Néel-VBS transition in a $S = 1/2$ honeycomb lattice antiferromagnet

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Nordita Workshop
July 22 2014
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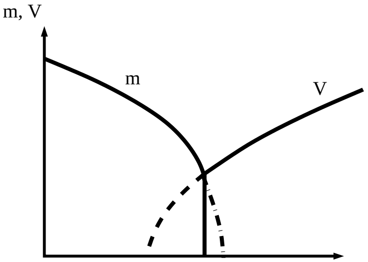
Thinking about symmetry breaking transitions: Landau theory

- Symmetry-breaking state characterized by long-range correlations of "order-parameter" $\hat{O}$
- Onset of these long-range correlations studied phenomenologically
- Landau free energy F
  Keep all symmetry allowed analytic terms in $\hat{O}$
- Neglecting derivatives (fluctuations):
  phase transition $\rightarrow$ change in minimum of F

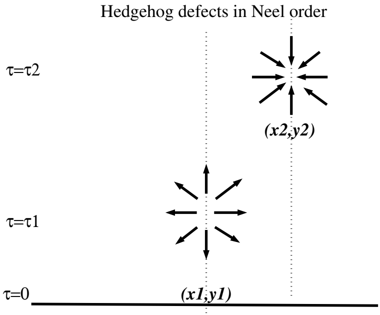
Néel-VBS transitions on the square-lattice: Landau Theory

- Neel ordered state spontaneously breaks spin rotation symmetry
- Valence bond solid spontaneously breaks lattice translation symmetry
- Standard Landau theory argument $\rightarrow$ First order transition or intermediate phase with co-existing orders or intermediate phase with no order...



Berry-phases of hedgehogs in Néel state

- Senthil *et. al.* (2004): Need to think beyond Landau theory if Berry phases in $\exp(-F)$
  Haldane: phase $0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}$ associated with topological defects on 4-sublattices of plaquettes on square lattice



Narrowing down possibilities

- Implication of phase factors:
  Hedgehog creation operator has same symmetries as columnar/plaquette VBS order parameter Ψ.
  If proliferation of hedgehogs destroys Néel order, it must create columnar/plaquette VBS order at same time!
  Such transitions generically expected to be *"direct"*

"Deconfined" scenario for continuous direct transition

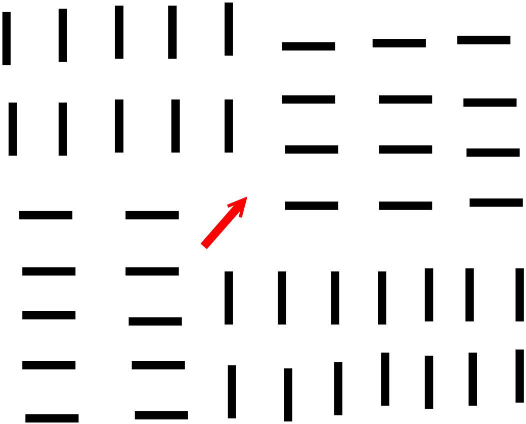
- CP^1 language: $\hat{n} = z^\dagger_\alpha \vec{\sigma}_{\alpha\beta} z_\beta$, with $n = 2$-component complex z_α coupled to compact $U(1)$ gauge field A.
- Hedgegogs $\rightarrow$ monopoles of A
- Phase-factor $\rightarrow$ only quadrupled monopoles in coarse-grained description
- IF four-fold monopoles irrelevant at Motrunich-Vishwanath non-compact (NC)CP^1 (all monopoles forbidden) critical point
  Néel-VBS transition continuous, described by NCCP^1 critical point
  System cannot immediately choose between columnar VBS order and plaquette VBS order
  Senthil *et. al.* (2004)

Are four-fold monopoles irrelevant?

