Kavli Institute for Theoretical Physics

Disentangling Quantum Many-body Systems: Computational and Conceptual Approaches

Seminar, December 15, 2010

Deconfined spinons at the Néel-VBS transition in two dimensions

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Outline

Introduction

- **Conventional T>0 quantum-criticality in 2D antiferromagnets**
- **Scaling behavior at putative deconfined quantum-critical point**
  - Neel - VBS transition in "J-Q" model
  - Observed (QMC) scaling anomalies; T=0 and T>0
  - Phenomenological spinon-gas model

Results and analysis

- **Locating the critical point in the J-Q model and dimerized models**
- **T>0 correlation length at criticality**
- **Evidence for continuous transition (J-Q) with weak scaling violations**
- **Low-energy phenomenology; spinon and magnon gas model**
  - Low-T forms of magnetic susceptibility and specific heat
  - QMC data fits; critical J-Q and dimerized models
  - Effective spin (S≈1/2) of the excitations in the J-Q model

Other related issues (time permitting)

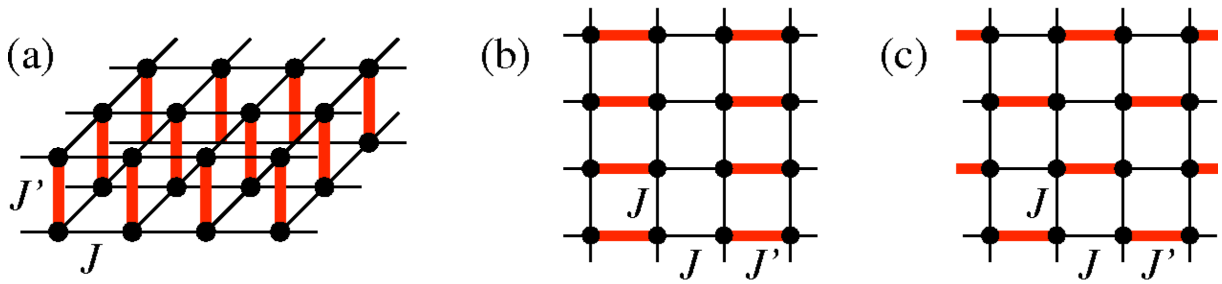
- **Critical examination of the first-order scenario**
  - comparing with the first-order transition into staggered VBS
- **VBS fluctuations and emergent U(1) symmetry**

key papers: arXiv:1010.2522 PRL 104, 177201 (2010), PRB 80, 180414 (2009)

Conventional O(3) transition in 2D antiferromagnets

Theory: Chakravarty, Halperin, Nelson (1989), Chubukov, Sachdev, Ye (1994)

Realized in dimerized S=1/2 Heisenberg models

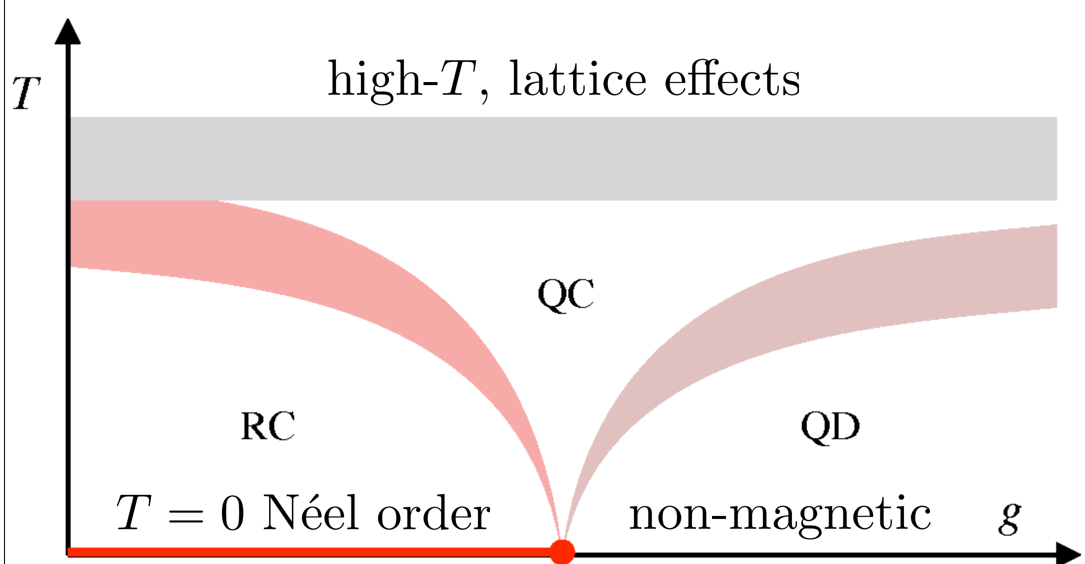


$$H = J\sum_{\langle ij\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J'\sum_{\langle ij\rangle'} \mathbf{S}_i \cdot \mathbf{S}_j$$

Neel - non-magnetic T=0 transition vs **g=J'/J**

- plain singlet-product (+ fluct) state for $g>g_c$

cross-over "phase diagram"



3D O(3) (Heisenberg) universality

T>0 **quantum-critical regime**

- magnons (S=1) remain as the elementary excitations at the critical point
- dynamic exponent z=1
- scaling behavior:

$$\xi \propto T^{-1}$$
$$\chi \propto T$$
$$C \propto T^2$$

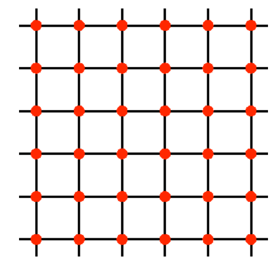
- confirmed by QMC
- some issues remain in (c)

Deconfined Neel-VBS transition in 2D antiferromagnets

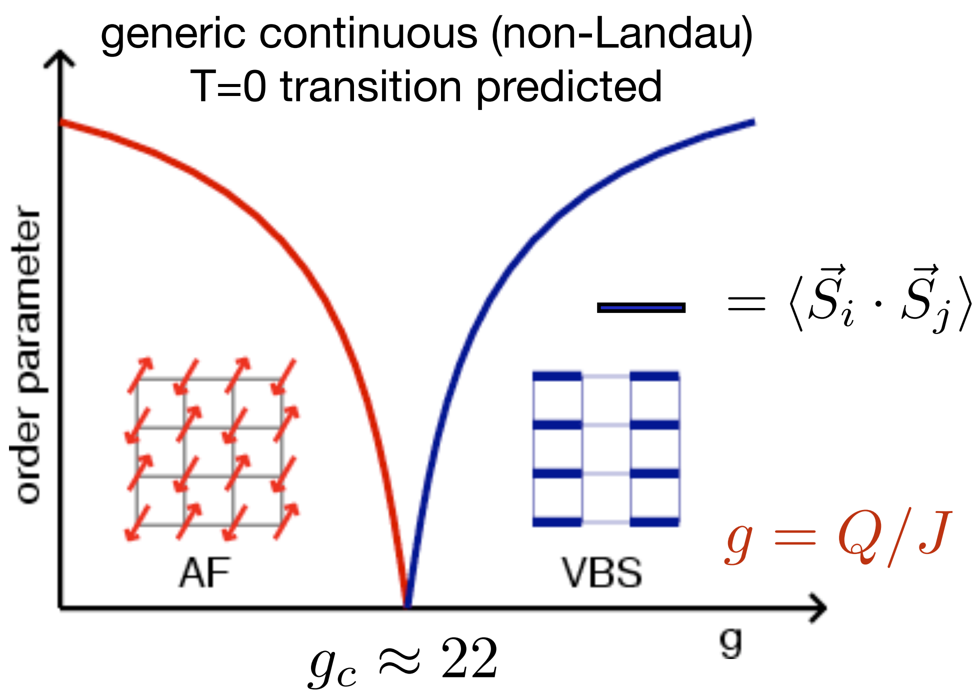
Theory: Senthil, Vishwanath, Balents, Sachdev, Fisher, Science 303, 1490 (2004)

Neel-VBS transition realized in the “J-Q” model (square lattice)
AWS, PRL 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
  - unlike frustrated systems (traditional play ground for VBS physics)

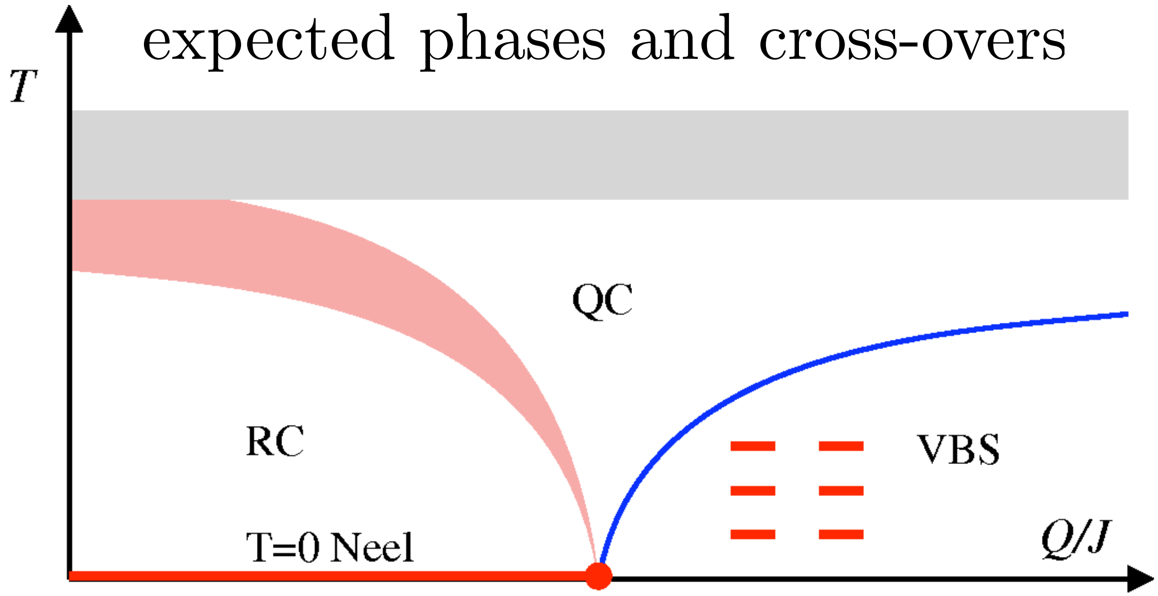


QMC in agreement with theory:
- dynamic exponent z=1
- “large” exponent $\eta_{spin} \approx 0.35$
- emergent U(1) VBS symmetry

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

recent large-scale studies do
not find any evidence for 1st-order
- instead: log-corrections

Question: Consequences of spinons in T>0 QC regime?



J-Q QMC results:

Standard QC forms

$$\xi \propto T^{-1}$$

$$\chi \propto T$$

are **weakly violated.**
Specific heat obeys the standard form

$$C \propto T^2$$

Phenomenological model of a spinon gas at T>0

- bosonic spinons, linearly dispersing at T=0; **ε(k)=ck**
- thermal length Λ(T); assuming free spinons for q>1/Λ
  - contributions to thermodynamics from these spinons

Infrared momentum cut-off 1/Λ equivalent to thermal gap Δ=1/Λ

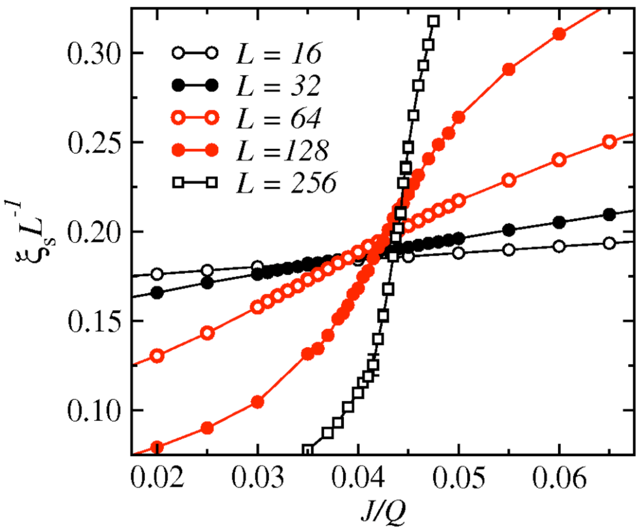
$$\epsilon(\mathbf{k}) = \sqrt{\mathbf{c^2 k^2 + \Delta^2}}$$

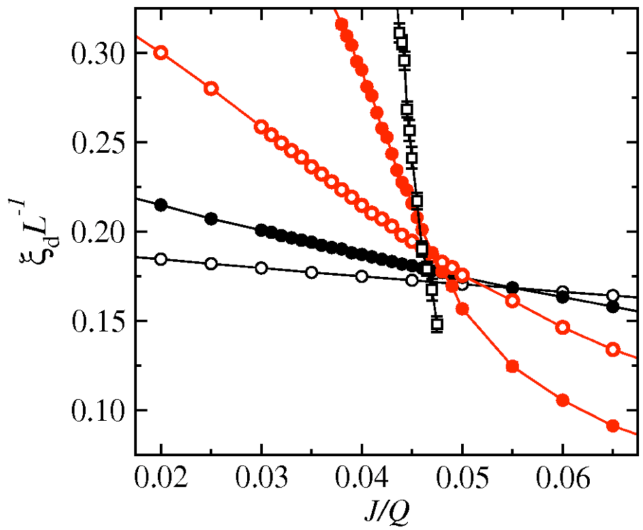
J-Q model: critical **ξ diverges faster than 1/T** as T→0 (Δ/T→0) ➡

