Projective Symmetry Group Classification of Chiral Spin Liquids

Kagome Heisenberg model: New materials and Quantum Spin Liquids

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Phys. Rev. B 92, 060407(R) (2015)

+ work in progress

D. Boldrin, Fåk, Enderle, **SB**, Ollivier, Rols, Manuel, and Wills

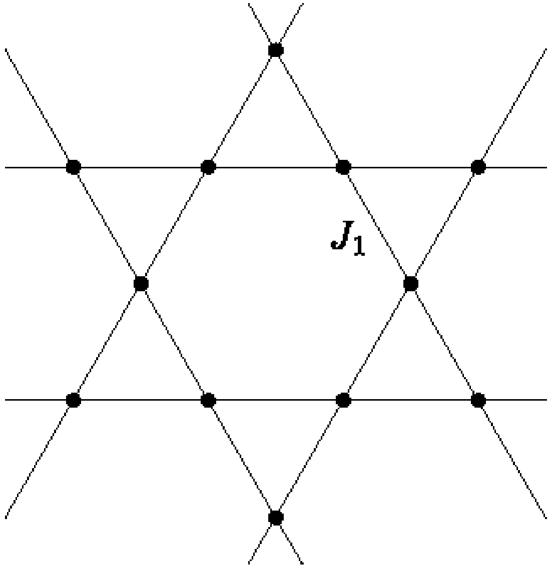
Phys. Rev. B 91, 220408(R) (2015)

AGENCE NATIONALE DE LA RECHERCHE ANR

Outline

- New quantum magnets on the Kagomé lattice:
  From Herbertsmithite to Kapellasite and Haydeeite
- Evidence for gapless quantum spin liquid (QSL) phase in Kapellasite
- Classical Heisenberg models
- Parton construction, projective symmetry group, and chiral spin liquids (CSL)
- SU(2) gauge flux, QSL order parameters
- Results, phase diagram, structure factors
- Conclusion & outlook

Strong Mott insulators (S=1/2) on the Kagome lattice



1. Herbertsmithite [$ZnCu_3(OH)_6Cl_2$]

   - No ordering down to mK , gapless spin excitations
   - Nearest-neighbor AF Heisenberg model J ~ 200 K
   - Recently: single crystals

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2. Kapellasite [polymorph]

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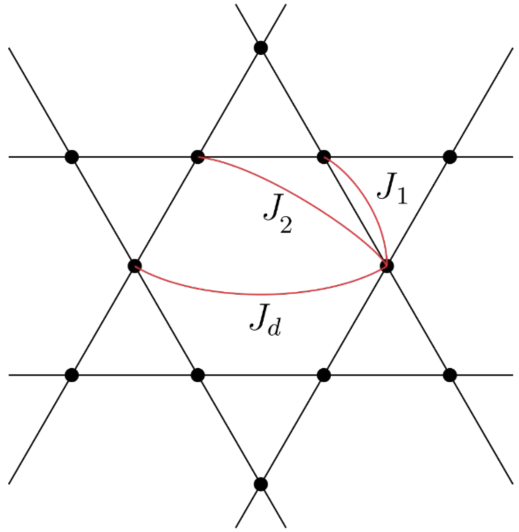
- Weak ferro Curie-Weiss temp Θ_{CW} ~ 9 K
- Farther-neighbor Heisenberg exchange: J_1 ~ -12 K, J_2 ~ -4 K, J_d ~ 16 K
- Powder samples



B. Bernu et al, PRB 87, 155107 (2013).

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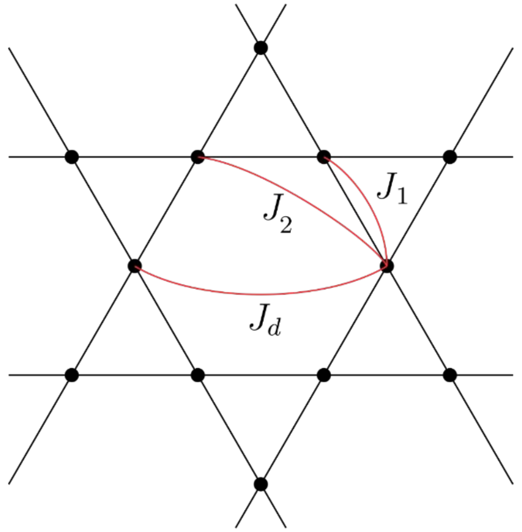

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3. Haydeeite [Zn -> Mg]

- Ferro ordering at T_C ~ 4 K
- Ferro Curie-Weiss temp Θ_{CW} ~ 25 K
- Powder samples

- Spin-waves to neutron scattering fits: J_1 ~ -38 K, J_2 ~ 0, J_d ~ 11 K
- Small/neglible DM interaction

D. Boldrin, **SB** et al, PRB 91, 220408(R) (2015)

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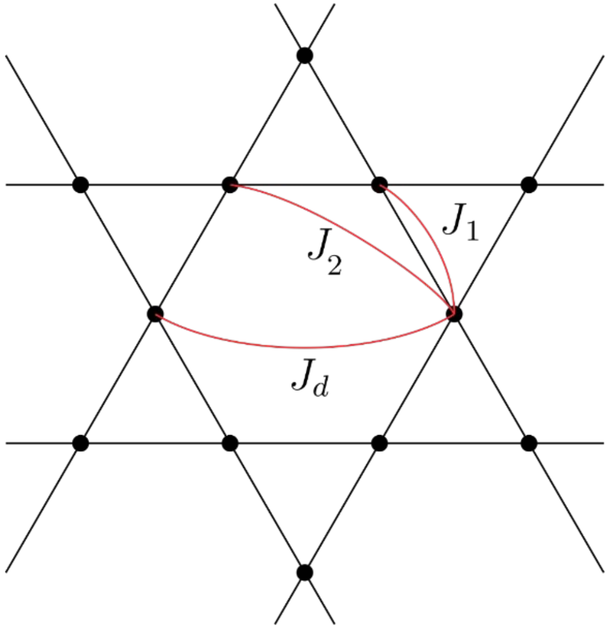

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E. Kermarrec et al, PRB 90, 205103 (2014).