- In large-n limit of NCCP^{n-1} theory: All monopoles irrelevant.
- When $n = 1$: "NCCP^0" theory of single charged boson.
  Boson-vortex duality: q-fold monopole in $A \rightarrow q$-fold anisotropy in dual $d = 3$ XY model.
  Best numerical estimate: Irrelevant for $q = 4$ and higher.
- Irrelevant at $n = 1$, $n = \infty$.
  Most likely irrelevant at $n = 2$ case!

Completing the ciricle: spinon defects in columnar VBS order

- Levin and Senthil (2004): 'The CP^1 field $z_\alpha^\dagger$ creates $S = 1/2\ Z_4$ vortices in VBS order parameter.



Consequences

- Direct second order transition described by NCCP^1 theory
- For NCCP^1 theory: $z = 1$ $d = 2$
  Critical Neel order parameter correlations (equal time):
  $\langle \vec{n}(r)\vec{n}(0)\rangle_{\text{crit}} \sim r^{-(1+\eta_n)}$
  $\vec{n} = z^{\dagger}_{\alpha}\vec{\sigma}_{\alpha\beta}z_{\beta} \rightarrow$ large η_n (unlike usual critical points)
  Critical $\langle \Psi(r)\Psi(0)\rangle$ also with large η_V: 'Hedgehog Green function!

Hedgehogs in honeycomb Néel state

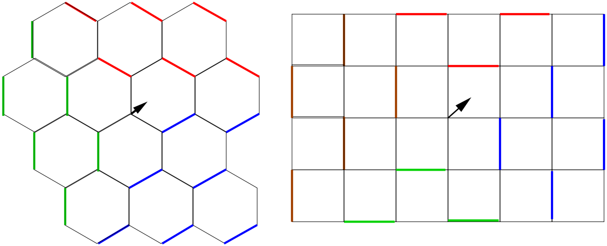
- Again, hedgehogs in $\hat{n}$ lead to non-trivial phase factors.
  Haldane: phase 0, $2\pi/3$, $4\pi/3$ associated with topological defects on 3-sublattices of hexagons of honeycomb lattice
- Implication of phase factors:
  Hedgehog creation operator corresponds to (complex) columnar/plaquette VBS order parameter Ψ on the honeycomb lattice
  If hedgehog-proliferation destroys Néel order, must seed columnar/plaquette VBS order
  Again: such transitions generically "direct"

Deconfined scenario for continuous direct transition

- Only 3-fold monopoles allowed in CP^1 description.
- IF three-fold monopoles irrelevant at Motrunich-Vishwanath non-compact (NC)CP^1 (all monopoles forbidden) critical point
  Néel-VBS transition continuous, described by NCCP^1 critical point
  System cannot immediately choose between columnar VBS order and plaquette VBS order

Dual picture

- $z^\dagger$ creates $S = 1/2$ Z_3 vortices in VBS order-parameter.

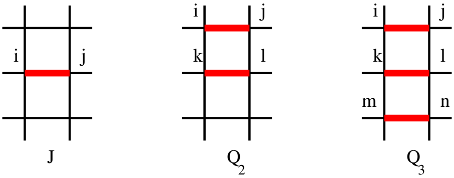


Are three-fold monopoles relevant at NCCP^1 transition?

- 3-fold anisotropy relevant at $n = 1$
  Known: $q = 3$ fold anisotropy in dual-XY model drives it to a weakly first-order transition.
- Irrelevant at $n = \infty$, relevant at $n = 1$ . . . What happens at $n = 2$??

Accessing Néel-VBS transitions

- Néel-VBS transitions in *unfrustrated* spin models
  Sandvik 2007



$$H_{JQ_2} = -J \sum_{\langle ij \rangle} P_{\langle ij \rangle} - Q \sum_{\langle ij \rangle || \langle kl \rangle} P_{\langle ij \rangle} P_{\langle kl \rangle}$$

$$H_{JQ_3} = -J \sum_{\langle ij \rangle} P_{\langle ij \rangle} - Q \sum_{\langle ij \rangle || \langle kl \rangle || \langle rs \rangle} P_{\langle ij \rangle} P_{\langle kl \rangle} P_{\langle rs \rangle}$$

where $P_{\langle ij \rangle} = (\frac{1}{4} - \vec{S}_i \cdot \vec{S}_j)$

Initial controversy for Néel-VBS transition on square lattice

Apparently second order direct transition between two phases

- Sandvik (2007): JQ_2 model using singlet-sector ground-state projection algorithm in valence bond basis ($T = 0$ results directly)
- Melko & Kaul (2008): JQ_2 using Quantum Monte Carlo at inverse temperature $\beta Q \approx L$ for $L \times L$ square lattice

