Quantum Monte Carlo Methods at Work for Novel Phases of Matter
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Quantum Monte Carlo simulations of "deconfined" quantum criticality at the 2D Néel-VBS transition

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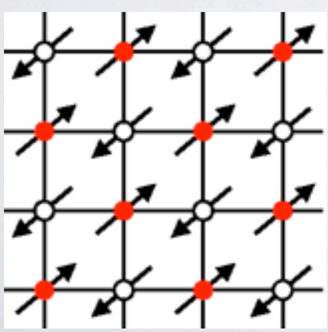
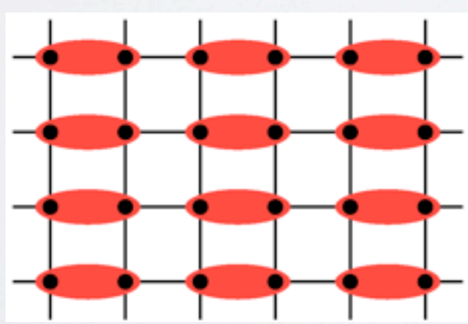
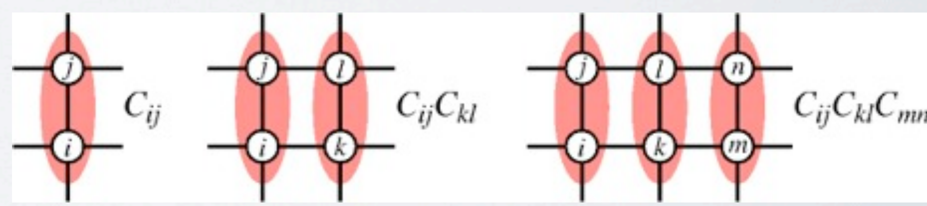
Outline

- 2D Heisenberg model; T=0 long-range Néel order
- Conventional Néel - paramagnet quantum phase transition
- Valence-bonds-solid (VBS) order and “deconfined” criticality
- Microscopic realizations; J-Q model
- Insights from QMC simulations; SU(2) and SU(N) models
- Emergent U(1) symmetry of the near-critical VBS state
- First-order scenario vs log corrections





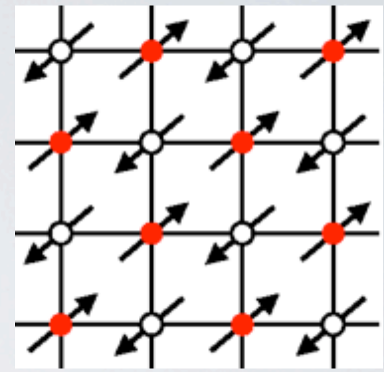


Long-range antiferromagnetic order in the 2D S=1/2 Heisenberg model

Sublattice magnetization

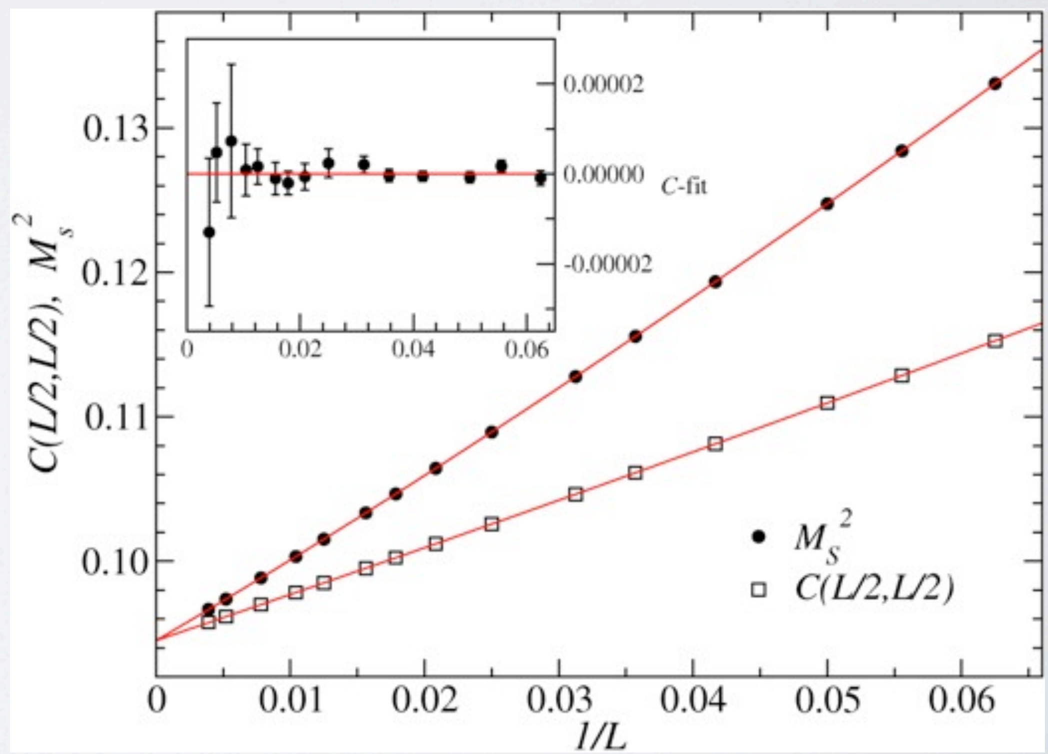
$$\mathbf{H} = \mathbf{J} \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \mathbf{S_i} \cdot \mathbf{S_j}$$

$$\vec{m}_s = \frac{1}{N}\sum_{i=1}^{N} \phi_i \vec{S}_i, \quad \phi_i = (-1)^{x_i+y_i} \quad \text{(2D square lattice)}$$



Long-range order: **$\langle m_s^2 \rangle > 0$ for $N \to \infty$**

Rigorous proof of ordered ground states for S>1/2
- no analytical proof for S=1/2
- **quantum Monte Carlo** is the only unbiased way to compute m_s
  - finite-size calculation
  - no approximations
  - extrapolation to infinite size



Reger & Young 1988:

$$m_s = 0.30(2)$$

$$\approx 60\ \%\ \text{of classical value}$$

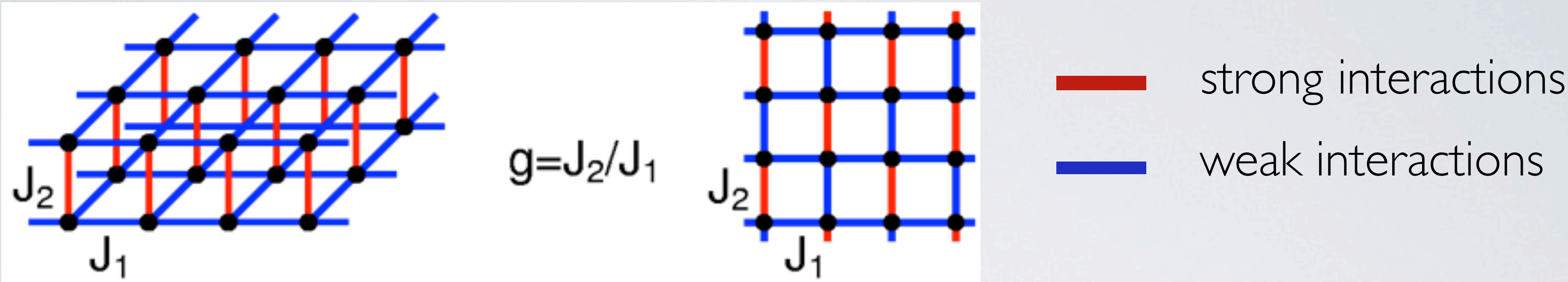
Sandvik & Evertz 2010:

$$m_s = 0.30743(1)$$

Conventional quantum phase transitions

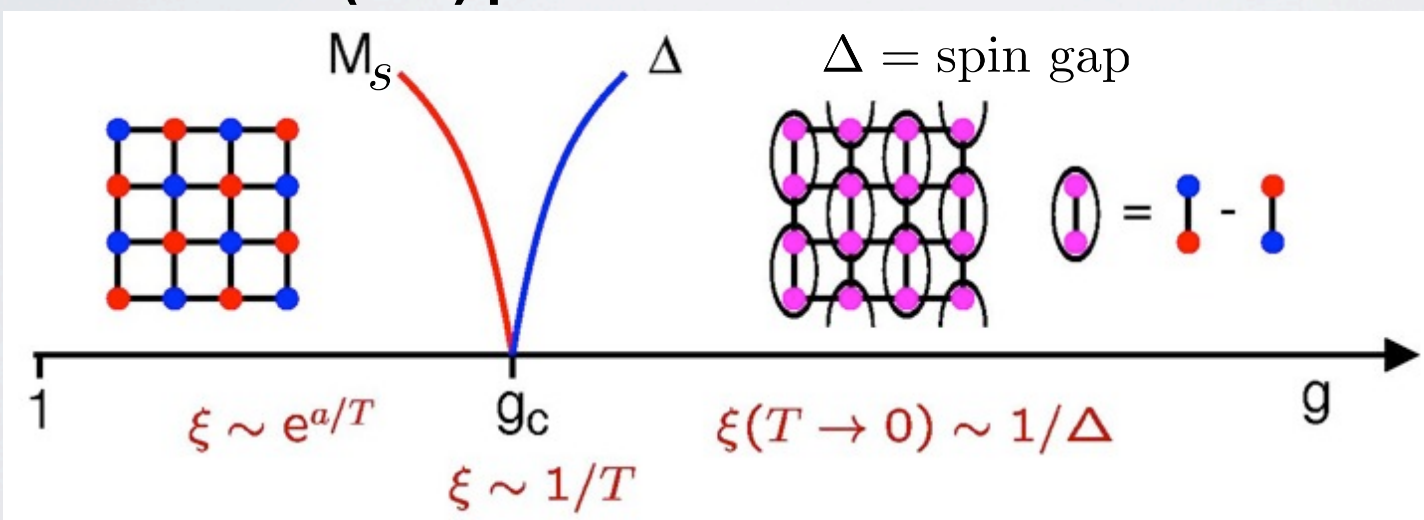
Example: Dimerized S=1/2 Heisenberg models

- every spin belongs to a dimer (strongly-coupled pair)
- many possibilities, e.g., bilayer, dimerized single layer



Singlet formation on strong bonds ➙ Neel - disordered transition

Ground state (T=0) phases



2D quantum Heisenberg map onto (2+1)D classical Heisenberg (Haldane)
⇒ 3D classical Heisenberg (O3) universality class; QMC confirmed

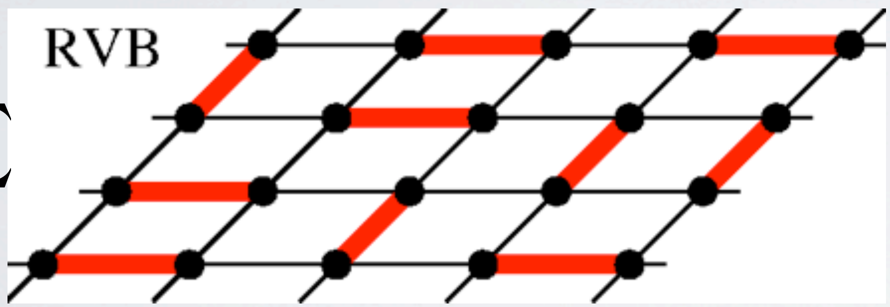
Experimental realization (3D system): $TlCuCl_3$

More complex non-magnetic states; systems with 1 spin per unit cell

$$\mathbf{H} = \mathbf{J} \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \mathbf{S_i} \cdot \mathbf{S_j} + \mathbf{g} \times \cdots$$

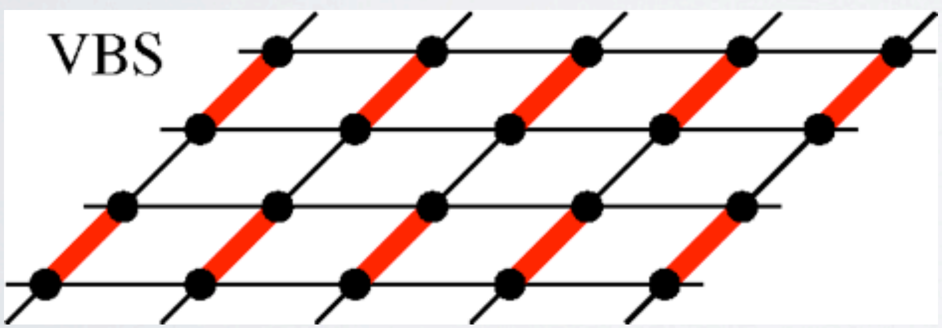
- **non-trivial non-magnetic ground states are possible, e.g.,**
  - ➡ resonating valence-bond (RVB) spin liquid
  - ➡ valence-bond solid (VBS)

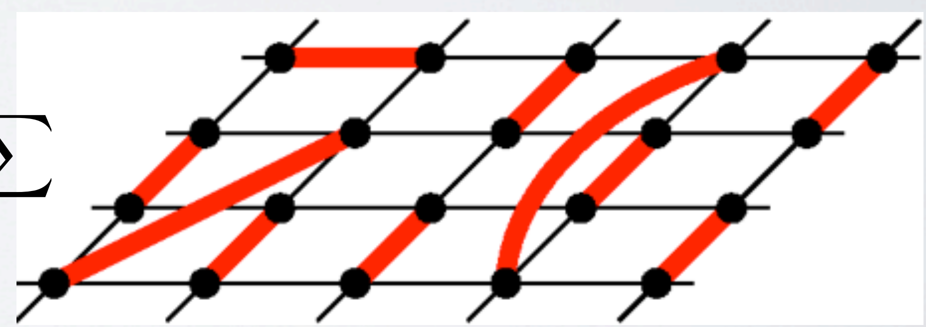
Non-magnetic states often have natural descriptions with **valence bonds**

$\sum$ 

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

The basis including bonds of all lengths is **overcomplete** in the singlet sector



$\sum$ 

In the 2D Néel state the bond-length (*r*) probability has the form: $P(r) \propto \frac{1}{r^3}$

- non-magnetic states dominated by short bonds

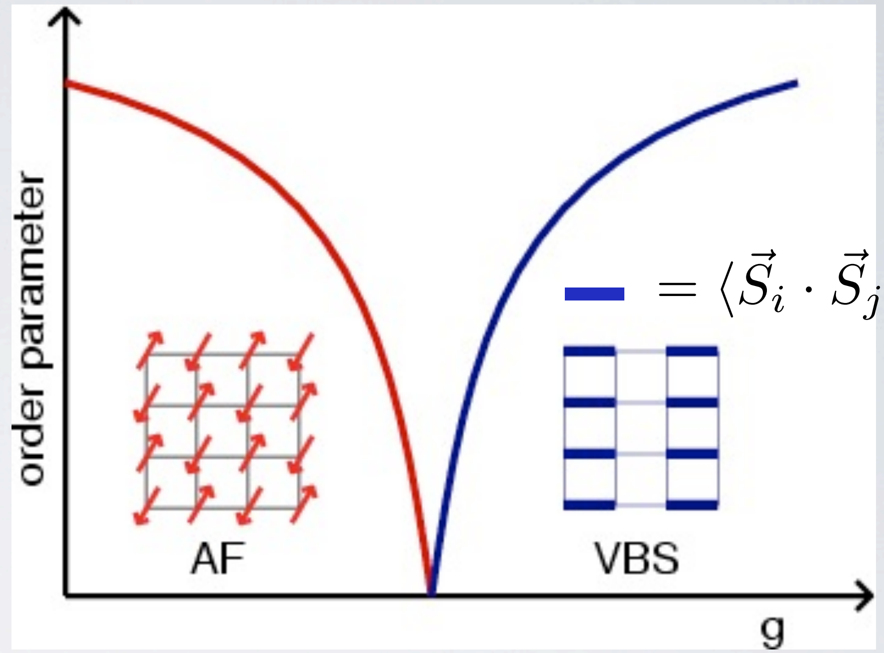
VBS states and deconfined quantum criticality

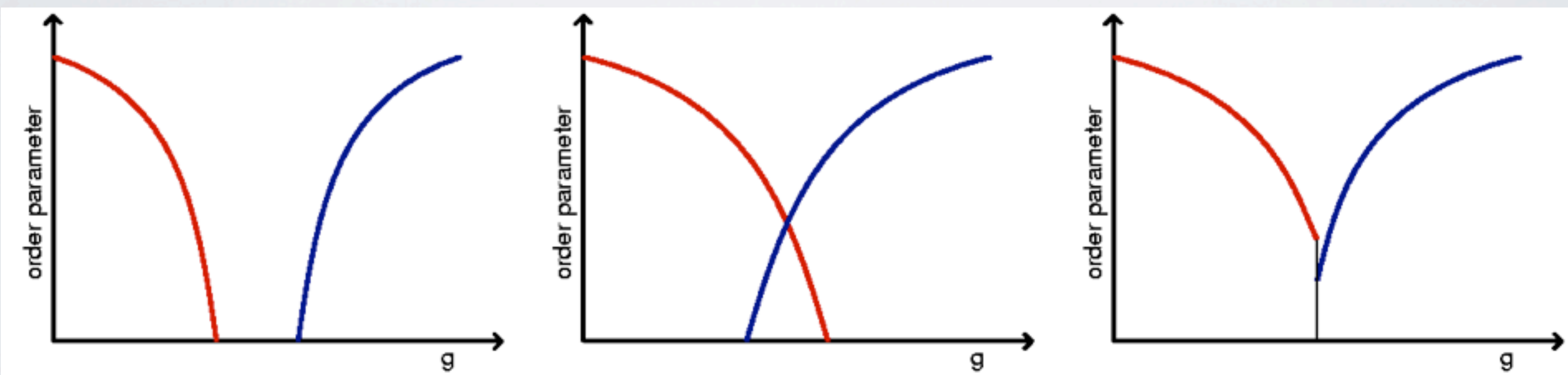
Senthil, Vishwanath, Balents, Sachdev, Fisher, Science 303, 1490 (2004)

$$\mathbf{H} = \mathbf{J} \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \mathbf{S_i} \cdot \mathbf{S_j} + \mathbf{g} \times \cdots$$

