Title: Scaling with two divergent lengths in deconfined quantum criticality

Date: May 24, 2017 02:00 PM

URL: http://pirsa.org/17050007

Abstract: <p>The existence of a deconfined quantum-critical point [1] between the standard antiferromagnet
and a valence-bond solid in 2D S=1/2 quantum magnets has been controversial, in part due to
anomalous finite-size scaling behaviors observed in quantum Monte Carlo simulations interpreted by some as signs of a first-order transition. I will discuss a new finite-size scaling hypothesis in which a scaling function of two divergent length scales [the standard correlation length and a length-scale related to an emergent U(1) symmetry of the valence-bond solid] has a limiting form implying unconventional finite-size scaling behaviors, while maintaining conventional scaling in the thermodynamic limit [2]. This proposal goes beyond the standard scenario of a dangerously irrelevant perturbation as a source of the second length scale in, e.g., classical 3D clock models. Quantum Monte Carlo simulations of the J-Q model (a spin-1=2 Heisenberg model extended with certain multi-spin interactions) are in full agreement with the proposed scaling form, suggesting that deconfined quantum-criticality is an even richer phenomenon than initially imagined. Since finite temperature T plays the role of a finite imaginary-time dimension in quantum systems, the anomalous scaling behavior impacts also the scaling in the quantum-critical \fan" at T > 0. This is also observed in the J-Q model.

[1] H. Shao, W. Guo, and A. W. Sandvik, Science 352, 213 (2016).
[2] T. Senthil, A. Vishwanath, L. Balents, S. Sachdev, M. P. A. Fisher, Science 303, 1490 (2004).</p>

Perimeter Institute, Colloquium, May 24, 2017

Scaling with two divergent lengths in deconfined quantum-criticality

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BOSTON UNIVERSITY

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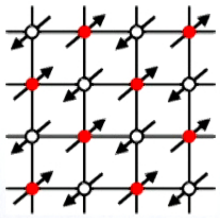
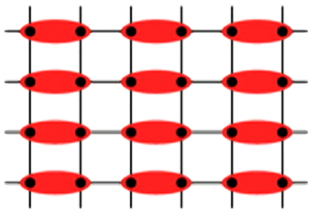
To be discussed:

- 2D quantum antiferromagnets (Heisenberg, J-Q models)
- order and criticality of the ground state
- finite-size scaling in simulation studies
- **two divergent length scales at Néel-VBS transition**





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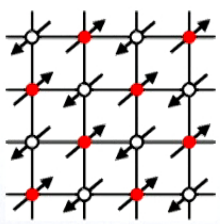

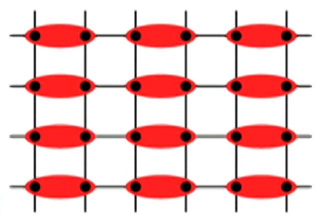

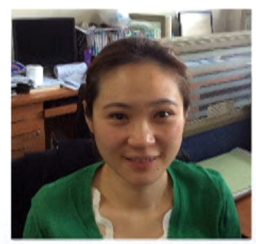

Hui Shao

Wenan Guo

BOSTON UNIVERSITY

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

Classical and quantum phase transitions

Classical (thermal) phase transition

- Fluctuations regulated by temperature T>0

Quantum (ground state, T=0) phase transition

- Quantum fluctuations regulated by parameter g in Hamiltonian

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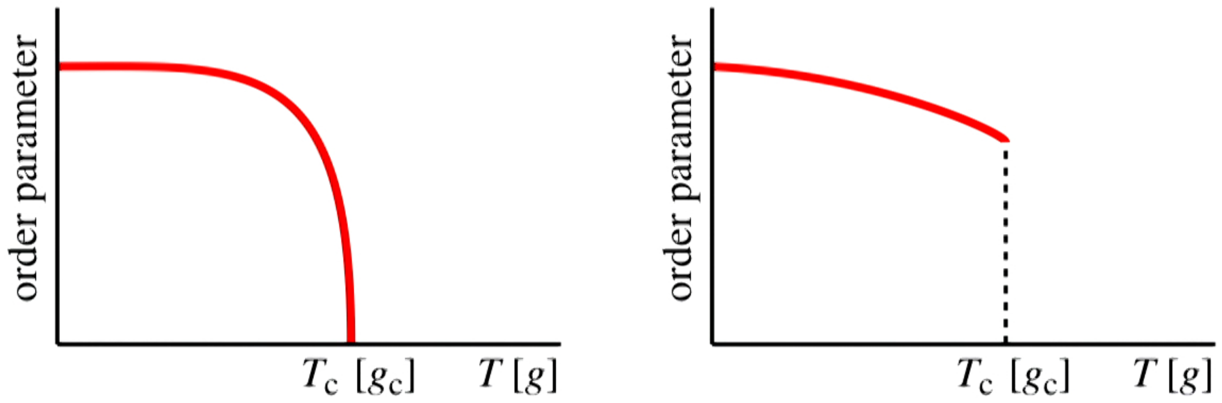

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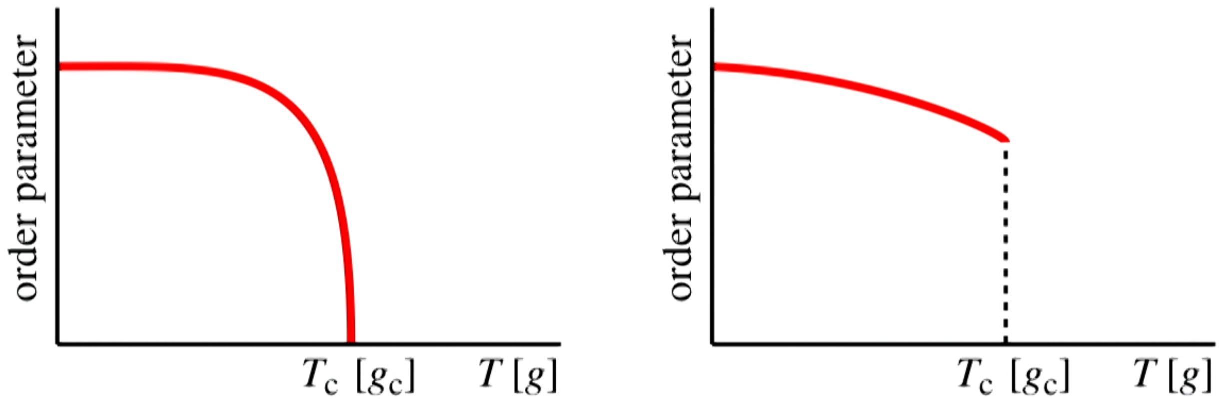

- <u>first-order (discontinuous):</u> **finite correlation length ξ** as $g \to g_c$ or $T \to T_c$
- <u>continuous:</u> correlation length diverges:

$$\xi \sim |g-g_c|^{-\nu} \text{ or } \xi \sim |T-T_c|^{-\nu}$$

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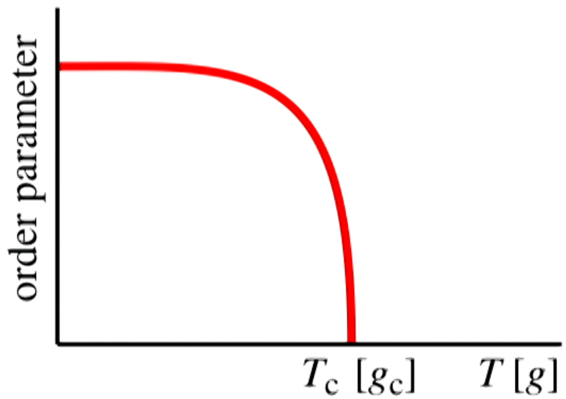

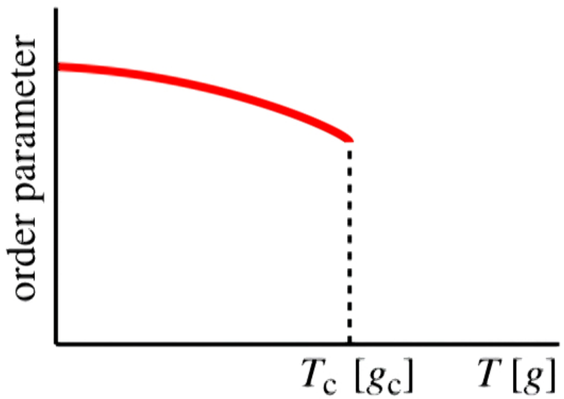

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This talk: Continuous T=0 transitions in 2D quantum antiferromagnets

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$$H = \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \qquad S = 1/2 \text{ spins}$$

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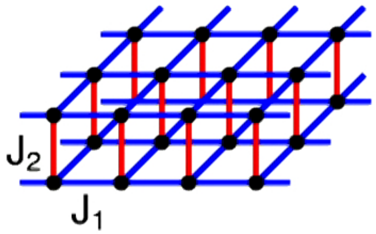

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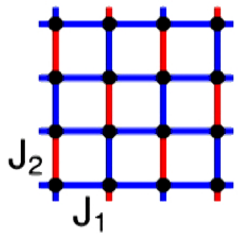

strong interactions (red)

weak interactions (blue)

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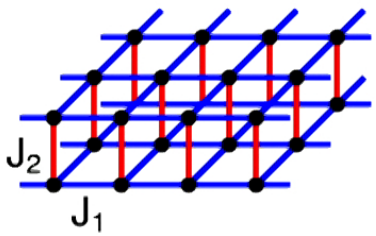

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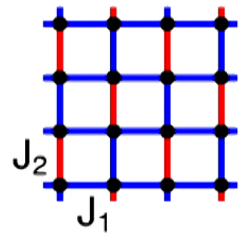
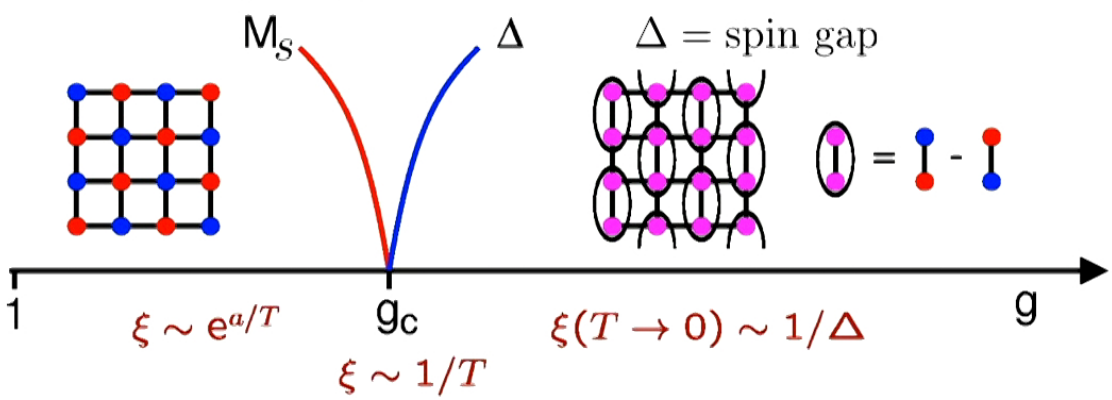


strong interactions

weak interactions

Singlet formation on strong bonds → Néel - disordered transition

Ground state (T=0) phases



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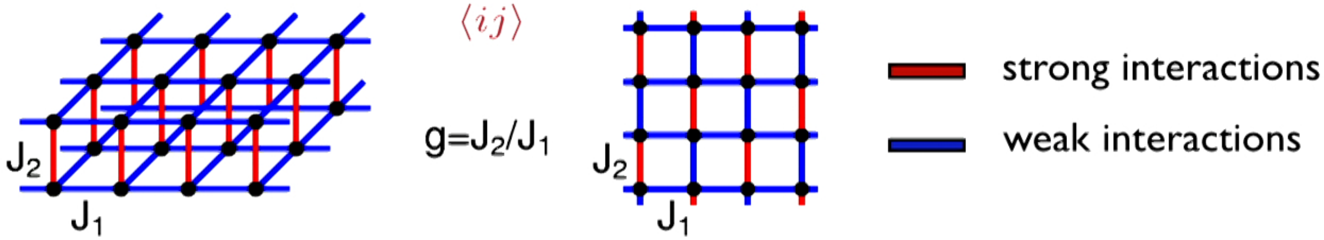

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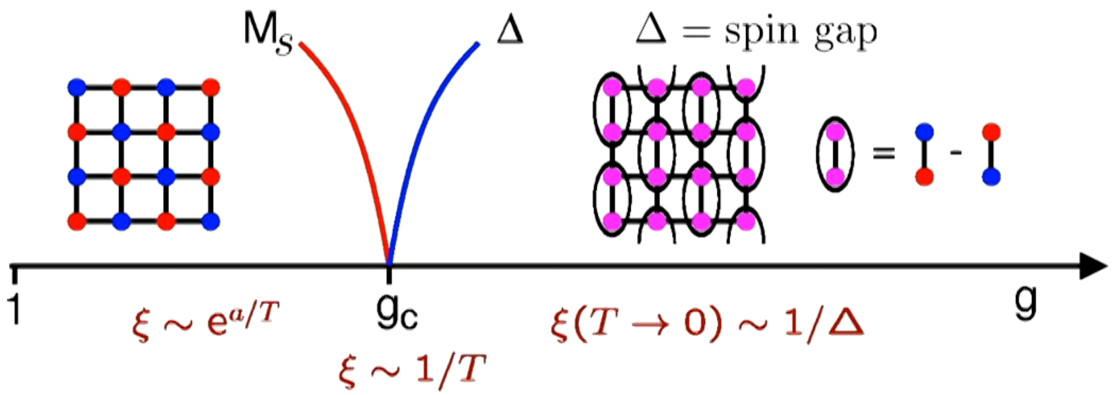
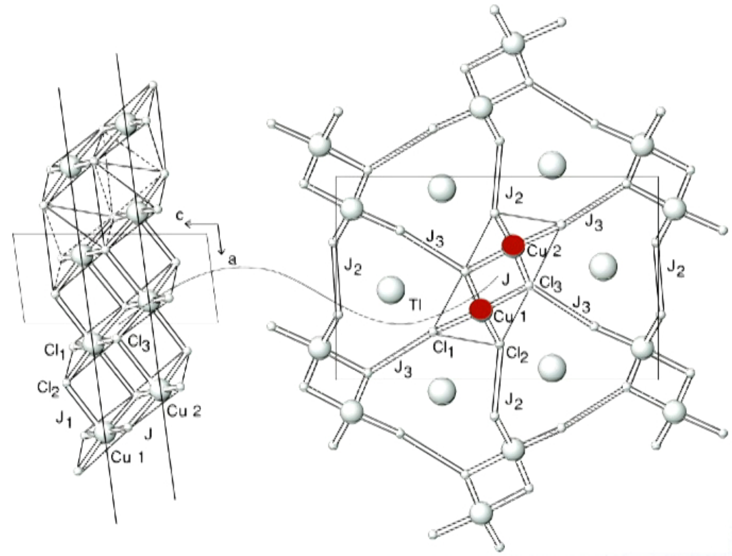


Transition in 3D O(3) Universality class

$TlCuCl_3$

3D Network of **spin dimers**

- couplings depend on pressure



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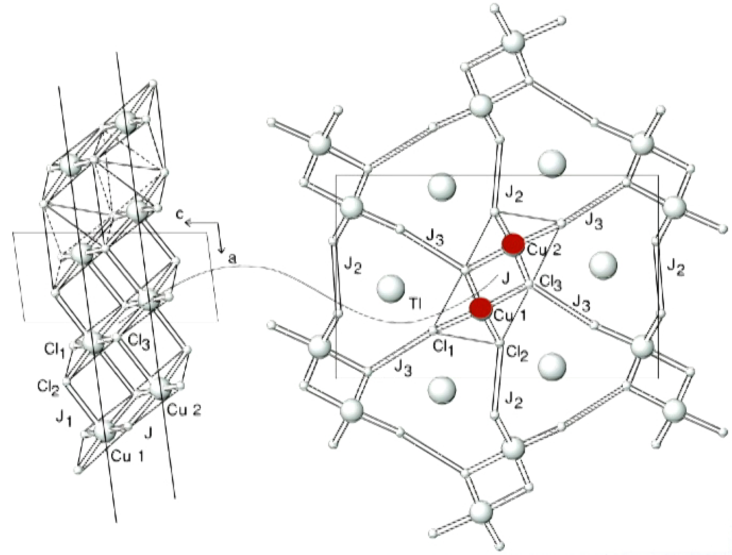

The spins on an isolated Cu dimer form a singlet $\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$

nature physics

ARTICLES

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Quantum and classical criticality in a dimerized quantum antiferromagnet

P. Merchant[1], B. Normand[2], K. W. Krämer[3], M. Boehm[4], D. F. McMorrow[1] and Ch. Rüegg[1,5,6]*

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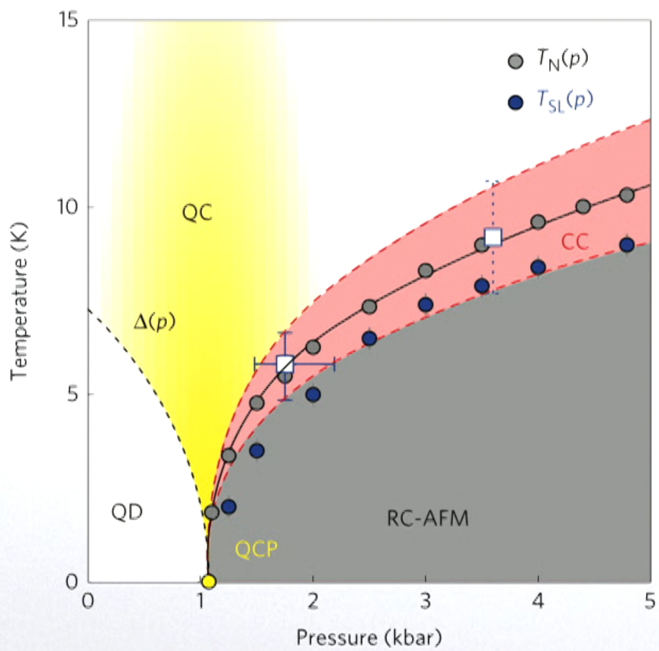

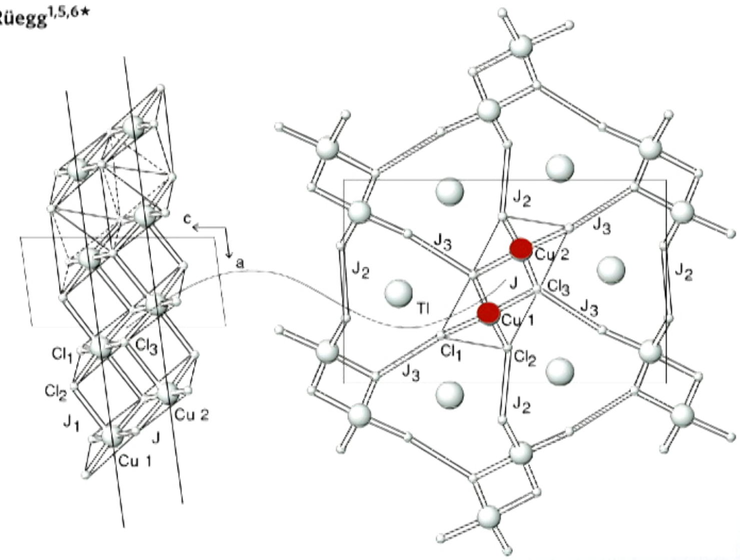

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Experimental realization of Néel - quantum-paramagnetic transition

