Monte Carlo simulations of deconfined quantum-criticality

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Outline

- ➪ Exotic Neel-VBS transition; **deconfined quantum-criticality**
- ➪ S=1/2 Heisenberg model with four-spin interactions
- ➪ Quantum Monte Carlo in the valence bond basis
- ➪ Simulation Results; VBS phase, critical behavior
- ➪ **Emergent U(1) symmetry**

Funded by the NSF

National Science Foundation
WHERE DISCOVERIES BEGIN

Deconfined quantum criticality

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

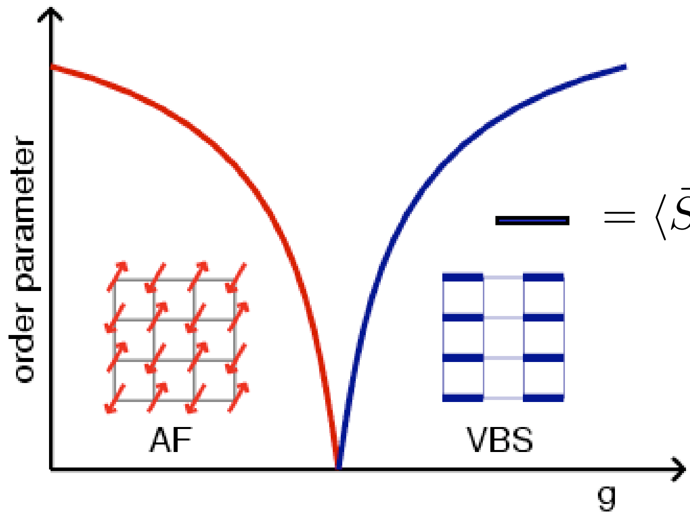
Continuous quantum phase transition (T=0) between two ordered phases

➢ Neel to valence-bond-solid (VBS)

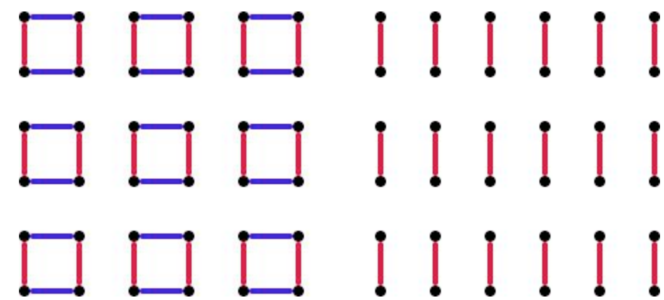
➢ Deconfined spinons at critical point

➢ Confined spinons ➞ Neel or VBS order

$$H = \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j + \ldots. \quad g = g(\{J_{ij}, \ldots\})$$



$$= \langle \vec{S}_i \cdot \vec{S}_j \rangle$$



Two types of critical VBS fluctuations

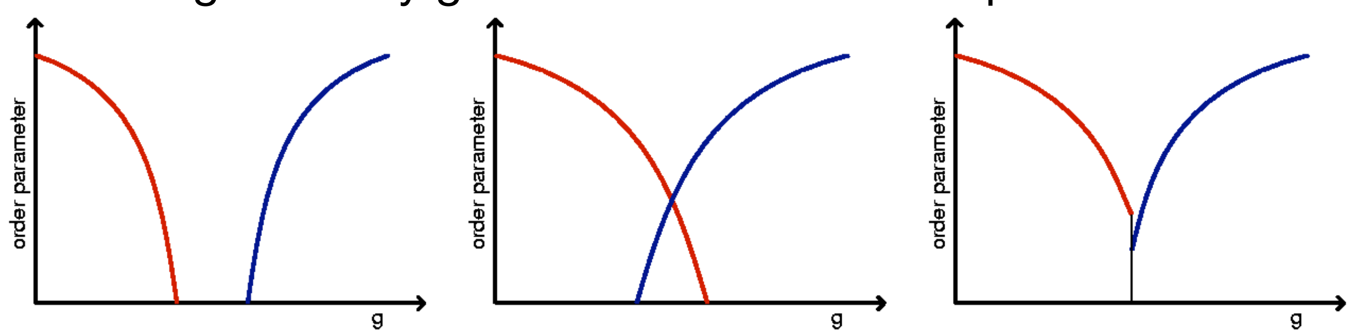
➢ plaquette and columnar

➢ Z_4 symmetry irrelevant at critical point

➢ **emergent U(1) symmetry**

Outside the Ginzburg-Landau-Wilson phase transition framework

➢ GLW generically gives first-order or two separate transitions



Do deconfined quantum-critical points exist?

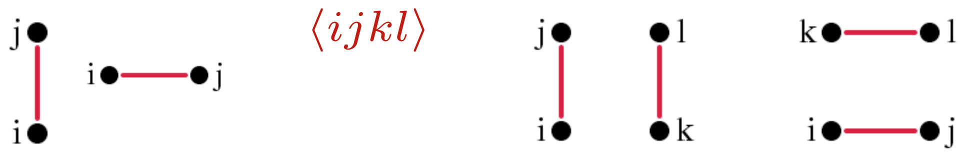
- ➢ Do they exist in nature? Can they be identified in numerical studies?
- ➢ First step: Find model hamiltonians exhibiting Neel-VBS transition
- ➢ VBS phases of quantum spin systems have been studied for a long time [Read and Sachdev, PRL (1988)]
- ➢ Why have Neel-VBS transitions not been fully characterized yet?

Models exhibiting both Neel and VBS phases are typically frustrated

- ➢ Sign problems for quantum Monte Carlo
- ➢ Only very small lattices can be studied (exact digonalization)
- ➢ No unbiased numerical methods for this class of systems
- ➢ Only approximate numerical/analytical results available

2D Heisenberg model with 4-spin term

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



- ➢ Studied using QMC projector method in the valence bond basis
- ➢ Turns out to have a Neel-VBS transition for J/Q≈0.04

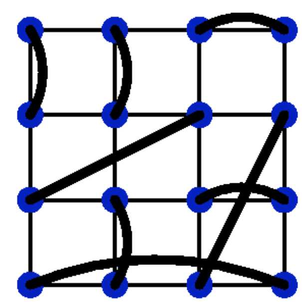
[AWS, arXiv:cond-mat/0611343 (to appear in PRL)]

Projector MC in the valence bond basis

[Liang, 1990; Santoro & Sorella, 1998; AWS, Phys. Rev. Lett 95, 207203 (2005)]

$$|\Psi\rangle = \sum_k f_k |(a_a, b_1)(a_2, b_2)\cdots(a_{N/2}, b_{N/2})\rangle$$

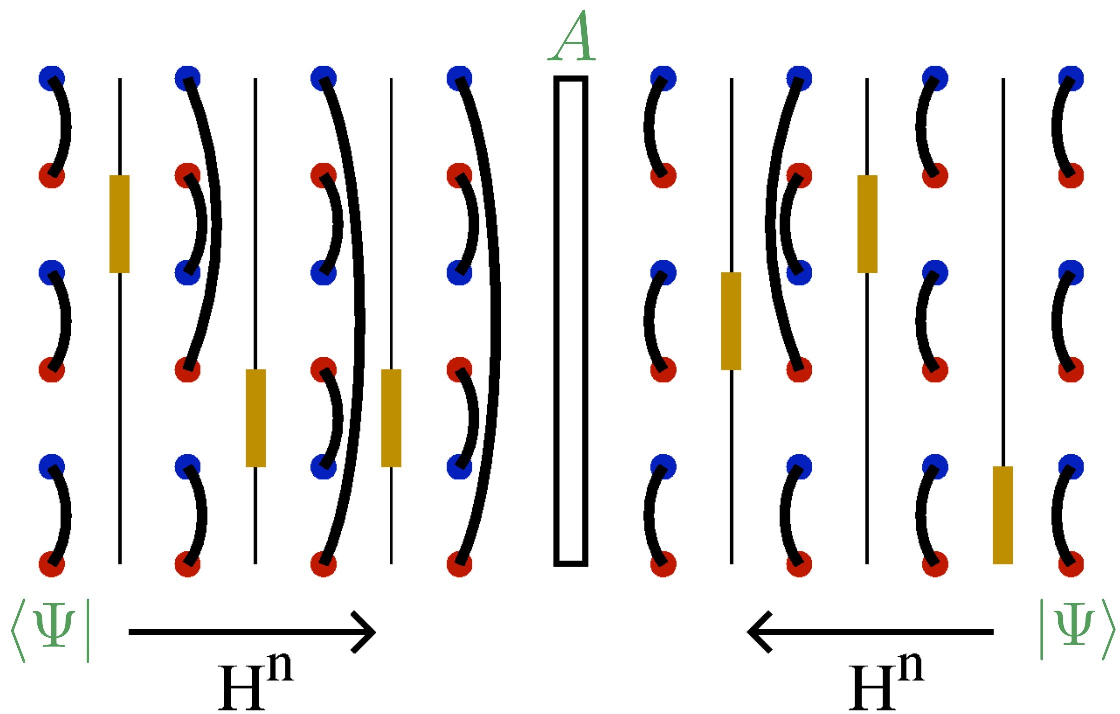
$$(a_i, b_i) = (\uparrow_i\downarrow_j - \downarrow_i\uparrow_j)/\sqrt{2}$$



