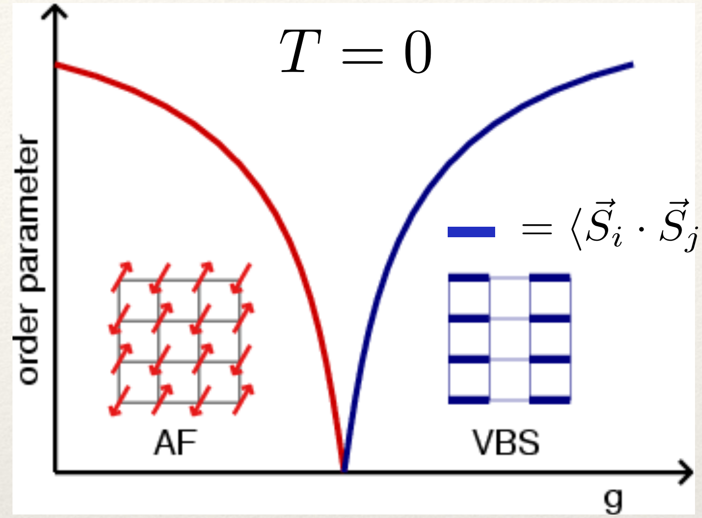
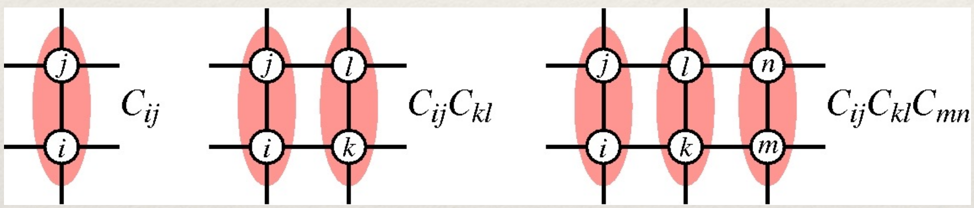
2D: Deconfined quantum criticality

Senthil, Vishwanath, Balents, Sachdev, Fisher (Science 2004)
(+ many previous works; Read & Sachdev, Sachdev & Murthy, Motrunich & Vishwanath….)

Continuous AF - VBS transition at T=0
- would be violation of Landau rule
- first-order would normally be expected
- role of topological defects



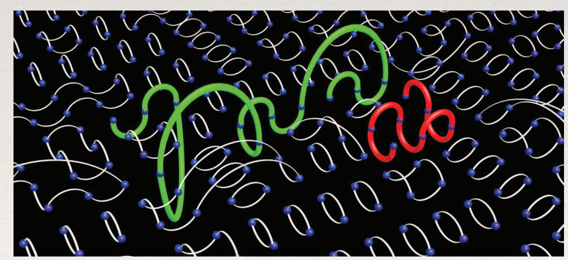
Numerical (QMC) tests using J-Q models



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

The "J-Q" model with two projectors is (Sandvik, PRL 2007)

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

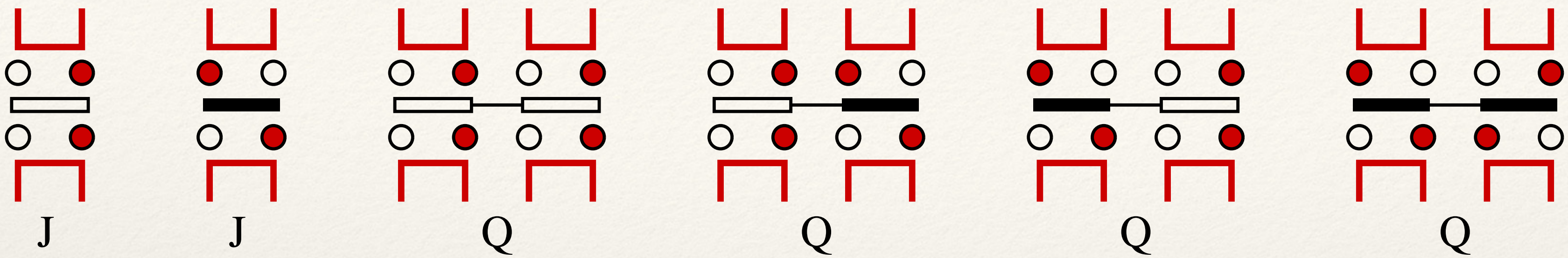


- Has Néel-VBS transition, appears to be continuous
- Not a realistic microscopic model for materials
- "Designer Hamiltonian" for VBS physics and AF-VBS transition

- **Unusual scaling properties** [Shao, Guo, Sandvik (Science 2016)]

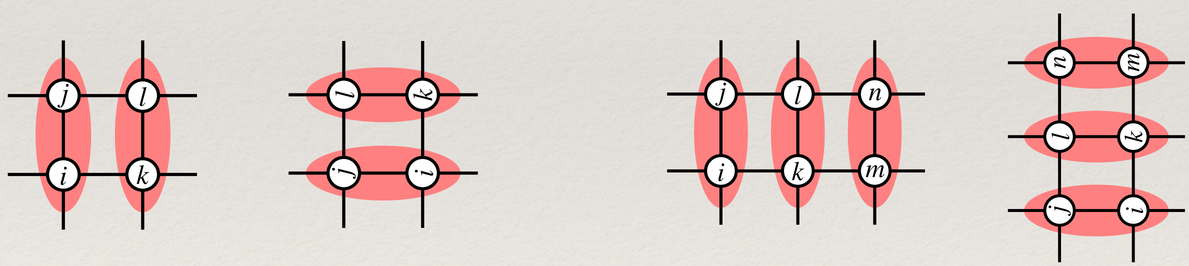
SSE and projector methods can be easily generalized for J-Q

J- and Q-vertices through which loops enter and exit at the individual 2-spin diagonal and off-diagonal parts

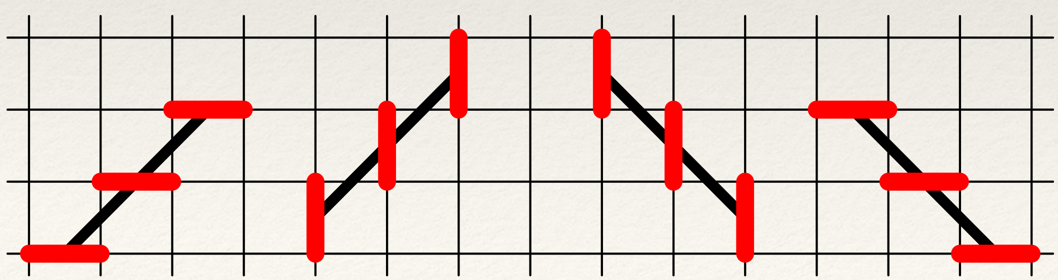


The 1D J-Q model has critical-dimerized transition of exactly the same kind as in the J_1-J_2 Heisenberg chain

2D J-Q models with first-order and (apparently) continuous transitions (deconfined quantum criticality) can be constructed



Continuous transitions



first-order transition

Operator coding for J-Q models

Slide by Ying Tang, Trieste School 2012

- **JQ3 Model**

$$H = -J \sum_{<ij>} \mathbf{C_{ij}} - Q \sum_{<ijklmn>} \mathbf{C_{ij} C_{kl} C_{mn}}$$

J Operator (<J> = J/2)

	0	0	0	0		0	0	0	1

Q Operator (<Q> = Q/8)

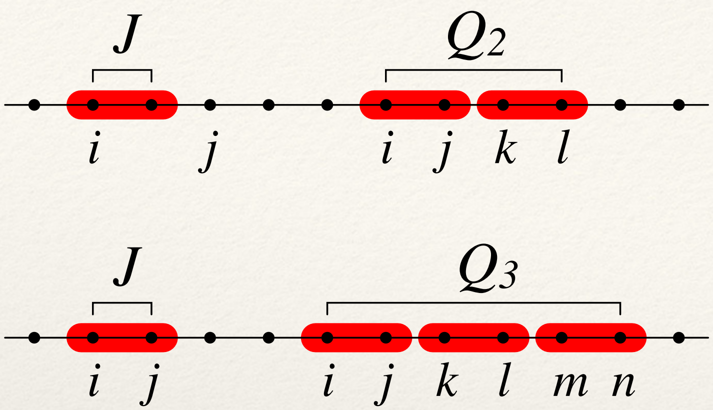
	1	0	0	0		1	1	0	0
	1	0	0	1		1	1	0	1
	1	0	1	0		1	1	1	0
	1	0	1	1		1	1	1	1

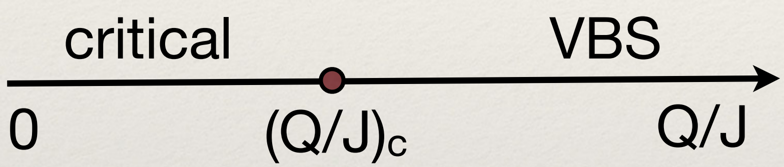
$$(-H)^m = \sum_{\{\alpha,a\}} \prod_{l=1}^{m} \hat{O}^{a}_{i^\alpha_l j^\alpha_l} = \sum_{\{\alpha\}} P_{\{\alpha\}}$$

Linked vertex list and loop update:

- direct generaization of data structure and procedure for Heisenberg

Related 1D system:
VBS state in J-Q chains

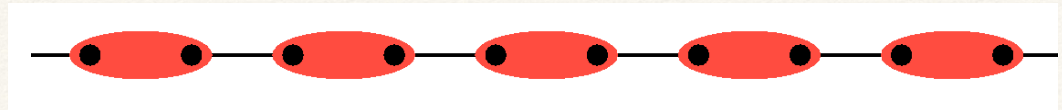




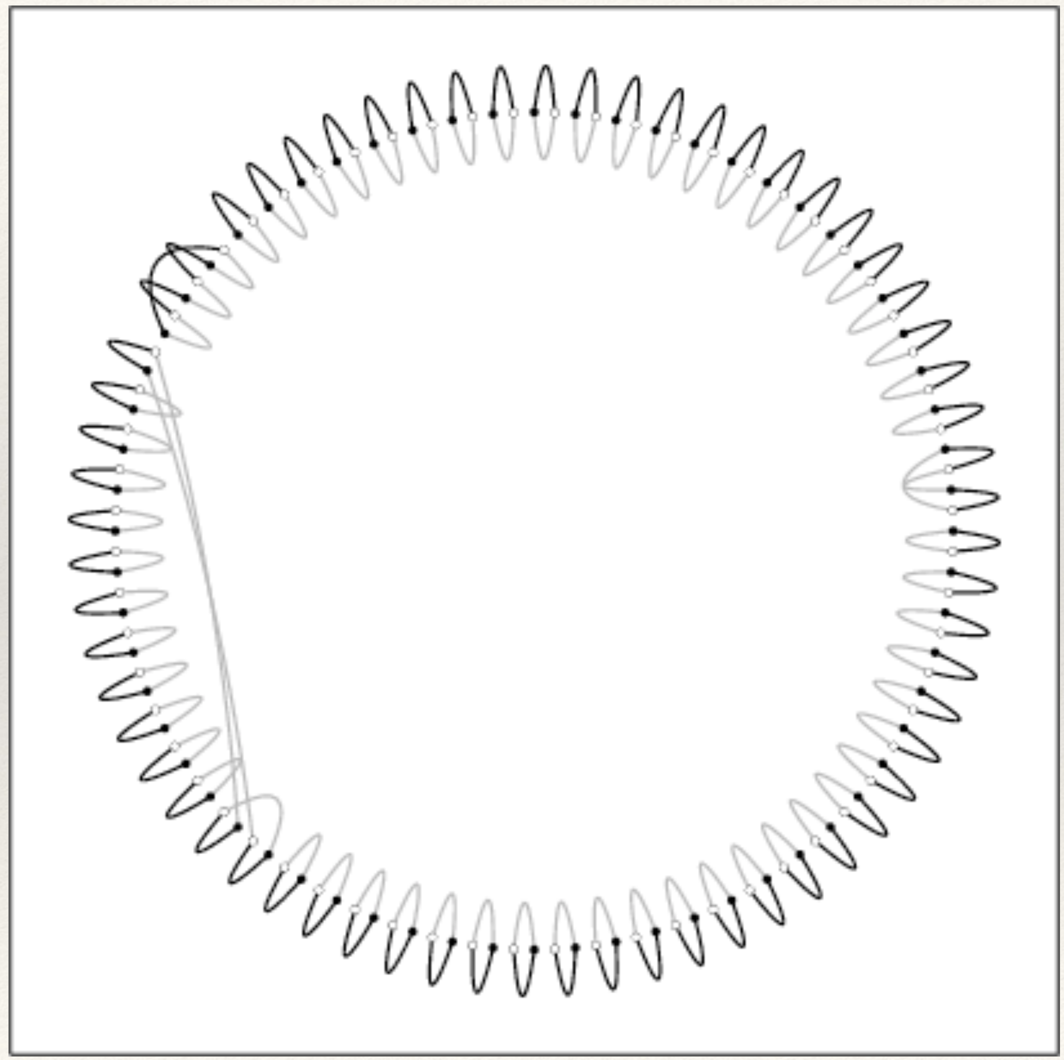
Exactly the same physics (quantum phases and phase transition) as in J_1-J_2 Heisenberg chain

Evolution of VBS state during projector QMC (J=0)

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

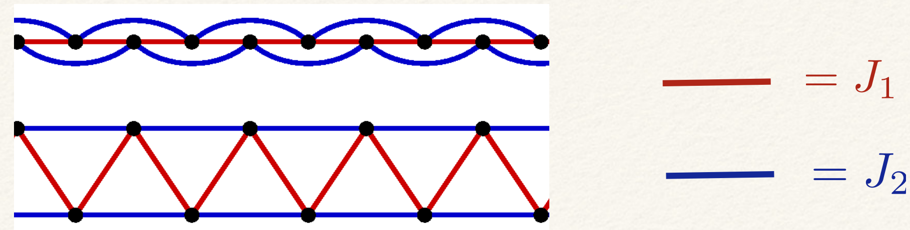


VBS phase - always with fluctuations



Heisenberg chain with frustrated interactions

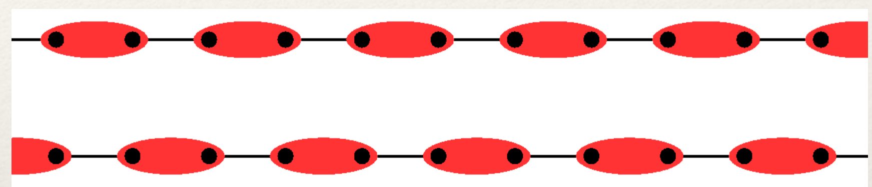
$$H = \sum_{i=1}^{N} \left[J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_i \cdot \mathbf{S}_{i+2} \right]$$



For the special point $J_2/J_1=0.5$, this model has an exact solution

Singlet-product states

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



It is not hard to show that these are eigenstates of H

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

The system has this kind of order (with fluctuations, no exact solution) for all $J_2/J_1>0.2411$..... This is a **quantum phase transition** between

- a critical state
- a valence-bond-solid (VBS) state

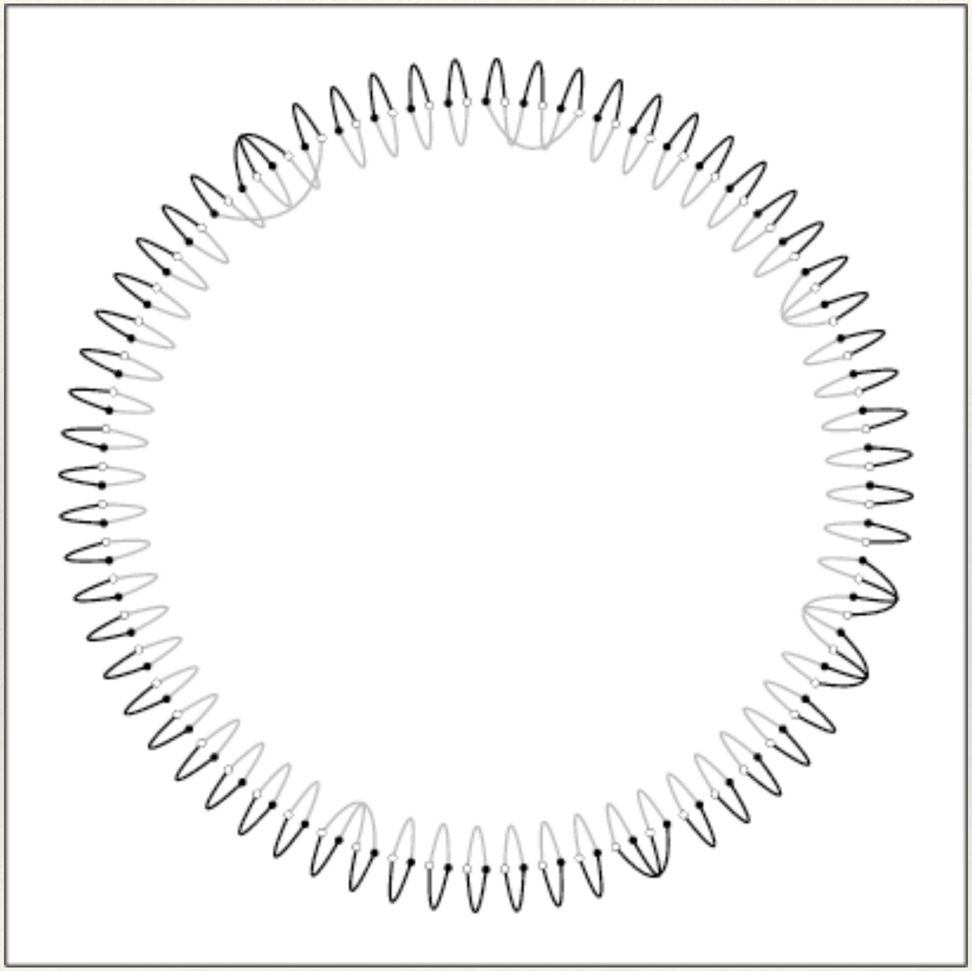
The symmetry is not broken for finite N

- the ground state is a superposition of the two ordered states

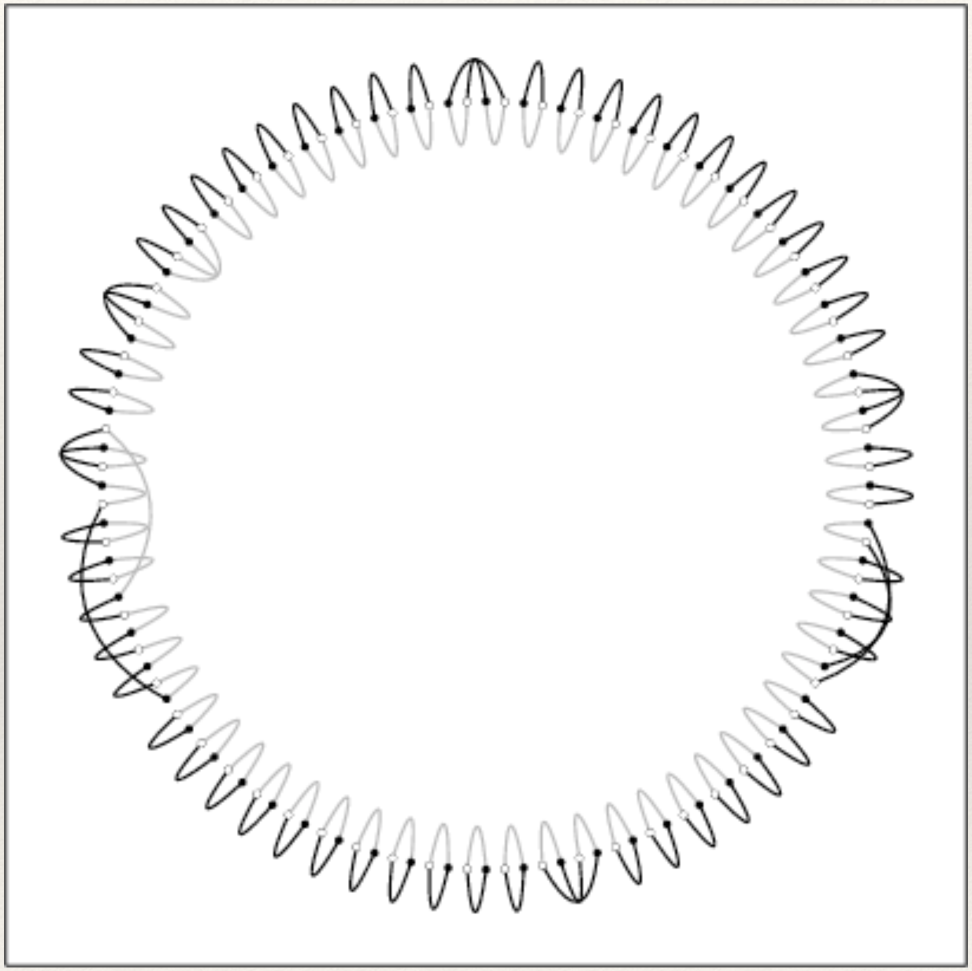
$$|\Psi_0\rangle \sim |\Psi_A\rangle + |\Psi_B\rangle, \qquad |\Psi_1\rangle \sim |\Psi_A\rangle - |\Psi_B\rangle$$

