# Quantum criticality with two length scales
# 两尺度量子临界性

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# Collaborators

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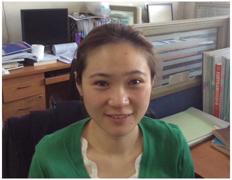


- Anders W. Sandvik, Boston University

References:

1. Science 354, 213 (2016).

2. PRB 91, 094426 (2015).

# outline

Background

Unconventional scaling form with two-length scales

Quantum Monte Carlo methods

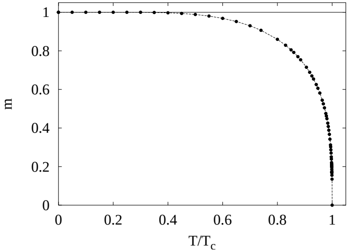
Numerical results

Anomalous critical scaling at finite temperature

Conclusions

# Thermal phase transitions

- At critical point, thermal fluctuations: divergent length scale leads to singularity
- Quantum mechanics is largely irrelevant




3D Ising FM-Paramagnetic transition (MC simulation)

- The coarse grained continuum field description: Landau-Ginzburg-Wilson Hamiltonian

$$H(\mathbf{\Phi}) = \int \mathrm{d}\mathbf{r}((\nabla\mathbf{\Phi})^2 + s\mathbf{\Phi}^2 + u(\mathbf{\Phi}^2)^2); \quad \mathcal{Z} = \int \mathcal{D}\mathbf{\Phi}\ \mathrm{e}^{-H(\mathbf{\Phi})}$$

  $\mathbf{\Phi}$ is the order parameter, $s$ is a function of $T$.
- Meanfield: $\mathbf{\Phi}^2 = -s/2u$ for $T < T_c \quad (s \sim s'(T - T_c))$.
- well understood within Wilson's RG framework;
  - longrange order $\langle \mathbf{\Phi} \rangle \neq 0$: spontaneous symmetry breaking
  - universality class: symmetry and dimensions

# Quantum phase transitions

- happens at zero temperature, when adapt $g$ in $H = H_0 + gH_I$; $[H_0, H_I] \neq 0$, continueous transition
- at $g_c$, the correlation length diverges, due to quantum fluctuations
- path integral maps $D$-dim quantum systems onto classical field theories in $(D+1)$-dim

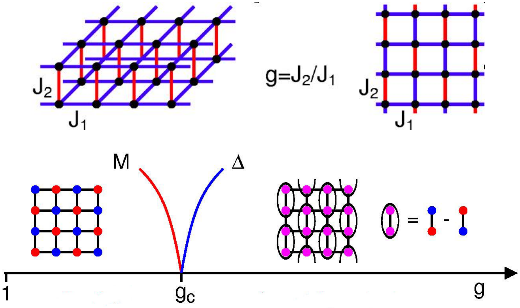
$$\mathcal{S}(\mathbf{\Phi}) = \int \mathrm{d}\mathbf{r}\mathrm{d}\tau((\partial_\tau \mathbf{\Phi})^2 + v^2(\nabla_x \mathbf{\Phi})^2 + s\mathbf{\Phi}^2 + u(\mathbf{\Phi}^2)^2)$$

$$Z = \int \mathcal{D}\mathbf{\Phi} \;\; \mathrm{e}^{-\mathcal{S}(\mathbf{\Phi})}$$

- many of these transitions can be understood in the conventional Landau-Ginzburg-Wilson framework

- for example: AF Néel-Paramagnetic transition

  $H_0$ is AF Heisenberg Hamiltonian, $g = J_2/J_1$




  - 3D classical Heisenberg universality class: confirmed by QMC
  - Experimental realized

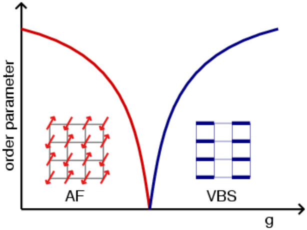
However, many strongly-correlated quantum materials seem to defy such a description and call for new ideas

**for example, continuous transition from Néel to VBS state**

# Deconfined quantum criticality

**describes the direct continuous transition from Néel to VBS in 2D**

Senthil, Vishwanath, Balents, Sachdev, Fisher; Science (2004)




- violates the "Landau rule":
  - Néel-param should be in the 3D O(3) universality class;
  - away from VBS should be in the 3D O(2) universality class.