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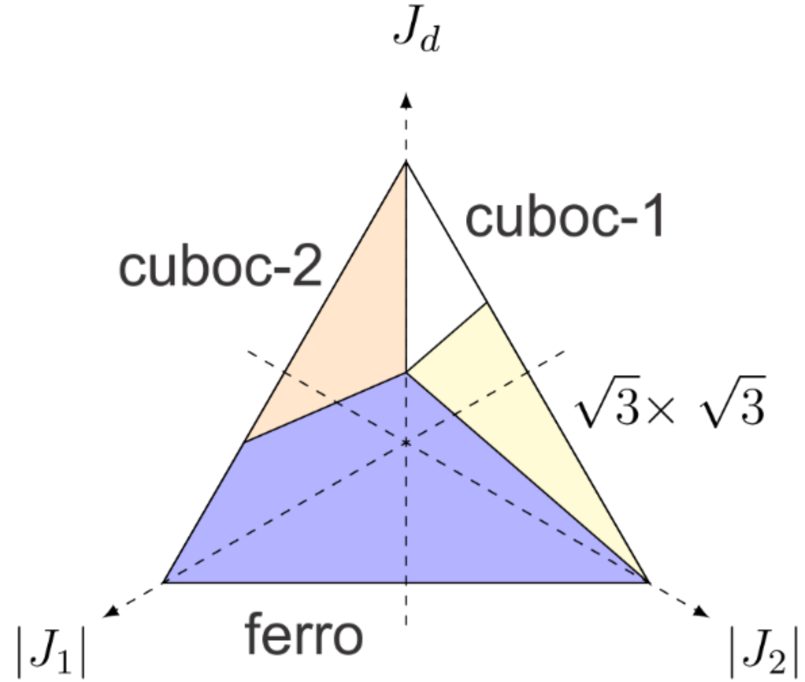
$$H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_d \sum_{\langle i,j \rangle_d} \mathbf{S}_i \cdot \mathbf{S}_j$$

➡ Evidence for a gapless ground state with unbroken spin rotation & lattice translation (quantum spin liquid)

Phase diagram of *classical* J_1-J_2-J_d Kagome Heisenberg model



$$|J_1|+|J_2|+J_d = 1$$

$$J_1 < 0,\ J_2 < 0,\ J_d > 0$$

Messio, Lhuillier, Misguich, PRB 83, 184401 (2011).

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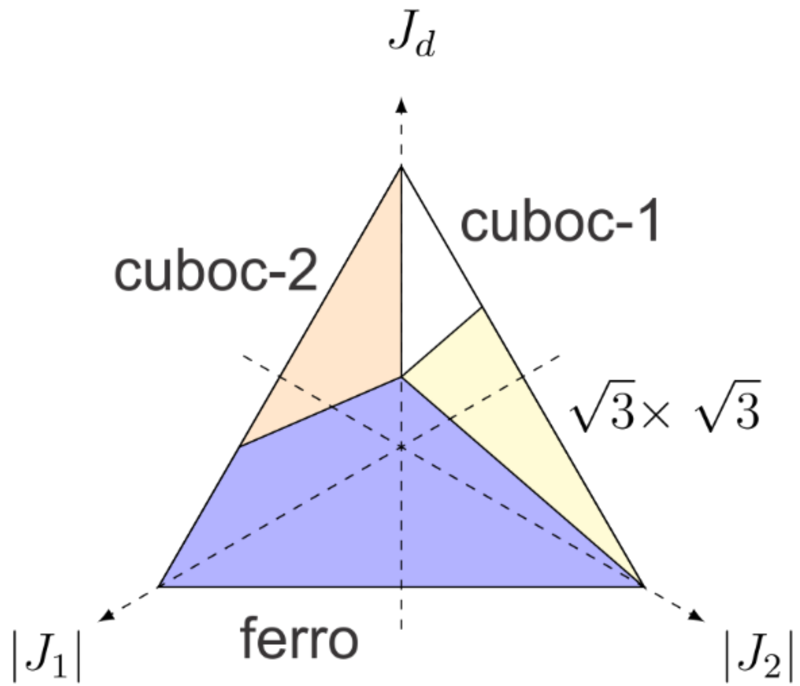

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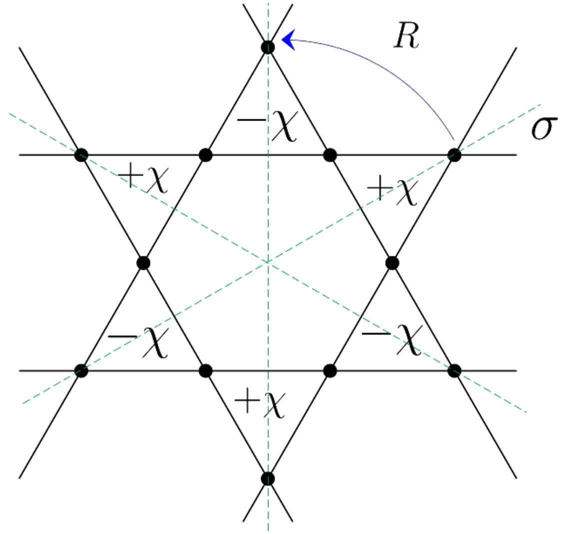
cuboc-1,-2: non-planar spin order with $\chi = \boldsymbol{S}_1\cdot(\boldsymbol{S}_2 \times \boldsymbol{S}_3) \neq 0$
12 site unit cell

Spontaneous breaking of time-reversal, (up to) lattice reflections and lattice rotations