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

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

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  - ➡ resonating valence-bond (RVB) spin liquid
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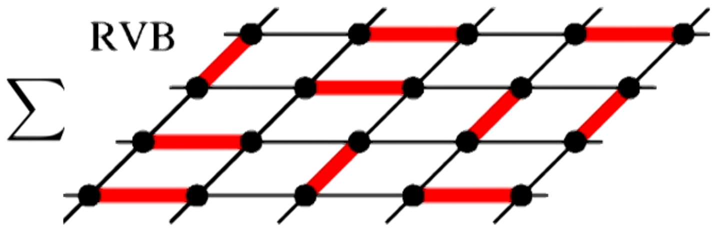

$$= (\uparrow_i \downarrow_j - \downarrow_i \uparrow_j)/\sqrt{2}$$

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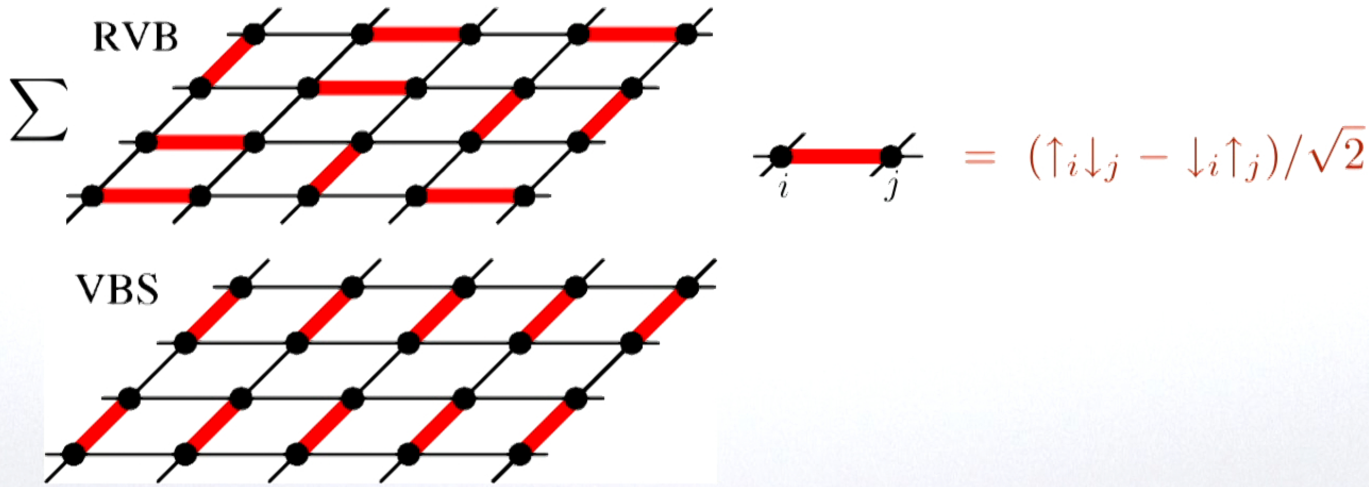

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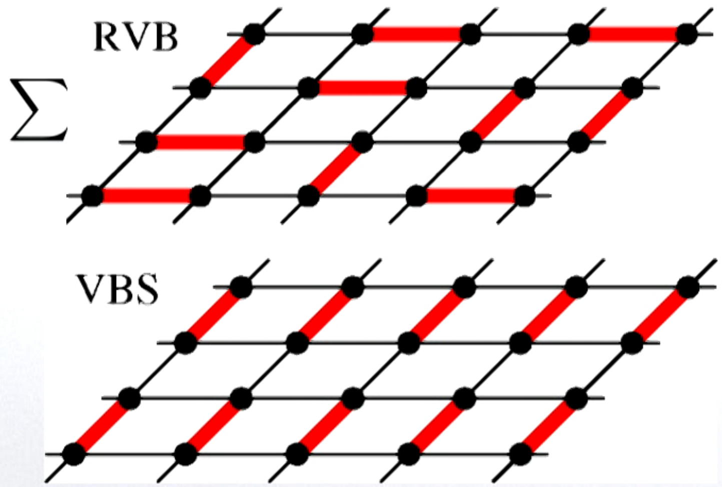

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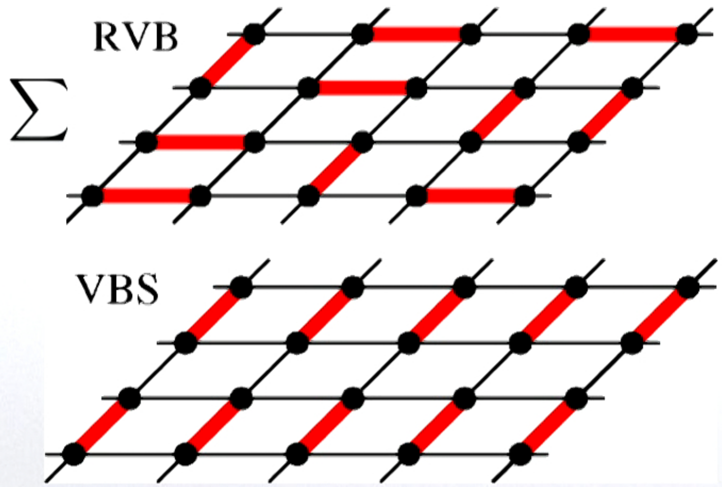

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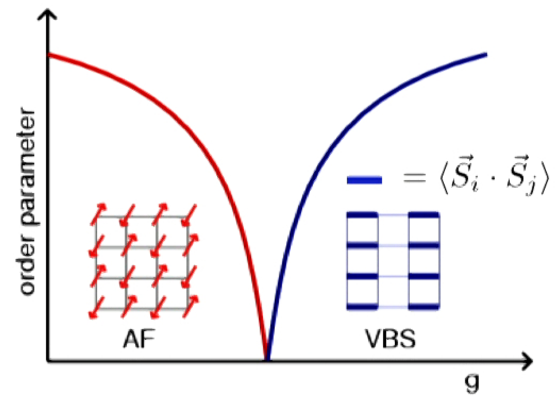
The Néel - VBS transition may be “beyond LGW”

Deconfined quantum criticality

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



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Continuous Néel - VBS transition proposed

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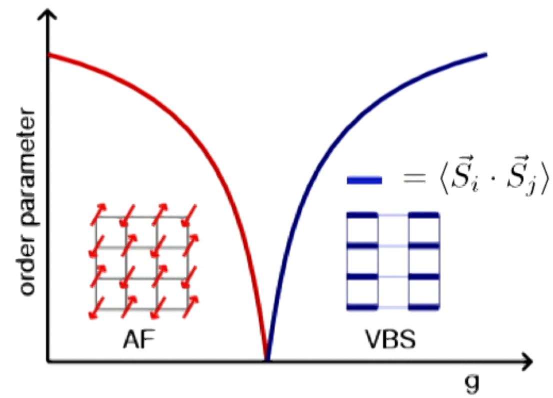

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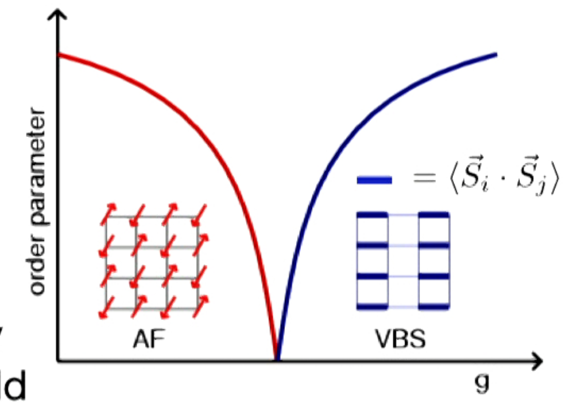
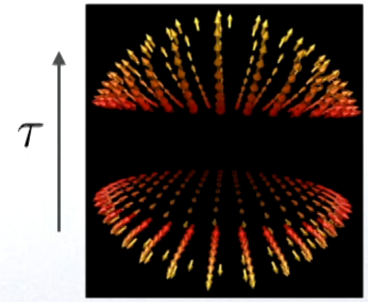
- "dangerously irrelevant" topological defects
- universality: 3D defect-suppressed O(3)
- topological defects relevant in VBS state only
- both order parameters emerge from same field





Graph:Senthil et al.

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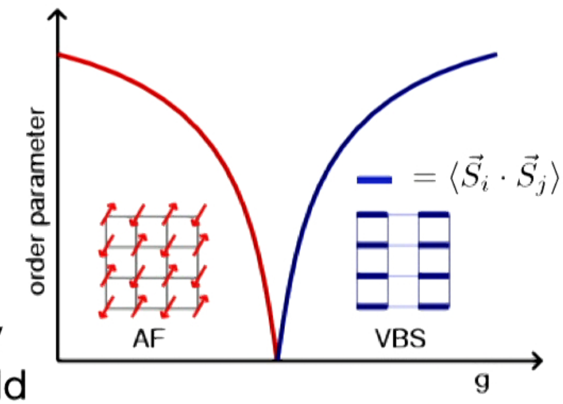

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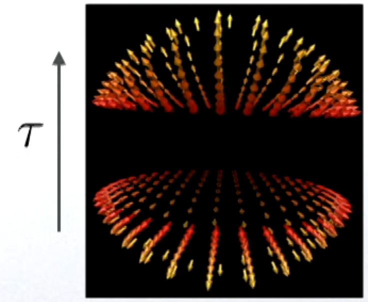

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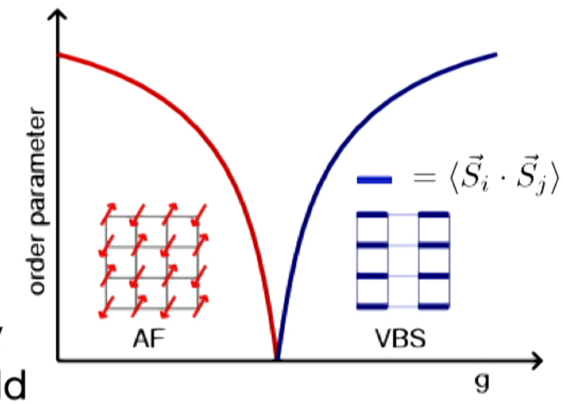

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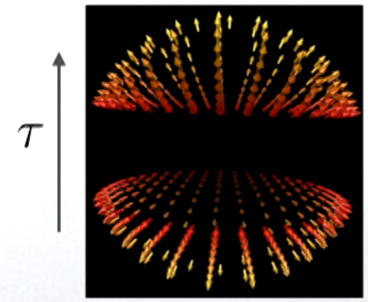

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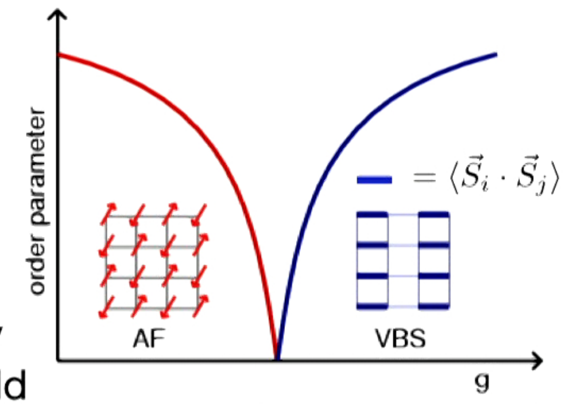

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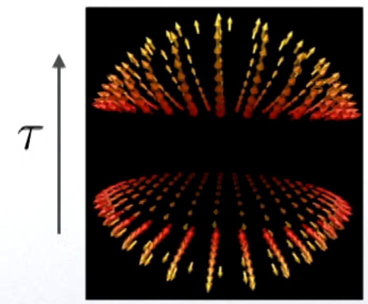

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Consequences of two divergent length scales?

Dangerously irrelevant perturbations

Classical phase transitions with two divergent length scales

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Jose, Kadanoff, Kirkpatrick, Nelson, PRB 1977

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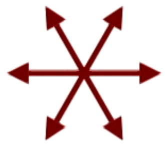

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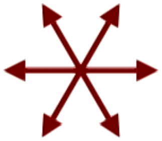

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h term is dangerously irrelevant

- does not change criticality
- changes ordered state (different symmetry breaking)

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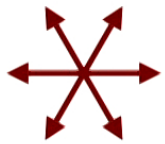

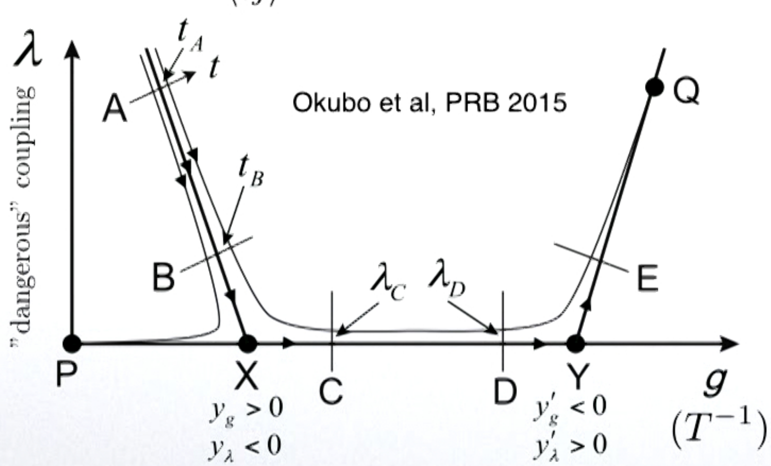

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- changes ordered state (different symmetry breaking)

Fixpoints:

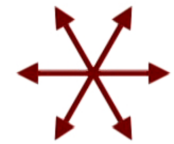
P = paramagnet
X = 3D XY critical point
Y = U(1) symmetry breaking
Q = Z_q symmetry breaking

Dangerously irrelevant perturbations

Classical phase transitions with two divergent length scales

- correlation length $\xi \propto (g - g_c)^{-\nu}$ and larger cross-over length $\xi' \propto (g - g_c)^{-\nu'}$
- known in many classical systems (e.g., 3D clock models)

Jose, Kadanoff, Kirkpatrick, Nelson, PRB 1977



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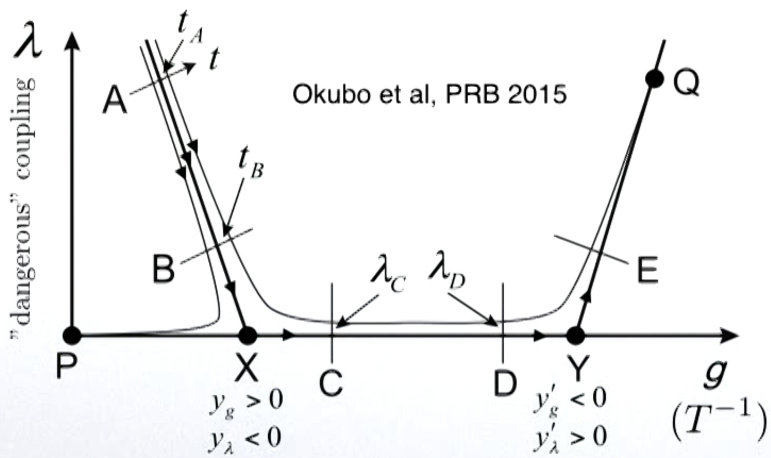

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Cross-over from XY ordering to clock ordering at length scale ξ'

MC simulations of classical 3D clock model

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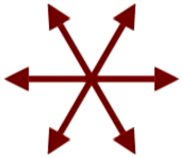
Restricted to q clock angles



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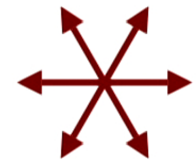

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Standard order parameter **(m_x,m_y)**

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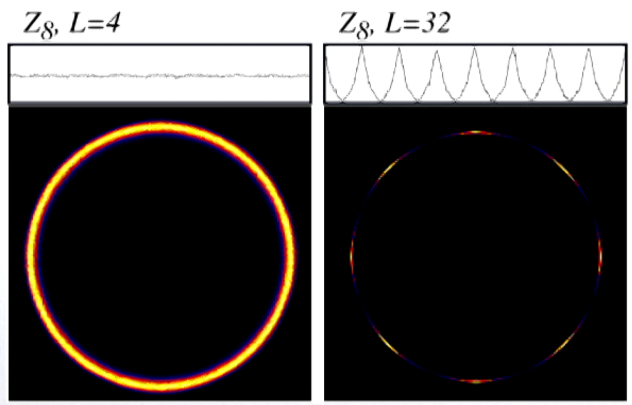

Lou, Balents, Sandvik, PRL 2007

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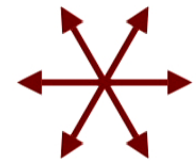

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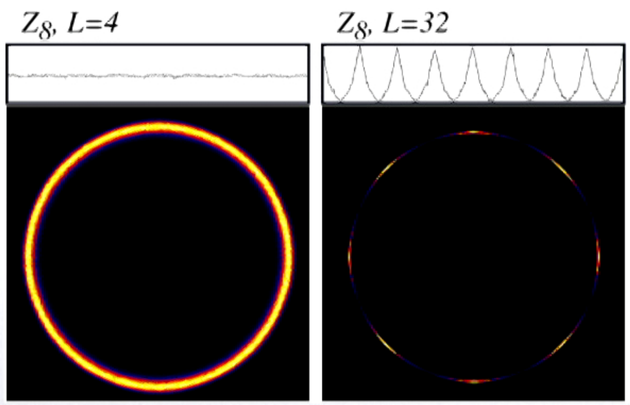

Lou, Balents, Sandvik, PRL 2007

Angular anisotropy quantified by "angular order parameter":

$$m_q = \int_0^{2\pi} d\Theta \cos(q\Theta) P(\Theta)$$

$m_q > 0$ only if q-fold anisotropy

Studying RG flows in MC simulations

H. Shao, W. Guo, A. W. Sandvik (work in progress)

XY fixed point can be studied using the Binder cumulant of m

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

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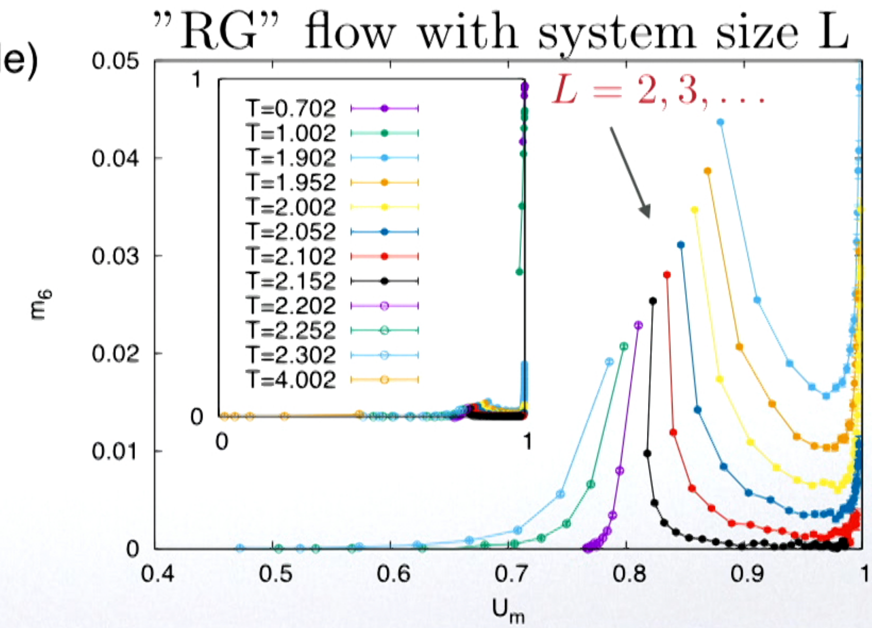