J-Q chains: VBS with more fluctuations and critical state

$J/Q = 0.5$



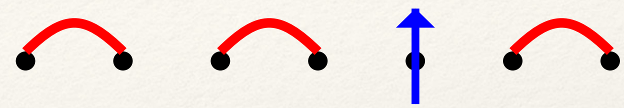
$J/Q = (J/Q)_c \approx 6$

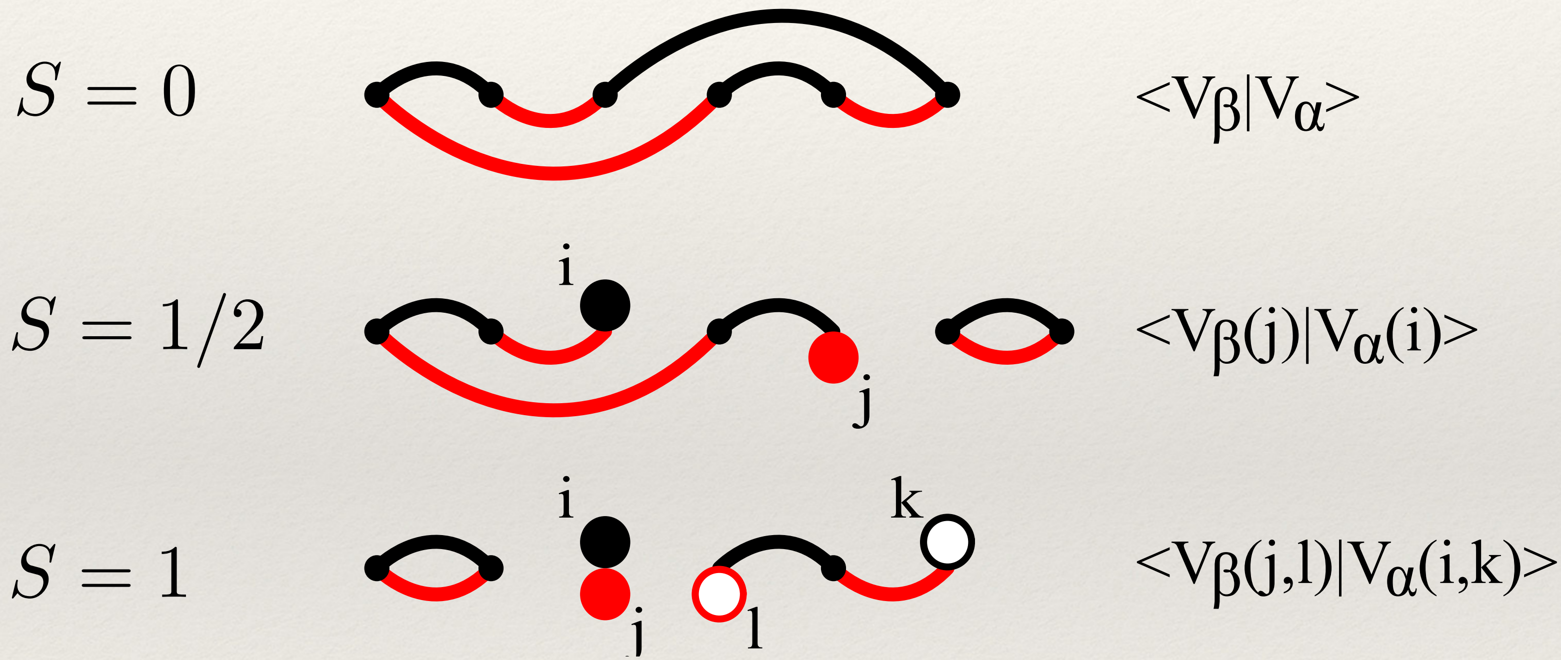


Extended valence-bond basis for S>0 states

Consider $S^z=S$

- for even N spins: N/2-S bonds, 2S unpaired "up" spins
- for odd: (N-2S)/2 bonds, 2S unpaired spins
- transition graph has 2S open strings





Overlaps and matrix elements involve loops and strings

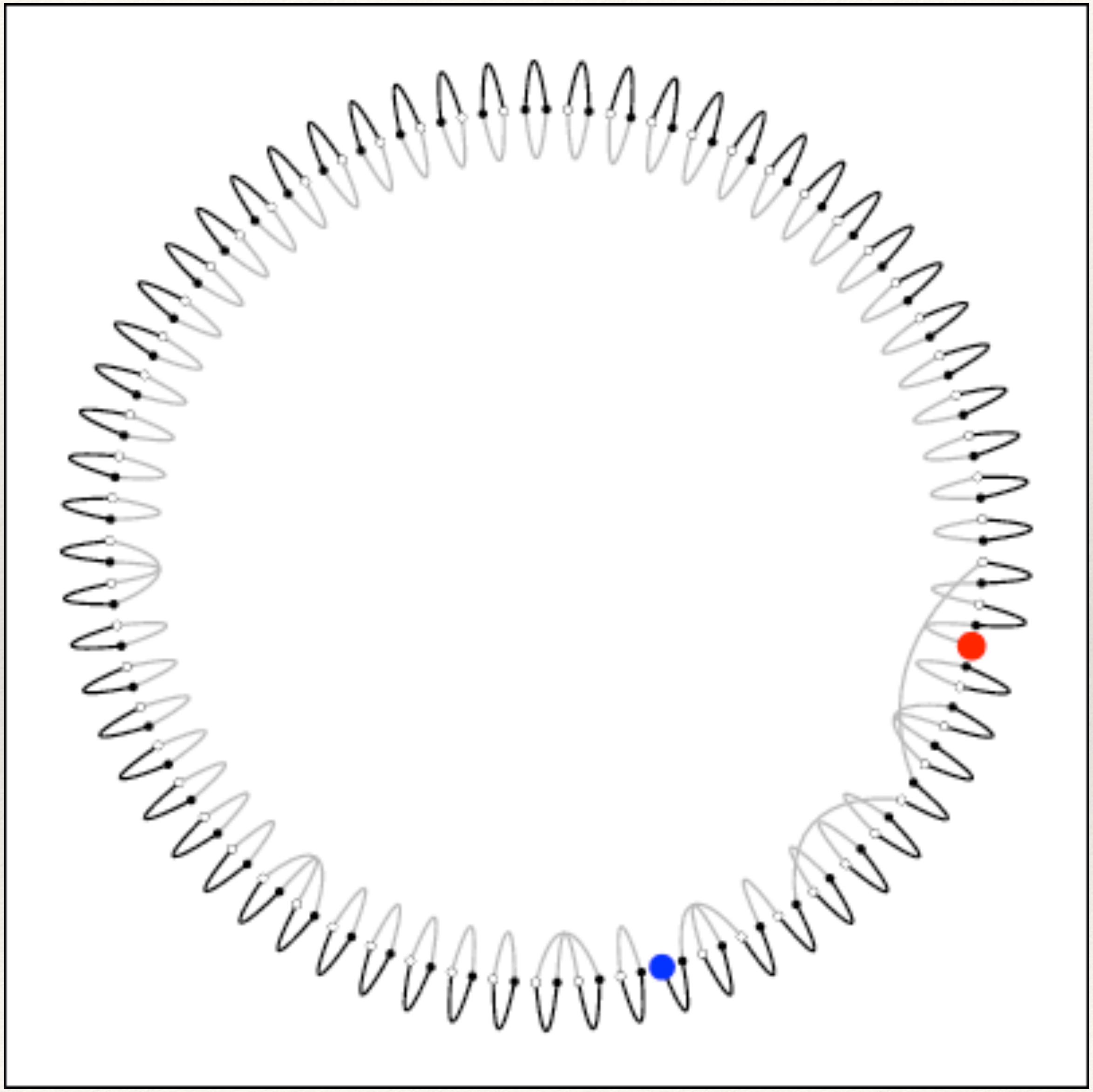
- very simple generalizations of the S=0 case
- loops have 2 states, strings have 1 state