    ($Z_4$ anisotropy is dangerously irrelevant)

Léonard and Delamotte, PRL 2015

Néel order parameter

$$\mathbf{m}_s = \frac{1}{N}\sum_i (-1)^{x_i+y_i}\mathbf{S}_i$$

VBS order parameter $(D_x, D_y)$

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

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

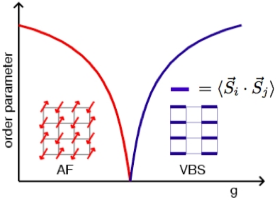
New physics

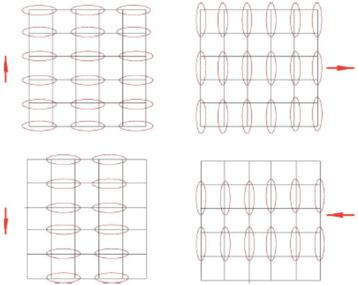
- Order parameters of the Néel state and the VBS state are NOT the fundamental objects, they are composites of fractional quasiparticles carrying $S = 1/2$

# Physical picture from VBS side

Levin and Senthil, PRB 70, 2004

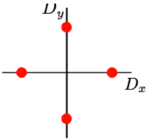
VBS: 4 symmetry broken ground states



similar to classical 4-state clock model

$$H = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j), \quad \theta_i = n\pi/2, \;\; n = 0, 1, 2, 3$$



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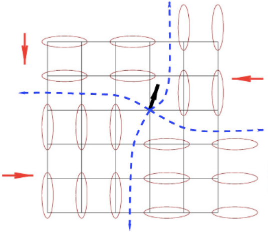
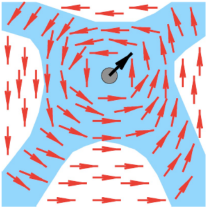




- Blue-shaded regions are domain walls
- The thickness $\xi'$ diverges faster than $\xi$
- emergent $U(1)$ symmetry; same as 4-state clock model ($Z_4$anisotropy is dangerously irrelevant)

- At the core of the $Z_4$ vortex, there is a spinon: unpaired spin
- different from 4-state clock model

- Spinons bind together in the VBS state (confinement) and condensate the Néel state, deconfine at the critical point leading to a continuous phase transition
- New universality: neither O(2) nor O(3)

# Deconfined quantum criticality

Field-theory description with spinor field **z**

- Order parameters of the Néel state are composites of spinons

$$\mathbf{\Phi} = z^\dagger \boldsymbol{\sigma} z$$

  $z$: spinor field (2-component complex vector); $\boldsymbol{\sigma}$: Pauli

- Non-compact $CP^1$ action

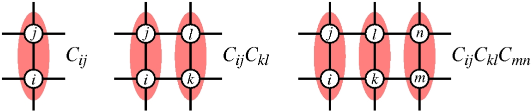
- Only SU(N) generalization can be sloved when $N \to \infty$, nonperturbative numerical simulations are required to study small $N$

- The most natural physical realization of the Néel-VBS transition for SU(2) spins is in **frustrated quantum magnets** however, notoriously difficult to study numerically: sign problem in QMC

# Designer Hamiltonian: *J*-*Q* model

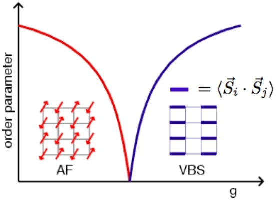
Sandvik designs the *J*-*Q* model (2007)

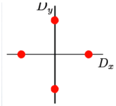
$$H = -J \sum_{\langle ij \rangle} C_{ij} - Q \sum_{\langle ijkl \rangle} C_{ij} C_{kl}, \quad C_{ij} = (\frac{1}{4} - \mathbf{S}_i \cdot \mathbf{S}_j)$$




Lattice symmetries are kept ($J - Q_2$ version similar)

- large $Q$, columnar VBS
- small $Q$, Néel
- No sign problem
- ideal for QMC study of the DQC physics




Sandvik, PRL 98, 227202(2007)

