Abstract: Motivated by spin-wave continuum (SWC) observed in recent neutron scattering experiments in Herbertsmithite, we use Gutzwiller-projected wave functions to study dynamic spin structure factor of spin liquid states on the kagome lattice. As their ground state, spin-1 excited states for spin liquids are represented by Gutzwiller-projected two-spinon excited wave functions. We investigate three different spin liquid candidates, spinon Fermi-surface spin liquid (FSL), Dirac spin liquid (DSL) and random-flux spin liquid (RSL). We find that DSL has no explicit contradiction with experiments. Besides a fractionalized spin moment, DSL has a fractionalized crystal momentum which is also detectable directly in the neutron scattering measurements.
Recent progress on high Tc superconductivity and related problems

Fractional spin-wave continuum in kagome spin liquid states

Jia-Wei Mei

JWM and X.G. Wen, coming soon ....
Outline:

- **Motivation**
  quantum spin liquid is a key ingredient of high Tc superconductivity

- **Fractional spin-wave continuum in kagome spin liquid states**
  Neutron scattering experiments, spin fractionalization, crystal momentum fractionalization

- **New kagome material**
  Selective doping Barlowite (Cu4(OH)6FBr), LDA, Cu3Mg(OH)6FBr, Cu3Zn(OH)6FBr
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An End to the Drought of Quantum Spin Liquids
-- P.A. Lee

Ordered spins. (Left) Néel’s picture of antiferromagnet ordering with an alternate spin-up–spin-down pattern across the lattice. (Right) Quantum fluctuations lead to mutual spin flips, which Landau argued would disorder Néel’s state.

Quantum AF ($J > 0$) spin model

\[ H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \]

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Quantum AF ($J > 0$) spin model

$$H = J \sum_{\langle ij \rangle} S_i \cdot S_j$$

Spin liquid:
- no spin order at 0K;
- Long range entangled;
- Symmetry fractionalization;

Herbertsmithite (Y. Lee group)
$H = J \sum_{\langle i,j \rangle} S_i \cdot S_j$  
Spin wave, Slave particle mean field + VMC, MERA, DMRG, PEPS, ED ...

Possible ground state candidates: valence-bond solds, gapless or gapped QSLs ...

DMRG: Z2 spin liquid with small singlet gap $\Delta s \approx 0.05J$ and triplet gap $\Delta t \approx 0.1J$.

S. Yan et al, Science (2011)

VMC (Gutzwiller-projected wave functions): U(1) Dirac spin liquid

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- It has a spin-wave continuum (SWC) spectrum over a large momentum and energy;
- The magnetic intensity is low in the elementary BZ and high in the extended region of magnetic BZ;
- The integrated intensity up to 11 meV only accounts for 20% of total spin moment and the SWC extends up to $2 \sim 3J$;
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$$H = J \sum_{\langle ij \rangle} S_i \cdot S_j$$

Slave particle decomposition:

$$S_i^a = \frac{1}{2} \sum_{\alpha \beta} f_{i\alpha}^\dagger \sigma^a f_{i\beta}$$

Mean field Hamiltonian:

$$H_{MF} = -\sum_{\langle ij \rangle} (\chi_{ij} f_{i\sigma}^\dagger f_{j\sigma} + H.C.)$$

Ground state:

$$|\Psi\rangle = \mathcal{P}_G |\Psi_{MF}^{\chi_{ij}}\rangle$$

Spin-1 excited states:

$$|\Psi_{ij}^{S=1}\rangle = \mathcal{P}_G f_{e_i\uparrow}^\dagger f_{e_j\downarrow} |\Psi_{MF}^{\chi_{ij}}\rangle$$
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*Ground-state Assumption*

$$|\Psi_{ij}^{S=1}\rangle = \mathcal{P}_G f_{e_i}^{\dagger} f_{e_j} |\Psi_{MF}^{X_{ij}}\rangle$$

*Excited-state Assumption*

The projected Hamiltonian system

$$\mathbb{H}(i'j', ij) = \langle i'j' | H | ij \rangle, \quad \mathbb{O}(i'j', ij) = \langle i'j' | ij \rangle$$

MC strategy: single Markov chain for spin configuration samplings.

$$S(q, i\omega_n) = \int_0^\beta d\tau e^{i\omega_n\tau} \frac{1}{N} \sum_{ij} e^{iq \cdot r_{ij}} \langle T_\tau S_i^- (\tau) S_j^+ (0) \rangle_0$$

Since spin operator commute with Gutzwiller projection operator,

$$S(q, \omega) = \sum_n \delta(\omega - (\epsilon_n - \epsilon_0)) |\phi_n\rangle \mathcal{P}_G ^* |\Psi_{MF}^{X_{ij}}\rangle^2$$

$$\mathbb{H}|\phi_n\rangle = \epsilon_n \mathbb{O}|\phi_n\rangle$$

Tao Li and Fan Yang, PRB(2010)
Best trial GPWF: Dirac spin liquid (DSL)

"Q1=Q2 states", Sachdev (1992)

\[ |\Psi\rangle = \mathcal{P}_G |\Psi_{MF}^{X_{ij}}\rangle \]

Crystal momentum fractionalization:

\[ T_1 T_2 = -T_2 T_1 \]
Random-flux spin liquid (RSL)

ω=0.05J

ω=0.5J
S(q,ω) along high symmetry directions

Full ω-integrated S(q, ω) = S(q)

Partial ω-integrated S(q, ω) from 0 to 0.6J
**S(q,ω) along high symmetry directions**

Low energy $ω_0$ magnetic intensity

- FSL has a gap at M points;
- FSL and RSL have low energy peaks around K points;
- DSL has low energy peaks at M and M' points.
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Dashed line: MF

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| \chi_{ij} | = 0.43J
New kagome antiferromagnet

(a) Barlowite

(b) $J \approx 180 \text{ K}$

$\text{Cu}^{2+} \rightarrow \text{Zn}^{2+}$

arXiv: 1504.00521
New kagome antiferromagnet

![Diagram of kagome antiferromagnet with energy levels and atomic configurations]

arXiv: 1504.00521

\[ J \approx 180 \text{ K} \]

Cu2⁺ → Mg2⁺
Cu2⁺ → Zn2⁺
Summary:

• Dirac spin liquid is very likely in Herbertsmithite. A crystal momentum fractionalization is also potential detectable in neutron scattering experiments.

• Selective doping Barlowite varieties (Cu3Mg(OH)6FBr and Cu3Zn(OH)6FBr) are promising for new kagome materials with much less imperfection.