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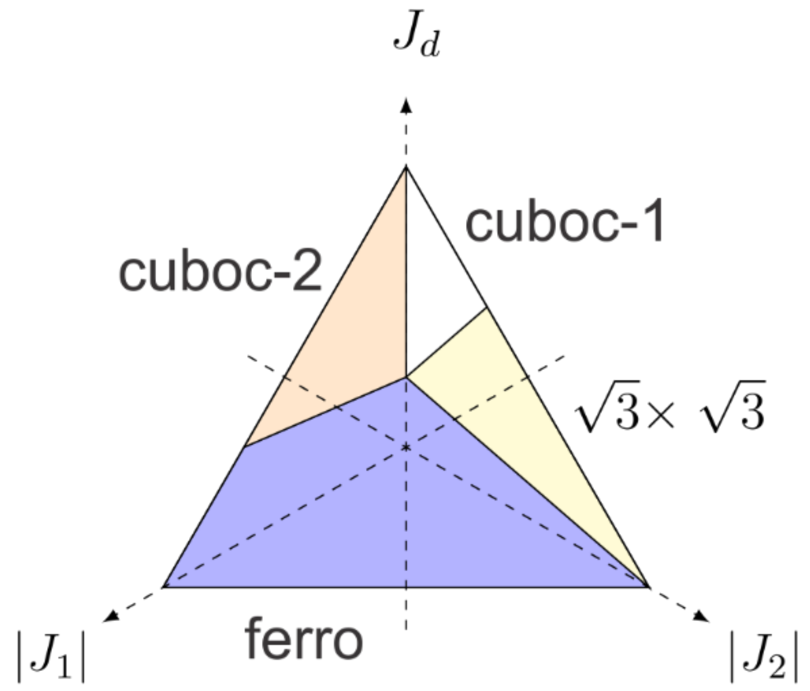

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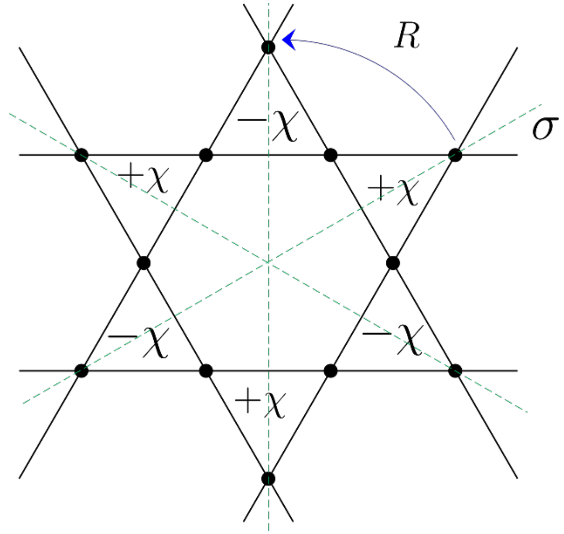


What happens in the case of quantum spin S=1/2?

Is the elusive chiral spin liquid realized in Kapellasite?

Kalmeyer and Laughlin, PRL 59, 2095 (1987).

Wen, Wilczek, Zee, PRB 39, 11413 (1989).

Yang, Warman, Girvin, PRL 70, 2641 (1993).

Construction & Classification of Chiral Spin Liquids

1. Fractionalization of spin into spinons f_α , carrying ΔS = 1/2 (magnons ΔS=1)
(f_α : spinon/"Abrikosov fermion" creation operator)

spinon doublet: $\boldsymbol{f} = (f_\uparrow, f_\downarrow)^T$ $2S_a = \boldsymbol{f}^\dagger \sigma_a \boldsymbol{f}$ $\boldsymbol{S}^2 = \frac{3}{4} n[2-n]$

enlarged local Hilbert space:

$\{|\uparrow\rangle, |\downarrow\rangle\} \Rightarrow \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$ constraint/physical subspace: $n = \boldsymbol{f}^\dagger \boldsymbol{f} \equiv 1$

gauge doublet: $\boldsymbol{\psi} = (f_\uparrow, f_\downarrow^\dagger)^T$ $2G_a = \boldsymbol{\psi}^\dagger \sigma_a \boldsymbol{\psi}$ constraint: $G_a = 0$

gauge transformation: $\boldsymbol{\psi} \mapsto g\boldsymbol{\psi}, \; g \in \mathrm{SU}(2)$: leaves spin S_a invariant

Affleck et al, PRB 38, 745 (1988).
Marston et al, PRB 39, 11538 (1989).

⇨ emergent local SU(2) (gauge) symmetry
in enlarged spinon Hilbert space

$$\boldsymbol{\psi} = (f_\uparrow, f_\downarrow^\dagger)^T$$

$$\boldsymbol{\psi} \mapsto g\boldsymbol{\psi}, \; g \in \mathrm{SU}(2)$$

Projective symmetry group: How can actual symmetries be represented in spinon space?

X.-G. Wen, PRB 65, 165113 (2002).

e.g. time-reversal: $\Theta(\boldsymbol{\psi}) = \varepsilon\boldsymbol{\psi}^* \xrightarrow{g_\Theta = \varepsilon^T} \boldsymbol{\psi}^*$ $\qquad \varepsilon = i\sigma_2$

$$H = \sum_{ij} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \qquad 2S_a = \boldsymbol{f}^\dagger \sigma_a \boldsymbol{f}$$

+ approximation scheme

⇨ Quadratic spinon Hamiltonian (= singlet "ansatz")

$$H_0 = \sum_{ij} \xi_{ij} f^\dagger_{i\alpha} f_{j\alpha} + \Delta_{ij} f_{i\uparrow} f_{j\downarrow} + \text{h.c.} = \sum_{ij} \boldsymbol{\psi}^\dagger_i u_{ij} \boldsymbol{\psi}_j + \text{h.c.} \qquad \boldsymbol{\psi} = (f_\uparrow, f^\dagger_\downarrow)^T \quad u_{ij} = \begin{pmatrix} \xi_{ij} & \Delta_{ij} \\ \Delta^*_{ij} & -\xi^*_{ij} \end{pmatrix}$$

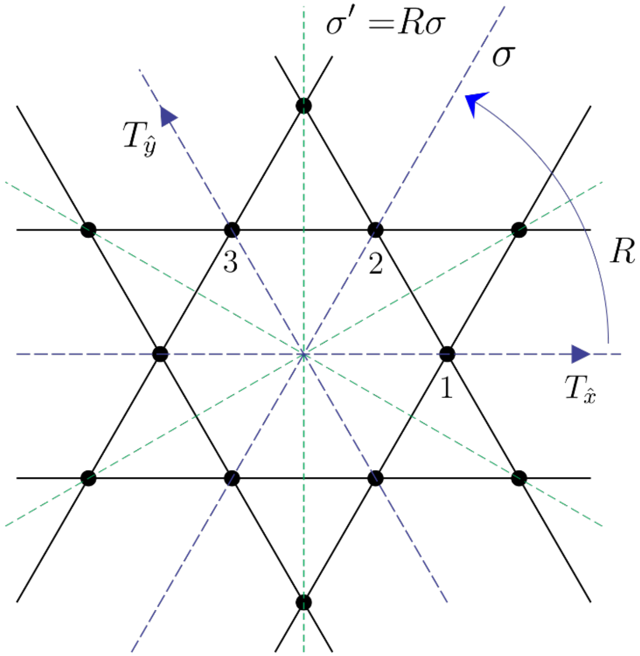
"Ansatz": $u = \{u_{ij}\}$

Symmetries: $\mathrm{SG}_{\tau_\sigma,\tau_R} = \{T_{\hat{x}}, T_{\hat{y}}, \sigma\Theta^{\tau_\sigma}, R\Theta^{\tau_R}\}$ (+ spin rot)

