Correlations and Coherence in Quantum Systems, Évora, October 8-12, 2012

Exploring Quantum Fluctuations and Quantum Phase transitions in Spin Systems

Anders W. Sandvik, Boston University

Collaborators:

- Ribhu Kaul (U of Kentucky)
- Naoki Kawashima (ISSP, U of Tokyo)
- Jie Lou (BU \rightarrow ISSP \rightarrow Fudan U)
- Arnab Sen (BU → Max Planck, Dresden)

Related review article:

- R. K. Kaul, R. G. Melko, A. W. Sandvik, arXiv:1204.5405 (to appear in Annual Review of Condensed Matter Physics)





Outline

- Antiferromagnet-paramagnet quantum phase transition
- Valence-bonds-solid (VBS) order and "deconfined" criticality
- Microscopic realizations; J-Q model
- Insights from QMC simulations; SU(2) and SU(N) models
- Time permitting: Emergent U(1) symmetry of the near-critical VBS



Conventional Neel-paramagnet quantum phase transition

Example: Dimerized S=1/2 Heisenberg models

- every spin belongs to a dimer (strongly-coupled pair)
- many possibilities, e.g., bilayer, dimerized single layer



Singlet formation on strong bonds → Neel - disordered transition Ground state (T=0) phases



⇒ 3D classical Heisenberg (O3) universality class; QMC confirmed

Example of QMC finite-size scaling scaling with QMC data dimerized single-layer Heisenberg model



According to theory, spin stiffness at the critical point should scale

0.25

$$\rho_s \sim \frac{1}{L} \to L \rho_s \text{ constant}$$

Allows accurate determination of the critical point (curve crossings)

More complex non-magnetic states; systems with 1 spin per unit cell

$$\mathbf{H} = \mathbf{J} \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} \mathbf{S}_{\mathbf{i}} \cdot \mathbf{S}_{\mathbf{j}} + \mathbf{g} \times \cdots$$

non-trivial non-magnetic ground states are possible, e.g.,

- resonating valence-bond (RVB) spin liquid
- ➡ valence-bond solid (VBS)

Non-magnetic states often have natural descriptions with valence bonds



$$= (\uparrow_i \downarrow_j - \downarrow_i \uparrow_j)/\sqrt{2}$$

The basis including bonds of all lengths is **overcomplete** in the singlet sector





non-magnetic states dominated by short bonds

VBS states and "deconfined" quantum criticality

Read, Sachdev (1989),...., Senthil, Vishwanath, Balents, Sachdev, Fisher (2004)

$$\mathbf{H} = \mathbf{J} \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} \mathbf{S}_{\mathbf{i}} \cdot \mathbf{S}_{\mathbf{j}} + \mathbf{g} \times \cdots$$

Neel-VBS transition in 2D

- generically continuous
- violating the "Landau rule" stating 1st-order transition

Description with spinor field

(2-component complex vector)



$$\Phi = z_{\alpha}^{*} \sigma_{\alpha\beta} z_{\beta} \qquad \text{gauge redundancy: } z \to e^{i\gamma(r,\tau)} z$$
$$S_{z} = \int d^{2}r d\tau \left[|(\partial_{\mu} - iA_{\mu})z_{\alpha}|^{2} + s|z_{\alpha}|^{2} + u(|z_{\alpha}|^{2})^{2} + \frac{1}{2e_{0}^{2}}(\epsilon_{\mu\nu\lambda}\partial_{\nu}A_{\lambda})^{2} \right]$$

A is a U(1) symmetric gauge field

• CP¹ action (non-compact)

- large-N calculations for CP^{N-1} theory
- proposed as critical theory separating Neel and VBS states
- describes VBS state when additional terms are added

Competing scenario: first-order transition (Kuklov et al., 2008)

In what systems can Neel-VBS transition be studied with QMC? <u>VBS states from multi-spin interactions</u> (Sandvik, 2007)

The Heisenberg interaction is equivalent to a singlet-projector $C_{ij} = \frac{1}{4} - \vec{S}_i \cdot \vec{S}_j$ $C_{ij} |\phi_{ij}^s\rangle = |\phi_{ij}^s\rangle, \quad C_{ij} |\phi_{ij}^{tm}\rangle = 0 \quad (m = -1, 0, 1)$

- 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-Q2" 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
- Intended to study Néel-VBS transition (universal physics)

