Nematic quantum paramagnet in spin-1 square lattice models

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Acknowledgments

- Prof. Dung-Hai Lee, UC Berkeley

- Prof. Kivelson, Stanford

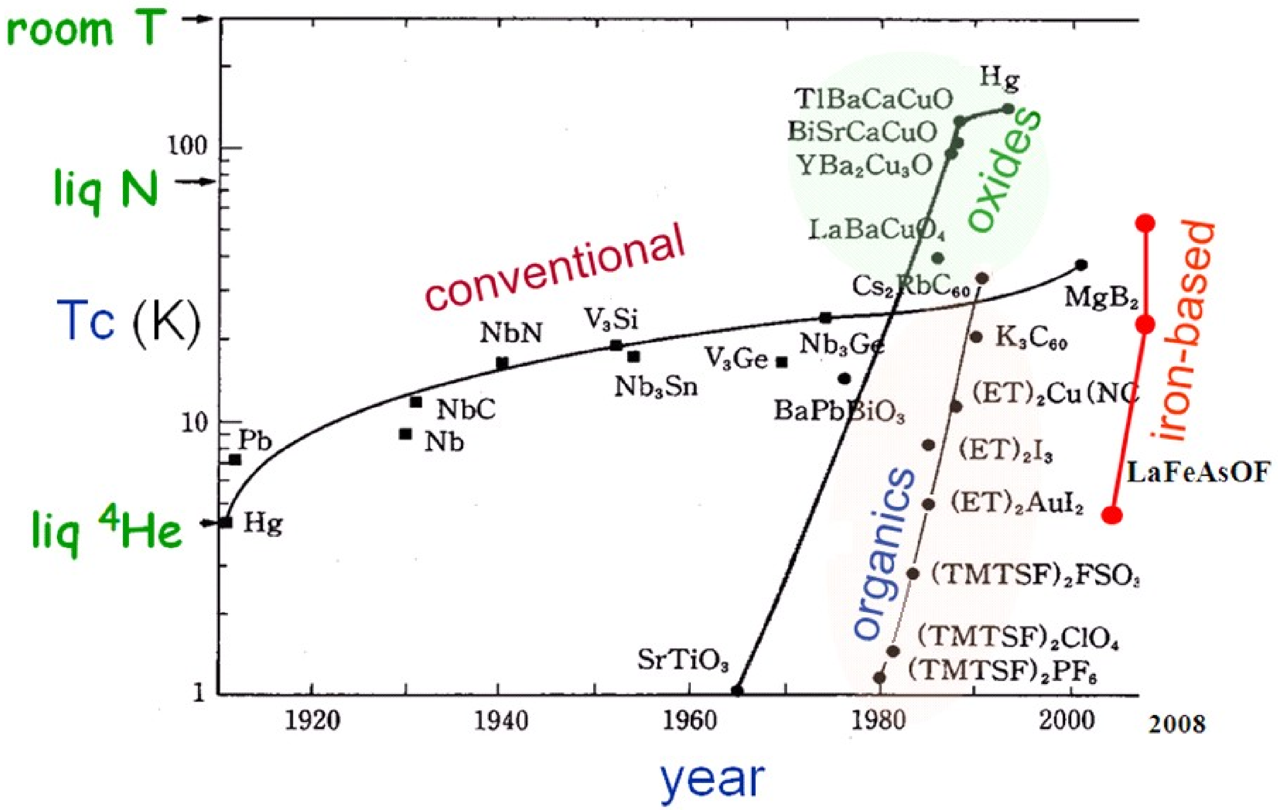
- Discussions with Prof. Tao Xiang, IOP CAS

Outline

- Motivation
- Theory
- Numerical results
- Summary

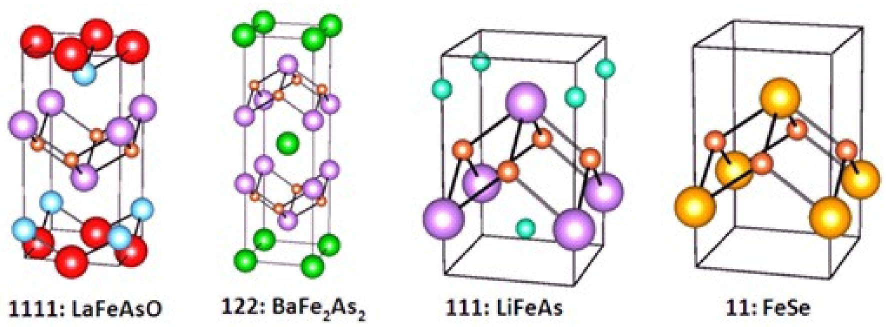
Motivation: experimental

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

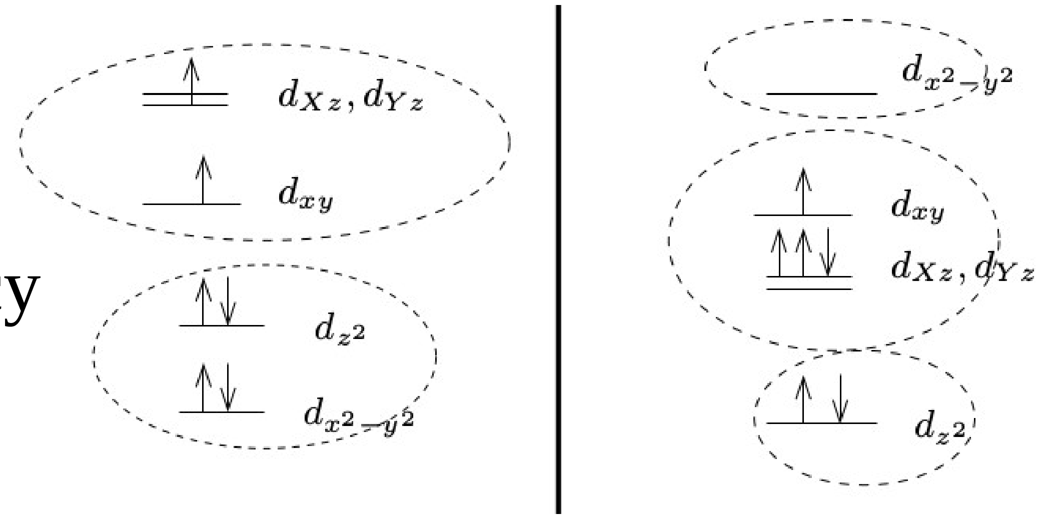


Motivation: experimental

- Fe-based high Tc superconductors(FeSC)
  - Common structure: X-Fe_2-X tri-layer (X=As, P, Se, Te), Fe square lattice.

