Deconfined spinons at the Néel-VBS transition in two dimensions

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Outline

Introduction

• Conventional T>0 quantum-criticality in 2D antiferromagnets
• Scaling behavior at putative deconfined quantum-critical point
  - Neel - VBS transition in “J-Q” model
  - Observed (QMC) scaling anomalies; T=0 and T>0
  - Phenomenological spinon-gas model

Results and analysis

• Locating the critical point in the J-Q model and dimerized models
• T>0 correlation length at criticality
• Evidence for continuous transition (J-Q) with weak scaling violations
• Low-energy phenomenology; spinon and magnon gas model
  - Low-T forms of magnetic susceptibility and specific heat
  - QMC data fits; critical J-Q and dimerized models
  - Effective spin (S≈1/2) of the excitations in the J-Q model

Other related issues (time permitting)

• Critical examination of the first-order scenario
  - comparing with the first-order transition into staggered VBS
• VBS fluctuations and emergent U(1) symmetry

Conventional O(3) transition in 2D antiferromagnets


Realized in dimerized S=1/2 Heisenberg models

\[
H = J \sum_{\langle ij \rangle} S_i \cdot S_j + J' \sum_{\langle ij \rangle'} S_i \cdot S_j
\]

Neel - non-magnetic T=0 transition vs \( g = J'/J \)
• plain singlet-product (+ fluct) state for \( g > g_c \)

T>0 quantum-critical regime
• magnons (S=1) remain as the elementary excitations at the critical point
• dynamic exponent \( z = 1 \)
• scaling behavior:
  \[
  \xi \propto T^{-1} \\
  \chi \propto T \\
  C \propto T^2
  \]
• confirmed by QMC
• some issues remain in (c)

3D O(3) (Heisenberg) universality
Deconfined Neel-VBS transition in 2D antiferromagnets


Neel-VBS transition realized in the “J-Q” model (square lattice)
AWS, PRL 98, 227202 (2007)

\[ H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - Q \sum_{\langle ijk \ell \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4}) (\mathbf{S}_k \cdot \mathbf{S}_l - \frac{1}{4}) \]

- no sign problems in QMC simulations
  - unlike frustrated systems (traditional play ground for VBS physics)

QMC in agreement with theory:
- dynamic exponent \( z = 1 \)
- “large” exponent \( \eta_{\text{spin}} \approx 0.35 \)
- emergent U(1) VBS symmetry

weakly 1st-order transition argued by
Jiang et al., JSTAT, P02009 (2008)
Kuklov et al., PRL 101, 050405 (2008)

recent large-scale studies do not find any evidence for 1st-order
- instead: log-corrections
**Question:** Consequences of spinons in T>0 QC regime?

Phenomenological model of a spinon gas at T>0

- bosonic spinons, linearly dispersing at T=0; $\varepsilon(k) = c k$
- thermal length $\Lambda(T)$; assuming free spinons for $q>1/\Lambda$
  - contributions to thermodynamics from these spinons

Infrared momentum cut-off $1/\Lambda$ equivalent to thermal gap $\Delta=1/\Lambda$

$$\varepsilon(k) = \sqrt{c^2 k^2 + \Delta^2}$$

**J-Q QMC results:**

- Standard QC forms
  - $\xi \propto T^{-1}$
  - $\chi \propto T$
  - are weakly violated.

Specific heat obeys the standard form

$$C \propto T^2$$

**J-Q model:** critical $\xi$ diverges faster than $1/T$ as $T \to 0$ ($\Delta/T \to 0$)

- infrared divergent integral leads to weak $T \to 0$ divergence (log) of $\chi/T$
- weaker correction to $T^2$ form of C
**T=0 critical couplings:** Dimensionless quantities should scale as $L$
- Correlation lengths, Binder cumulants, spin stiffness ($L\rho_s$),...
- Curves vs coupling for different $L$ cross at critical point

**J-Q model**
Spin and dimer correlation lengths (second moment def)
Critical-point estimates

J-J’ model: \((J'/J)_c=1.90948(4)\), (using \(J'/J=1.9095\))
J-Q model: \((J/Q)_c=0.04498(3)\), (using \(J/Q=0.0450\))

**T>0 critical spin correlation length**

- \(L\) up to 512; converged to thermodynamic limit for \(T\) considered

\[
\xi = \frac{1}{q} \sqrt{\frac{S(Q)}{S(Q - q)}} - 1,
q = \frac{2\pi}{L}
\]