Project out the ground state

$$(-H)^n|\Psi\rangle \to c_0|E_0|^n|0\rangle \qquad \langle A\rangle = \frac{\langle\Psi|(-H^*)^n A(-H)^n|\Psi\rangle}{\langle\Psi|(-H^*)^n(-H)^n|\Psi\rangle}$$

Example 2D Heisenberg model: $H = -\sum_{\langle ij\rangle} H_{ij}, \quad H_{ij} = -(\mathbf{S}_i\cdot\mathbf{S}_j - \frac{1}{4})$



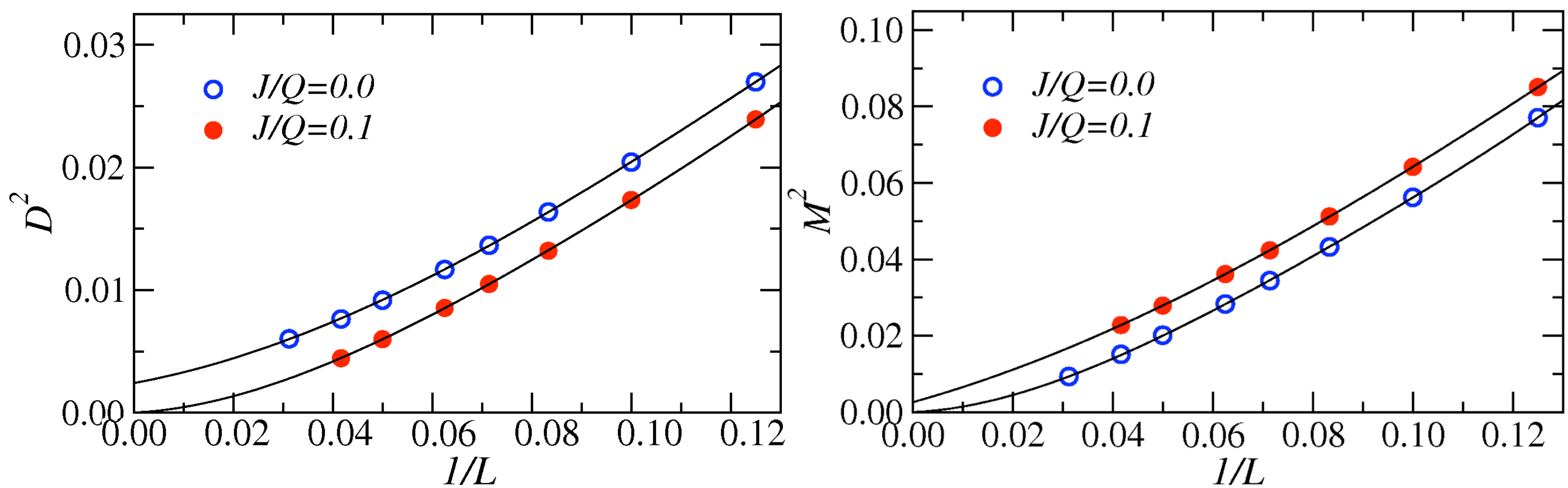
J-Q model; is there a VBS phase?

- VBS order parameter - columnar dimer-dimer correlations

$$D^2 = \frac{1}{N^2}\sum_{i,j} = \langle(\mathbf{S}_i\cdot\mathbf{S}_{i+\hat{x}})(\mathbf{S}_j\cdot\mathbf{S}_{j+\hat{x}})\rangle(-1)^{(x_i-x_j)}$$

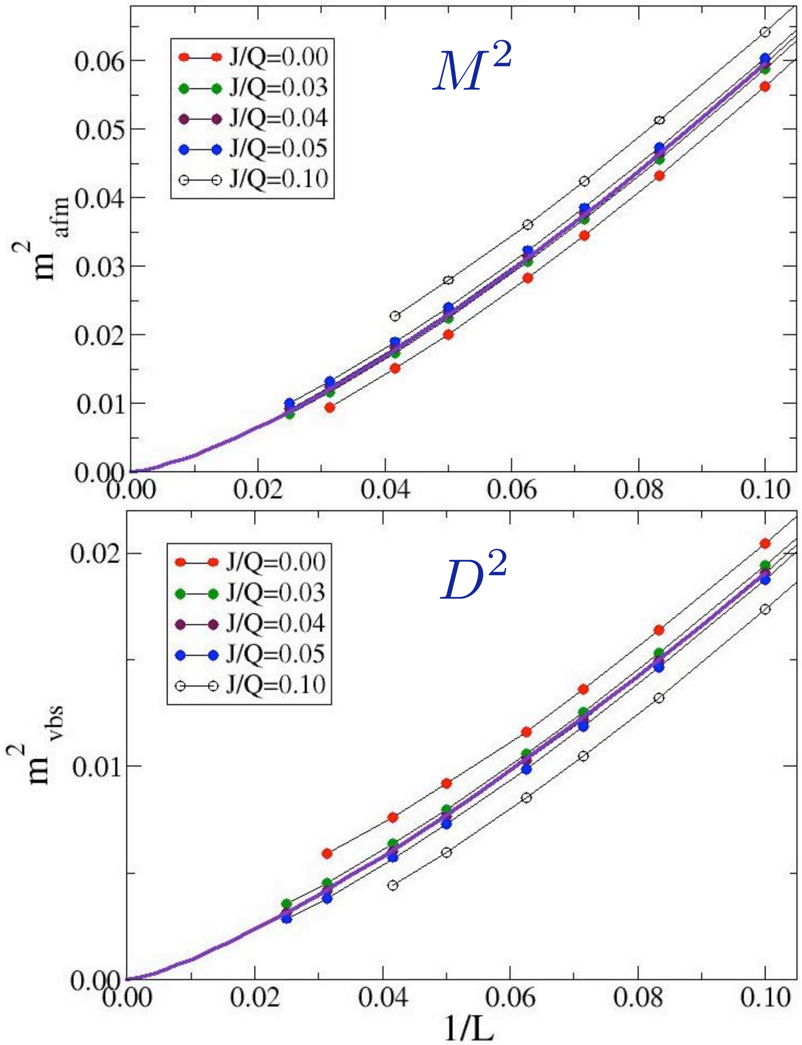
- Sublattice magnetization - staggered spin-spin correlations

$$M^2 = \frac{1}{N^2}\sum_{i,j}\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle(-1)^{(x_i-x_j+y_i-y_j)}$$



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

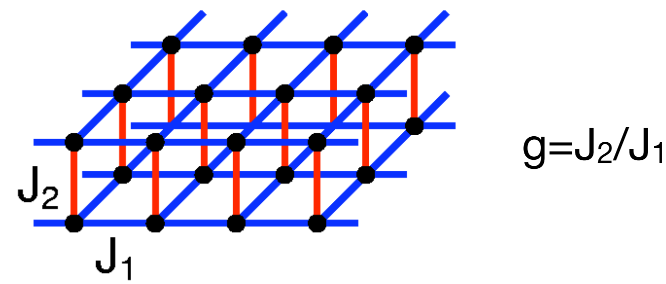
Do the VBS and AFM orders vanish at the same point?