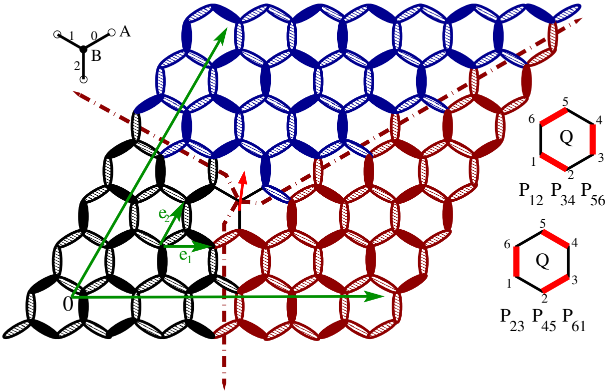
Conflicting claim of first order behaviour

- Jiang *et. al.* (2008)

Evidence for/against deconfined criticality

- Lou, Sandvik, & Kawashima (2009).
  No sign of first order behavour.
- Universality: Both H_{JQ_2} and H_{JQ_3} yield *same* exponents.
- $\eta_s \approx 0.34$, $\eta_d \approx 0.20$, $\nu \approx 0.68$.
- Main worry: Drifts in "universal" "dimensionless" quantities at transition
  Could be flow to first-order (Jiang *et. al.* 2008), log-violations (Sandvik, Banerjee *et. al.*), large corrections to scaling (Kaul) . . .

Our work:

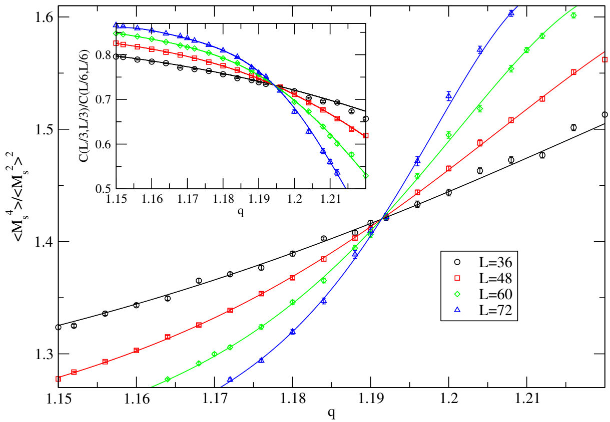


JQ model designed to have columnar/plaquette VBS phase

Method

- Singlet sector $\{|s\rangle\}$ of $2N$ spin $S = 1/2$ moments spanned by overcomplete bipartite (AB) valence bond basis.
- Start with arbitrary singlet state $|v_0\rangle$ and compute $\langle v_0|(-H)^m \hat{O}(-H)^m|v_0\rangle / \langle v_0|(-H)^{2m}|v_0\rangle$ stochastically.
  Sandvik (2005)
- Note: Gives ground state expectation value of operator $\hat{O}$ for 'large enough' m (in practice $m \sim \text{Volume} \times \Delta_S^{-1}$)
- Crucial: Efficient importance sampling algorithm for stochastic sampling of contributions to $\langle v_0'|(-H)^m|v_0\rangle$
  Sandvik & Evertz (2010)

Evidence for continuous transition(s)