$\tau_R = 0, \tau_\sigma = 0$: Symmetric QSL

$\tau_R = 0, \tau_\sigma = 1$: "Kalmeyer-Laughlin" CSL

$\tau_R = 1$: Staggered-flux CSL



Interpretations/uses of $H_0(u)$:

1. Low-energy effective theory;

   Invariant gauge group (IGG_u): U(1) [$f_j \mapsto e^{i\varphi} f_j$] or $\mathbb{Z}_2$ [$f_j \mapsto -f_j$]

2. Self-consistent saddle point of H

3. Tool to construct variational spin w.f. by Gutzwiller projection (VMC): $|\psi\rangle = \prod_j n_j[2-n_j] |\psi_0\{u_{ij}\}\rangle$

Gauge-invariant characterization of ansatz $u = \{u_{ij}\}$; $u_{ij} \mapsto g_i u_{ij} g_j^\dagger$ $g_j \in \mathrm{SU}(2)$

SU(2) gauge flux: $P_1^{\mathcal{C}} = \prod_{\mathcal{C}} u_{ij} = u_{12} u_{23} \ldots u_{q1}$ $P_j \mapsto g_j P_j g_j^\dagger$

Lee, Nagaosa, Wen, RMP 78, 17 (2006).

$$\mathrm{Tr} P_j = \begin{cases} \cos\theta, & q \ \text{ even,} \\ i\sin\theta, & q \ \text{ odd.} \end{cases}$$

flux angle θ

Spin order parameter?

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flux angle θ

Spin order parameter?

$$u_{ij} \sim \langle \Psi_i \Psi_j^\dagger \rangle \qquad \Psi = (\boldsymbol{\psi}, \epsilon\boldsymbol{\psi}^*) = \begin{pmatrix} f_\uparrow & f_\downarrow \\ f_\downarrow^\dagger & -f_\uparrow^\dagger \end{pmatrix}$$

flux operator: $\hat{P}_1^{\mathcal{C}} = \prod_{\mathcal{C}} \Psi_i \Psi_j^\dagger$ $\mathrm{Tr}[:\hat{P}_1:] = -\mathrm{Tr}[\,\underline{S}_1 \underline{S}_2 \dots \underline{S}_q]$ $\underline{S} = S^a \sigma_a$

$$q = 3 \ : \qquad \mathrm{Tr}[:\hat{P}_1:] = i\,\boldsymbol{S}_1 \cdot (\boldsymbol{S}_2 \wedge \boldsymbol{S}_3)$$

Projective symmetry group (PSG)

1. Algebraic PSG: Classes of representations of the symmetry group SG in the gauge group $\mathcal{G}=\{g\},\ g=\otimes g_j\ , g_j\ \in\mathrm{SU}(2)$

$$Q\colon \mathrm{SG} \mapsto \mathcal{G}$$
$$x \mapsto g_x$$

Equivalence of reps:

$$Q^1 \sim Q^2 \iff \exists g \in \mathcal{G}\ \text{ s.t. } Q^1 = gQ^2g^\dagger$$

Algebraic relations in SG respected *up to IGG*, e.g.: $\sigma^2 = 1 \implies g_\sigma(\boldsymbol{r})g_\sigma(\sigma\boldsymbol{r}) \in \mathrm{IGG}\ \{\pm 1\}$

IGG: Invariant Gauge Group
(here: $\mathbb{Z}_2$ classification)

2. Invariant PSG: Ansatz u respecting SG for each PSG class

action of symmetry x on ansatz : $Q_x(u_{ij}) = (-)^{\tau_x} g_x(i) u_{x^{-1}(ij)} [g_x(j)]^\dagger$

$$Q_x(u) = u \qquad \text{for all } x \text{ in SG}$$

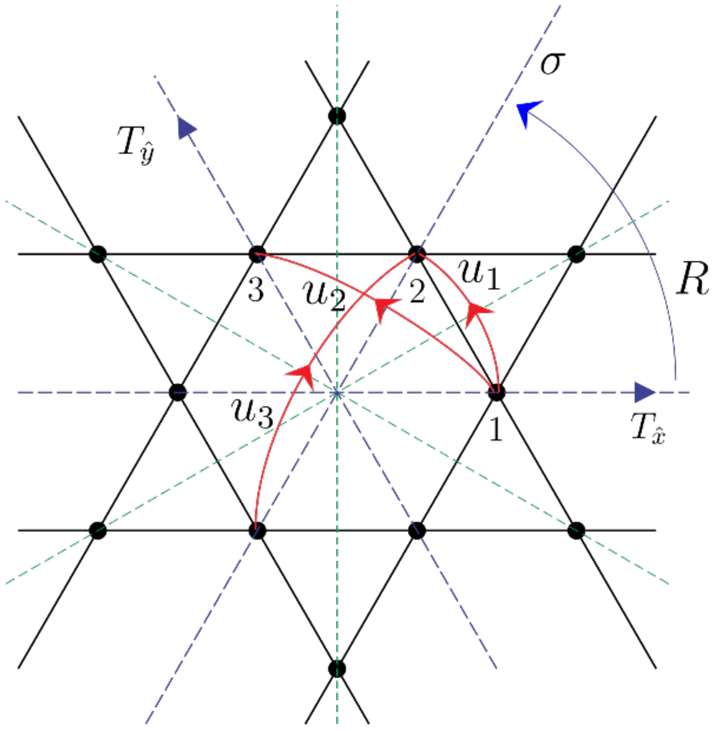
Projective symmetry group (PSG): Kagome

Symmetries: $\mathrm{SG}_{\tau_\sigma,\tau_R} = \{T_{\hat{x}}, T_{\hat{y}}, \sigma\Theta^{\tau_\sigma}, R\Theta^{\tau_R}\}$

