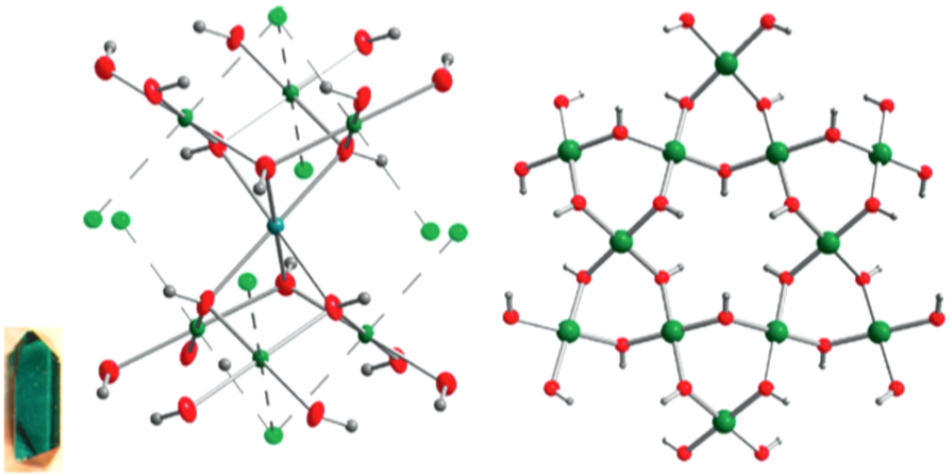
Title: Fractional spin-wave continuum in spin liquid states on the kagome lattice

Date: Jul 10, 2015 11:00 AM

URL: http://pirsa.org/15070063

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 ….

Z. Liu, X.L. Zou, JWM and F. Liu, arXiv: 1504.00521

PERIMETER INSTITUTE

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 ($Cu_4(OH)_6FBr$), LDA, $Cu_3Mg(OH)_6FBr$, $Cu_3Zn(OH)_6FBr$

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 ($Cu_4(OH)_6FBr$), LDA, $Cu_3Mg(OH)_6FBr$, $Cu_3Zn(OH)_6FBr$

Outline:

- Motivation

  quantum spin liquid is a key ingredient of high Tc superconductivity

- Fractional spin-wave continuum in kagome spin liquid states

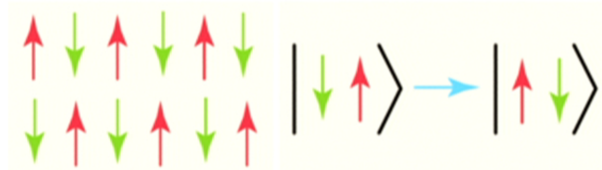
  Neutron scattering experiments, spin fractionalization, crystal momentum fractionalization

- New kagome material

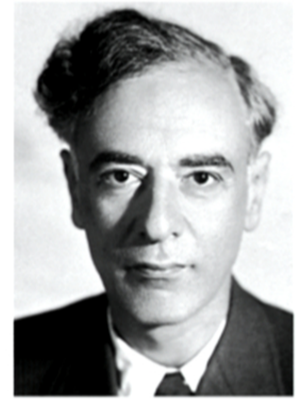
  Selective doping Barlowite ($Cu_4(OH)_6FBr$), LDA, $Cu_3Mg(OH)_6FBr$, $Cu_3Zn(OH)_6FBr$

Louis Neel

An End to the Drought of Quantum Spin Liquids
-- P.A. Lee



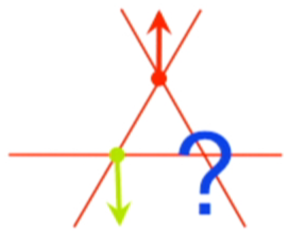
Ordered spins. (**Left**) Néel's picture of antiferro-magnet ordering with an alternate spin-up–spin-down pattern across the lattice. (**Right**) Quantum fluctuations lead to mutual spin flips, which Landau argued would disorder Néel's state.



Lev Landau

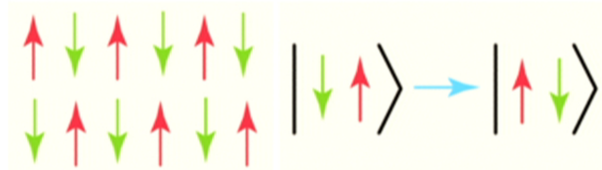
Quantum AF ($J > 0$) spin model

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

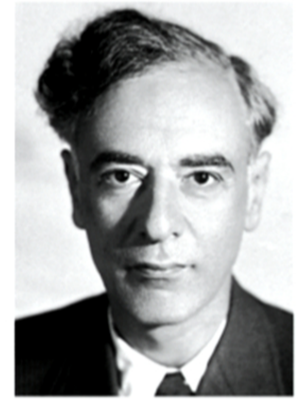


Louis Neel

An End to the Drought of Quantum Spin Liquids -- P.A. Lee, Science (2008)



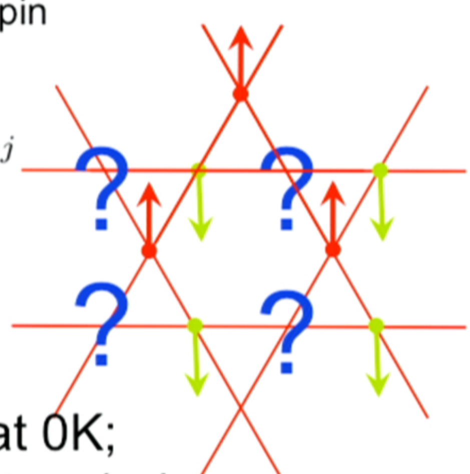
Ordered spins. (**Left**) Néel's picture of antiferromagnet ordering with an alternate spin-up–spin-down pattern across the lattice. (**Right**) Quantum fluctuations lead to mutual spin flips, which Landau argued would disorder Néel's state.