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

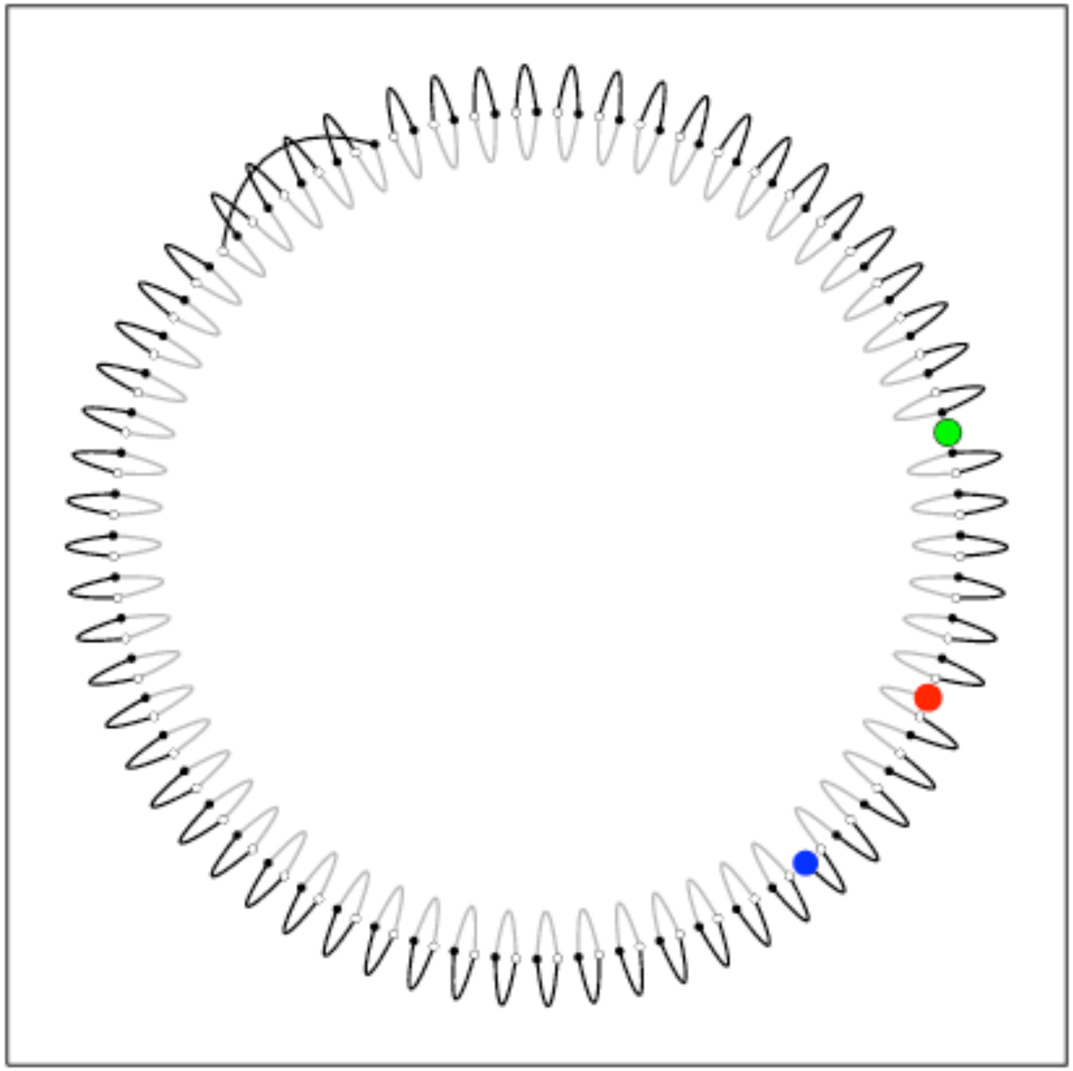
- one spin (spinon) doesn't belong to any bond
- bra and ket spinons at different locations; non-orthogonality

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

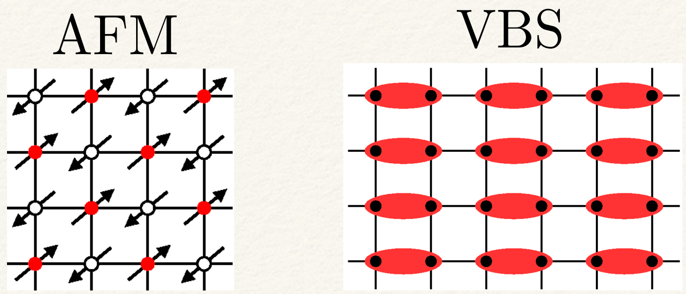
- the spinon is not just the unpaired spin



Two spinons in 1D VBS are deconfined (no confining potential)
- 2 separated (deconfined) sets of bra/ket spinons



Phase transition in the 2D J-Q model



Staggered magnetization

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

Dimer order parameter (D_x,D_y)

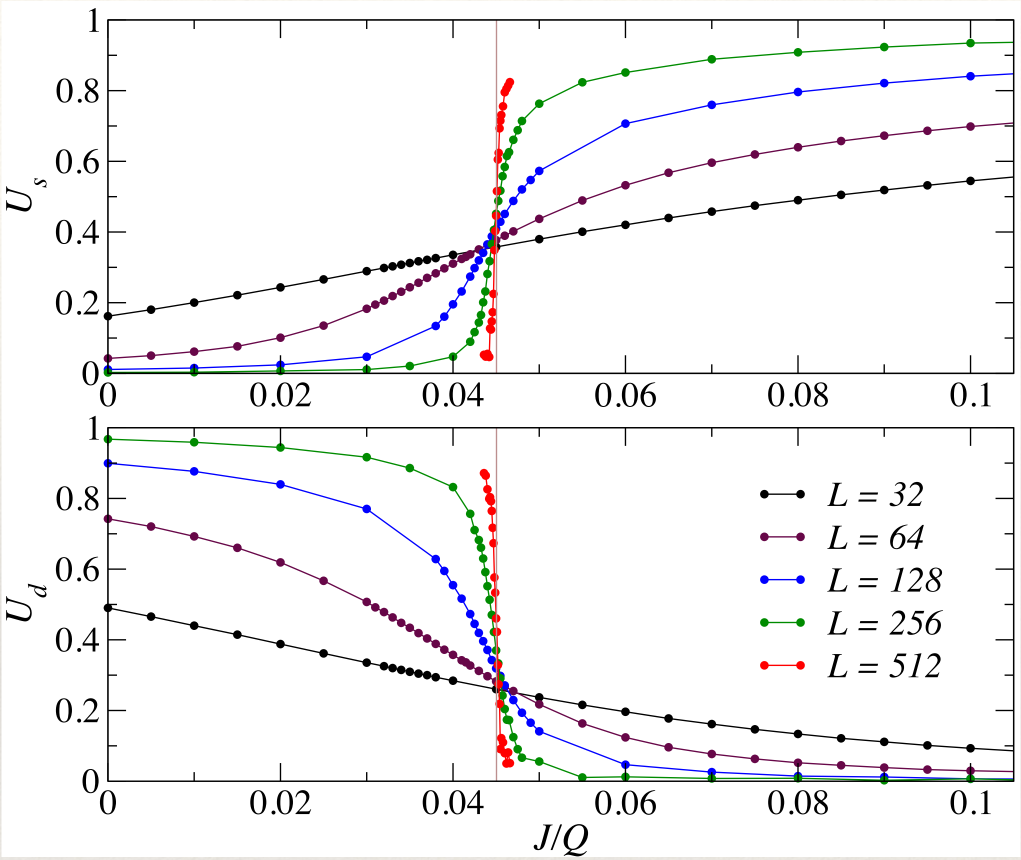
$$D_x = \frac{1}{N}\sum_{i=1}^{N}(-1)^{x_i}\mathbf{S}_i\cdot\mathbf{S}_{i+\hat{x}}$$

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

Binder cumulants:

$$U_s = \frac{5}{2}\left(1-\frac{1}{3}\frac{\langle M_z^4\rangle}{\langle M_z^2\rangle^2}\right)$$

$$U_d = 2\left(1-\frac{1}{2}\frac{\langle D^4\rangle}{\langle D^2\rangle^2}\right)$$



U_s → 1, U_d → 0 in AFM phase

U_s → 0, U_d → 1 in VBS phase

Behaviors of crossing points → exponents

Phenomenological two-length scaling

[Shao, Guo, Sandvik (Science 2016)]

Competing scenario:

- weak first-order transition
- non-unitary conformal field theory

Exponent ν: crossing-point analysis

H. Shao, W. Guo, A. W. Sandvik (Science 2016)

Binder ratio of the AF order parameter

$$R_1 = \frac{\langle m_{sz}^2 \rangle}{\langle |m_{sz}| \rangle^2}$$

- **Crossing of $R_1(g,L)$, $R_1(g,rL)$**, g=J/Q,
  g*(L), analyze size dependence (using r=2)

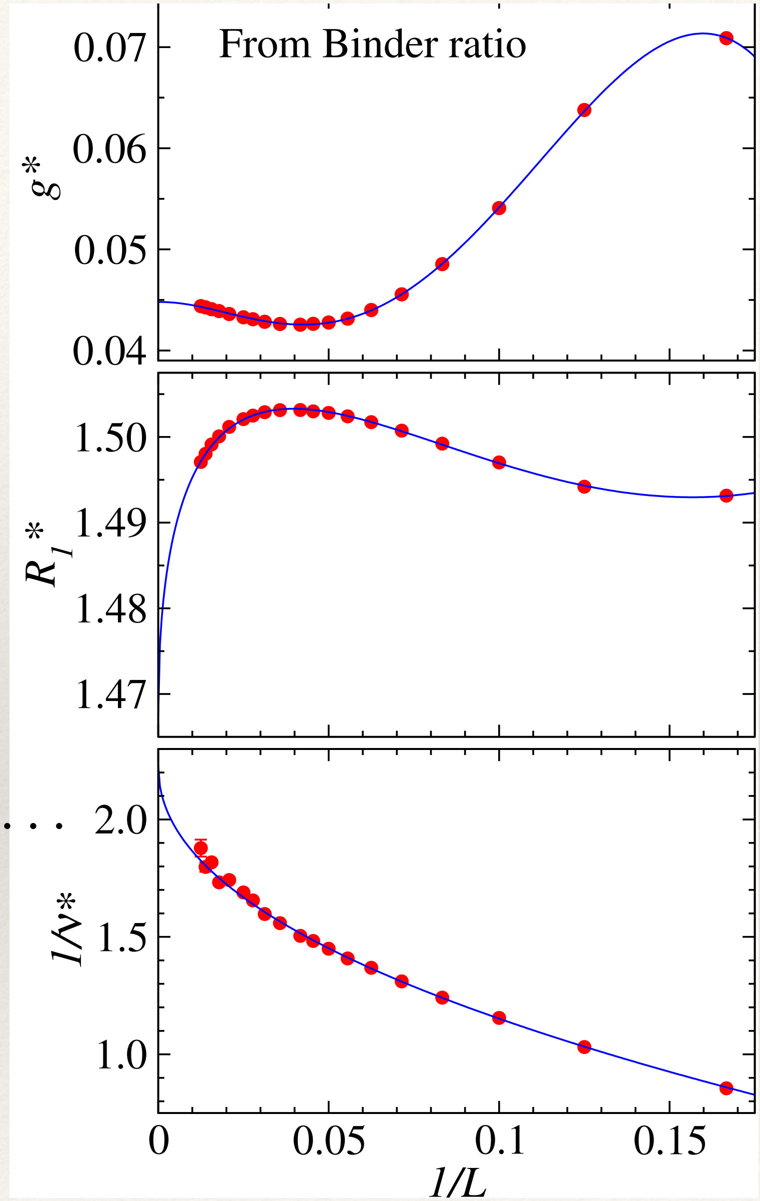
$$g^*(L) = g_c + aL^{-(1/\nu+\omega)} + \ldots$$

$$R_1^*(L) = R_{1c} + aL^{-\omega} + \ldots$$

$$\frac{1}{\nu^*} = \ln[s(g^*,rL)/s(g^*,L)] = \frac{1}{\nu}\ln(r) + aL^{-\omega} + \ldots$$

$$s(g,L) = dR_1(g,L)/dg \quad \text{(slope)}$$

- Small correction exponent; ω ≈ 0.5
- ν = 0.45 +/- 0.01



Improved results

[Sandvik & Zhao, Chin. Phys. Lett. 2020]