# Finite-size scaling

- Correlation length divergent for $T \to T_c$: $\xi \propto |\delta|^{-\nu}, \delta = T - T_c$(or $g - g_c$)
- Other singular quantity: $A(T, L \to \infty) \propto |\delta|^{\kappa} \propto \xi^{-\kappa/\nu}$
- For L-dependence at $T_c$ just let $\xi \to L$: $A(T \approx T_c, L) \propto L^{-k/\nu}$
- Close to critical point: $A(T, L) = L^{-\kappa/\nu} g(L/\xi) = L^{-\kappa/\nu} f(\delta L^{1/\nu})$

For example

$$\chi(T, L \to \infty) \propto \delta^{-\gamma}$$

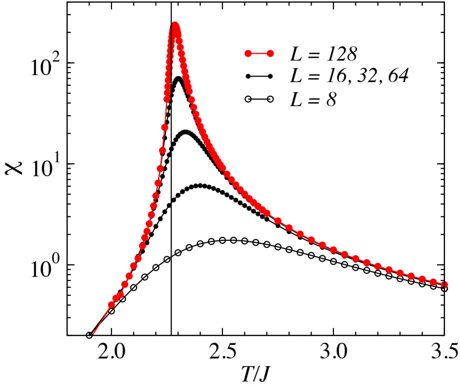
data collapse

$$\chi(T, L) L^{-\gamma/\nu} = f(\delta L^{1/\nu})$$

2D Ising model, use $\gamma = 7/4, \nu = 1$

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

When these are not known, treat as fitting parameters



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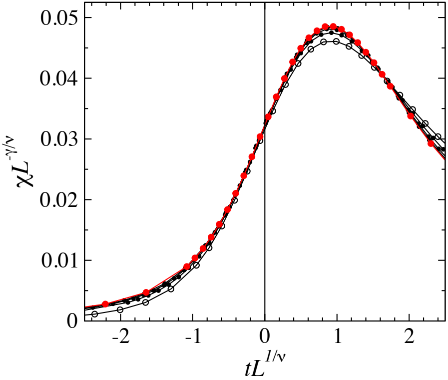


# systematic critical-point analysis

- include corrections to scaling are included (RG theory); $u_i$ are irrelevant fields

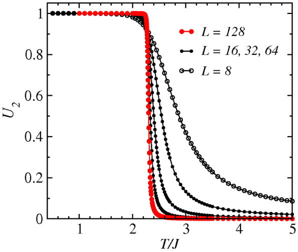
$$AL^{\kappa/\nu} = f(\delta L^{1/\nu}, u_1 L^{-\omega_1}, u_2 L^{-\omega_2}, \dots)$$

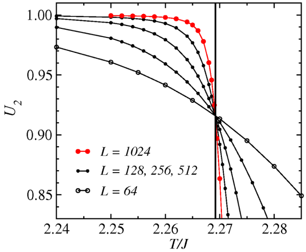
Binder cumulant $U = \frac{1}{2}(3 - \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2})$, dimensionless $\kappa = 0$

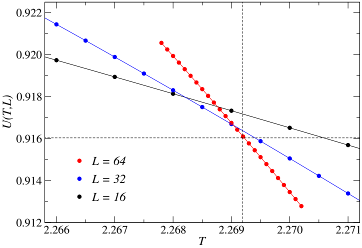
$$U = f(\delta L^{1/\nu}, u_1 L^{-\omega_1}, u_2 L^{-\omega_2}, \dots)$$