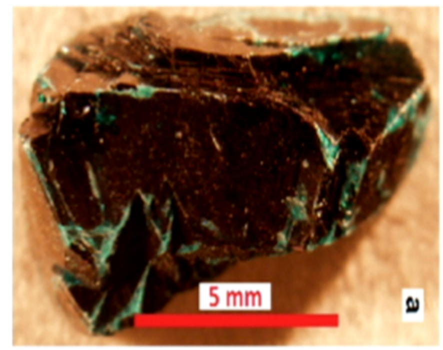


Lev Landau

Quantum AF ($J > 0$) spin model

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

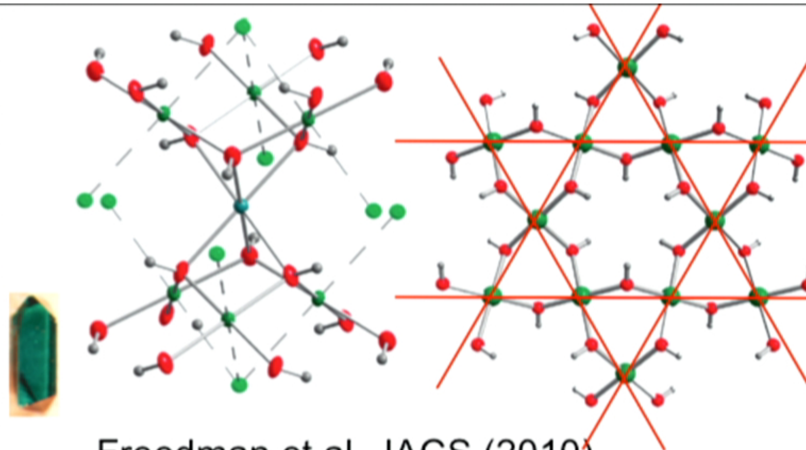


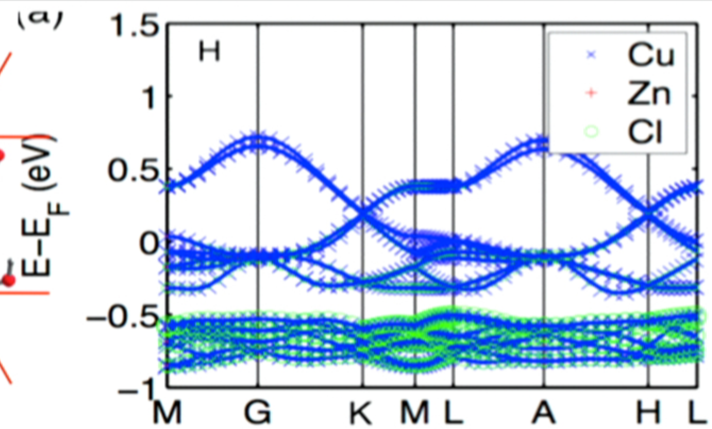


Herbertsmithite (Y. Lee group)

Spin liquid:

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





Freedman et al, JACS (2010)

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

Spin wave, Slave particle mean field + VMC, MERA, DMRG, PEPS, ED ...

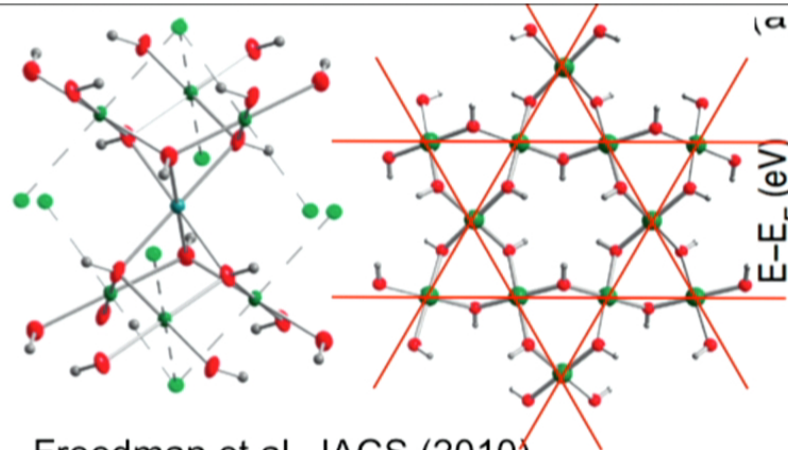
Possible ground state candidates: valence-bond solds, gapless or gapped QSLs ...

