# Quantum criticality with two length scales

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References:

- 1. Science: DOI: 10.1126/science.aad5007
- 2. PRB 91, 094426 (2015).

## outlines

#### Background

Deconfined quantum criticality introduction to finite-size scaling J-Q model and scaling violation

#### QMC study of deconfined criticality

Quantum Monte Carlo methods spinon deconfinement and critical exponents VBS domain wall thickness critical scaling with two lengths and phenomenological explanation

Anomalous critical scaling at Finite temperature

Conclusions

# Thermal phase transitions

- At critical point, divergent length scale leads to singularity, which is the result of thermal fluctuations
- Quantum mechanics is largely irrelevant



3D Ising FM-Paramagnetic transition (MC simulation)

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

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

where  $\Phi$  is the order parameter, *s* is a function of *T*.

- Meanfield:  $\Phi^2 = -s/2u$  for  $T < T_c(s \sim s'(T T_c))$ .
- 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<sub>c</sub>*, the correlation length diverges, due to quantum fluctuations
- ▶ path integral maps *D*-dim quantum systems onto classical field theories in *D* + 1-dim

$$S(\Phi) = \int dV d\tau ((\partial_{\tau} \Phi)^2 + v^2 (\nabla_x \Phi)^2 + s \Phi^2 + u(\Phi^2)^2)$$
$$Z = \int \mathcal{D}\Phi \ e^{-S(\Phi)}$$

many of these transitions can be understood in the conventional Landau-Ginzburg-Wilson framework ▶ for example: AF Néel-Paramagnetic transition H<sub>0</sub> is AF Heisenberg Hamiltonian, g = J<sub>2</sub>/J<sub>1</sub>



- 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

# Non-trivial non-magnetic ground state

► Valence bond  $\frac{1}{i} = (\uparrow_i \downarrow_j - \downarrow_i \uparrow_j)/\sqrt{2}$ 

- resonating valence-bond (RVB) spin liquid exotic state without any long-range order
- valence-bond solid (VBS) breaking the translation and rotation symmetry of the lattice

VBS order parameter  $(D_x, D_y)$ 

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

#### valence-bond state: the overcomplete basis







$$\langle \mathbf{m}_s \rangle = \langle \frac{1}{N} \sum_i \mathbf{S}_i (-1)^{x_i + y_i} \rangle = 0$$

# Deconfined quantum criticality

#### describe the direct continuous transition from Néel to VBS

in 2D Read and Sachdev, 1989; Senthil, Vishwanath, Balents, Sachdev, Fisher (2004)



• the direct continous transition violates the "Landau rule":

Néel-param should be in 3D O(3) universality class;

but transition away from VBS sould be in 3D O(2) ( $Z_4$ anisotropy is dangerously irrelevant, Léonard and Delamotte, PRL 2015) universality class.

either first order or a phase in between

 reason: Berry phase related interference effect in path integral, complex statistical weight in the field theories, NOT like classical statistical systems

New physics is called

# Deconfined quantum criticality

Field-theory description with spinor field  $\boldsymbol{z}$ 

• 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

$$\boldsymbol{\Phi} = \boldsymbol{z}_{\alpha}^* \boldsymbol{\sigma}_{\alpha\beta} \boldsymbol{z}_{\beta}$$

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

$$S_{z} = \int \mathrm{d}r^{2} \mathrm{d}\tau [|(\partial_{\mu} - iA_{\mu})z_{\alpha}|^{2} + s|z_{\alpha}|^{2} + u(|z_{\alpha}|^{2})^{2}) + \kappa(\epsilon_{\mu\nu\lambda}\partial_{\nu}A_{\lambda})^{2}]$$

A is a U(1) symmetric gauge field; related to the VBS order parameter  $(D_x, D_y)$ Non-compact  $CP^1$  action

