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New perspectives on deconfined quantum criticality



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Advancing Research in Basic Science and Mathematics

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Outline

Deconfined quantum criticality

- Néel to VBS quantum phase transition (field theory)
- Concept of "Dangerously irrelevant" perturbations
- Valence-bond solids (VBS) and models hosting them
 - J-Q model (no QMC sign problem)

Introduction to finite-size scaling

- 2D Ising model

QMC study of deconfined criticality

- emergent U(1), RG flows
- critical exponents
- VBS domain walls
- critical scaling with two divergent lengths
- phenomenological explanation of scaling anomalies

Revision of conventional quantum-critical scaling forms





Field theory description; brief summary

Standard low-energy theory of $quax_{\mu} = (x, y, \tau)$ tiferromagnet

$$S = \int d^{d}r d\tau \frac{1}{2} [c^{2} (\partial_{r} \phi)^{2} + (\partial_{\tau} \phi)^{2} + m_{0} \phi^{2} + u_{o} (\phi^{4})]^{\vec{n}(x_{\mu})}$$

Can describe Neel to featureless paramations $\mathcal{L}_{\sigma} = \frac{1}{2g} |\partial_{\mu} \vec{n}|^{2}$ ition - VBS pattern or topological order cannol $\mathcal{L}_{\sigma} = \mathcal{L}_{\sigma} |\partial_{\mu} \vec{n}|^{2}$ by φ

Topological defects (hedgehogs) in field configurations:

- suppressed in the Neel state
- proliferate in the quantum paramagnet

The VBS state corresponds to a certain condensation of topological defects

- requires a description beyond φ^4 theory

Neel vector described by spinors z; $\phi = z_{\alpha}^* \sigma_{\alpha\beta} z_{\beta}$

 - coupled to U(1) gauge field where hedgehogs correspond to monopoles
 - VBS on square lattice arises from condensation of quadrupled monopoles Murthy & Sachdev 1991, Read & Sachdev 1991

Nature of the Neel - VBS transition remained unknown...



 $\vec{n}(x_{\mu})$





Graph:Senthil et al.

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PHYSICAL REVIEW LETTERS

Striped Phase in a Quantum XY Model with Ring Exchange

A.W. Sandvik,^{1,2} S. Daul,^{3,*} R. R. P. Singh,⁴ and D. J. Scalapino²

QMC study of 2D S=1/2 XY model with plaquette flip (partial ring exchange)

$$H = -J \sum_{\langle ij \rangle} B_{ij} - K \sum_{\langle ijkl \rangle} P_{ijkl},$$
$$B_{ij} = S_i^+ S_j^- + S_i^- S_j^+ = 2(S_i^x S_j^x + S_i^y S_j^y)$$

$$P_{ijkl} = S_i^+ S_j^- S_k^+ S_l^- + S_i^- S_j^+ S_k^- S_l^+,$$

First-order transition would be expected for superfluid (XY magnet) to VBS transition

No discontinuities detected



Motivated re-examination of the field theory

Deconfined quantum criticality $\mathcal{L}_{\sigma} = \frac{1}{2\pi} |\partial_{\mu}\vec{n}|^{2}$

 $|\vec{n}(x_{\mu})$

 $\vec{n}(x_{\mu})$

O(3) transition with suppressed topological defects in MC simulations - changes universality class

Motrunich and Vishwanath 2004 (+ earlier work in particle physics)

Topological defects may be "dangerously irrelevant" at the 2D Neel - VBS transition

- universality of defect suppressed O(3)
- topological defects relevant in VBS state only

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

$$S_{z} = \int d^{2}r d\tau \left[\left| (\partial_{\mu} - iA_{\mu})z_{\alpha} \right|^{2} + s|z_{\alpha}|^{2} + u(|z_{\alpha}|^{2})^{2} + \frac{1}{2e_{0}^{2}}(\epsilon_{\mu\nu\lambda}\partial_{\nu}A_{\lambda})^{2} \right]$$

- non-compact (defect-free) CP¹ model
- large-N calculations for SU(N) CP^{N-1} theory

Continuous transition found for large N

- violation of Landau rule
- expected first-order transition between ordered states

Is the transition really continuous for N=2 (small N)?