**J-J’ model:** expected \(1/T\) divergence

**J-Q model:** faster than \(1/T\) divergence

- logarithmic or power correction (data consistent with either form)
Conclusion from previous T=0 and T>0 calculations
AWS, PRL 104, 177201 (2010)

logarithmic corrections to quantum-critical scaling
\[
\rho_s \sim \frac{\ln(L/L_0)}{L} \quad (T \to 0)
\]
\[
\chi \sim T[1 + a \ln(1/T)] \quad (L \to \infty)
\]

Could the behavior indicate \( z \neq 1 \)?
\[
\xi \sim T^{-(1/z)}
\]
\[
\chi \sim T^{2/z-1}
\]
\[
\rho_s \sim L^{-z}
\]

\( \xi \) gives \( z \approx 0.82 \)
- consistent with \( \rho_s(L) \)
- inconsistent with \( \chi(T) \)
  - demands \( \chi/T \to 0 \) for \( T \to 0 \)

Some unconventional reason
- marginal operator causing logs?
Can we find relationships between the different anomalies?  
• can this provide a fingerprint for spinons?

Gas of non-interacting spinons (S=1/2) or magnons (S=1) at T>0

\[
\epsilon_\pm(k) = \sqrt{c^2k^2 + \Delta^2} \pm \mu B \equiv \epsilon(k) \pm \mu B \quad \text{(B = magnetic field)}
\]

\[
\mu = 1/2 \text{ (spinons)}, \quad \mu = 1 \text{ (magnons)}
\]

Magnetization to linear order (bosonic excitations)

\[
M = \mu F \int \left( \frac{1}{e^{\epsilon_-/T} - 1} - \frac{1}{e^{\epsilon_+/T} - 1} \right) \frac{d^2k}{(2\pi)^2}
\]

\[
= -2\mu^2 FB \int \frac{\partial n}{\partial \epsilon} \frac{d^2k}{(2\pi)^2}
\]

\[
= \mu^2 F \frac{TB}{4\pi c^2} \int_0^\infty \frac{xdx}{\sinh^2 \left[ \frac{1}{2} \sqrt{x^2 + (\Delta/T)^2} \right]}
\]

**F is a degeneracy factor:** F=2 (spinons/anti-spinons), F=1 (magnons)  
Conventional quantum-criticality: \(\Delta/T \rightarrow m \approx 0.96\) (Chubukov & Sachdev 1994)  
• computed using large-N calculations (nonlinear \(\sigma\)-model)  
In the J-Q model (deconfined criticality?): \(\Delta/T \rightarrow 0\) (\(\log^{-1}(1/T)\) or \(T^a\))  
• infrared divergent integral; significant consequences
\[
\int_{0}^{\infty} \frac{xdx}{\sinh^{2}\left(\frac{1}{2}\sqrt{x^{2}+p^{2}}\right)} = \frac{4p}{1-e^{-p}} - 4\ln(e^{p} - 1) \quad p = \Delta/T
\]

Using these gaps for spinon (S=1/2) and magnon (S=1) calculations:

\[
\Delta_{1/2}/T = 1/(T\xi) = (T/mc)^{a} \quad (mc \text{ and } a \text{ from J-Q QMC data})
\]

\[
\Delta_{1}/T = m = 0.96 \quad \text{(Chubukov & Sachdev)}
\]

Gives the low-T magnetic susceptibility

\[
\chi_{1} = \left(1.0760/\pi c^{2}\right)T
\]

\[
\chi_{1/2} = \frac{T}{2\pi c^{2}} \left[1 + a \ln\left(\frac{mc}{T}\right) + \frac{1}{24} \left(\frac{T}{mc}\right)^{2a}\right]
\]

Specific heat

\[
C_{S} = (2S + 1) F \int \epsilon(k) \frac{\partial n(\epsilon)}{\partial T} \frac{d^{2}k}{(2\pi)^{2}}
\]

\[
C_{1} = \left[36\zeta(3)/5\pi c^{2}\right]T^{2} \quad \text{(Chubukov & Sachdev)}
\]

\[
C_{1/2} = \frac{2T^{2}}{\pi c^{2}} \left[6\zeta(3) - \left(\frac{T}{c}\right)^{2a} \left[\frac{3}{2} + a + a(1 + a) \ln\left(\frac{c}{T}\right)\right]\right]
\]
QMC data fits: J-J’ (magnon forms) and J-Q models (spinon forms)