# Physical picture

Levin and Senthil, PRB 70, 2004

At the core of the  $Z_4$  vortex, there is a spinon



Blue-shaded regions are domain walls (Not a line). The thickness  $\xi_{DW}$  diverges faster than the correlation length  $\xi$ : two length scales , emergent U(1) symmetry



 Spinons bind together in the VBS state (confinement) and condensate the Néel state, deconfine at the critical point leading to a continuous phase transition

- Only SU(N) generalization can be sloved when N → ∞, 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

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



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

• large *Q*, columnar VBS

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

small Q, Néel

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



- No sign problem for QMC simulations,
- ideal for QMC study of the DQC physics

Sandvik, PRL 98, 227202(2007)

## Finite-size scaling

- Correlation length divergent for  $T \to T_c$ :  $\xi \propto |\delta|^{-\nu}, \delta = T T_c$
- Other singular quantity:  $A(T,L 
  ightarrow \infty) \propto |\delta|^\kappa \propto \xi^{-\kappa/
  u}$
- 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  $\gamma = 7/4, \nu = 1$  $T_c = 2/\ln(1 + \sqrt{2}) \sim 2.2692$ When these are not known, treat as fitting parameters



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## systematic critical-point analysis

• consider a quantity with  $\kappa = 0$ , or, with known  $\kappa/\nu$ 

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

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

• (almost) size-independent at T<sub>c</sub> leads to crosssings at T<sub>c</sub>

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





Drift in (L, 2L) crossing points

 scaling corrections in crossings

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

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

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

$$Q(T,L) = f(\delta L^{1/\nu}, uL^{-\omega})$$



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

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





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

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  $\rightarrow$  single continous transition!

- J-Q<sub>2</sub> model;  $q_c = 0.961(1)$   $\eta_s = 0.35(2); \eta_d = 0.20(2);$  $\nu = 0.67(1)$
- J-Q<sub>3</sub> 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



# scaling violation

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

$$\begin{split} \rho_{s}(\delta,L) &= L^{-\nu(d+z-2)/\nu}f(\delta L^{1/\nu}), \qquad \chi(\delta,L) = L^{-\nu(d-z)/\nu}f(\delta L^{1/\nu}) \\ \text{At critical point: } \rho_{s} \propto L^{-(d+z-2)} = L^{-z}, \qquad \chi \propto L^{-(d-z)} \\ z &= 1 \text{ for } J\text{-}Q \text{ model}, \rho_{s}L \text{ and } \chi L \text{ should be constants at } q_{c} \\ & \int_{a_{d}}^{0.55} \int_{a_{d}}^{0.45} \int_{a_{d}}^{0.25} \int_{a_{d}}^{0.45} \int_{a_{d}}^{0.150} \int_{a_{d}}^{0.46} \int_{a_{d}$$

- $z \neq 1$  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 et al arXiv: 1506.06798

In this talk, we will try to resolve this puzzle

- study the deconfinement of spions
- VBS domain wall thickness
- introduce scaling form with two-length scales and give phenomenological explanation
- anomalous critical scaling at finite temperature

# Quantum Monte Carlo method

#### General idea of QMC :

• rewrite a quantum-mechanical trace or expectation value into a classical form

$$\langle A \rangle = \frac{\text{Tr}\{Ae^{-\beta H}\}}{\text{Tr} e^{-\beta H}} \text{ or } \frac{\langle \Psi | A | \Psi \rangle}{\langle \Psi | \Psi \rangle} \rightarrow \frac{\sum_{c} A_{c} W_{c}}{\sum_{c} W_{c}}$$

 $W_c$  is the weight of a configuration,  $A_c$  is the estimator of A.