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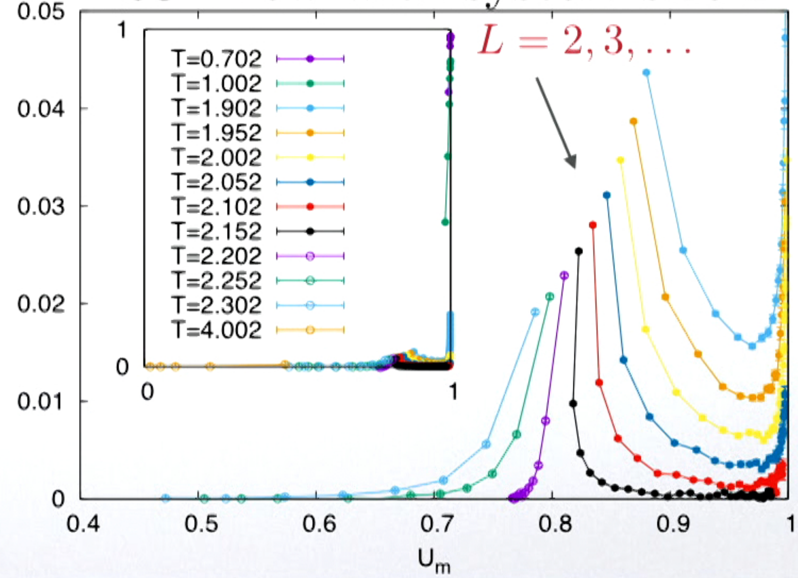
In principle the length scale ξ' can be extracted from the flows

"RG" flow with system size L



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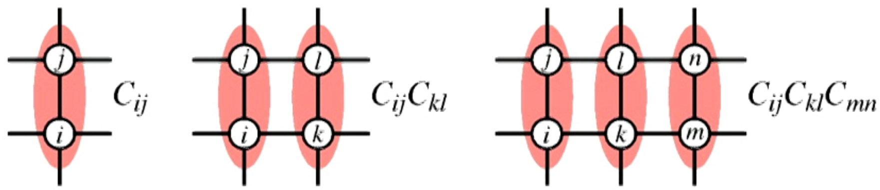

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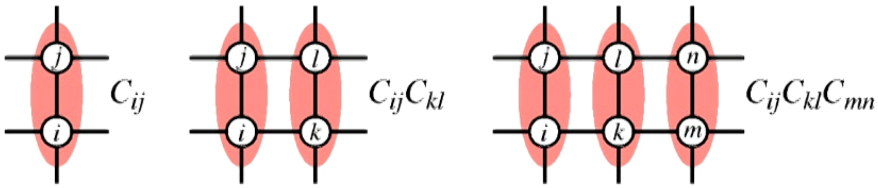

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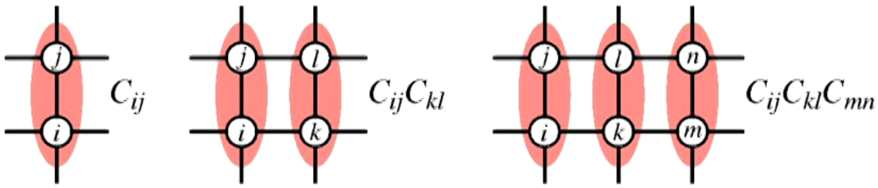

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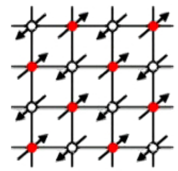
- Has Néel-VBS transition, appears to be continuous
- Not a realistic microscopic model for materials
- "Designer Hamiltonian" for VBS physics and Néel-VBS transition

Critical behavior of the J-Q model

Staggered magnetization

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



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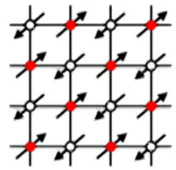

Dimer order parameter (D_x,D_y)

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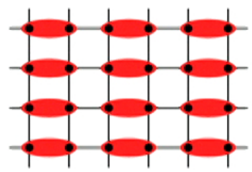

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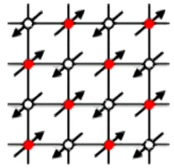

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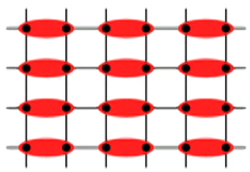

Compute squared order parameters

$$\langle M^2\rangle,\quad \langle D^2\rangle = \langle D_x^2 + D_y^2\rangle$$

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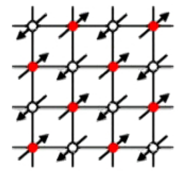

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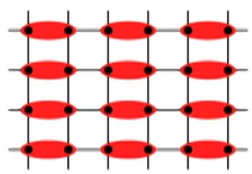

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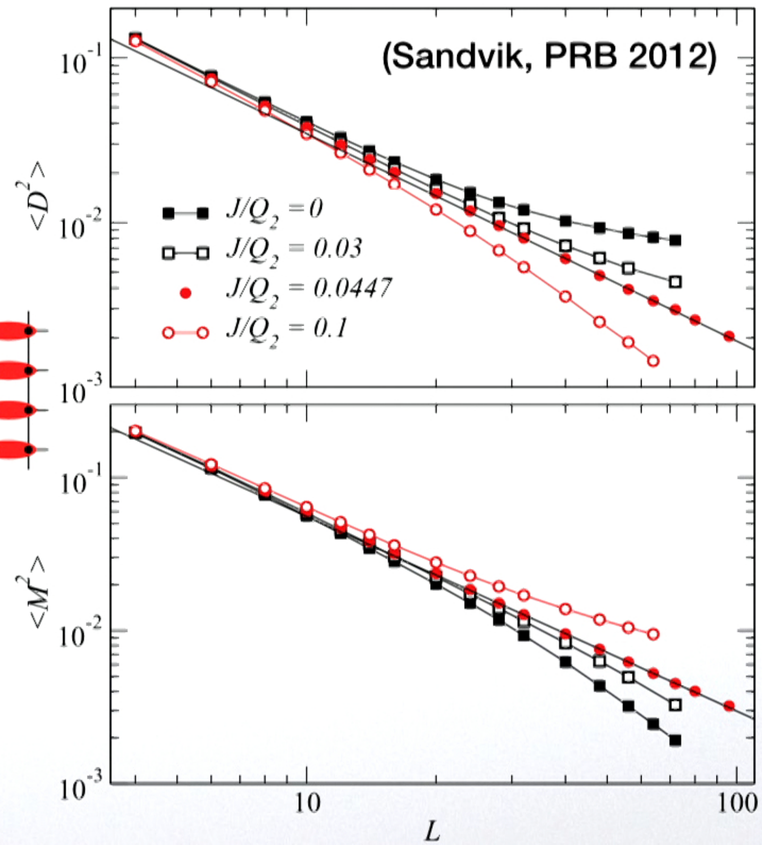

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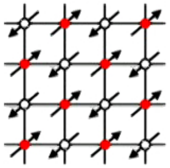

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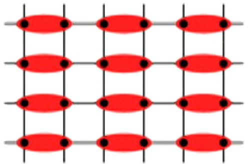

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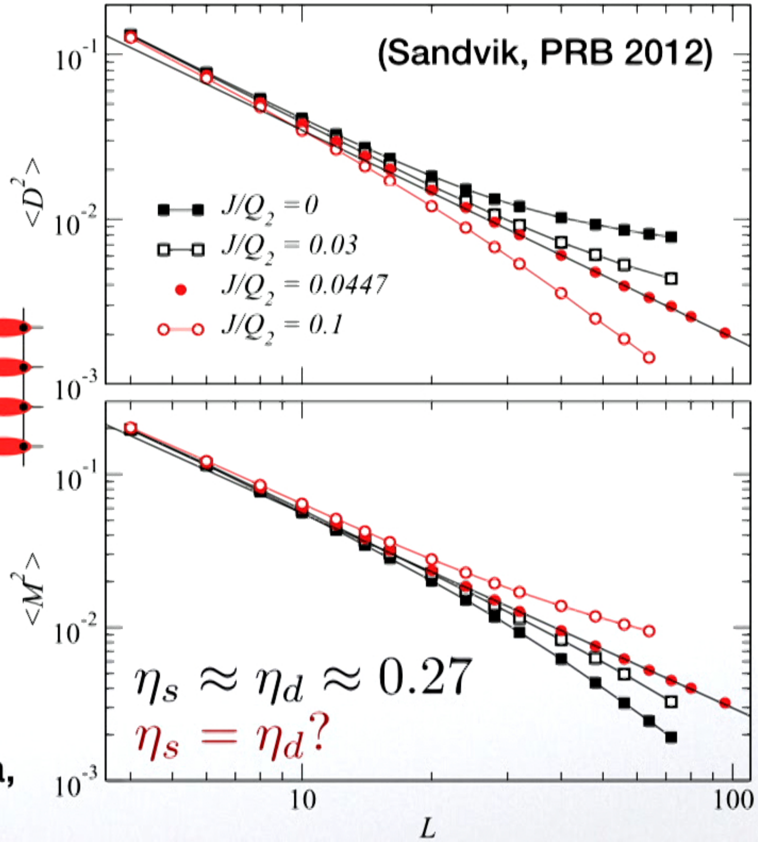
Emergent SO(5) symmetry?

[Nahum, Serna, Chalker, Ortuno, Somoza, PRL 2015]



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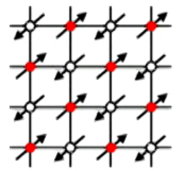

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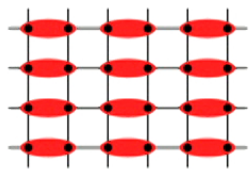

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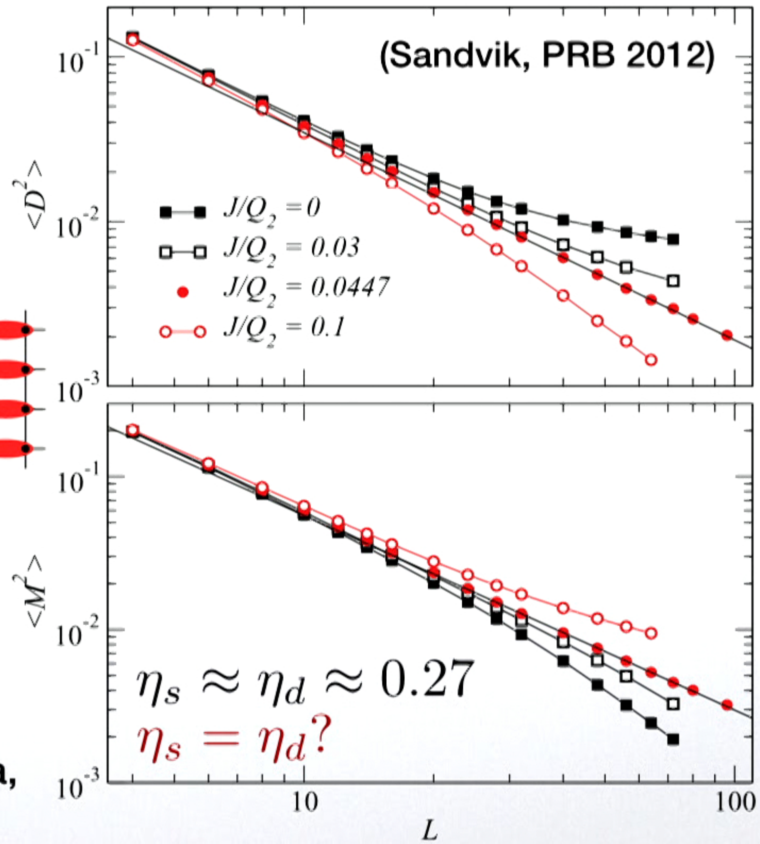

How can we study two divergent lengths?

Expected RG flows in DQC scenario

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

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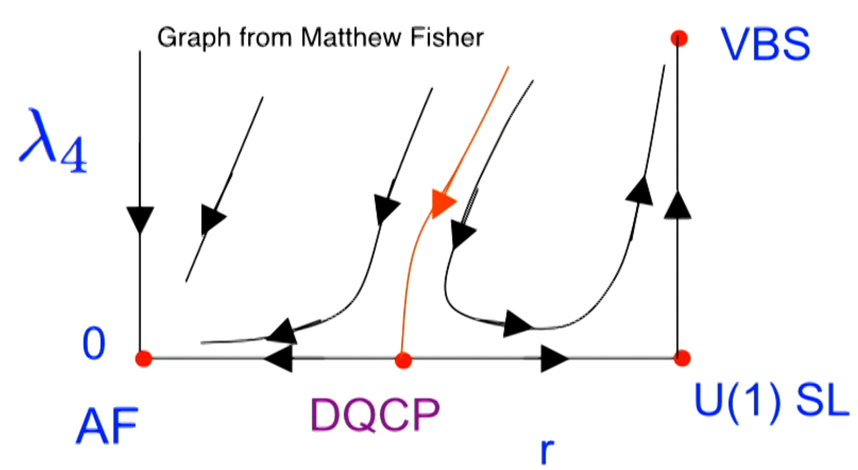

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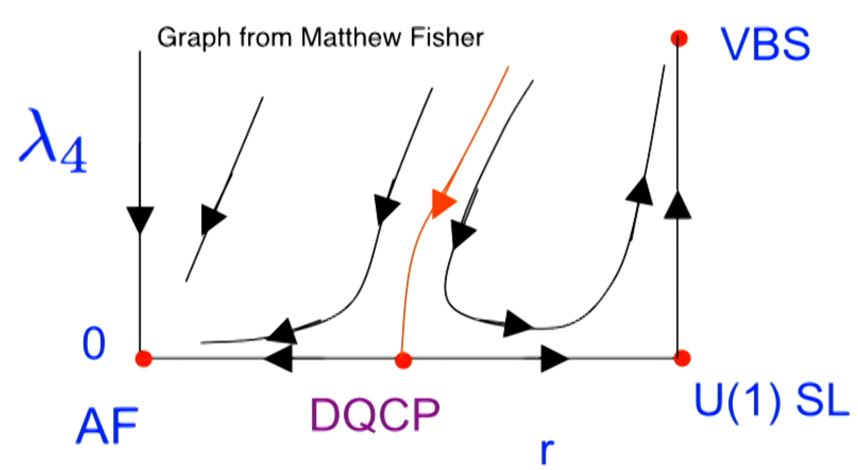

Non-compact CP¹ model

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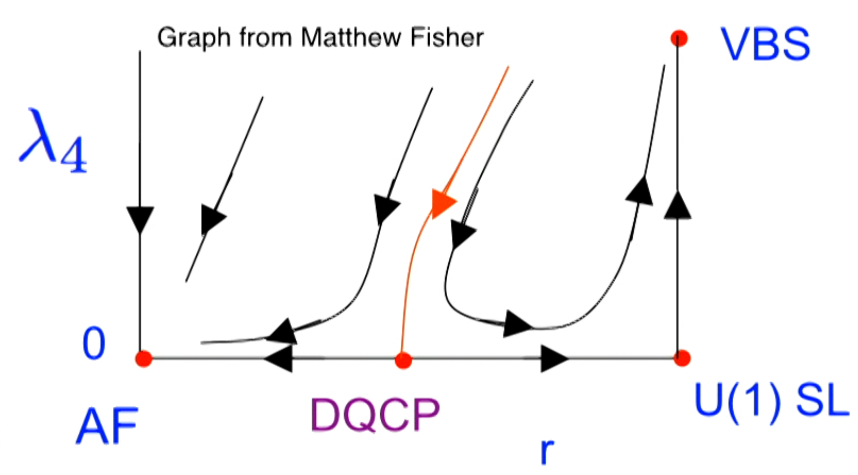

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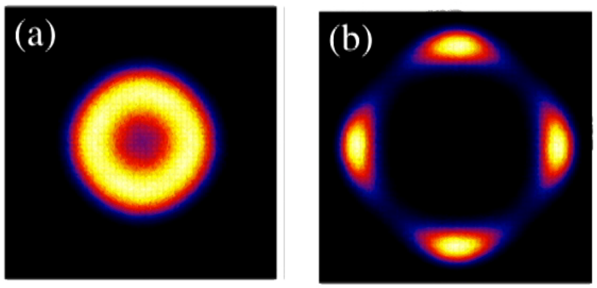
Goal: Test scenario and obtain quantitative results using numerics

Emergent U(1) and RG flows in the J-Q_3 model

P(D_x,D_y): Emergent U(1) symmetry



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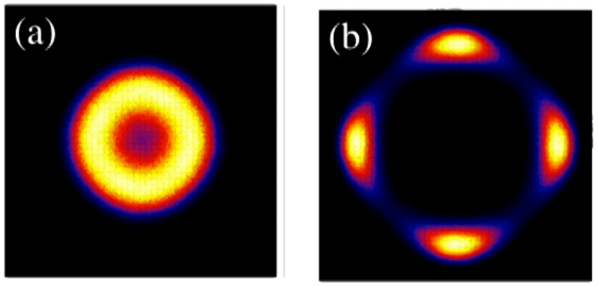

Define D_4 as in the clock model
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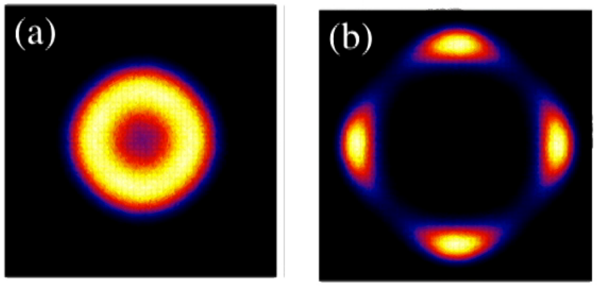

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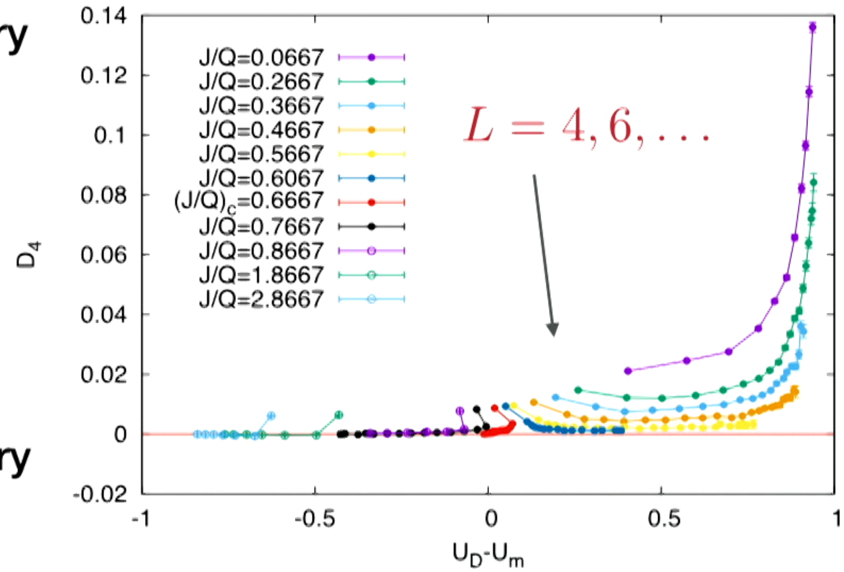