Neel-VBS transition in 2D

- generically continuous
- violating the “Landau rule” stating 1st-order transition
- field theory: non-compact CP^1
- large-N calculations for CP^{N-1}





Landau-Ginzburg paradigm:

direct transition between states breaking unrelated symmetries is 1st-order

- except at fine-tuned multi-critical points

Spinon confinement in a VBS state: standard picture

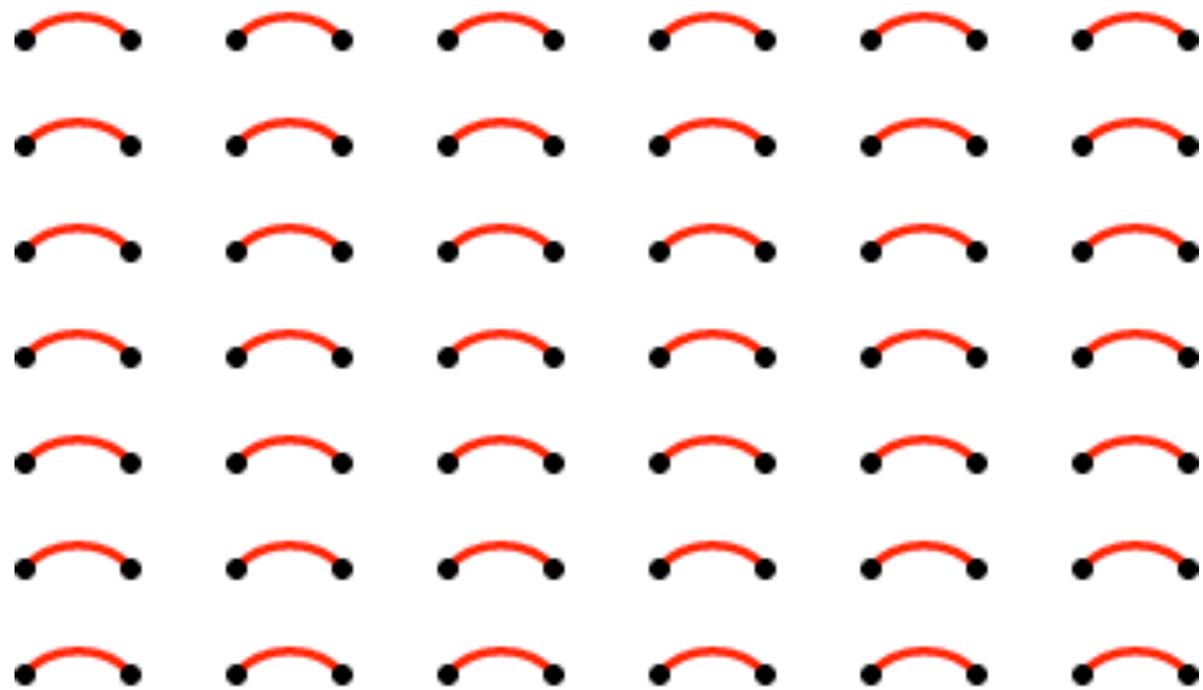
A spinon is an S=1/2 excitation

The VBS ground state is a singlet

An S=1 (“triplon”) excitation can be regarded as a bound state of two spinons

- confined spinons
- confinement due to “string” in VBS background

How is the confinement modified by VBS fluctuations?



What is the length-scale of confinement?

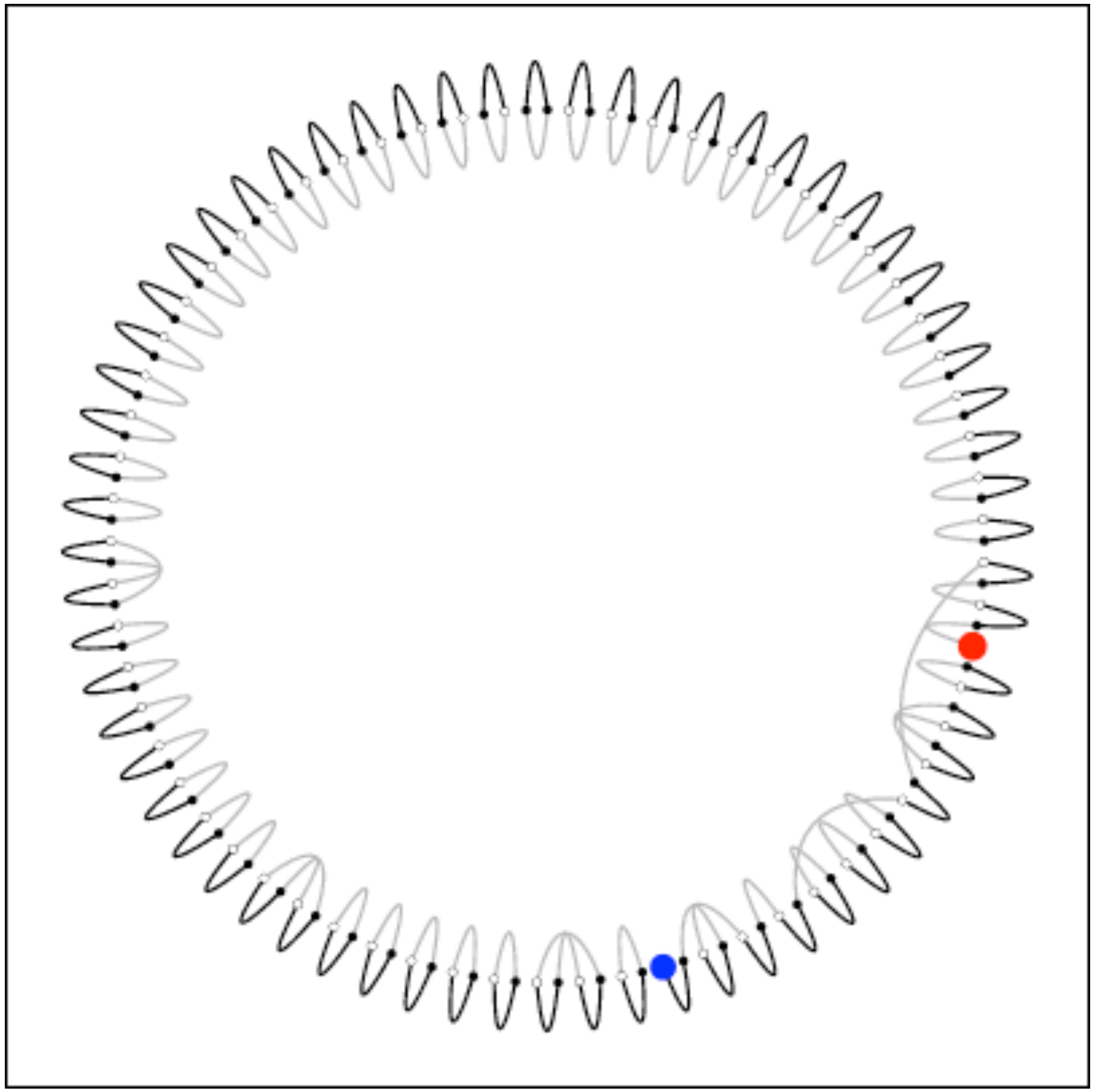
What are the actual VBS fluctuations like?

What happens at the VBS-Neel transition?

In what model can this be studied on large lattices with QMC?
- frustrated systems have sign problems
- **are there sign-problem free models with Neel-VBS transitions?**

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

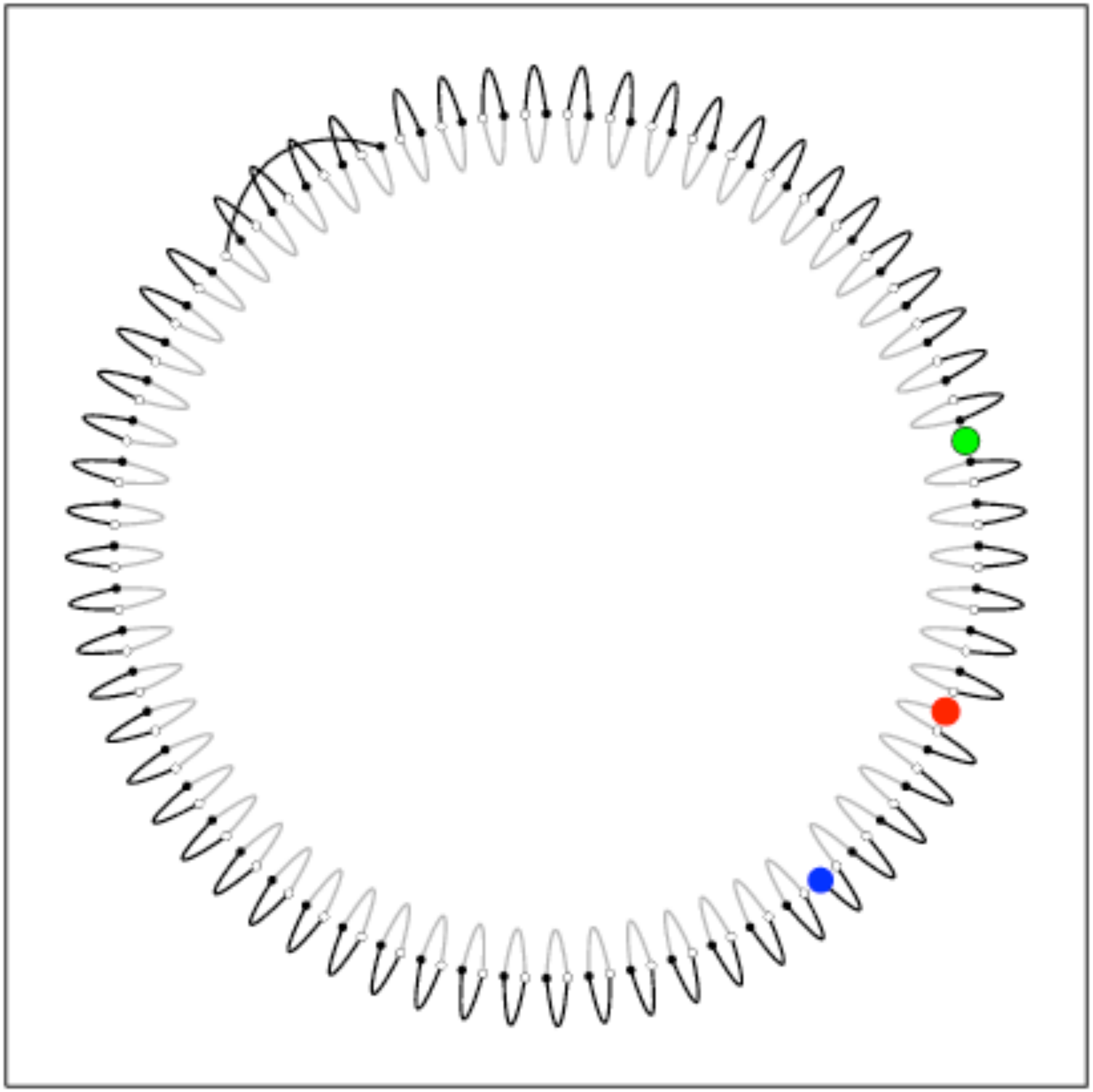
- one spin (spinon) doesn’t belong to any bond
- bra and ket spinons at different locations; non-orthogonality



Y. Tang and AWS, Phys. Rev. Lett. 107, 157201 (2011)

Two spinons in 1D VBS are deconfined (no confining potential)

- 2 separated (deconfined) sets of bra/ket spinons

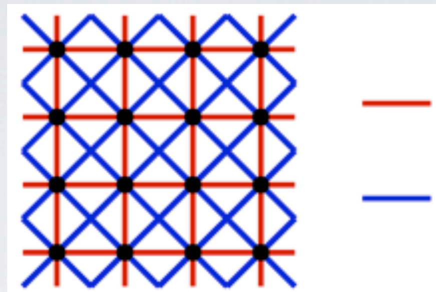


2D VBS states from frustrated interactions

Quantum phase transitions as some coupling (ratio) is varied (T=0)

- J_1-J_2 Heisenberg model is the prototypical example

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

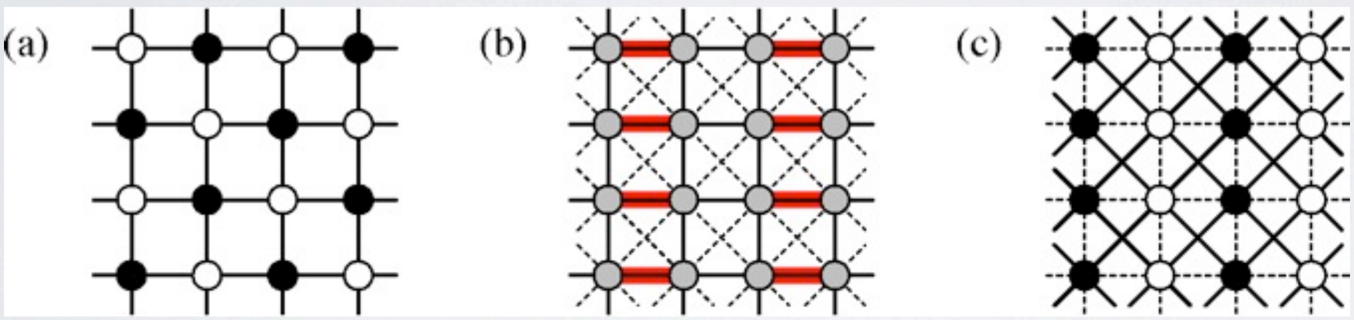


$= J_1$

$= J_2$

$$g = J_2/J_1$$

- Ground states for small and large g are well understood
  - Standard **Néel order up to g≈0.45; collinear magnetic order for g>0.6**



$0 \leq g < 0.45$ $\quad$ $0.45 \leq g < 0.6$ $\quad$ $g > 0.6$

- A non-magnetic state exists between the magnetic phases
  - Most likely a columnar VBS
  - Some calculations (interpretations) suggest RVB spin liquid
- 2D and 3D frustrated models are challenging
  - no generally applicable unbiased methods (numerical or analytical)
  - QMC sign problem

VBS states from multi-spin interactions

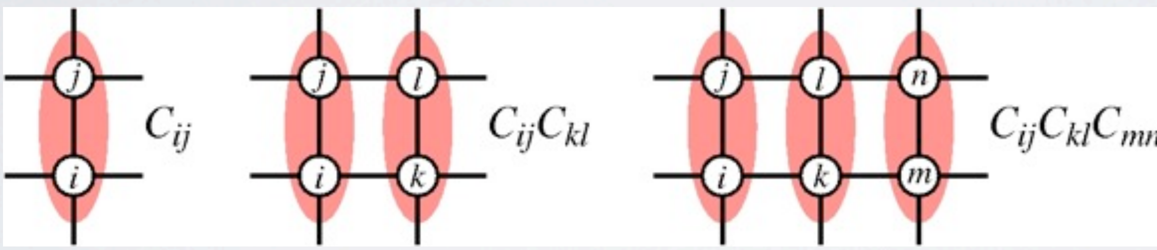
Sandvik, Phys. Rev. Lett. 98, 227202 (2007)

The Heisenberg interaction is equivalent to a singlet-projector

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

$$C_{ij}|\phi^s_{ij}\rangle = |\phi^s_{ij}\rangle, \qquad C_{ij}|\phi^{tm}_{ij}\rangle = 0 \quad (m = -1, 0, 1)$$

- we can construct models with products of singlet projectors
- no frustration in the conventional sense (QMC can be used)
- correlated singlet projection reduces the antiferromagnetic order



+ all translations and rotations

The "J-Q" model with two projectors is

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

- Has Néel-VBS transition, appears to be continuous
- Not a realistic microscopic model for materials
- Intended to study Néel-VBS transition (universal physics)

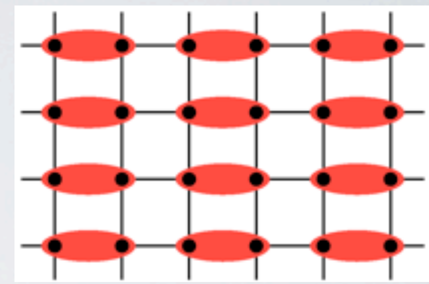
Néel-VBS transition in the J-Q model

T=0 projector QMC results (no approximations; finite size)

Sandvik, PRL 2007; Lou, Sandvik, Kawashima, PRB (2009)

VBS vector order parameter (D_x,D_y) (x and y lattice orientations)