$$g_x = \mathbb{1}_2$$
$$g_y = (\epsilon_2)^x \mathbb{1}_2$$
$$g_\sigma(x,y) = (\epsilon_2)^{xy} g_\sigma$$
$$g_R(x,y) = (\epsilon_2)^{xy+y(y+1)/2} g_R$$

$$\epsilon_2 = \pm 1$$

no.	g_σ	g_R	ϵ_σ	$\epsilon_{R\sigma}$	ϵ_R	sym
1	$\mathbb{1}_2$	$\mathbb{1}_2$	$+$	$+$	$+$	SU(2)
2	$i\sigma_3$	$\mathbb{1}_2$	$-$	$-$	$+$	U(1)
3	$\mathbb{1}_2$	$i\sigma_3$	$+$	$-$	$-$	U(1)
4	$i\sigma_3$	$i\sigma_3$	$-$	$+$	$-$	U(1)
5	$i\sigma_2$	$i\sigma_3$	$-$	$-$	$-$	$\mathbb{Z}_2$



⇨ 10 PSG classes on Kagome

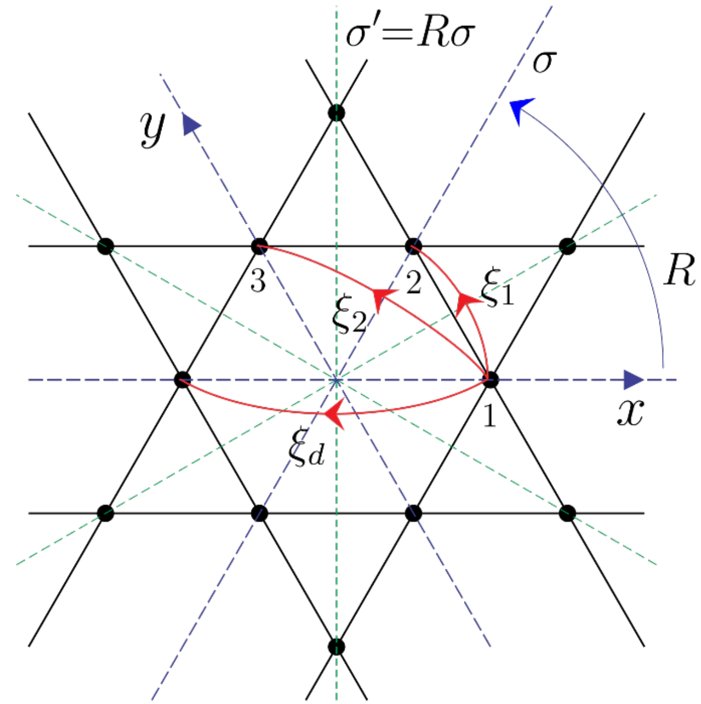
List of U(1) chiral spin liquids resulting from PSG construction

no	τ_σ	τ_R	ϵ_2	g_σ	g_R	β_1	β_2	β_d	Description
1	0	0	+	$\mathbb{1}_2$	$\mathbb{1}_2$	0	0	0	large Fermi surface
2	0	0	−	$\mathbb{1}_2$	$\mathbb{1}_2$	0	0	x	Dirac spect. [1]
3	1	1	+	$\mathbb{1}_2$	$\mathbb{1}_2$	0	$\pi/2$	x	triangular FS
4	1	1	+	$i\sigma_2$	$i\sigma_2$	0	β_2	0	large FS
5	1	1	−	$\mathbb{1}_2$	$\mathbb{1}_2$	0	$\pi/2$	0	Dirac spectrum
6	1	1	−	$i\sigma_2$	$i\sigma_2$	0	β_2	x	FS/Dirac
7	0	1	+	$\mathbb{1}_2$	$\mathbb{1}_2$	$\pi/2$	0	$\pi/2$	triangular FS
8	0	1	+	$\mathbb{1}_2$	$i\sigma_2$	β_1	0	β_d	large FS
9	0	1	−	$\mathbb{1}_2$	$\mathbb{1}_2$	$\pi/2$	0	x	kagome FS
10	0	1	−	$\mathbb{1}_2$	$i\sigma_2$	β_1	0	x	FS/Dirac
11	0	1	−	$i\sigma_2$	$\mathbb{1}_2$	β_1	x	0	Dirac spectrum
12	1	0	+	$i\sigma_2$	$\mathbb{1}_2$	β_1	β_2	0	large FS
13	1	0	−	$i\sigma_2$	$i\sigma_2$	$\pi/2$	β_2	$\pi/2$	CSL A
14	1	0	−	$\mathbb{1}_2$	$i\sigma_2$	β_1	$\pi/2$	β_d	CSL B
15	1	0	−	$i\sigma_2$	$\mathbb{1}_2$	β_1	β_2	$\pi/2$	fully gapped [2]

Algebraic PSG : $g_x = \mathbb{1}_2;\ \ g_y = (\epsilon_2)^x \mathbb{1}_2;\ \ g_\sigma;\ \ g_R$

Invariant PSG : $\xi_1 = \rho_1\, e^{i\beta_1}$; $\xi_d = \rho_d\, e^{i\beta_d}$

$\xi_2 = \rho_2\, e^{i\beta_2}$ x $\Rightarrow \xi = 0$



[1] Ran et al, PRL 98, 117205 (2007)

[2] Hastings, PRB 63, 014413 (2000); Marston and Zeng, JAP 69, 5962 (1991)