- infrared divergent integral leads to weak T→0 divergence (log) of χ/T
- weaker correction to T^2 form of C

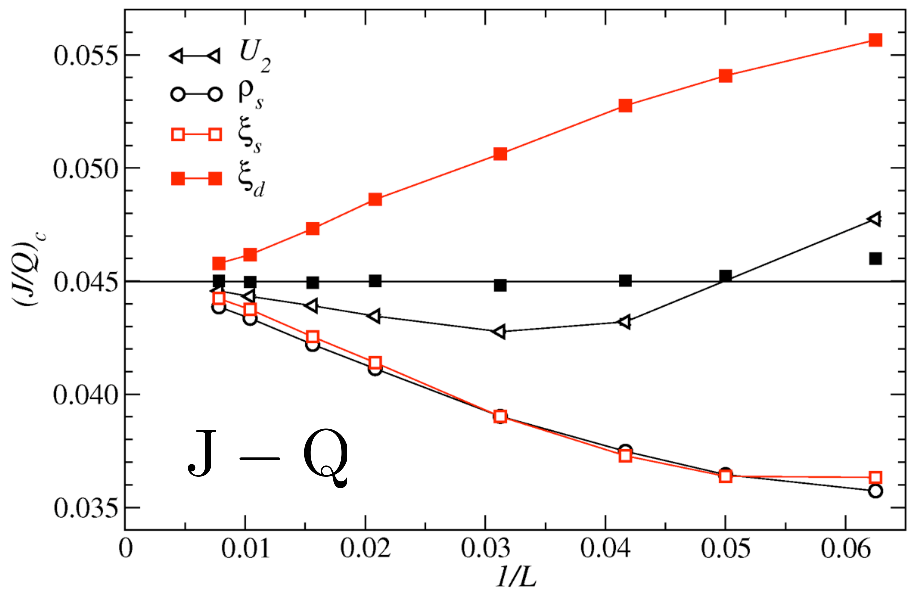
T=0 critical couplings: dimensionless quantities should scale as L

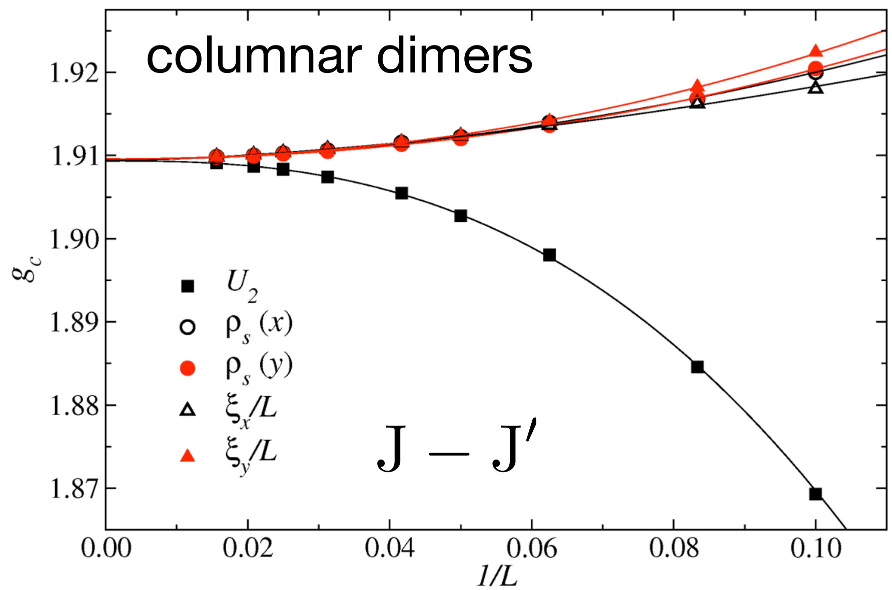
- correlation lengths, Binder cumulants, spin stiffness ($L\rho_s$),...
- curves vs coupling for different L cross at critical point





J-Q model
spin and dimer
correlation
lengths (second
moment def)





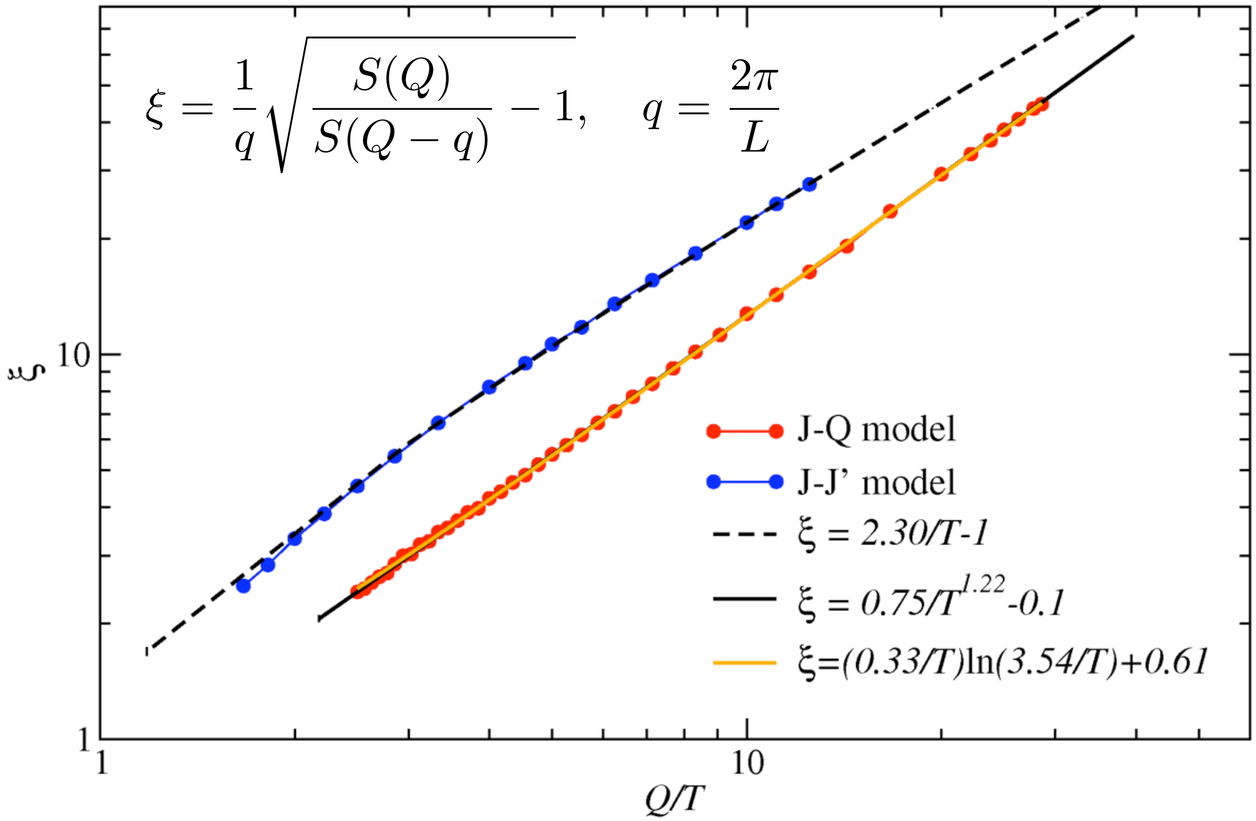
Critical-point estimates

J-J' model: $(J'/J)_c$=1.90948(4), (using J'/J=1.9095)

J-Q model: $(J/Q)_c$=0.04498(3), (using J/Q=0.0450)

T>0 critical spin correlation length

- L up to 512; converged to thermodynamic limit for T considered



J-J' model: expected 1/T divergence

J-Q model: faster than 1/T divergence

- logarithmic or power correction (data consistent with either form)

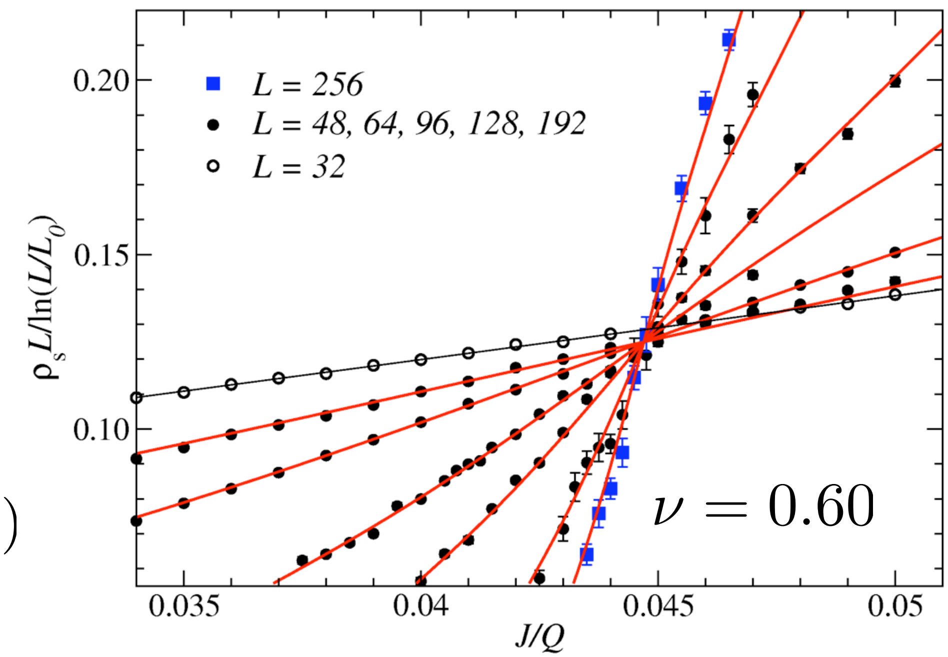
Conclusion from previous T=0 and T>0 caculations

AWS, PRL 104, 177201 (2010)

logarithmic corrections to quantum-critical scaling

$$\rho_s \sim \frac{\ln(L/L_0)}{L} \quad (T \to 0)$$

$$\chi \sim T[1 + a\ln(1/T)] \quad (L \to \infty)$$

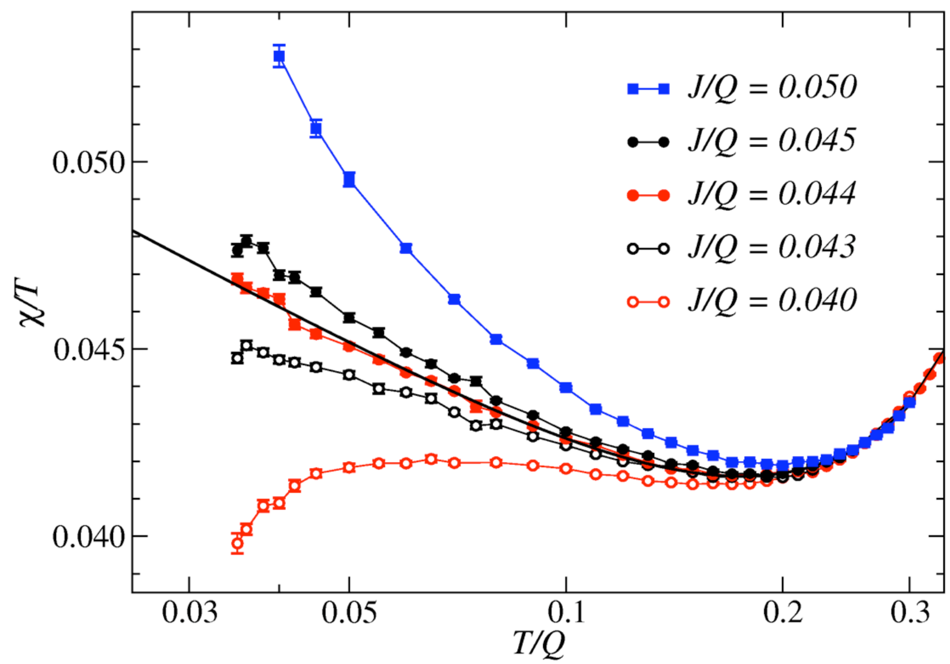


Could the behavior indicate z≠1?

$$\xi \sim T^{-(1/z)}$$

$$\chi \sim T^{2/z-1}$$

$$\rho_s \sim L^{-z}$$



ξ gives z≈0.82

- consistent with $\rho_s(L)$
- inconsistent with $\chi(T)$
  - demands $\chi/T \to 0$ for $T \to 0$

Some unconventional reason

- marginal operator causing logs?

Can we find relationships between the different anomalies?

- can this provide a fingerprint for spinons?