• There are many different ways of doing it: Worldline (worm), SSE, Fermion determinant, ···

# SSE Quantum Monte Carlo method

 A SSE configuration: spin state + operator string

-1 +1 -1 -1 +1 -1 +1 +1



- diagonal and loop updates
- observables and estimators
  - ► energy estimator : number of operators, H<sub>c</sub> = −n/β
  - spin stiffness estimator : winding number fluctuations

$$p_s = rac{\langle W_{lpha}^2 
angle}{L^{d-2} eta}$$

• staggered magnetization:  $m_{sz} = \sum_{i} (-1)^{i_x + i_y} s_{iz} / N$ 

# Projector Quantum Monte Carlo method

#### For ground state calculations

Apply the imaginary time evolution operator to an initial state

$$U( au o \infty) |\Psi_0
angle o |0
angle$$

where  $U(\tau)=(-H)^{\tau}$  or  $U(\tau)=\exp\left(-H\tau\right)$ 

$$\left[ \langle A \rangle = \frac{\langle \Psi_0 | U(\tau) A U(\tau) | \Psi_0 \rangle}{\langle \Psi_0 | U(\tau) U(\tau) | \Psi_0 \rangle} \to \frac{\sum_c A_c W_c}{\sum_c W_c} \right]$$

 $A_c$  is the estimator of A.

# Projector Quantum Monte Carlo method

using VB basis (in the singlet sector)

$$|\Psi\rangle = \sum_{\nu} f_{\nu} |\nu\rangle, \qquad |\nu\rangle = |(a_1, b_1) \cdots (a_{N/2}, b_{N/2})\rangle$$





- take  $U(\tau) = \exp(-\tau H)$ , SSE representation  $\rightarrow Z = \sum_{c} W_{c}$
- loop update algorithm are used



## **Expectation values**

- energy estimator:  $H_c = -n/2\tau$
- correlation functions computed using transition graphs



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

 $\phi_{ij} = \pm 1, \, i, j$  on the same/different sublattice

# spinons and Deconfinement of spinons

- The excitations of VBS carry S = 1
  - bound spinon pair
  - confining string
- The confining string weakens as *q<sub>c</sub>* is approached
  - deconfinement

The distance  $\Lambda$  diverages,  $\propto \xi_{DW}(?)$ 



QMC simulations can be carried out in the S = 1 space

## Extend valence-bond basis to total spin S > 0 states

Tang and Sandvik PRL 2011, Banerjee and Damle JSTAT 2010

Consider  $S_z = S$ 

• for even N spins: N/2 - S bonds, 2S upaired "up" spins



• transition grap has 2*S* open strings study spinon bound states and unbinding The two-spinon distance in the J- $Q_2$  model

A QMC transition graph representing  $\langle \psi_L | \psi_R \rangle$  of S = 1 states

- two strings (spinons) in a background of loops formed by valence bonds.
- two strings represent two spinons in bound state



J-Q model in deep VBS phase

animation at VBS

# J-Q model at the critical point

animation at  $q_c$ 

# The two-spinon distance in the *J*-*Q*<sub>2</sub> model

# Define the size of spinon bound state $\Lambda$ as root-mean-square string distance



#### Crossing-point analysis of $\Lambda/L$

- We find that Λ/L at q<sub>c</sub> is dimensionless, like the Binder ratio R<sub>1</sub> of Néel order parameter.
- The crossing points of (L, 2L) converge monotonicly

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

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

• we find  $q_c = 0.04463(4), \nu' = 0.58(2)$ 

Transition is associated with spinon deconfinement

# The Binder ratio in the *J*-*Q*<sup>2</sup> model



Similar crossing-point analysis of the Binder ratio

- From Binder ratio, we have  $\nu = 0.446$  which controls the correlation.
- what is  $\nu'$ ?
  - DQC theory: two diverging length scales

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

 ν/ν' = 0.77(3) agrees with the result obtained from the VBS domain-Wall energy calculations suggesting ν' is the domain wall thickness exponent fundamental lenght scale: domain wall thickness

In some classical systems (clock models, XY model with symmetry breaking field) the thickness of a domain wall is larger than the correlation length

$$\xi \sim \delta^{-\nu}, \qquad \xi_{DW} \sim \delta^{-\nu'}, \qquad \nu' > \nu$$