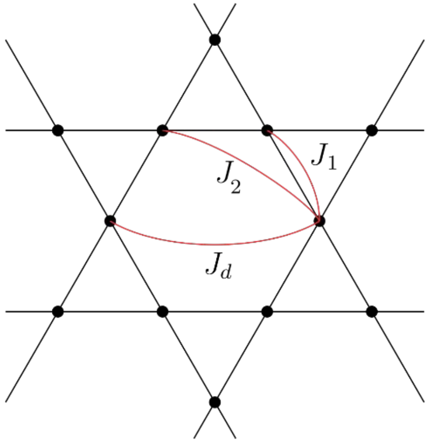
Phase diagram

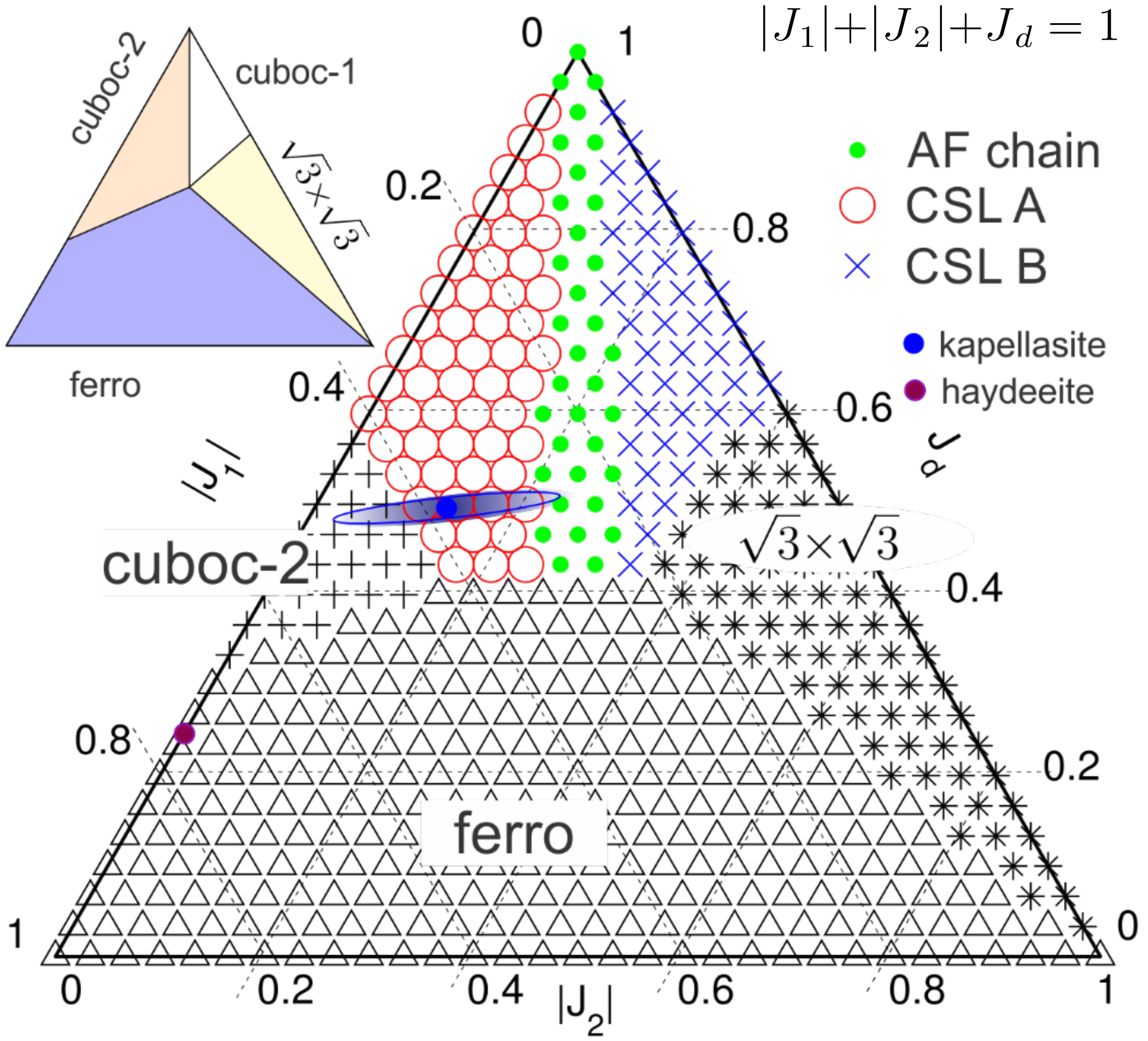
Comparison of projected U(1) CSL w.f.

$$|\psi\rangle = \prod_j n_j[2-n_j]|\psi_0\rangle$$

with correlated Neel states

$$|\mathrm{Neel}\rangle = \exp\{\sum_{ij} \mathcal{J}_{ij} S_i^z S_j^z\} \prod_k |S_k\rangle$$





Spin model

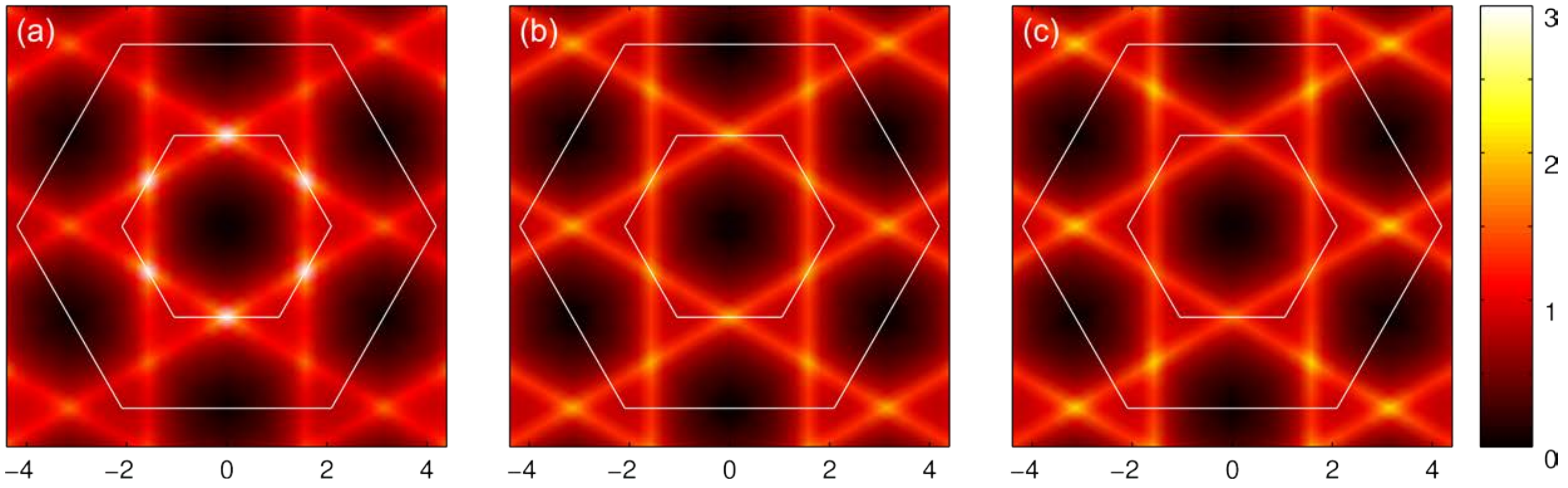
$$H = J_1 \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j\rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_d \sum_{\langle i,j\rangle_d} \mathbf{S}_i \cdot \mathbf{S}_j$$

with $J_1 < 0,\ J_2 < 0,\ J_d > 0$

Physical properties of QSL phases

Static structure factor S(q)

