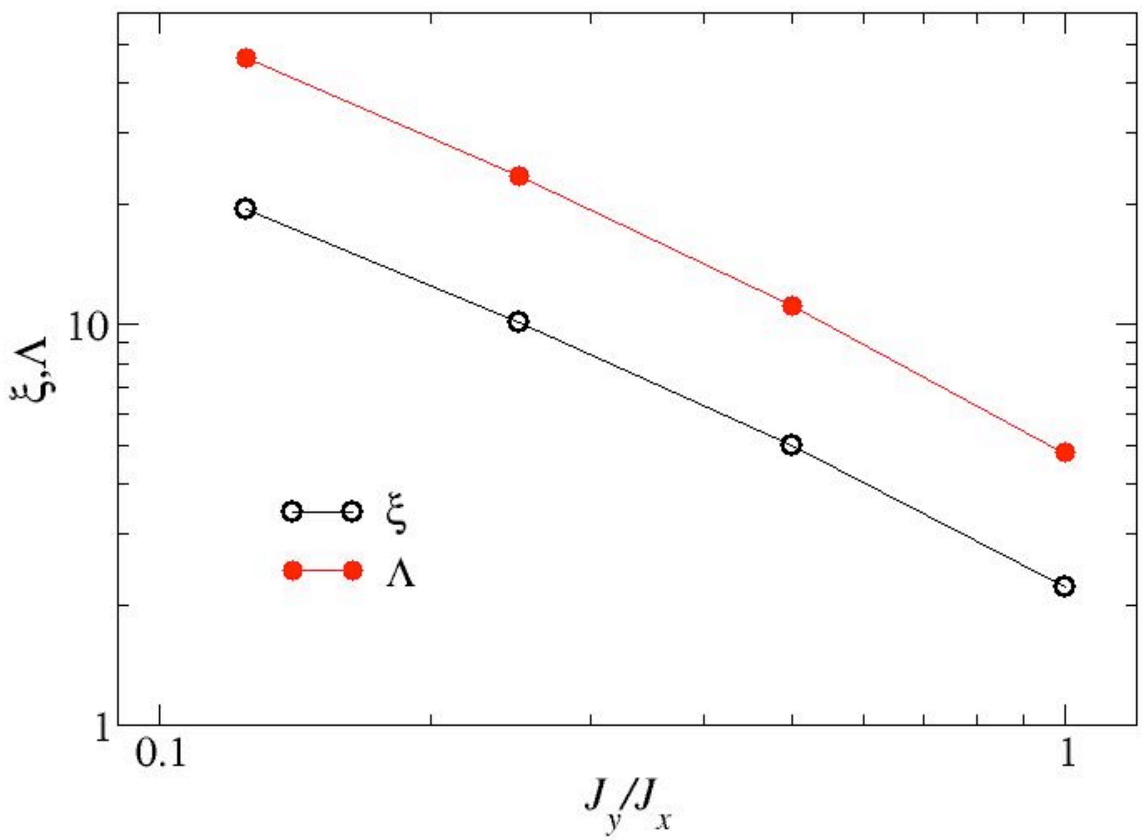


A.W. Sandvik, manuscript in preparation

Spinon deconfinement for $J_y/J_x \rightarrow 0$

ξ = spin correlation length

Λ = confinement length (average triplet size)



In this case

$\Lambda \propto \xi$

At a deconfined quantum-critical point

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

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 model

- Finite-size behavior indicated deconfined quantum-critical point
- Same exponents for two models; strengthens the case
- Emergent U(1) symmetry; cross-over quantified

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