Gas of non-interacting spinons (S=1/2) or magnons (S=1) at T>0

$$\epsilon_{\pm}(k) = \sqrt{c^2k^2 + \Delta^2} \pm \mu B \equiv \epsilon(k) \pm \mu B$$ (B = magnetic field)

$$\mu = 1/2 \text{ (spinons)}, \quad \mu = 1 \text{ (magnons)}$$

Magnetization to linear order (bosonic excitations)

$$\begin{aligned} M &= \mu F \int \left(\frac{1}{e^{\epsilon_-/T} - 1} - \frac{1}{e^{\epsilon_+/T} - 1} \right) \frac{d^2k}{(2\pi)^2} \\ &= -2\mu^2 FB \int \frac{\partial n}{\partial \epsilon} \frac{d^2k}{(2\pi)^2} \\ &= \mu^2 F \frac{TB}{4\pi c^2} \int_0^\infty \frac{x\,dx}{\sinh^2[\frac{1}{2}\sqrt{x^2 + (\Delta/T)^2}]} \end{aligned}$$

F is a degeneracy factor; F=2 (spinons/anti-spinons), F=1 (magnons)

Conventional quantum-criticality: **$\Delta/T \to m \approx 0.96$** (Chubukov & Sachdev 1994)

- computed using large-N calculations (nonlinear σ-model)

In the J-Q model (deconfined criticality?): **$\Delta/T \to 0$** ($\log^{-1}(1/T)$ or T^a)

- infrared divergent integral; significant consequences

$$\int_0^\infty \frac{x dx}{\sinh^2(\frac{1}{2}\sqrt{x^2+p^2})} = \frac{4p}{1-\mathrm{e}^{-p}} - 4\ln(\mathrm{e}^p - 1) \qquad p = \Delta/T$$

Using these gaps for spinon (S=1/2) and magnon (S=1) calculations:

$$\Delta_{1/2}/T = 1/(T\xi) = (T/mc)^a$$ (***mc*** and ***a*** from J-Q QMC data)

$$\Delta_1/T = m = 0.96$$ (Chubukov & Sachdev)

Gives the low-T **magnetic susceptibility**

$$\chi_1 = (1.0760/\pi c^2)T$$

$$\chi_{1/2} = \frac{T}{2\pi c^2}\left[1 + a\ln\left(\frac{mc}{T}\right) + \frac{1}{24}\left(\frac{T}{mc}\right)^{2a}\right]$$

Specific heat

$$C_S = (2S+1)F\int \epsilon(k)\frac{\partial n(\epsilon)}{\partial T}\frac{d^2k}{(2\pi)^2}$$

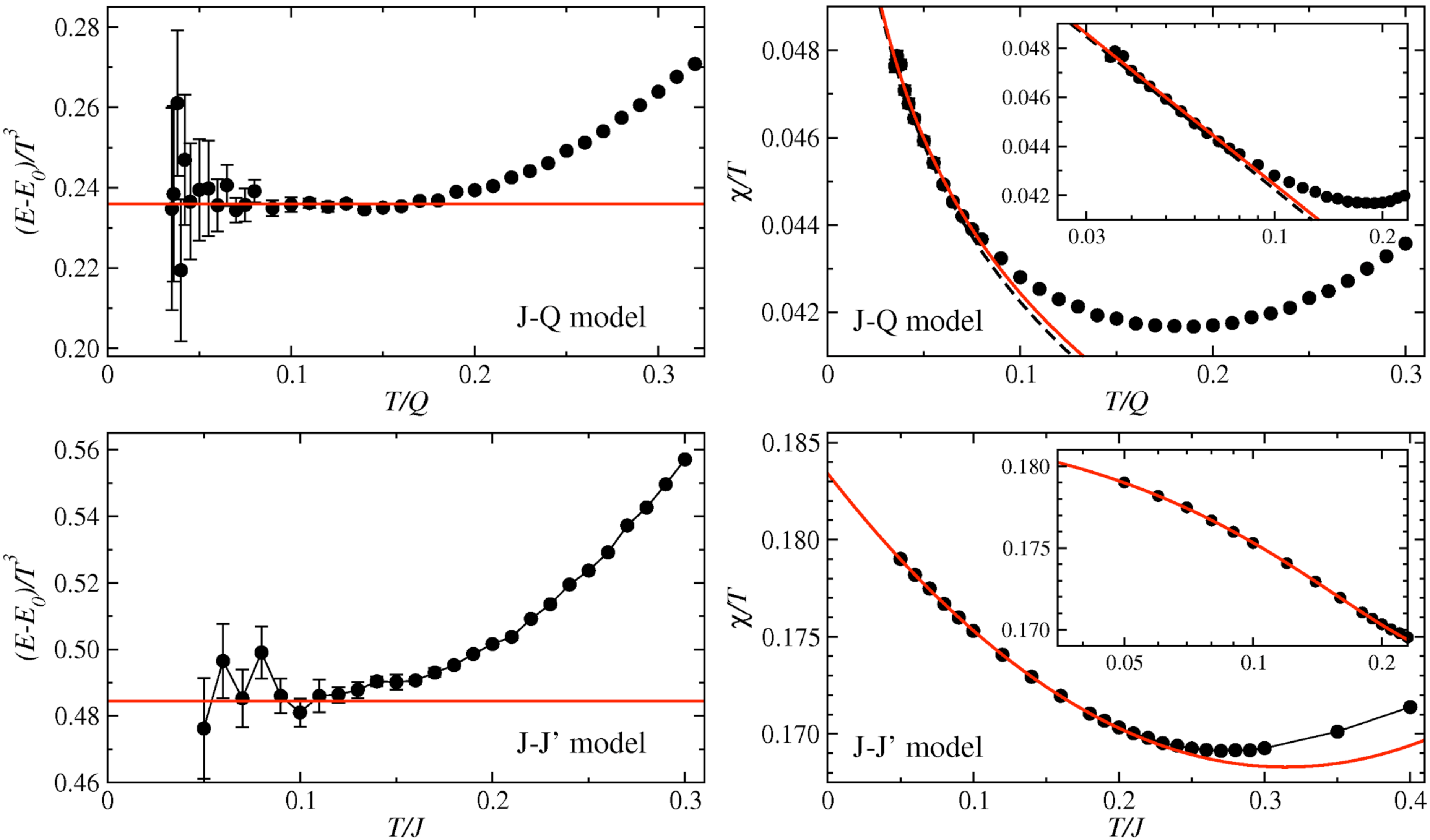
$$C_1 = [36\zeta(3)/5\pi c^2]T^2$$ (Chubukov & Sachdev)

$$C_{1/2} = \frac{2T^2}{\pi c^2}\left[6\zeta(3) - \left(\frac{T}{c}\right)^{2a}\left[\frac{3}{2} + a + a(1+a)\ln\left(\frac{c}{T}\right)\right]\right]$$

QMC data fits: J-J' (magnon forms) and J-Q models (spinon forms)

- **J-J':** velocity fitted in E/T^3, polynomial fit for X/T (velocities agree to 2%)
- **J-Q:** velocity is fitted; values from X/T and C agree within 2%

$$(\mathbf{E}-\mathbf{E_0})/\mathbf{T^3} \qquad \chi/\mathbf{T}$$



J-Q model: effective spin of the excitations

Under the assumption of spinons, S=1/2, μ=1/2, F=2 (spinon/anti-spinon):

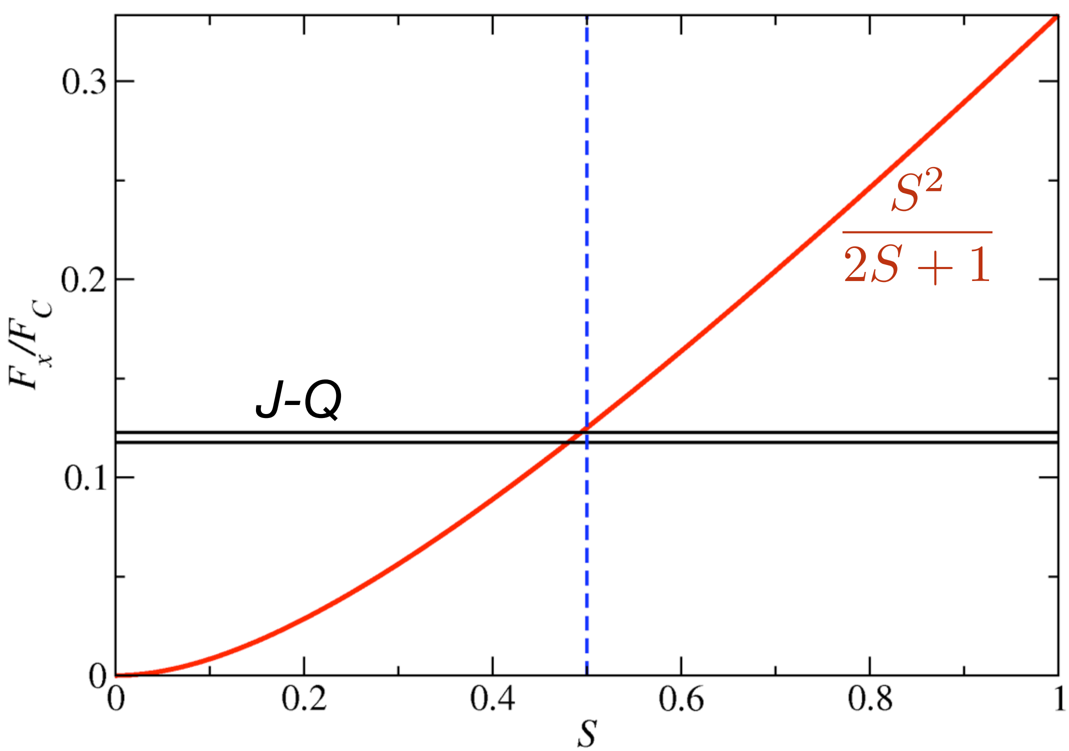
$$F_\chi = \frac{\mu^2 F}{c_\chi^2} \approx 0.074, \qquad F_C = \frac{(2S+1)F}{c_C^2} \approx 0.615$$

$$c_\chi = 2.60$$
$$c_C = 2.55$$

Should have $c_\chi = c_C$. S≠1/2? For both spinons (S=1/2) and magnons (S=1)

$$\mu = S^{-1}, \quad F = 1/S \quad \rightarrow \quad \frac{F_\chi}{F_C} = \frac{S^2}{2S+1}$$

Treat S as continuous variable and find effective S given the J-Q data:



The J-Q results are consistent with S=1/2 (spinons) but not consistent with S=1 (magnons)

Could this be a coincidence?

- assumed Δ=1/ξ
- may be Δ=*d*/ξ, *d*≈1
- results depend weakly on *d*

Independent estimate of the velocity would be good

- can be done
  - imaginary time correlations

Could the transition be first-order?

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

From an antiferromagnet to a valence bond solid: evidence for a first order phase transition

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

Deconfined Criticality: Generic First-Order Transition in the SU(2) Symmetry Case

One can never, strictly speaking, rule out a very weak first-order transition

- **but are there any real signs of this in the J-Q model?**

The above studies were based on scaling of winding numbers

- claimed signs of phase coexistence (finite spin stiffness and susceptibility)

$$\begin{aligned}\langle W^2\rangle &= \langle W_x^2\rangle + \langle W_y^2\rangle + \langle W_\tau^2\rangle \\ &= 2\beta\rho_s + \frac{4N}{\beta}\chi\end{aligned}$$

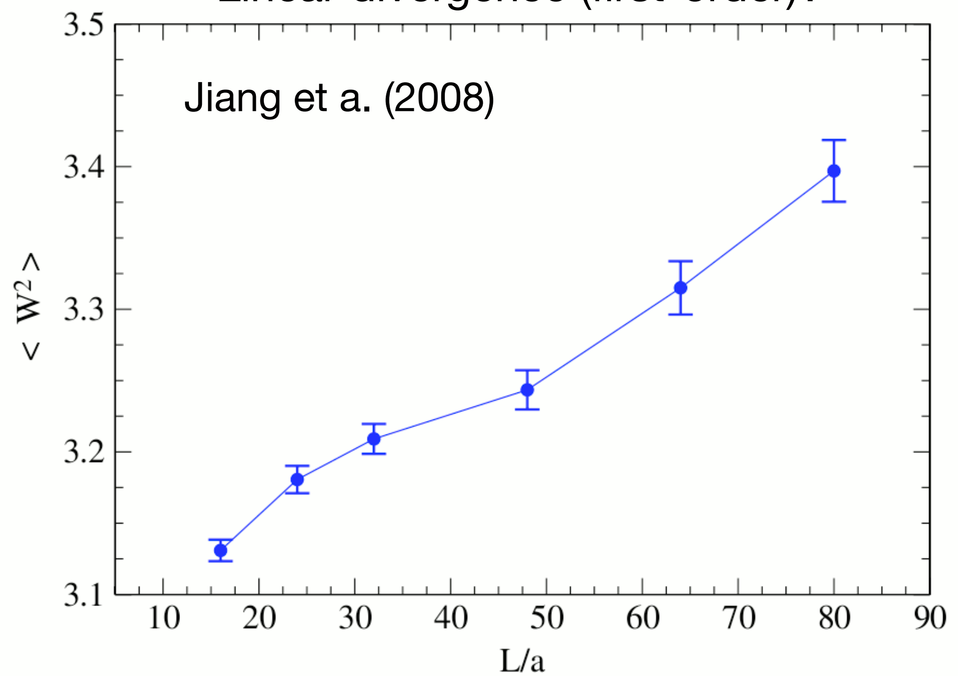
At at a critical point

$$z = 1, \beta \propto L \rightarrow$$

$$\rho_s \propto L^{-1}, \quad \chi \propto L^{-1}$$

$$\rightarrow \quad \langle W^2\rangle = \text{constant}$$

Linear divergence (first-order)?