(Sandvik, 2007; Lou, Sandvik, Kawashima, 2009)

VBS vector order parameter (D_x, D_y) (x and y lattice orientations)

T=0 projector QMC results (no approximations; finite size)

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

Néel order parameter (staggered magnetization)

Néel-VBS transition in the J-Q model

$$\vec{M} = \frac{1}{N} \sum_{i} (-1)^{x_i + y_i} \vec{S}_i$$

No symmetry-breaking in simulations; study the squares

$$M^2 = \langle \vec{M} \cdot \vec{M} \rangle, \quad D^2 = \langle D_x^2 + D_y^2 \rangle$$

Finite-size scaling: a critical squared order parameter (A) scales as

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

Data "collapse" for different system sizes L of AL^{1+η} graphed vs (q-q_c)L^{1/v}







J-Q₂ model; q_c=0.961(1) $\eta_s = 0.35(2)$ $\eta_d = 0.20(2)$ $\nu = 0.67(1)$ J-Q₃ model; q_c=0.600(3)

 $\eta_s = 0.33(2)$ $\eta_d = 0.20(2)$ $\nu = 0.69(2)$

Exponents universal (same within error bars)



Making connections with field theory

The non-compact CP^{N-1} model has been studied for large N

large-N expansion, SU(N) symmetry

Senthil et al. (2004), Kaul & Sachdev (2009)

$$\eta_s = 1 - \frac{32}{\pi^2 N} + \dots$$

$$SU(2) \rightarrow SU(N)$$

• older results, using relationship between monopoles in the field theory and the VBS order parameter Read & Sachdev (1989)

 $\eta_d = 0.2492 \times N - 1 + \dots$

How can we test these results?

QMC studies of spin hamiltonians with SU(N) spins

2D SU(N) Heisenberg model [Harada et al. (2003), Beach et al. (2010)]

- Fundamental and conjugate repr. of SU(N) on A,B sublattices
- No sign problem in QMC
- Same repr. used in analytical large-N calculations
- Neel ground state for N<5, VBS for N=5,6,...

J-Q models with SU(N) spins

Lou, Sandvik, Kawashima, PRB (2009)

Heisenberg model (Q=0) has Neel ground state for N=2,3,4 \Rightarrow

Neel - VBS transition vs Q/J

Model, symmetry	η_s	η_d	ν
$J-Q_2$, SU(2)	0.35(2)	0.20(2)	0.67(1)
$J-Q_3$, SU(2)	0.33(2)	0.20(2)	0.69(2)
$J-Q_2$, SU(3)	0.38(3)	0.42(3)	0.65(3)
$J-Q_2, SU(4)$	0.42(5)	0.64(5)	0.70(2)

How can we reach larger N to really study the large-N limit?



J1-J2 Heisenberg model with SU(N) spins (Kaul, Sandvik, PRL 2012)

Ferromagnetic 2nd-neighbor couplings enhance Neel order

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



 $J_1 > 0$ $= J_2 < 0$

SU(N) generalization:

$$H = -\frac{J_1}{N} \sum_{\langle ij \rangle} P_{ij} - \frac{J_2}{N} \sum_{\langle \langle ij \rangle \rangle} \Pi_{ij}$$

 $P_{ij} = SU(N)$ singlet projector $\Pi_{ij} =$ permutation operator

There is Neel order for all N>4
Neel - VBS transition accessible with QMC for large N



Comparing results: J₁-J₂, J-Q, NCCP^{N-1}



Conclusion: Trends for large N show excellent agreement

- QMC results predict size of the next 1/N corrections
- Field-theory challenge: Compute the next correction

Nature of the VBS fluctuations in the J-Q model - SU(2) Joint probability distribution P(D_x,D_y) of x and y VBS order

$$D^{2} = \langle D_{x}^{2} + D_{y}^{2} \rangle, \quad D_{x} = \frac{1}{N} \sum_{i=1}^{N} (-1)^{x_{i}} \mathbf{S}_{i} \cdot \mathbf{S}_{i+\hat{x}}, \quad D_{y} = \frac{1}{N} \sum_{i=1}^{N} (-1)^{y_{i}} \mathbf{S}_{i} \cdot \mathbf{S}_{i+\hat{y}}$$

The squared order parameter cannot distinguish between:



J-Q₂ model, J=0, L=128



Magnitude of D has formed but the VBS "angle" is fluctuating

VBS fluctuations in the theory of deconfined quantum-critical points [Senthil et al., 2004]

- > plaquette and columnar VBS are almost degenerate
- > tunneling barrier seperating 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 (related to spinon confinement length)

Creating a more rubust VBS order - the J-Q3 model

J. Lou, A.W. Sandvik, N. Kawashima, PRB (2009)



$$H = -J\sum_{\langle ij\rangle} C_{ij} - Q_3 \sum_{\langle ijklmn\rangle} C_{ij} C_{kl} C_{mn}$$

$$C_{ij} = \frac{1}{4} - \vec{S}_i \cdot \vec{S}_j$$
$$q = \frac{Q_3}{J + Q_3}$$

This model has a more robust VBS phasecan the symmetry cross-over be detected?

 $\begin{array}{c}
q = 0.635 \\
(q_c \approx 0.60) \\
L = 32
\end{array}$ $\begin{array}{c}
q = 0.85 \\
L = 32
\end{array}$

Analysis of the VBS symmetry cross-over (J-Q₃ model)

J. Lou, A.W. Sandvik, N. Kawashima, PRB (2009)

Z₄-sensitive VBS order parameter

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



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





Signs of Z₄ 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)



The simulations take a long time to rotate the VBS angle L=128: 10^5 measurements require > 1 day of computation



building 100×10⁵ measurements

10⁵ measurements

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
- emergent U(1) symmetric VBS order parameter

SU(N) J-Q model and J₁-J₂ Heisenberg model

critical correlation exponents approach large-N results

Relation to deconfined quantum-criticality of Senthil et al.

- Main features in good agreement
 - z=1 scaling
 - "large" anomalous dimension η_{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 analytically
- difficult to extend to N=2 (3,4) in analytical work
- could there be log-corrections for N=2 (or general "small" N)?
 - claimed recently by Nogueira & Sudbo (arXiv 2011)

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 Kuklov, Matsumoto, Prokof'ev, Svistunov, Troyer, PRL 101, 050405 (2008) 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)



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 $W_x = W_y = W_\tau = 0$



Sandvik, PRL 104, 177201 (2010)

Logarithmic divergence of <W²>

scaling correction (not 1st-order)



Let's look at a well known signal of a first-order transition:

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

Binder ratio

Binder cumulant

 $U_2 = (5 - 3Q_2)/2$

Size independent (curve crossings) at criticality

U₂ < 0 at a first-order transition

 no signs of U₂<0 in SSE QMC results for L up to 256

Phase coexistence

leads to $U_2 \rightarrow -\infty$ at 1st-order trans





Example of a first-order Néel - VBS transition

J-Q model with staggered VBS phase [A. Sen, A. Sandvik, PRB (2010)]
no local VBS fluctuations favoring emergent U(1) symmetry



Any signs of coexistence in the standard J-Q VBS distributions?

• L=128 data close to the transition

J/Q=0.040



0.1

J/Q=0.046

logarithmic corrections

$$\rho_s \sim \frac{\ln(L/L_0)}{L} \quad (T \to 0)$$

$$\gamma \sim T[1 + c \ln(1/T)] \quad (L \to \infty)$$

$$\chi \sim T[1 + a \ln(1/T)] \quad (L \to \infty)$$

Governed by the dynamic exponent z (=1 in the theory)

Could the behavior indicate z≠1?

$$\begin{aligned} \xi &\sim T^{-(1/z)} \\ \chi &\sim T^{2/z-1} \\ \rho_s &\sim L^{-z} \end{aligned}$$

ξ gives z≈0.82

- consistent with $\rho_s(L)$
- inconsistent with χ(T)
 - demands $\chi/T \rightarrow 0$ for $T \rightarrow 0$

Most likely z=1

- logs also in impurity response Banerjee, Damle, Alet, PRB 2010
- marginal operator causing logs?

T>0 quantum-criticality - conventional O(3) case

Theory: Chakravarty, Halperin, Nelson (1989), Chubukov, Sachdev, Ye (1994) Realized in various dimerized S=1/2 Heisenberg models

Neel - non-magnetic T=0 transition vs g=J'/J

plain singlet-product (+ fluct) state for g>gc

cross-over "phase diagram"

T high-T, lattice effects QC QD T = 0 Néel order non-magnetic g 3D O(3) (Heisenberg) universality

T>0 quantum-critical regime

 magnons (S=1) remain as the elementary excitations at the critical point

$$\xi \propto T^{-1}$$

 $\chi \propto T$

$$C~\propto~T^2$$

- confirmed by QMC
- some issues remain in (c)

Consequences of spinons at T>0 in the J-Q model?