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



Néel order parameter (staggered magnetization)

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

No symmetry-breaking in simulations; study the squares

$$M^2 = \langle \vec{M}\cdot\vec{M}\rangle, \qquad D^2 = \langle D_x^2 + D_y^2\rangle$$

Finite-size scaling: a critical squared order parameter (A) scales as

$$A(L,q) = L^{-(1+\eta)}f[(q-q_c)L^{1/\nu}]$$

coupling ratio

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

Data "collapse" for different system sizes L of $AL^{1+\eta}$ graphed vs $(q-q_c)L^{1/\nu}$

J-Q_2 model; q_c=0.961(1)

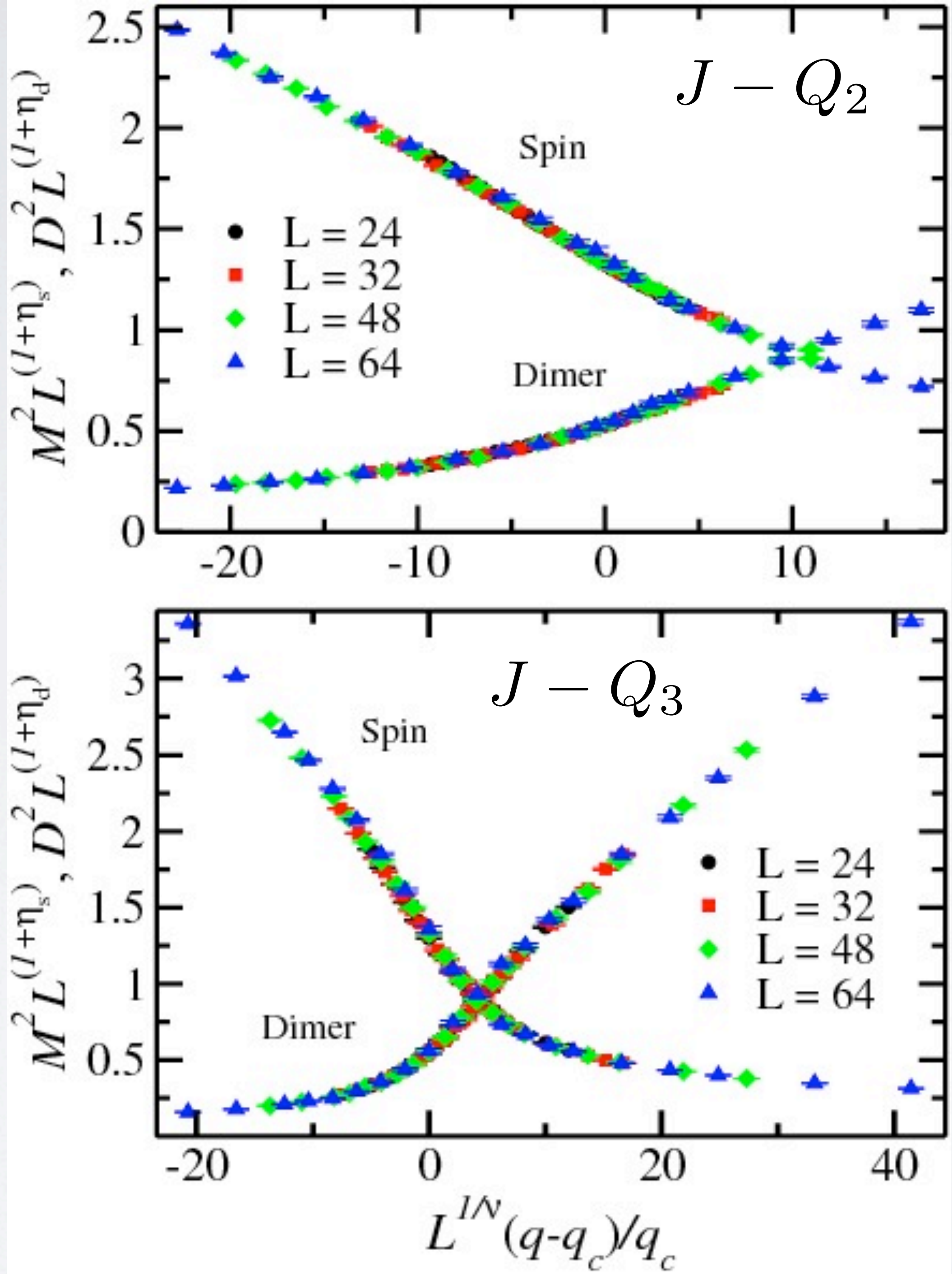
$$\eta_s = 0.35(2)$$
$$\eta_d = 0.20(2)$$
$$\nu = 0.67(1)$$

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)

η_s “large” in agreement with theory



Making connections with field theory results

The non-compact CP^{N-1} model has been studied for large N

- large-N expansion, SU(N) symmetry (N+1 components)

Senthil et al. (2004), Kaul & Sachv (2009)

$$\eta_s = 1 - \frac{32}{\pi^2 N} + \ldots$$

- older results, using relationship between monopoles in the field theory and the VBS order parameter Read & Sachdev (1989)

$$\eta_d = 0.2492 \times N - 1 + \ldots$$

How can we test these results?

QMC studies of spin hamiltonians with SU(N) spins

2D SU(N) Heisenberg model [Harada, Kawashima, Troyer (2003)]

- Fundamental and conjugate repr. of SU(N) on A,B sublattices
- No sign problem in QMC
- Same repr. used in large-N calculations
- Neel ground state for N<5, VBS for N=5,6,...

J-Q models with SU(N) spins

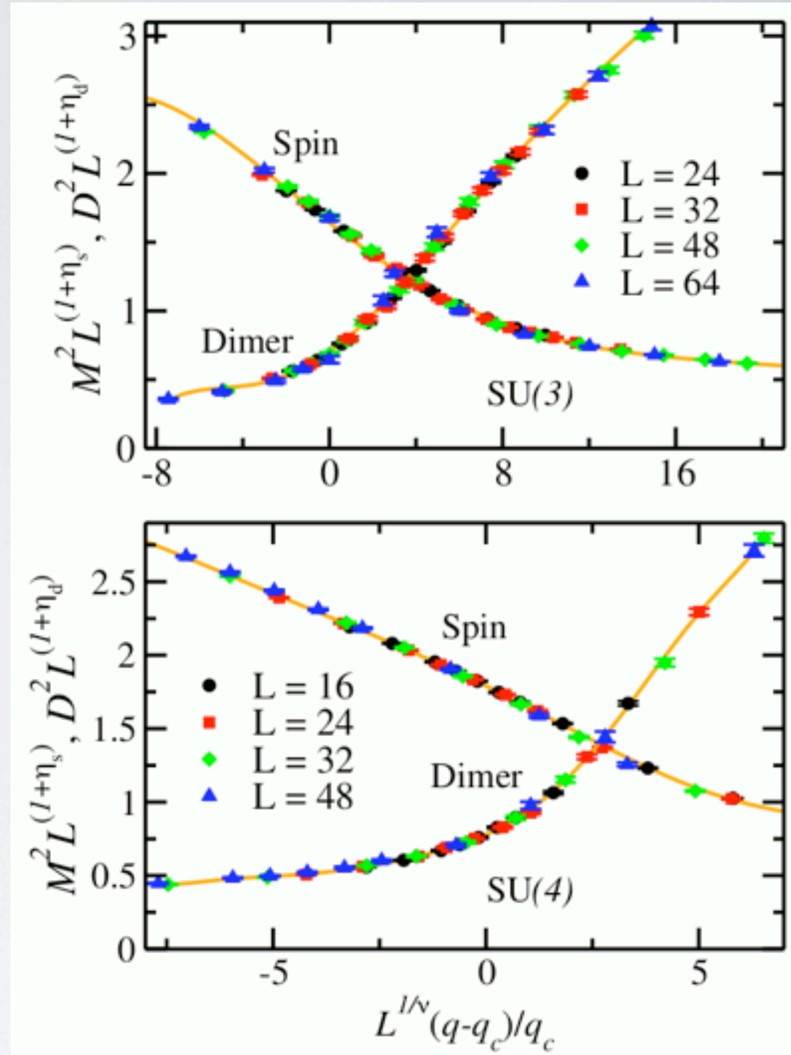
Lou, Sandvik, Kawashima, PRB (2009)

Heisenberg model (Q=0) has Neel ground state for N=2,3,4 ⇒

Neel - VBS transition vs Q/J

Model, symmetry	η_s	η_d	ν
J-Q_2, SU(2)	0.35(2)	0.20(2)	0.67(1)
J-Q_3, SU(2)	0.33(2)	0.20(2)	0.69(2)
J-Q_2, SU(3)	0.38(3)	0.42(3)	0.65(3)
J-Q_2, SU(4)	0.42(5)	0.64(5)	0.70(2)

How can we reach larger N to really study the large-N limit?



$$\eta_s = 1 - \frac{32}{\pi^2 N} + \ldots$$

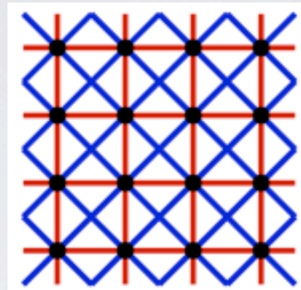
$$\eta_d = 0.2492 \times N - 1 + \ldots$$

J_1-J_2 Heisenberg model with SU(N) spins

Kaul & Sandvik (2011)

Ferromagnetic 2nd-neighbor couplings enhance Neel order

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



— $= J_1 > 0$

— $= J_2 < 0$

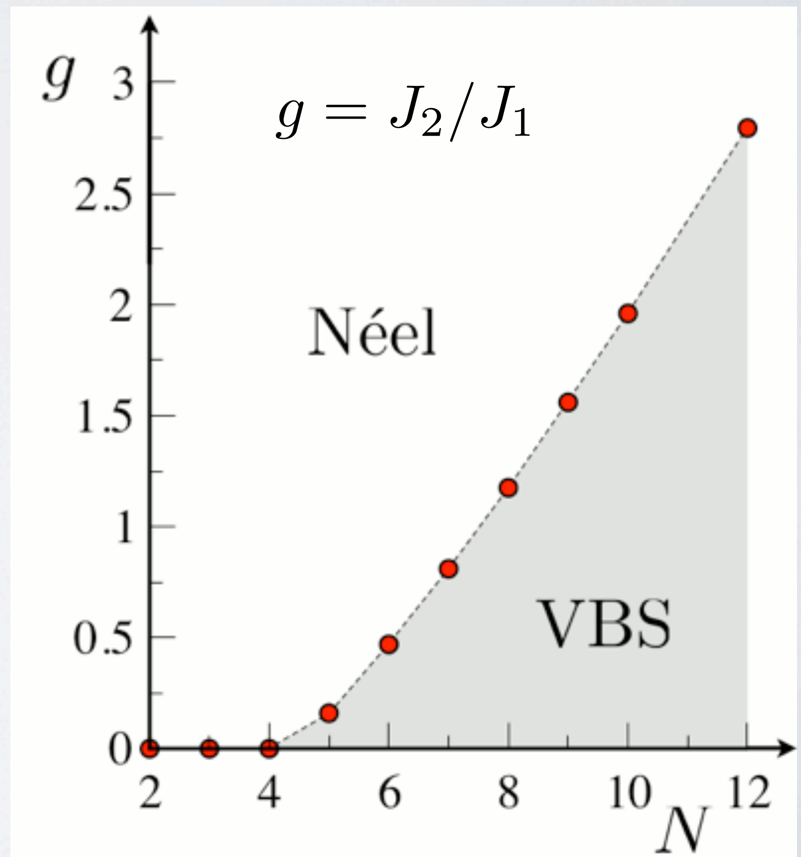
SU(N) generalization:

$$H = -\frac{J_1}{N} \sum_{\langle ij \rangle} P_{ij} - \frac{J_2}{N} \sum_{\langle\langle ij \rangle\rangle} \Pi_{ij}$$

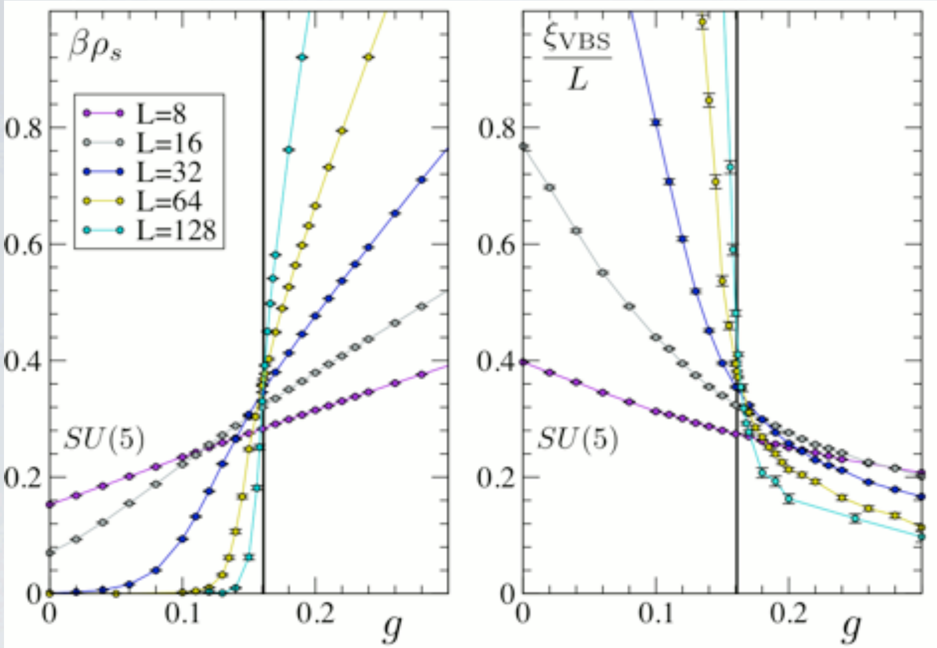
P_{ij} = SU(N) singlet projector
Π_{ij} = permutation operator

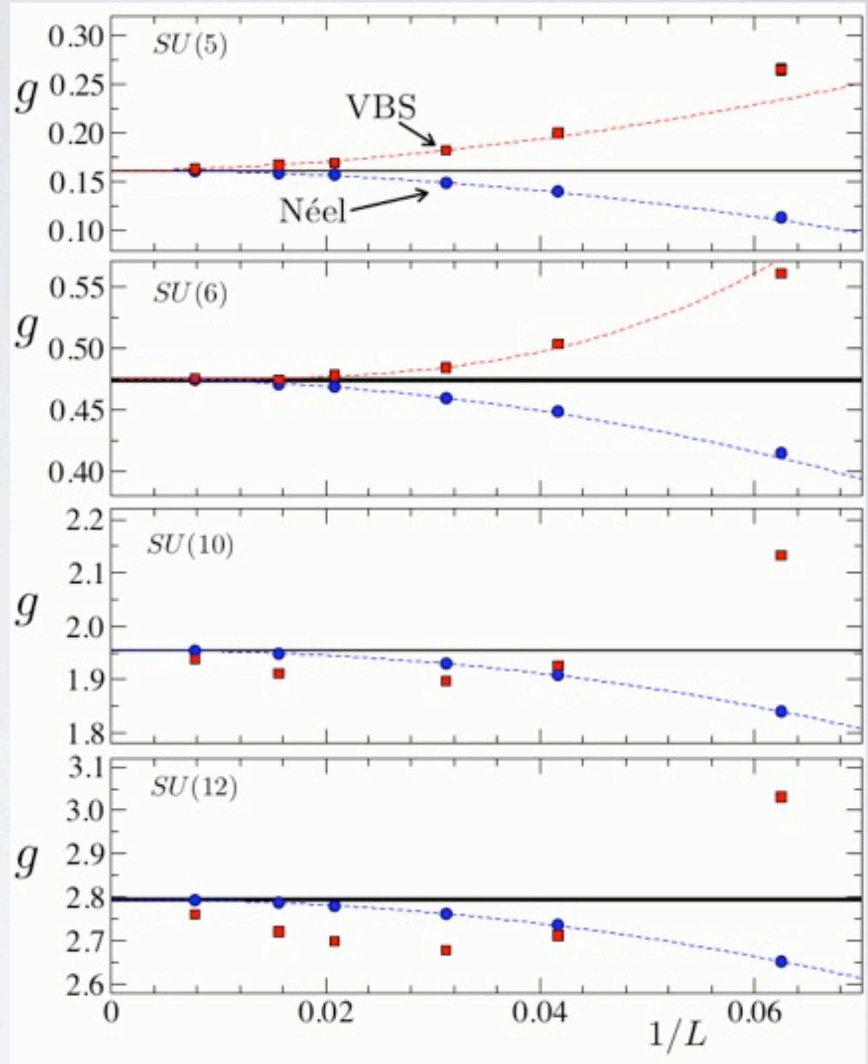
There is Neel order for all N>4

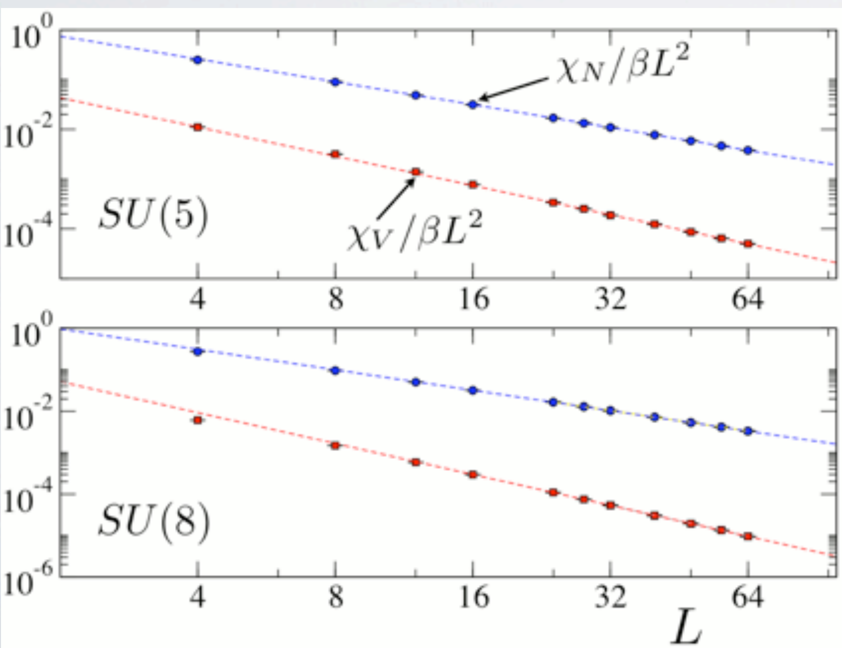
- Neel - VBS transition accessible with QMC for large N