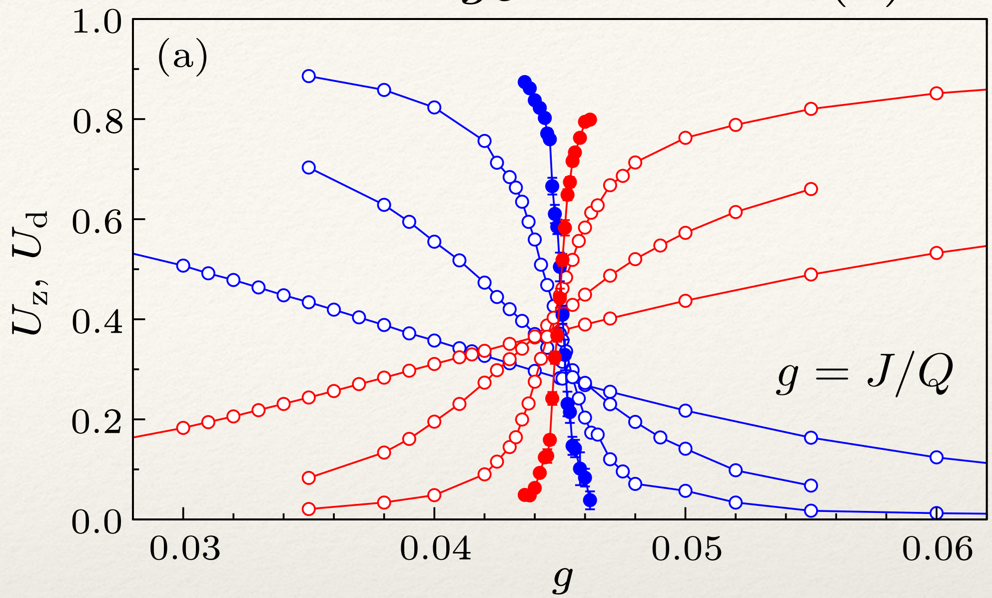
Binder cumulants give critical point

- slopes used to define $1/\nu$

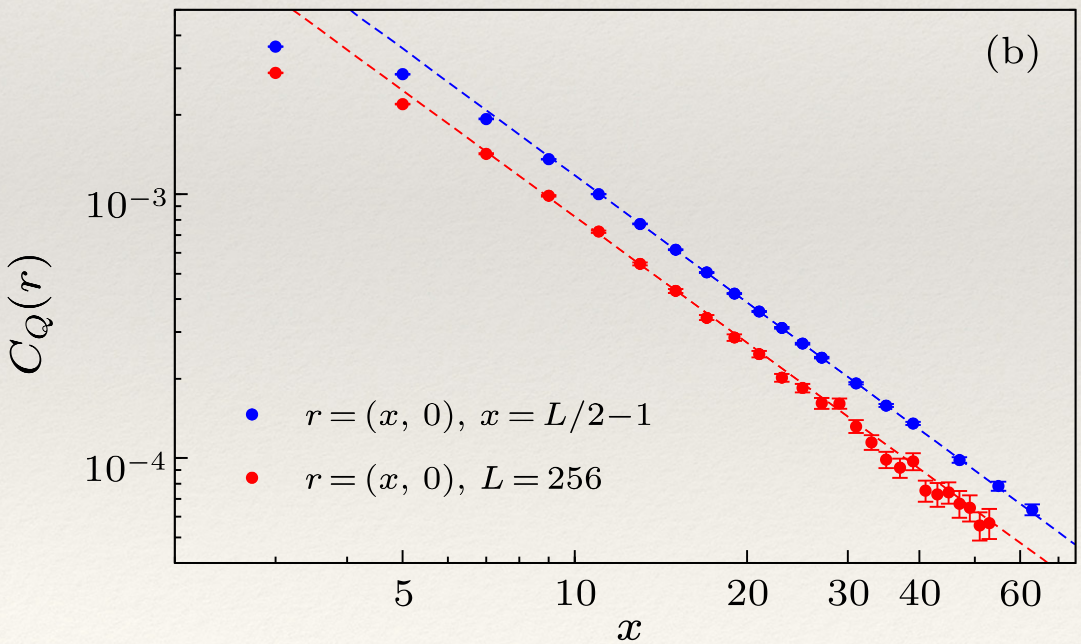
$$\frac{1}{\ln(2)} \ln\left(\frac{U'(2L)}{U'(L)}\right) \to \frac{1}{\nu}$$

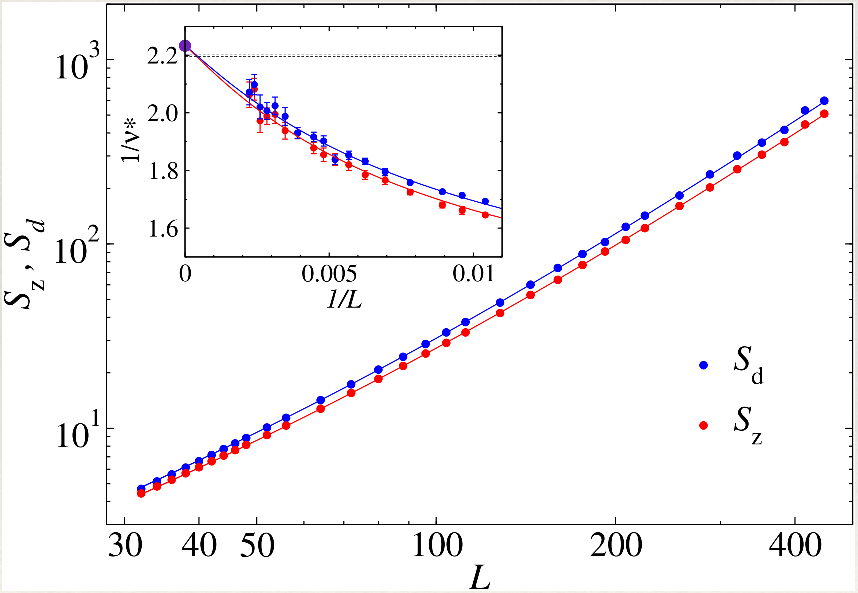
We can also calculate correlations of the relevant J and Q terms in H

$L \to \infty: \; g_c = 0.04510(2)$



Q-Q correlations:





Mutual consistency between two ways of calculating $1/\nu$

The VBS order parameter

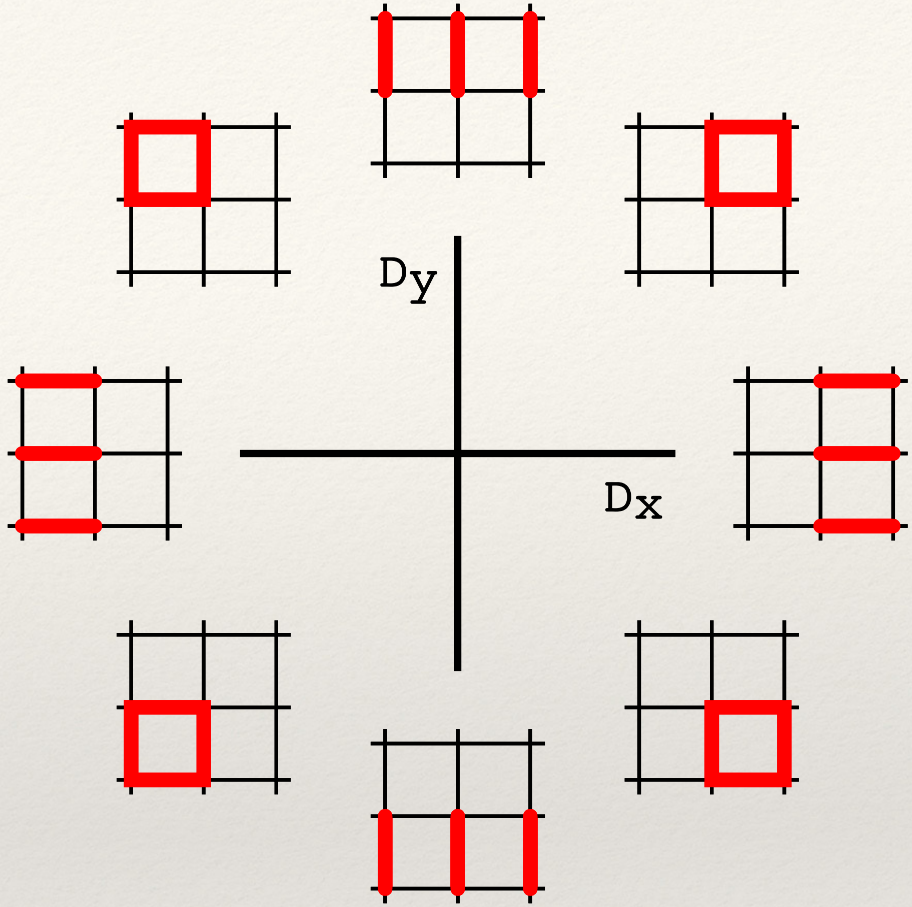
Dimer order parameter

$$D_x = \frac{1}{N}\sum_{x,y}(-1)^x \mathbf{S}_{x,y}\cdot\mathbf{S}_{x+1,y}$$

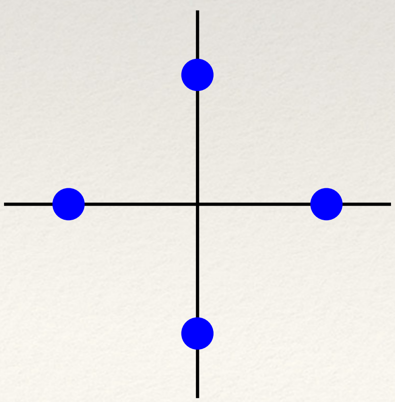
$$D_y = \frac{1}{N}\sum_{x,y}(-1)^y \mathbf{S}_{x,y}\cdot\mathbf{S}_{x,y+1}$$