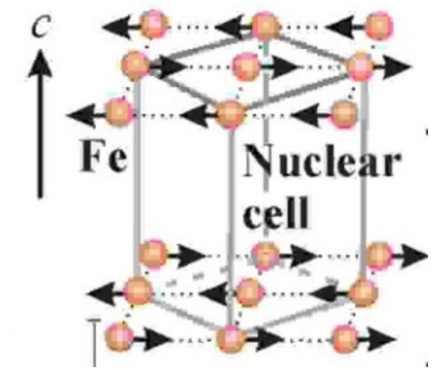


  - Nominally Fe^{2+} ($3d^6$), low-spin state would be spin-1 with orbital degeneracy (in tetragonal phase)

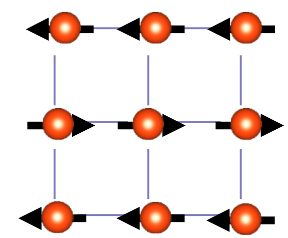


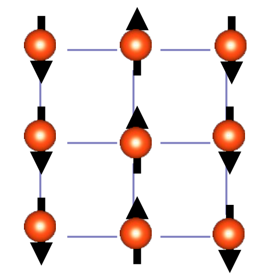
Motivation: experimental

- 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]

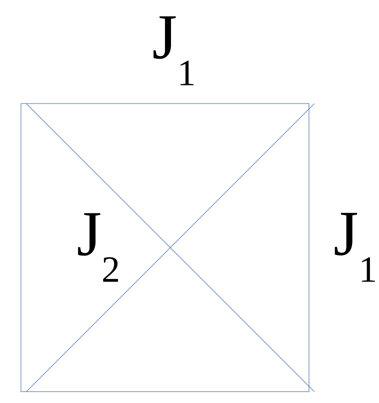


LaFeAsO
Cruz et al. Nature'08



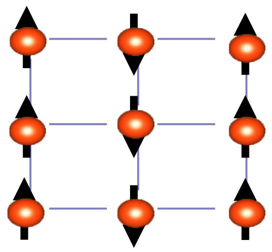


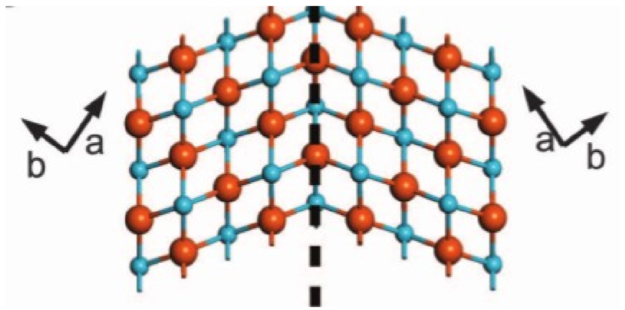
$$J_1 \sum_{\langle ij \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$