Recent large-scale QMC results

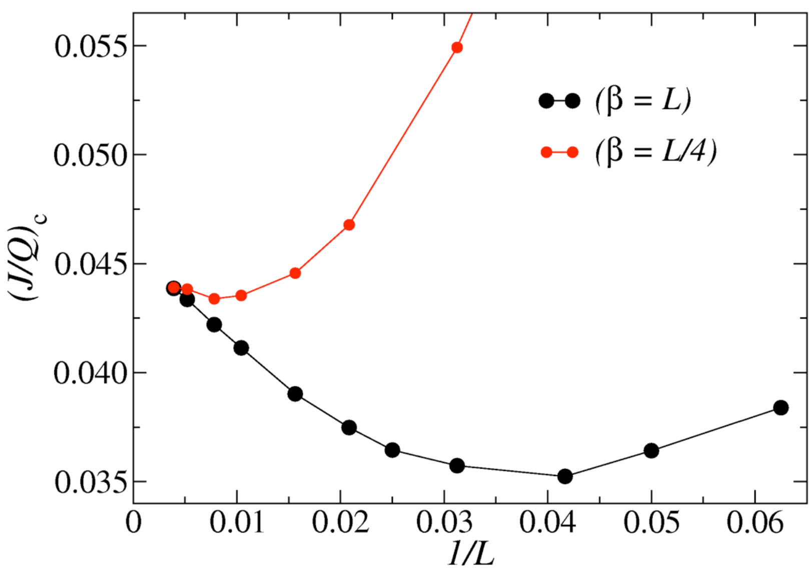
AWS, Phys. Rev. Lett. 104, 177201 (2010)

- Stochastic series expansion
- up to 256×256 lattices

$$\beta \propto L \ (\beta = L,\ \beta = L/4)$$

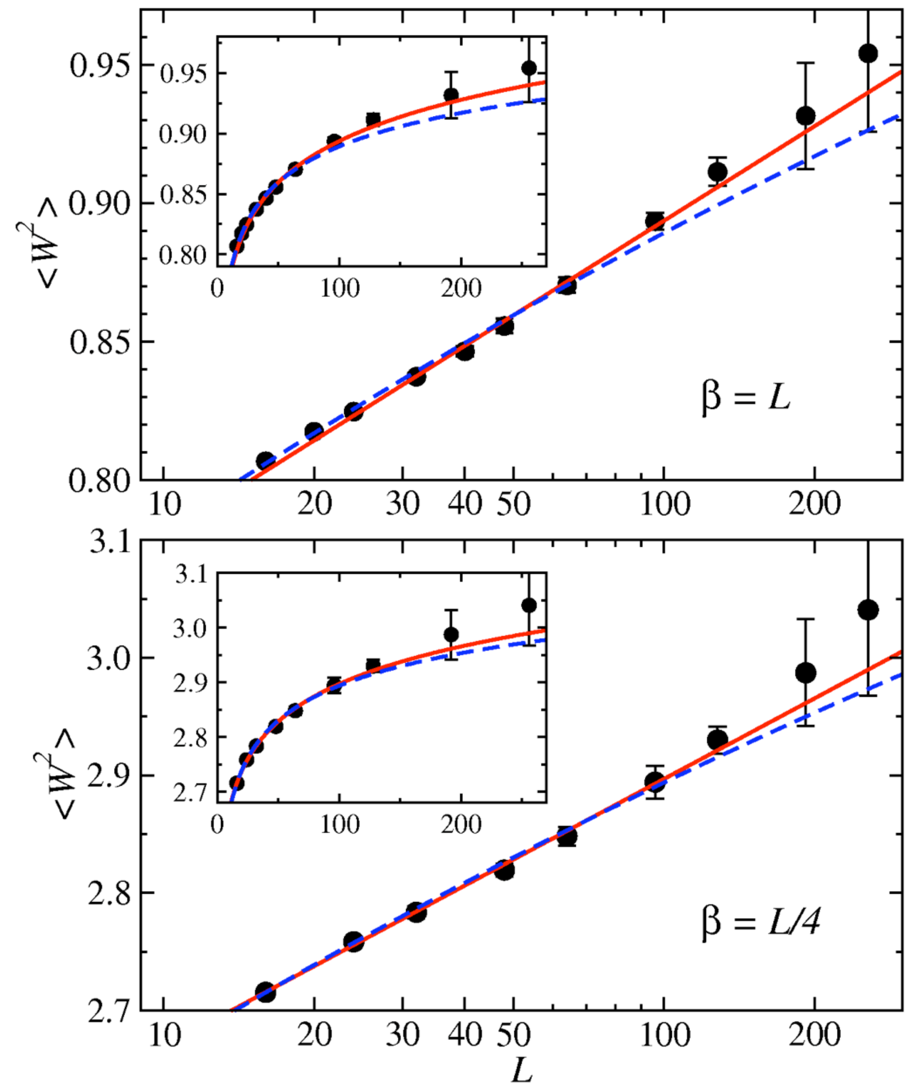
Same finite-size definition of critical point as used by Kuklov et al. and Jiang et al.

- fixed probability of the generated configurations having $W_x=W_y=W_\tau=0$



Logarithmic divergence of <W²>!

- scaling correction (not 1st-order)



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

Binder ratio

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

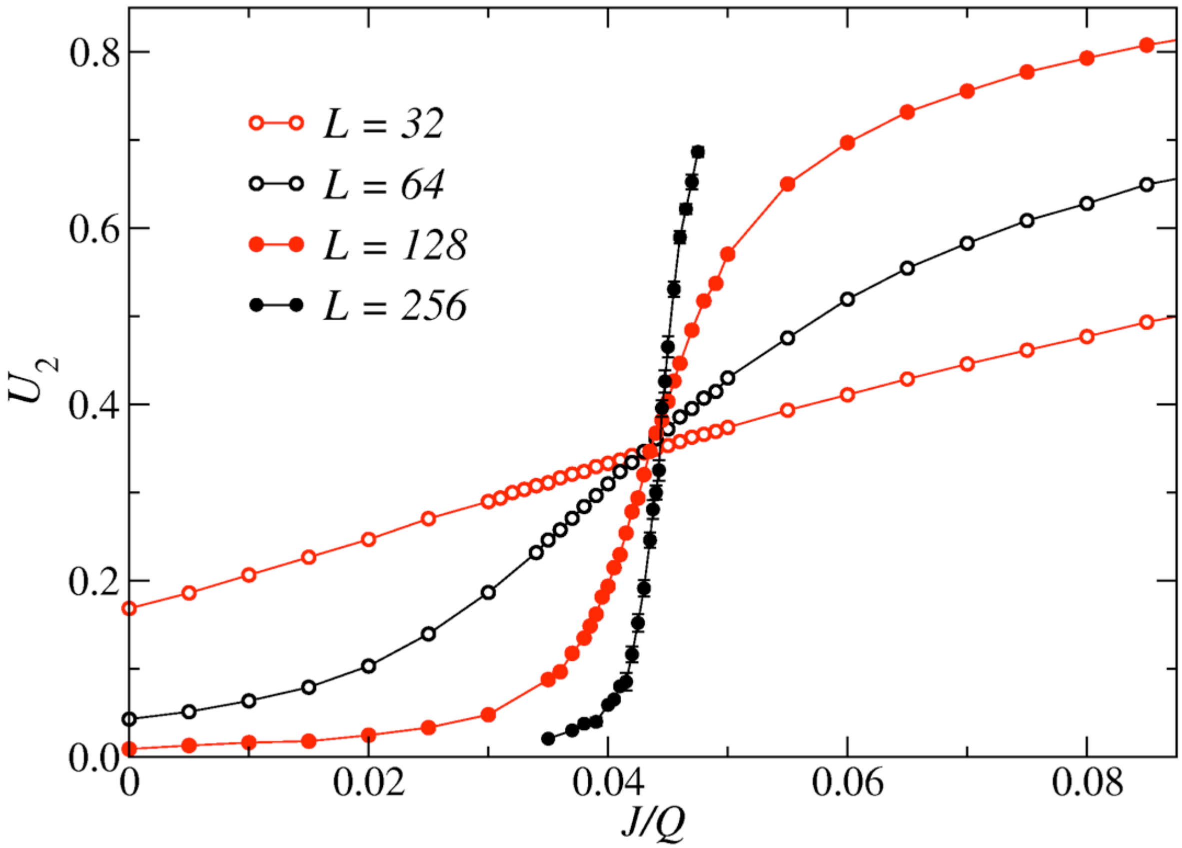
Binder cumulant

$$U_2 = (5 - 3Q_2)/2$$

Size independent (curve crossings) at criticality

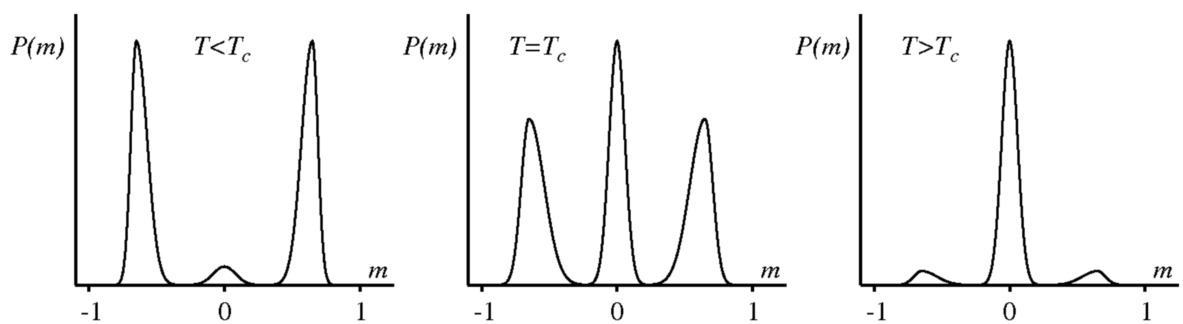
$U_2 < 0$ at a first-order transition

- no signs of $U_2<0$ in SSE results for L up to 256



Phase coexistence leads to $U_2 \to -\infty$ at 1st-order trans.

Example: Scalar order parameter at classical transition

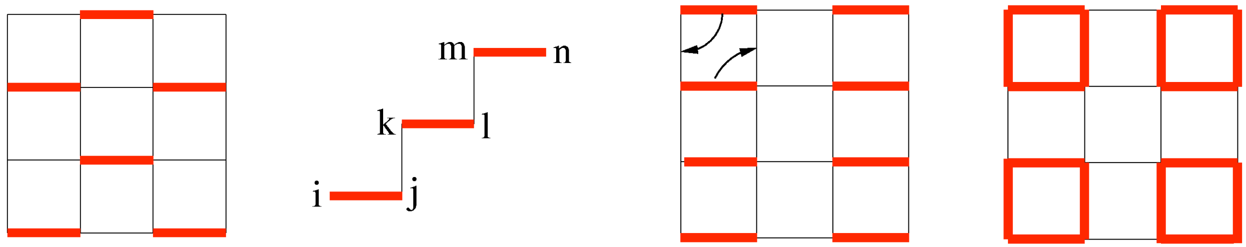


Example of a first-order Neel - VBS transition

J-Q model with staggered VBS phase [A. Sen, AWS, PRB (2010)]

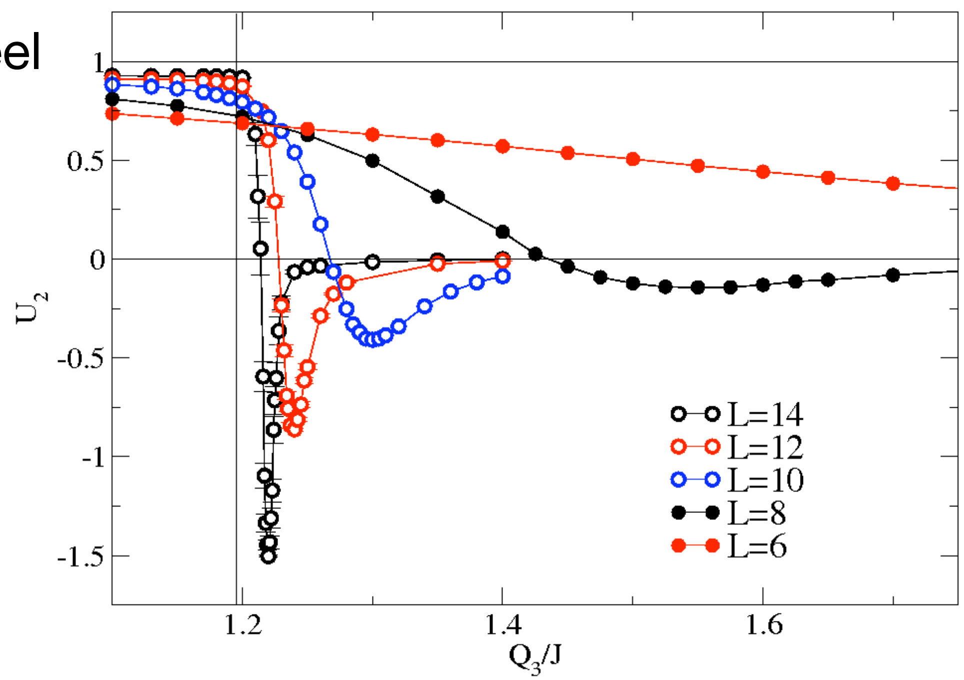
- no local VBS fluctuations favoring emergent U(1) symmetry

$$H = -J \sum_{\langle ij \rangle} C_{ij} - Q_3 \sum_{\langle ijklmn \rangle} C_{ij} C_{kl} C_{mn} \qquad C_{ij} = \frac{1}{4} - \vec{S}_i \cdot \vec{S}_j$$