|y|





Detour: Dangerously irrelevant perturbations

DQC scenario has two divergent length scales on VBS side

- correlation length $\xi \propto (g g_c)^{-\nu}$ and emergent U(1) length $\xi' \propto (g g_c)^{-\nu'}$
- due to dangerously-irrelevant perturbation which causes VBS
- known in many classical systems (e.g., 3D clock models)
 Jose, Kadanoff, Kirkpatrick, Nelson, PRB 1977



h is dangerously irrelevant

- does not change critical point
- changes ordered state

Fixpoints:

- **P** = paramagnet
- X = 3D XY critical point
- Y = XY symmetry breaking
- **Q** = **Z**_q symmetry breaking

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

RG flows can be observed in MC simulations

MC simulations of classical 3D clock model

$$H = -J \sum_{\langle ij \rangle} \cos(\Theta_i - \Theta_j)$$
 Restricted to q clock angles

Standard order parameter (mx,my)

$$m_x = \frac{1}{N} \sum_{i=1}^{N} \cos(\Theta_i) \qquad m_y = \frac{1}{N} \sum_{i=1}^{N} \sin(\Theta_i)$$



Probability distribution $P(m_x, m_y)$ shows cross-over from U(1) to Z_q for T<T_c



Lou, Balents, Sandvik, PRL 2007

Can be quantified with "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

$$U_m = 2 - \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2} \qquad \qquad U_m = \begin{cases} \\ \end{bmatrix}$$

$$= \left\{ \begin{array}{c} 0, \\ 0.77... \\ 1, \end{array} \right.$$

in paramagnet at critical point in ordered phase



Flows to these values with the system size (inverse energy scale)

Use m_q to quantify the degree of Z_q symmetry

 related to the dangerously irrelevant coupling

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

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

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

$\lambda_{4} \qquad \qquad VBS$





Goal: Test scenario and obtain quantitative results using numerics

VBS state in frustrated 2D Heisenberg model

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



$$g = J_2/J_1$$

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



- A non-magnetic state exists between the magnetic phases
 - Some recent calculations suggest spin liquid
 - Most likely a VBS (what kind? Columnar or plaquette?)

2D frustrated models are challenging: QMC sign problems, DMRG/tensors still difficult

VBS states from multi-spin interactions

Sandvik, PRL 2007

The Heisenberg interaction is equivalent to a singlet-projector

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

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



+ all translations and rotations

The "J-Q" model with two projectors is

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

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

Use to test the deconfined quantum-criticality scenario

Critical behavior of the J-Q model



Need to compute the exponents more systematically

Emergent U(1) and RG flows in the J-Q₃ model

 \mathbf{D}_{4}

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

(a)



Define D₄ as in the clock model to quantify degree of Z₄ symmetry

Use Binder cumulants for Neel (Um) and dimer order (UD)

- U_D - U_m shows flows to phases and dqc point

Shows similarity with the clock models

- but clock models only have one ordered phase
- different universality expected

Use systematic finite-size scaling approach for exponents



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

Finite-size scaling hypothesis (general)

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



2D Ising universality class $\gamma = 7/4, \ \nu = 1$ Critical T known

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

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

Systematic critical-point analysis

Binder cumulant

- dimensionless
- size-independent at $T_{\mbox{\scriptsize c}}$

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



Curves cross asymptotically at Tc

Systematic crossing-point analysis



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

Correlation-length exponent v

Can be extracted from the slope of the Binder cumulant

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

Evaluate at crossing point for sizes (L,2L)

Fit to power-law correction

Extrapolation stable, gives exponent 1/v=1.0001(7)(exact = 1)



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

Curve-crossings ↔ "phenomenological renormalization" (Fisher)

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

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





Exponent v: crossing-point analysis

H. Shao, W. Guo, A. W. Sandvik (unpublished)



- Small correction exponent; $\omega \approx 0.5$
- -v = 0.45 + 0.01

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

0.05

 $\mathbf{0}$

0.1

1/L

0.15

Two length scales - VBS domain walls

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



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



Do finite-size scaling studies of VBS domain walls

Warm-up: classical systems, single length scale ($\xi' = \xi$)

General scaling theory (following Fisher et al., PRB 1989)

Classical d-dimensional system, free-energy density (singular part)

$$f(\delta, L) = \xi^{-d} Y(\xi/L), \quad \xi \sim \delta^{-\nu}$$

Excess free energy in presence of domain wall

$$\Delta F(\delta, L) = \xi^{-d} \tilde{Y}(\xi/L) L^d$$

We can also see that

$$\Delta F(\delta, L) = \rho(\delta) \left(\frac{\phi}{\xi}\right)^2 \xi L^{d-1}$$

