Quantum criticality with two length scales

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References:


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

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

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

\(\Phi\) 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 \(\langle \Phi \rangle \neq 0\): spontaneous symmetry breaking
  - universality class: symmetry and dimensions
Quantum phase transitions

• happens at zero temperature, when adapt $g$ in $H = H_0 + gH_I$; $[H_0, H_I] \neq 0$, continuous 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

\[ S(\Phi) = \int \text{d}r \text{d}\tau ((\partial_\tau \Phi)^2 + v^2 (\nabla_x \Phi)^2 + s\Phi^2 + u(\Phi^2)^2) \]

\[ Z = \int \mathcal{D}\Phi \ e^{-S(\Phi)} \]

• many of these transitions can be understood in the conventional Landau-Ginzburg-Wilson framework
for example: AF Néel-Paramagnetic transition
\( H_0 \) 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


\[ m_s = \frac{1}{N} \sum_i (-1)^{x_i+y_i} S_i \]

VBS order parameter \((D_x, D_y)\)

\[ D_x = \frac{1}{N} \sum_{i=1}^{N} (-1)^{x_i} S_i \cdot S_{i+\hat{x}}, \]
\[ D_y = \frac{1}{N} \sum_{i=1}^{N} (-1)^{y_i} S_i \cdot S_{i+\hat{y}} \]

New physics

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

- 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
Physical picture from VBS side

Levin and Senthil, PRB 70, 2004

VBS: 4 symmetry broken ground states

\[ H = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j), \quad \theta_i = n\pi/2, \quad n = 0, 1, 2, 3 \]
Physical picture from VBS side

Levin and Senthil, PRB 70, 2004

- At the core of the $\mathbb{Z}_4$ 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
- Blue-shaded regions are domain walls
- The thickness $\xi'$ diverges faster than $\xi$
- emergent $U(1)$ symmetry; same as 4-state clock model ($\mathbb{Z}_4$ anisotropy is dangerously irrelevant)
- 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
  \[ \Phi = z^\dagger \sigma z \]

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

\[
H = -J \sum_{\langle ij \rangle} C_{ij} - Q \sum_{\langle ijkl \rangle} C_{ij} C_{kl}, \quad C_{ij} = \left( \frac{1}{4} - S_i \cdot S_j \right)
\]

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 $\gamma = 7/4, \nu = 1$

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

When these are not known, treat as fitting parameters
Finite-size scaling

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When these are not known, treat as fitting parameters
systematic critical-point analysis

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

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

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

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

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

2D Ising model; MC results
Drift in \((L, 2L)\) crossing points

- scaling corrections in crossings

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

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

\(\omega\): unknown correction to scaling, free exponent in fits
● correlation-length exponent $\nu$

can be extracted from the slope of $U$: $s(T, L) = \frac{dU(T,L)}{dT}$

$$\ln\left(\frac{s(T^*, 2L)}{s(T^*, L)}\right) / \ln 2 = \frac{1}{\nu} + aL^{-\omega} + \cdots$$
numerical study of the J-Q model
Many numerical results support DQC scenario

FSS of squared order parameter\((A)\)

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

Data ”collapse”: \(M^2\) and \(D^2\) simultaneously \(\rightarrow\) 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

\[\text{Alet and Damle, PRB 2013 Kaul et al., PRL 2014}\]
However, scaling violation

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

Conventional FSS

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

At critical point:

$$\rho_s \propto L^{-(d+z-2)} = L^{-z}, \quad \chi \propto L^{-(d-z)}$$

$z = 1$ 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**

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

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

- **We propose**

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

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 \( q_c \)

**NOT** \( \rho_s \propto L^{-(d+z-2)} \), **BUT** \( \rho_s \propto L^{-(d+z-2)\nu'/\nu'} \)
phenomenological explanation of our scaling form
General scaling theory for $\rho_s$, single length scale


Free energy density scales

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

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

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

- $\tilde{Y}$ 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

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

- the excess energy due to a twist along apace:

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

which means

\[ \tilde{Y}_s \sim \left(\frac{\xi}{L}\right)^a \left(\frac{\xi'}{L}\right)^{2-a} \]

- 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 \( \xi = L^{\nu'/\nu} \),

\[ \rho_s \sim L^{-(d+z-2)\nu'/\nu'} \]
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 \( U(\tau) = \exp(-H\tau) \)

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

\( A_c \) is the estimator of \( A \).
Projector Quantum Monte Carlo method

- using VB basis

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

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

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

\[ \langle S_i \cdot S_j \rangle = \begin{cases} 0, & (i)_L(j)_L \\ \frac{3}{4} \phi_{ij}, & (i,j)_L \end{cases} \]
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

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

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

- what is $\nu'$ obtained from confinement length $\Lambda$?
  - DQC theory: VBS domain wall thickness
    $$\xi \propto (q - q_c)^{-\nu}, \quad \xi' \propto (q - q_c)^{-\nu'}, \quad \nu' > \nu$$

- $\nu/\nu' = 0.77(3)$ 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
  \[
  \delta F = F_{\text{wall}} - F_{\text{uniform}}
  \]
  \[
  \kappa = \frac{\delta F}{L^{d+z-1}}
  \]

\[
\langle S_i \cdot S_j \rangle
\]
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,
  
  \[
  \rho_s \propto \frac{1}{\xi}, \quad \Lambda \propto \xi', \quad \kappa \propto \frac{1}{\xi \xi'} \propto \delta^{\nu+\nu'}
  \]

- translate to finite size at $q_c$:
  
  When $\xi'$ reaches $L$, $\xi$ saturates at
  
  \[
  \xi^{\nu/\nu'} = L^{\nu/\nu'}
  \]

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

  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

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

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

\[ \xi \sim \xi'^{\nu/\nu'}, \nu/\nu' \approx 0.47, \nu' \text{ is universal} \]

Léonard and Delamotte, PRL 2015
Further evidence for unconventional scaling according to our scaling form

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

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

- 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 $\nu/\nu'$:

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

![Graphs showing scaling behavior](image)
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!