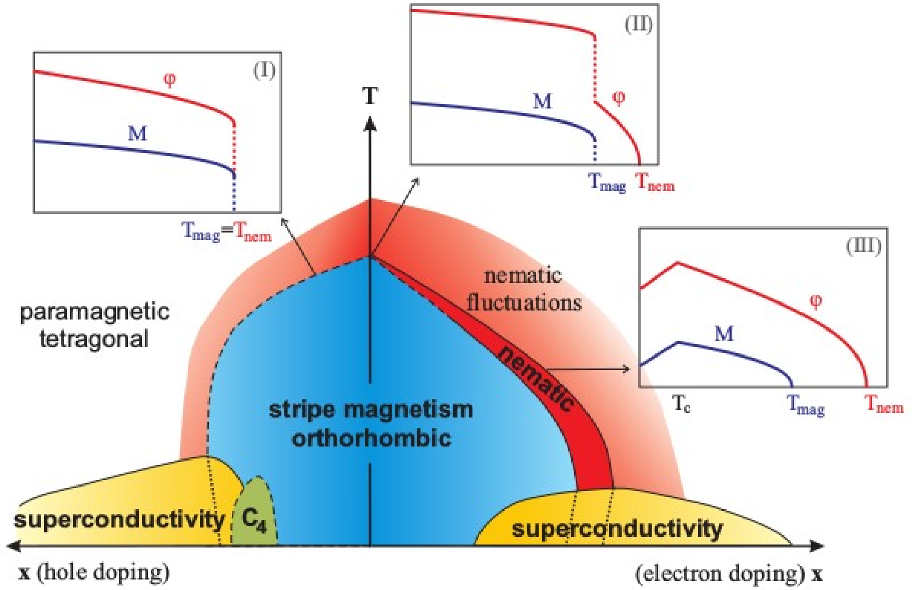
Motivation: experimental

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





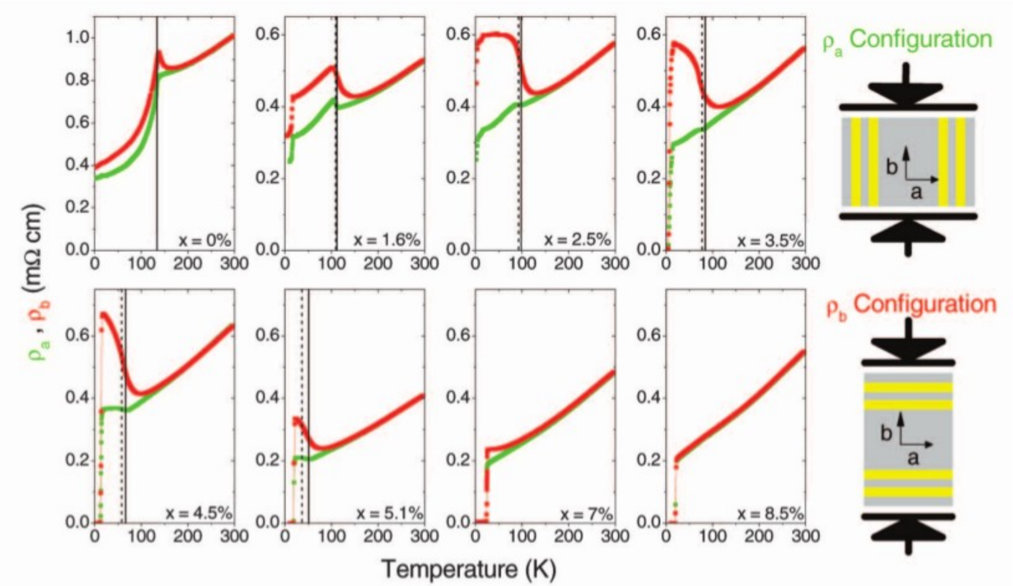
Chu et al. Science 329, 824 (2010)



Fernandes et al. Nat.Phys.'14

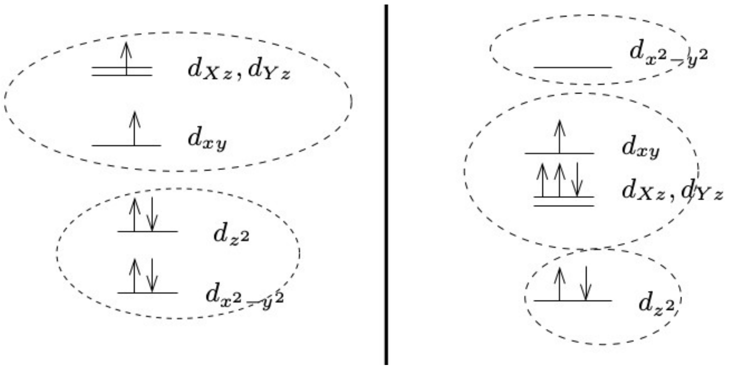
Motivation: experimental

- Typical FeSC materials
  - lattice distortion is small ($\sim 10^{-3}$), electronic properties has significant C_4 breaking: nematicity



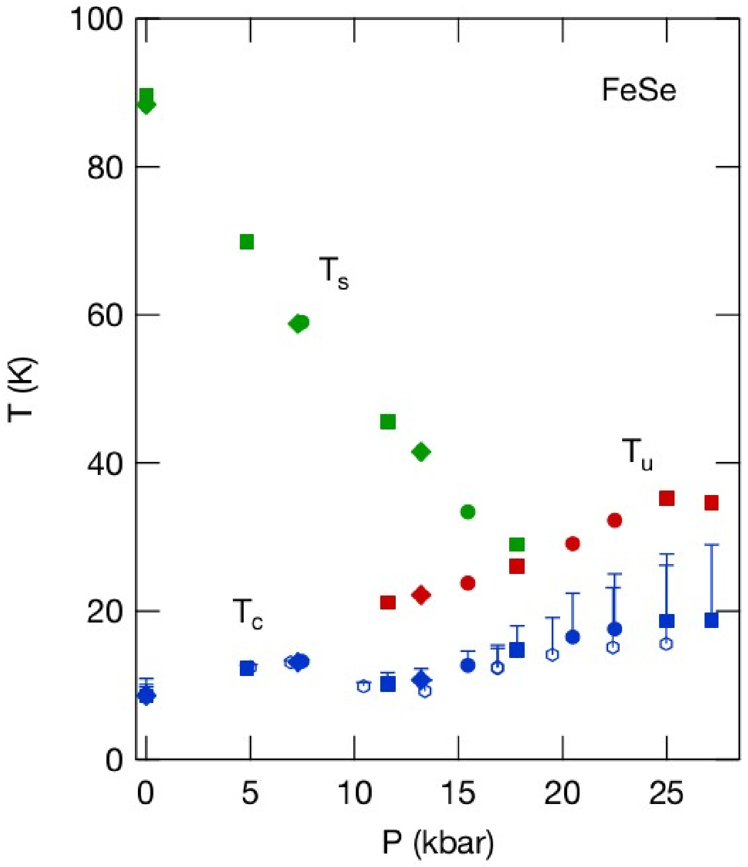
Ba(Fe,Co)As, Chu et al. Science 329,824(2010).

  - 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]? ...



Motivation: experimental

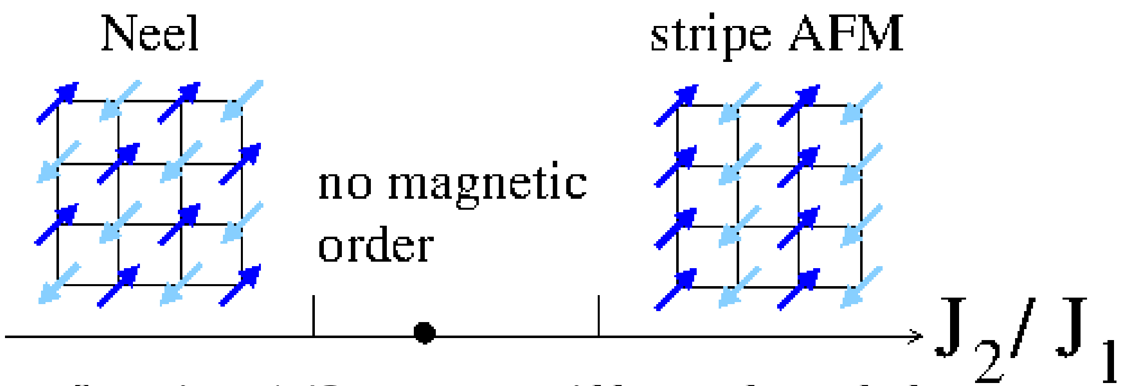
- Atypical FeSC: FeSe
  - Superconducting without doping [Tc~8K]
  - No magnetic order
  - Has orthorhombic structural transition [Tc~90K]
  - Pressure can induce AFM order [Bendele et al'12, Terashima et al'15]