- **J-J’**: velocity fitted in $E/T^3$, polynomial fit for $\chi/T$ (velocities agree to 2%)
- **J-Q**: velocity is fitted; values from $X/T$ and $C$ agree within 2%

\[
\frac{(E - E_0)}{T^3}
\]

\[
\chi/T
\]
**J-Q model: effective spin of the excitations**

Under the assumption of spinons, S=1/2, μ=1/2, F=2 (spinon/anti-spinon):

\[ F_\chi = \frac{\mu^2 F}{c^2_\chi} \approx 0.074, \quad F_C = \frac{(2S + 1)F}{c^2_C} \approx 0.615 \]

\[ c_\chi = 2.60 \quad c_C = 2.55 \]

Should have \( c_\chi = c_C \). \( S \neq 1/2 ? \) For both spinons (S=1/2) and magnons (S=1)

\[ \mu = S^{-1}, \quad F = 1/S \quad \rightarrow \quad \frac{F_\chi}{F_C} = \frac{S^2}{2S + 1} \]

Treat S as continuous variable and find effective S given the J-Q data:

The J-Q results are consistent with S=1/2 (spinons) but not consistent with S=1 (magnons)

**Could this be a coincidence?**

- assumed \( \Delta = 1/\xi \)
- may be \( \Delta = d/\xi, \ d \approx 1 \)
- results depend weakly on d

Independent estimate of the velocity would be good
- can be done
  - imaginary time correlations
Could the transition be first-order?

Jiang, Nyfeler, Chandrasekharan, Wiese, JSTAT, P02009 (2008)
From an antiferromagnet to a valence bond solid: evidence for a first order phase transition
Deconfined Criticality: Generic First-Order Transition in the SU(2) Symmetry Case

One can never, strictly speaking, rule out a very weak first-order transition
• but are there any real signs of this in the J-Q model?

The above studies were based on scaling of winding numbers
• claimed signs of phase coexistence (finite spin stiffness and susceptibility)

\[
\langle W^2 \rangle = \langle W_x^2 \rangle + \langle W_y^2 \rangle + \langle W_\tau^2 \rangle \\
= 2\beta \rho_s + \frac{4N}{\beta} \chi
\]

At at a critical point
\[
z = 1, \beta \propto L \rightarrow \\
\rho_s \propto L^{-1}, \chi \propto L^{-1} \\
\rightarrow \langle W^2 \rangle = \text{constant}
\]
Recent large-scale QMC results

- Stochastic series expansion
- up to 256×256 lattices

$$ \beta \propto L \ (\beta = L, \ \beta = L/4) $$

Same finite-size definition of critical point as used by Kuklov et al. and Jiang et al.
- fixed probability of the generated configurations having $W_x=W_y=W_T=0$

Logarithmic divergence of $\langle W^2 \rangle$!
- scaling correction (not 1st-order)
Let’s look at a well known signal of a first-order transition:

**Binder ratio**

\[ Q_2 = \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2} \]

**Binder cumulant**

\[ U_2 = \frac{5 - 3Q_2}{2} \]

Size independent (curve crossings) at criticality

\( U_2 < 0 \) at a first-order transition

- no signs of \( U_2 < 0 \) in SSE results for \( L \) up to 256

**Phase coexistence**

leads to \( U_2 \rightarrow -\infty \) at 1st-order trans.
Example of a first-order Neel - VBS transition

J-Q model with staggered VBS phase  [A. Sen, AWS, PRB (2010)]

- no local VBS fluctuations favoring emergent U(1) symmetry

\[ H = -J \sum \langle ij \rangle C_{ij} - Q_3 \sum \langle ijklnm \rangle C_{ij}C_{kl}C_{mn} \]

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

- clear signs of phase coexistence

For Neel order
Any signs of coexistence in the standard J-Q VBS distributions?
• L=128 data close to the transition

\[ J/Q = 0.040 \]
$J/Q = 0.041$
$J/Q = 0.042$
$J/Q = 0.043$
J/Q = 0.044
$J/Q = 0.045$
$J/Q = 0.046$
Exponents: T=0 results obtained with valence-bond QMC algorithm