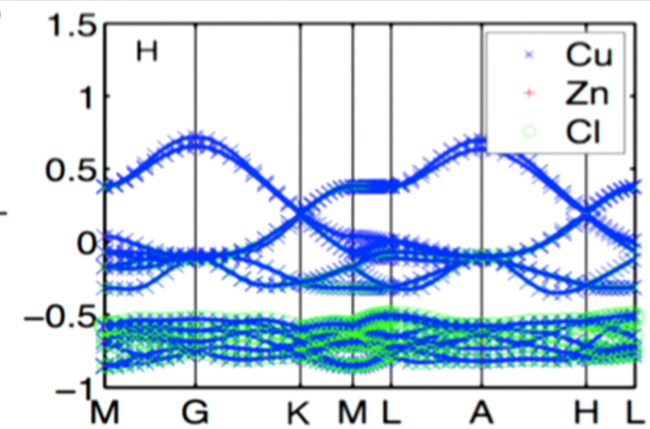
DMRG: Z2 spin liquid with small singlet gap $\Delta s \approx 0.05J$ and triplet gap $\Delta t \approx 0.1J$.

S. Yan et al, Science (2011)

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

Y. Ran et al, PRL (2007)





Freedman et al, JACS (2010)

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

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)

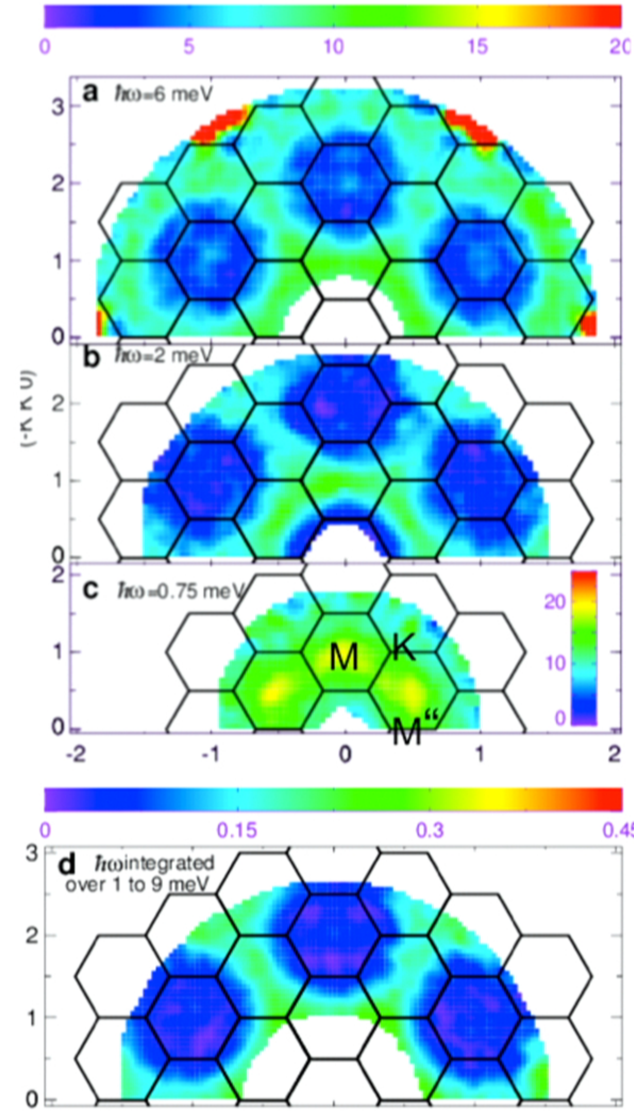
VMC (Gutzwiller-projected wave functions): U(1) Dirac spin liquid

Y. Ran et al, PRL (2007)

T. Han et al, Nature (2012)

Properties in neutron scattering: J~17 meV

- 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 2~3J;
- The magnetic intensity is almost energy independent between 1.5 meV and 11 meV;
- Magnetic intensity is quite flat in momentum and has no sharp dispersing boundary edge;
- The low energy pattern of intensity varies in momentum and low energy peaks (at M) are connected through M";

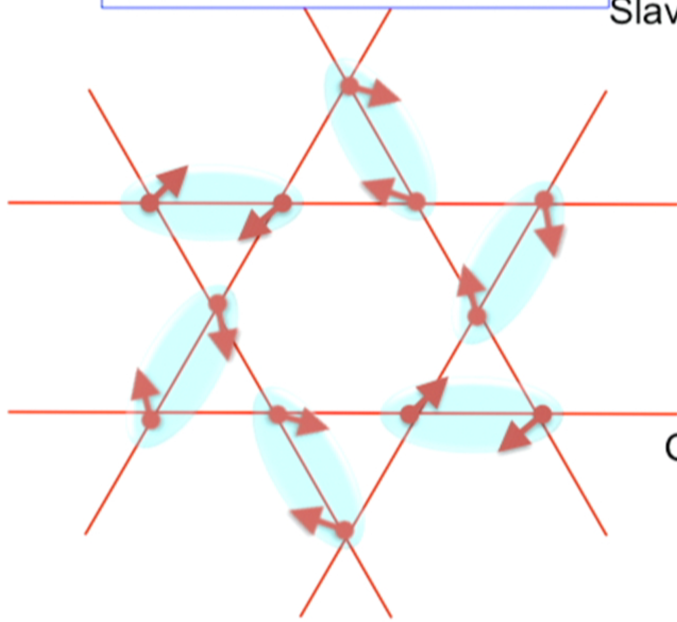


Gutzwiller-Projected Wave Function (GPWF)

Quantum AF ($J > 0$) spin model:

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

T.M. Rice, P.W. Anderson ...