H. Shao, W. Guo, A. W. Sandvik
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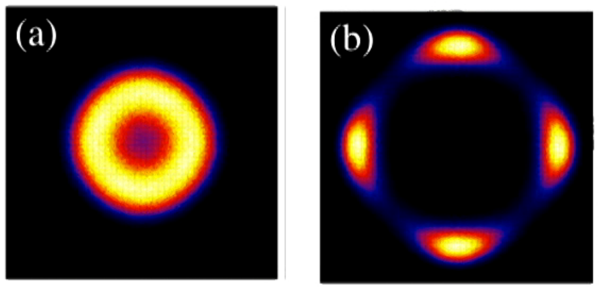

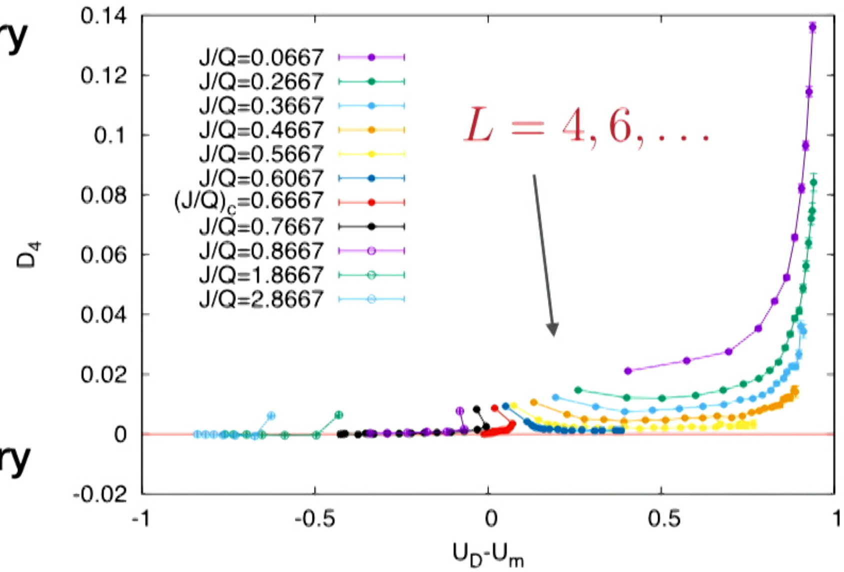

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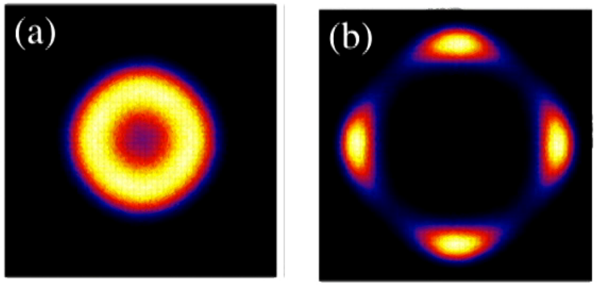

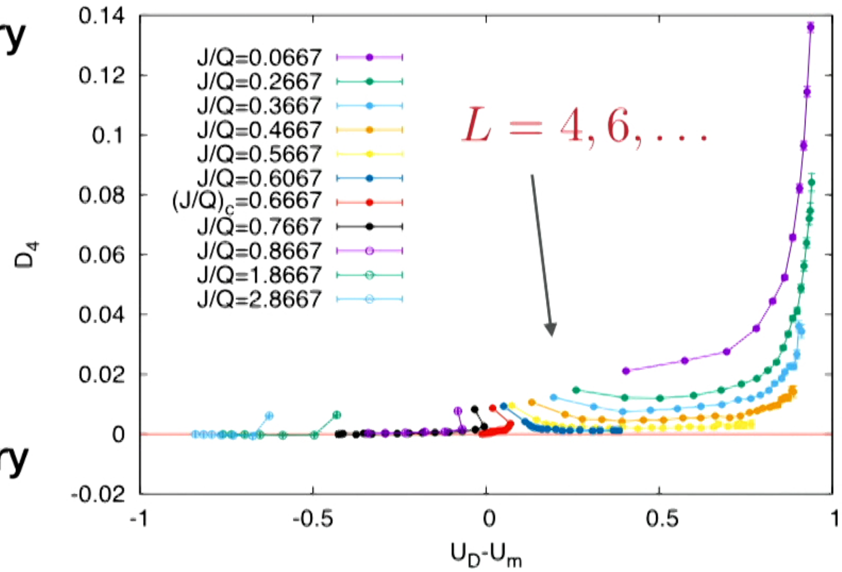

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Use systematic finite-size scaling approach for exponents

Finite-size scaling (one divergent length)

Correlation length divergent for T → T_c $\xi \propto |\delta|^{-\nu}, \quad \delta = T - T_c$

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Other singular quantity: $A(L \to \infty) \propto |\delta|^{\kappa} \propto \xi^{-\kappa/\nu}$

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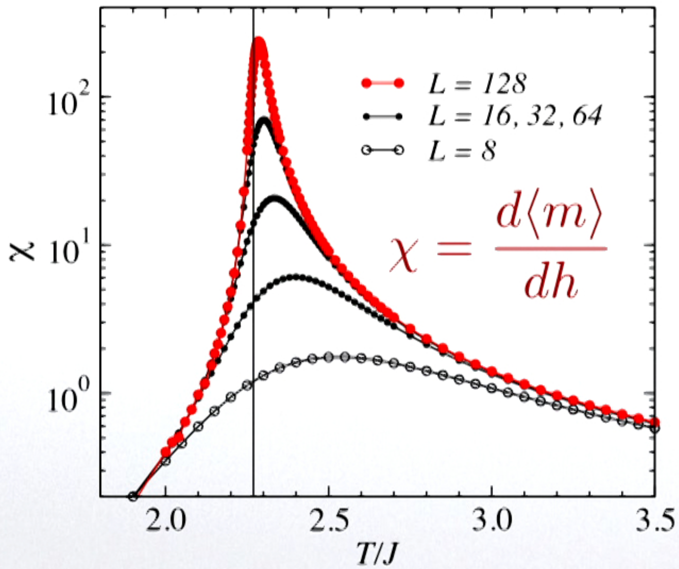

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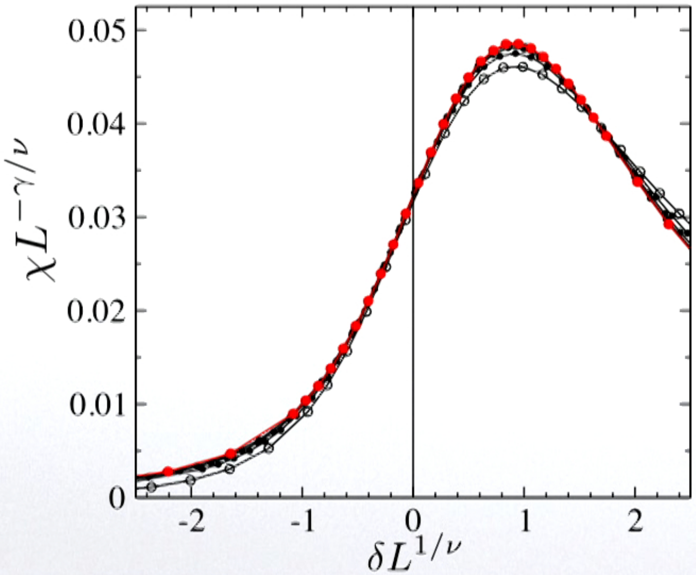

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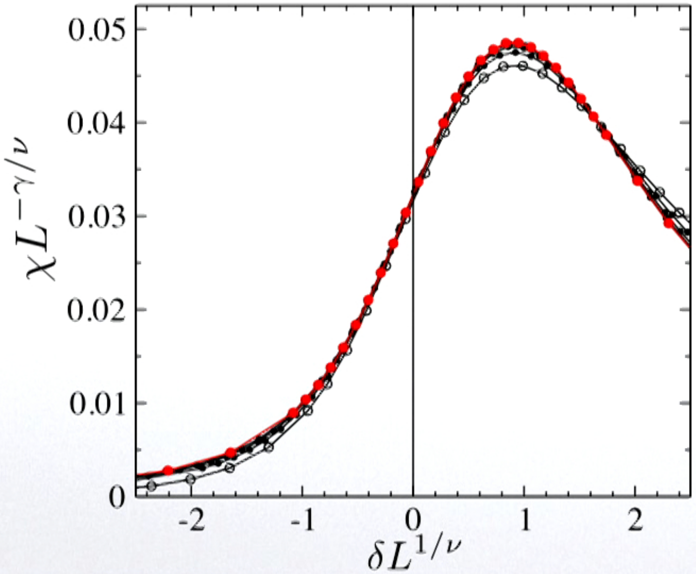

2D Ising universality class

$\gamma = 7/4, \quad \nu = 1 \quad (\kappa = -\gamma)$

Critical T known

$T_c = 2/\ln(1+\sqrt{2}) \approx 2.2692$

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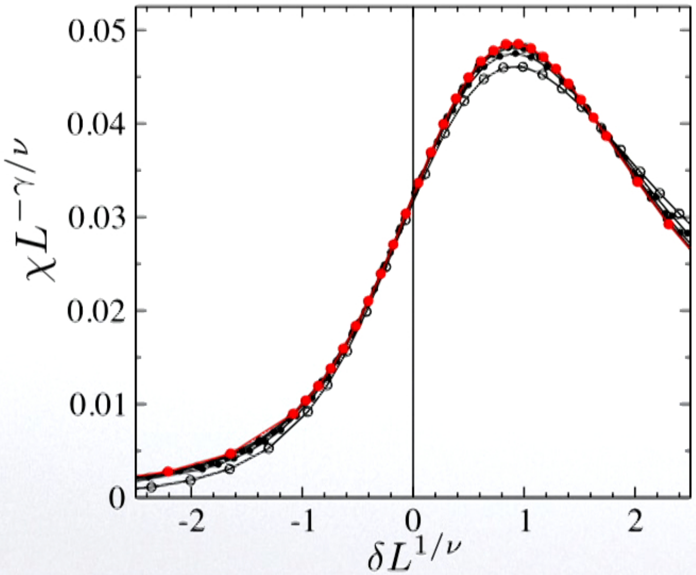

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When these are not known,
treat as fitting parameters
- or extract in other way

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Systematic critical-point analysis

Binder cumulant
- dimensionless
- size-independent at T_c

$$U = \frac{1}{2}\left(3 - \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2}\right)$$

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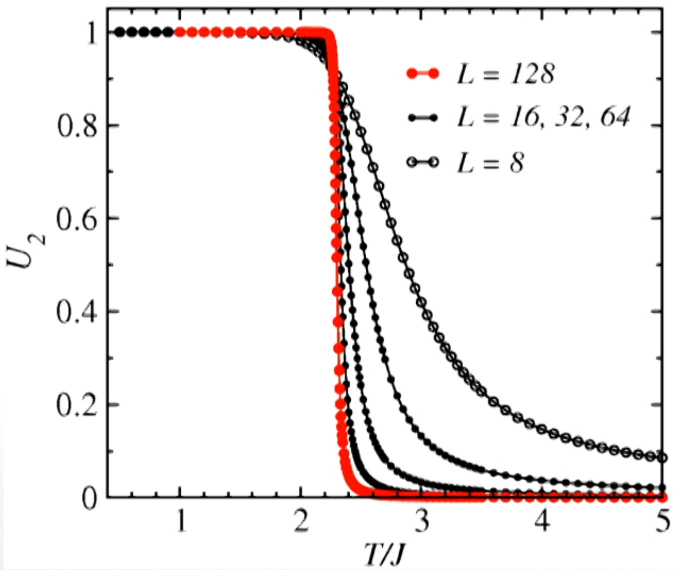
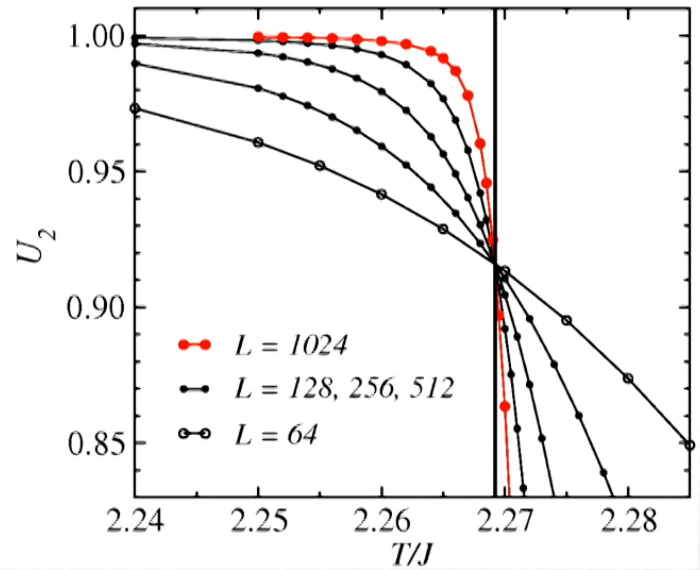
2D Ising model: MC results





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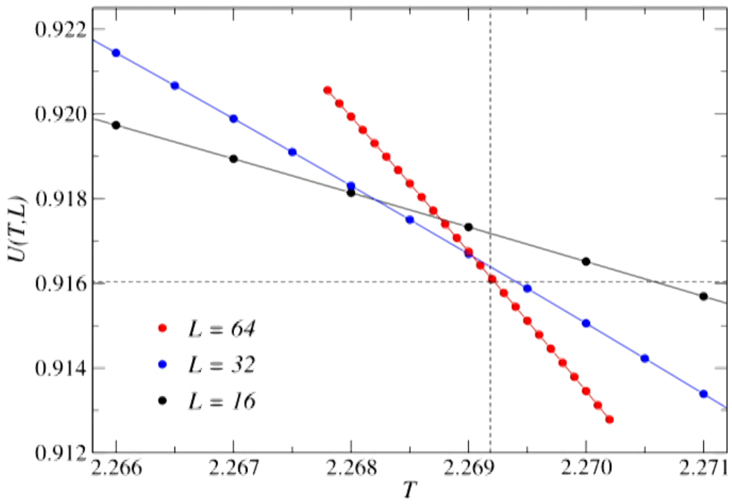

Drift in crossing point expected
- scaling correction

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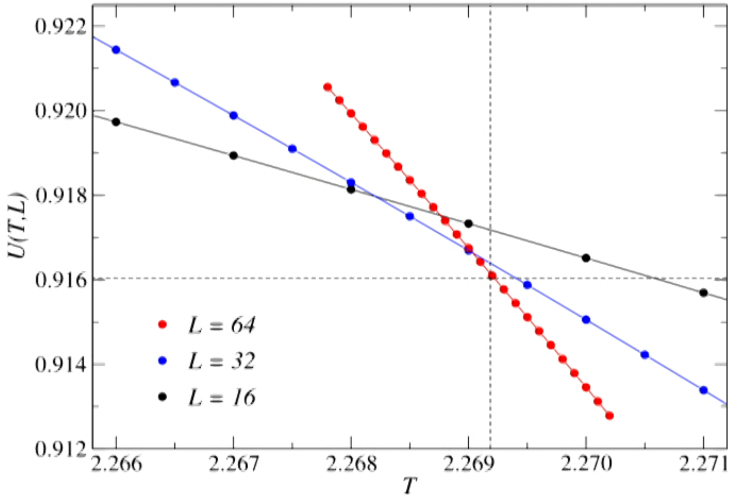

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Fit (L,2L) crossing-points
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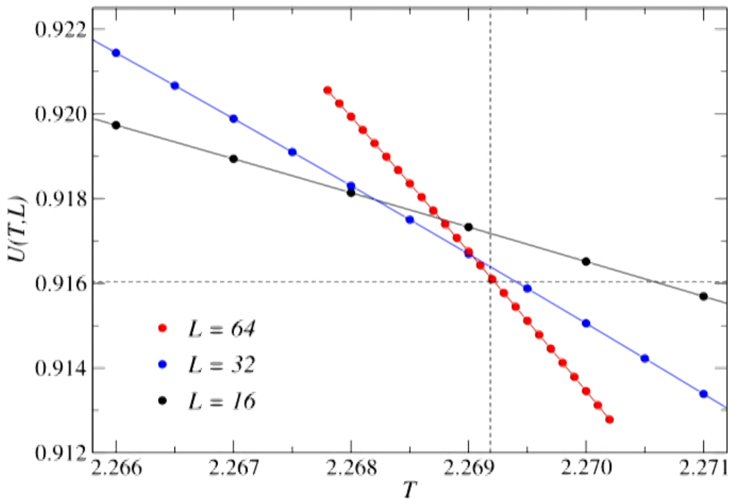

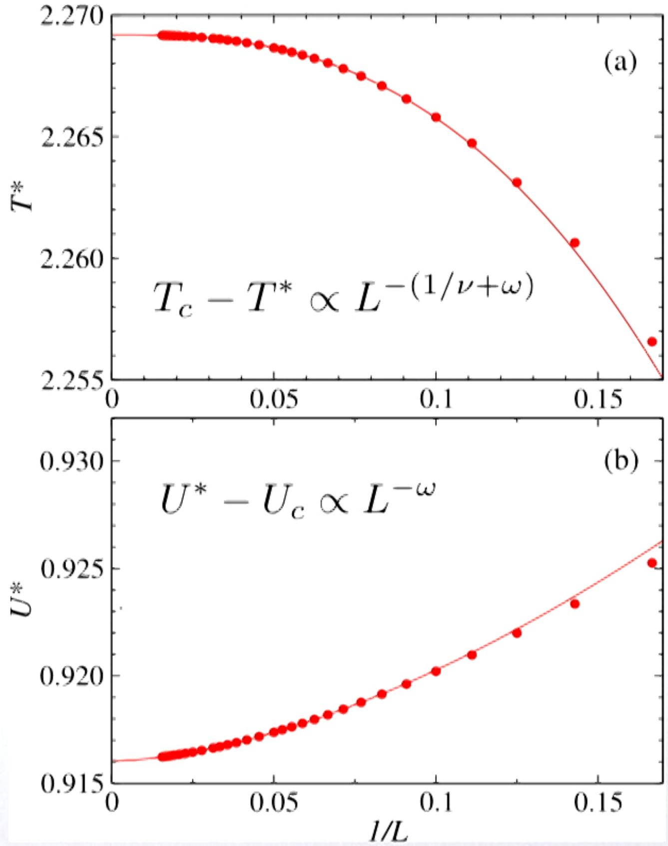

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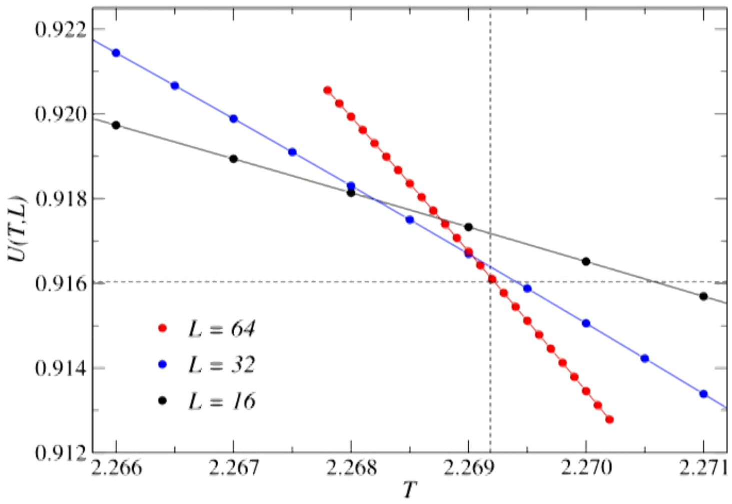

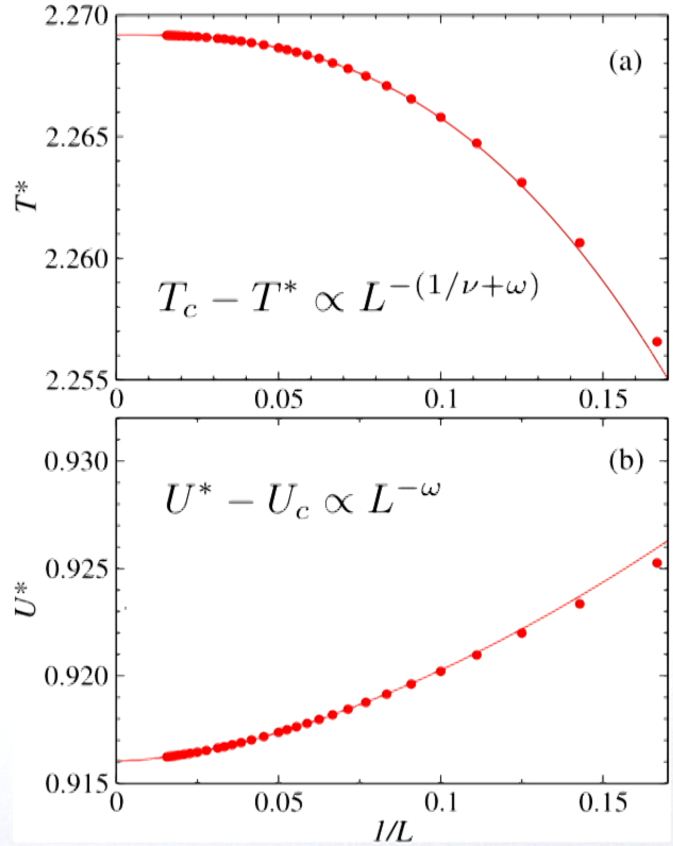

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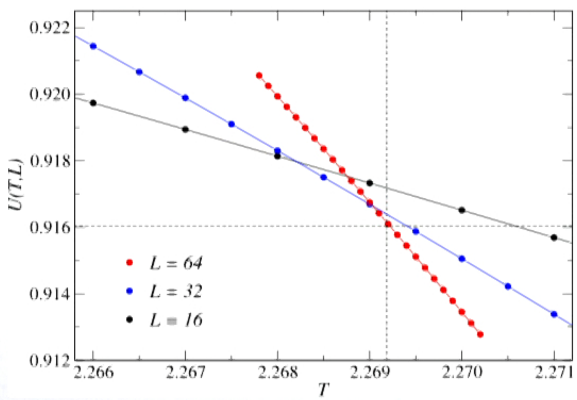
Fit with L_{min}=12: T_c=2.2691855(5). Correct T_c=2.2691853...