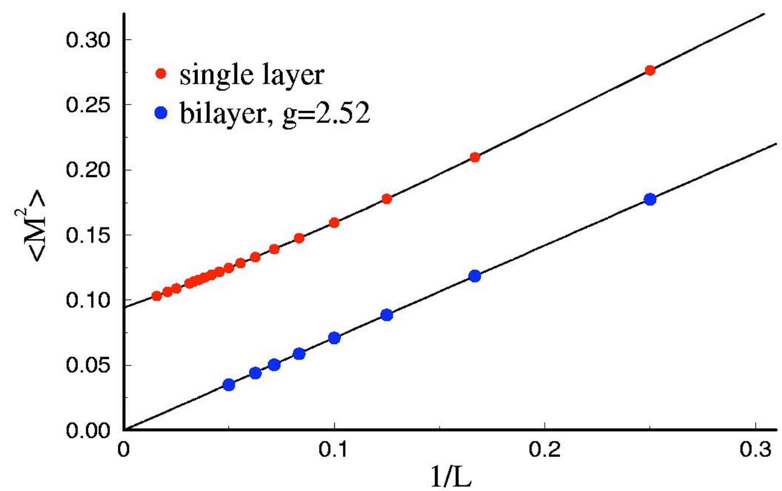


Both vanish at J/Q≈0.04

scale as $(1/L)^{z+\eta}$ with $z+\eta\approx 1.3$

Compare with O(3) transition in Heisenberg bilayer





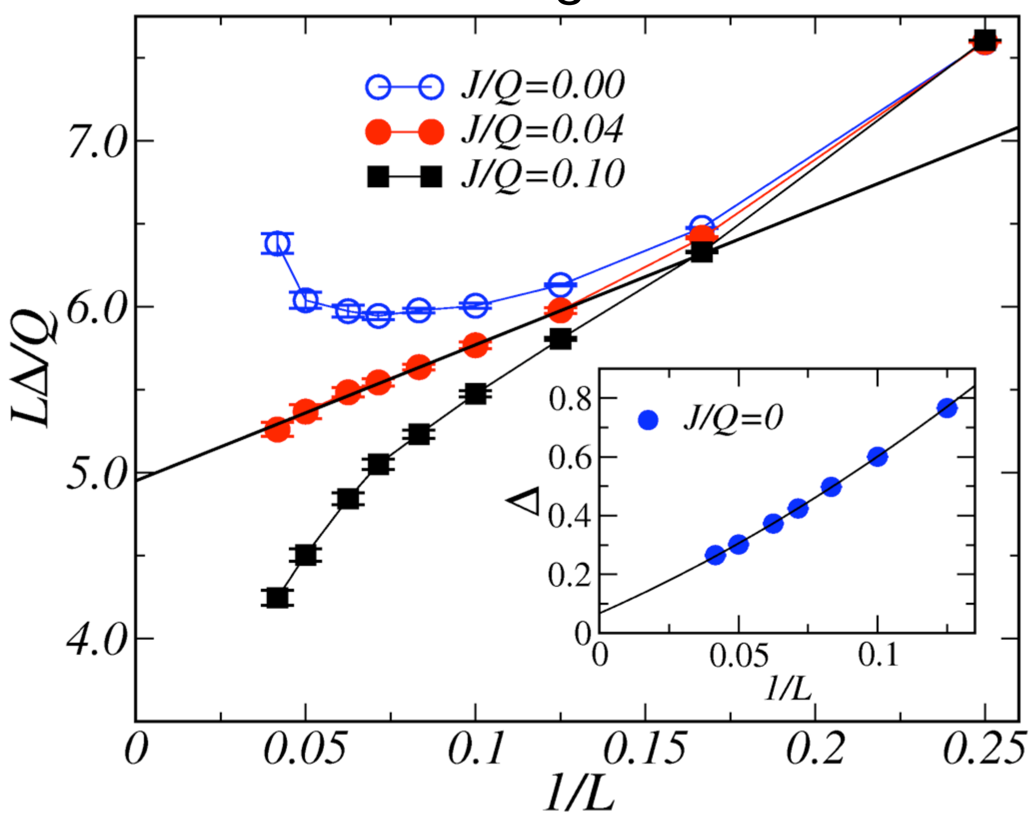
$z+\eta\approx 1.03$, $z=1$, $\eta\approx 0.03$

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 $L\Delta$



Critical gap scaling:

$$\Delta(L) = \frac{a_1}{L} + \frac{a_2}{L^2} + \cdots$$

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

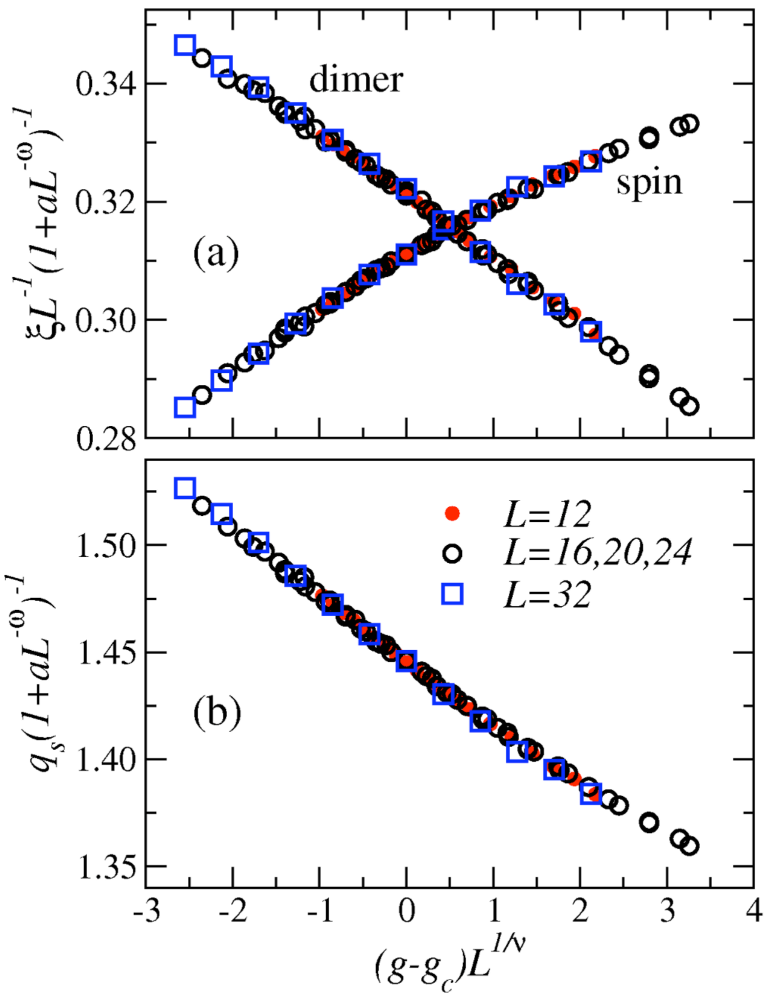
- z=1 field theory and "large" η predicted (Senthil et al.)

Finite-size scaling

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

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

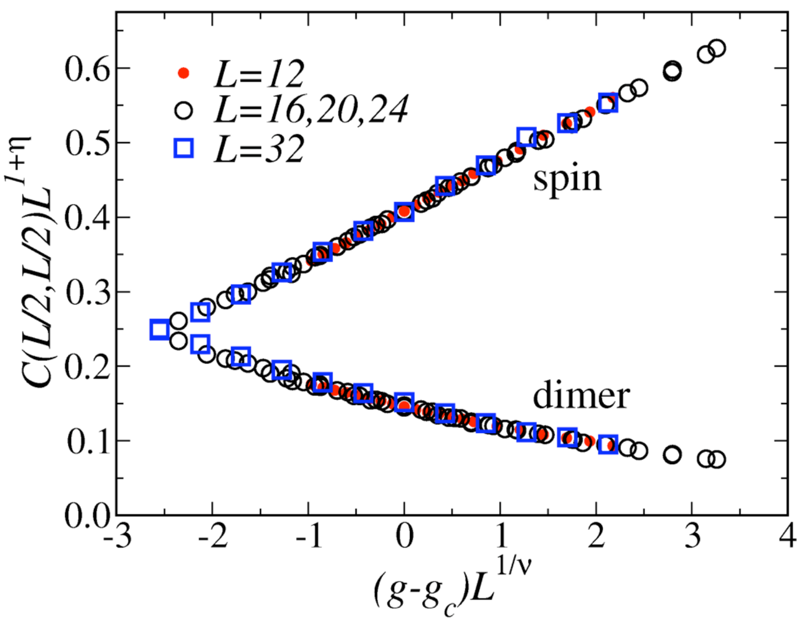
long-distance spin and dimer correlations: $C_{s,d}(L/2,L/2)$



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

(with subleading corrections)

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



Any other evidence for deconfined quantum-criticality?