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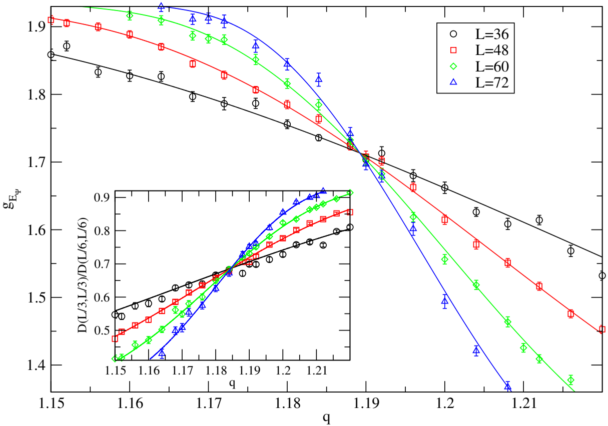
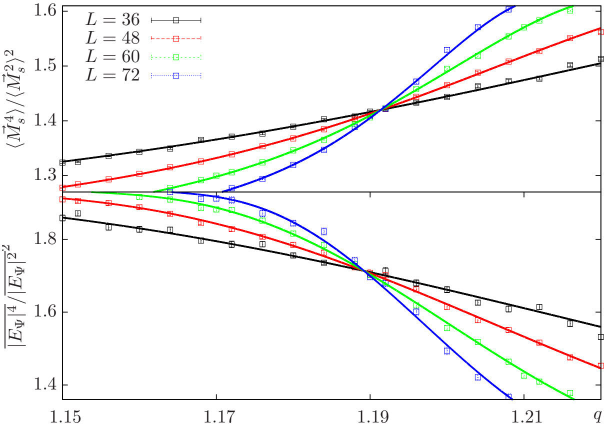


Do the transitions coincide?



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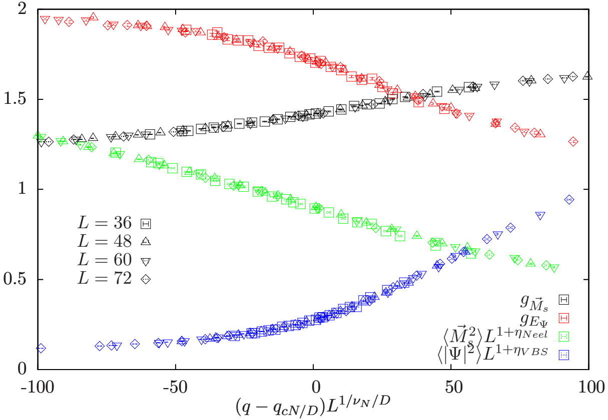
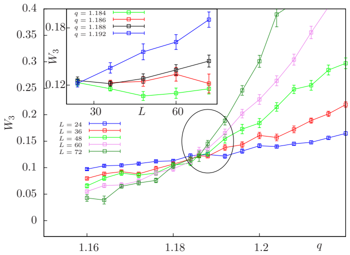


Single deconfined critical point?

- $q_{cN} \approx 1.1936(24)$
- $q_{cD} \approx 1.1864(28)$
  slightly outside each-other's error bars
- $\nu_N \approx 0.51(3)$
- $\nu_D \approx 0.55(4)$
  agree within errors
- $g_N^* \approx 1.42(1)$
  agrees with value at square-lattice deconfined transition
- $\eta_N \approx 0.30(5)$
- $\eta_V \approx 0.28(8)$

Minimal explanation: Single deconfined critical point

But: Three-fold anisotropy at critical point



Analogy with 4-fold anisotropy in 3d XY model

- Similar behaviour seen over reasonable length-scales for 4 fold anisotropy at $d = 3$ XY critical point
  (Lou, Balents, Sandvik)

Acknowledgements

- Collaborators:
  Argha Banerjee (TIFR) & Arun Paramekanti (Toronto)
  Sumiran Pujari & Fabien Alet (Toulouse)
- Computational resources of TIFR Mumbai and LPTMS Toulouse.
- CEFIPRA (Indo-French) postdoc. funding for Sumiran Pujari