Nematic quantum paramagnet in spin-1 square lattice models

Fa Wang (王垡)
Peking University

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Outline

- Motivation
- Theory
- Numerical results
- Summary
Motivation: experimental

- Fe-based high Tc superconductors (FeSC): [Hosono et al'08]
Motivation: experimental

- Fe-based high Tc superconductors (FeSC)
  - Common structure: X-Fe\(_2\)-X tri-layer (X=As, P, Se, Te), Fe square lattice.
  
  - Nominally Fe\(^{2+}\) (3d\(^6\)), low-spin state would be spin-1 with orbital degeneracy (in tetragonal phase)
Motivation: experimental

- Typical FeSC materials
  - Parent compounds have stripe AFM order, which breaks 4-fold rotation symmetry
  - Magnetism can be explained by $J_1$-$J_2$ and related models [Yildirim'08 ...; review Dai'15]

\[ J_1 \sum_{\langle ij \rangle} S_i \cdot S_j + J_2 \sum_{\langle\langle ij \rangle\rangle} S_i \cdot S_j \]
Motivation: experimental

• Typical FeSC materials
  - Tetragonal to orthorhombic \((a \neq b)\) structural transition (breaking of 4-fold rotation \(C_4\) symmetry) at or slightly above AFM order temperature

Fernandes et al. Nat.Phys.’14
Motivation: experimental

- Typical FeSC materials
  - lattice distortion is small (~$10^{-3}$), electronic properties has significant $C_4$ breaking: nematicity
  - driving force of nematicity? [review Fernandes et al'14]
    - orbital order: $n_{xz} \neq n_{yz}$, [Singh'08, Kontani&Onari'12]?
    - magnetic correlation [Fang et al'08, Xu et al.'08]? ...

Ba(Fe,Co)As, Chu et al. Science 329,824(2010).
Motivation: experimental

- Atypical FeSC: FeSe
  - Superconducting without doping \([T_c \sim 8\text{K}]\)
  - No magnetic order
  - Has orthorhombic structural transition \([T_c \sim 90\text{K}]\)
  - Pressure can induce AFM order \([\text{Bendele et al.'12, Terashima et al.'15}]\)
Motivation: theoretical

• Long-standing question: nature of nonmagnetic phase for square $J_1$-$J_2$ Heisenberg model
  
  – There is a nonmag phase between Neel and stripe AFM [Chandra&Doucot'88]
  
  Neel
  
  stripe AFM
  
  no magnetic order
  
  $J_2/ J_1$
  
  – Nature of spin-1/2 case still under debate: gapped spin liquid [Jiang&Yao&Balents'12] valence bond solid(VBS) or gapless [Gong et al.'14]
Motivation: theoretical

- DMRG for spin-1 $J_{1x} - J_{1y} - J_2$ model [Jiang et al'09]
  - Nonmag phase for $0.525 < J_2/J_1 < 0.555$
Motivation: questions to answer

- Nature of nonmag phase of spin-1 square lattice $J_1$-$J_2$ Heisenberg model
  A: nematic quantum paramagnet (break $C_4$ only)

- Nature of phase transitions to magnetic orders
  A: possibly Landau-forbidden continuous quantum phase transition to Neel

- Relevance of this nonmag phase to FeSe
  A: might be driving force of nematicity in FeSe
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Theoretical treatment: argument

- Haldane's argument [Haldane'88]
  - Disordering Neel order will proliferate monopole of Neel order parameter \( n(r) \sim (-1)^{x+y} S(r) \)
  - monopole: skyrmion # changing event in space-time, monopole charge is the change of skyrmion number
  - skyrmion number: number of times the unit vector \( n(r) \) wraps around Bloch sphere
    \[
    \frac{1}{4\pi} \int \int dx dy \, n \cdot (\partial_x n \times \partial_y n)
    \]
    Example of \( q_m = 1 \) monopole
Theoretical treatment: argument