- (almost) size-independent at $T_c$ leads to crosssings at $T_c$

2D Ising model; MC results





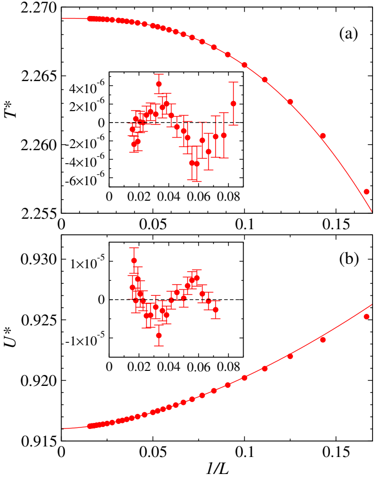

Drift in $(L, 2L)$ crossing points

- scaling corrections in crossings

$$T^*(L) = T_c + aL^{-(1/\nu+\omega)}$$

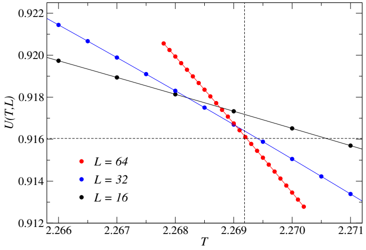
$$U^*(L) = U_c + bL^{-\omega}$$

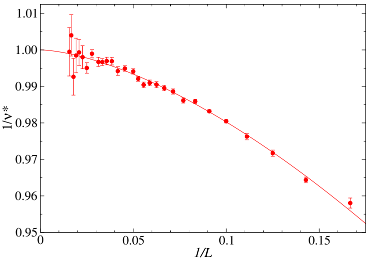
$\omega$: unkown correction to scaling, free exponent in fits



- correlation-length exponent $\nu$
  can be extracted from the slope of $U$: $s(T,L) = \frac{\mathrm{d}U(T,L)}{\mathrm{d}T}$

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



**numerical study of the J-Q model**

# Many numerical results support DQC scenario

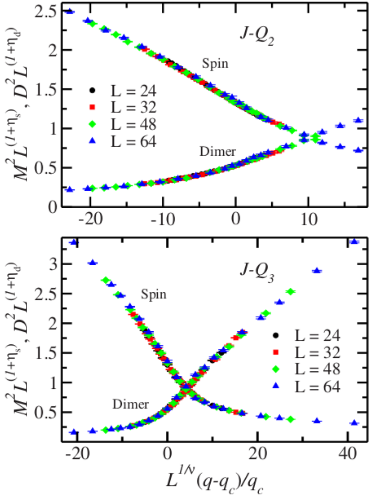
FSS of squared order parameter(A)

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

Data "collapse": $M^2$ and $D^2$ simutaneously → single continuous transition!

- $J$-$Q_2$ model; $q_c = 0.961(1)$
  $\eta_s = 0.35(2); \eta_d = 0.20(2);$
  $\nu = 0.67(1)$
- $J$-$Q_3$ model; $q_c = 0.600(3)$
  $\eta_s = 0.33(2); \eta_d = 0.20(2);$
  $\nu = 0.69(2)$ Lou,Sandvik and Kawashima, PRB 2009
- Comparable results for honeycomb J-Q model

Alet and Damle, PRB 2013 Kaul et al., PRL 2014



# However, scaling violation

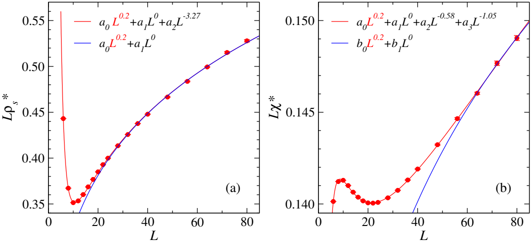
Spin stiffness $\rho_s \propto \delta^{\nu(d+z-2)}$ and susceptibility $\chi \propto \delta^{(d-z)\nu}$

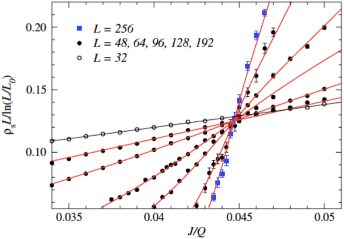
Conventional FSS

$$\rho_s(\delta, L) = L^{-\nu(d+z-2)/\nu} f(\delta L^{1/\nu}), \qquad \chi(\delta, L) = L^{-\nu(d-z)/\nu} f(\delta L^{1/\nu})$$

At critical point: $\boxed{\rho_s \propto L^{-(d+z-2)} = L^{-z}, \quad \chi \propto L^{-(d-z)}}$

$z = 1$ for $J$-$Q$ model, $\rho_s L$ and $\chi L$ should be constants at $q_c$




- $z \neq 1$ **does not work**
- **large scaling corrections?** Sandvik PRL 2010, Bartosch PRB 2013
- **weak first-order transition?** Chen et al PRL 2013