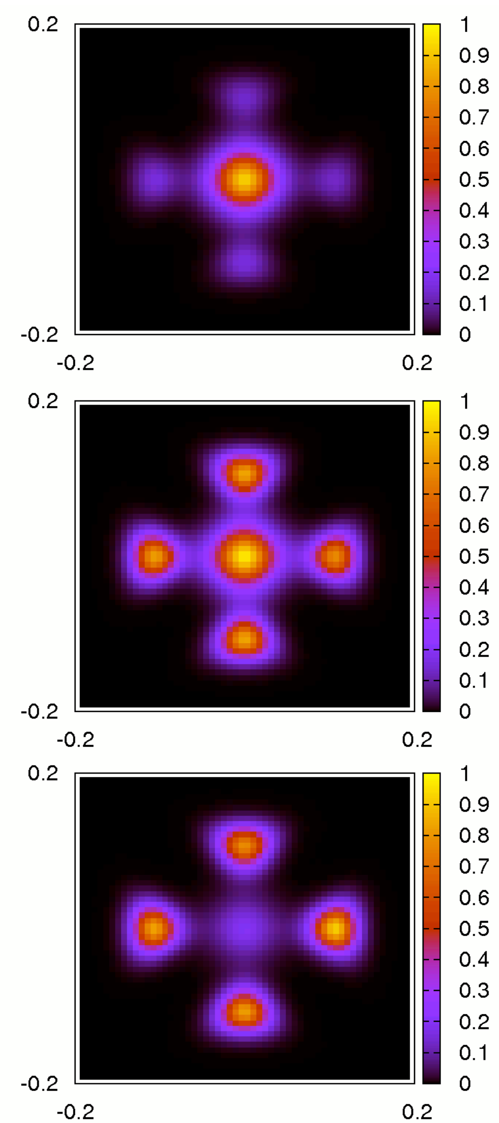


- clear signs of phase coexistence

For Neel order



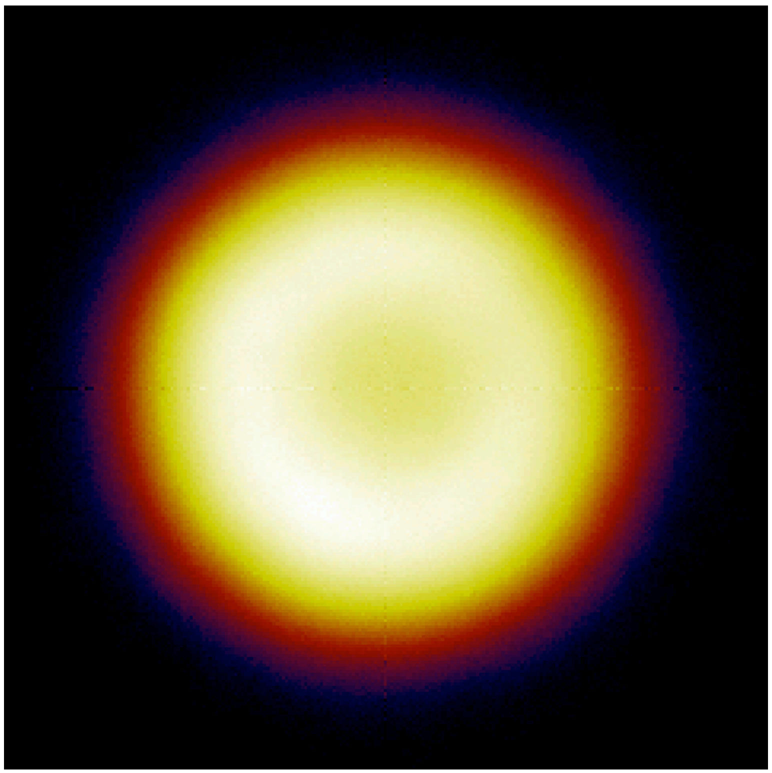
VBS

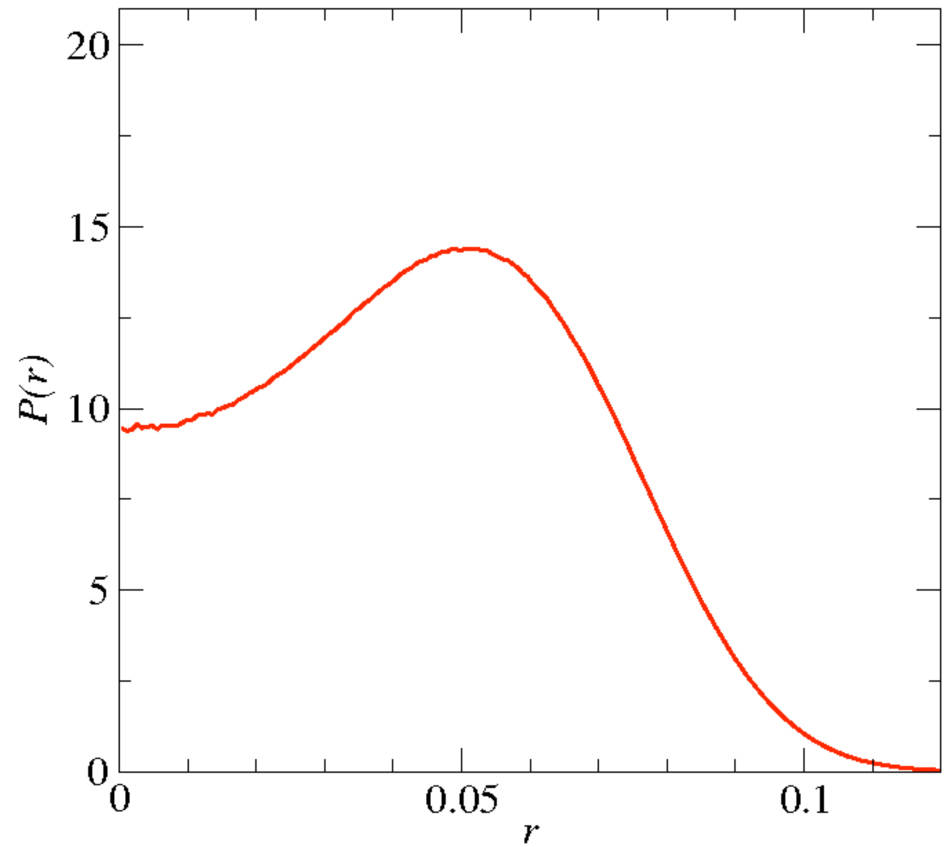


Any signs of coexistence in the standard J-Q VBS distributions?