J_1-J_2 SU(N): critical points from curve crossings (T=1/L)

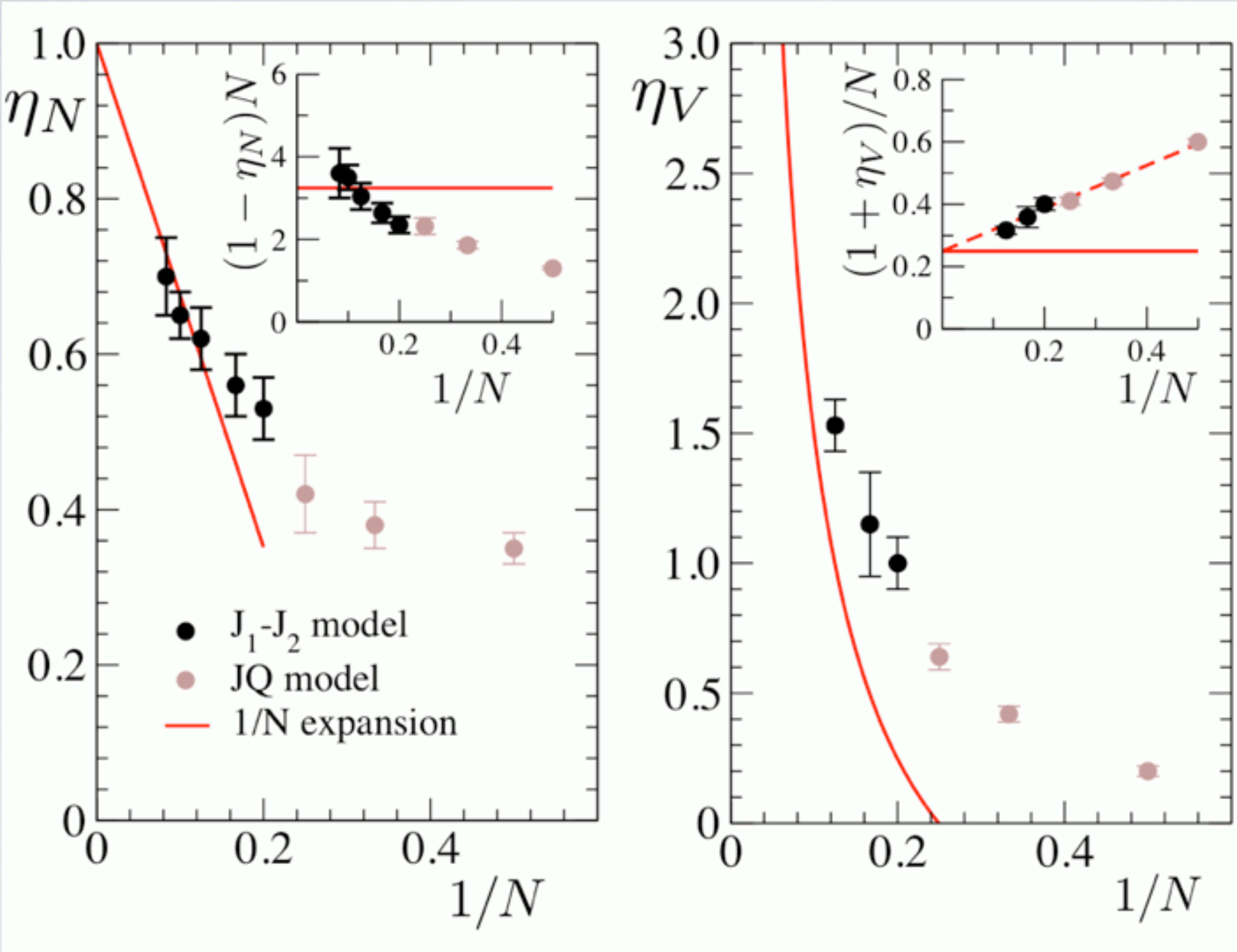






← critical correlation exponents from susceptibilities at g_c

Comparing results: J_1-J_2, J-Q, $NCCP^{N-1}$



Conclusion: Trends for large N show excellent agreement

- QMC results predict size of the next 1/N corrections

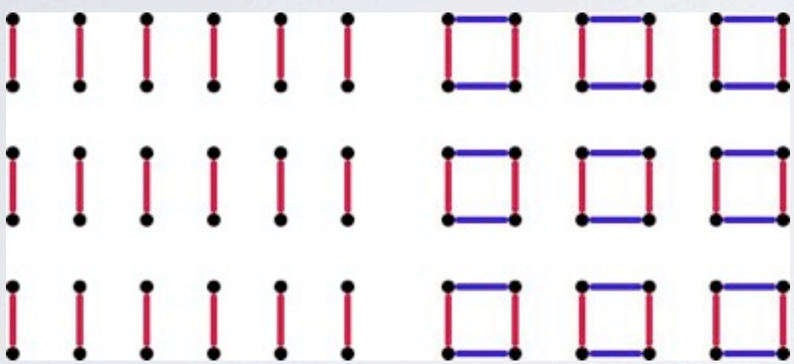
Nature of the VBS fluctuations in the J-Q model - SU(2)

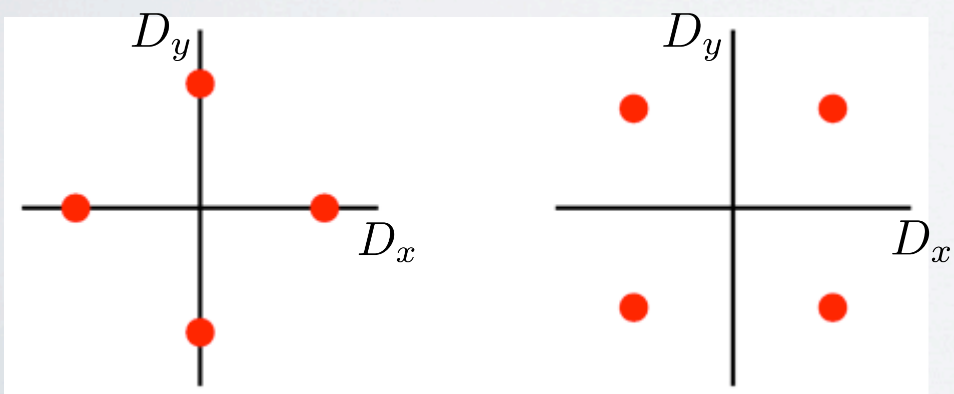
Joint probability distribution **$P(D_x,D_y)$** of x and y VBS order

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

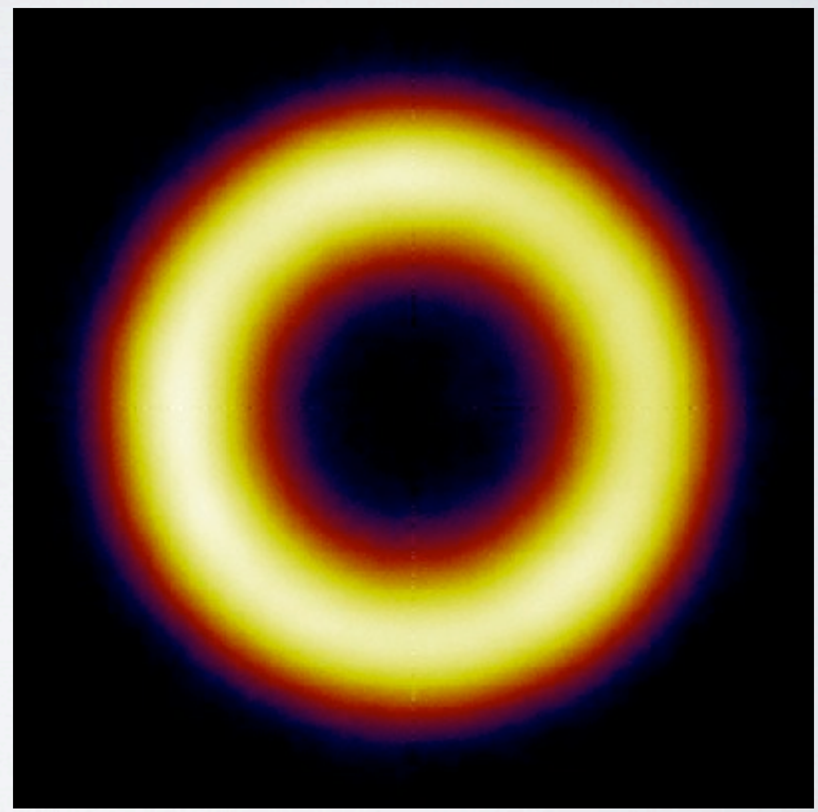
The squared order parameter cannot distinguish between:

columnar plaquette





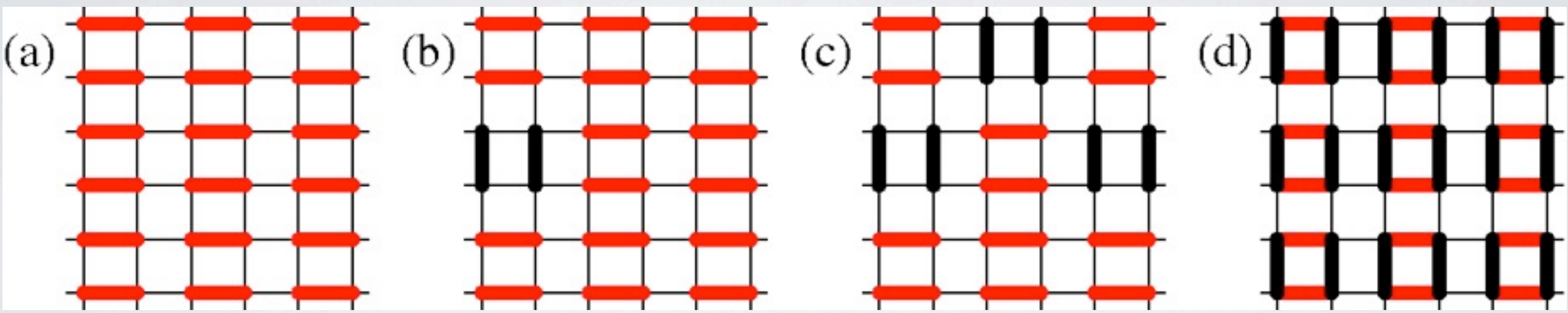
J-Q_2 model, J=0, L=128



Magnitude of D has formed but the VBS “angle” is fluctuating

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

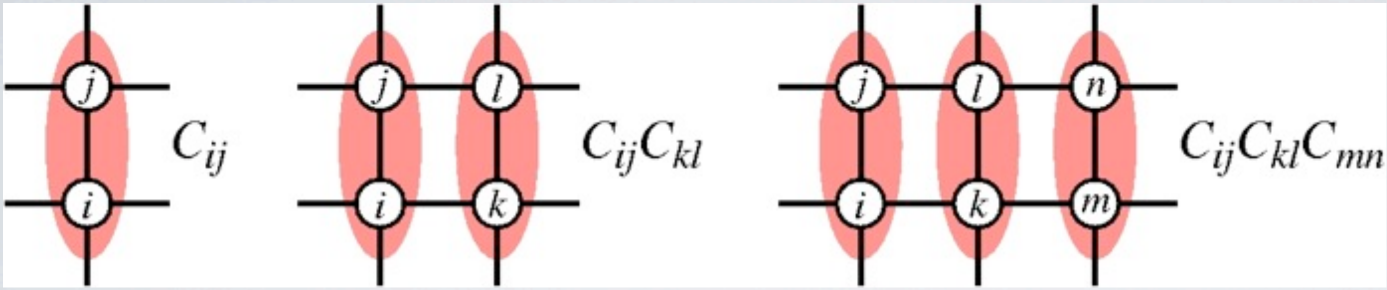


➢ **emergent U(1) symmetry**
➢ **ring-shaped distribution expected in the VBS phase for small systems**

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

Creating a more rubust VBS order - the J-Q$_3$ model

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



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

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

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

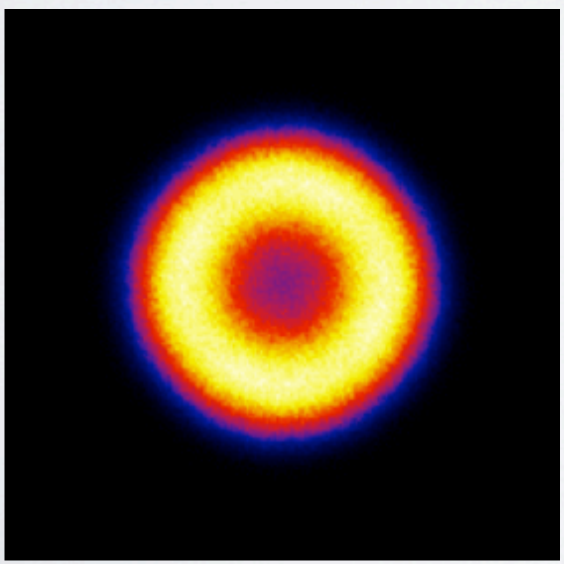
This model has a more robust VBS phase

- can the symmetry cross-over be detected?

$q = 0.635$

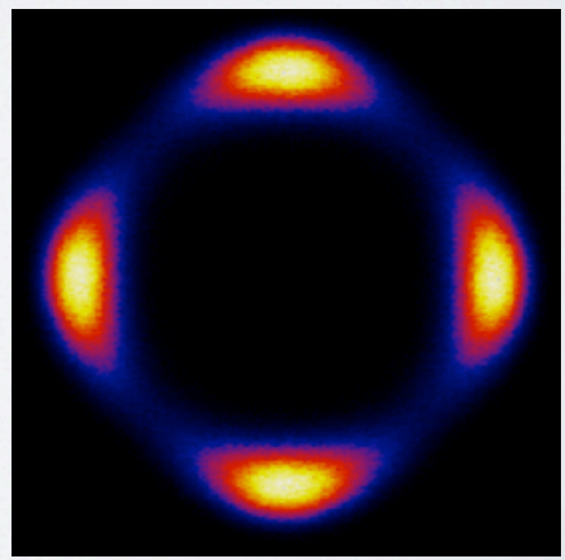
$(q_c \approx 0.60)$

$L = 32$



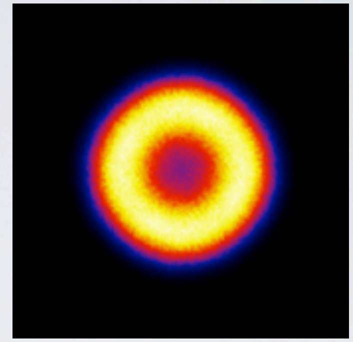
$q = 0.85$

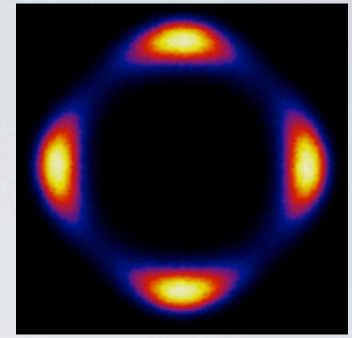
$L = 32$



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

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

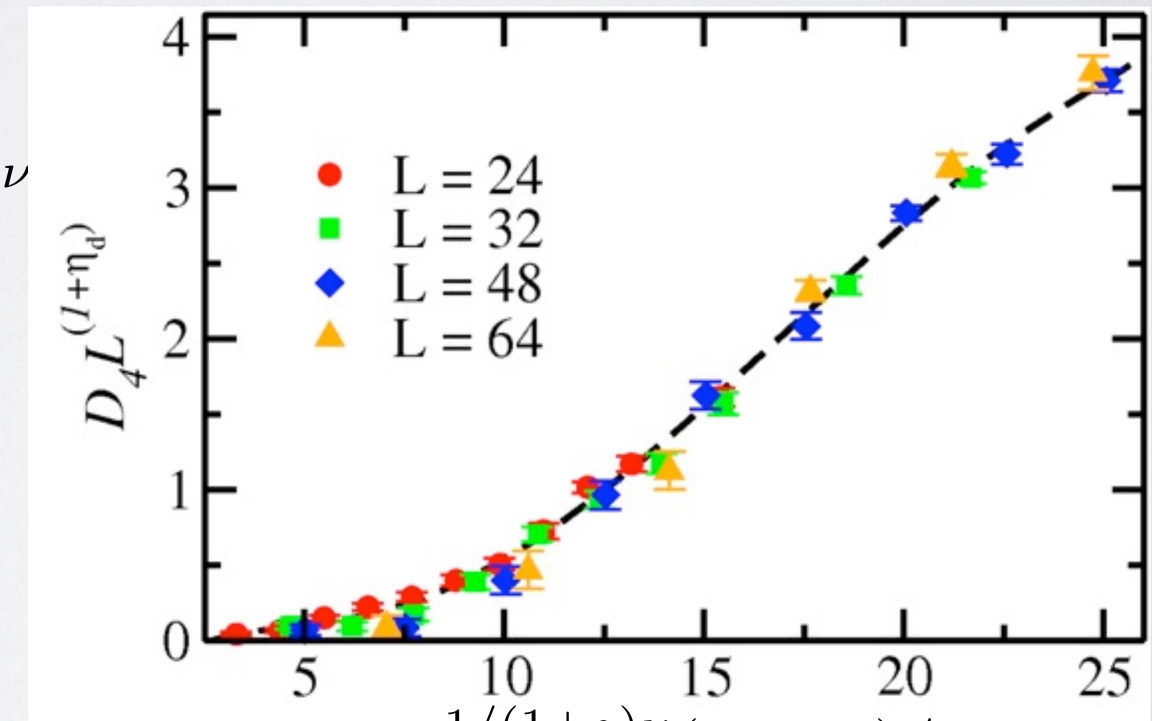
Finite-size scaling gives U(1) (deconfinement) length-scale