T.Terashima et al. arXiv:1502.03548

Motivation: theoretical

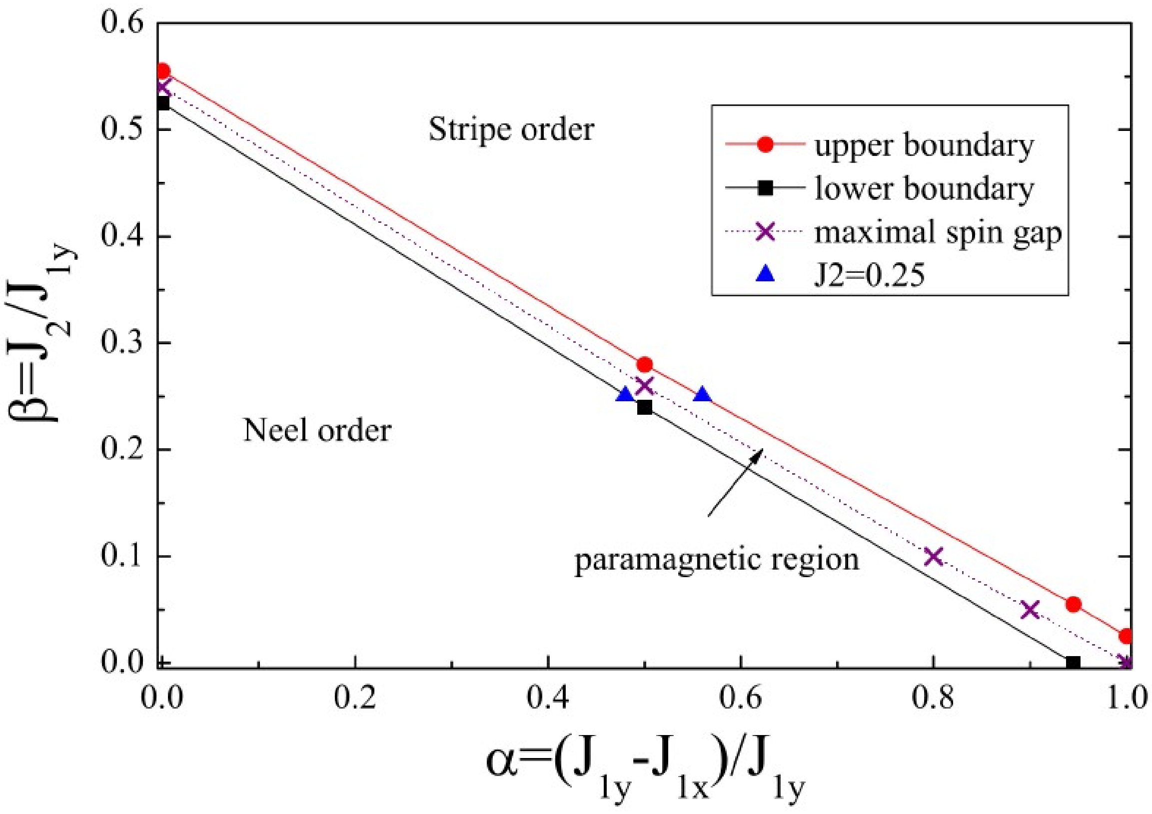
- Long-standing question: nature of nonmagnetic phase for square J_1-J_2 Heisenberg model
  - There is a nonmag phase between Neel and stripe AFM [Chandra&Doucot'88]



  - 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]

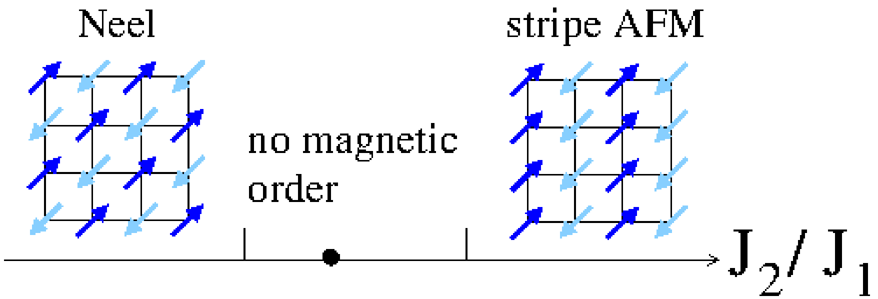
Motivation: theoretical

- 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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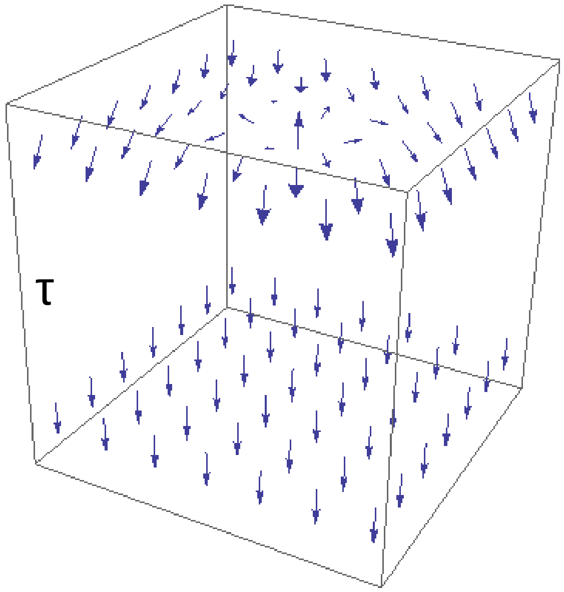
Theoretical treatment: argument