CSL A   quasi 1D phase   CSL B



+ gapless continuum of spin ex

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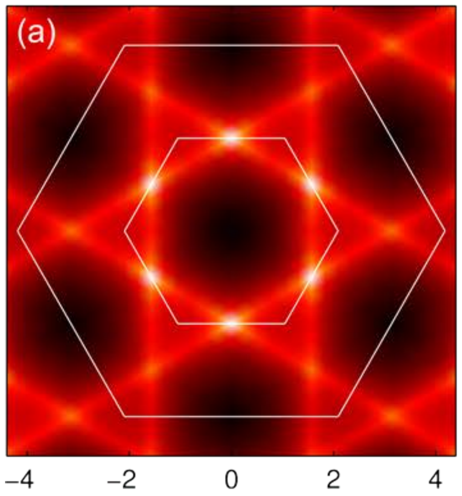

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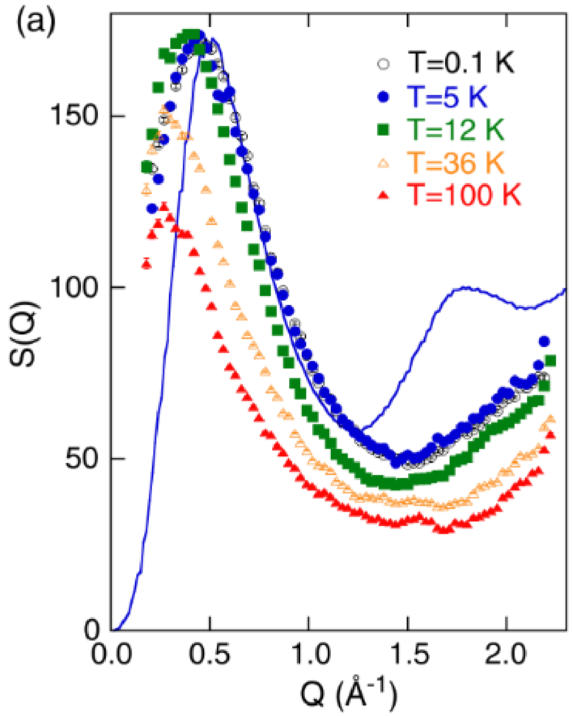

B. Fåk et al, PRL 109, 037208 (2012).

Conclusions & outlook

- PSG classification for Kagome
- Exhaustive list of fermionic CSL states
- Variational phase diagram of physically relevant Heisenberg model
- "CSL A" consistent with neutron scattering on Kapellasite
- Interesting dimensional crossover 1D to 2D
- Further directions: chiral Z_2 liquids, AF J_1-J_2 (Herbertsmithite), …
- PSG classifications for triangular, honeycomb, ...

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Thank you!