Standard QC forms

 $\xi \propto T^{-1}$

 $\propto T$

 $C~\propto~T^2$

 χ

are **weakly violated.** Specific heat obeys the standard form

Phenomenological model of a spinon gas at T>0

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

Infrared momentum cut-off 1/ ξ equivalent to thermal "gap" Δ =1/ ξ

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

<u>J-Q model</u>: critical **\xi diverges faster than 1/T** as T \rightarrow 0 (Δ /T \rightarrow 0) \blacktriangleright

- infrared divergent integral leads to weak T \rightarrow 0 divergence (log) of χ/T
- weaker correction to T² form of C

Т

Spin correlation lengths; J-J' (columnar) and J-Q models

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

J-J' model: expected 1/T divergence **J-Q model:** faster than 1/T divergence

• logarithmic or power correction (data consistent with either form)

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

$$\epsilon_{\pm}(k) = \sqrt{c^2 k^2 + \Delta^2} \pm \mu B \equiv \epsilon(k) \pm \mu B$$
 (B = magnetic field)
 $\mu = 1/2$ (spinons), $\mu = 1$ (magnons)

Magnetization to linear order (bosonic excitations)

$$M = \mu F \int \left(\frac{1}{e^{\epsilon_-/T} - 1} - \frac{1}{e^{\epsilon_+/T} - 1}\right) \frac{d^2k}{(2\pi)^2}$$
$$= -2\mu^2 F B \int \frac{\partial n}{\partial \epsilon} \frac{d^2k}{(2\pi)^2}$$
$$= \mu^2 F \frac{T B}{4\pi c^2} \int_0^\infty \frac{x dx}{\sinh^2 \left[\frac{1}{2}\sqrt{x^2 + (\Delta/T)^2}\right]}$$

F is a degeneracy factor; F=2 (spinons/anti-spinons), F=1 (magnons)

<u>Conventional quantum-criticality</u>: $\Delta/T \rightarrow m \approx 0.96$ (Chubukov & Sachdev 1994) • computed using large-N calculations (nonlinear σ -model)

In the J-Q model (deconfined criticality?): $\Delta/T \rightarrow 0$ (log⁻¹(1/T) or T^a) • infrared divergent integral; significant consequences

$$\int_0^\infty \frac{x dx}{\sinh^2(\frac{1}{2}\sqrt{x^2 + p^2})} = \frac{4p}{1 - e^{-p}} - 4\ln(e^p - 1) \qquad p = \Delta/T$$

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

$$\Delta_{1/2}/T = 1/(T\xi) = (T/mc)^a$$
 (*mc* and *a* from J-Q QMC data)
 $\Delta_1/T = m = 0.96$ (Chubukov & Sachdev)

Gives the low-T magnetic susceptibility

$$\chi_1 = (1.0760/\pi c^2)T$$

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

Specific heat

$$\begin{split} C_S &= (2S+1)F \int \epsilon(k) \frac{\partial n(\epsilon)}{\partial T} \frac{d^2k}{(2\pi)^2} \\ C_1 &= [36\zeta(3)/5\pi c^2]T^2 \qquad \text{(Chubukov \& Sachdev)} \\ C_{1/2} &= \frac{2T^2}{\pi c^2} \left[6\zeta(3) - \left(\frac{T}{c}\right)^{2a} \left[\frac{3}{2} + a + a(1+a)\ln\left(\frac{c}{T}\right) \right] \right] \end{split}$$

QMC data fits: J-J' (magnon forms) and J-Q models (spinon forms)

- J-J': velocity fitted in E/T³, polynomial fit for X/T (velocities agree to 2%)
- J-Q: only velocity is fitted; values from X/T and C agree within 2%

J-Q model: effective spin of the excitations

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

$$F_{\chi} = \frac{\mu^2 F}{c_{\chi}^2} \approx 0.074, \qquad F_C = \frac{(2S+1)F}{c_C^2} \approx 0.615 \qquad \begin{array}{l} c_{\chi} = 2.60\\ c_C = 2.55 \end{array}$$

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

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

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