 ϕ = total order-parameter "twist" ρ = stiffness constant

Consistency between the two expressions for ΔF requires $\ { ilde Y} \sim$

$$\frac{\xi}{L}, \quad \rightarrow$$

$$\Delta F \sim \xi^{-(d-1)} L^{d-1}$$

Test with Monte Carlo simulations

Monte Carlo simulations: 2D, 3D Ising models

We have developed efficient "multi-canonical" MC method for calculating $\Delta F(L) = F_{wall}(L) - F_{uniform}(L)$

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

Finite-size scaling exactly at the critical point $(T=T_c)$:

 $\xi \to L$ $\kappa(L) \sim L^{-(d-1)}$

MC data analysis:

- assume κ ~ L^{-p}



Agreement with expectation $p \rightarrow d-1$ when $L \rightarrow \infty$



Quantum system + two length scales

Quantum-critical point

- dynamic exponent z; $d \rightarrow d+z$
- F becomes ground-state energy E₀

Generalizing the Fisher et al. approach to 2 lengths:

Energy in the thermodynamic limit should be controlled by ξ , since

$$\xi^{-(d+z)} >> \xi'^{-(d+z)}$$

 $\Delta E_0(\delta, L) = \xi^{-(d+z)} \tilde{Y}(\xi/L, \xi'/L) L^d$

Two divergent lengths

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



$$\Delta E_0(\delta, L) = \rho(\delta) \left(\frac{\phi}{\xi'}\right)^2 \xi' L^{d-1}$$

Consistency between the two relationships requires

$$\tilde{Y} \sim \frac{L}{\xi'} \frac{\xi^2}{L^2} = \frac{\xi^2}{\xi' L} \to \Delta E_0 \sim \xi^{-(d+z-2)} \xi'^{-1} L^{d-1}$$

$$\kappa \sim \xi^{-(d+z-2)} \xi'^{-1}$$

Deconfined quantum criticality: d=2, z=1 $\rightarrow \kappa \sim \xi^{-1} \xi^{-1}$

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

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

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



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

Ambiguity in finite-size scaling: option 1) $\xi \rightarrow L$, $\xi' \rightarrow L^{\nu'/\nu}$: $\kappa \sim L^{-(1+\nu'/\nu)}$ option 2) $\xi \rightarrow L$, $\xi' \rightarrow L$: $\kappa \sim L^{-2}$ option 3) $\xi' \rightarrow L$, $\xi \rightarrow L^{\nu/\nu'}$: $\kappa \sim L^{-(1+\nu/\nu')}$

Results show option 3 (exponent < 2): v/v' \approx 0.715 +/- 0.015 $p(L) = \ln[\kappa(L)/\kappa(2L)]/\ln(2) \rightarrow 1 + \nu/\nu'$



This result demonstrates explicitly two divergent length scales! - different from the standard "dangerously irrelevant" perturbation

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

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



The "dangerously irrelevant" perturbation in the J-Q model is more serious ("super-dangerous"?)

Deconfinement of spinons

Nature of magnetic excitations

- The VBS state is confined
- confining string
- excitations carry S=1
- "triplon" = bound spinon pair
- The confining string weakens as the critical point is approached
- deconfinement
- spinon (S=1/2) excitations
 liberated at the critical point



What is the size Λ of the bound spinon pair?

The theory predicts $\Lambda \sim \xi'$ (or possibly $\xi < \Lambda < \xi'$)

QMC simulations can be carried out in the valence-bond basis

- lowest state in each spin sector, S=0,1,2,...
- S=1 state used to study triplons and spinons

Test the scaling of the spinon bound state in the J-Q model

Ground-state projector QMC with valence bonds

Liang PRB 1989; Sandvik PRL 2005, Sandvik, Evertz PRB 2010

Project valence bonds with H^m or exp(-βH) Expectation values (correlation functions) computed using transition graphs



Put the spins back in a way compatible with the valence bonds (singlets) and sample in a combined space of spins and bonds



Loop updates similar to those in finite-T methods (world-line and stochastic series expansion methods)