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

$a = 0.20 \pm 0.05$

$SU(3): a = 0.6 \pm 0.2$

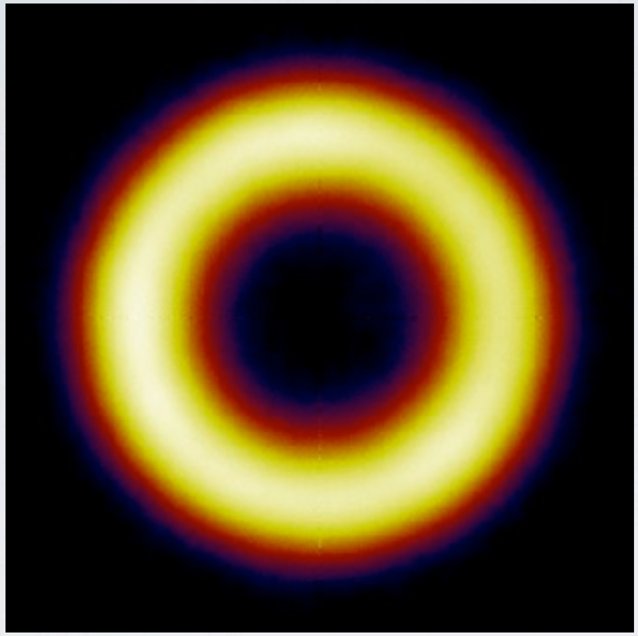
$SU(4): a = 0.5 \pm 0.2$

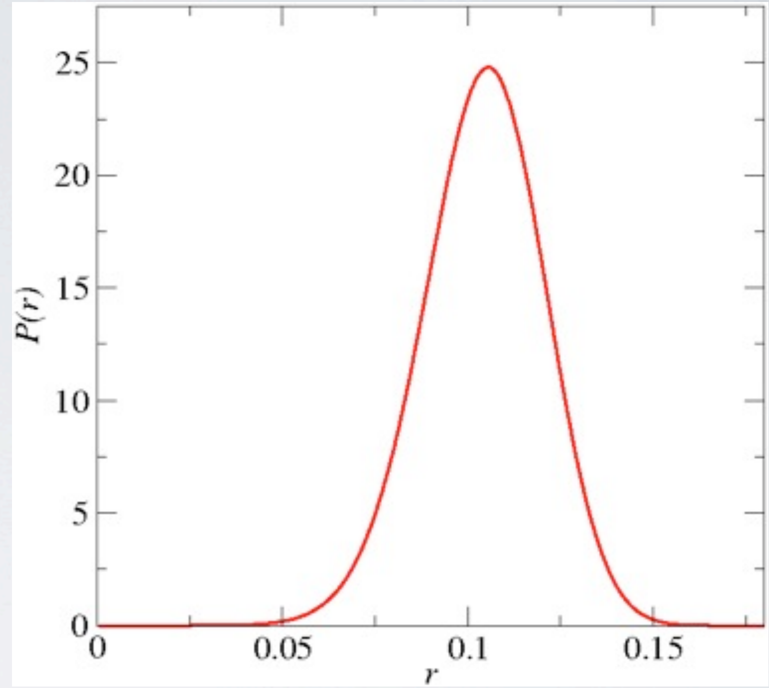


$L^{1/(1+a)\nu}(q-q_c)/q_c$

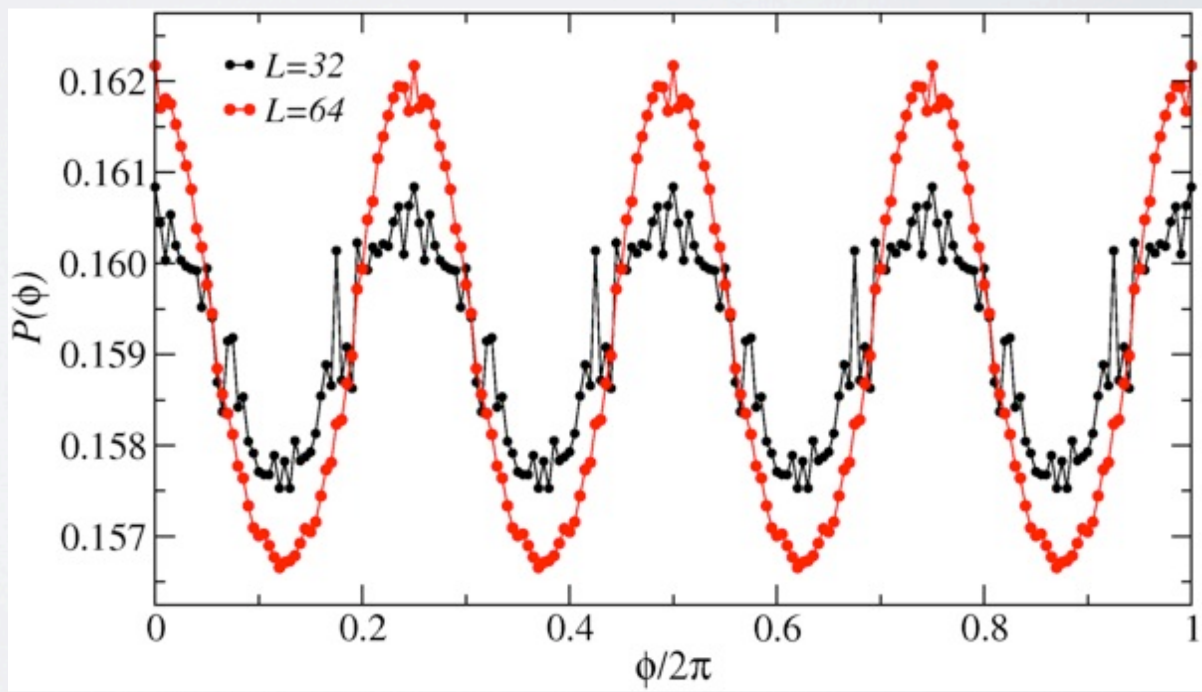
Signs of Z_4 symmetry in the original J-Q model?

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



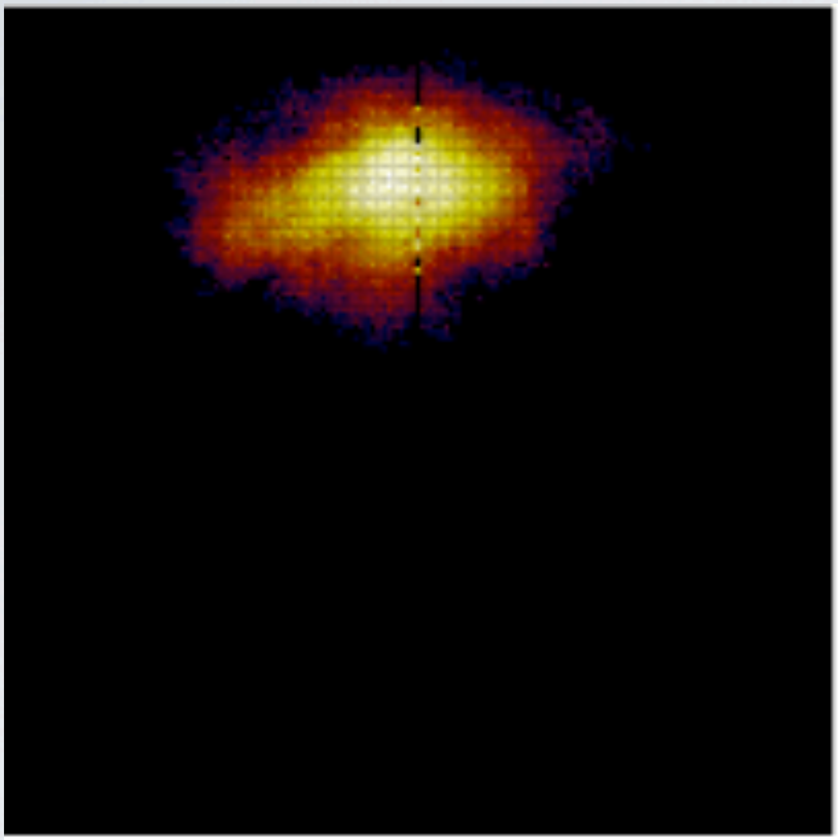


L=32, L=64; J=0
Weak but statistically significant angular dependence consistent with **columnar VBS** (L=128 still too noisy)

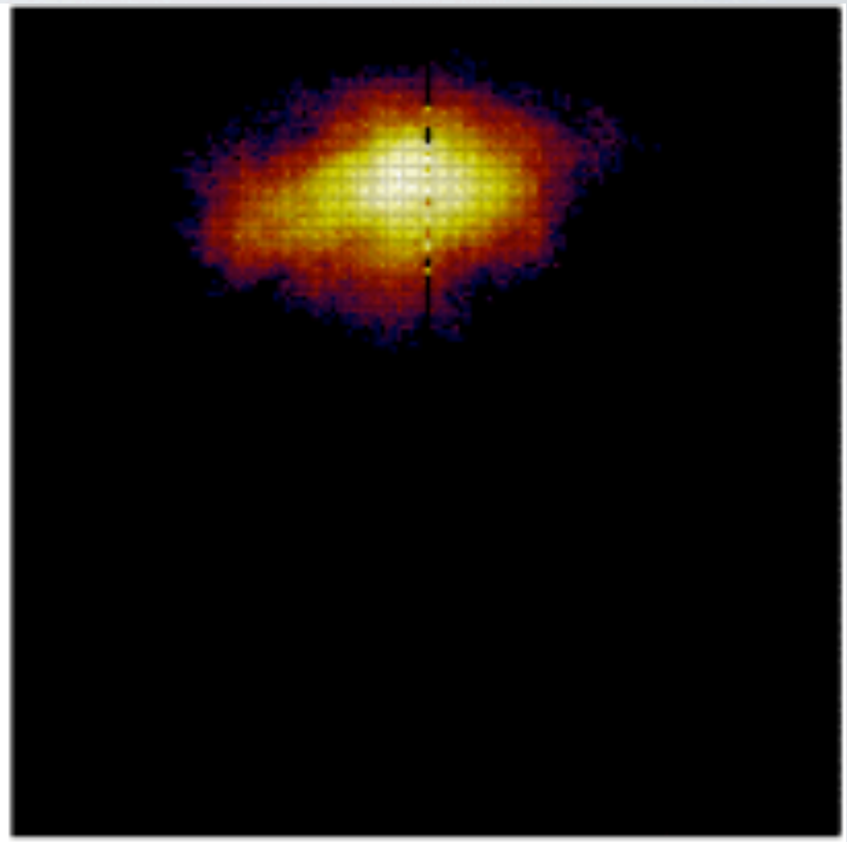


The simulations take a long time to rotate the VBS angle

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



building 100×10^5 measurements



10^5 measurements

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)

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

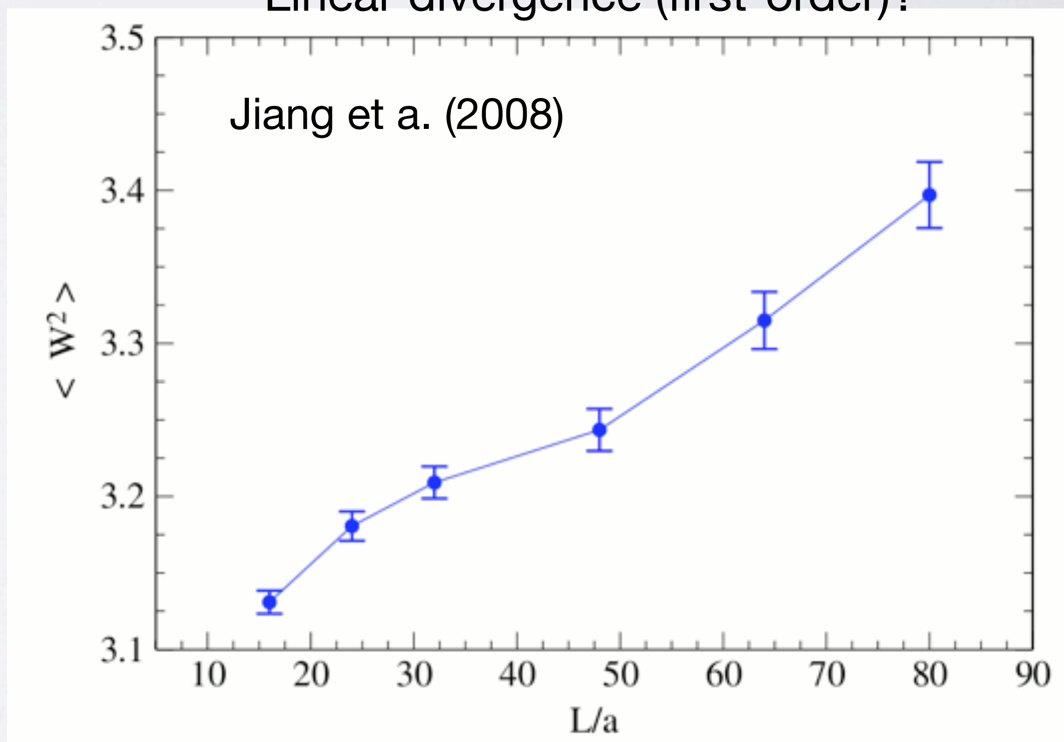
At at a critical point

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

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

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

Linear divergence (first-order)?