- Haldane's argument [Haldane'88]
  - Disordering Neel order will proliferate monopole of Neel order parameter $\boldsymbol{n}(\boldsymbol{r}) \sim (-1)^{x+y}\boldsymbol{S}(\boldsymbol{r})$
  - monopole: skyrmion # changing event in space-time, monopole charge is the change of skyrmion number
  - skyrmion number: number of times the unit vector $\boldsymbol{n}(\boldsymbol{r})$ wraps around Bloch sphere

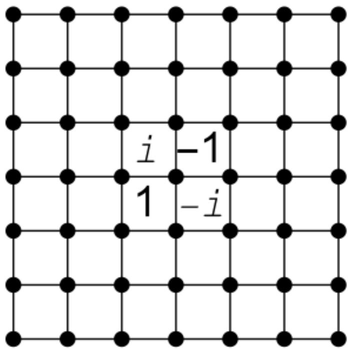
$$\frac{1}{4\pi}\int\int \mathrm{d}x\mathrm{d}y\,\boldsymbol{n}\cdot(\partial_x\boldsymbol{n}\times\partial_y\boldsymbol{n})$$



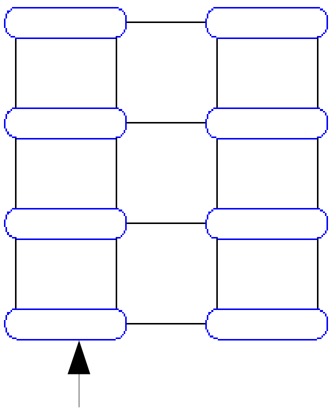
Example of q_m=1 monopole

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



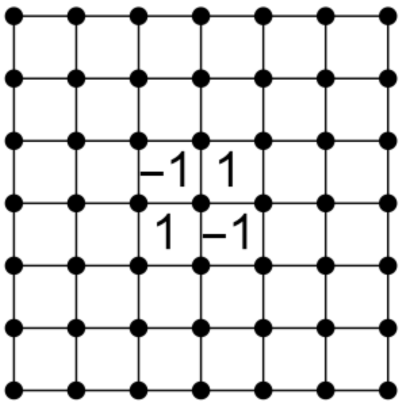
Phase factor for charge q_m=1 monopoles



singlet (valence bond)

Theoretical treatment: argument

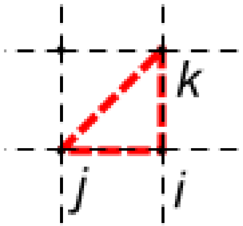
- Haldane's argument applied to spin-1
  - monopole Berry phase (for charge q_m=1)



  - 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

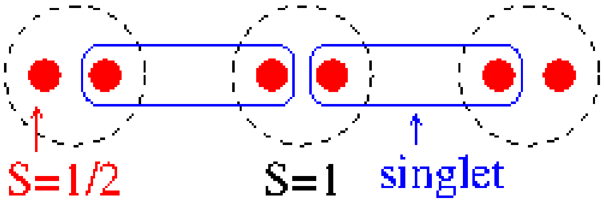
- Parent Hamiltonian of nematic quantum paramagnet (due to Prof. Kivelson)

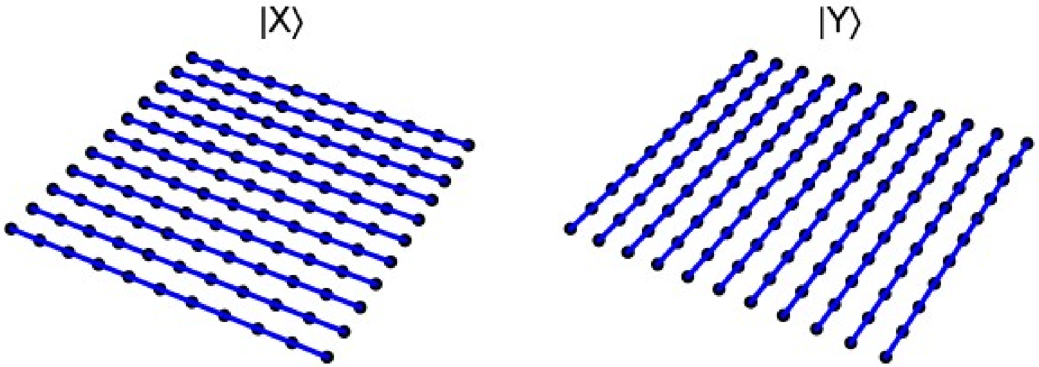


$$H_K = K \sum_{\langle jik \rangle} P_3(\boldsymbol{S}_i + \boldsymbol{S}_j + \boldsymbol{S}_k)$$

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

  - Horizontal/vertical AKLT chains are two ground states
    - AKLT state [Affleck et al'87]:





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

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

$$\hat{\phi} \propto (n_x, n_y, n_z, v_x, v_y) \qquad v_x \sim (-1)^x(\boldsymbol{S}_{(x,y)}\cdot\boldsymbol{S}_{(x+1,y)} - \boldsymbol{S}_{(x,y)}\cdot\boldsymbol{S}_{(x-1,y)})$$

$$S_{O(3)\times C_{4v}} = \int \mathrm{d}^2x\mathrm{d}\tau\left(\frac{1}{2g_n}|\partial_\mu\boldsymbol{n}|^2 + \frac{1}{2g_v}|\partial_\mu\boldsymbol{v}|^2\right) + \ldots$$

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

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

  - 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

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

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

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

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

$$v_1' = \frac{v_x^2 - v_y^2}{\sqrt{v_x^2+v_y^2}},\quad v_2' = \frac{2v_xv_y}{\sqrt{v_x^2+v_y^2}}$$

Theoretical treatment: field theory

- Field theory for possible continuous transition from nematic paramagnet to Neel state
  - In terms of ***Φ'***=(***n***,***v'***), the action has WZW term similar to the spin-1/2 case

$$S_1[\hat{\phi}'] = \; S_{O(3)\times Z_2\times Z_2}[\hat{\phi}'] - 2\pi\frac{3}{8\pi^2}\int \mathrm{d}u\mathrm{d}^2x\mathrm{d}\tau\, \epsilon^{abcdf}\phi'_a\partial_x\phi'_b\partial_y\phi'_c\partial_\tau\phi'_d\partial_u\phi'_f.$$

