S=1 "QSL" in a Ni-based multilayer triangular system Gang Chen CU Boulder

- Motivation
- Theory
- Prediction



FIG. 1: (Color online) Powder XRD patterns (crosses) at 295 K for the $Ba_3NiSb_2O_9$ polytypes: (a) 6H-A, (b) 6H-B, and (c) 3C. Solid curves are the best fits obtained from Rietveld refinements using FullProf. Schematic crystal structures for the $Ba_3NiSb_2O_9$ polytypes: (d) 6H-A, (e) 6H-B, and (f) 3C, red octahedra represents Sb(M') site and blue octahedra represents $Ni_{2/3}Sb_{1/3}(M)$ site. Magnetic lattices composed of Ni^{2+} ions for the $Ba_3NiSb_2O_9$ polytypes: (g) 6H-A, (h) 6H-B, and (i) 3C.







FIG. 2: (Color online) (a) Temperature dependencies of the DC magnetic susceptibility (χ) for the Ba₃NiSb₂O₉ polytypes. Inset: Temperature dependencies of $1/\chi$. The solid lines on $1/\chi$ data represent Curie-Weiss fits. For 6H-B phase, χ (open squares) is obtained by subtracting 1.7% Ni²⁺ orphan spin's contribution (crosses) from the as measured data (solid squares).

FIG. 3: (Color online) (a) Temperature dependencies for the magnetic specific heat (C_M) for all three Ba₃NiSb₂O₉ polytypes. Solid lines are the fits as described in the main text. Inset: variation in magnetic entropy ΔS below 30 K.

Works of other groups: I





FIG. 2. The phase boundary between SL GS's with p+ip and d+id pairing. (a) The spin susceptibility $\tilde{\chi}_{xx}$ in the d+id phase as a function of D/J for K/J = 0.55. The susceptibility is normalized by the average density of states, $\bar{\nu} = (\nu_x + \nu_z)/2$, where ν_x is calculated without the gap. (b) Gapped (dashed red line) and ungapped (blue line) Fermi surfaces of x, y, and z-fermions for K/J = 0.55, D/J = 0.8.

ArXiv 1108.3070

Works of other groups: II

$$\hat{S}_{i}^{\mu} = \frac{1}{2} \sum_{\alpha,\beta=\uparrow,\downarrow} \sum_{a=1,2} f_{\alpha,a,i}^{\dagger} \sigma_{\alpha\beta}^{\mu} f_{\beta,a,i}.$$
$$\hat{n}_{i} = \sum_{a=1,2} \sum_{\alpha=\uparrow,\downarrow} f_{\alpha,a,i}^{\dagger} f_{\alpha,a,i} = 2,$$
$$\hat{\tau}^{\mu} = \sum_{\alpha,j} f_{\alpha,a,j}^{\dagger} \tau_{ab}^{\mu} f_{\alpha,b,i} = 0.$$

$$\hat{\tau}^{\mu} = \sum_{\alpha,a,b} f^{\dagger}_{\alpha,a,i} \tau^{\mu}_{ab} f_{\alpha,b,i} = 0.$$

$$\begin{aligned} \mathrm{U}(1)_c &: f_{\alpha,a,i} \to e^{i\theta_i} f_{\alpha,a,i}; \\ \mathrm{SU}(2)_o &: f_{\alpha,a,i} \to [e^{i\vec{\theta_i}\cdot\vec{\tau}/2}]_{ab} f_{\alpha,b,i}. \end{aligned}$$



FIG. 1: *a*, The spin liquid we are considering contains a quadratic band touching at $\vec{k} = 0$ (hexagon), and Dirac points (squares) at the corners of the Brillouin zone. *b*, with a nonzero and small nematic order $N_1 > 0$, the quadratic band touching is split into two Dirac points, and the locations of the other Dirac points are shifted.

ArXiv 1110.3328

Crystal structure



 $\Theta_{CW} = -75.6K$

Model



FIG. 1. (Color online) The bilayer triangular lattice (on left) is equivalent to a single layer honeycomb lattice (on right). A (in dark red) and B (in light blue) denote two triangular lattice (on left) or two sublattices of honeycomb lattice (on right). J_1 , J_2 are interlayer and intralayer exchange, respectively.

$$\begin{aligned} \mathcal{H}_{\text{ex}} &= J_1 \sum_{\langle ij \rangle \in AB} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle ij \rangle \in AA \text{ or } BB} \mathbf{S}_i \cdot \mathbf{S}_j, \\ \mathcal{H}_{\text{ani}} &= D \sum (S_i^z)^2, \end{aligned}$$

i

Phase diagram

b



FIG. 2. (Color online) Zero temperature phase diagram determined from the SPE. In the figure, "IC"=incommensurate spin order, "Néel"= Néel state, "QP"=quantum paramagnet. Shaded region (in blue) is the expected parameter regime for the 6H-B compound.



$$\sum_{\mathbf{b}\}} \cos(\mathbf{q}_{\perp} \cdot \mathbf{b}) = (\frac{J_1}{J_2})^2 - 3,$$