Emergent U(1) symmetry predicted; should show up in the VBS order-parameter close to the critical point (on the VBS side)

➪ for L below a length scale Λ at which Z_4 anisotropy becomes relevant

Analogy: 3D classical XY model with Z_4 anisotropy

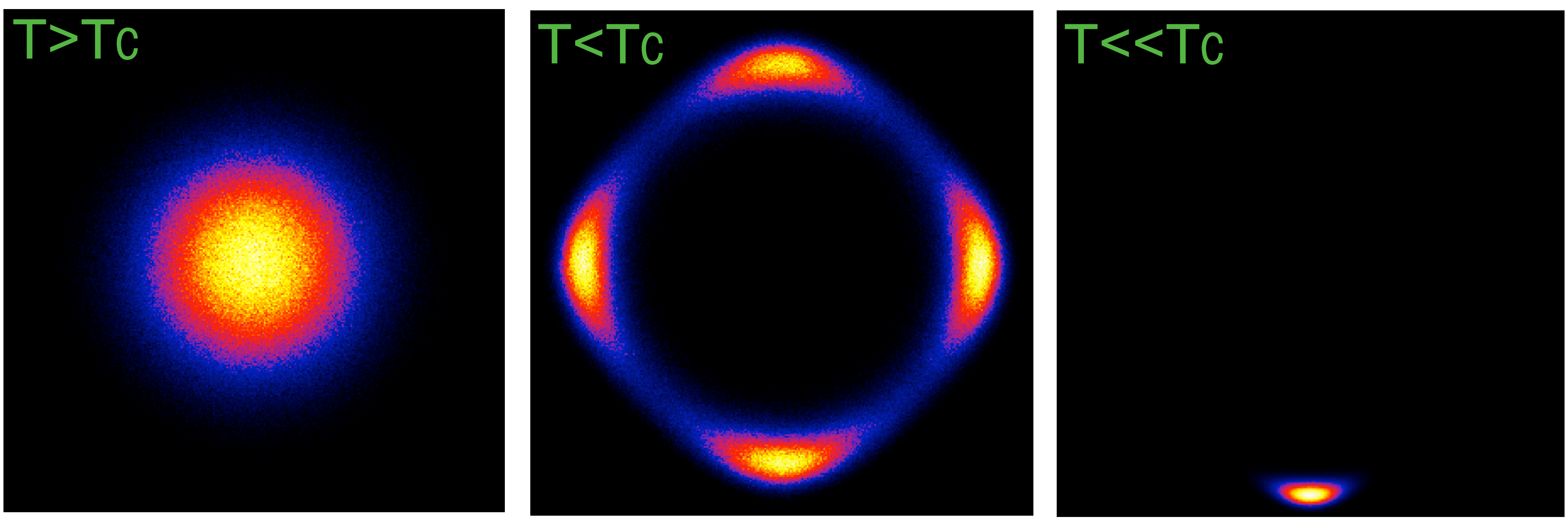
[Jie Lou and AWS, ArXiv:0704.1472]

$$H = -J \sum_{\langle i,j \rangle} \cos(\Theta_i - \Theta_j) - h \sum_i \cos(4\Theta_i)$$

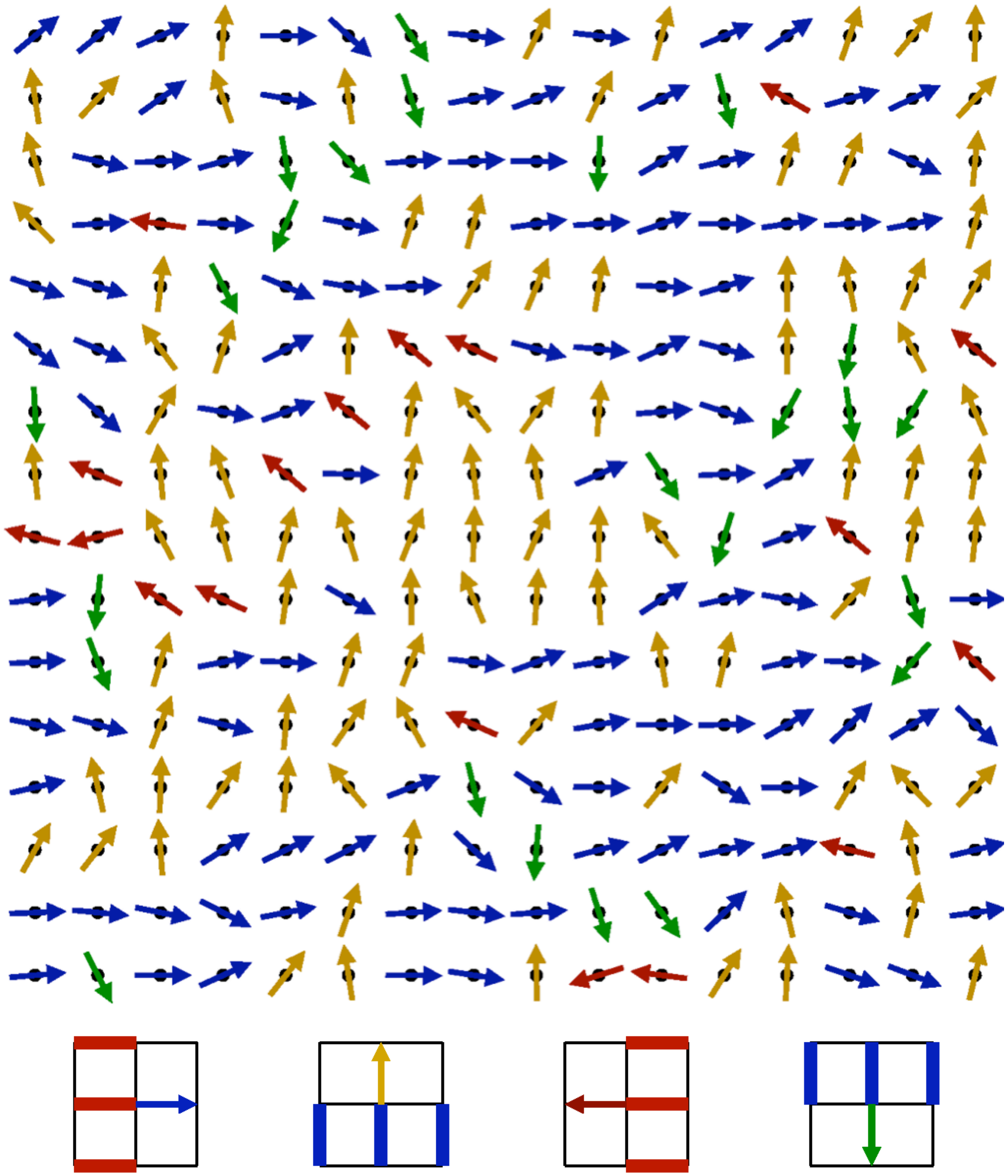
➪ the anisotropy h is known to be marginally irrelevant

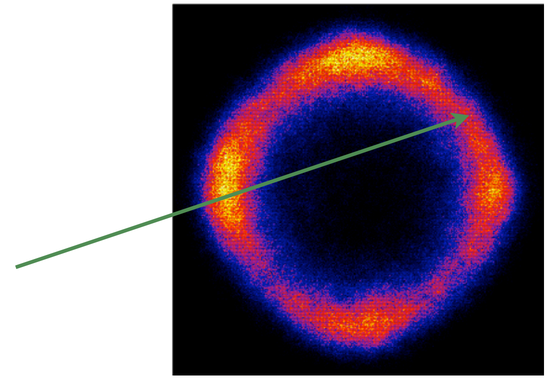
➪ Universality class unaffected, but ordered state reflects Z_4 term

➪ seen in 2D histogram P(Mx,My) $M_x = \frac{1}{N}\sum_i \cos(\Theta_i), \quad M_y = \frac{1}{N}\sum_i \sin(\Theta_i)$



Mx≈My Configuration (one layer); h/J=1



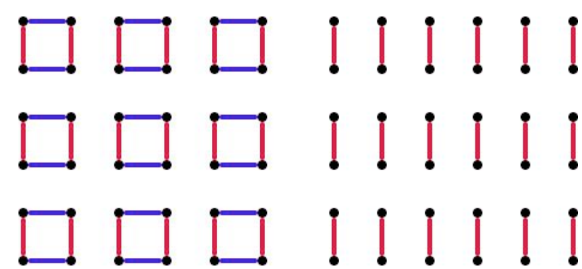


4 orientations (colors)

➪ correspond to the
4 ways of arranging
VBS order in J-Q model

1 or 2 directions dominate on the “U(1) circle”

➪ corresponds to mixing
of two types of VBS



J-Q model

Correlations between x and y VBS order parameters

The simulations sample the ground state;

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

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

$$D_x = \frac{\langle V_k | \mathbf{S}_i \cdot \mathbf{S}_{\mathbf{i}+\hat{\mathbf{x}}} | V_p \rangle}{\langle V_k | V_p \rangle} \qquad D_y = \frac{\langle V_k | \mathbf{S}_i \cdot \mathbf{S}_{\mathbf{i}+\hat{\mathbf{y}}} | V_p \rangle}{\langle V_k | V_p \rangle}$$