Collect histograms $P(D_x,D_y)$ with valence-bond basis QMC

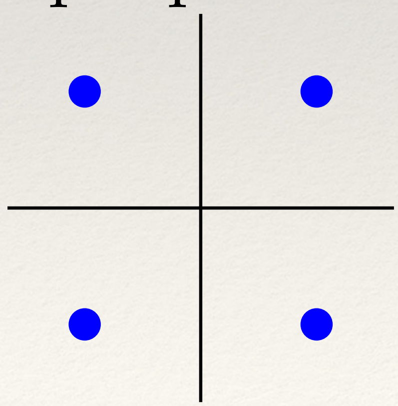
Two possible types of order patterns distinguished by histograms

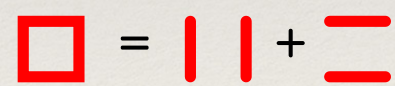


columnar



plaquette



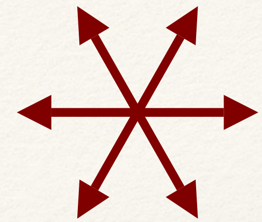


Finite-size fluctuations
- amplitude
- angular

Analogy with classical 3D clock model

$$H = -J \sum_{\langle ij \rangle} \cos(\Theta_i - \Theta_j) - h \sum_i \cos q\Theta_i$$ (soft clock model)

$$H = -J \sum_{\langle ij \rangle} \cos(\Theta_i - \Theta_j)$$ q clock angles (hard clock model)

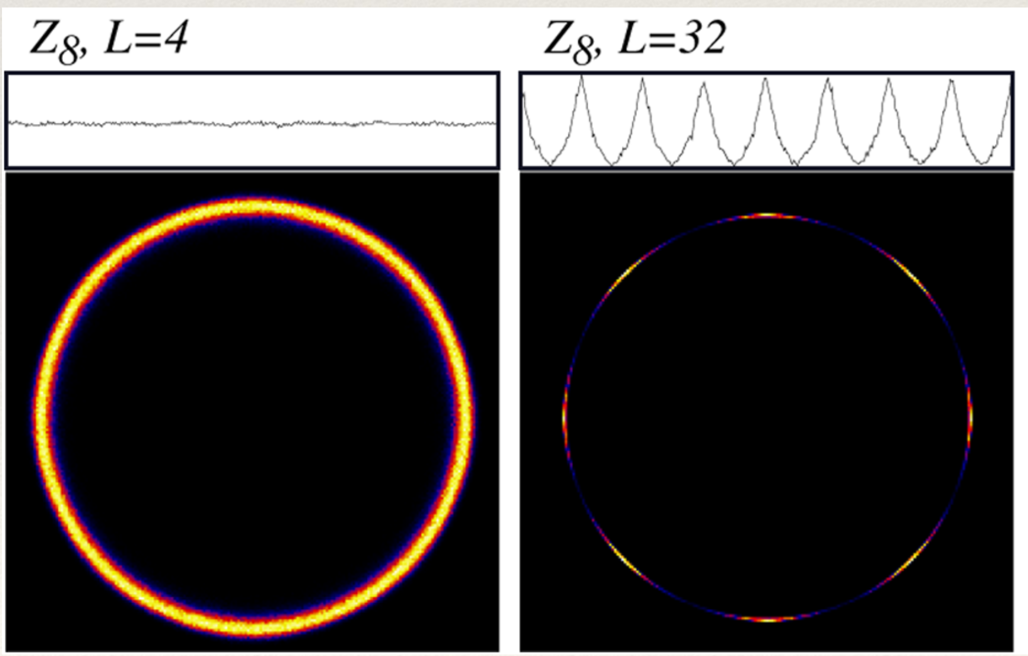


$q = 6$

Standard order parameter **(m_x,m_y)**

$$m_x = \frac{1}{N}\sum_{i=1}^{N} \cos(\Theta_i) \qquad m_y = \frac{1}{N}\sum_{i=1}^{N} \sin(\Theta_i) \quad \rightarrow \ \text{global angle } \theta$$

Probability distribution $P(m_x,m_y)$ shows cross-over from U(1) to Z_q for $T<T_c$



Lou, Balents, Sandvik, PRL 2007

Can be quantified with "angular order parameter":

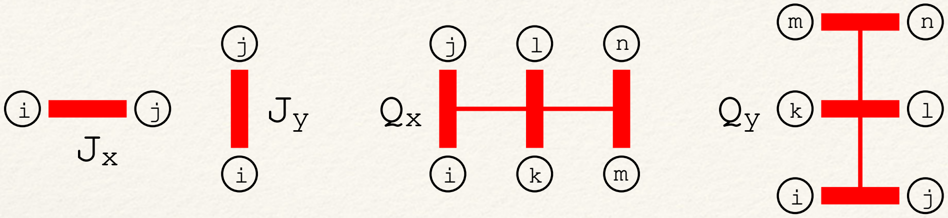
$$\phi_q = \int_0^{2\pi} d\theta \cos(q\theta) P(\theta)$$

$\varphi_q > 0$ only if q-fold anisotropy

Finite-size scaling of φ_q can be used to extract length scale $\xi' > \xi$ and associated scaling dimension y_q [Lecture by Hui Shao]

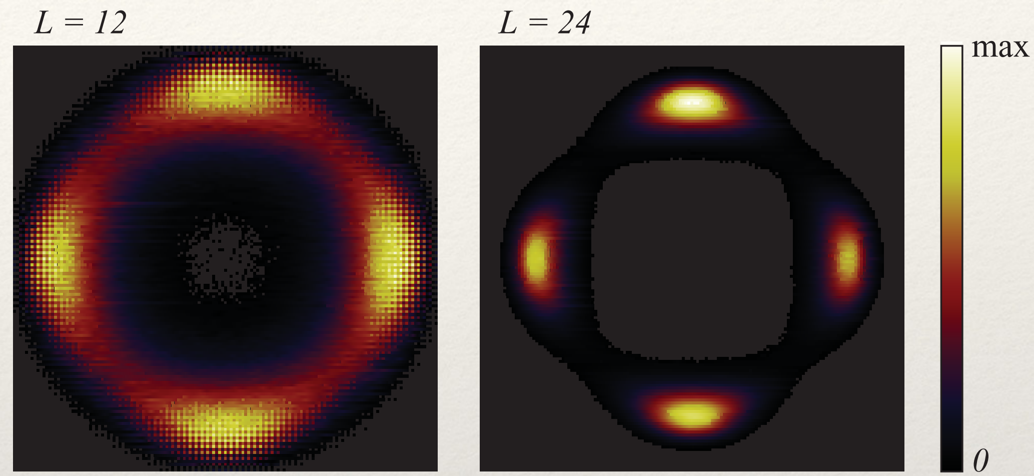
Emergent U(1) symmetry of columnar VBS order

Realize stronger VBS order with J-Q_3 model



J-Q_3 model
$J_x=J_y$, $Q_x=Q_y$

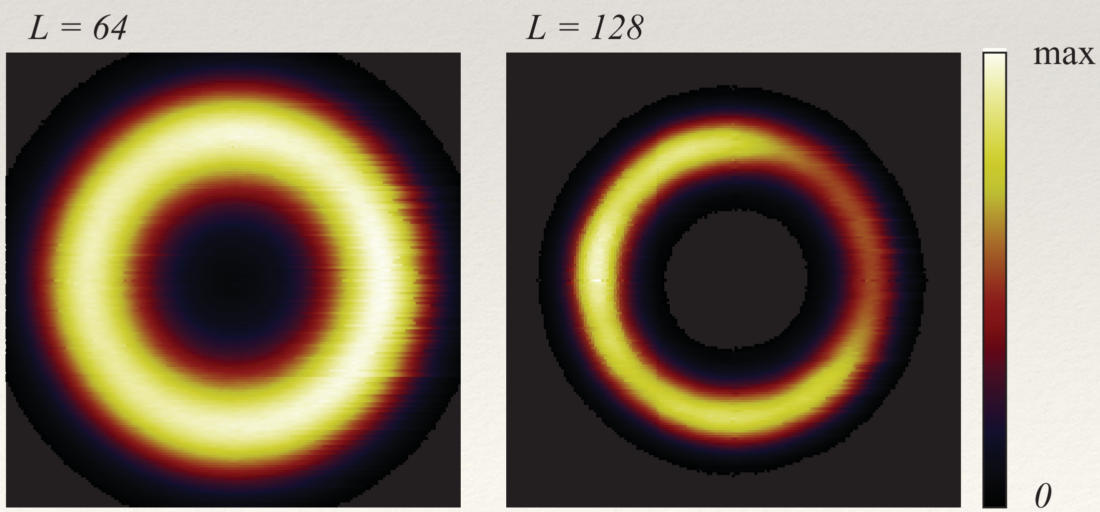
Lou, Sandvik, Kawashima, PRB (2009),
Sandvik, PRB (2012)