Recent large-scale QMC results

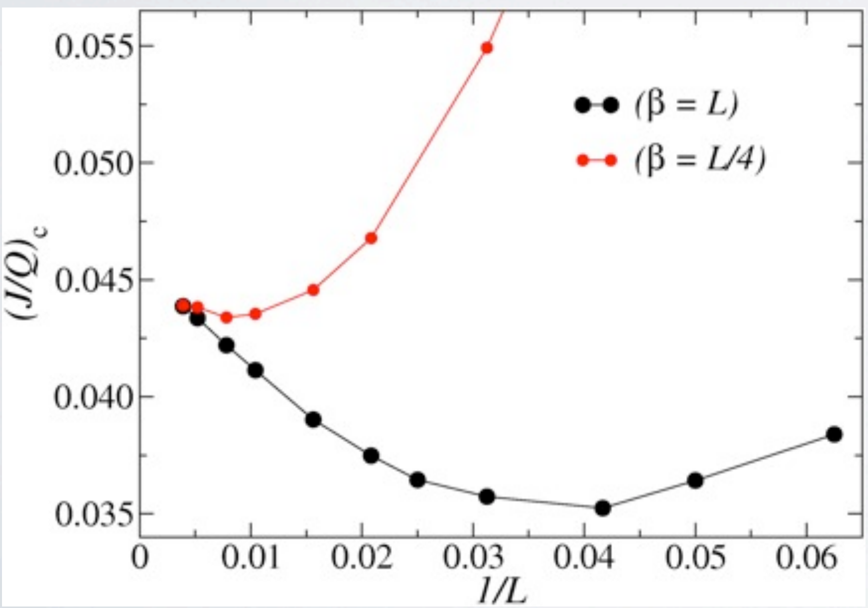
Sandvik, PRL 104, 177201 (2010)

- Stochastic series expansion
- up to 256×256 lattices

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

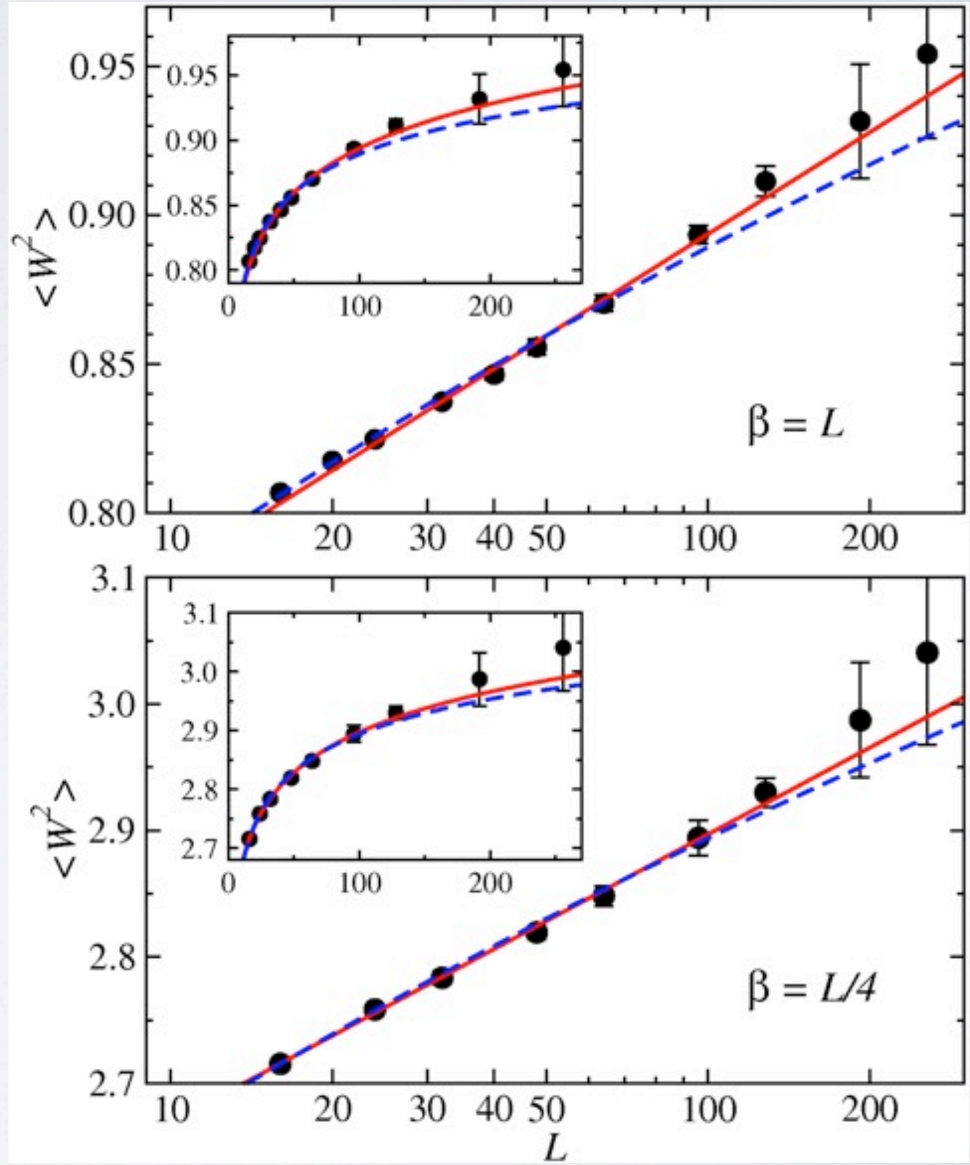
Same finite-size definition of critical point as used by Kuklov et al. and Jiang et al.

- 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

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

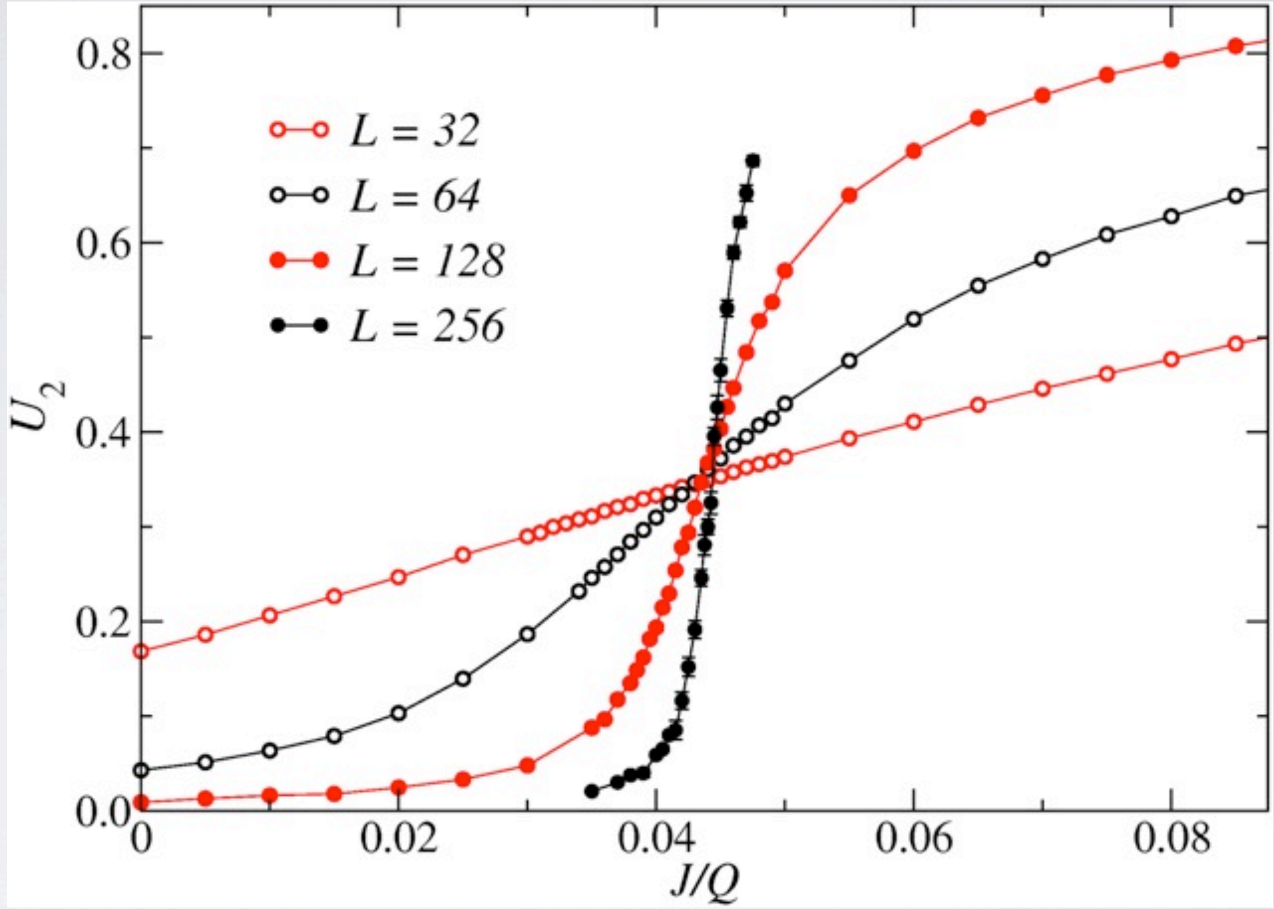
Binder cumulant

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

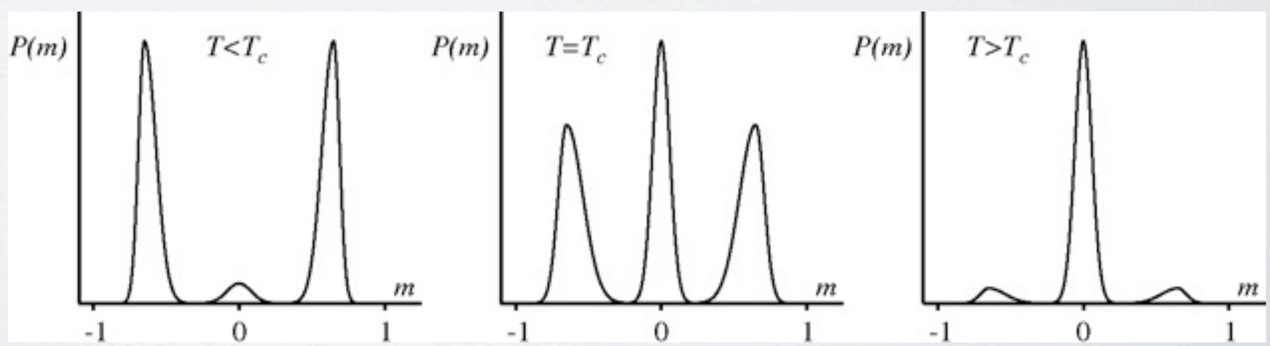
Size independent (curve crossings) at criticality

$U_2 < 0$ at a first-order transition

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



Example: Scalar order parameter at classical transition



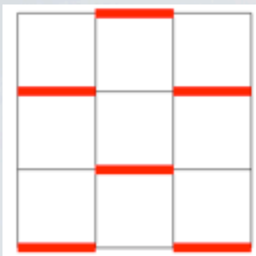
Phase coexistence leads to $U_2 \to -\infty$ at 1st-order trans

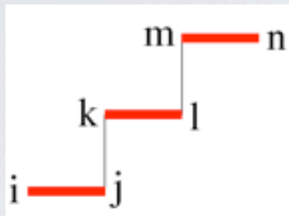
Example of a first-order Néel - VBS transition

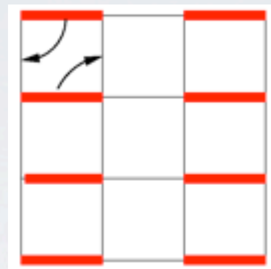
J-Q model with staggered VBS phase [A. Sen, A. Sandvik, PRB (2010)]

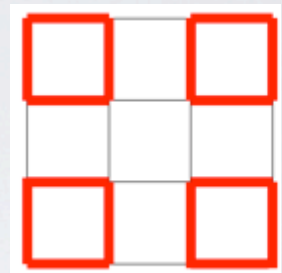
- no local VBS fluctuations favoring emergent U(1) symmetry