**The enigmatic current state is well summed up in Nahum PRX, 2015**

In this talk, we will try to resolve this puzzle by

- **introducing a new scaling form with two-length scales**
- **showing numerical evidences**
  - **direct simulations of the deconfinement of spions**
  - **critical scaling of VBS domain wall energy, spin stiffness and susceptibility**
- **anomalous critical scaling at finite temperature**

Unconventional scaling form with two lengths

# Unconventional scaling form with two lengths

Two divergent lengths tuned by one parameter:

$$\xi \propto \delta^{-\nu}, \quad \xi' \propto \delta^{-\nu'}$$

Consider FSS of a quantity $A \propto \delta^{\kappa}$

- Conventional scenario

$$A(\delta, L) = L^{-\kappa/\nu} f(\delta L^{1/\nu}, \delta L^{1/\nu'}), \quad \boxed{A(\delta = 0, L) \propto L^{-\kappa/\nu}}$$

$L \to \infty, f(\delta L^{1/\nu}, \delta L^{1/\nu'}) \to (\delta L^{1/\nu})^{\kappa}$, recovers $A \propto \delta^{\kappa}$

- We propose

$$A(\delta, L) = L^{-\kappa/\nu'} f(\delta L^{1/\nu}, \delta L^{1/\nu'}), \quad \boxed{A(\delta = 0, L) \propto L^{-\kappa/\nu'}}$$

when $L \to \infty, f(\delta L^{1/\nu}, \delta L^{1/\nu'}) \to (\delta L^{1/\nu'})^{\kappa}$ leads to $A \propto \delta^{\kappa}$

**For example**: spin stiffness $\rho_s \propto \delta^{\nu(d+z-2)}, \kappa = \nu(d+z-2)$. At $q_c$

$$\boxed{\text{NOT } \rho_s \propto L^{-(d+z-2)}, \quad \text{BUT} \quad \rho_s \propto L^{-(d+z-2)\nu/\nu'}}$$

phenomenological explanation of our scaling form

# General scaling theory for $\rho_s$, single length scale

Fisher et al PRB,40,546(1989)

Free energy density scales

$$f_s(\delta, L, \beta) \sim \xi^{-(d+z)} Y(\frac{\xi}{L}, \frac{\xi^z}{\beta}), \qquad \xi \sim \delta^{-\nu}$$

- $\rho_s \frac{\Delta^2 \phi}{L^2}$ is the excess energy due to a twist along apace:

$$\Delta f(\delta, L, \beta) \sim \xi^{-(d+z)} \tilde{Y}(\frac{\xi}{L}, \frac{\xi^z}{\beta}) \sim \rho_s \frac{\pi^2}{L^2}$$

- $\tilde{Y}$ has to behave like $(\xi/L)^2$, thus

$$\rho_s \sim \xi^{2-(d+z)}$$

- replacing $\xi$ to $L$, we have $\rho_s \sim L^{-(d+z-2)}$

# Two length scales scenario

Free energy density scales

$$f_s(\delta, L, \beta) \sim \xi^{-(d+z)} Y(\frac{\xi}{L}, \frac{\xi^z}{\beta}, \frac{\xi'}{L}, \frac{\xi'^z}{\beta})$$

- the excess energy due to a twist along apace:

$$\rho_s(\frac{\Delta\phi}{L})^2 \sim \Delta f(\delta, L, \beta) \sim \xi^{-(d+z)} \tilde{Y}_s(\frac{\xi}{L}, \frac{\xi^z}{\beta}, \frac{\xi'}{L}, \frac{\xi'^z}{\beta})$$

which means

$$\tilde{Y}_s \sim (\frac{\xi}{L})^a (\frac{\xi'}{L})^{2-a}$$

- The larger correlation length $\xi'$ reaches $L$ first, so $L = \xi'$

we have $a = 2$, and

$$\rho_s \sim \xi^{-(d+z-2)}$$

but, since $L = \xi'$, $\xi$ saturates at $\xi = L^{\nu/\nu'}$,

$$\boxed{\rho_s \sim L^{-(d+z-2)\nu/\nu'}}$$

# Projector Quantum Monte Carlo method: ground state $S=0$

Apply the imaginary time evolution operator to an initial state

$$U(\tau \to \infty)|\Psi_0\rangle \to |0\rangle$$

where $U(\tau) = (-H)^\tau$ or $U(\tau) = \exp(-H\tau)$

$$\boxed{\langle A\rangle = \frac{\langle\Psi_0|U(\tau)AU(\tau)|\Psi_0\rangle}{\langle\Psi_0|U(\tau)U(\tau)|\Psi_0\rangle} \to \frac{\sum_c A_c W_c}{\sum_c W_c}}$$