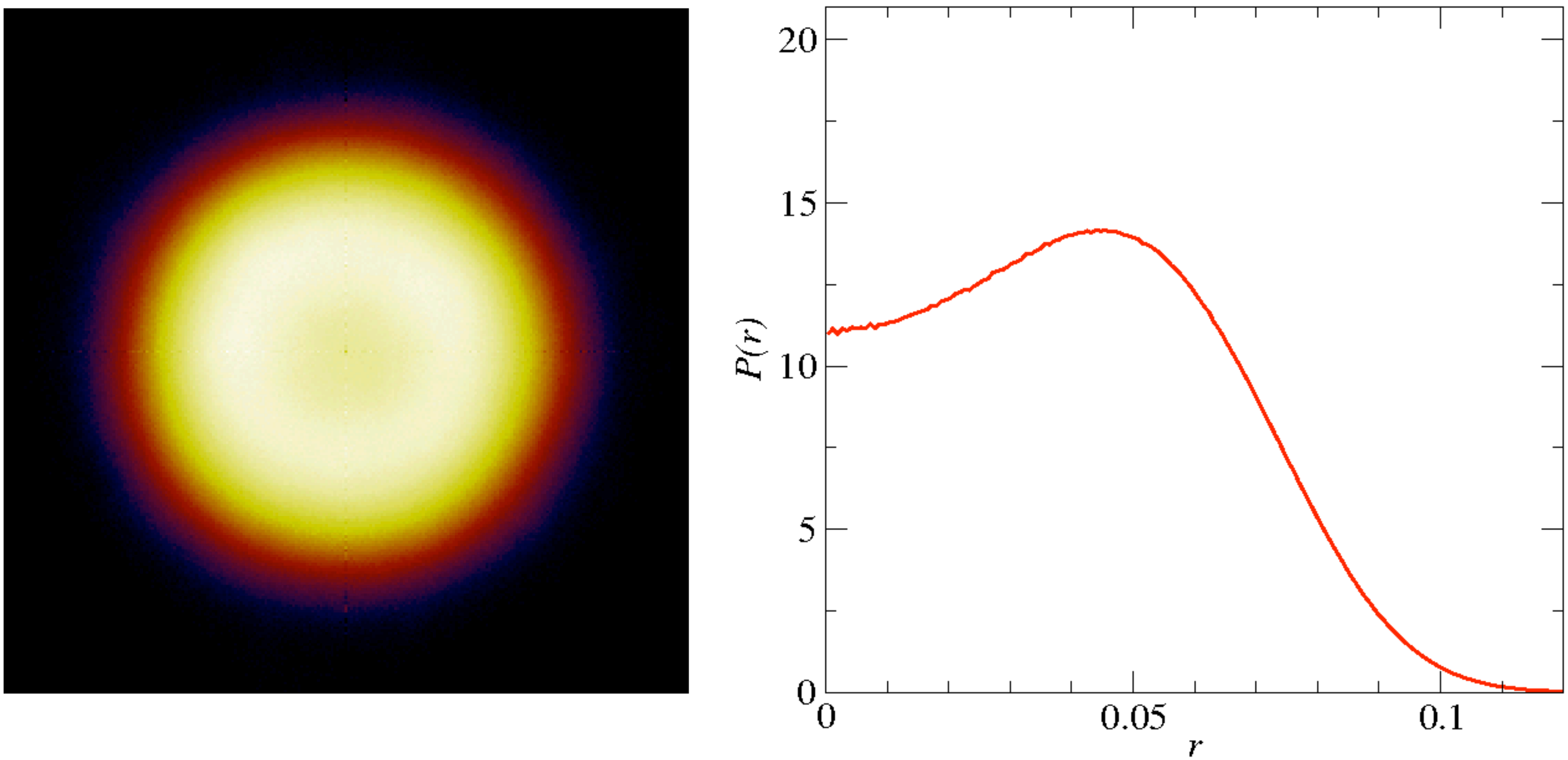
- L=128 data close to the transition

J/Q=0.040

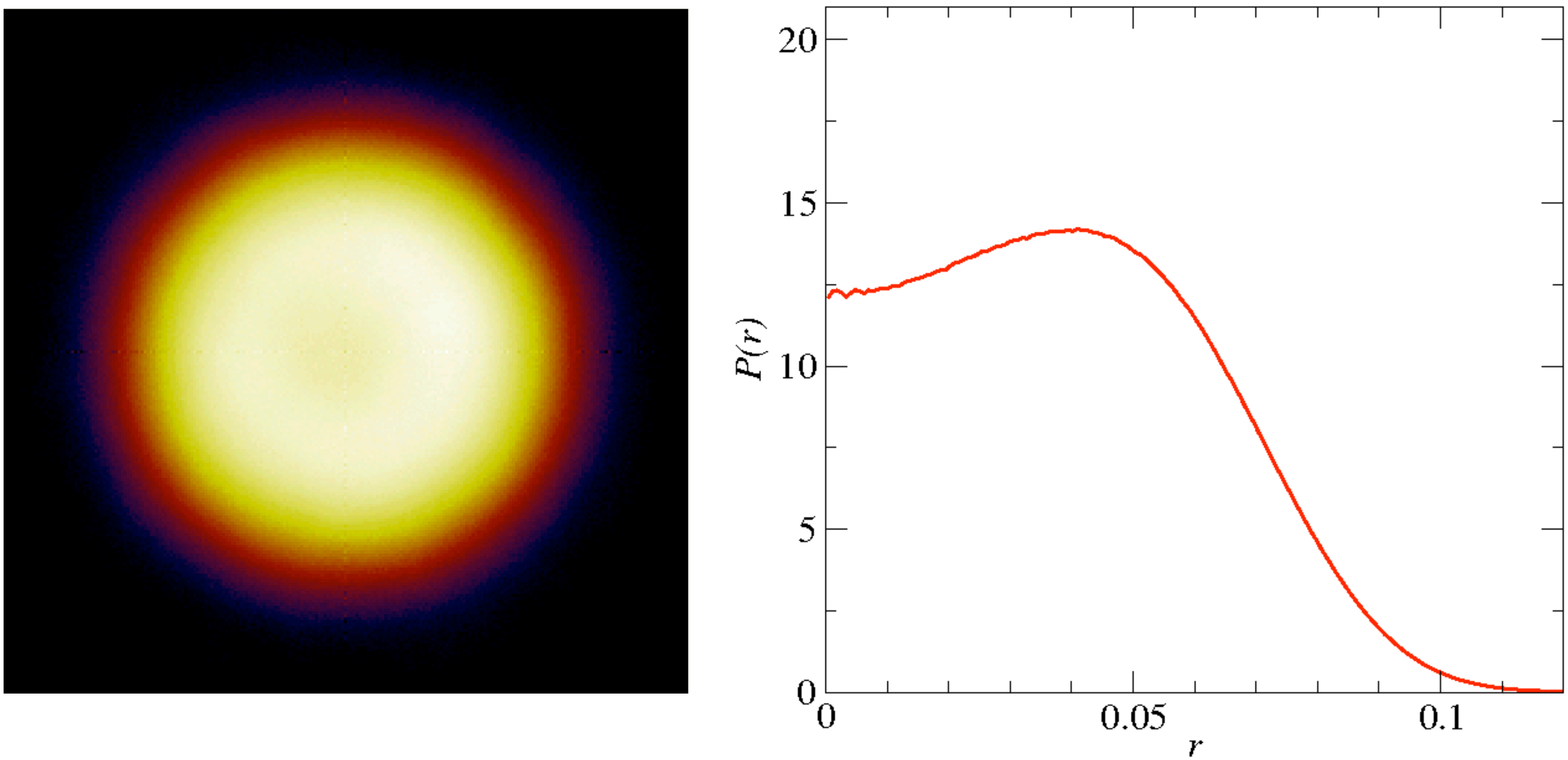




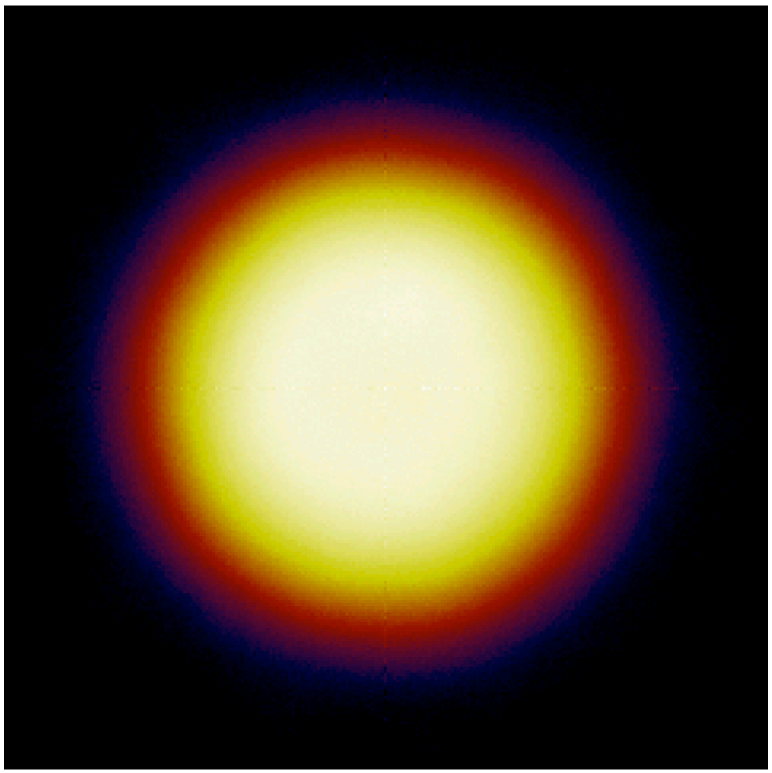
J/Q=0.041

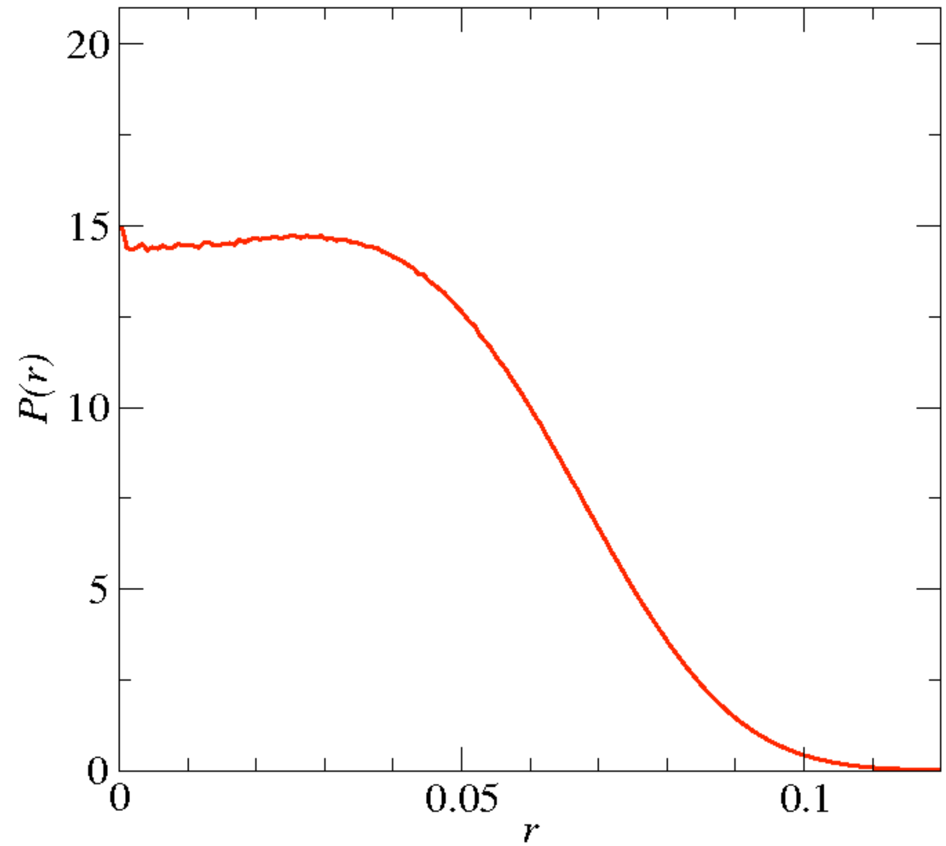


J/Q=0.042

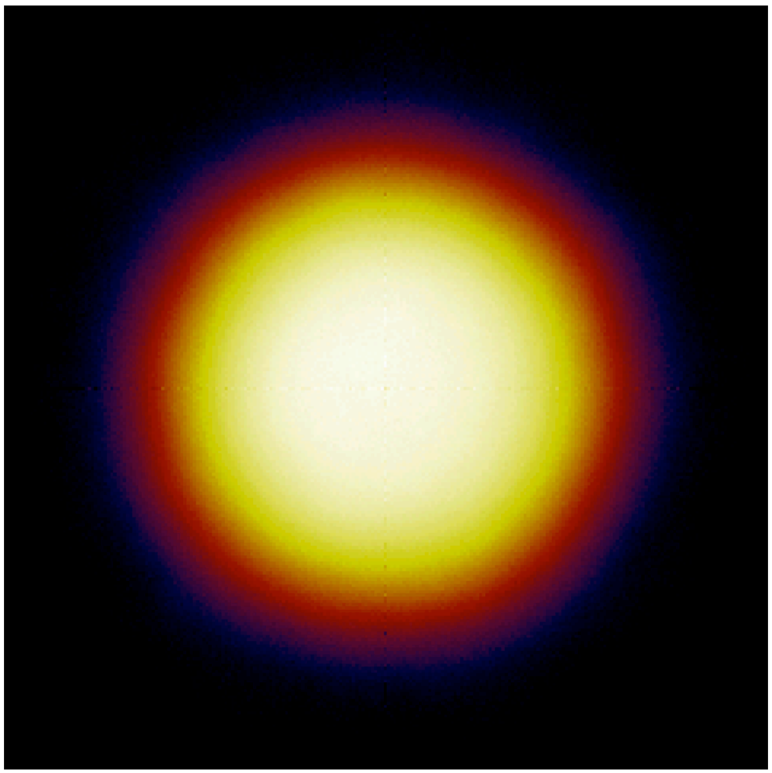


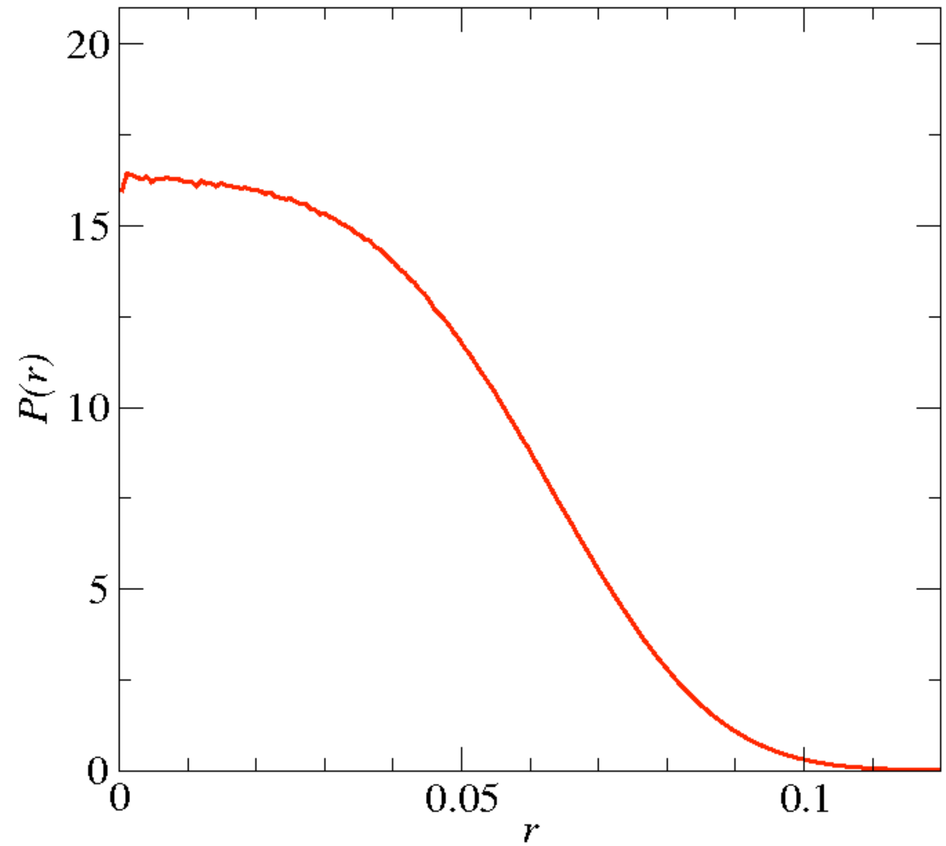
J/Q=0.043



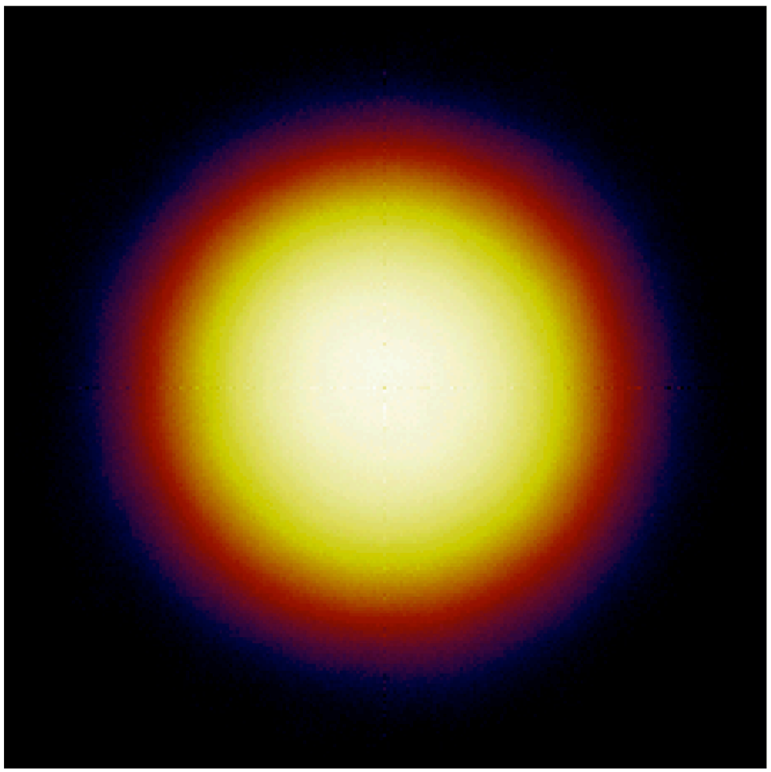


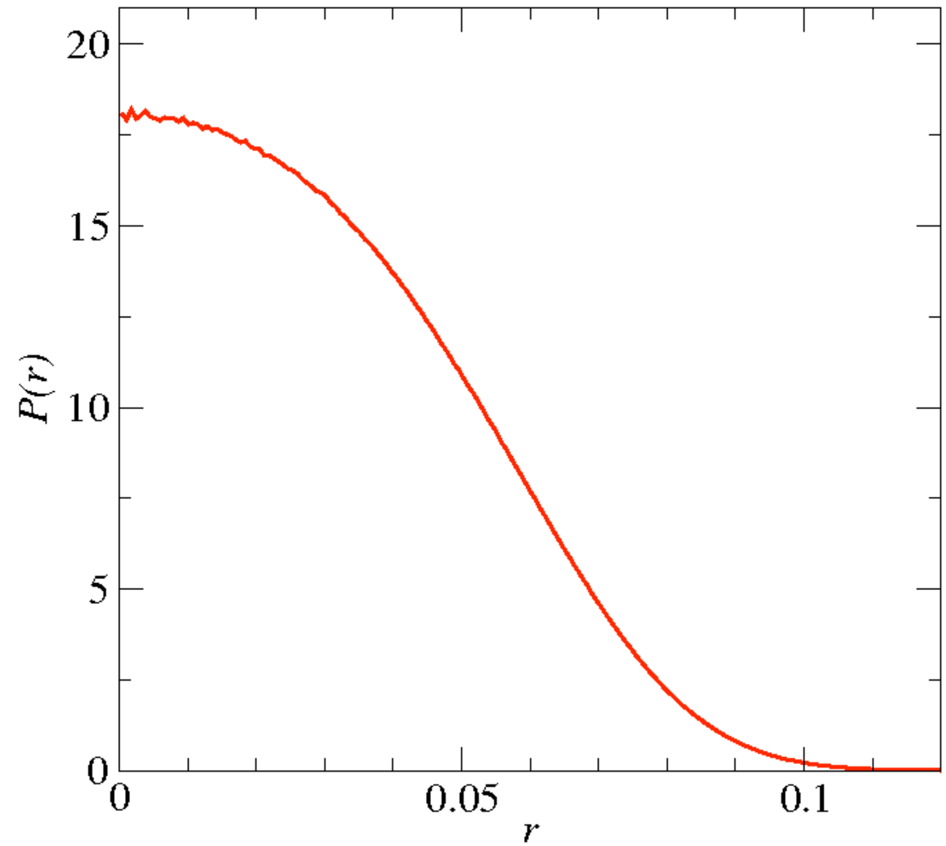
J/Q=0.044



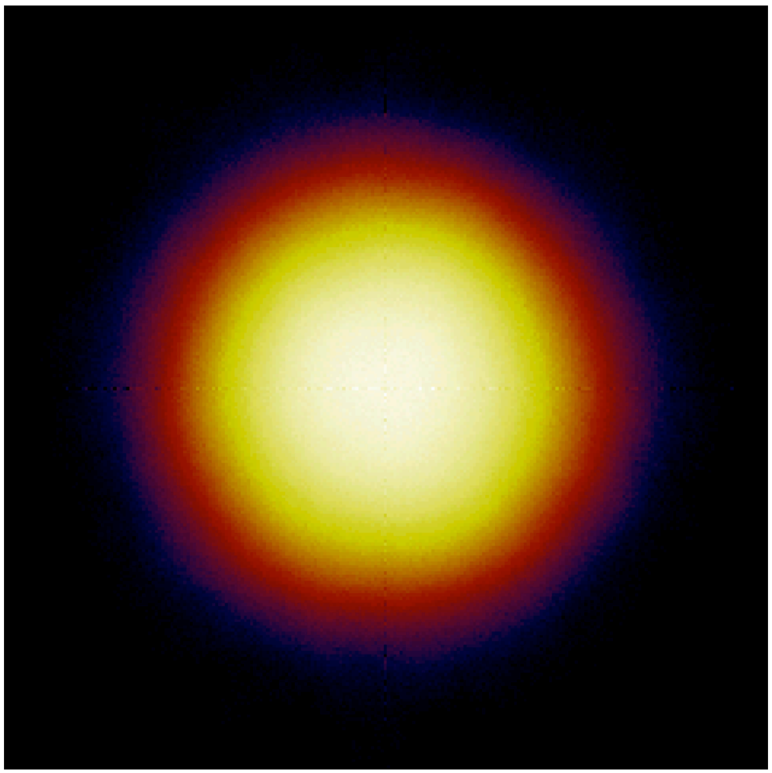


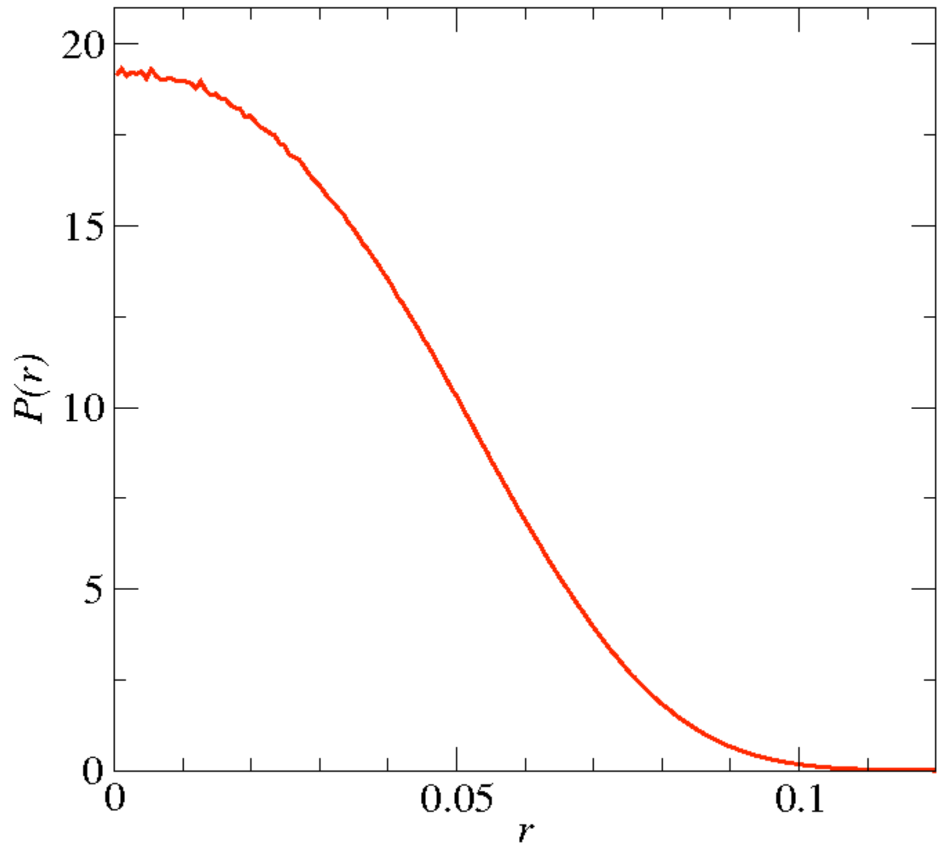
J/Q=0.045





J/Q=0.046





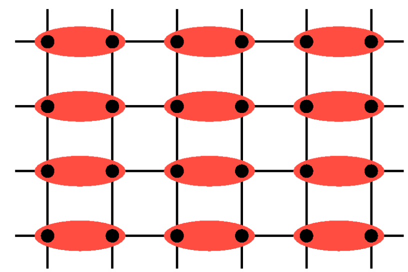
Exponents: T=0 results obtained with valence-bond QMC algorithm

AWS, PRL 2007; J. Lou, AWS, N. Kawashima, PRB (2009)

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

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

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



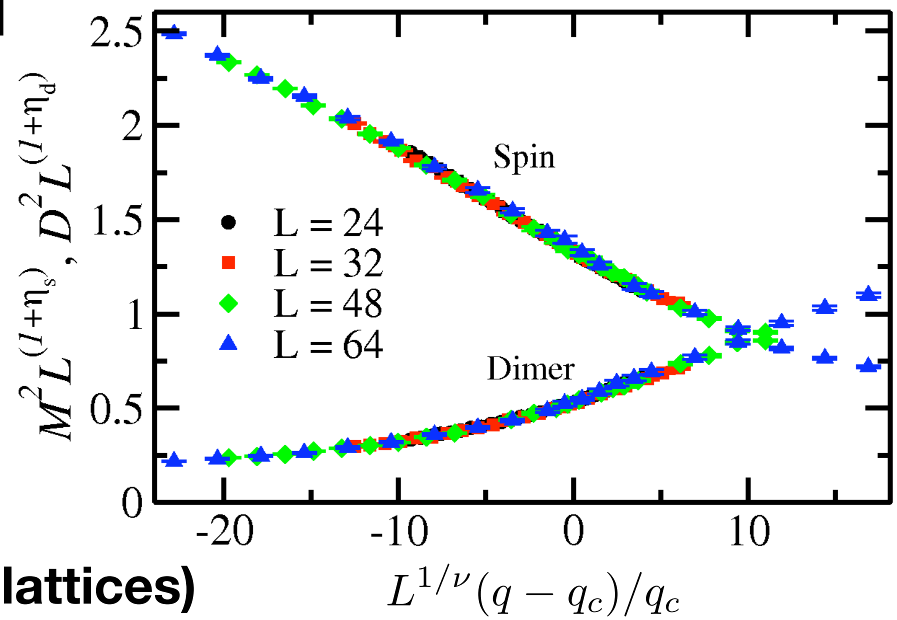