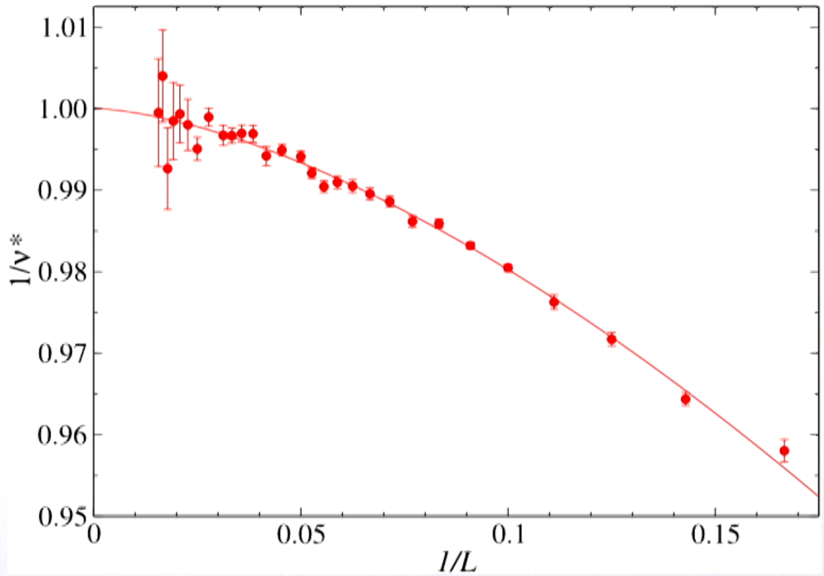
Correlation-length exponent ν

Can be extracted from the slope of the Binder cumulant

$$s(L,T) = \frac{dU(L,T)}{dT}$$

$$\frac{1}{\ln(2)} \ln\left(\frac{s(2L,T^*)}{s(L,T^*)}\right) = \frac{1}{\nu} + aL^{-\omega} + \dots$$





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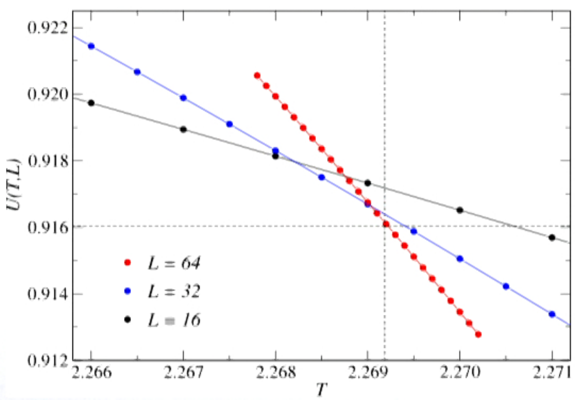

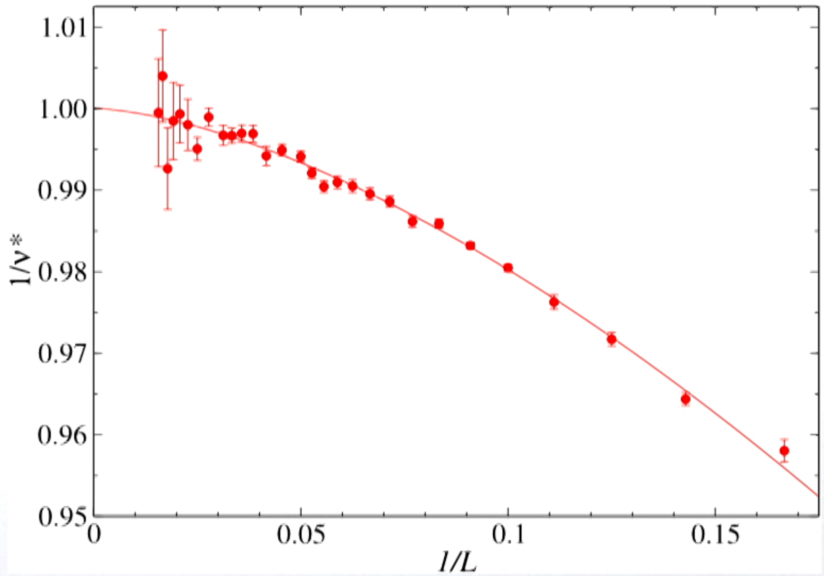

Extrapolated exponent
1/ν=1.0001(7)

Note: exponent ω is large here → fast convergence

J-Q model: Exponent ν from crossing-point analysis

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

Binder ratio of the spin order parameter

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

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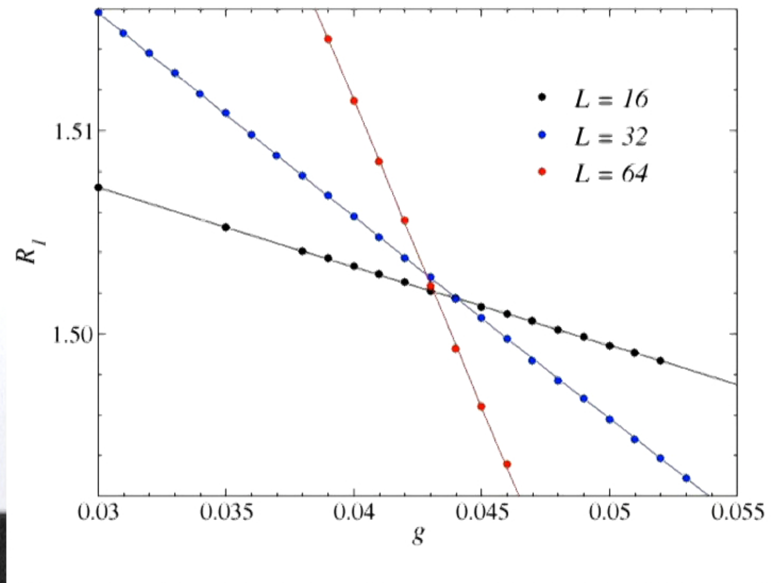

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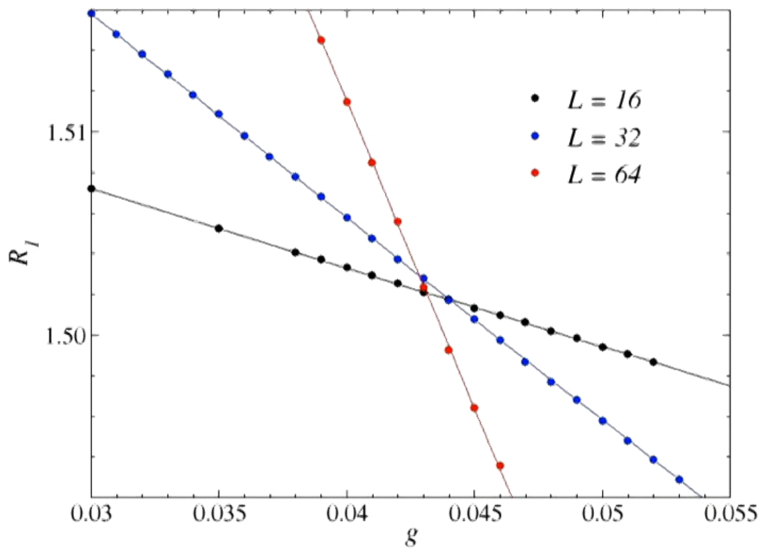

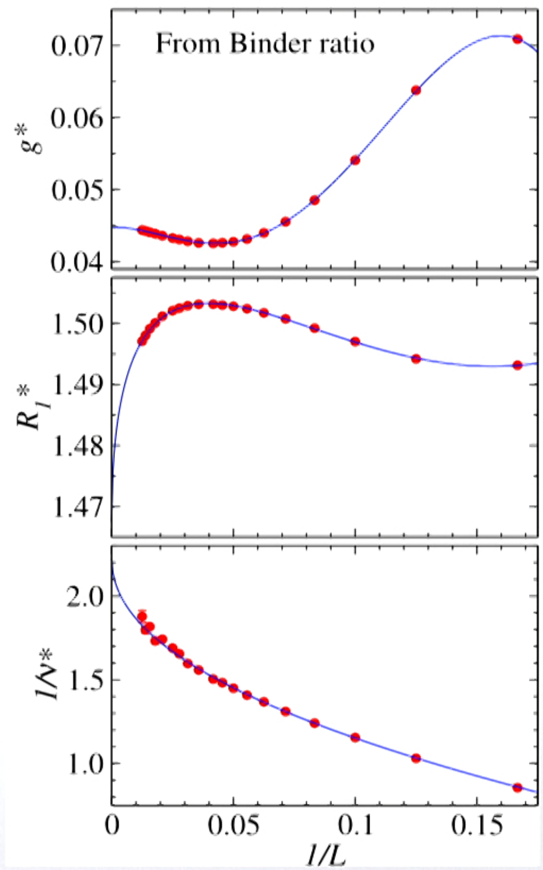

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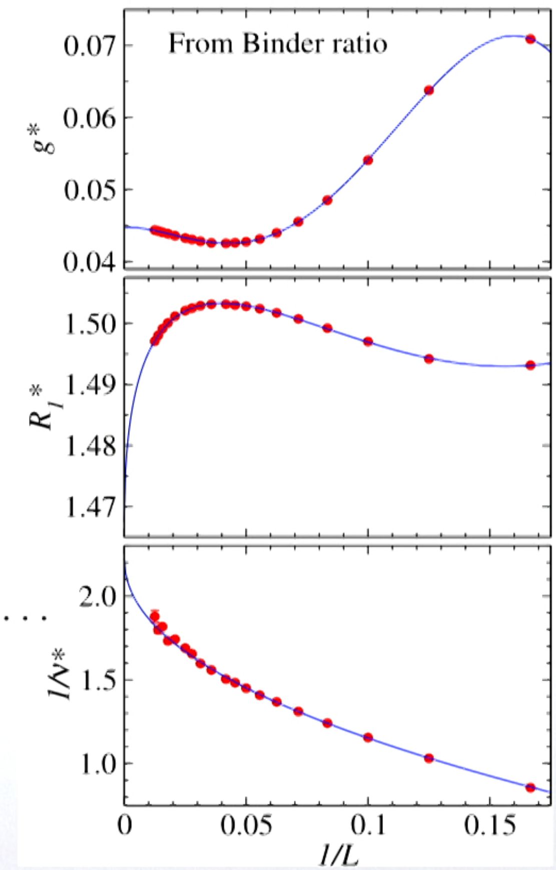
$$s(g,L) = dR_1(g,L)/dg \quad \text{(slope)}$$

- **Small correction exponent; ω ≈ 0.4**
- **ν = 0.45 +/- 0.01**



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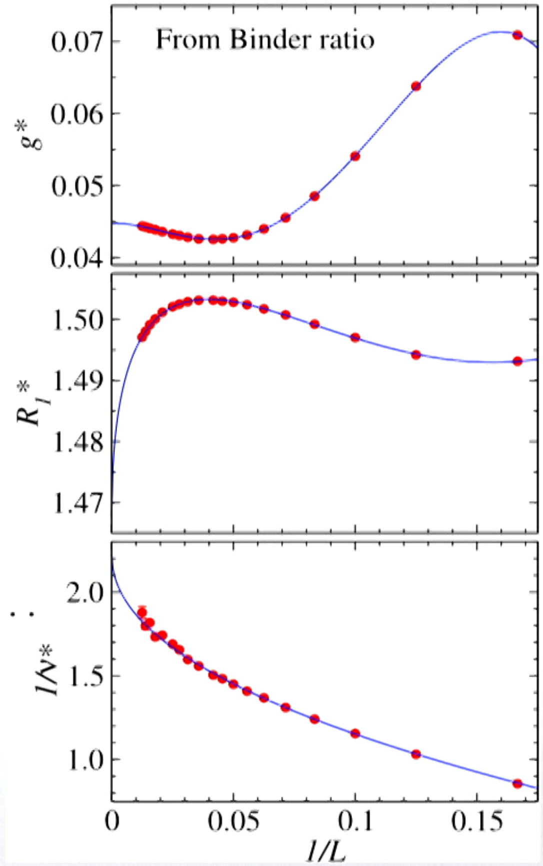


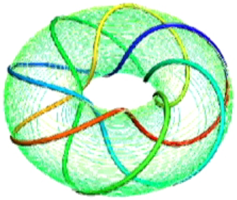
No sign of first-order transition (then ν=1/3 in finite-size scaling)

Anomalous scaling behavior - weak first-order transition?

First-order scenario: Prokofe'v, Svistunov, Kuklov, Troyer,... (2008-2013)
Jiang, Nyfeler, Chandrasekharan,Wiese (2008)

Anomalous scaling of winding numbers

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



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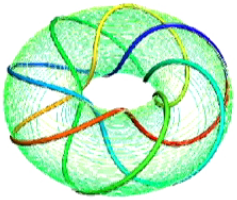

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$\rightarrow \langle W^2\rangle = \text{constant}$

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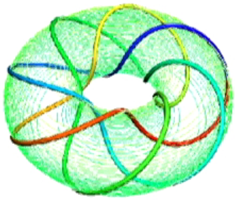

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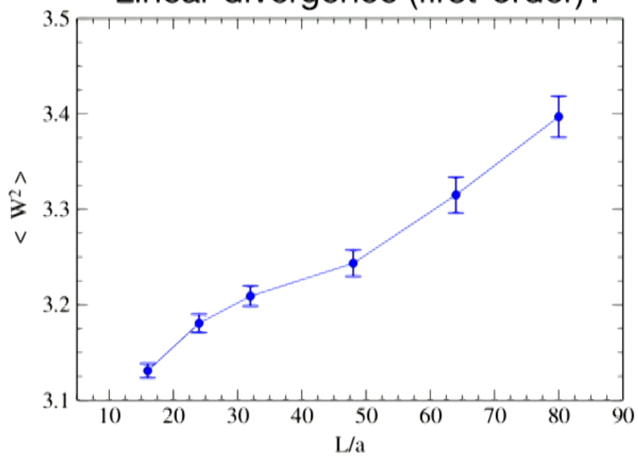

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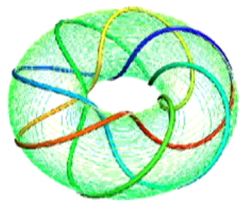

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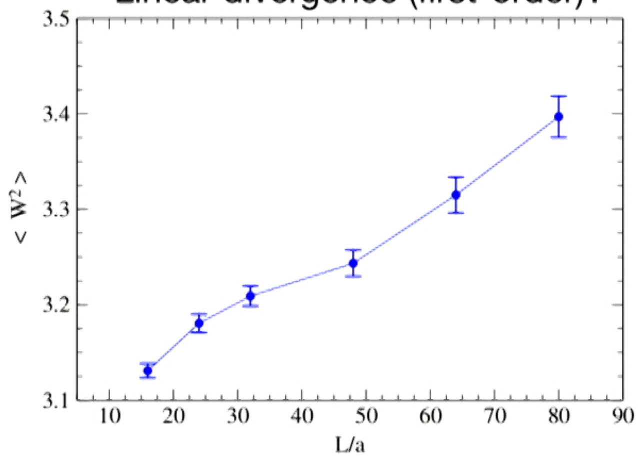
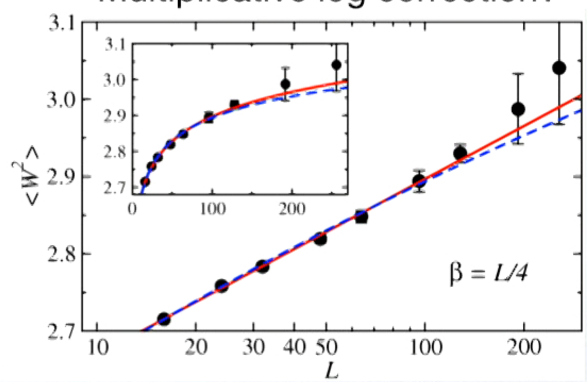


Jiang et al. (2008)

Multiplicative log correction?



