Monte Carlo simulations of deconfined quantum-criticality

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Outline
- Exotic Neel-VBS transition; deconfined quantum-criticality
- $S=1/2$ Heisenberg model with four-spin interactions
- Quantum Monte Carlo in the valence bond basis
- Simulation Results; VBS phase, critical behavior
- Emergent $U(1)$ symmetry

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Continuous quantum phase transition (T=0) between two ordered phases

- Neel to valence-bond-solid (VBS)
- Deconfined spinons at critical point
- Confined spinons → Neel or VBS order

\[
H = \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j + \ldots \quad g = g(\{J_{ij}, \ldots\})
\]

Two types of critical VBS fluctuations
- plaquette and columnar
- \(\mathbb{Z}_4\) symmetry irrelevant at critical point
- emergent \(U(1)\) symmetry

Outside the Ginzburg-Landau-Wilson phase transition framework
- GLW generically gives first-order or two separate transitions
Do deconfined quantum-critical points exist?

- Do they exist in nature? Can they be identified in numerical studies?
- First step: Find model hamiltonians exhibiting Neel-VBS transition

- VBS phases of quantum spin systems have been studied for a long time [Read and Sachdev, PRL (1988)]
- Why have Neel-VBS transitions not been fully characterized yet?

Models exhibiting both Neel and VBS phases are typically frustrated

- Sign problems for quantum Monte Carlo
- Only very small lattices can be studied (exact diagonalization)
- No unbiased numerical methods for this class of systems
- Only approximate numerical/analytical results available

2D Heisenberg model with 4-spin term

\[ H = J \sum_{\langle ij \rangle} S_i \cdot S_j - Q \sum_{\langle ijkl \rangle} (S_i \cdot S_j - \frac{1}{4})(S_k \cdot S_l - \frac{1}{4}) \]

- Studied using QMC projector method in the valence bond basis
- Turns out to have a Neel-VBS transition for \( J/Q \approx 0.04 \)

Projector MC in the valence bond basis


\[ |\Psi\rangle = \sum_k f_k |(a_1, b_1)(a_2, b_2) \cdots (a_{N/2}, b_{N/2})\rangle \]

Projector out the ground state

\[ (-H)^n |\Psi\rangle \rightarrow c_0 |E_0|^n |0\rangle \]

\[ \langle A \rangle = \frac{\langle \Psi|(-H^*)^n A (-H)^n |\Psi\rangle}{\langle \Psi|(-H^*)^n (-H)^n |\Psi\rangle} \]

Example 2D Heisenberg model:

\[ H = -\sum_{\langle ij \rangle} H_{ij}, \quad H_{ij} = -(S_i \cdot S_j - \frac{1}{4}) \]
J-Q model; is there a VBS phase?

✦ VBS order parameter - columnar dimer-dimer correlations

\[ D^2 = \frac{1}{N^2} \sum_{i,j} \langle (\mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}})(\mathbf{S}_j \cdot \mathbf{S}_{j+\hat{x}}) \rangle (-1)^{(x_i-x_j)} \]

✦ Sublattice magnetization - staggered spin-spin correlations

\[ M^2 = \frac{1}{N^2} \sum_{i,j} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle (-1)^{(x_i-x_j+y_i-y_j)} \]

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➤ J/Q=0.0 → VBS

➤ J/Q=0.1 → antiferromagnet
Do the VBS and AFM orders vanish at the same point?

Both vanish at $J/Q \approx 0.04$

scale as $(1/L)^{z+\eta}$ with $z+\eta \approx 1.3$

Compare with $O(3)$ transition in Heisenberg bilayer

$g = J_2/J_1$

$z+\eta \approx 1.03$, $z=1$, $\eta \approx 0.03$
Singlet-triplet gap scaling $\rightarrow$ Dynamic exponent $z$

$z$ relates length and time scales:

$$\omega_q \sim |q|^z \quad \text{finite size} \rightarrow \Delta \sim L^{-z}$$

There is an improved estimator for the gap in the VB basis QMC

$\Delta \sim L^{-z}$

$z=1$ $\Rightarrow$ $\eta \approx 0.3$: consistent with deconfined quantum-criticality

- $z=1$ field theory and "large" $\eta$ predicted (Senthil et al.)
Finite-size scaling

Correlation lengths (spin, dimer): $\xi_{s,d}$

Binder ratio (for spins): $q_s = \frac{\langle M^4 \rangle}{\langle M^2 \rangle^2}$

long-distance spin and dimer correlations: $C_{s,d}(L/2,L/2)$

All scale with a single set of critical exponents at $g_c \approx 0.04$
(with subleading corrections)

$\nu = 0.78(3), \eta = 0.26(3)$
Any other evidence for deconfined quantum-criticality?