  - v'_1 is the nematic order parameter: momentum=0, changes sign under C_4 ($v_x \to v_y \to -v_x$),
  - If anisotropy disfavors v'_2, theory reduces to O(3)*Z2 NLσM with Θ(=π)-term of 4-component Ω=(***n***,v'_1),

$$S = \cdots + i\frac{\Theta}{2\pi^2}\int \mathrm{d}^2x\mathrm{d}\tau\ \epsilon^{abcd}\Omega_a\partial_x\Omega_b\partial_y\Omega_c\partial_\tau\Omega_d$$

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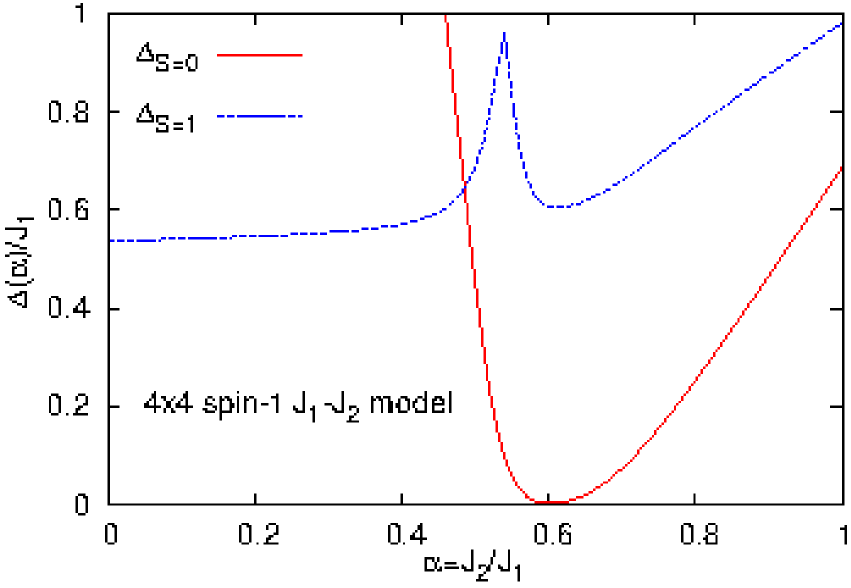
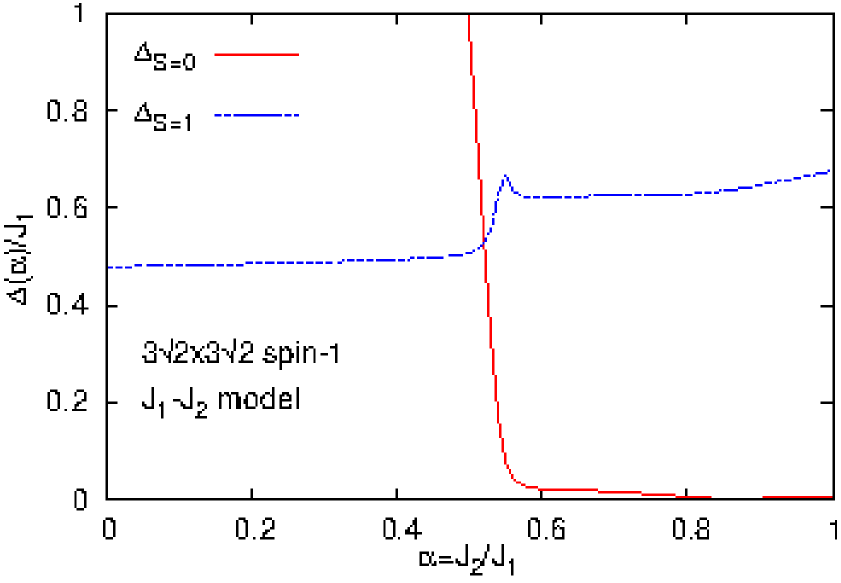
Numerical results

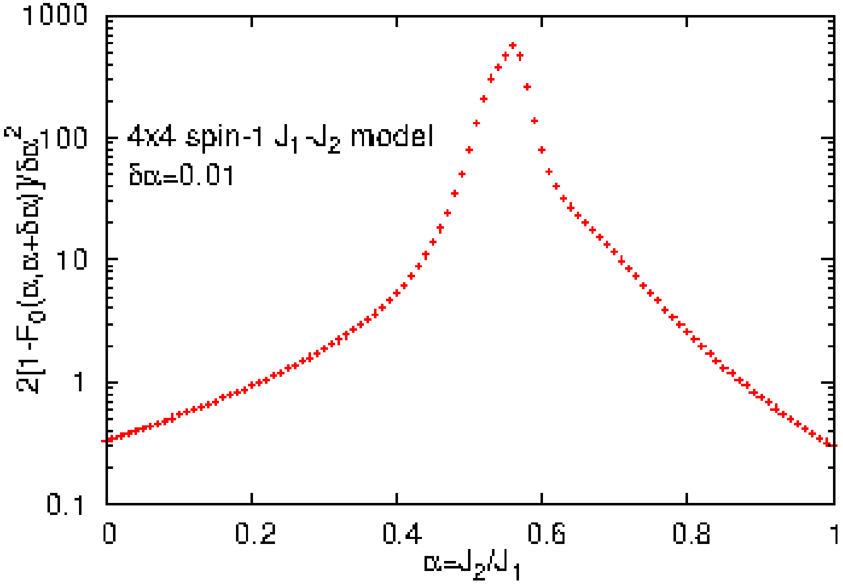
- Exact diagonalization of J_1-J_2 model:
  - Hint of nematic paramagnet from singlet and spin gap: large spin gap, vanishingly small singlet gap.