#### VBS domain wall behaves similarly



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

 $\phi = \pi/2$   $\phi = \pi$ 

two kinds of VBS domain walls are imposed in open-boundary systems

 $\pi$  wall splits into two  $\pi/2$  walls

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





1/I

At deconfined critical point  $q_c$ ,  $\kappa \propto L^{-b}$ ,  $b \approx 1.80(1)$ 

Shao, Guo and Sandvik, PRB 2015

# 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.



we have  $b = 1 + \nu/\nu'$ , and  $\nu/\nu' = 0.80(1)$ 

- The only other estimate from analysis of the emergent U(1) symmetry:  $\nu/\nu'=0.83((4),$  J. Lou et al PRB 80, 180414(R)(2009)

# Domain wall scaling in classical model

3D q-state clock model(q > 3): basic example of dangerously irrelevant perturbation

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

• 
$$\theta$$
 restriction:

The prediction for the domain wall energy in  $L \rightarrow \infty$ 

$$\kappa \sim \frac{1}{\xi \xi_{DW}}$$

But, finite-size scaling at  $T_c$  shows

 $\kappa \sim L^{-2} \neq L^{-(1+\nu/\nu')}$  The dangerously irrelevant perturbation in the J-Q model is more serious

 $\xi \sim \xi_{DW}^{
u/
u'}, 
u/
u' pprox 0.47, 
u'$  is

universal Léonard and Delamotte, PRL 2015



## Quantum criticality with two lengths

Two divergent lengths tuned by one parameter:

$$\xi \propto \delta^{-
u}, \ \ \xi' \propto \delta^{-
u'}$$

A quantity  $A \propto \delta^{\kappa}$ , finte-size scaling of A

Conventional scenario

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

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

• We propose

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

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

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

$$ho_s \propto L^{-(d+z-2)}$$
 or  $ho_s \propto L^{-(d+z-2)
u/
u'}$ 

# General scaling theory for $\rho_s$ and $\chi$ , 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  $\rho_s \sim L^{-(d+z-2)}$ 

• Simmilarly,  $\chi \frac{\Delta^2 \phi}{\beta^2}$  is the excess energy density needed to enforce the twist, which means  $\tilde{Y} \sim \xi^{2z}/\beta^2$ 

$$\chi \sim \xi^{2z-(d+z)}, \qquad \chi \sim L^{-(d-z)}$$

## Two correlation lengths 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

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

The larger correlation length  $\xi'$  reaches *L* first, so  $L \sim \xi' \sim \delta^{-\nu'}$ , we have a = 2, and

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

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

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

Similarly, we have

$$\chi \sim L^{-(d-z)\nu/\nu'}$$

## Evidence for unconventional scaling in J-Q model We have



- this unexplains drifts in  $L\rho_s$  and  $\chi L$  in J-Q and other models (z = 1, d = 2)
- Behavior was interpreted as flow to first-order transition is due to unconventional scaling!

## Anomalous critical scaling at finite Temperature

Quantum critical point at T = 0 governs the behavior in a T > 0 region which expands out from  $(g_c, T = 0)$ : experimentally important



#### Anomalous critical scaling at finite Temperature

- $\beta = 1/T$  is also a 'finite-size':  $L \rightarrow \beta^{1/z}$
- convetional scaling (z = 1 for J-Q)

• new scaling with  $\nu/\nu'$ :

 $\xi_{_T} \propto T^{u'/
u}$ ;  $\chi \sim L^{u/
u'}$  leads to  $\chi_{_T} \propto T^{
u/
u'}$ 



# Conclusions

- Two length scales observed explicitly in the J-Q model
- No sign of first-order transition in the J-Q model
- Simple two-length scaling hypothesis explains scaling violation of spin stiffness and susceptibility
- For *T* > 0 we find scaling laws from finite-size scaling forms experimentally important

# Thank you !