Questions

Is there an emergent U(1) symmetry at the transition

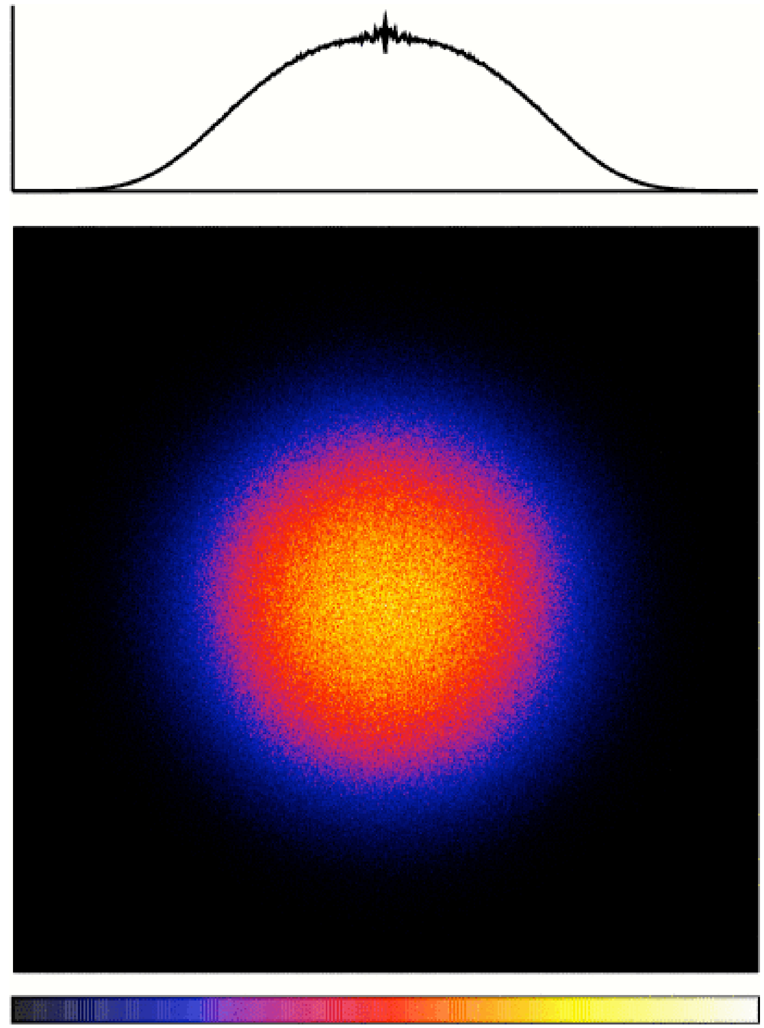
➩ rotational, U(1), vs 4-fold, Z_4, symmetry of $P(D_x,D_y)$

Is the transition weakly first order?

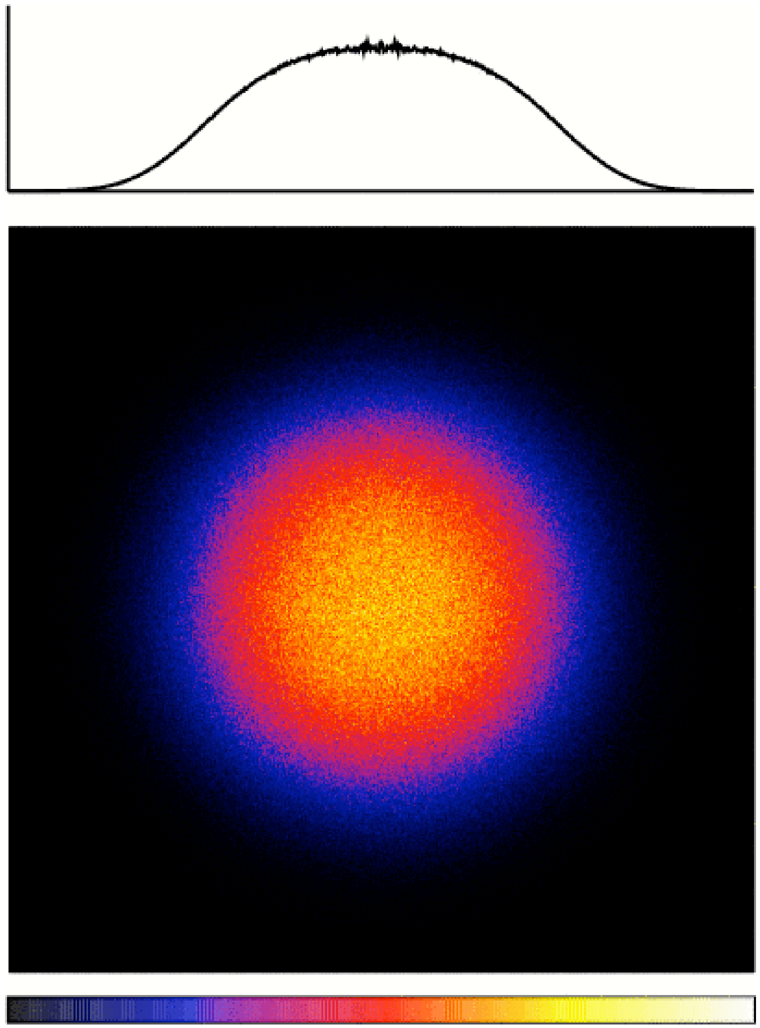
➩ coexistence of Neel and VBS should show up in $P(D_x,D_y)$ as a central peak coexisting with 4 VBS maxima