(Sandvik, PRL 2010)
Also consistent with power-law

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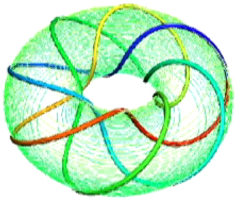

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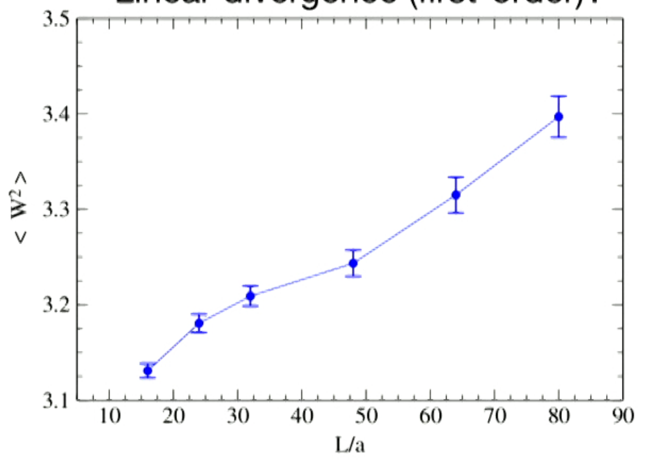

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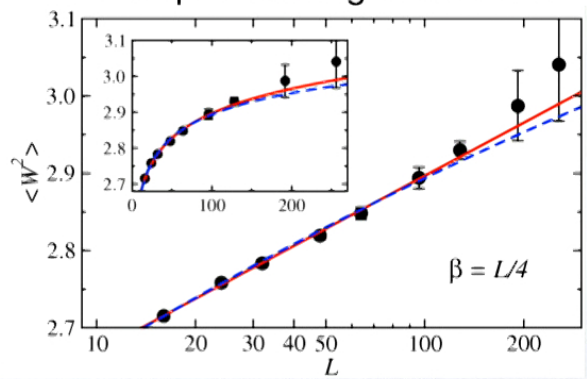

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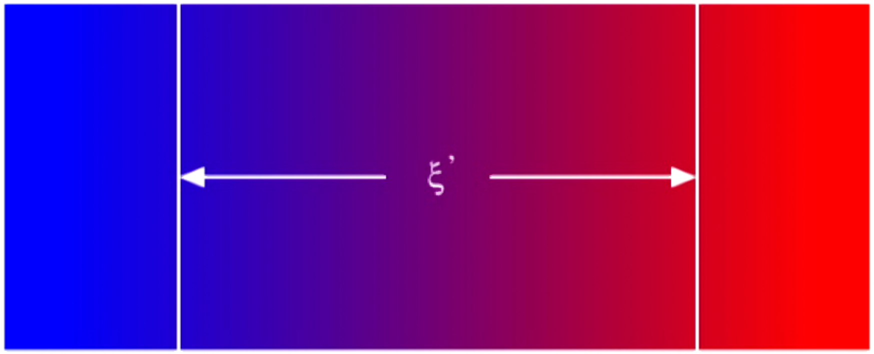
Could the anomalous behavior be a consequence of two length scales?

Two length scales - VBS domain walls

In some classical systems (clock models,...) the thickness of a domain wall is larger than the correlation length: $\xi \sim \delta^{-\nu}, \quad \xi' \sim \delta^{-\nu'}, \quad \nu' > \nu$



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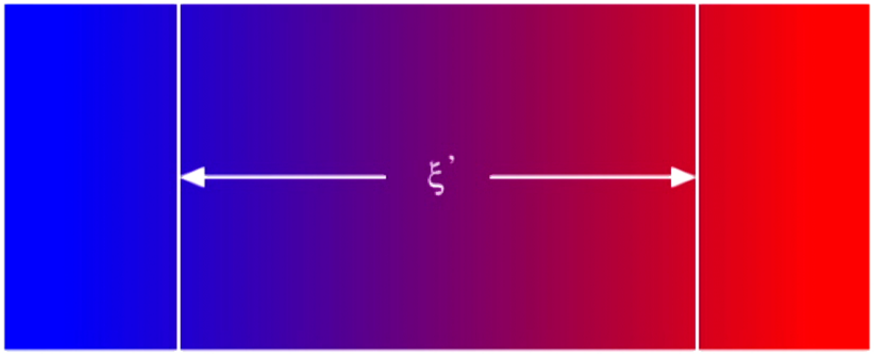

Free-energy cost of wall:

$\Delta F \sim \xi^{d-2} \xi'^{-1} L^{d-1}$

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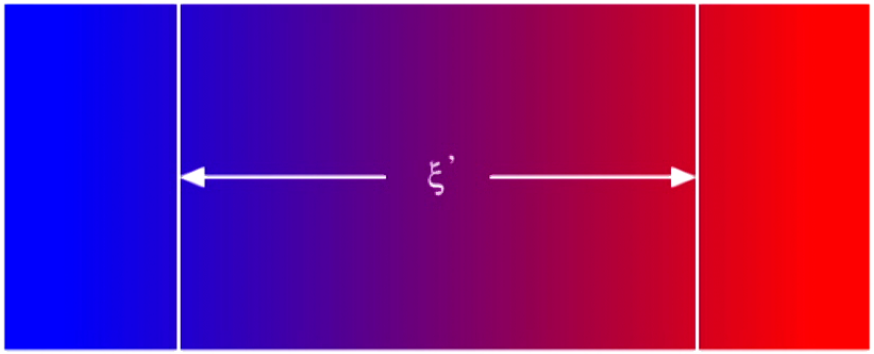

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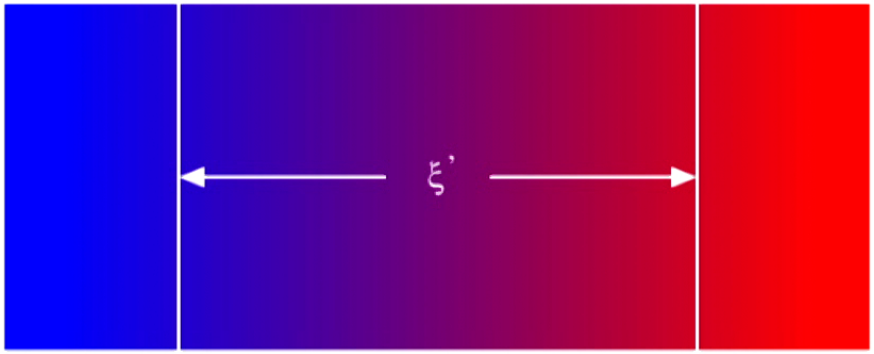

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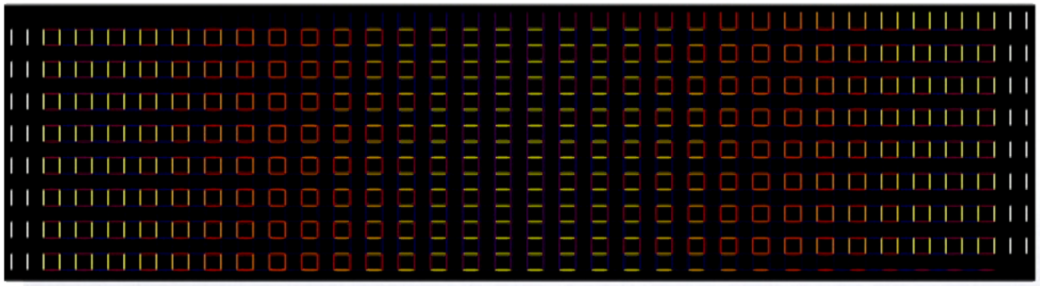
Deconfined quantum-criticality: VBS domain wall should have this property



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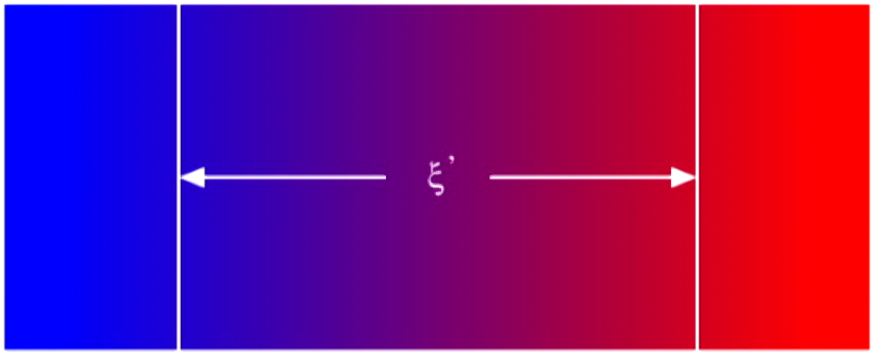

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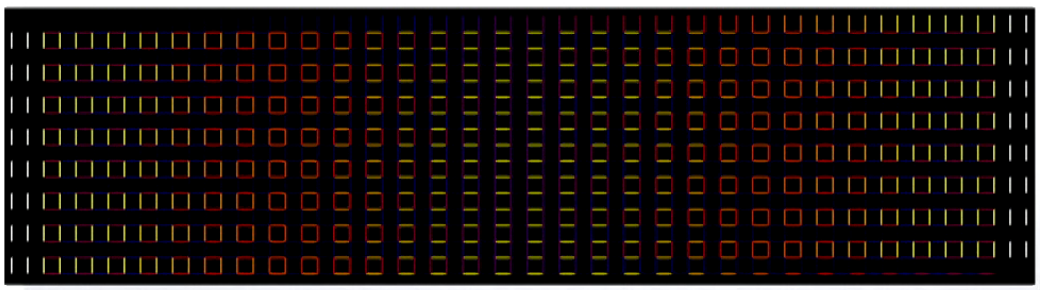


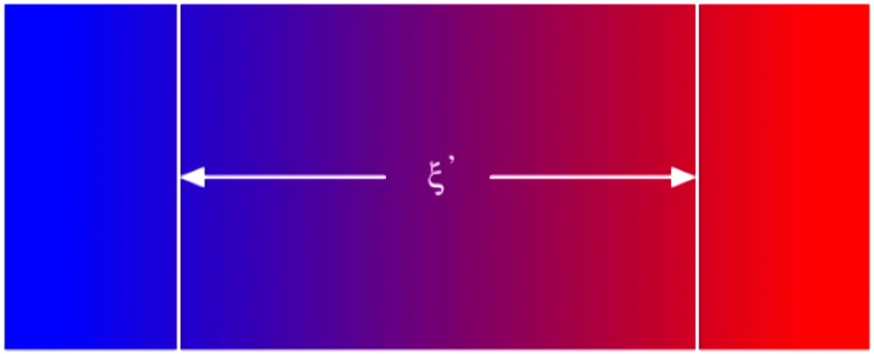
Ground state energy cost of wall:

$$\kappa \sim \xi^{-1}\xi'^{-1}$$

(Senthil et al.)

Two length scales - VBS domain walls

In some classical systems (clock models,...) the thickness of a domain wall is larger than the correlation length: $\xi \sim \delta^{-\nu}, \quad \xi' \sim \delta^{-\nu'}, \quad \nu' > \nu$



Free-energy cost of wall:

$\Delta F \sim \xi^{d-2} \xi'^{-1} L^{d-1}$

Define: $\kappa = \Delta F / L^{d-1}$

$\kappa \sim \xi^{d-2} \xi'^{-1}$

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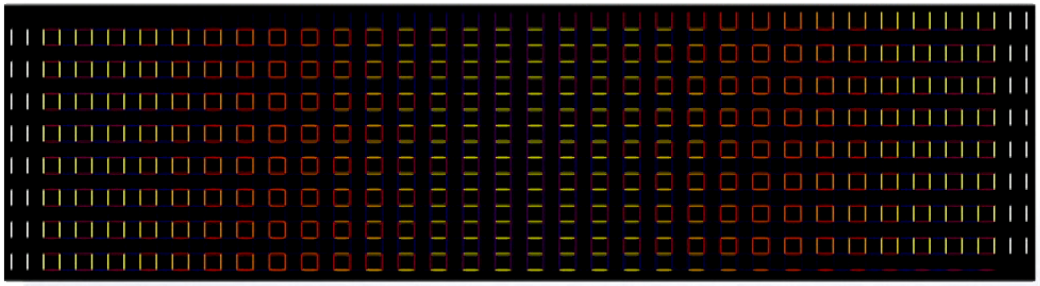

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➜ finite-size scaling studies of clock/VBS domain walls

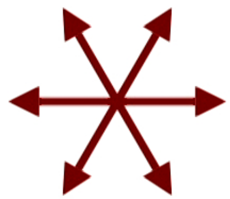
Domain-wall energy in the 3D clock model

3D q-state clock model (q>3)

- basic example of dangerously irrelevant perturbation [to U(1) symmetry]

$$H = -J \sum_{\langle ij \rangle} \cos(\Theta_i - \Theta_j)$$

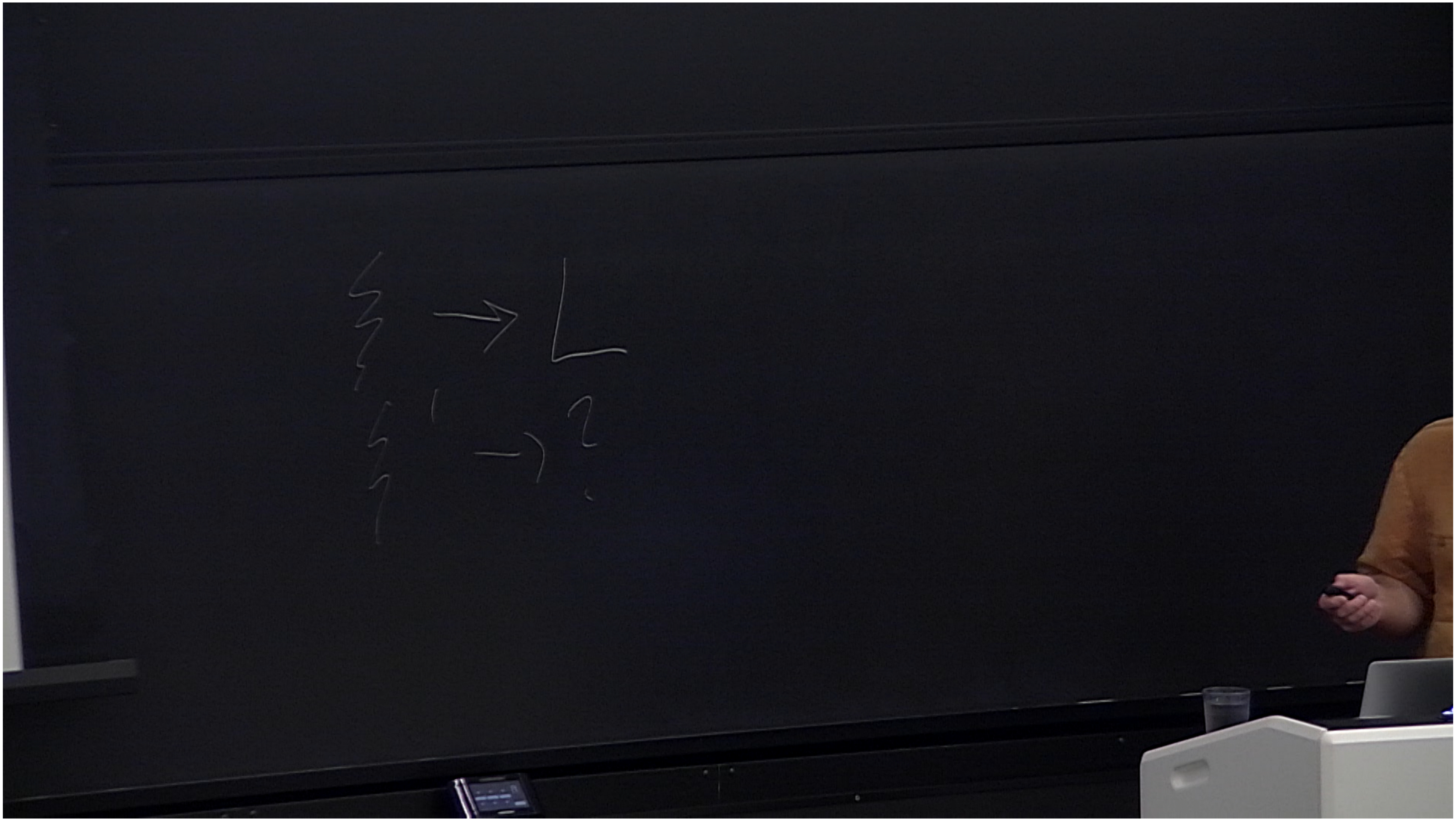
- restriction to "clock" angles



$$q = 6$$

The prediction for the domain wall energy in the thermodynamic limit is

$$\kappa \sim \frac{1}{\xi} \frac{1}{\xi'}$$



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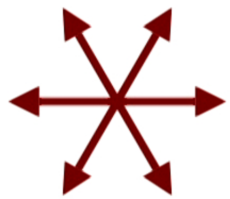

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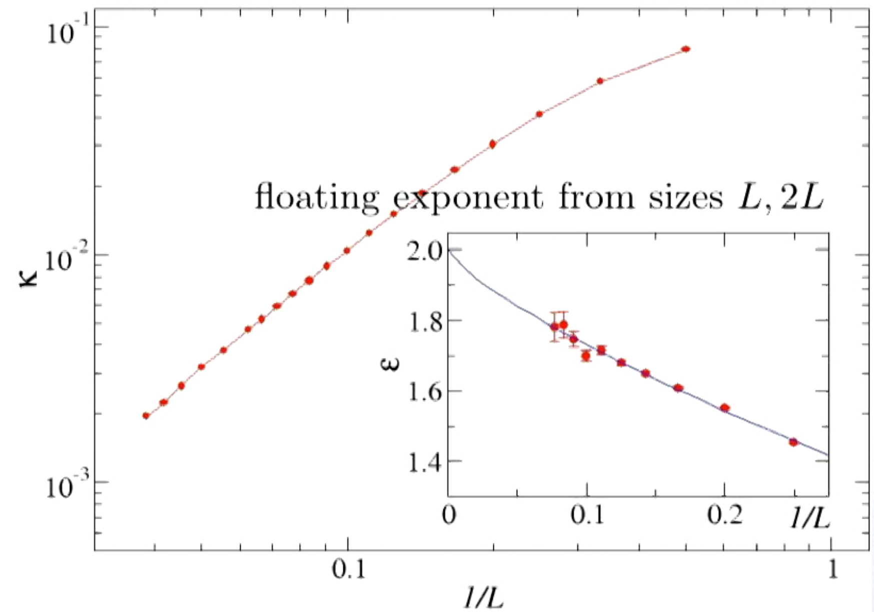
Finite-size scaling at Tc shows

$$\kappa \sim L^{-2}$$

$$\xi' \sim \xi^{\nu'/\nu}, \quad \nu'/\nu \approx 2 \quad (q = 6)$$



VBS Domain-wall scaling in the critical J-Q model

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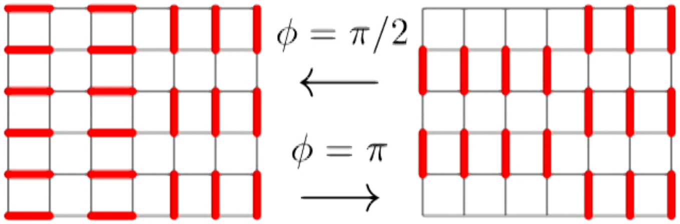
Two kinds of VBS domain walls can be imposed in open-boundary systems



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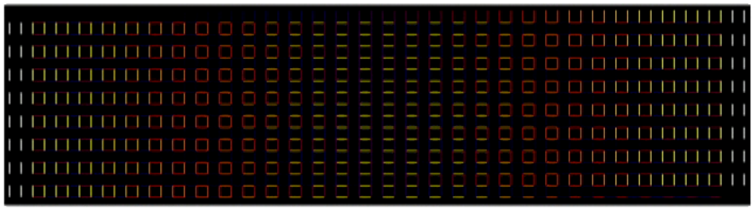