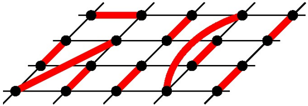
$A_c$ is the estimator of $A$.

# Projector Quantum Monte Carlo method

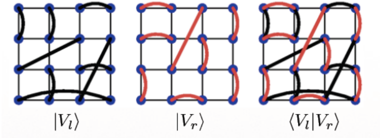
- using VB basis

$$|\Psi\rangle = \sum_v f_v |v\rangle, \qquad |v\rangle = |(a_1, b_1)\cdots(a_{N/2}, b_{N/2})\rangle$$

$|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle/\sqrt{2}$

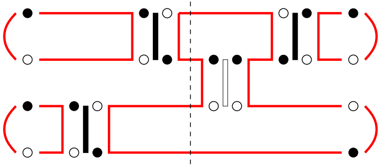
$\sum$ 

expectation values: transition graphs




$$\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = \begin{cases} 0, & (i)_L(j)_L \\ \frac{3}{4}\phi_{ij}, & (i,j)_L, \end{cases}$$

- take $U(\tau) = \exp(-\tau H)$, SSE representation $\rightarrow Z = \sum_c W_c$
- loop update algorithm are used



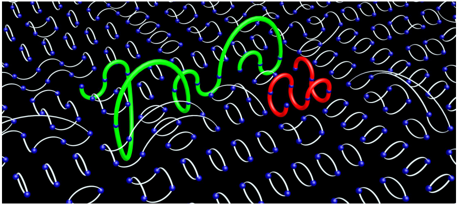
# study spinons

**extend valence-bond basis to total spin $S = 1$ states**

Tang and Sandvik PRL 2011, Banerjee and Damle JSTAT 2010

$2S$ upaired ”up” spins

- two spinons are two strings in a background of valence bond loops

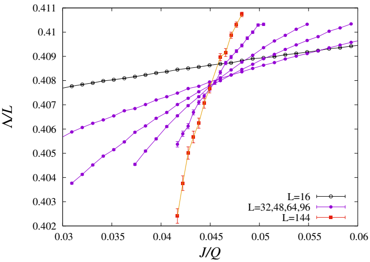


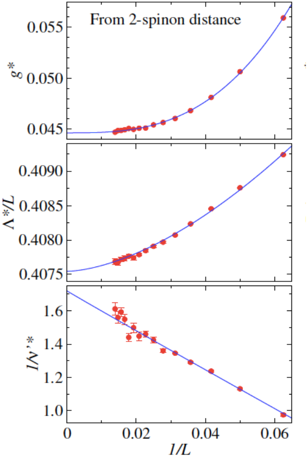
- **study spinon bound states and unbinding**

# Numerical results

# The two-spinon distance in the $J$-$Q_2$ model

size of spinon bound state $\Lambda \equiv$ root-mean-square string distance




- suppose $\Lambda \propto \xi' \propto \delta^{-\nu'}$, according to our new FSS, $\Lambda(q_c, L) \propto L$, $\Lambda(q_c, L)/L = $ constant
- $(L, 2L)$ crossing points converge monotonically

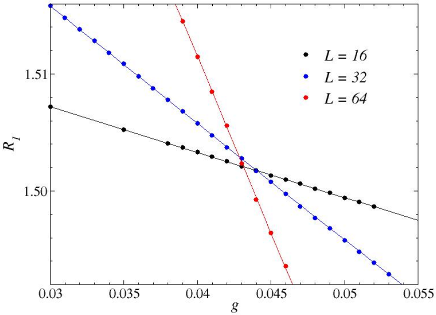
$$g^* - q_c \propto L^{-(1/\nu' + \omega)}, \quad \Lambda^*(L)/L - R \propto L^{-\omega}$$