Results: L=32 lattices

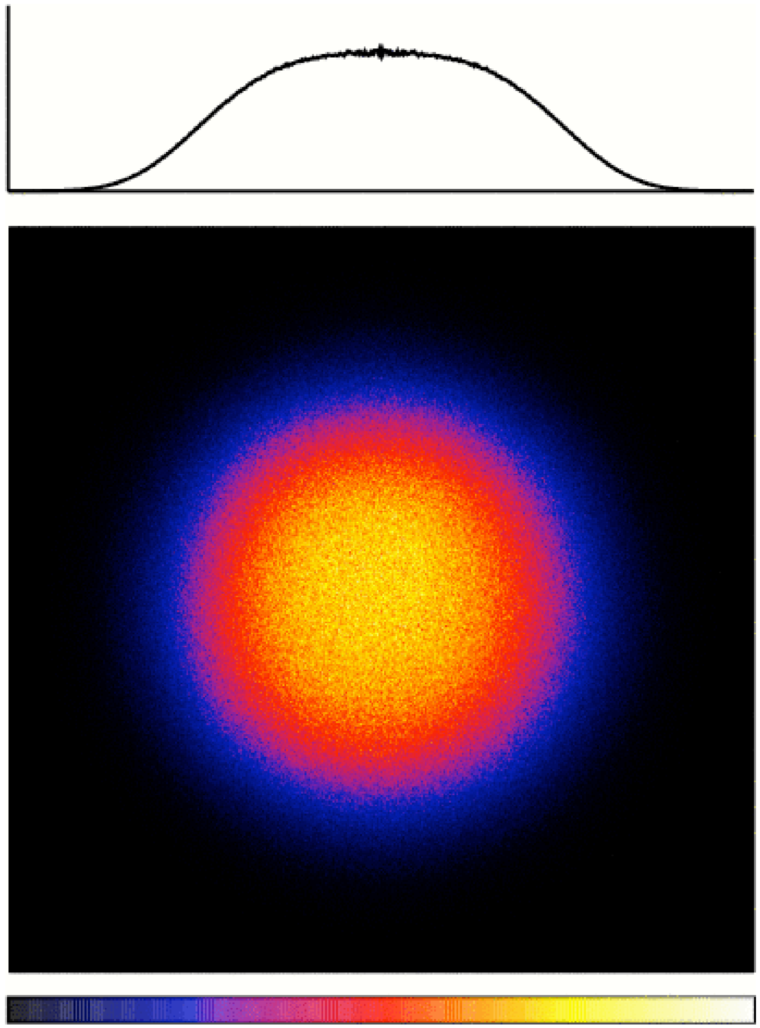
J/Q=0.45



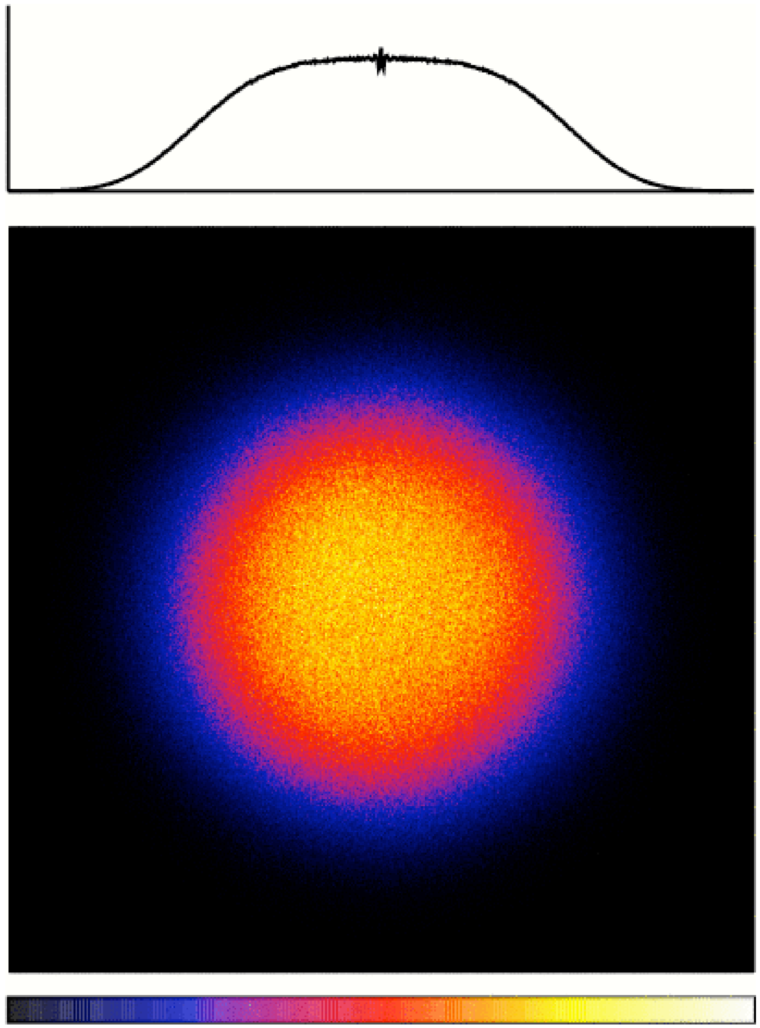
J/Q=0.40



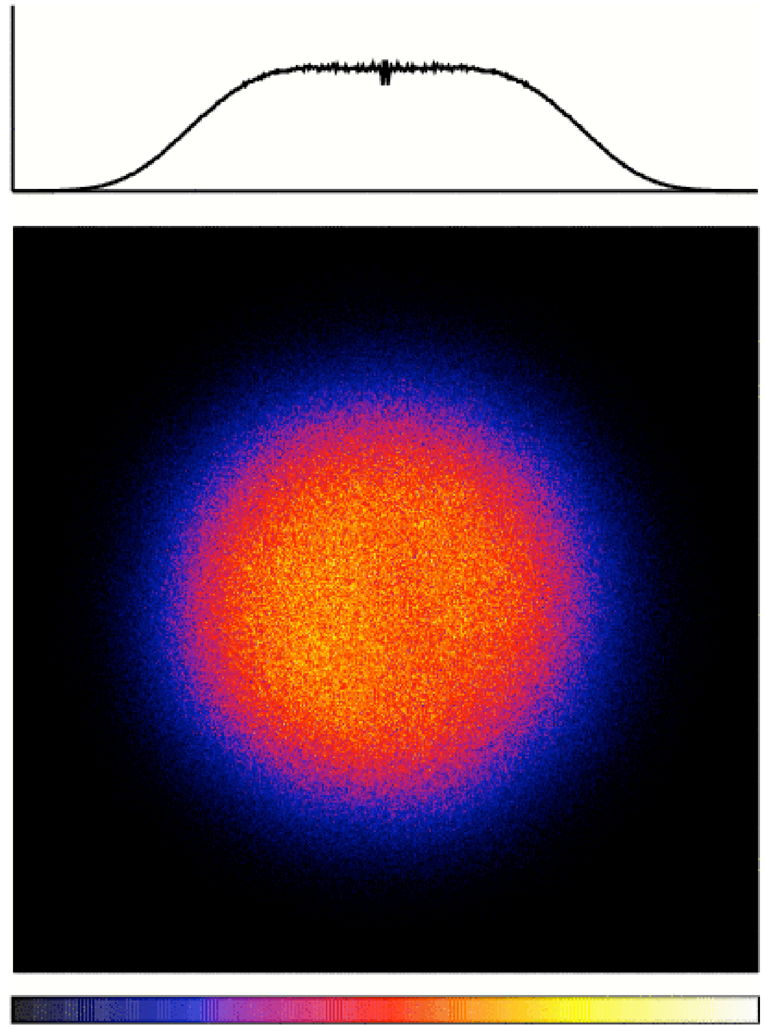
$J/Q = 0.35$



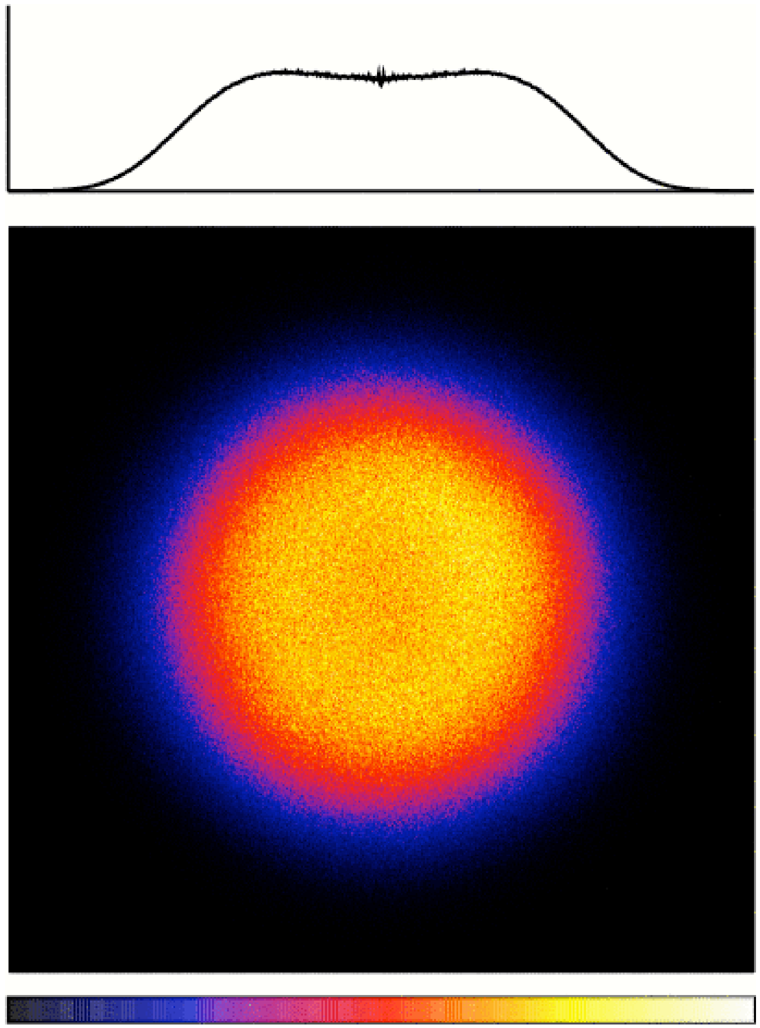
J/Q=0.30



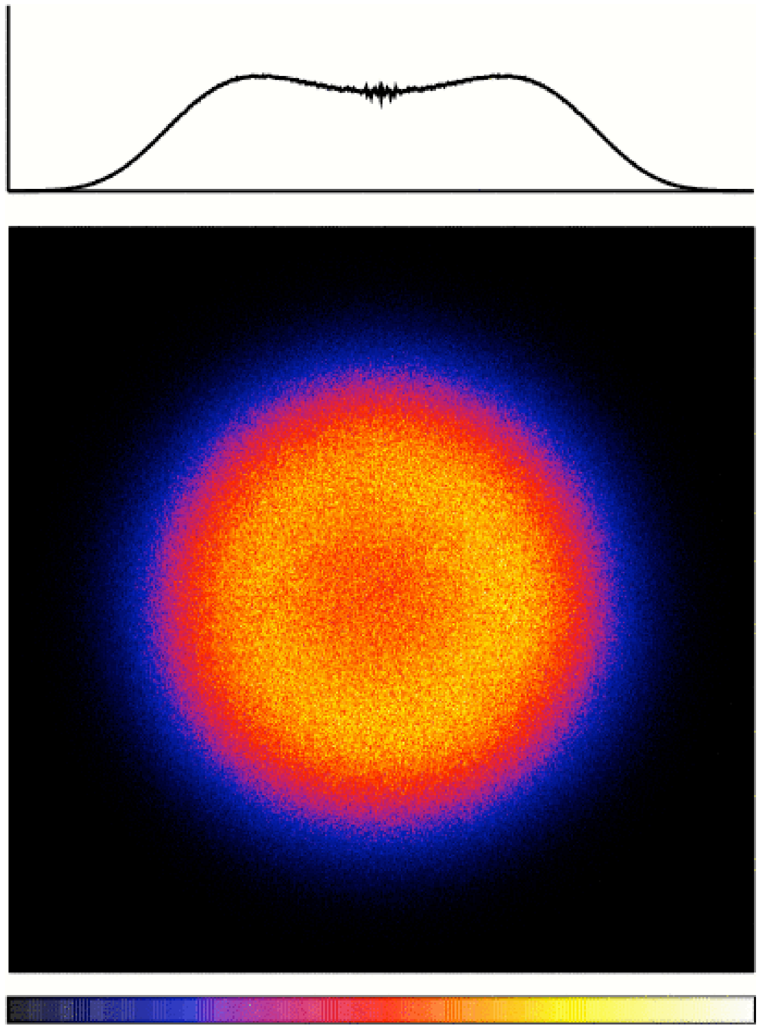
J/Q=0.25



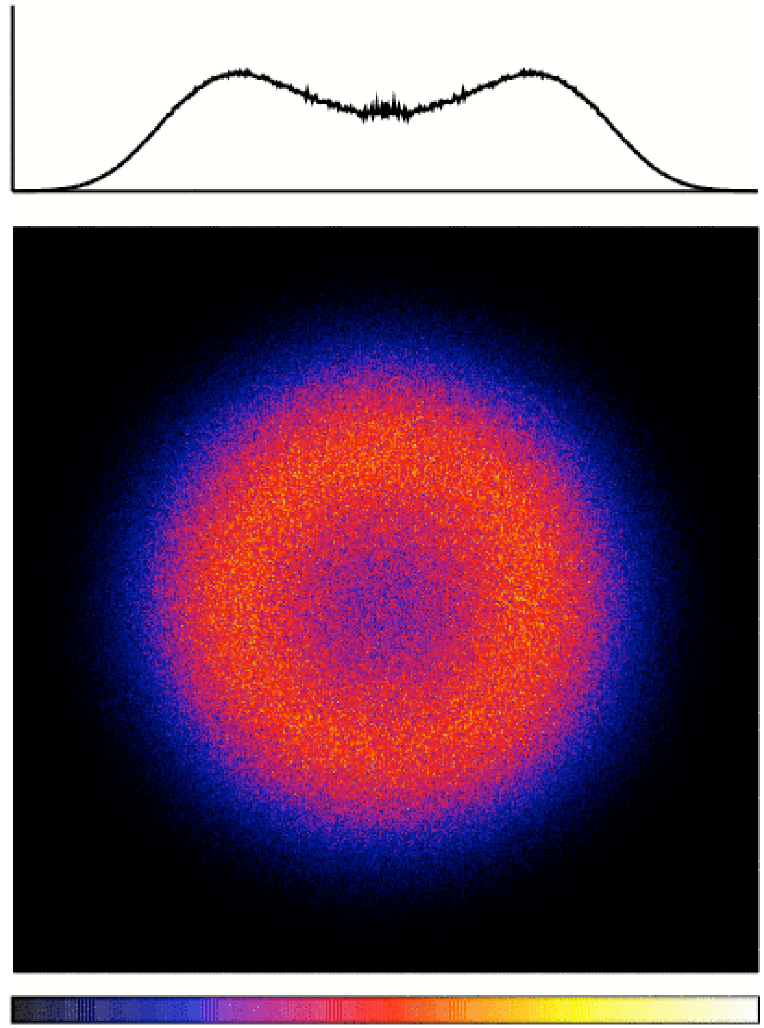
$J/Q=0.20$



J/Q=0.10



$J/Q=0.00$ **No signs of Z_4 anisotropy!**



Return to classical Z_q model to explore the cross-over from U(1) to Z_q order-parameter

Order parameter quantifying U(1) emergence

Magnetization in terms of the probability distribution