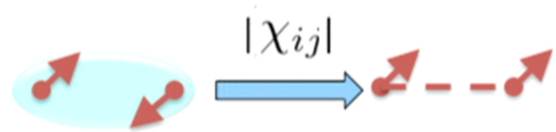
Slave particle decomposition:

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

Mean field Hamiltonian:

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

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



Spin-1 excited states: $|\Psi_{ij}^{S=1}\rangle = \mathcal{P}_G f_{e_i\uparrow}^\dagger f_{e_j\downarrow} |\Psi_{\mathrm{MF}}^{\chi_{ij}}\rangle$

Gutzwiller-Projected Wave Function (GPWF)

Quantum AF ($J > 0$) spin model: $$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$|\Psi\rangle = \mathcal{P}_G |\Psi_{\mathrm{MF}}^{\chi_{ij}}\rangle$$ *Ground-state Assumption*

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

The projected Hamiltonian system $\{\mathbb{H}, \mathbb{O}\}$ Tao Li and Fan Yang, PRB(2010)

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

MC strategy: single Markov chain for spin configuration samplings.

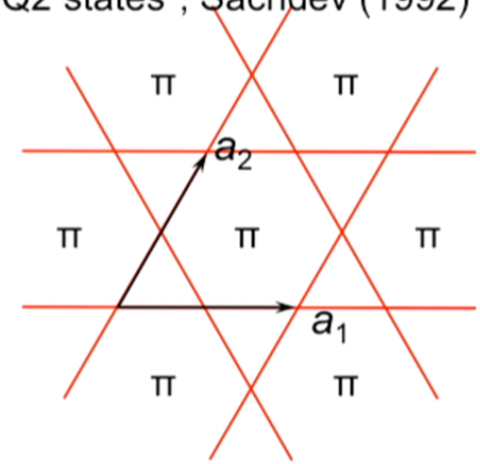
$$S(\mathbf{q}, i\omega_n) = \int_0^{\beta} d\tau e^{i\omega_n \tau} \frac{1}{N} \sum_{ij} e^{i\mathbf{q}\cdot\mathbf{r}_{ij}} \langle T_\tau S_i^-(\tau) S_j^+(0)\rangle_0$$

Since spin operator commute with Gutzwiller projection operator,

$$S(\mathbf{q}, \omega) = \sum_n \delta(\omega - (\epsilon_n - \epsilon_0)) |\langle \phi_n | S_{\mathbf{q}}^+ \mathcal{P}_G |\Psi_{\mathrm{MF}}^{\chi_{ij}}\rangle|^2 \qquad \mathbb{H}|\phi_n\rangle = \epsilon_n \mathbb{O}|\phi_n\rangle$$

Best trial GPWF: Dirac spin liquid (DSL)

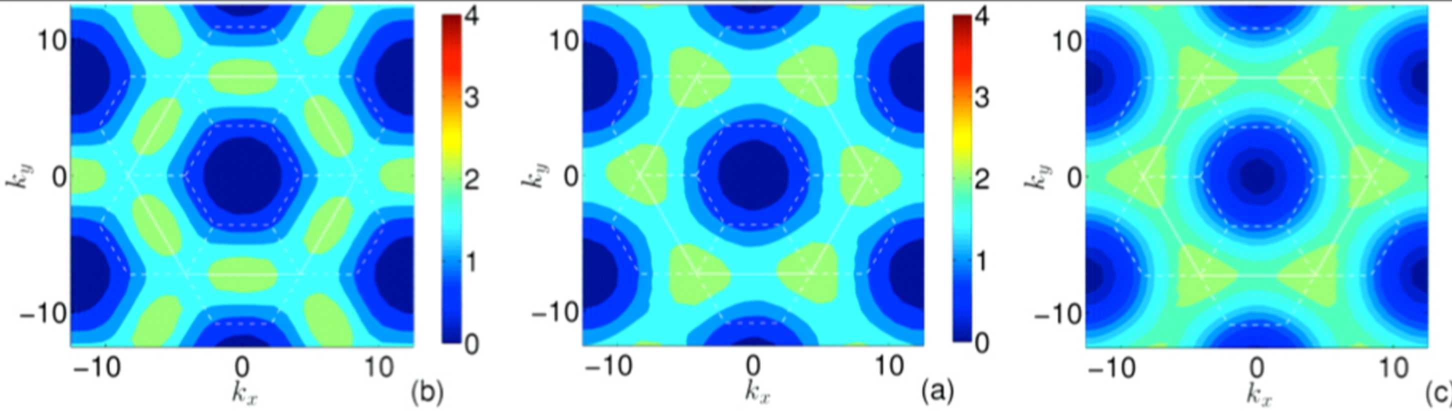
"Q1=Q2 states", Sachdev (1992)