Exponents $\eta_s$, $\eta_d$, and $\nu$ from the squared order parameters

\[
D^2 = \langle D_x^2 + D_y^2 \rangle, \quad D_x = \frac{1}{N} \sum_{i=1}^{N} (-1)^{x_i} S_i \cdot S_{i+x}, \quad D_y = \frac{1}{N} \sum_{i=1}^{N} (-1)^{y_i} S_i \cdot S_{i+y}
\]

\[
M^2 = \langle \vec{M} \cdot \vec{M} \rangle, \quad \vec{M} = \frac{1}{N} \sum_i (-1)^{x_i+y_i} \vec{S}_i
\]

Coupling ratio

\[
q = \frac{Q}{Q + J}
\]

- AF order for $q \to 0$
- VBS order for $q \to 1$

\[
(Q/J)_c \approx 24, \quad q_c \approx 0.961
\]

\[
\eta_s = 0.35(2) \quad \eta_d = 0.20(2) \quad \nu = 0.67(1)
\]

Analysis should be improved (larger lattices) in light of possible logarithmic corrections
**Columnar or plaquette VBS?**

QMC-sampled state in the valence-bond basis

\[ |0\rangle = \sum_k c_k |V_k\rangle \]

Joint probability distribution \( P(D_x, D_y) \) of x and y columnar VBS order parameters

\[
D_x = \frac{\langle V_k | \frac{1}{N} \sum_{i=1}^{N} (-1)^{x_i} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}} | V_p \rangle}{\langle V_k | V_p \rangle}
\]

\[
D_y = \frac{\langle V_k | \frac{1}{N} \sum_{i=1}^{N} (-1)^{y_i} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{y}} | V_p \rangle}{\langle V_k | V_p \rangle}
\]

4 peaks expected in VBS phase
- \( Z_4 \)-symmetry unbroken in finite system
**VBS fluctuations** in the theory of deconfined quantum-critical points
[Senthil et al., 2004]

- plaquette and columnar VBS are almost degenerate
- tunneling barrier separating the two
  - barrier increases with increasing system size $L$
  - barrier decreases as the critical point is approached

- emergent $U(1)$ symmetry
- ring-shaped distribution expected in the VBS phase for small systems
  \[ L < \Lambda \sim \xi^a, \; a > 1 \text{ (spinon confinement length)} \]
Signs of $Z_4$ symmetry in the original J-Q model?

$L=128, J=0$
$P(D_x, D_y)$

$L=32, L=64; J=0$
Weak but statistically significant angular dependence consistent with columnar VBS
($L=128$ still too noisy)
Creating a more robust VBS order - the J-Q$_3$ model


\[ H = -J \sum_{\langle ij \rangle} C_{ij} - Q_3 \sum_{\langle ijklnm \rangle} C_{ij}C_{kl}C_{mn} \]

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

This model has a more robust VBS phase
• can the symmetry cross-over be detected?

\[ q = 0.635 \quad (q_c \approx 0.60) \quad L = 32 \]

\[ q = 0.85 \quad L = 32 \]
Analysis of the VBS symmetry cross-over  (J-Q\textsubscript{3} model)


Z\textsubscript{4}-sensitive VBS order parameter

\[ D_4 = \int r \, dr \int d\phi P(r, \phi) \cos(4\phi) \]

Finite-size scaling gives U(1) (deconfinement) length-scale

\[ \Lambda \sim \xi^{1+a} \]
\[ \sim (q - q_c)^{(1+a)\nu} \]
\[ a = 0.20 \pm 0.05 \]
Conclusions

Large-scale QMC calculations of the J-Q model
• scaling behavior consistent with a continuous Neel-VBS transition
  - with weak scaling corrections; maybe logarithmic
• no signatures of first-order behavior
  - cannot be ruled out as a matter of principle, but seems unlikely
• a simple spinon gas pictures can account for the T>0 behavior
  - log-correction to susceptibility follows from anomalous length scale
  - effective-spin calculation in very good agreement with S=1/2 spinons

Relation to deconfined quantum-criticality of Senthil et al.
• Main features in good agreement
  - z=1 scaling
  - “large” anomalous dimension $\eta_{\text{spin}}$
  - emergent U(1) symmetry
• NCCP$^{N-1}$ field theory for large N
  [Senthil et al. (PRB 2004), Kaul & Sachdev (PRB 2008)]
  - no log-corrections found
  - difficult to extend to N=2 in analytical work
  - could there be log-corrections for N=2 (or general “small” N)?