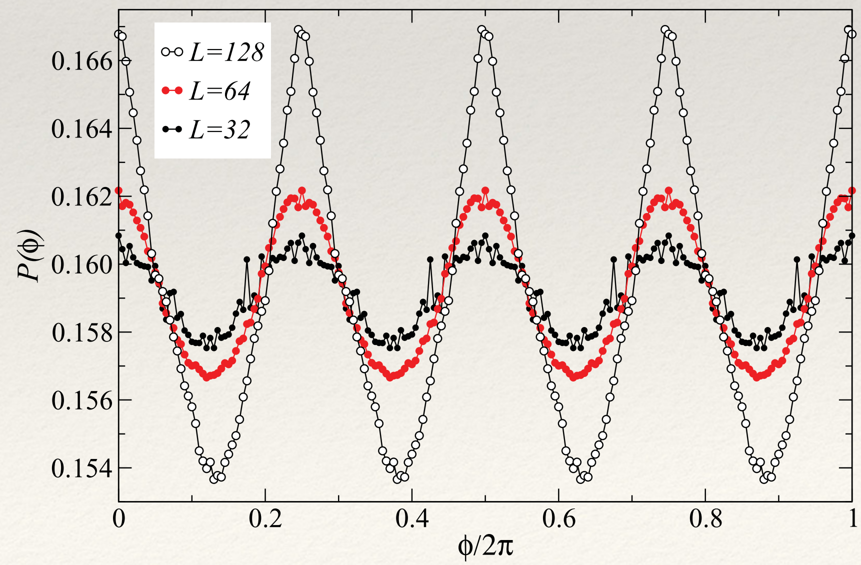


Strong columnar VBS when J/Q_3=0

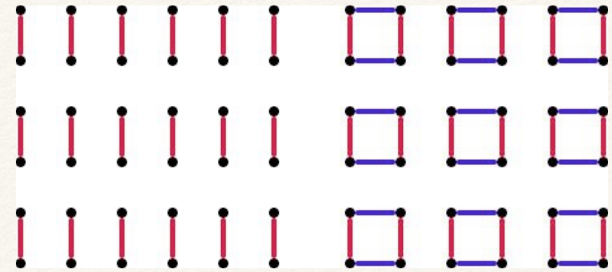
J-Q_2 model with J/Q_2=0

- weak columnar VBS
- very large angular fluctuations
- emergent U(1) symmetry



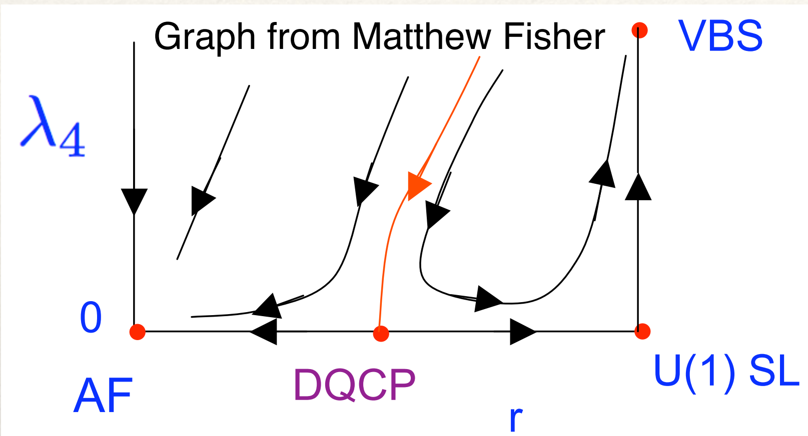


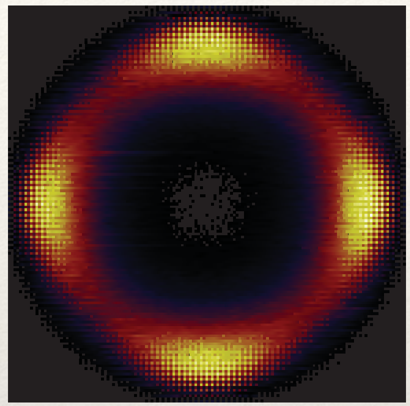
DQCP: In the field theory the VBS corresponds to condensation of topological defects (quadrupoled monopoles on square lattice)

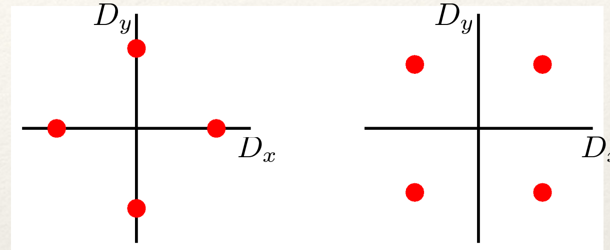


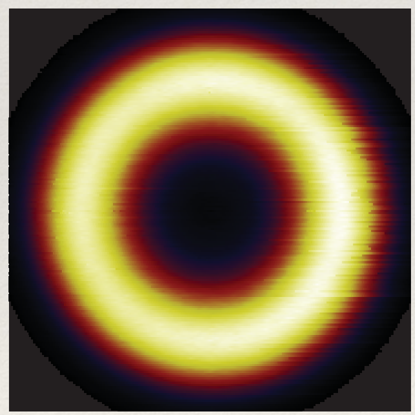
Analogy with 3D clock models: The topological defects should be dangerously irrelevant

Fugacity of topological defects λ_4



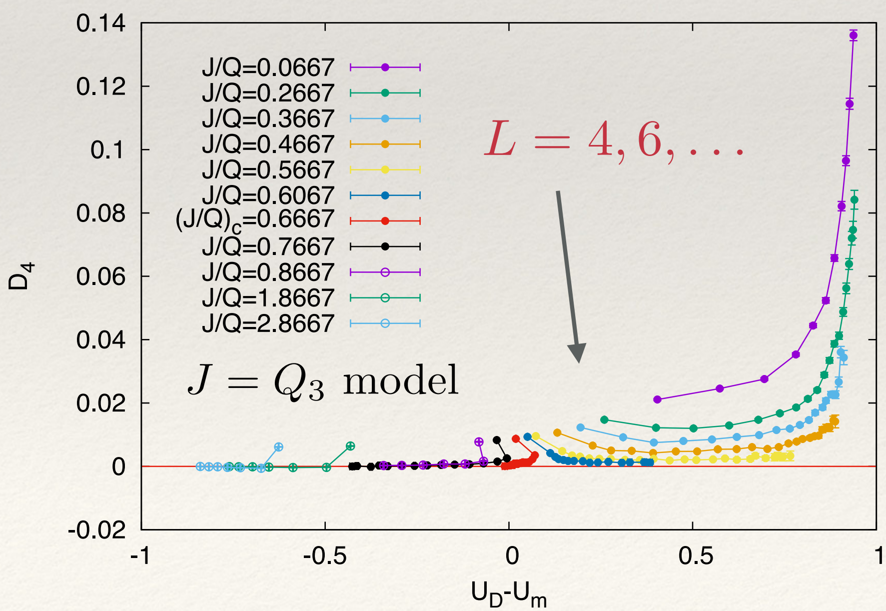






Ratio ν/ν' plays important in finite-size scaling

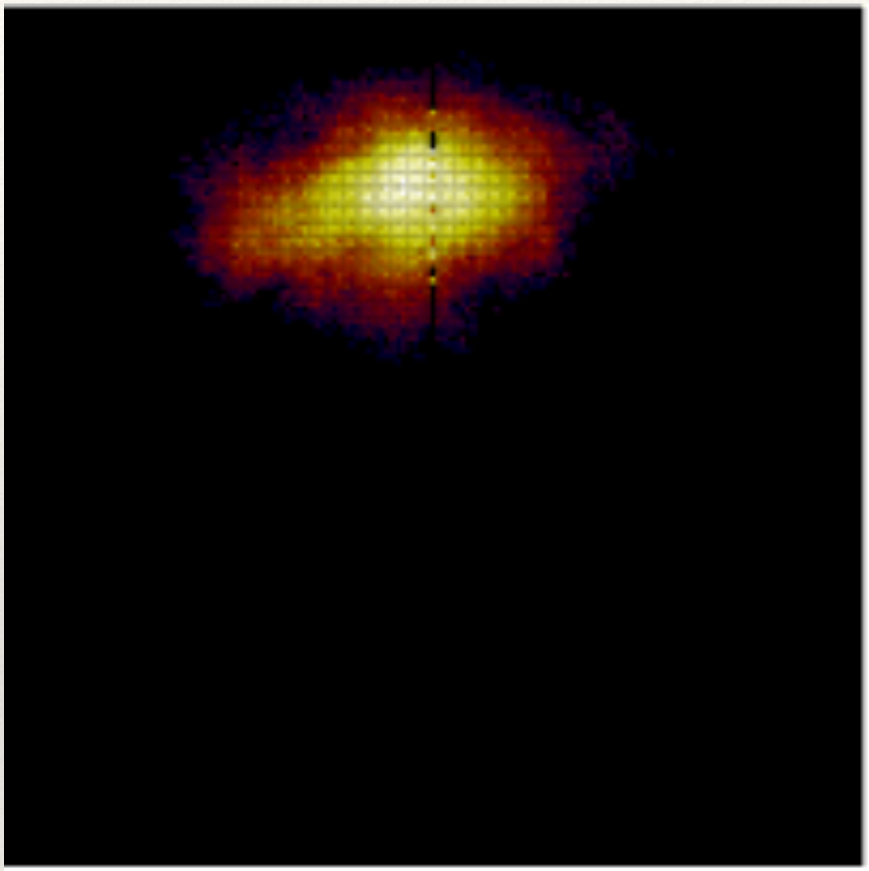
Shao, Guo, Sandvik (Science 2016)



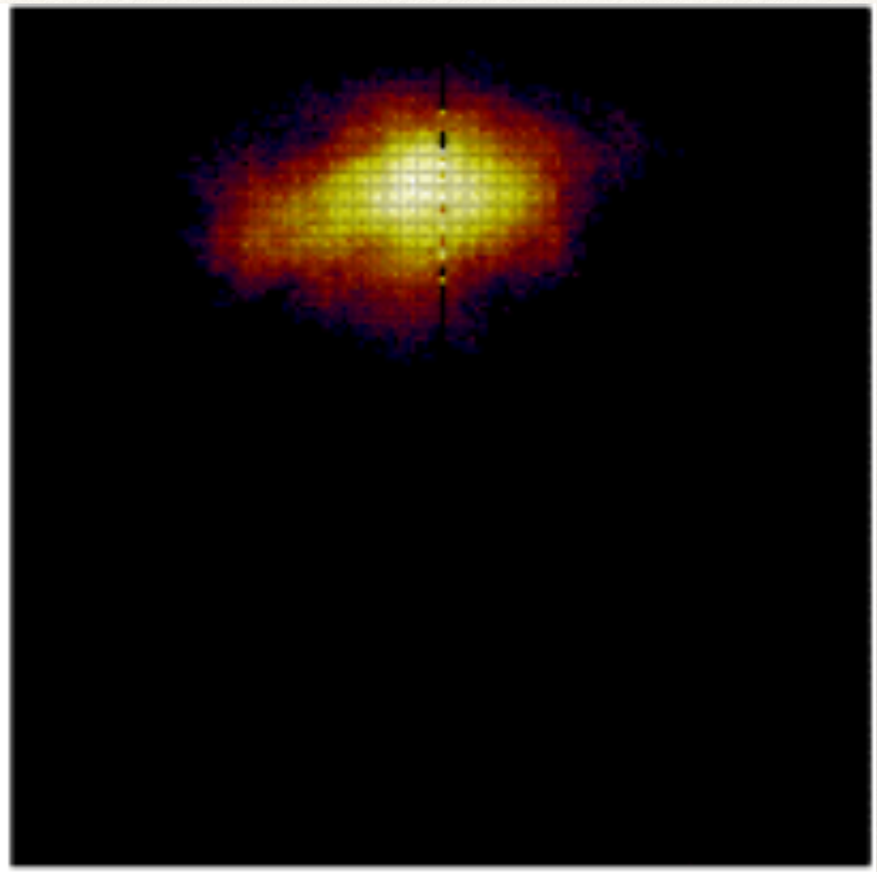
MC RG flows for J-Q_3 model
- work in progress