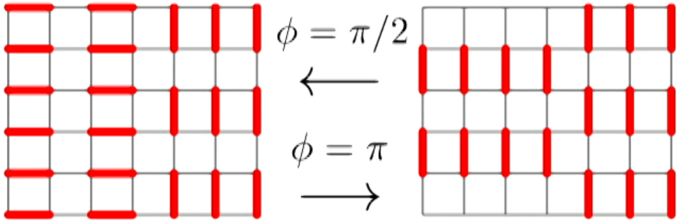

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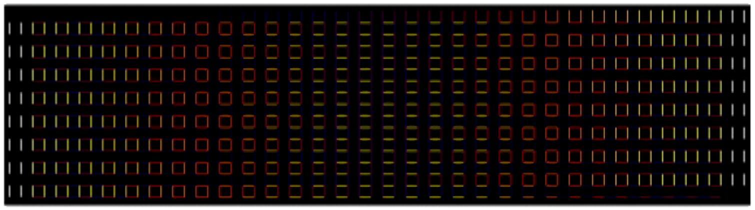

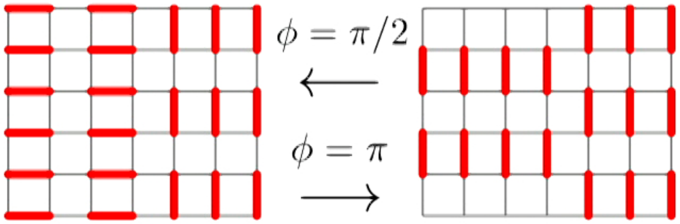

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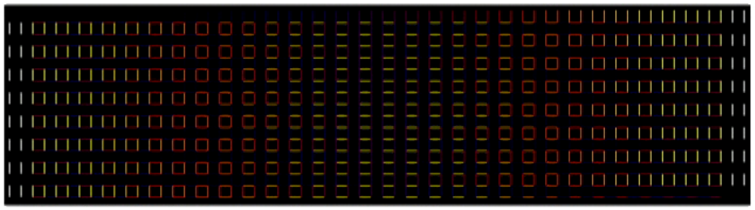

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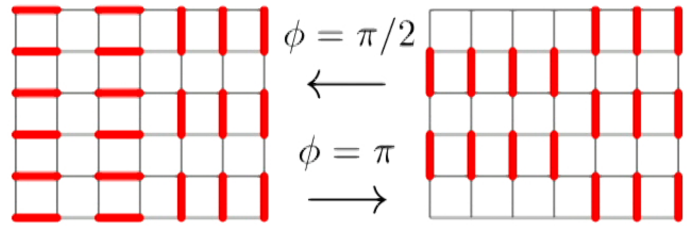

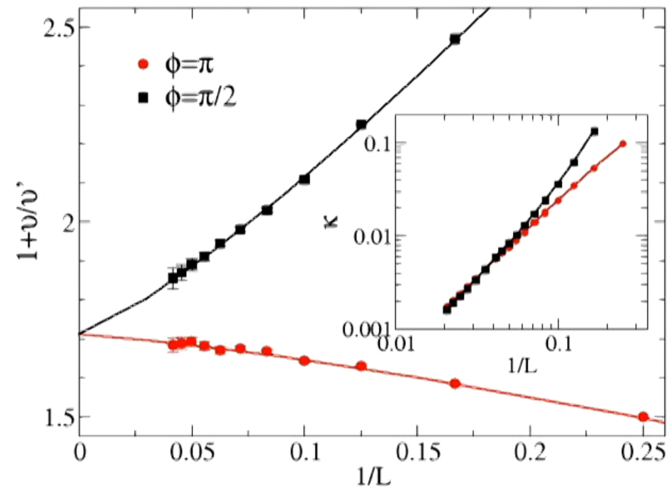

$$\ln[\kappa(L)/\kappa(2L)]/\ln(2) \to 1 + \nu/\nu'$$

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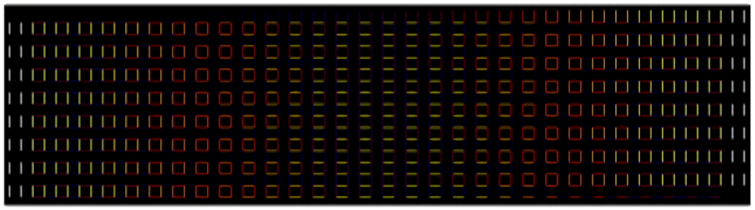

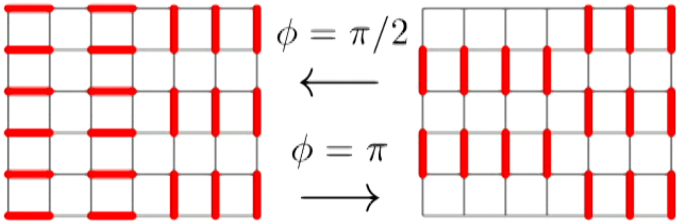

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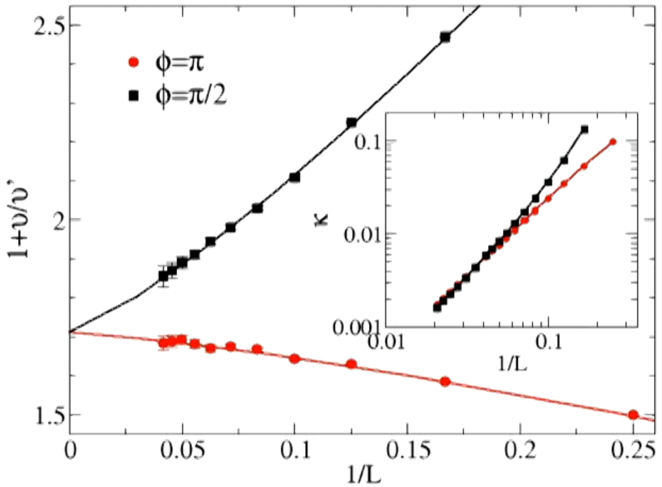

Ambiguity in finite-size scaling:

option 1) $\xi \rightarrow L$, $\xi' \rightarrow L^{\nu'/\nu}$: $\kappa \sim L^{-(1+\nu'/\nu)}$

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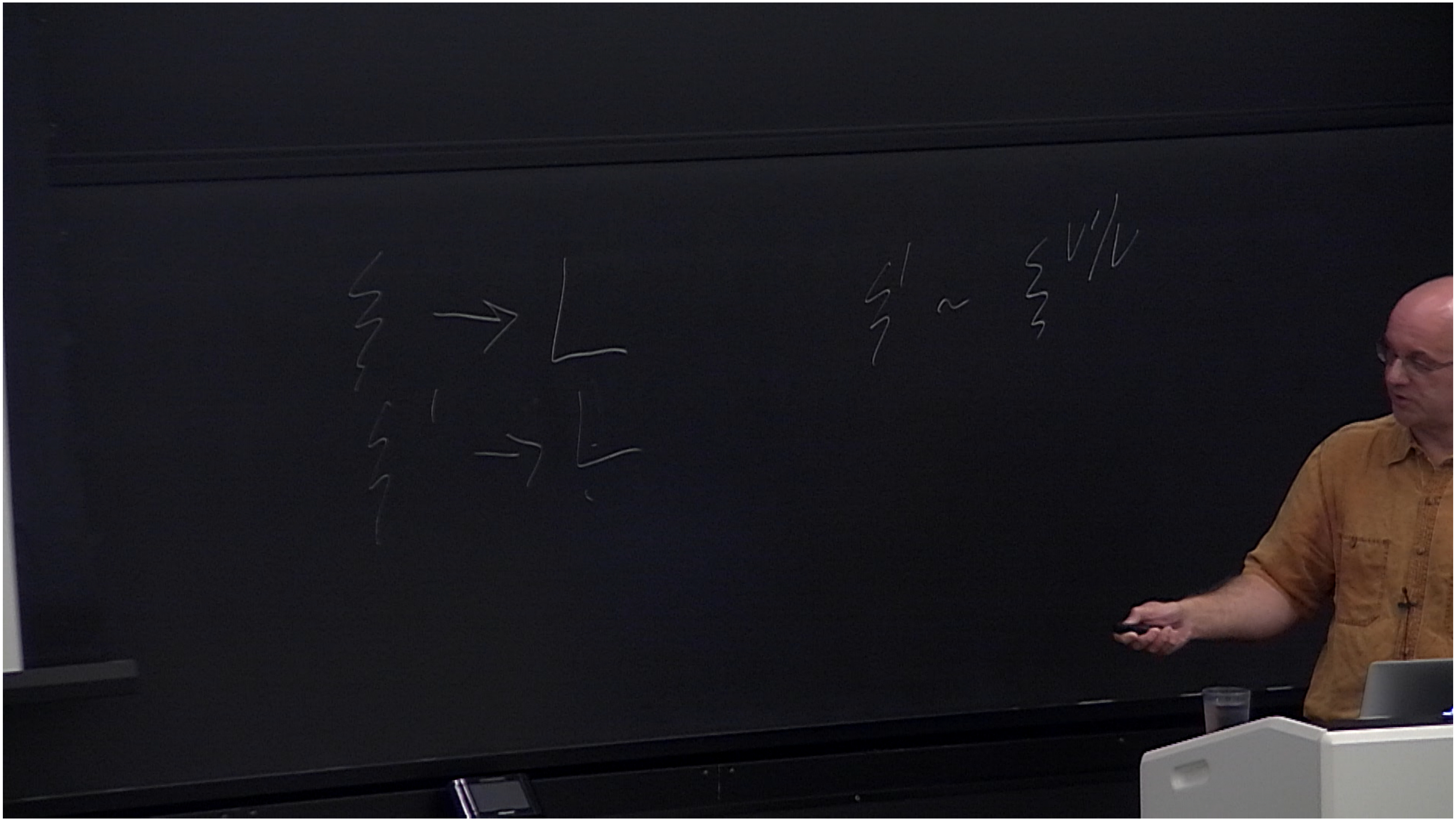
ξ → L
ξ' → L'
ξ' ~ ξ^{ν'/ν}

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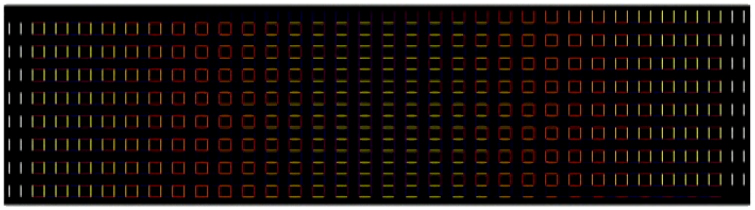

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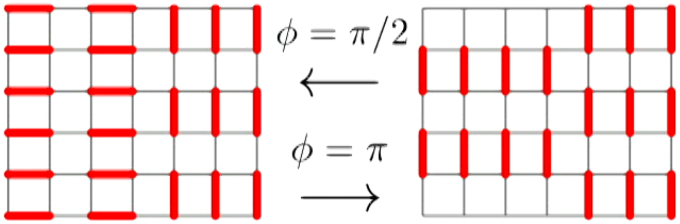
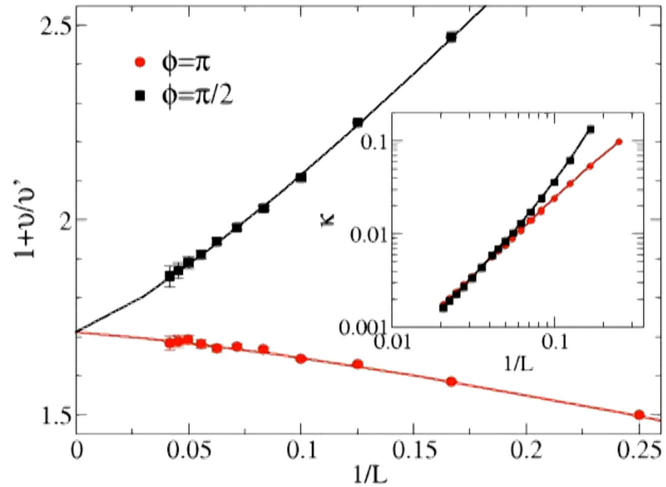
Results show option 3 (exponent < 2):

ν/ν' ≈ 0.715 +/- 0.015





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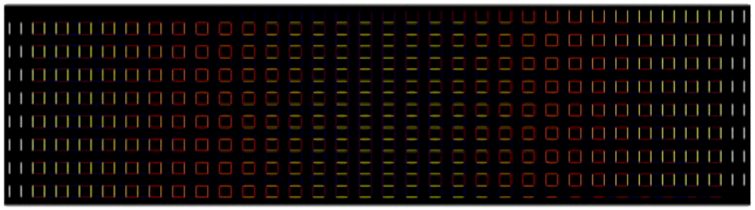

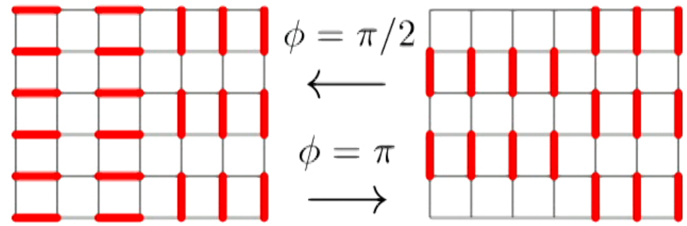

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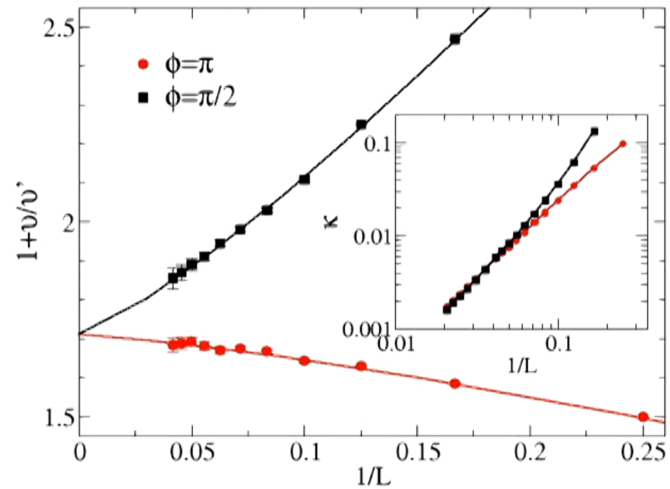

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Demonstrates explicitly two divergent length scales!

- different from standard "dangerously irrelevant" perturbation

Quantum criticality with two lengths

Quantum criticality with two lengths

Two divergent lengths tuned by one parameter: $\xi \propto \delta^{-\nu}, \quad \xi' \propto \delta^{-\nu'}$

Finite-size scaling of some quantity A. Thermodynamic limit: $A \propto \delta^{\kappa}$

Conventional scenario

$$A(\delta, L) = L^{-\kappa/\nu} f(\delta L^{1/\nu}, \delta L^{1/\nu'})$$

When L→∞: $f(\delta L^{1/\nu}, \delta L^{1/\nu'}) \to (\delta L^{1/\nu})^{\kappa}$

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The first scenario has so far been assumed
- unexplained drifts in $L\rho_s$ in J-Q and other models (z=1, d=2)

Evidence for unconventional scaling in J-Q model

(L,2L) crossing-point analysis of $L\rho_s$ and $L\chi$

The conventional scaling form

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

Replaced by new form

$$\rho_s, \chi \propto L^{-\nu/\nu'}$$

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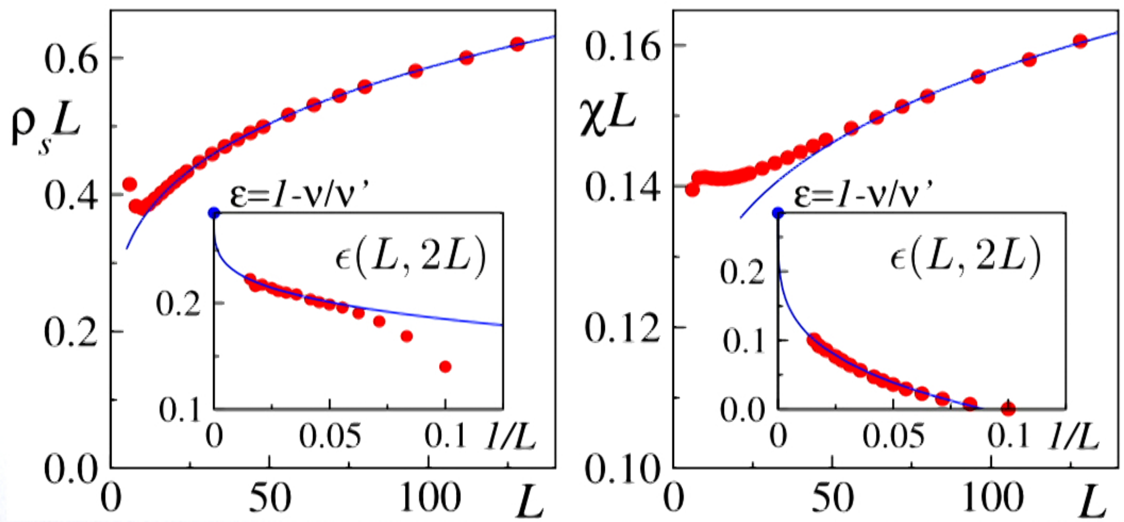

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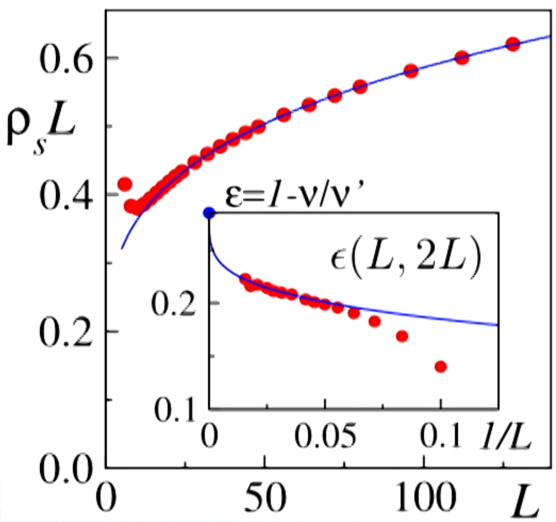

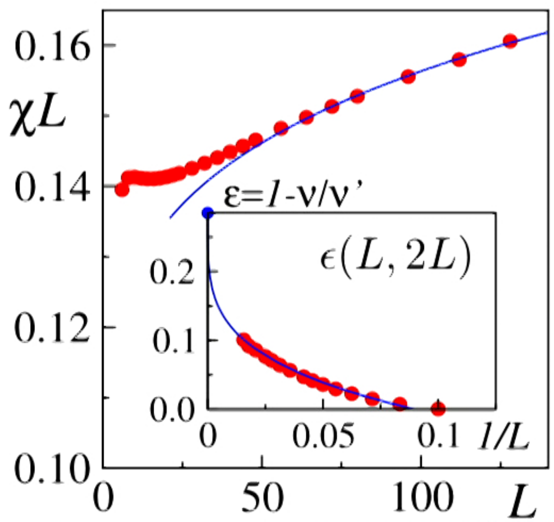

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Fixed; taken from domain-wall scaling fit

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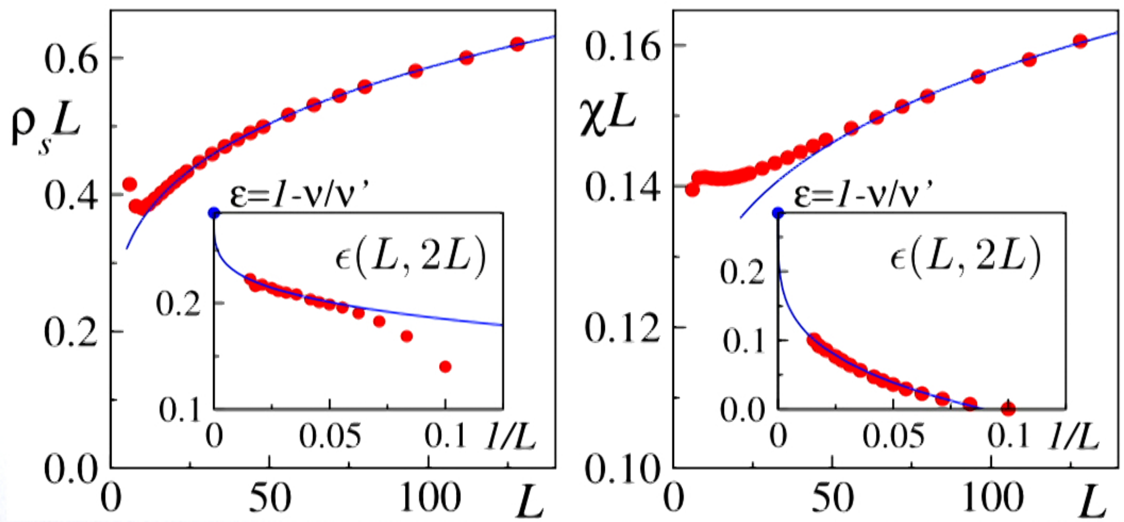

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Behavior interpreted (by some) as first-order transition is actually unconventional scaling related to two divergent lengths!