$$M = \int dr d\phi r^2 P(r,\phi)$$

Modified magnetization vanishing if not Z_q anisotropic

$$M^* = \int dr d\phi r^2 P(r,\phi)\cos(q\phi)$$

M^* should be controlled by the length scale Λ at which the Z_q term becomes relevant

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

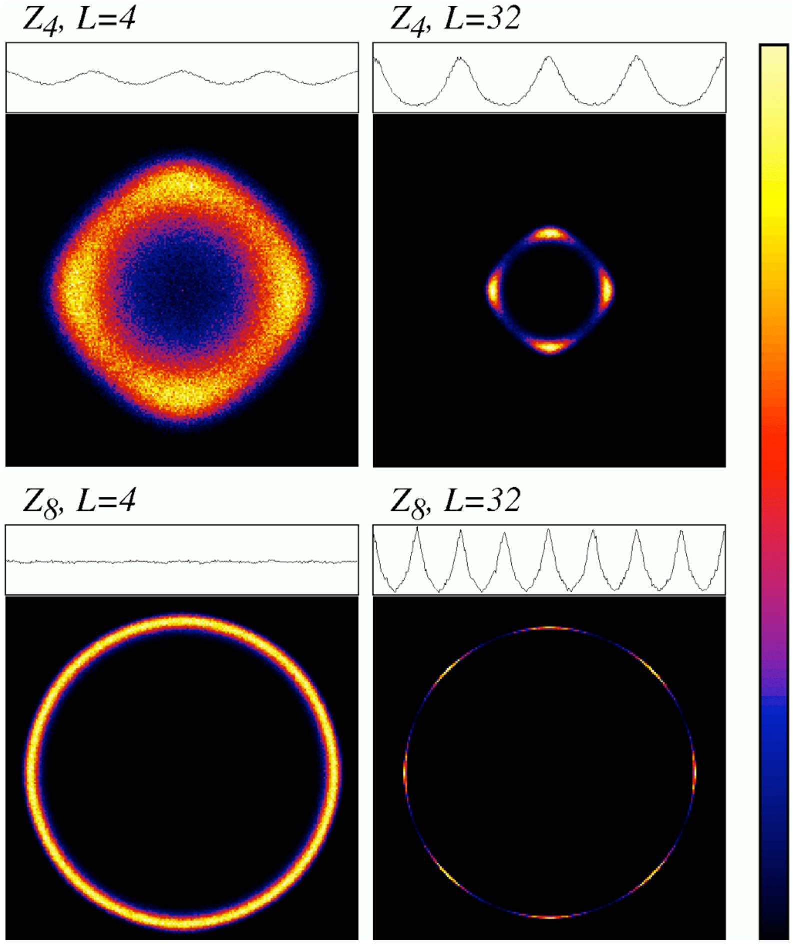
Finite-size scaling

$$M \sim L^{-(1+\eta)/2} f(tL^{1/\nu})$$

$$M^* \sim L^{-(1+\eta)/2} g(tL^{1/a\nu})$$

3D XY exponents

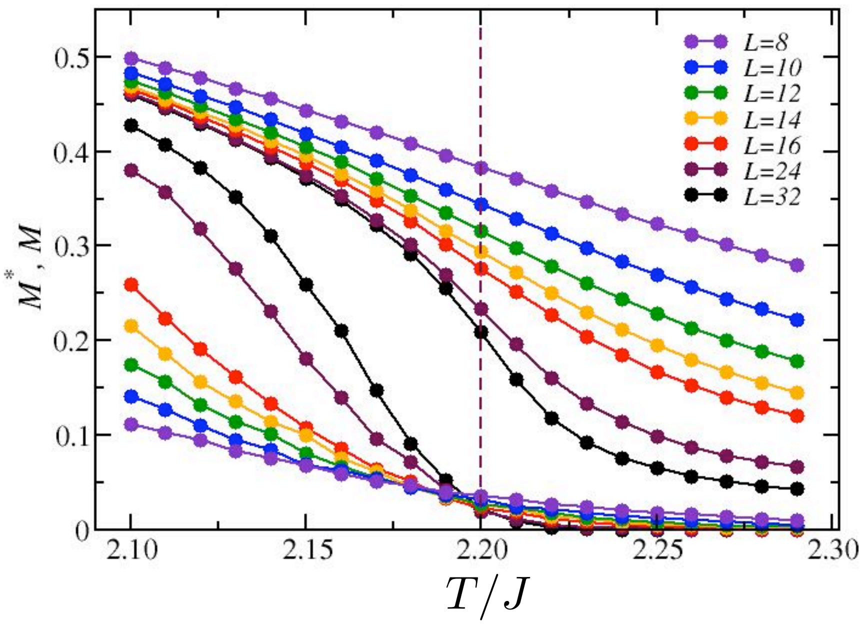
$$\nu \approx 0.67, \quad \eta \approx 0.04$$