- Haldane's argument [Haldane'88,Read&Sachdev'89]
  - monopole configurations contribute non-trivial Berry phase to the path integral, which depends on monopole spatial position and spin length $S$.
  - Spin-1/2: must proliferate $q_m = 0 \mod 4$ monopoles, skyrmion $# = 0, 1, 2, 3 \mod 4$ sectors become degenerate, break translation/rotation symmetry: (columnar) VBS

Phase factor for charge $q_m = 1$ monopoles

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Theoretical treatment: argument

- Haldane's argument applied to spin-1
  - monopole Berry phase (for charge \( q_m = 1 \))
  - Proliferation of \( q_m = 0 \) mod 2 monopoles, skyrmion number = 0, 1 mod 2 sectors are degenerate, breaks \( C_4 \), but not translation: nematic paramagnet.
Theoretical treatment: parent Hamiltonian

- Parent Hamiltonian of nematic quantum paramagnet (due to Prof. Kivelson)

\[ H_K = K \sum_{\langle jik \rangle} P_3(S_i + S_j + S_k) \]

\[ P_3(S) = \frac{1}{720} S^2(S^2 - 2)(S^2 - 6) = \begin{cases} 
1, \text{total spin}=3; \\
0, \text{otherwise}
\end{cases} \]

- Horizontal/vertical AKLT chains are two ground states

- AKLT state [Affleck et al'87]:

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Theoretical treatment: field theory

- Background: “deconfined quantum critical point” for spin-1/2 square lattice model [Tanaka&Hu'05, Senthil et al'06]
  - Landau-forbidden continuous quantum phase transition from Neel AFM($n$) to columnar VBS[$v=(v_x,v_y)$]
  - O(5) nonlinear sigma model with WZW term and anisotropy

\[
S_{\frac{1}{2}}[\hat{\phi}] = S_{O(3)\times C_{4v}}[\hat{\phi}] - 2\pi \frac{3}{8\pi^2} \int u^2 x \tau \epsilon^{abcdef} \phi_a \partial_x \phi_b \partial_y \phi_c \partial_{\tau} \phi_d \partial_u \phi_f.
\]

\[
\hat{\phi} \propto (n_x, n_y, n_z, v_x, v_y) \quad v_x \sim (-1)^x (S_{(x,y)} \cdot S_{(x+1,y)} - S_{(x,y)} \cdot S_{(x-1,y)})
\]

\[
S_{O(3)\times C_{4v}} = \int d^2xd\tau \left( \frac{1}{2g_n} |\partial_\mu n|^2 + \frac{1}{2g_v} |\partial_\mu v|^2 \right) + \ldots
\]
Theoretical treatment: field theory

- Field theory for possible continuous transition from nematic paramagnet to Neel state
  - Will also be a Landau-forbidden continuous transition
    - Neel AFM has $C_4$, breaks spin rotation symmetry; nematic paramagnet breaks $C_4$, has spin rotation.
    - View spin-1 as two ferromagnetic coupled spin-1/2
      \[ S_1[\hat{\phi}^{(1)}, \hat{\phi}^{(2)}] = S_{1/2}[\hat{\phi}^{(1)}] + S_{1/2}[\hat{\phi}^{(2)}] + \int d^2x d\tau \left( J_n \mathbf{n}^{(1)} \cdot \mathbf{n}^{(2)} + J_v \mathbf{v}^{(1)} \cdot \mathbf{v}^{(2)} \right). \]
      - Depending on sign of $J_n$, $J_v$, this may described transitions between different pairs of phases
Theoretical treatment: field theory

- Field theory for possible continuous transition from nematic paramagnet to Neel state

\[ S_1[\hat{\phi}^{(1)}, \hat{\phi}^{(2)}] = S_{\frac{1}{2}}[\hat{\phi}^{(1)}] + S_{\frac{1}{2}}[\hat{\phi}^{(2)}] + \int d^2x d\tau \left( J_n n^{(1)} \cdot n^{(2)} + J_v v^{(1)} \cdot v^{(2)} \right). \]