Quantum order-by-disorder

$$\mathbf{q}_{\perp} = \left(0, \frac{2}{\sqrt{3}} \cos^{-1}\left(\left(\frac{J_1}{2J_2}\right)^2 - \frac{5}{4}\right)\right), \text{ if } 1 < \frac{J_1}{J_2} < 3$$
$$\mathbf{q}_{\perp} = \left(2 \cos^{-1}\left(\frac{J_1}{2J_2} + \frac{1}{2}\right), \frac{2\pi}{\sqrt{3}}\right), \qquad \text{if } \frac{J_1}{J_2} < 1,$$

MFT:I



MFT:II



Map to rotor model

$$S_{i}^{z} \rightarrow n_{i} \text{ and } S_{i}^{+} \rightarrow \sqrt{2}e^{i\phi_{i}}, \qquad [\phi_{i}, n_{j}] = i\delta_{ij}.$$

$$\mathcal{H}_{\text{rotor}} = \frac{1}{2} \sum_{ij} J_{ij} [2\cos(\phi_{i} - \phi_{j}) + n_{i}n_{j}] + \sum_{i} Dn_{i}^{2}.$$

$$z = \int \mathcal{D}\Phi \prod_{i} \delta(|\Phi_{i}|^{2} - 1)e^{-S} \qquad (11)$$
with
$$S = \int_{\tau} \sum_{\mathbf{k}} (4D\mathbb{I} + 2\mathcal{J}_{\mathbf{k}})_{\mu\nu}^{-1} \sigma \Phi_{\mu,\mathbf{k}}^{*} \partial_{\tau} \Phi_{\nu,-\mathbf{k}} + \sum_{ij} J_{ij} \Phi_{i}^{*} \Phi_{j}$$

$$s_{\pm}(\mathbf{k}) = \sum_{\{\mathbf{b}\}} J_{2} \cos(\mathbf{k} + \mathbf{b}) \pm |J_{1}(1 + e^{ik_{z}}) \sum_{\{\mathbf{a}\}} e^{i\mathbf{k}\cdot\mathbf{a}}|$$
Saddle-point equation
$$\sum_{i=\pm} \int_{\mathbf{k}} \frac{2D + s_{i}(\mathbf{k})}{c_{i}(\mathbf{k})} \coth(\beta\epsilon_{i}(\mathbf{k})/2) = 2,$$

$$\epsilon_{\pm}(\mathbf{k}) = \sqrt{(\frac{2D + s_{i}(\mathbf{k})}{c_{i}(\mathbf{k})}} \cot(\beta\epsilon_{i}(\mathbf{k})/2) = 2,$$

$$\epsilon_{\pm}(\mathbf{k}) = \sqrt{(\frac{2D + s_{i}(\mathbf{k})}{c_{i}(\mathbf{k})}} \cot(\beta\epsilon_{i}(\mathbf{k})/2) = 2,$$

$$i\lambda_{i} = \frac{\beta}{2} \Delta (\frac{2D + s_{i}(\mathbf{k})}{c_{i}(\mathbf{k})} - \frac{2\beta}{2} \Delta ($$

MFT:II



Map to rotor model



Low-E spin excitation



FIG. 3. (Color online) The evolution of the low-energy spin excitations in $k_x \cdot k_y$ plane with $k_z = 0$ at the QCP. (a) $J_1 = 1.2J_2$, $D_c = 2.79J_2$, (b) $J_1 = J_2$, $D_c = 2.456J_2$, (c) $J_1 = 0.7J_2$, $D_c = 2.33J_2$, (d) $J_1 = 0$, $D_c = 2.01J_2$. Lattice constants in xy plane are set to be 1. (e) and the hexagon in (c) is the Brillouin zone (BZ) of the honeycomb lattice. When $J_1 > J_2$, the nodal line is centered in the middle of BZ. When $J_1 < J_2$, the nodal lines are centered around and eventually shrink to the corners of BZ in the limit $J_1 \rightarrow 0$. The " \bigstar " in (d) and (e) indicates the locations of the momenta with energy scale Λ_c (see the text).











FIG. 4. (Color online) The temperature dependence of specific heat. In the plot, $J_1 = 0.15J_2$. The critical $D_c = 2.018J_2$. For the curves in the plot, from top to bottom $D = 2.02J_2, 2.12J_2, 2.22J_2, 2.32J_2$. The dash lines are the linear fit for a range of data points.

Other prediction

1. NMR

's theory group 3. Crossover Gang 2. Neutron scattering

 S_{M} (JK⁻¹mol⁻¹)

0 T

9 T

Ф,

30

Б

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σ

10

20

r 0.99

T (K)

Spin Liquid State in the S = 1/2 Triangular Lattice Ba₃CuSb₂O₉

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(Received 12 October 2010; published 6 April 2011)



FIG. 1 (color). (a) Schematic crystal structure for $Ba_3CuSb_2O_9$; (b) The layer structure along the c axis; (c) The triangular lattice of Cu^{2+} in the *ab* plane.

g = 2.07 $\theta_{\rm CW} = -55 \ {\rm K}$ $z = 6, J/k_B = -2/3\theta_{CW} = 37$ K,



Summary

I. we study the spin-I multilayer triangular lattice magnet.

2. we propose the quantum criticality to be the origin of the puzzling spin liquid phenomena in Ni spin-I magnet.