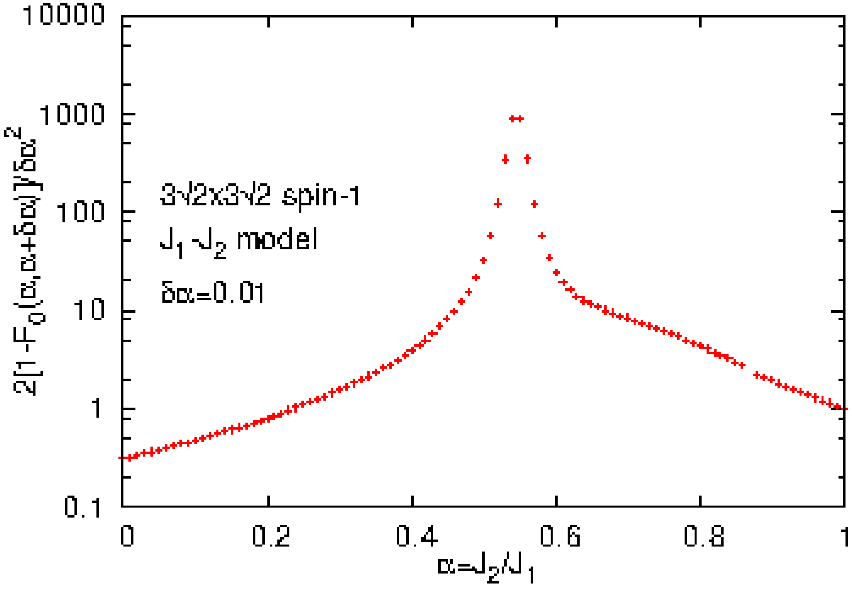




Numerical results

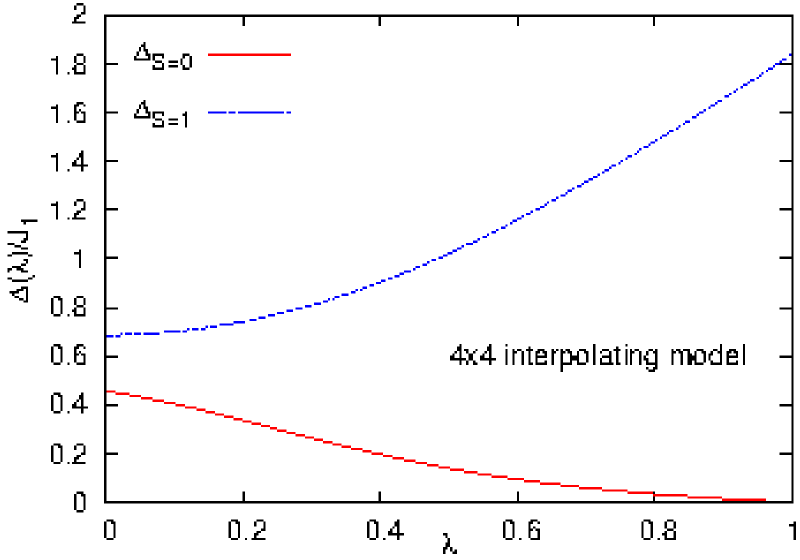
- Exact diagonalization J_1-J_2 model:
  - Hint of phase transitions from ground state fidelity susceptibility, fidelity is $F_0(\alpha, \alpha+\delta\alpha) \equiv |\langle\psi_0(\alpha)|\psi_0(\alpha+\delta\alpha)\rangle|$