Emergent U(1) symmetry predicted; should show up in the VBS order-parameter close to the critical point (on the VBS side)

- for L below a length scale $\Lambda$ at which $Z_4$ anisotropy becomes relevant

**Analogy:** 3D classical XY model with $Z_4$ anisotropy

[Jie Lou and AWS, ArXiv:0704.1472]

$$H = -J \sum_{\langle i,j \rangle} \cos(\Theta_i - \Theta_j) - h \sum_i \cos(4\Theta_i)$$

- the anisotropy $h$ is known to be marginally irrelevant
- Universality class unaffected, but ordered state reflects $Z_4$ term
- seen in 2D histogram $P(M_x, M_y)$

$$M_x = \frac{1}{N} \sum_i \cos(\Theta_i), \quad M_y = \frac{1}{N} \sum_i \sin(\Theta_i)$$

![Images showing histograms for $T>T_c$, $T<T_c$, and $T<<T_c$](image-url)
$M_x \approx M_y$ Configuration (one layer); $h/J = 1$

- **4 orientations (colors)**
  - correspond to the 4 ways of arranging VBS order in J-Q model
  - **1 or 2 directions dominate on the “U(1) circle”**
  - corresponds to mixing of two types of VBS
**J-Q model**

**Correlations between x and y VBS order parameters**

The simulations sample the ground state;

$$|0\rangle = \sum_k c_k |V_k\rangle$$

Graph joint probability distribution $P(D_x, D_y)$

$$D_x = \frac{\langle V_k | S_i \cdot S_{i+\hat{x}} | V_p \rangle}{\langle V_k | V_p \rangle} \quad \quad D_y = \frac{\langle V_k | S_i \cdot S_{i+\hat{y}} | V_p \rangle}{\langle V_k | V_p \rangle}$$

**Questions**

**Is there an emergent U(1) symmetry at the transition**

✓ rotational, U(1), vs 4-fold, $Z_4$, symmetry of $P(D_x, D_y)$

**Is the transition weakly first order?**

✓ coexistence of Neel and VBS should show up in $P(D_x, D_y)$ as a central peak coexisting with 4 VBS maxima

**Results:** L=32 lattices
$J/Q = 0.45$
$J/Q = 0.40$
$J/Q = 0.35$
\[ \frac{J}{Q} = 0.30 \]
$J/Q = 0.25$
$J/Q = 0.20$
$J/Q = 0.10$
$J(Q)=0.00$

No signs of $Z_4$ anisotropy!

Return to classical $Z_q$ model to explore the cross-over from $U(1)$ to $Z_q$ order-parameter
Order parameter quantifying U(1) emergence

Magnetization in terms of the probability distribution

\[ M = \int dr d\phi r^2 P(r, \phi) \]

Modified magnetization vanishing if not \( Z_q \) anisotropic

\[ M^* = \int dr d\phi r^2 P(r, \phi) \cos(q\phi) \]

\( M^* \) should be controlled by the length scale \( \Lambda \) at which the \( Z_q \) term becomes relevant

\[ \Lambda \sim \xi^a \sim t^{-a\nu} \]

Finite-size scaling

\[ M \sim L^{-(1+\eta)/2} f(tL^{1/\nu}) \]

\[ M^* \sim L^{-(1+\eta)/2} g(tL^{1/a\nu}) \]

3D XY exponents

\( \nu \approx 0.67, \quad \eta \approx 0.04 \)
Results: $Z_4$

\[ M \sim L^{-\frac{(1+\eta)}{2}} f(tL^{1/\nu}) \]

\[ M^* \sim L^{-\frac{(1+\eta)}{2}} g(tL^{1/\alpha\nu}) \]
$Z_6$

Results for $q=4,...,8 \Rightarrow$

\[ a_q \approx a_4 \left(\frac{q}{4}\right)^2, \quad a_4 \approx 1.07 \]

Agrees with RG, $\epsilon$-expansion (Oshikawa, PRB 2000)

Asymptotic $q\to\infty$ form:

\[ a_q = \frac{q^2}{10} \]
Summary & Conclusions

2D J-Q model; Heisenberg model with 4-spin interactions

- Results consistent with continuous Neel-VBS transition
- $z=1$, as required by deconfined theory
- Single set of exponents describe spin and dimer correl.
  - higher symmetry - SO(5) - at the critical point?
- $\eta$ is large ($\approx 0.26$) - consistent with prediction for DCQP
- Evidence of emergent U(1) symmetry

How does the $Z_4$ length $\Lambda$ diverge? $\Lambda \sim \xi^a$

- Larger lattices needed
- in 3D classical XY-$Z_4$ model, $a_4 \approx 1.07$
  - $a_q$ increases with $q$ for $Z_q$ model: $a_q \approx a_4 (q/4)^2$
  - in good agreement with $\epsilon$-expansion (Oshikawa)
- results indicate $a > a_4$ for J-Q model

J-Q model: “Ising model of deconfined quantum-criticality”