The simulations take a long time to rotate the VBS angle

L=128: 10^5 measurements require > 1 day of computation



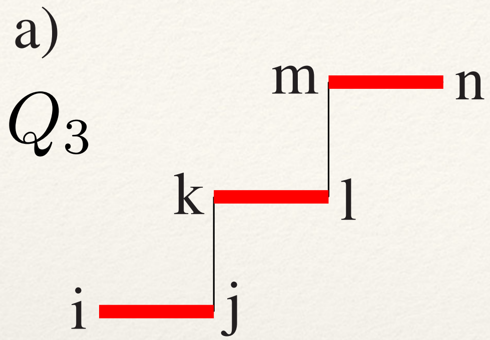
building 100×10^5 measurements

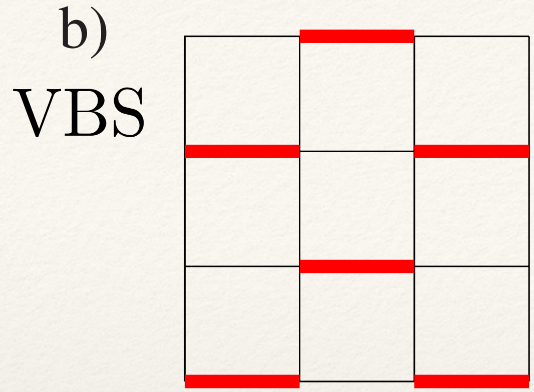


10^5 measurements

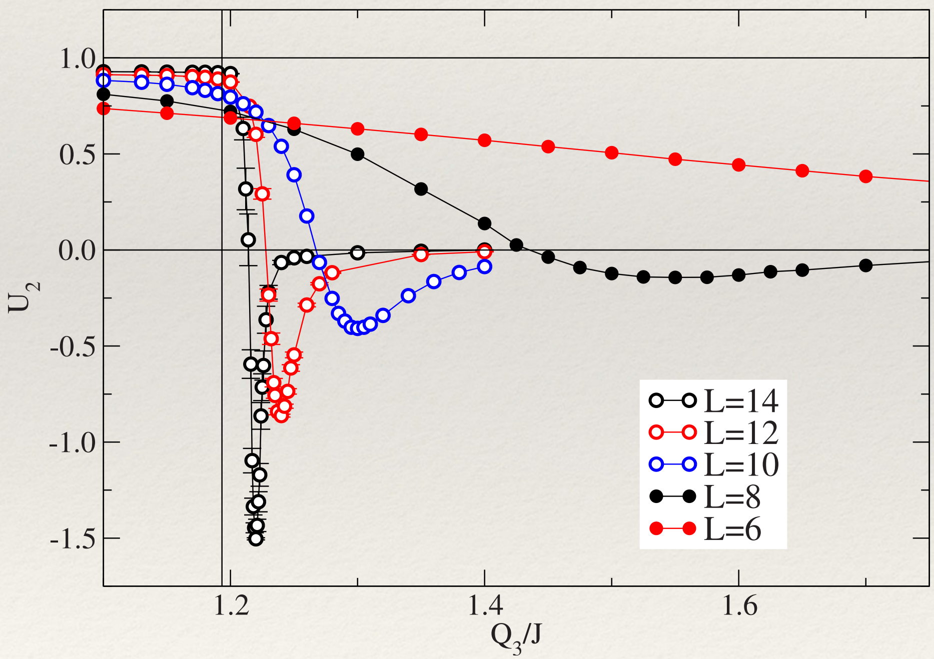
Conventional first-order transition

Staircase J-Q_3 model [Sen, Sandvik, PRB 2010]

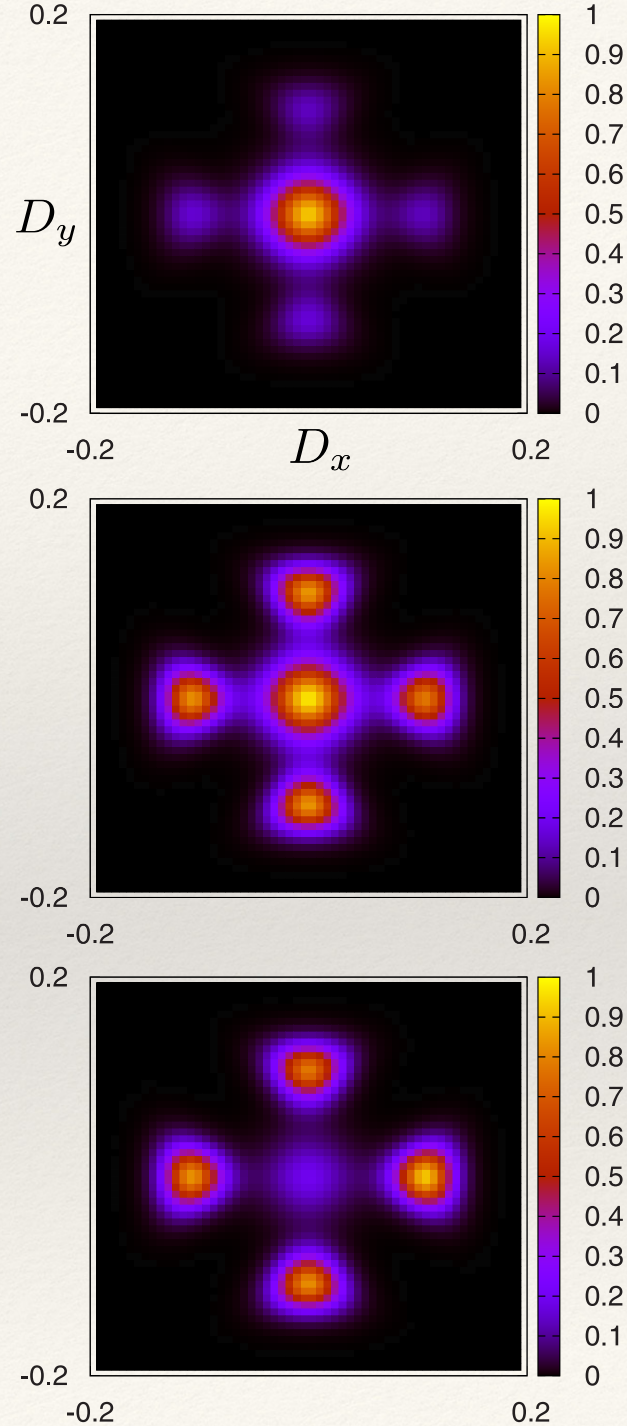




Binder cumulant of AFM order parameter



No emergent symmetry seen in $P(D_x,D_y)$

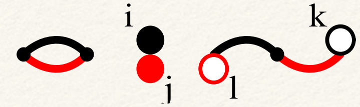


Negative Cumulant peak is a sign of phase coexistence; first-order transition

Spinons in the 2D J-Q model

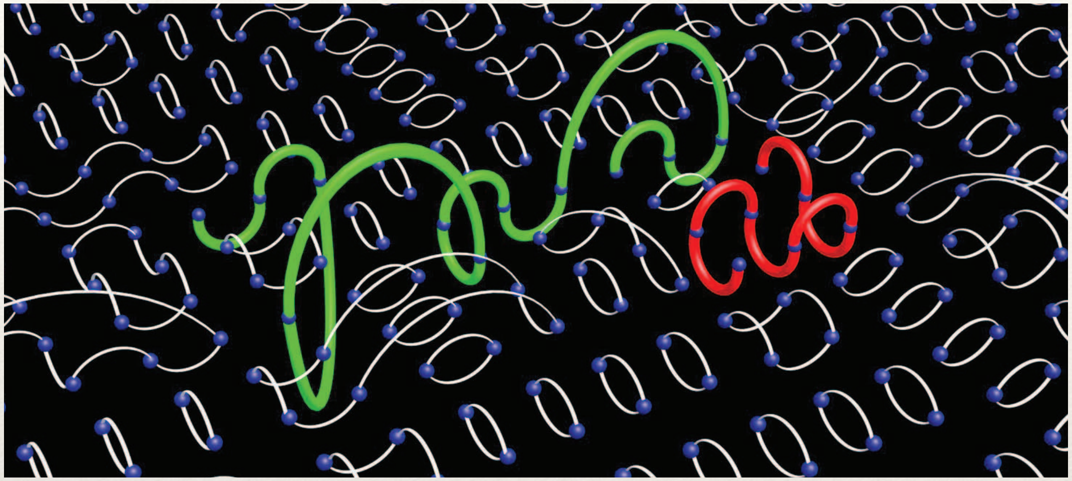
[Shao, Guo, Sandvik, Science 2016]

Recall extended VBS basis for S=1 excitation



$\langle V_\beta(j,l)|V_\alpha(i,k)\rangle$

Critical J-Q_2 model



The spinons can be considered as extended objects - strings in the transition graphs

- define mean distance Λ

- dΛ/dg for (L,2L) defines exponent

Exponent different from correlation-length exponent: $\nu' = 0.58 \pm 0.02$