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



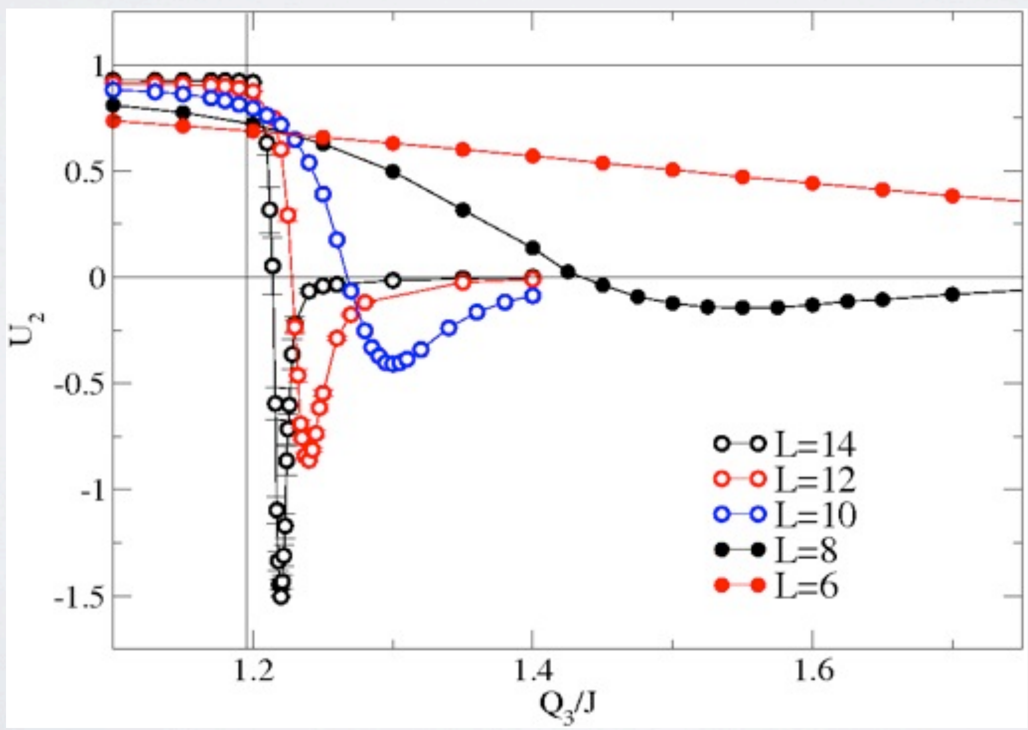




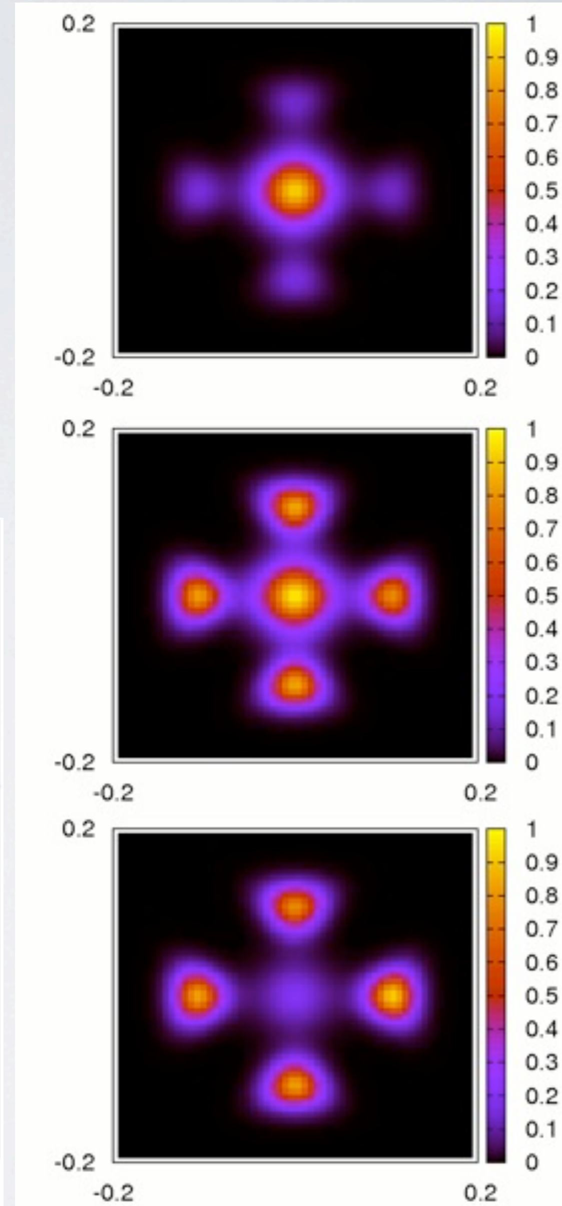


- clear signs of phase coexistence

Binder cumulant of the Neel order



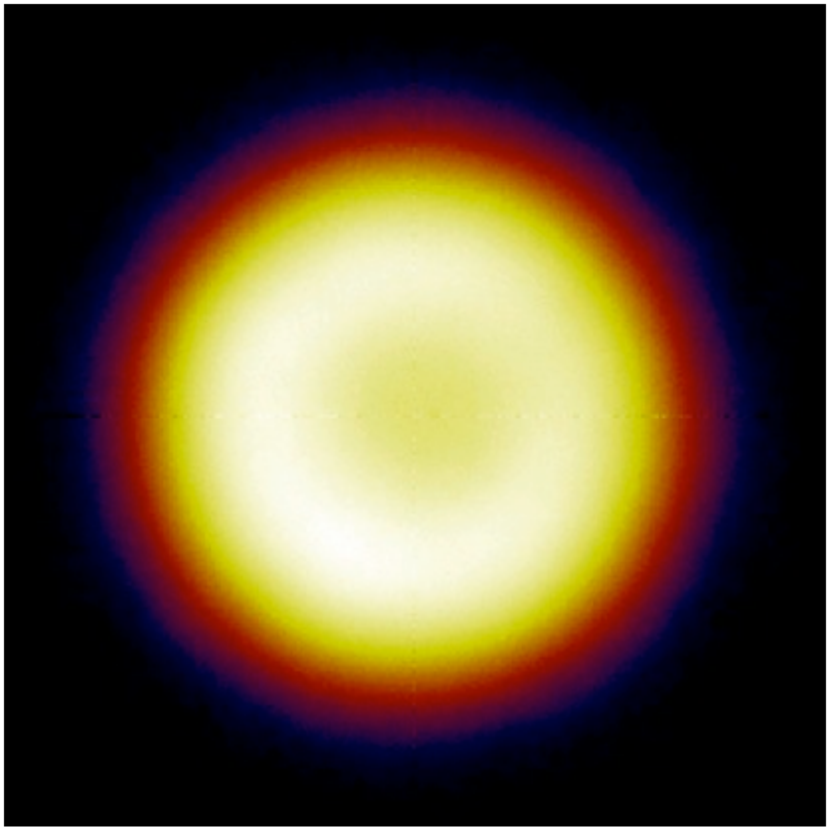
VBS

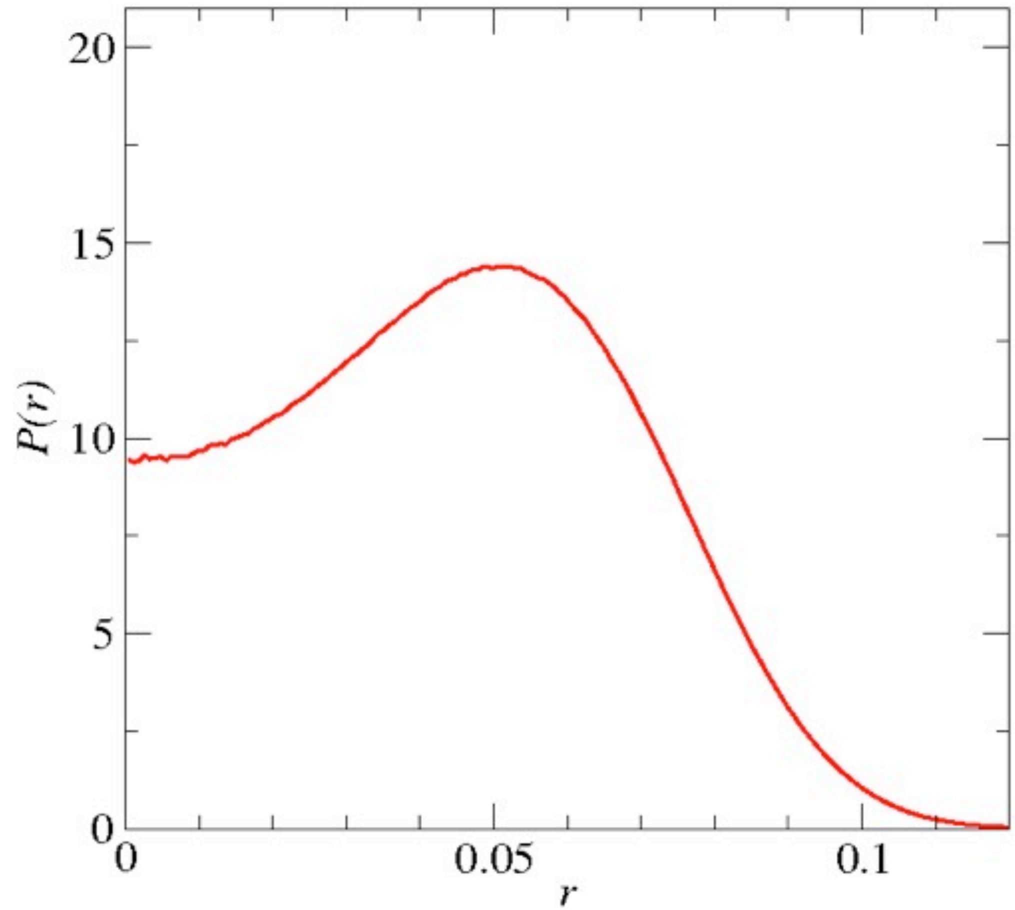


Any signs of coexistence in the standard J-Q VBS distributions?