Coupling ratio

$$q = \frac{Q}{Q+J}$$

- AF order for q→0
- VBS order for q→1

$$(Q/J)_c \approx 24, \quad q_c \approx 0.961$$

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



Analysis should be improved (larger lattices) in light of possible logarithmic corrections

Columnar or plaquette VBS?

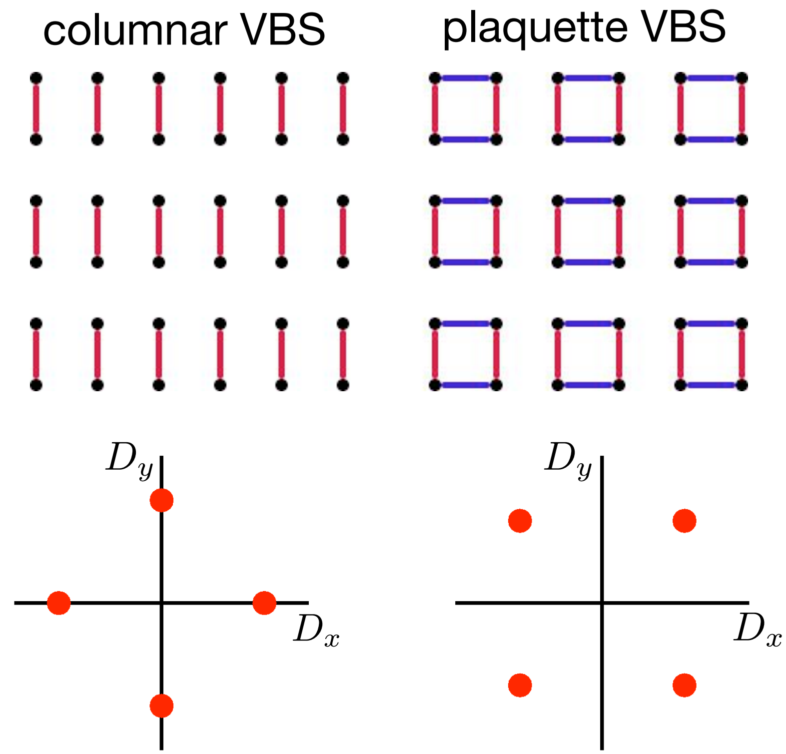
QMC-sampled state in the valence-bond basis

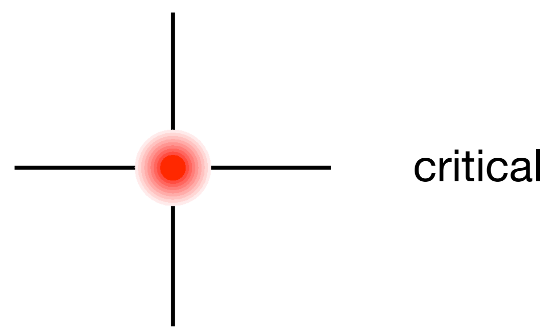
$$|0\rangle = \sum_k c_k |V_k\rangle$$

Joint probability distribution **$P(D_x,D_y)$** of x and y columnar VBS order parameters

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

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

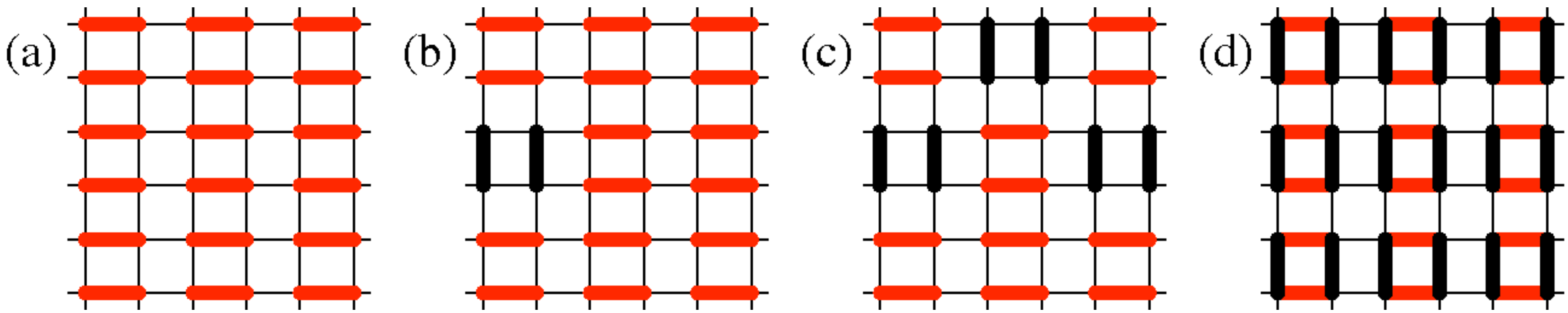




4 peaks expected in VBS phase
- Z_4-symmetry unbroken in finite system

VBS fluctuations in the theory of deconfined quantum-critical points
[Senthil et al., 2004]