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

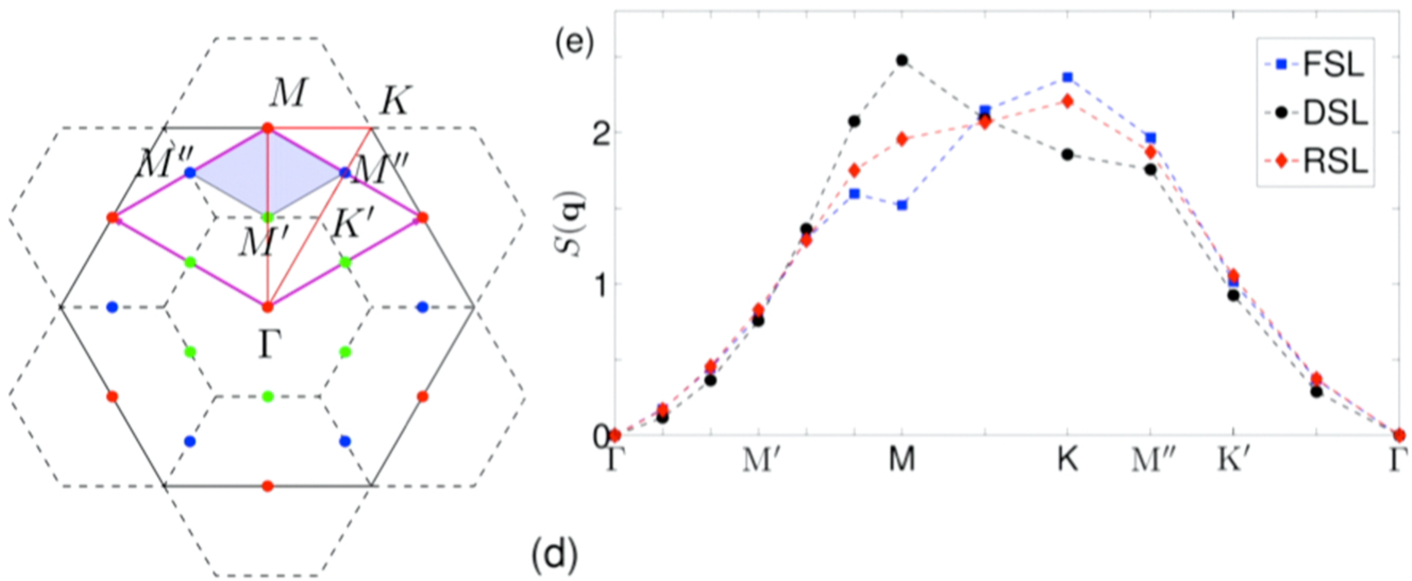
Crystal momentum fractionalization:

$$T_1 T_2 = -T_2 T_1$$



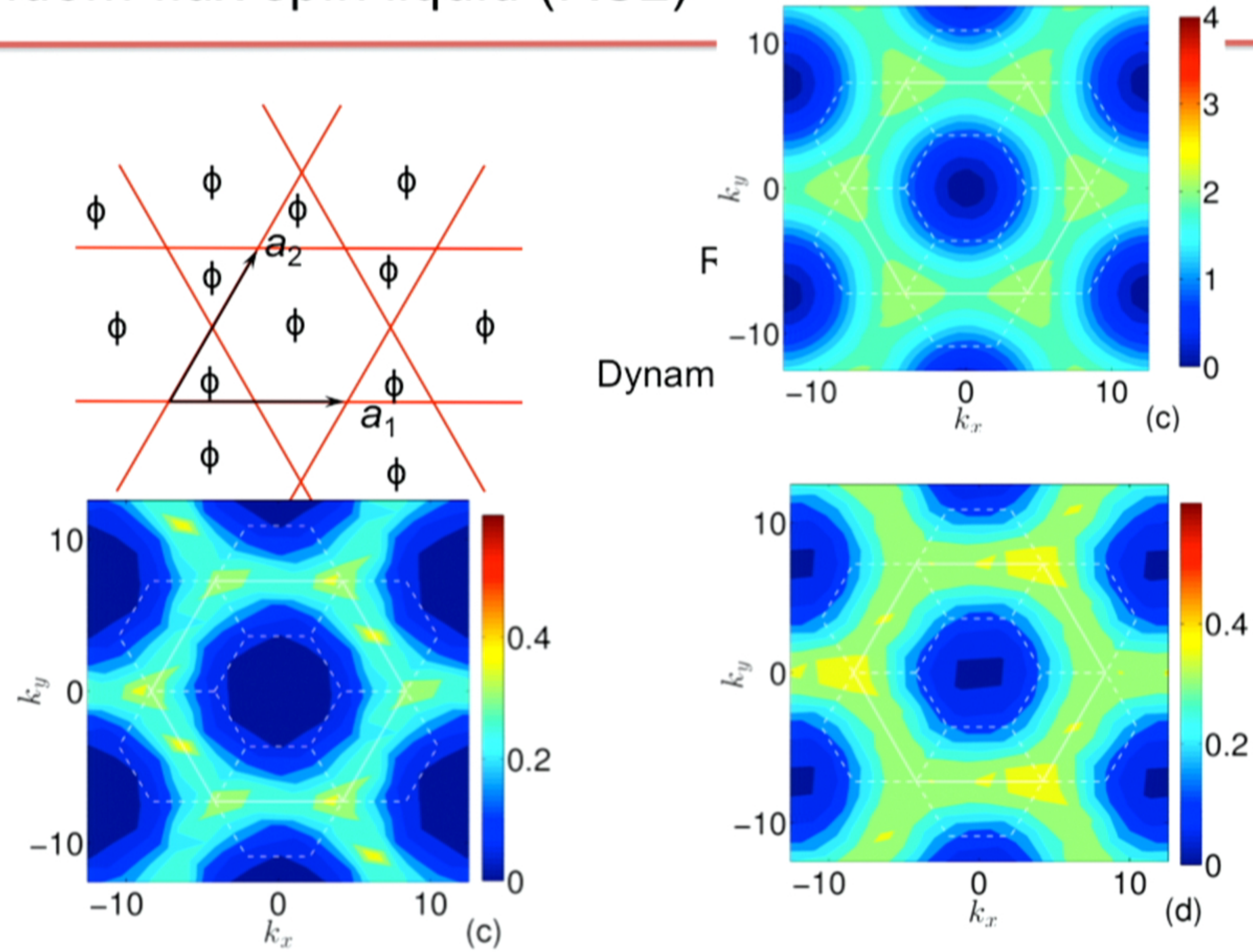
Dirac SL (DSL) Fermi-surface SL (FSL) Random-Flux SL (RSL)