"measure" using valence bonds

Total spin S=0 conserved, faster convergence than $T \rightarrow 0$ method

Access to spinons in QMC simulations

Extended valence-bond basis for S>0 states

Tang, Sandvik PRL 2011, Banerjee, Damle JSTAT 2010

Consider S^z=S

- for even N spins: N/2-S bonds, 2S unpaired "up" spins
- for odd: (N-2S)/2 bonds, 2S upnpaired spins

- transition graph has 2S open strings



Overlaps and matrix elements involve loops and strings

- very simple generalizations of the S=0 case
- loops have 2 states, strings have 1 state

Use to study spinon bound states and unbinding

J-Q model deep in VBS phase



transition graphs evolving in imaginary time

J-Q model at the critical point



transition graphs evolving in imaginary time

Exponent v' (confinement lengt)

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

Define Λ (size of spinon bound state) as root-mean-square string distance **Crossing-point analysis of \Lambda/L**

//L crossing points converge better
than in other cases (monotonic)

Slope analysis shows v' = 0.58(2) > v

⇒ Transition is associated with spinon deconfinement

v/v' = 0.77 +/- 0.03

In OK agreement with 0.715 +/- 0.015 from VBS domain-wall energy





How do the two divergent lengths affect other observables?

Anomalous scaling behavior

First-order scenario: Prokofe'v, Svistunov, Kuklov, Troyer,... (2008-2013) $\beta \propto L \ (\beta = L, \mathcal{B}$ **Anomalous scaling of winding numbers** $z = 1, \beta \propto L \rightarrow$ $\langle W^2 \rangle = \langle W_x^2 \rangle + \langle W_u^2 \rangle + \langle W_\tau^2 \rangle$ $\rho_s \propto L^{-1}, \quad \chi \propto L^{-1}$ $= 2\beta\rho_s + \frac{4N}{\beta}\chi$ $\rightarrow \langle W^2 \rangle = \text{constant}$ Linear divergence (first-order)? 3.5 Multiplicative log correction? 3.1 r 3.1 3.4 3.0 3.0 2.9 W² > °Å № 2.9 3.3 100 2002.8 3.2 $\beta = L/4$ 2.7 30 40 50 20 100 200 10 3.1 20 30 40 50 80 90 10 70 60 (Sandvik, PRL 2010) L/a Jiang et al. (2008)

Anomalous scaling or first-order transition?

Quantum criticality with two lengths

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

Two divergent lengths tuned by one parameter: $\xi \propto \delta^{-\nu}$, $\xi' \propto \delta^{-\nu'}$ Finite-size scaling of some quantity A. Thermodynamic limit: $A \propto \delta^{\kappa}$ **Conventional scenario**

$$\begin{split} A(\delta,L) &= L^{-\kappa/\nu} f(\delta L^{1/\nu}, \delta L^{1/\nu'}) \\ \text{When L} \to \infty: \ f(\delta L^{1/\nu}, \delta L^{1/\nu'}) \to (\delta L^{1/\nu})^{\kappa} \end{split}$$

Alternative scenario

$$\begin{split} A(\delta,L) &= L^{-\kappa/\nu'} f(\delta L^{1/\nu}, \delta L^{1/\nu'}) \\ \text{When L} \to \infty: \ f(\delta L^{1/\nu}, \delta L^{1/\nu'}) \to (\delta L^{1/\nu'})^{\kappa} \end{split}$$

Example: Spin stiffness: $\kappa = v(z+d-2)$. At criticality:

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

The first scenario has so far been assumed

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

Can alternative scaling form resolve the enigma?

Evidence for unconventional scaling in J-Q model

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

The conventional scaling form $\rho_s \propto L^{-(z+d-2)}$

Replaced by new form $\rho_s \propto L^{-(z+d-2)\nu/\nu'}$



Fixed; taken from

domwain-wall scaling fit

Behavior interpreted as first-order transition is actually unconventional scaling!

Finite-temperature behaviors are similarly affected

Unconventional T>0 critical scaling

Conjecture involving the two length-scale exponents:

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

 $\nu/\nu' \approx 0.72$

Fixed; taken from domain-wall scaling fit



Experimentally important revision of critical scaling

Conclusions

- Two length scales observed explicitly in the J-Q model
- No signs of first-order transition in the J-Q model
- Simple two-length scaling hypothesis explains anomalous scaling of spin stiffness and susceptibility
- conventional wisdoms 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 v/v'
- experimentally important
- How general is this kind of two-length criticality?