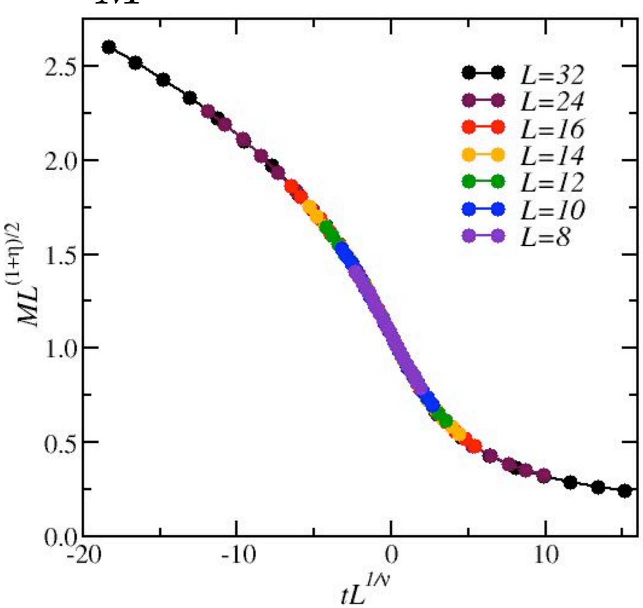
Results: Z_4

$$M \sim L^{-(1+\eta)/2} f(tL^{1/\nu})$$

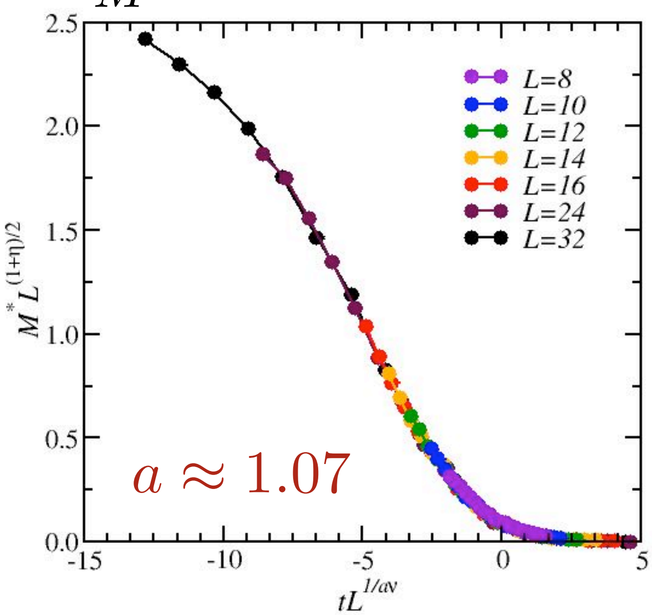
$$M^* \sim L^{-(1+\eta)/2} g(tL^{1/a\nu})$$



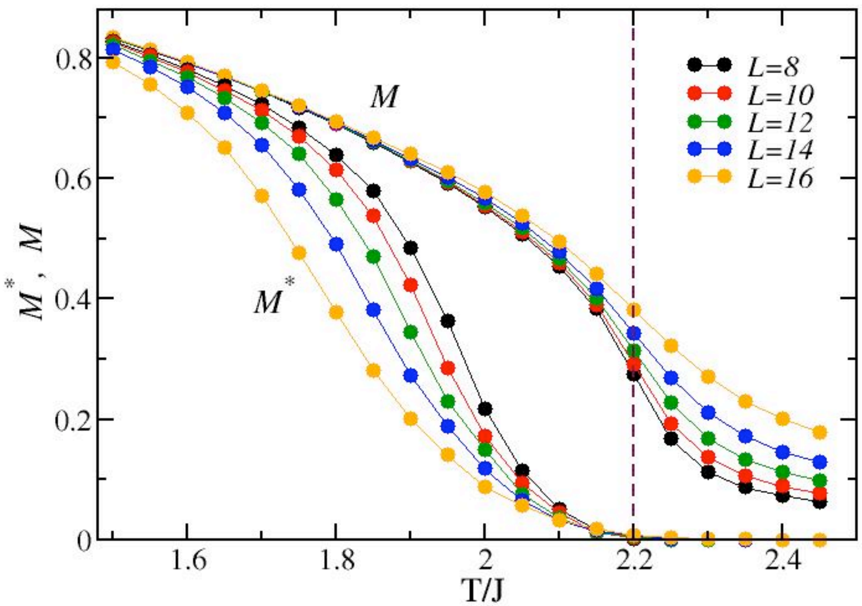
M



M^*



Z_6



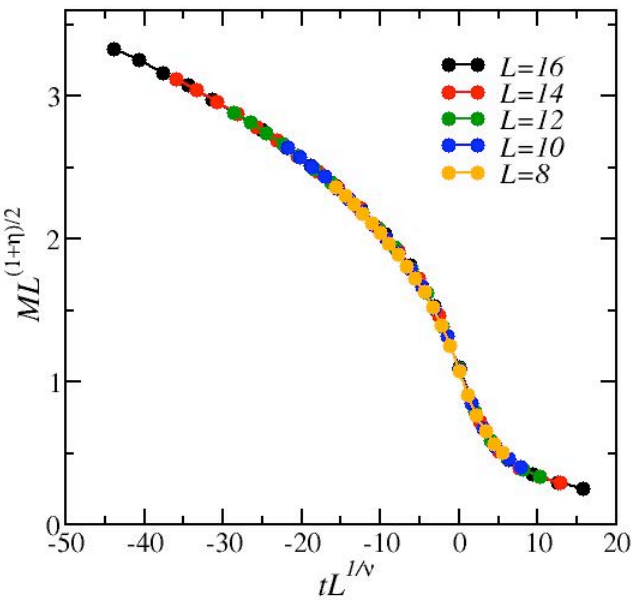
Results for q=4,...,8 ⇒

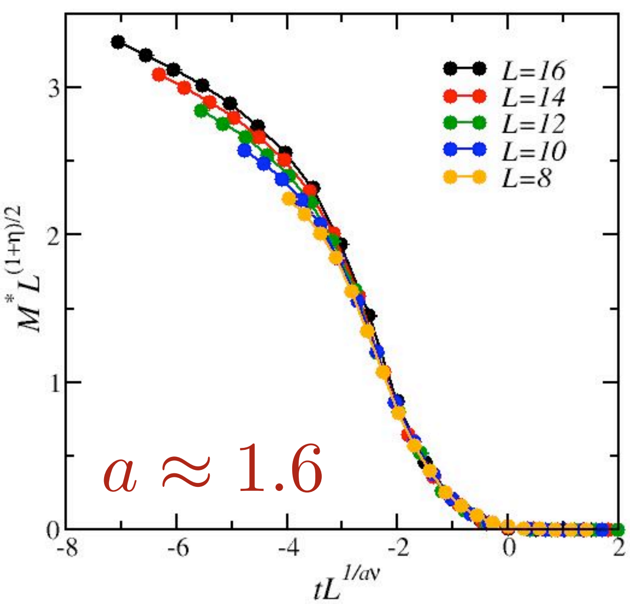
$a_q \approx a_4(q/4)^2, \quad a_4 \approx 1.07$

Agrees with RG, ϵ-expansion (Oshikawa, PRB 2000)

Asymptotic q→∞ form:

$a_q = q^2/10$





Summary & Conclusions

2D J-Q model; Heisenberg model with 4-spin interactions

- ➪ Results consistent with continuous Neel-VBS transition
- ➪ $z=1$, as required by deconfined theory
- ➪ Single set of exponents describe spin and dimer correl.
  - higher symmetry - SO(5) - at the critical point?
- ➪ η is large (≈0.26) - consistent with prediction for DCQP
- ➪ Evidence of emergent U(1) symmetry

How does the Z_4 length Λ diverge? $\Lambda \sim \xi^a$

- Larger lattices needed
- in 3D classical XY-Z_4 model, a_4≈1.07
  - a_q increases with q for Z_q model: $a_q \approx a_4(q/4)^2$
  - in good agreement with ϵ-expansion (Oshikawa)
- results indicate $a>a_4$ for J-Q model

J-Q model: "Ising model of deconfined quantum-criticality"