Equal-time spin structure factor S(q)



(d)

Random-flux spin liquid (RSL)

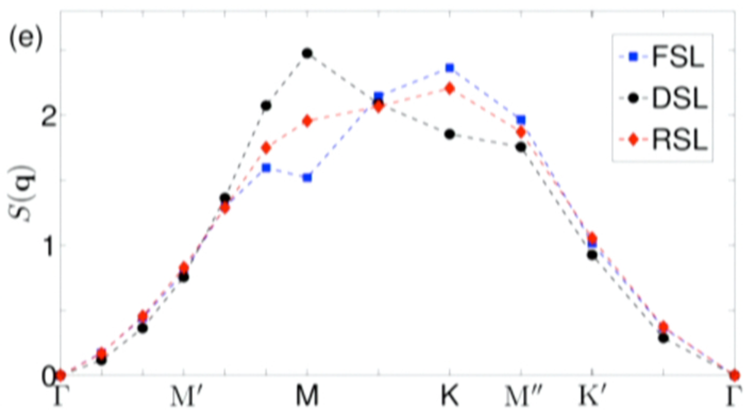


ω=0.05J

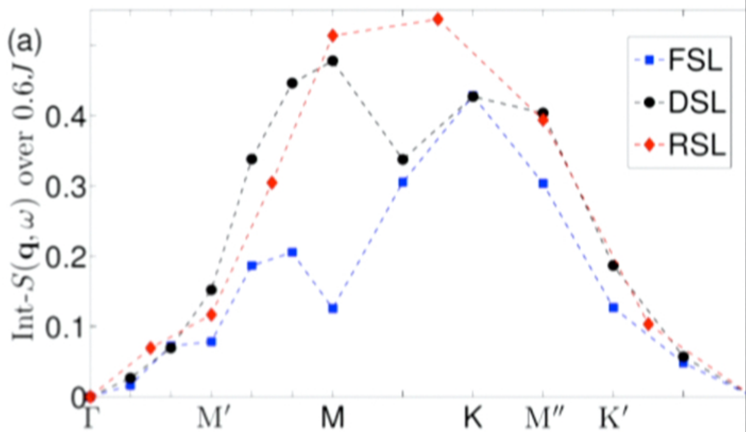
ω=0.5J

S(q,ω) along high symmetry directions

Full ω-integrated S(q, ω) = S(q)

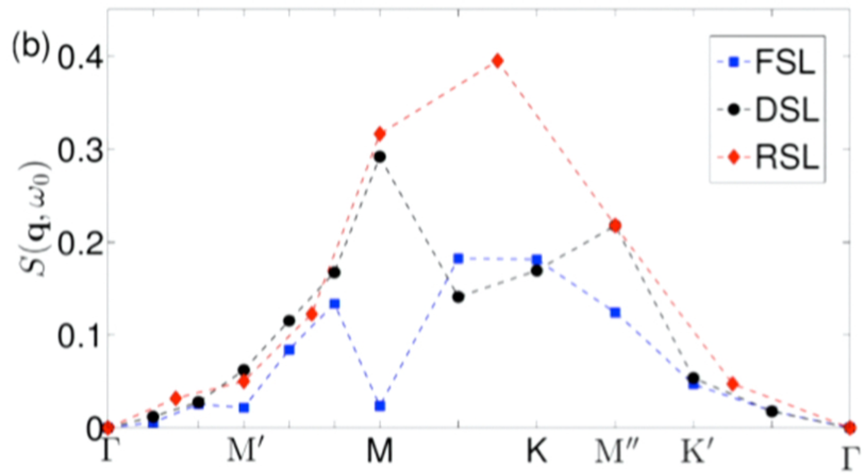


Partial ω-integrated S(q, ω) from 0 to 0.6J



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.