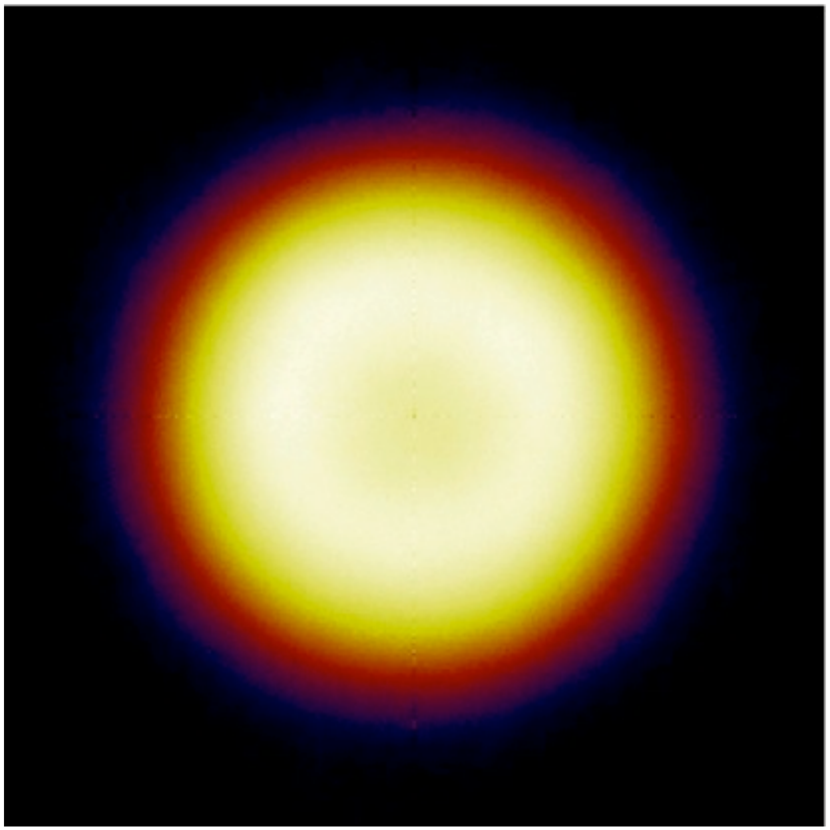
- L=128 data close to the transition

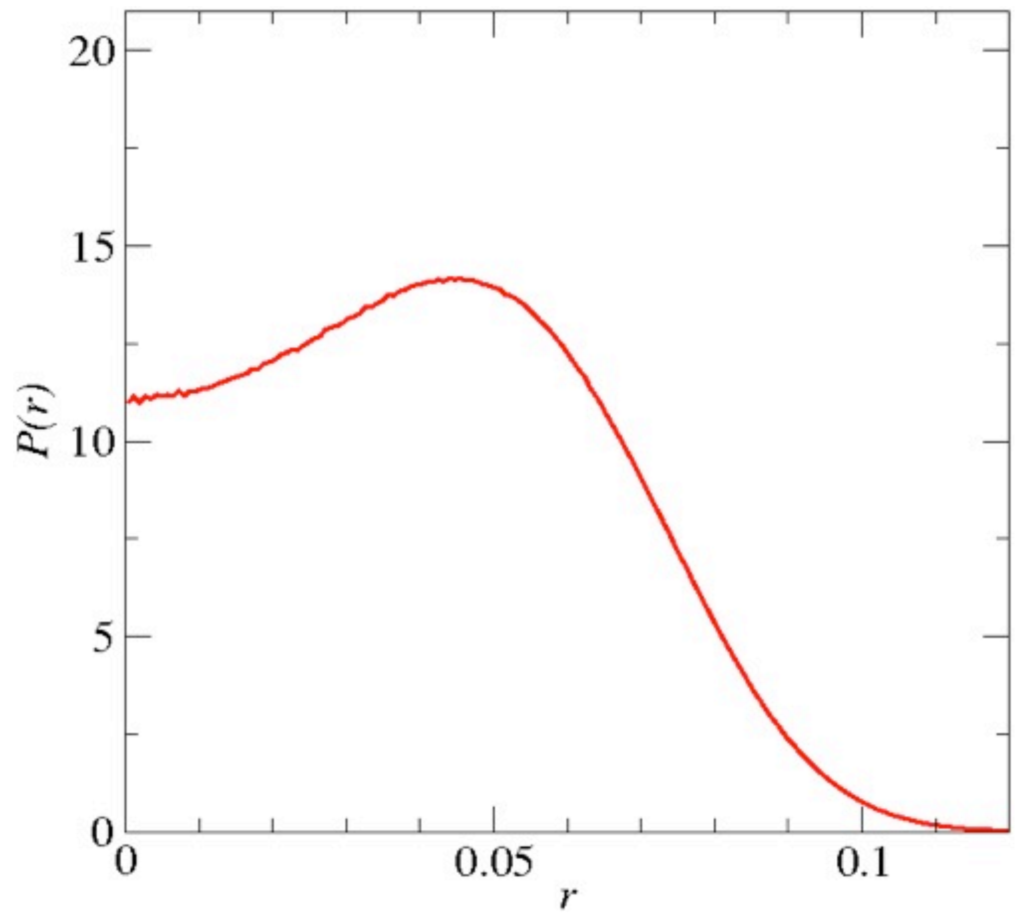
J/Q=0.040



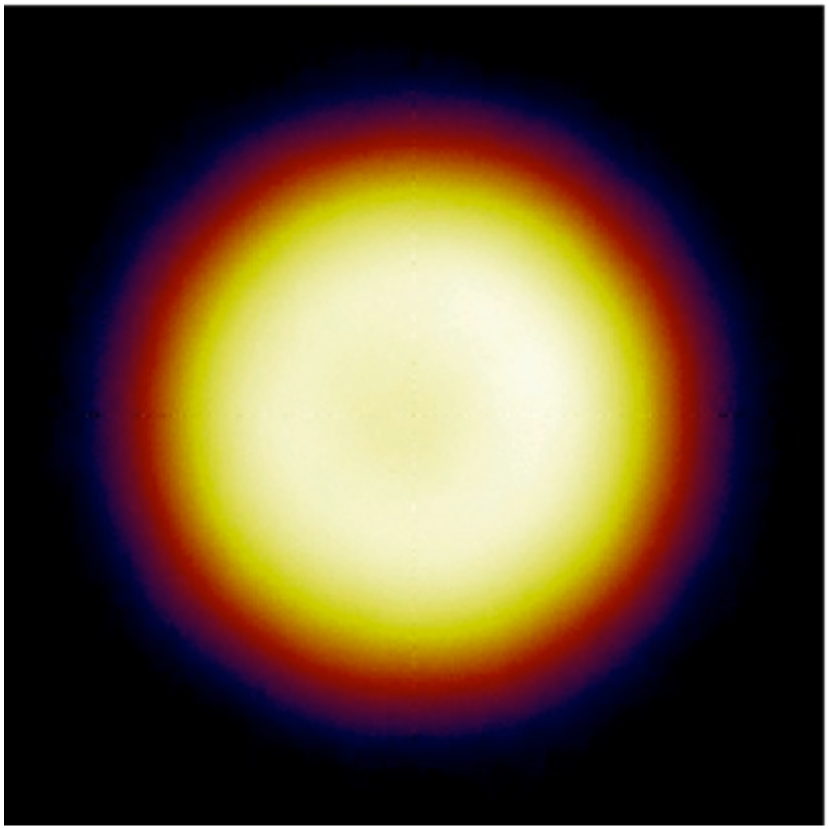


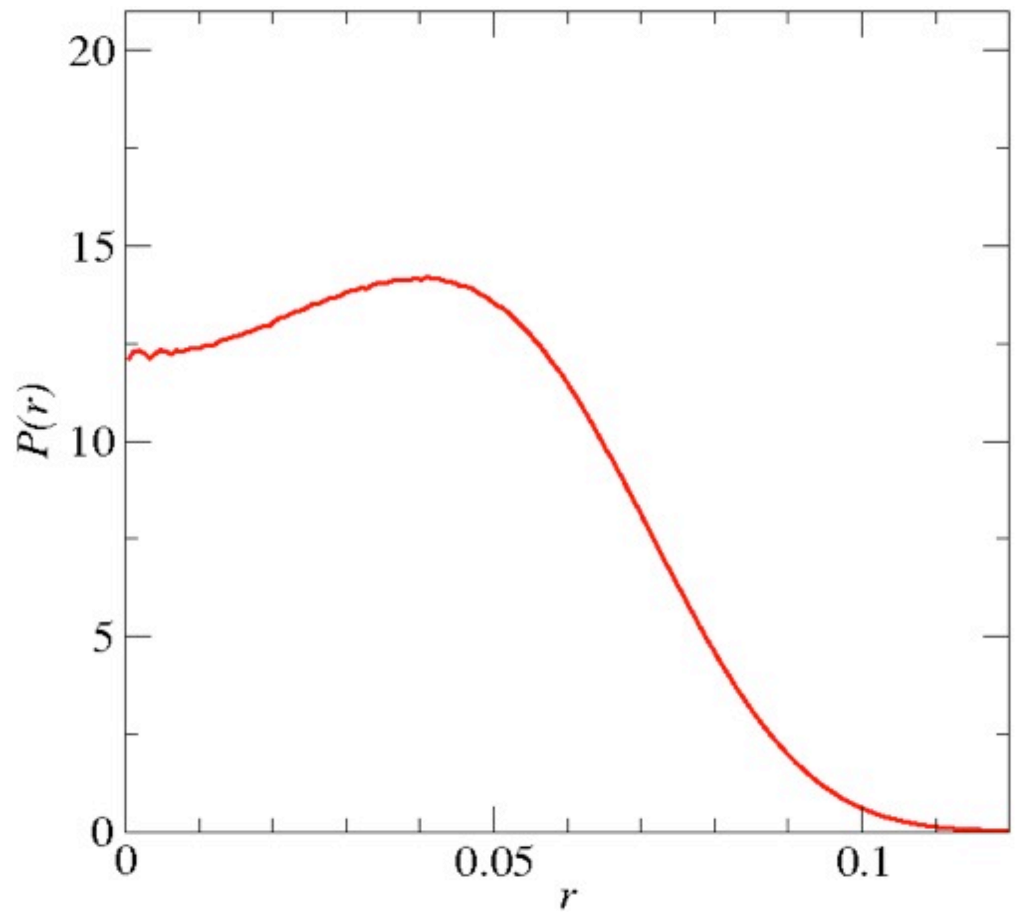
J/Q=0.041



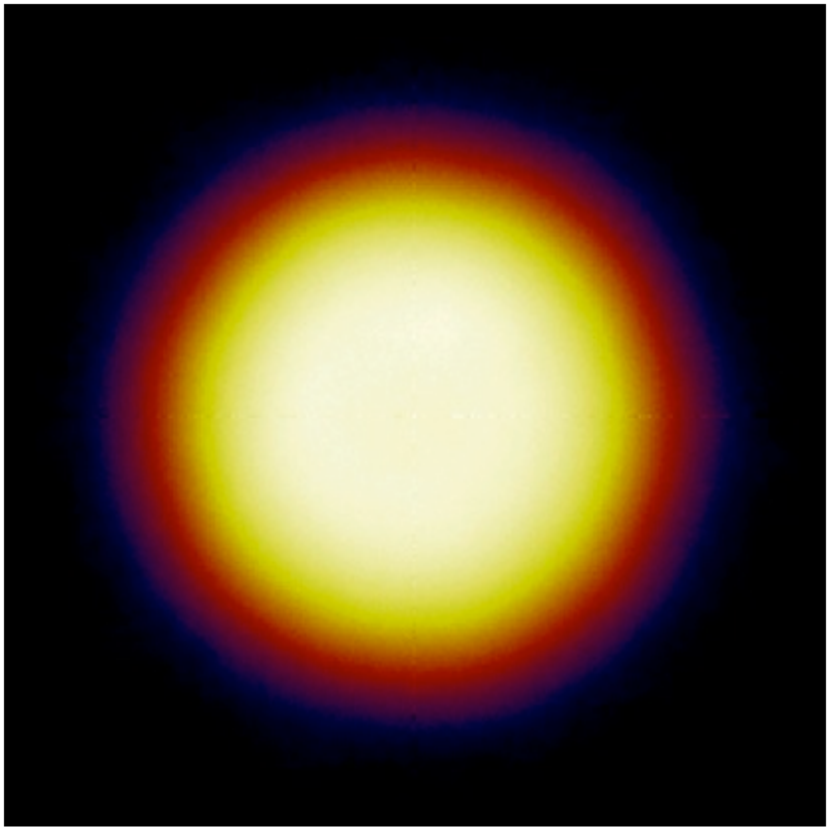


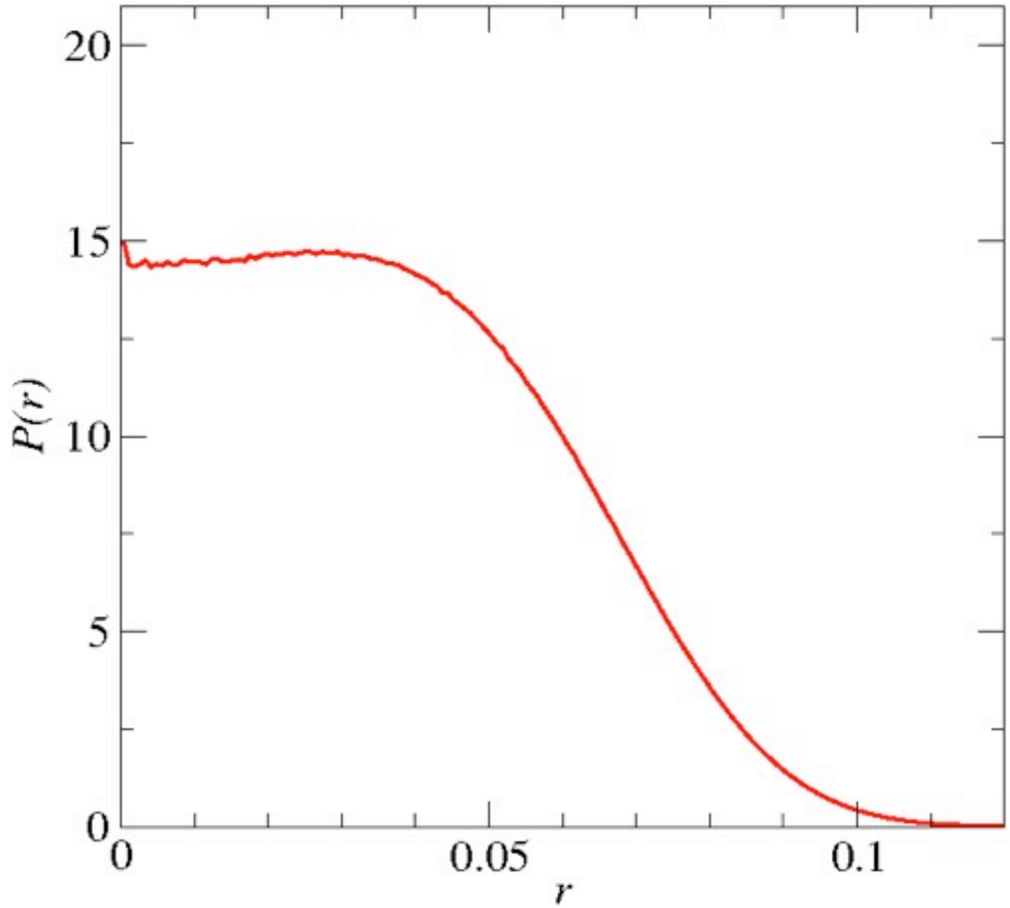
J/Q=0.042



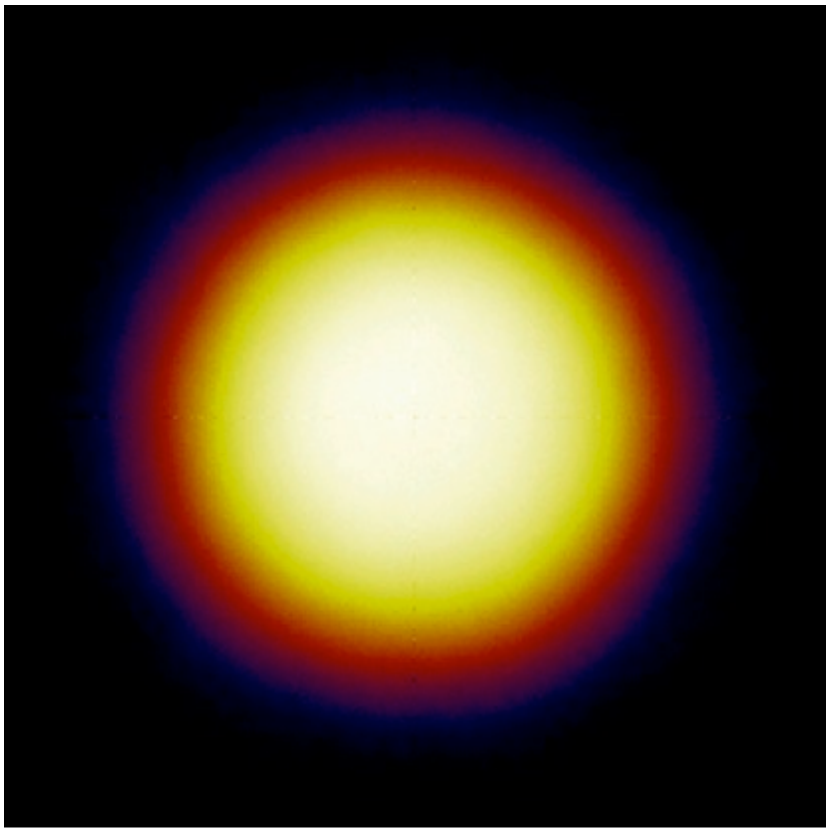


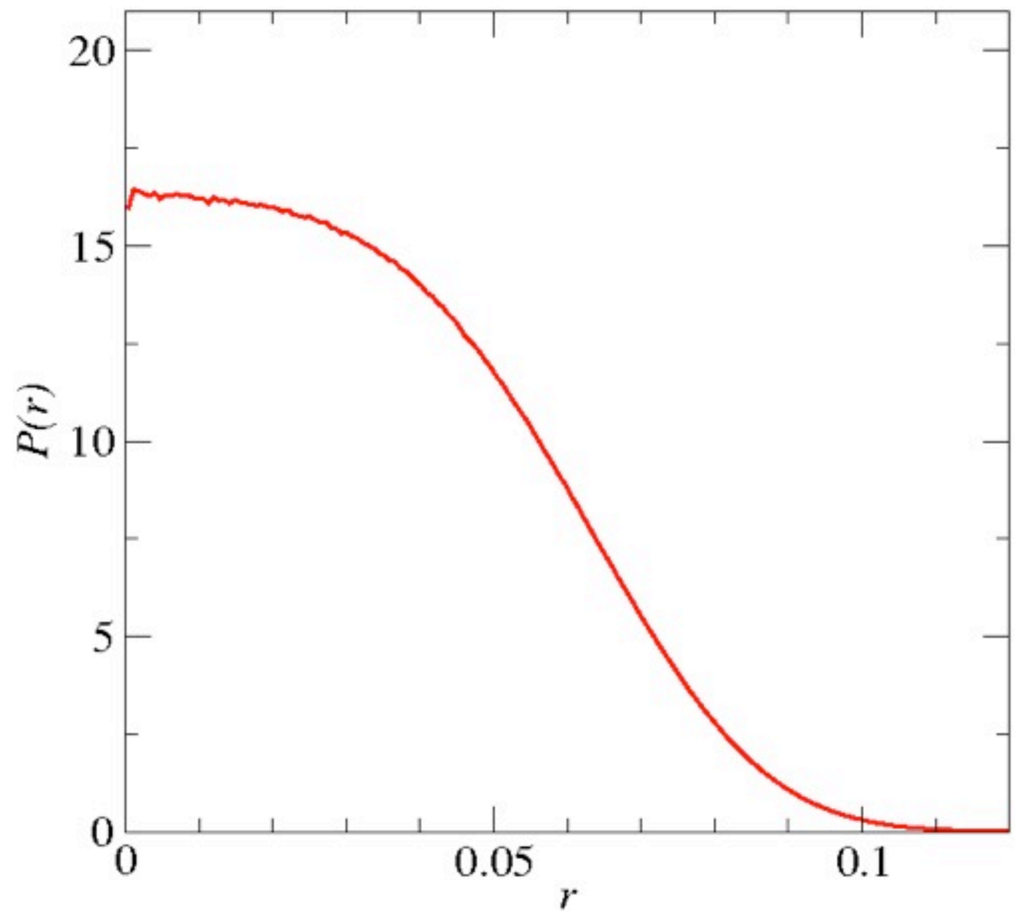
J/Q=0.043



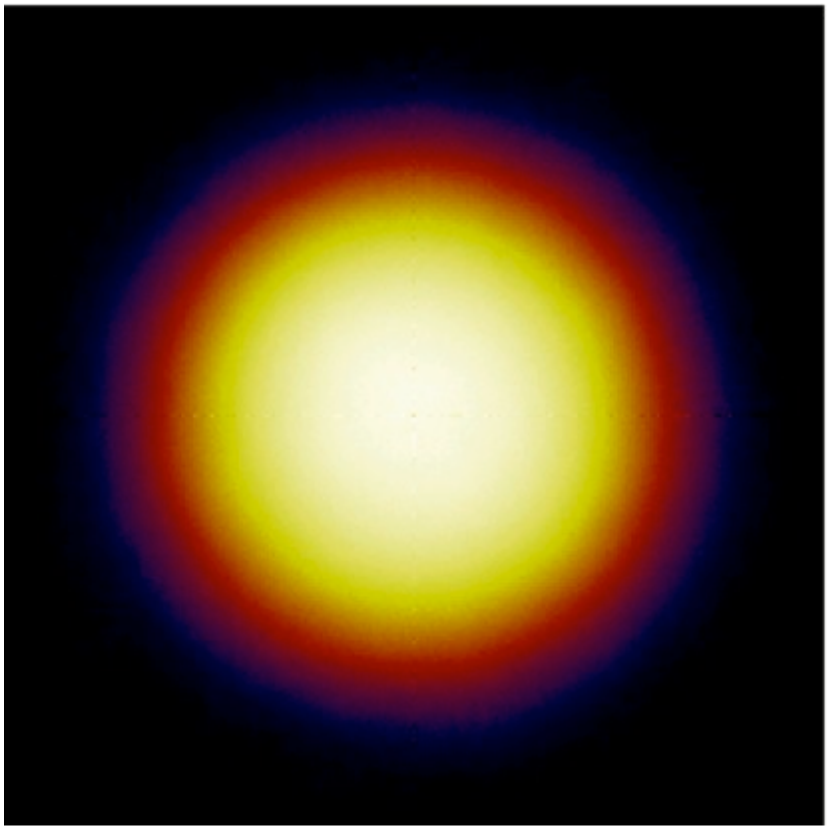


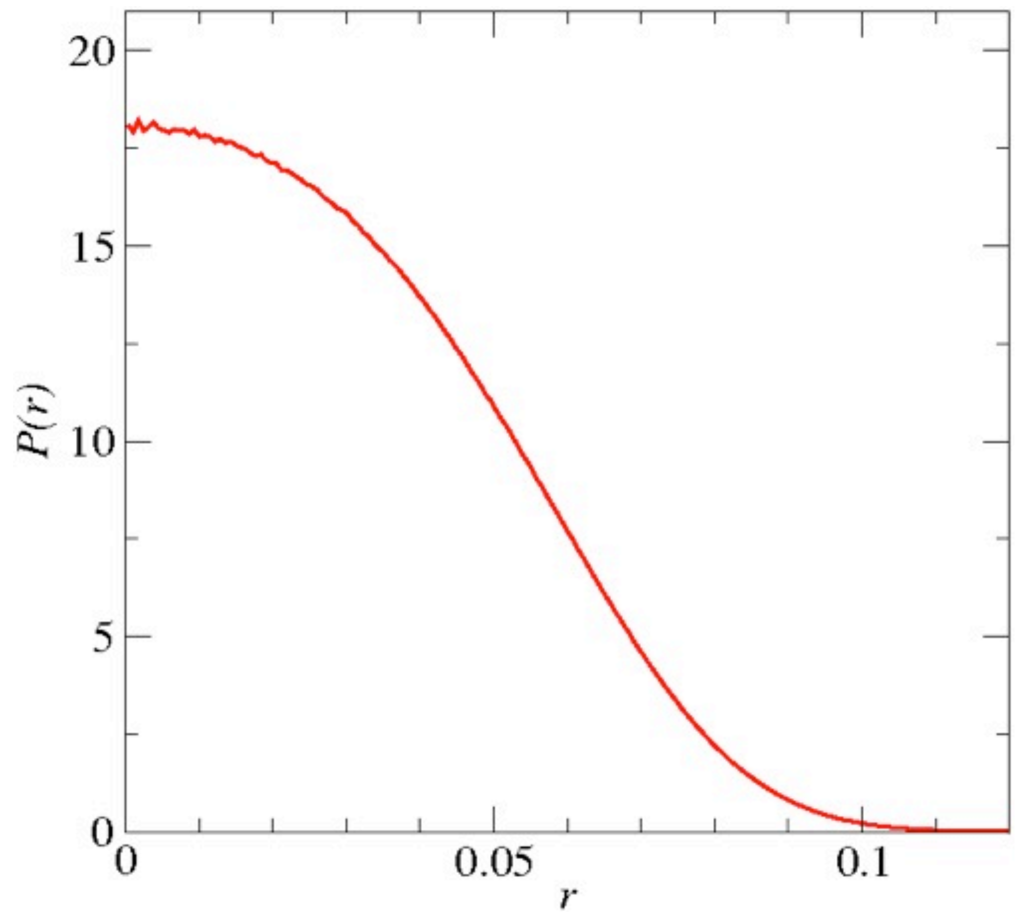
J/Q=0.044



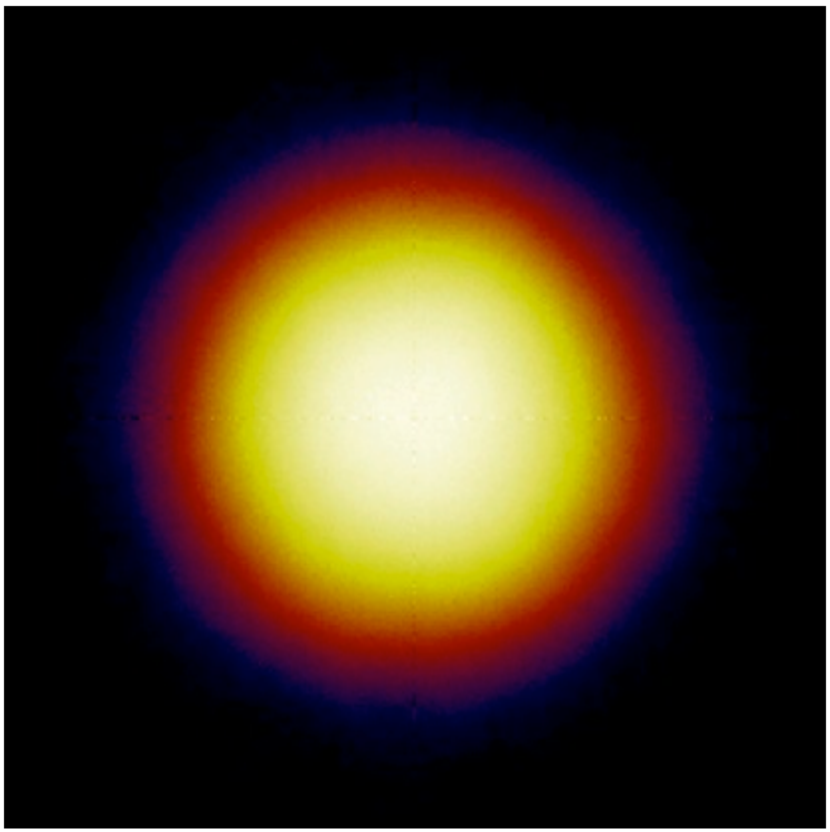


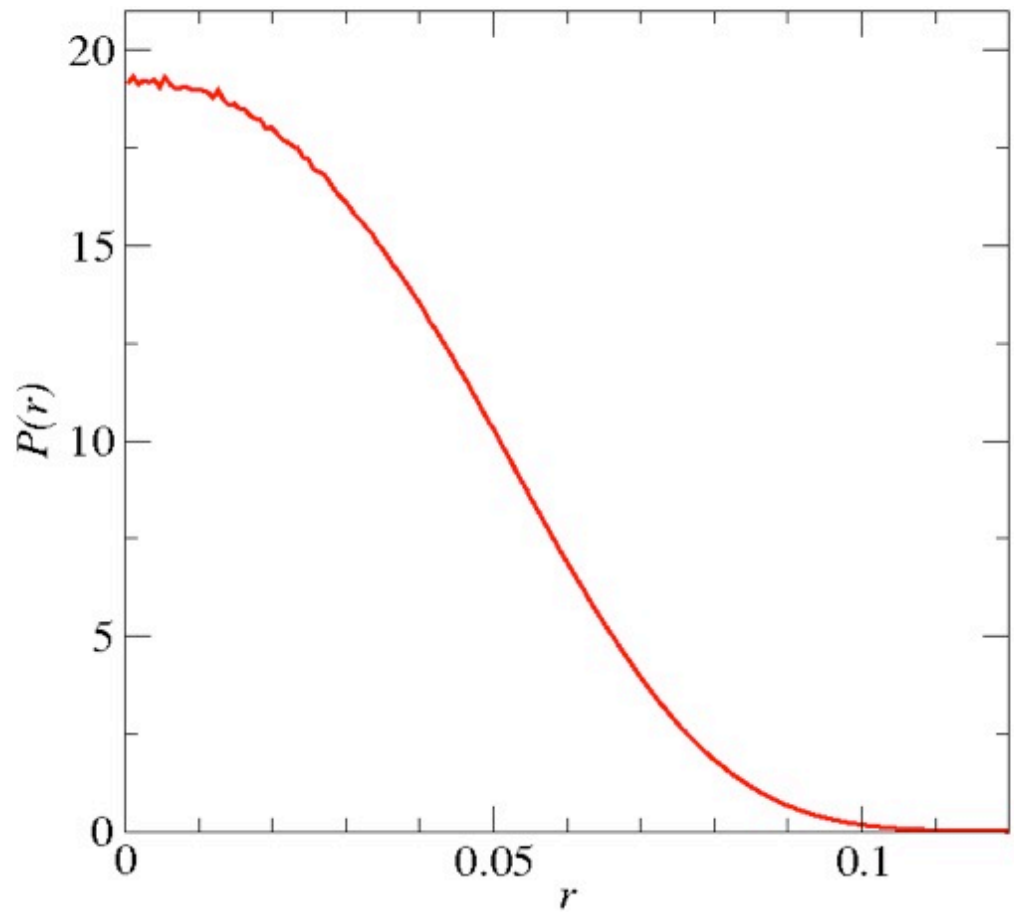
J/Q=0.045





J/Q=0.046





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
- **emergent U(1) symmetric VBS order parameter**

SU(N) J-Q model and J_1-J_2 Heisenberg model

- **critical correlation exponents approach large-N results**

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 analytically
  - difficult to extend to N=2 (3,4) in analytical work
  - could there be log-corrections for N=2 (or general "small" N)?
    - claimed recently by Nogueira & Sudbo (arXiv 2011)