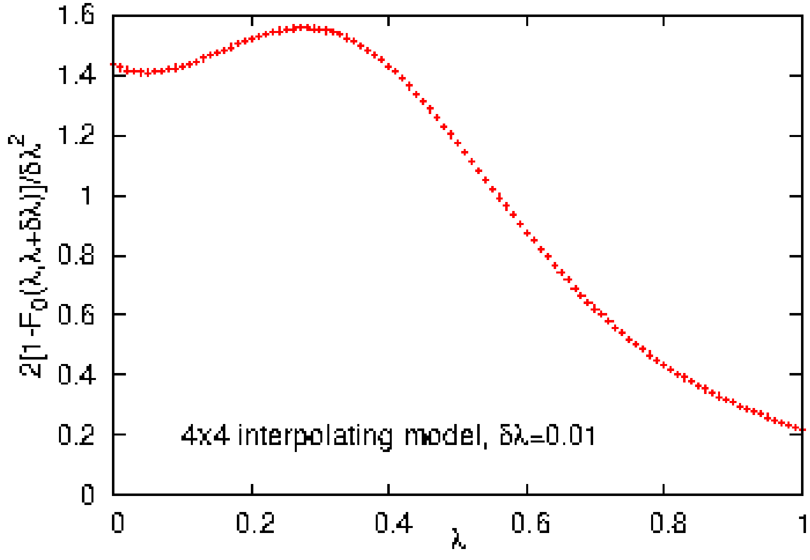




Numerical results

- Interpolating between parent Hamiltonian(λ=1) and J_1-J_2 model at J_2/J_1=0.5 (λ=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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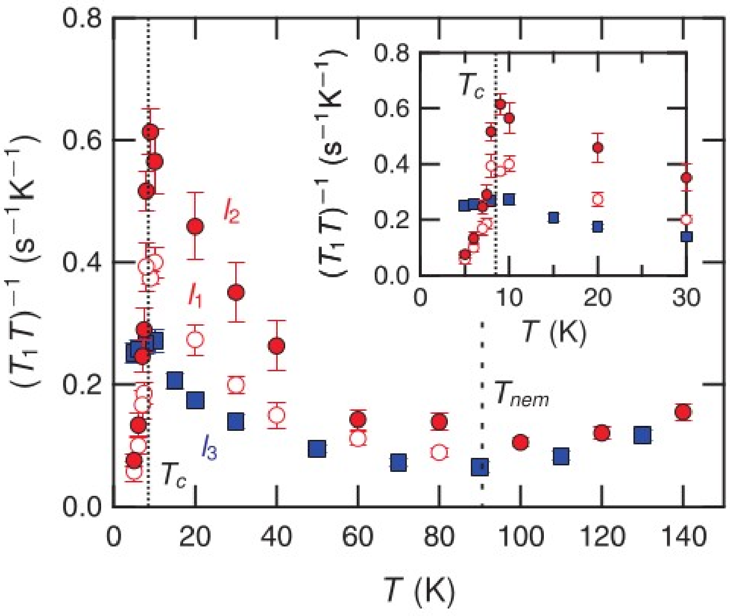
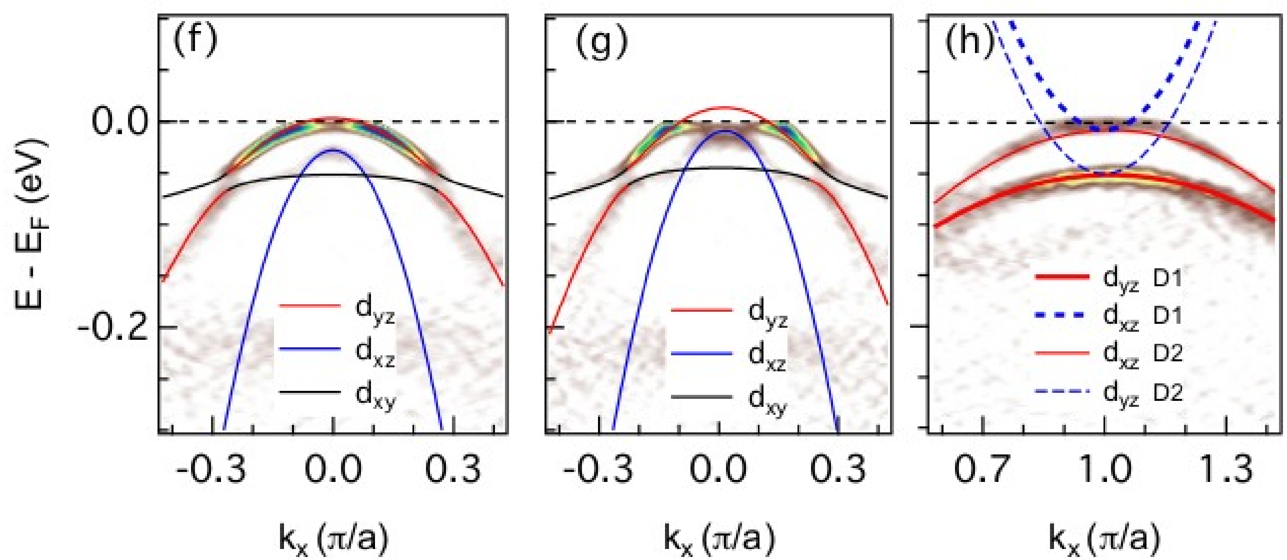
Discussion: possible relevance to FeSe

- 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 Ts~90K [Buchner et al'14], it was thus argued that the nematicity is not magnetism-driven.



Discussion: possible relevance to FeSe

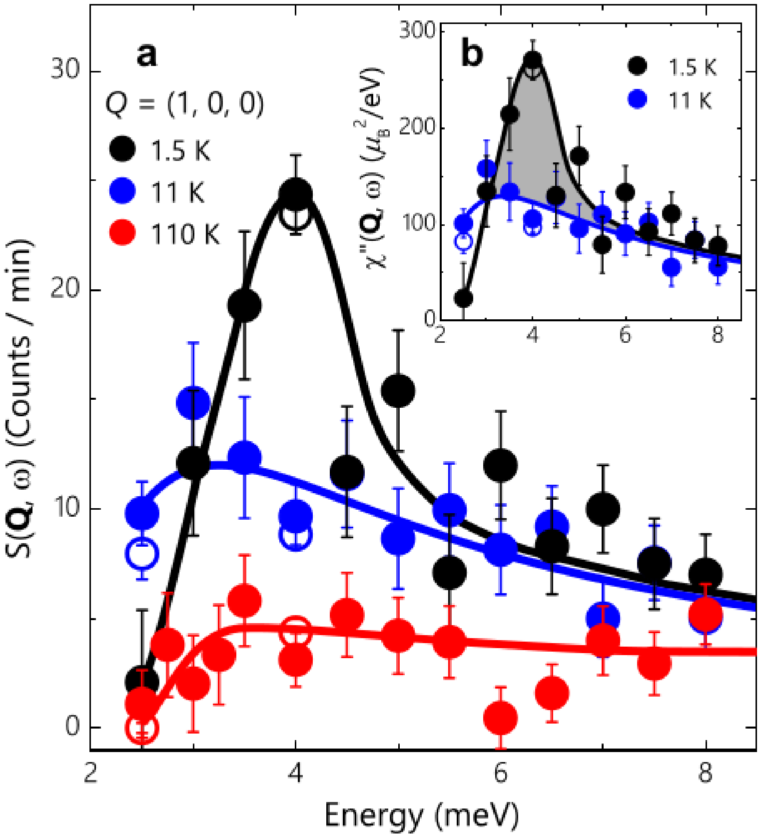
- Recent ARPES see momentum-dependent splitting of xz/yz orbitals, cannot be simple ferro-orbital order (xz,yz have different onsite potential) [Coldea et al'15; Ding et al'15; Zhang et al.'15]



Ding, et al. arXiv:1503.01390

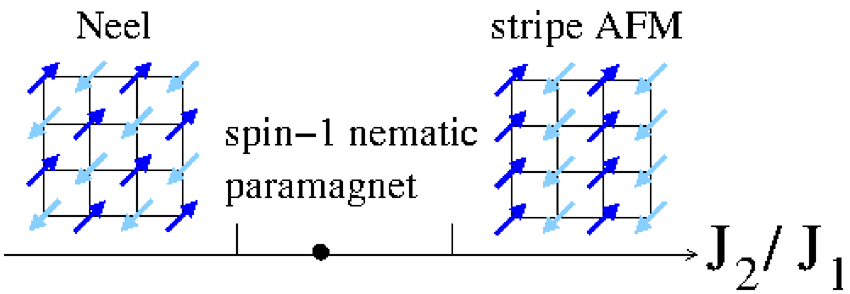
Discussion: possible relevance to FeSe

- 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!