- With \( J_n < 0, J_v > 0 \), low energy configs are \( n^{(1)}=n^{(2)}=n, v^{(1)}=-v^{(2)}=v \), in terms of \( \Phi=(n,v) \), action has WZW with doubled coefficient

\[ S_1[\phi] = \cdots - 2 \times 2\pi \frac{3}{8\pi^2} \int u^2 x \tau \epsilon^{abcd} \phi_a \partial_x \phi_b \partial_y \phi_c \partial_\tau \phi_d \partial_u \phi_f. \]

- \( v \) is not observable[antisym. w.r.t. exchange of (1)(2)] observable \( v'=(v_1,v_2) \), are bilinears of \( v \),

\[ v'_1 = \frac{v_x^2 - v_y^2}{\sqrt{v_x^2 + v_y^2}}, \quad v'_2 = \frac{2v_x v_y}{\sqrt{v_x^2 + v_y^2}}. \]
Theoretical treatment: field theory

- Field theory for possible continuous transition from nematic paramagnet to Neel state
  - In terms of $\Phi'=(n,v')$, the action has WZW term similar to the spin-1/2 case
    \[ S_1[\hat{\phi}'] = S_{O(3) \times Z_2 \times Z_2}[\hat{\phi}'] - 2\pi \frac{3}{8\pi^2} \int du \, dx \, d\tau \, \epsilon^{abcdef} \phi'_a \partial_x \phi'_b \partial_y \phi'_c \partial_{\tau} \phi'_d \partial_u \phi'_f. \]
  - $v'_1$ is the nematic order parameter:
    momentum=0, changes sign under $C_4$ ($v_x \rightarrow v_y \rightarrow -v_x$),
  - If anisotropy disfavors $v'_2$, theory reduces to $O(3) \ast Z_2$ NL$\sigma$M with $\Theta(=\pi)$-term of 4-component $\Omega=(n,v'_1)$,
    \[ S = \cdots + i \frac{\Theta}{2\pi^2} \int d^2x \, d\tau \, \epsilon^{abcd} \Omega_a \partial_x \Omega_b \partial_y \Omega_c \partial_{\tau} \Omega_d \]
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Numerical results

- Exact diagonalization of $J_1$-$J_2$ model:
  - Hint of nematic paramagnet from singlet and spin gap: large spin gap, vanishingly small singlet gap.
Numerical results

- Exact diagonalization $J_1-J_2$ model:
  - Hint of phase transitions from ground state fidelity susceptibility, fidelity is $F_0(\alpha, \alpha + \delta \alpha) \equiv |\langle \psi_0(\alpha) | \psi_0(\alpha + \delta \alpha) \rangle|$
Numerical results

- Interpolating between parent Hamiltonian ($\lambda=1$) and $J_1$-$J_2$ model at $J_2/J_1=0.5$ ($\lambda=0$):
  - DMRG of Jiang et al'09: $J_2/J_1=0.5$ should be Neel ordered
  - No strong sign of phase transition in small size ED:
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Discussion: possible relevance to FeSe

- Caveat: itinerant electrons in FeSe, may change universality [Xu et al'08]; orbital degrees of freedom ignored.

- NMR did not see low energy magnetic fluctuations above $T_s \sim 90K$ [Buchner et al'14], it was thus argued that the nematicity is not magnetism-driven.
Discussion: possible relevance to FeSe

- Recent ARPES see momentum-dependent splitting of xz/yz orbitals, cannot be simple ferro-orbital order (xz, yz have different onsite potential) [Coldea et al'15; Ding et al'15; Zhang et al.'15]

Discussion: possible relevance to FeSe

- Recent neutron scattering found low energy magnetic fluctuations at stripe wavevector [Jun Zhao et al'15]
Summary

- Nonmagnetic phase of spin-1 $J_1$-$J_2$ Heisenberg model on square lattice is nematic quantum paramagnet
  - According to Haldane-type argument & numerics
  - Possible Landau-forbidden continuous transition to Neel

- Magnetic fluctuation may still be the driving force of nematicity in FeSe, although it has no magnetic order and no very-low-energy spin fluctuation
  - Drive FeSe to Neel order?
Thank you!