T. Han et al, Nature (2012)

Properties in neutron scattering: $J \sim 17$ meV	DSL	FSL	RSL
• 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; short ranged spin liquid (RVB);	✔	✔	✔
• The integrated intensity up to 11 meV only accounts for 20% of total spin moment and the SWC extends up to 2~3J;	✔	✔	✔
• The magnetic intensity is almost energy independent between 1.5 meV and 11 meV; • Magnetic intensity is quite flat in momentum and has no sharp dispersing boundary edge; • The low energy pattern of intensity varies in momentum and low energy peaks (at M) are connected through M'';			

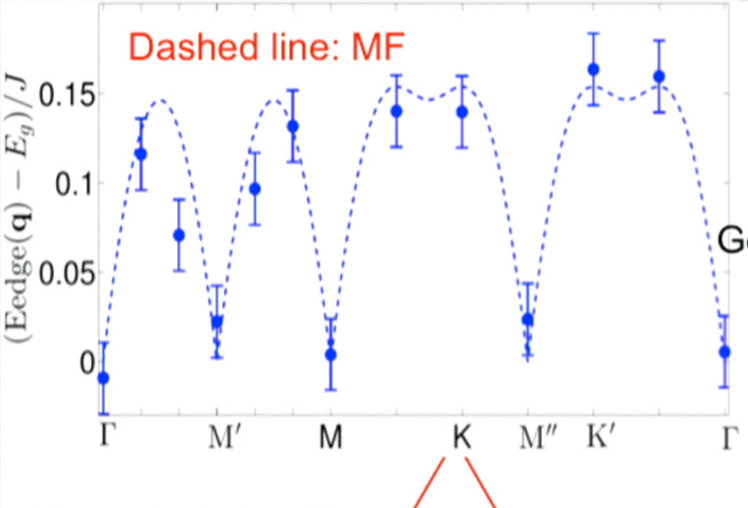
T. Han et al, Nature (2012)

Properties in neutron scattering: J ~ 17 meV	DSL	FSL	RSL
• 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; short ranged spin liquid (RVB);	✔	✔	✔
• The integrated intensity up to 11 meV only accounts for 20% of total spin moment and the SWC extends up to 2~3J;	✔	✔	✔
• The magnetic intensity is almost energy independent between 1.5 meV and 11 meV;	?✔	?✔	?✔
• Magnetic intensity is quite flat in momentum and has no sharp dispersing boundary edge;			
• The low energy pattern of intensity varies in momentum and low energy peaks (at M) are connected through M'';			

T. Han et al, Nature (2012)

Properties in neutron scattering: $J \sim 17$ meV	DSL	FSL	RSL
• 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; short ranged spin liquid (RVB);	✔	✔	✔
• The integrated intensity up to 11 meV only accounts for 20% of total spin moment and the SWC extends up to 2~3*J*;	✔	✔	✔
• The magnetic intensity is almost energy independent between 1.5 meV and 11 meV;	?✔	?✔	?✔
• Magnetic intensity is quite flat in momentum and has no sharp dispersing boundary edge;	?✔	? ✖	?✔
• The low energy pattern of intensity varies in momentum and low energy peaks (at M) are connected through M";	✔	✖	✖

Best trial GPWF: Dirac spin liquid (DSL)



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

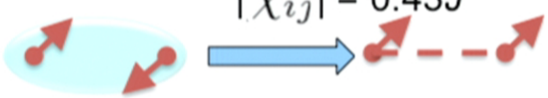
$$|\Psi_{ij}^{S=1}\rangle = \mathcal{P}_G f_{e_i\uparrow}^\dagger f_{e_j\downarrow}|\Psi_{\text{MF}}^{\chi_{ij}}\rangle$$

General eigen equation:

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

Mean field Hamiltonian:

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

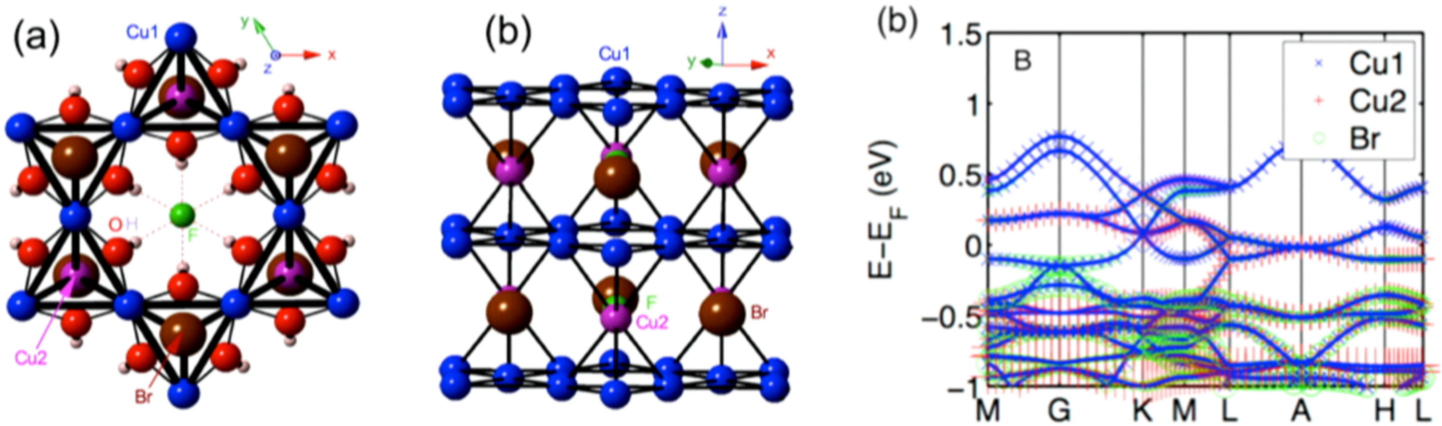


Crystal momentum fractionalization:

$$T_1 T_2 = -T_2 T_1$$

New kagome antiferromagnet

arXiv: 1504.00521



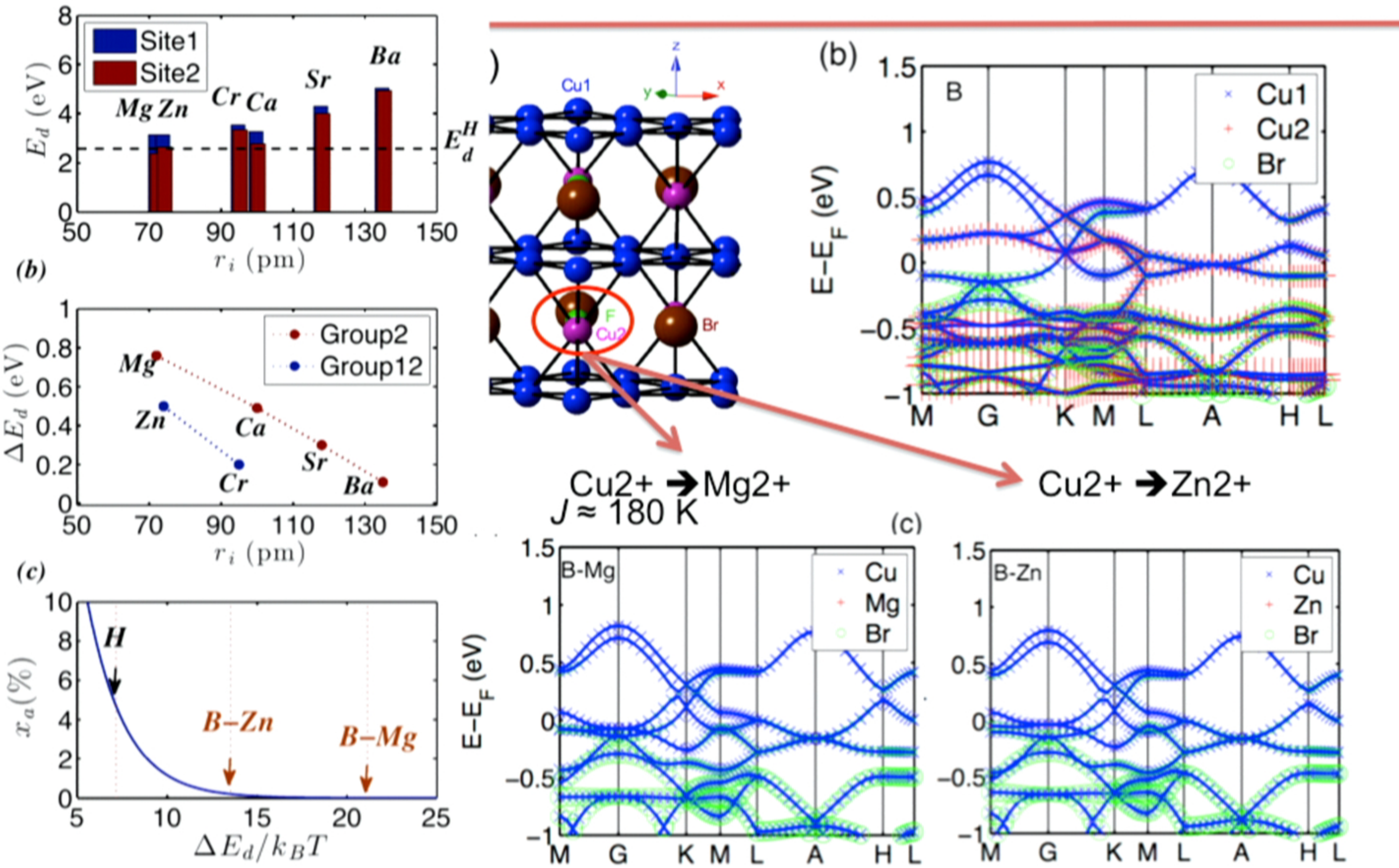
Barlowite

$J \approx 180$ K

Cu2+ ➔Zn2+

New kagome antiferromagnet

arXiv: 1504.00521



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.