Further tests of consistent scaling exponents

The expected behaviors including finite-size corrections are

$$\rho_s L = L^{\epsilon}(1 + a_1 L^{-\omega_1} + a_2 L^{-\omega_2} + \ldots)$$

$$\chi_u L = L^{\epsilon}(1 + b_1 L^{-\omega_1} + b_2 L^{-\omega_2} + \ldots)$$

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Leading power: $\epsilon = 1 - \nu/\nu' \approx 0.285$

Small leading correction exponent: $\omega_1 \approx 0.3$

The prefactors of the corrections depend on details:

- one can expect $a_i(r)$, $b_i(r)$
- r is the space-time aspect ratio; $\beta = L/r$
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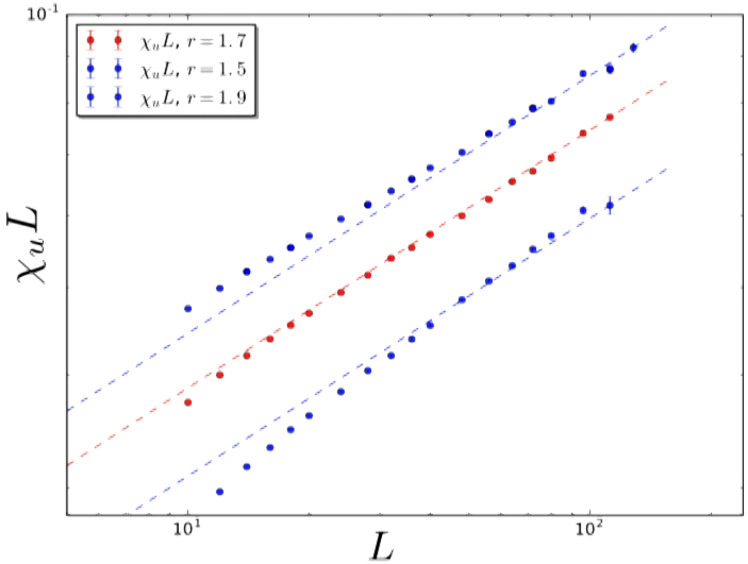
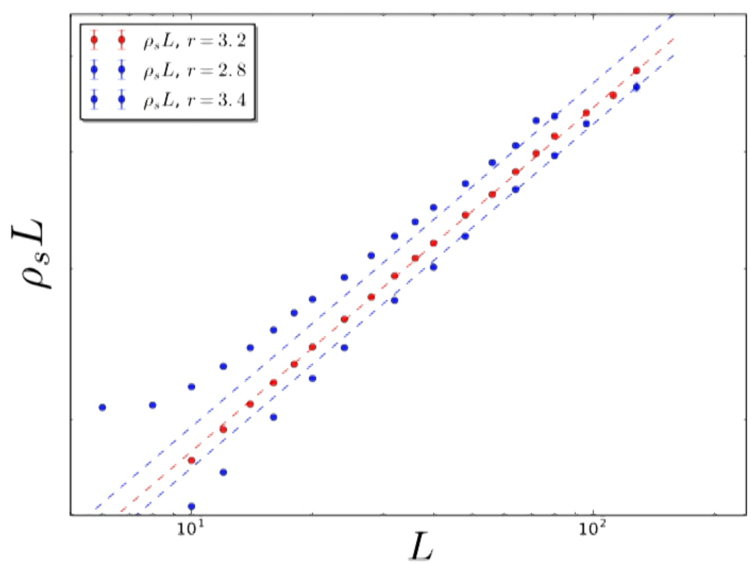
Calculations with different r to test for optimum
(Bowen Zhao, Hui Shao, AWS, work in progress)

Some preliminary results....

Results for different aspect ratios r





Apparent change in sign of the leading correction
- optimal aspect ratios r ≈ 1.7 (susceptibility), r ≈ 3.2 (spin stiffness)

Quantitative analysis

Three g-values close to the critical point, near-optimal aspect ratios

- exponent $\varepsilon=1-\nu/\nu'$ extracted from (L,2L) size pairs

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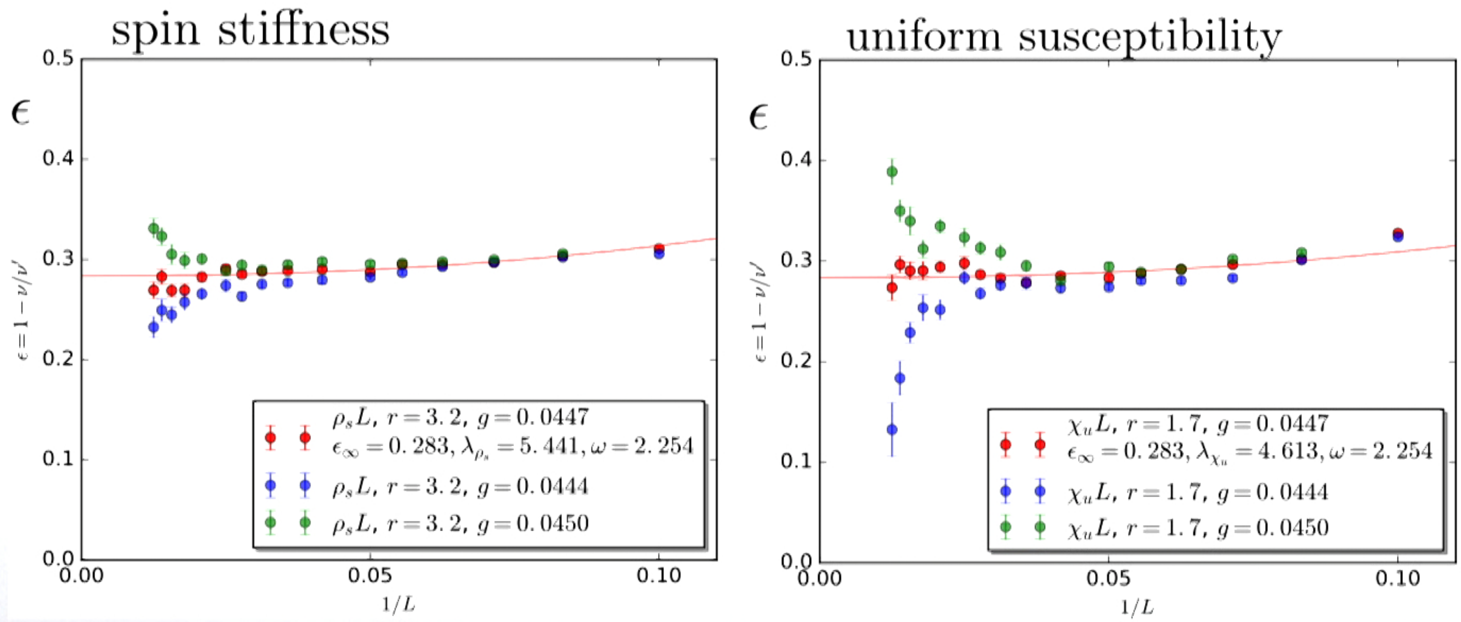

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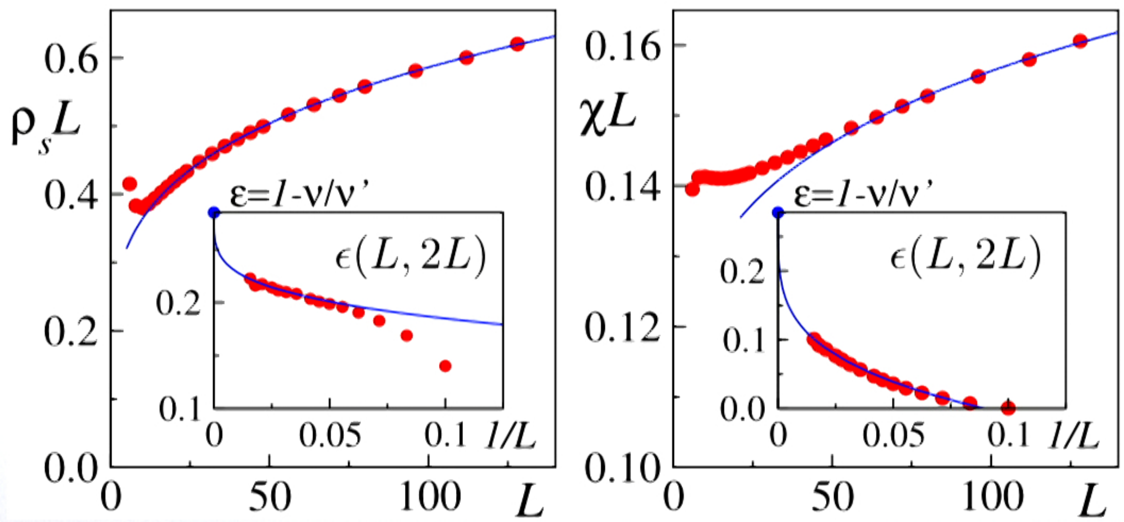

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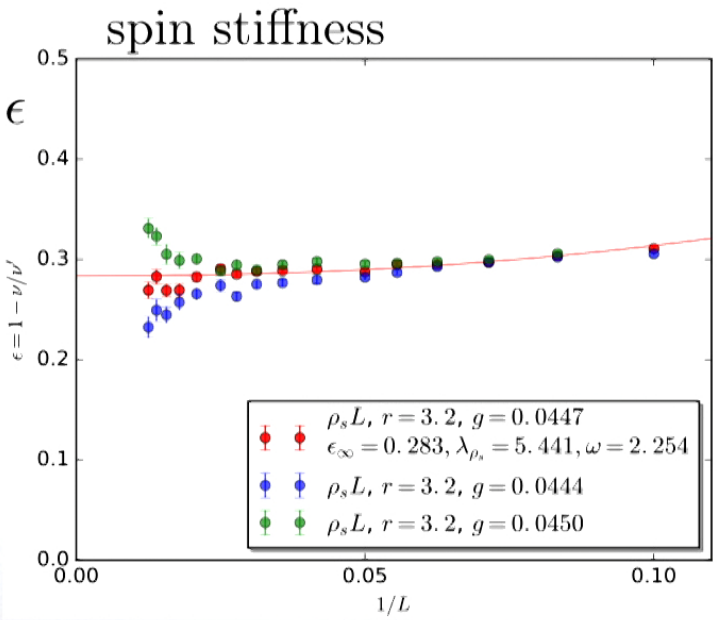

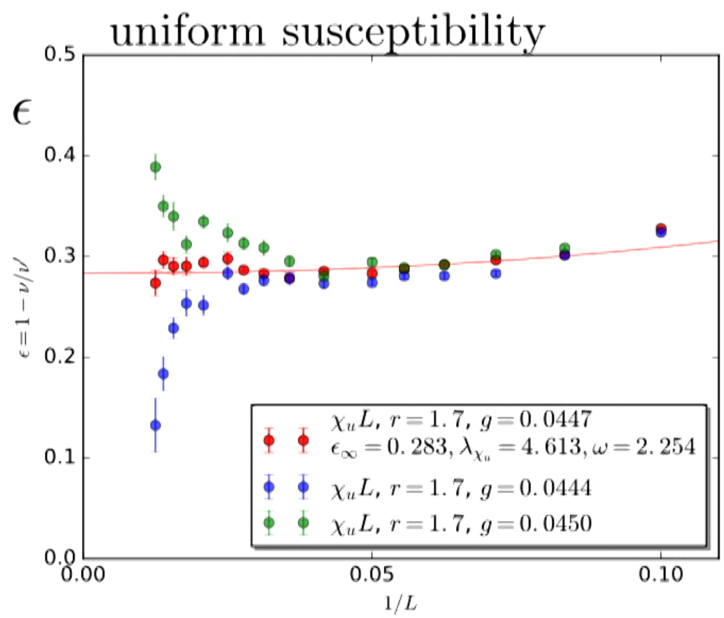

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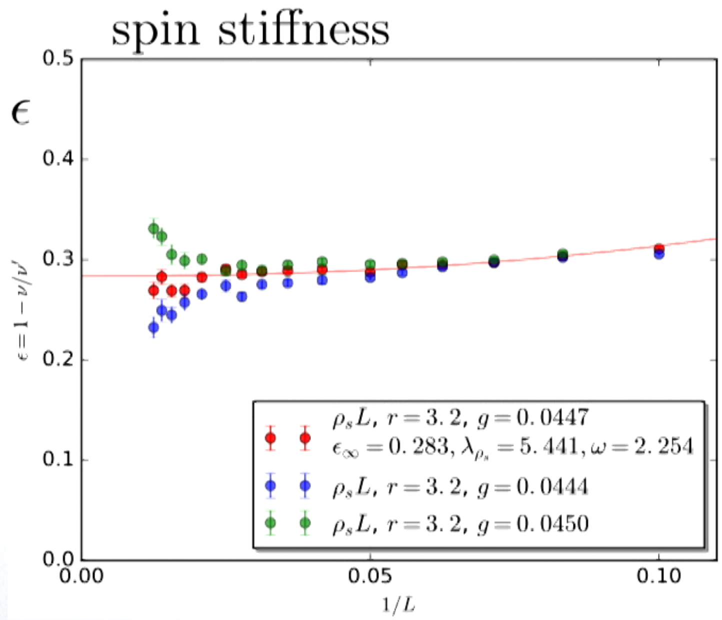

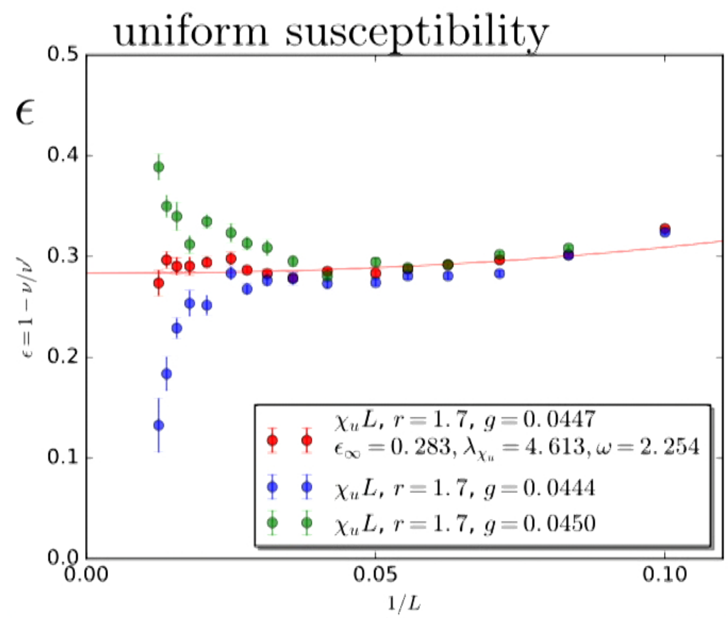

The critical point is very close to 0.0447

Exponent in full agreement with the domain-wall value

Unconventional T>0 critical scaling

Conjecture involving the two length-scale exponents:

$$\xi_T \propto T^{-1/(z\nu/\nu')}(1 + aT^{\omega_\xi}),$$
$$\chi_T \propto T^{(d/z-1)\nu/\nu'}(1 + bT^{\omega_\chi})$$

$$\nu/\nu' \approx 0.72$$

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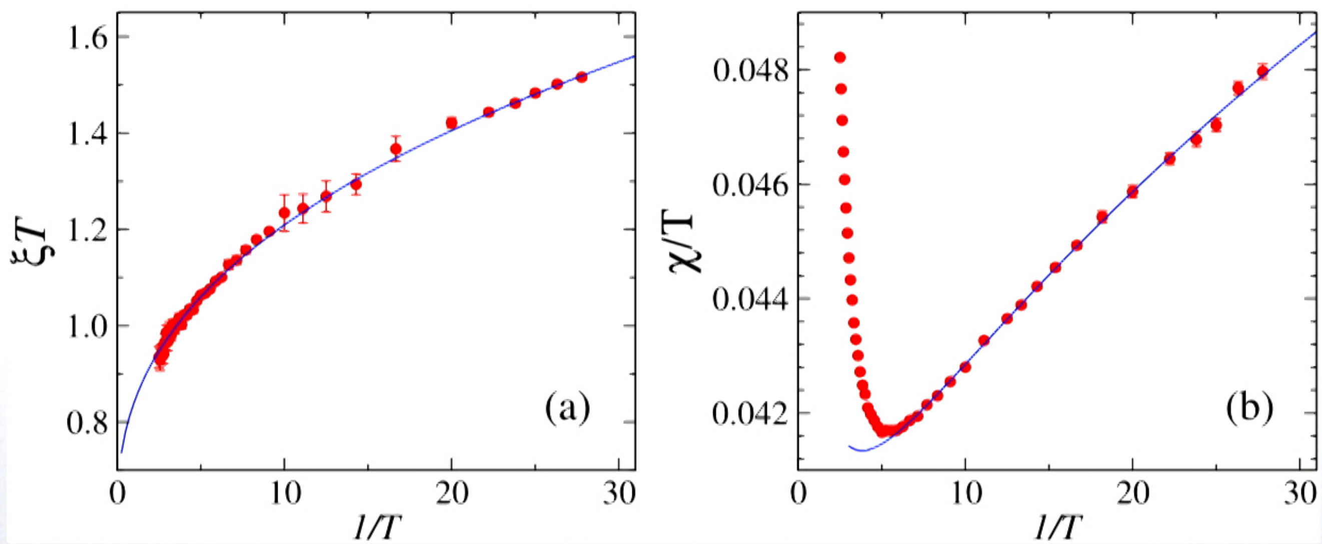

Conclusions

Two length scales observed explicitly in the J-Q model

No signs of first-order transition

Simple two-length scaling hypothesis explains anomalous scaling of spin stiffness and susceptibility
- conventional wisdoms need to be revised

Finite-temperature

- T>0 corresponds to thickness of quantum system in imaginary time
- scaling laws from finite-size scaling forms

Standard T>0 critical scaling forms have to be reconsidered
- existing J-Q results support unconventional forms with ν/ν'
- experimentally important

How general is this kind of two-length criticality?