$1/\nu'$ can be extracted from slopes at the crossing point

- $q_c = 0.04463(4), \nu' = 0.58(2)$

**Transition is associated with spinon deconfinement**

# The Binder ratio in the $J$-$Q_2$ model




Similar crossing-point analysis of the Binder ratio

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

- correlation length exponent $\nu = 0.446$, diffrent from $\nu'$

- what is $\nu'$ obtained from confinement length $\Lambda$?
  - DQC theory: VBS domain wall thickness

$$\xi \propto (q - q_c)^{-\nu}, \qquad \xi' \propto (q - q_c)^{-\nu'}, \qquad \nu' > \nu$$

  - $\nu/\nu' = 0.77(3)$ agrees with the result obtained from the VBS domain-Wall energy calculations
    suggesting $\nu'$ is the domain wall thickness exponent

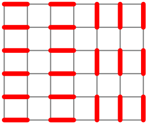
# VBS domain-wall scaling in the critical J-Q model

- VBS domain walls are imposed in open-boundary systems
- $\pi$ wall splits into two $\pi/2$ walls
- calculate domain-wall energy

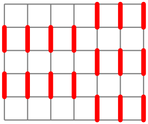
$$\delta F = F_{wall} - F_{uniform}$$

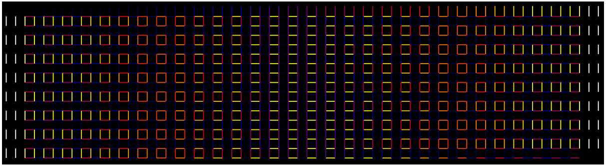
$$\kappa = \delta F / L^{d+z-1}$$

$\phi = \pi/2$



$\phi = \pi$





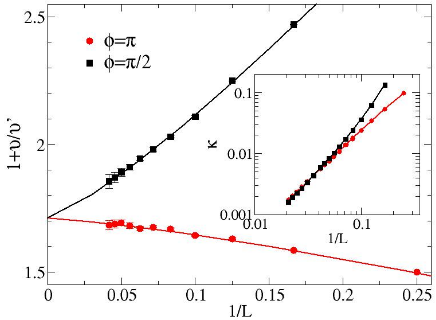
$\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$

# Scaling of $\kappa$ at deconfined critical point

- domain-wall energy can be expressed as $\kappa = \rho_s/\Lambda$
  $\rho_s$ is a stiffness: energy cost of a twist of the VB order
  $\Lambda$ is the width of the region over which the twist distributes.

- According to DQC theory,
  $\rho_s \propto 1/\xi$, $\Lambda \propto \xi'$,
  $$\boxed{\kappa \propto \frac{1}{\xi\xi'} \propto \delta^{\nu+\nu'}}$$
- translate to finite size at $q_c$:
  When $\xi'$ reaches $L$, $\xi$ saturates at
  $\xi'^{\nu/\nu'} = L^{\nu/\nu'}$

$$\boxed{\kappa(q_c) \propto L^{-(1+\nu/\nu')}}$$




we have $\nu/\nu' = 0.72(2)$

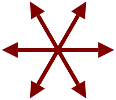
- predicted by our scaling form:
  $A(\delta, L) = L^{-\kappa/\nu'} f(\delta L^{1/\nu}, \delta L^{1/\nu'})$, $\quad A(\delta = 0, L) \propto L^{-\kappa/\nu'}$

# Compare to domain wall scaling in classical model

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

$$H = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j)$$

- $\theta$ restriction:

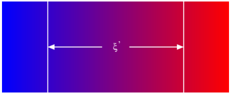


domain wall energy in $L \to \infty$

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

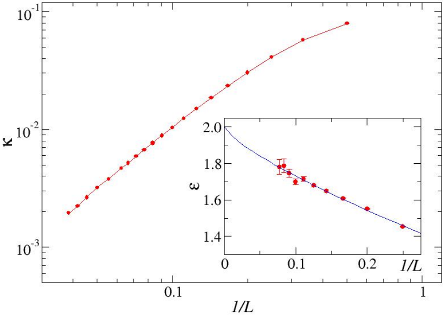
But, finite-size scaling at $T_c$ shows

$$\kappa \sim L^{-2} \neq L^{-(1+\nu/\nu')}$$




$\xi \sim \xi'^{\nu/\nu'}$, $\nu/\nu' \approx 0.47$, $\nu'$ is universal

Léonard and Delamotte, PRL 2015



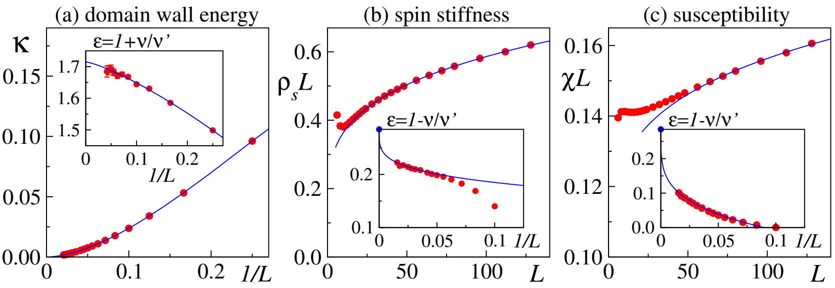

The dangerously irrelevant perturbation in the J-Q model is more serious

# Further evidence for unconventional scaling

according to our scaling form

$$\rho_s \sim L^{-(z+d-2)\nu/\nu'} \sim L^{-\nu/\nu'}, \quad \text{instead of } \rho_s \sim L^{-(z+d-2)} \sim L^{-1}$$

$$\chi \sim L^{-(d-z)\nu/\nu'} \sim L^{-\nu/\nu'}, \quad \text{instead of } \chi \sim L^{-(d-z)} \sim L^{-1}$$

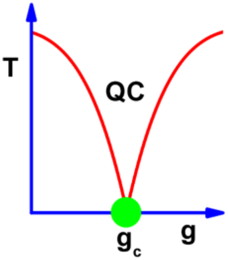



- This explains drifts in $L\rho_s$ and $\chi L$ in J-Q and other models ($z = 1, d = 2$)

# Anomalous critical scaling at finite Temperature

Quantum critical point at $T = 0$ governs the behavior in a $T > 0$ region which expands out from $(g_c, T = 0)$: $\xi > \Lambda_T \sim 1/T$, $\Lambda_T$ de Broglie wave length

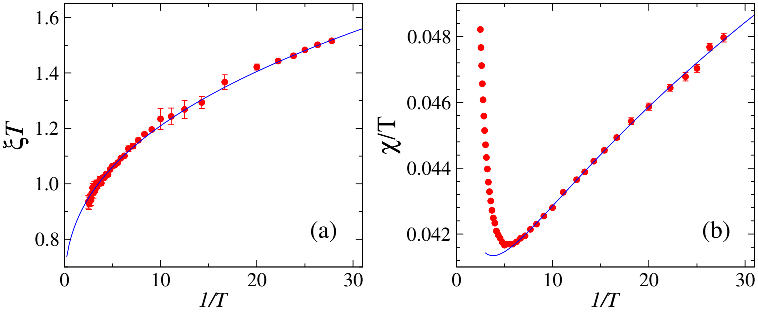
experimentally important



# Anomalous critical scaling at finite Temperature

- $\beta = 1/T$ is also a 'finite-size': $L \to \beta^{1/z}$
- conventional scaling ($z = 1$ for J-Q)
  - $\xi \sim L$ leads to $\xi_T \propto \beta^{1/z} = T^{-1}$,
  - $\chi \sim L^{-(d-z)}$ leads to $\chi_T \propto \beta^{-(d-z)/z} = T$
- new scaling with $\nu/\nu'$:

$\xi_T \propto T^{-\nu'/\nu}$; $\chi \sim L^{-\nu/\nu'}$ leads to $\chi_T \propto T^{\nu/\nu'}$



# conclusions

- Two length scales observed explicitly in the J-Q model
- Simple two-length scaling hypothesis explains scaling violation of spin stiffness and susceptibility
- we obtained the spinon deconfinement exponent $\nu'$
- For $T > 0$ we find scaling laws from finite-size scaling forms experimentally important

# Thank you !