➢ plaquette and columnar VBS are almost degenerate
➢ tunneling barrier seperating the two
- barrier increases with increasing system size L
- barrier decreases as the critical point is approached

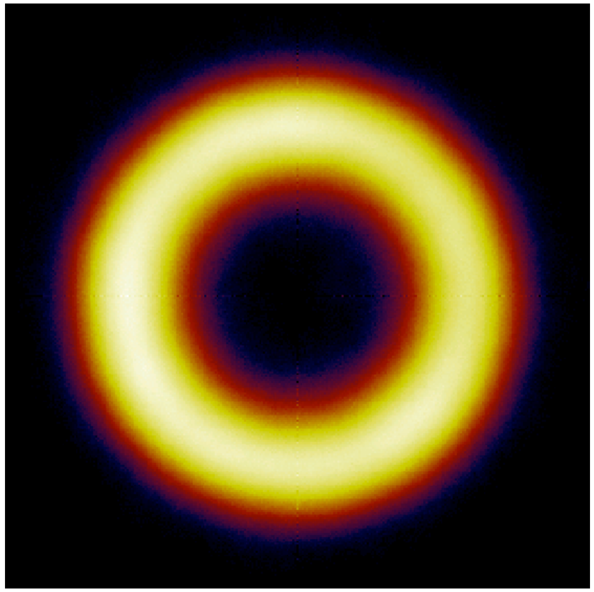


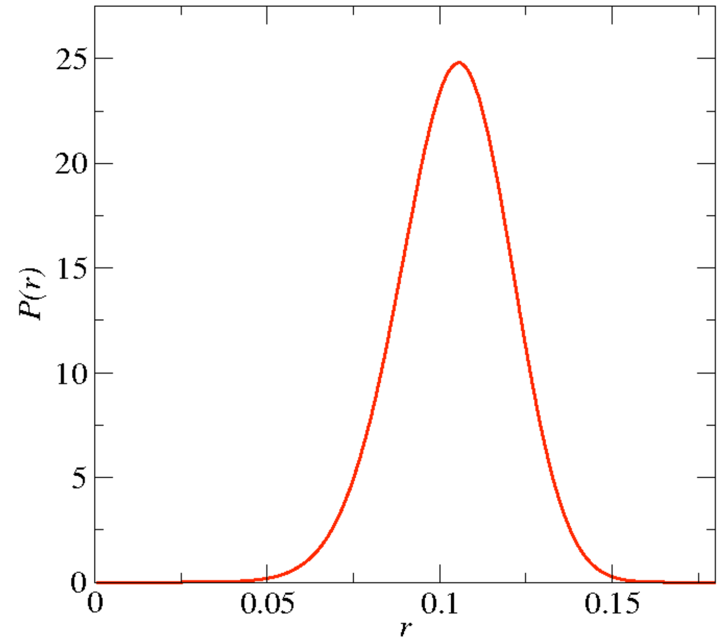
➢ **emergent U(1) symmetry**
➢ **ring-shaped distribution expected in the VBS phase for small systems**

$L < \Lambda \sim \xi^a$, $a > 1$ (spinon confinement length)

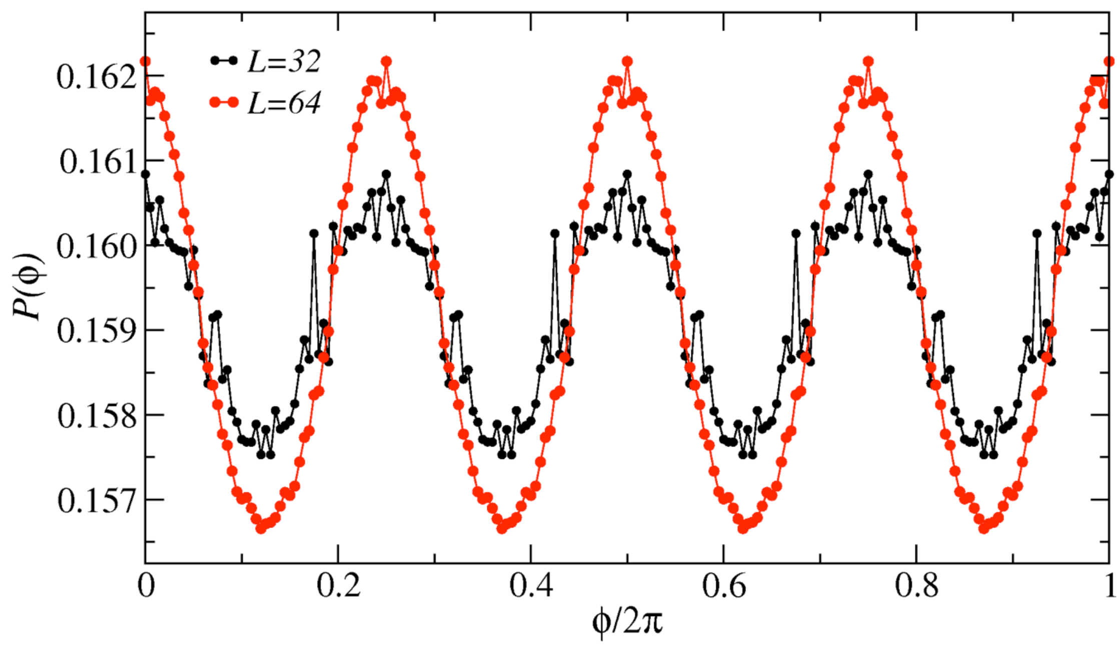
Signs of Z_4 symmetry in the original J-Q model?

L=128, J=0
P(D_x,D_y)



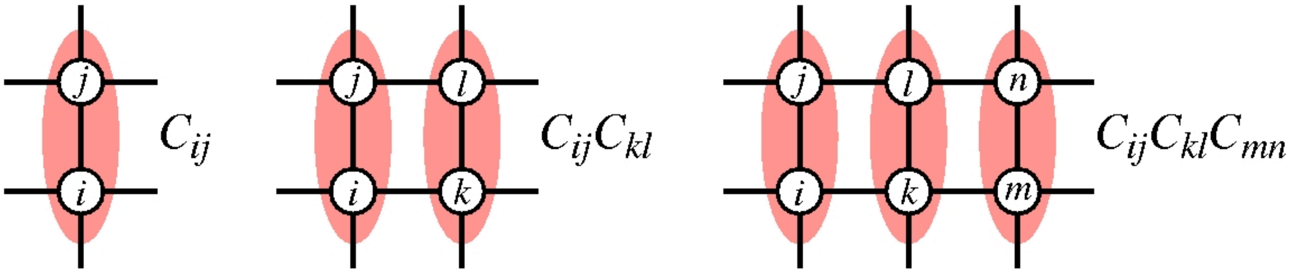


L=32, L=64; J=0
Weak but statistically significant angular dependence consistent with **columnar VBS**
(L=128 still too noisy)



Creating a more rubust VBS order - the J-Q_3 model

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



$$H = -J\sum_{\langle ij\rangle} C_{ij} - Q_3 \sum_{\langle ijklmn\rangle} C_{ij}C_{kl}C_{mn} \qquad C_{ij} = \frac{1}{4} - \vec{S}_i\cdot\vec{S}_j$$

$$q = \frac{Q_3}{J+Q_3}$$

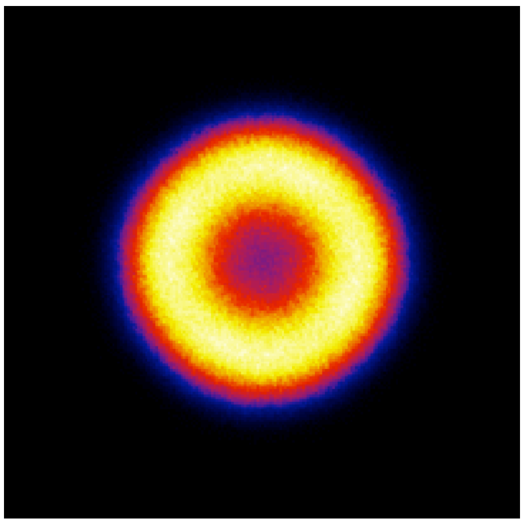
This model has a more robust VBS phase

- can the symmetry cross-over be detected?

$q = 0.635$

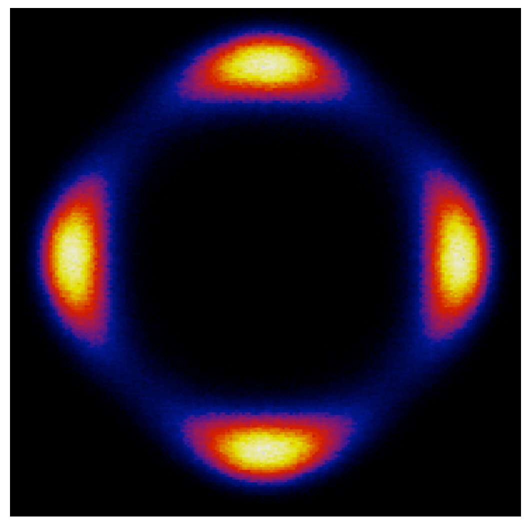
$(q_c \approx 0.60)$

$L = 32$



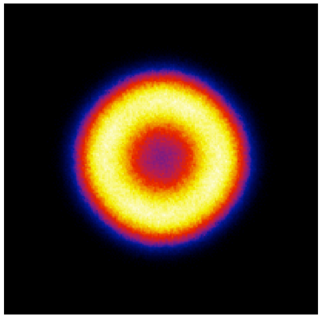
$q = 0.85$

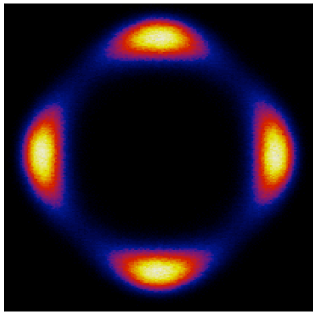
$L = 32$



Analysis of the VBS symmetry cross-over (J-Q_3 model)

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





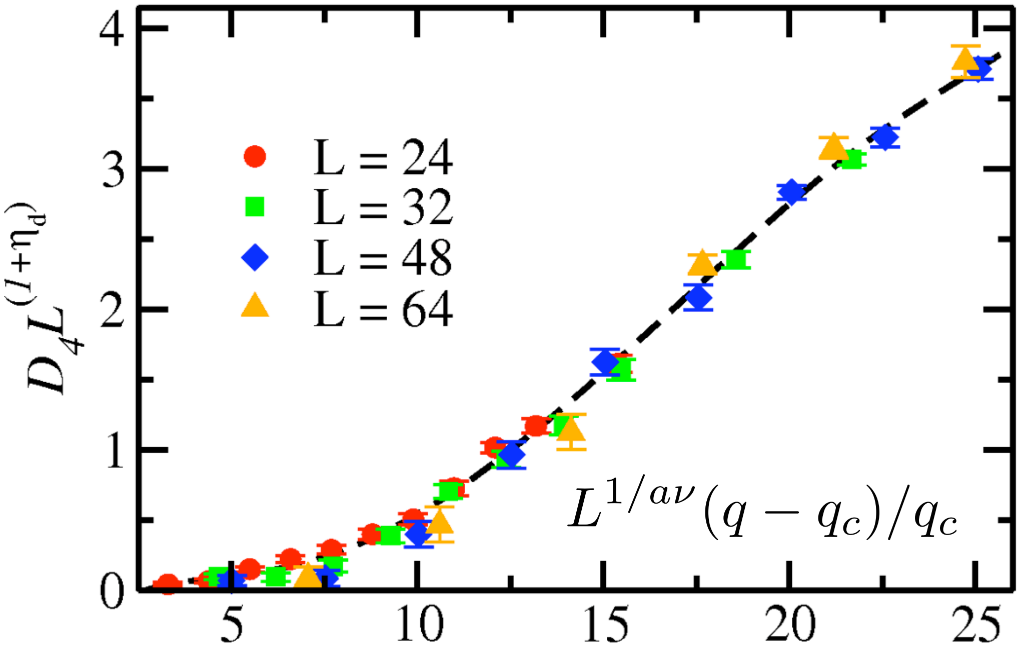
Z_4-sensitive VBS order parameter

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

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

$$\Lambda \sim \xi^{1+a}$$
$$\sim (q-q_c)^{-(1+a)\nu}$$

$$a = 0.20 \pm 0.05$$



Conclusions

Large-scale QMC calculations of the J-Q model

- **scaling behavior consistent with a continuous Neel-VBS transition**
  - with weak scaling corrections; maybe logarithmic
- **no signatures of first-order behavior**
  - cannot be ruled out as a matter of principle, but seems unlikely
- **a simple spinon gas pictures can account for the T>0 behavor**
  - log-correction to susceptibility follows from anomalous length scale
  - effective-spin calculation in very good agreement with S=1/2 spinons

Relation to deconfined quantum-criticality of Senthil et al.

- **Main features in good agreement**
  - z=1 scaling
  - "large" anomalous dimension η_{spin}
  - emergent U(1) symmetry
- **NCCP^{N-1} field theory for large N**
  [Senthil et al. (PRB 2004), Kaul & Sachdev (PRB 2008)]
  - no log-corrections found
  - difficult to extend to N=2 in analytical work
  - could there be log-corrections for N=2 (or general "small" N)?