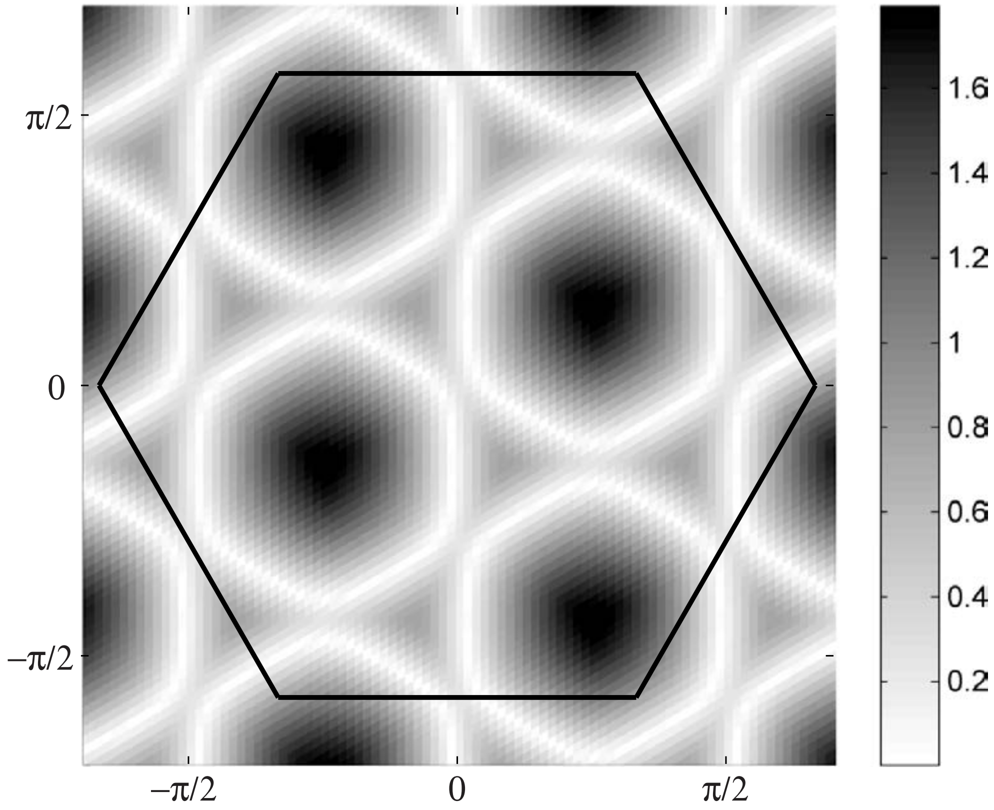

L. Messio


B. Bernu

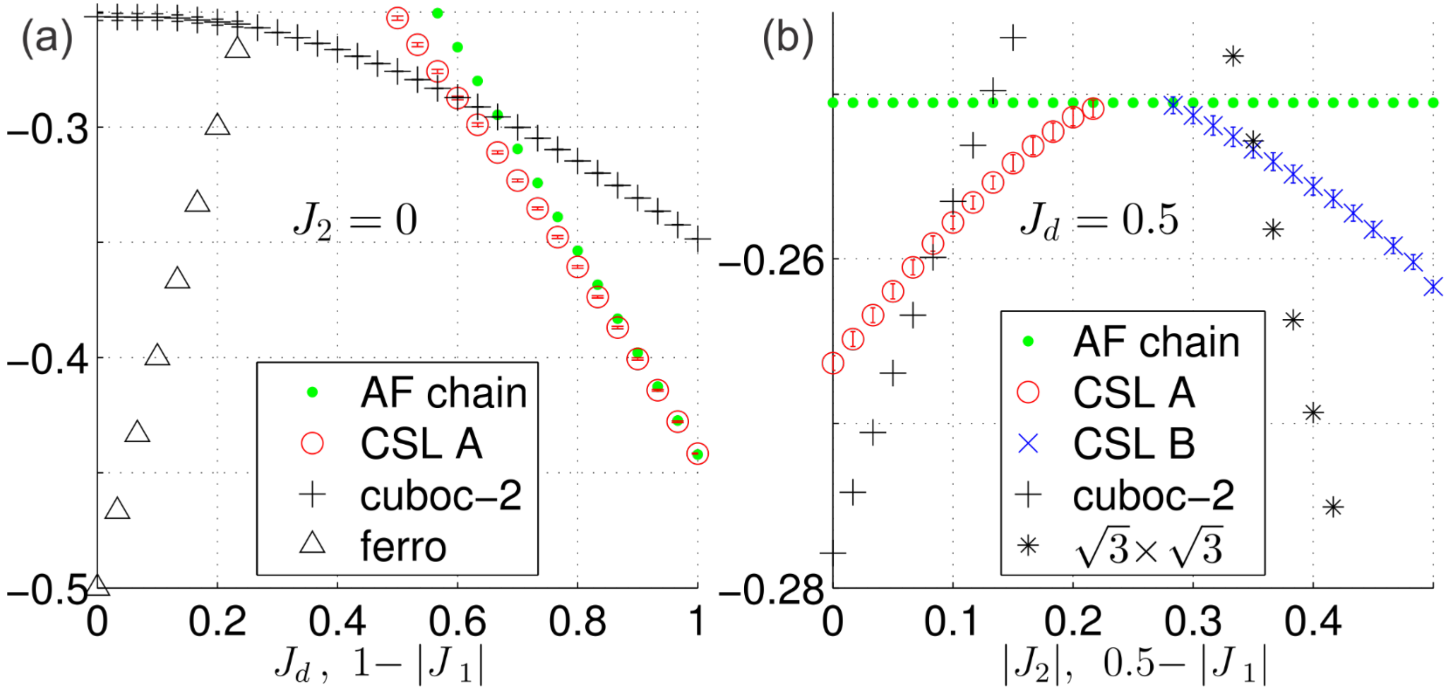

B. Fåk


C. Lhuillier

Spinon spectrum in CSL A (lowest band)



Variational energies

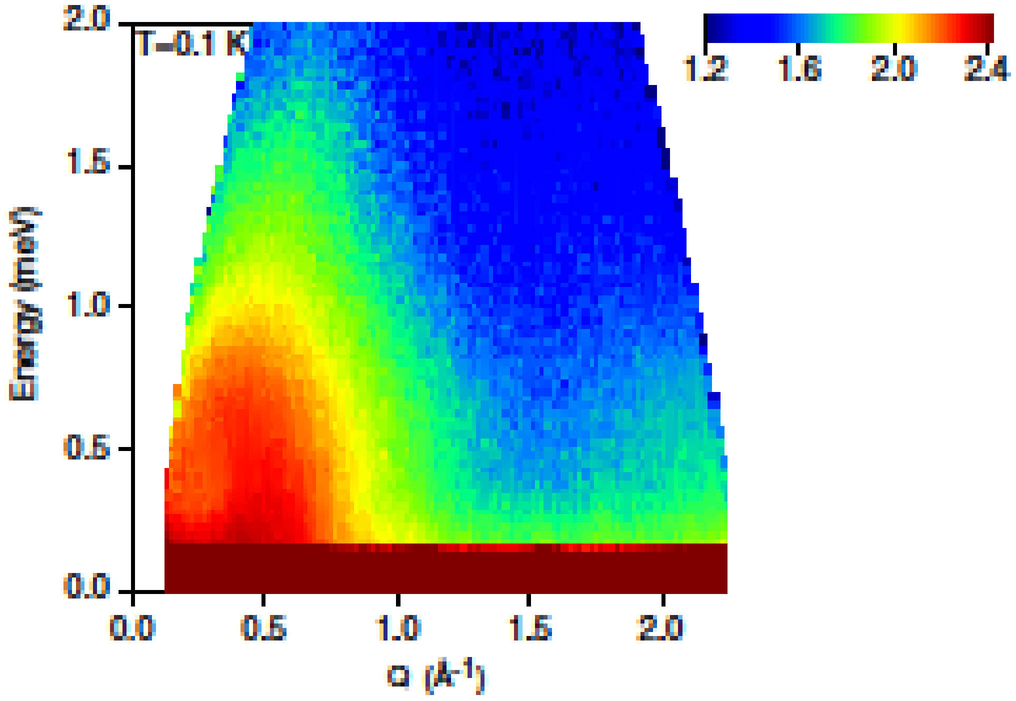


Kapellasite

- Neutron scattering: continuum of low-energy excitations
- Absence of frozen moments (muon SR, NMR)
- No transition down to 20 mK

R. H. Colman et al, Chem. Mater. 20, 6897 (2008); 22, 5774 (2010).

E. Kermarrec et al, PRB 90, 205103 (2014).



→ Evidence for a gapless ground state with unbroken spin rotation & lattice translation (quantum spin liquid)

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Kapellasite

Farther-neighbor spin exchange interactions

R. H. Colman et al, C.M. 20, 6897 (2008); 22, 5774 (2010).

O. Janson at al, PRL 101, 106403 (2008).

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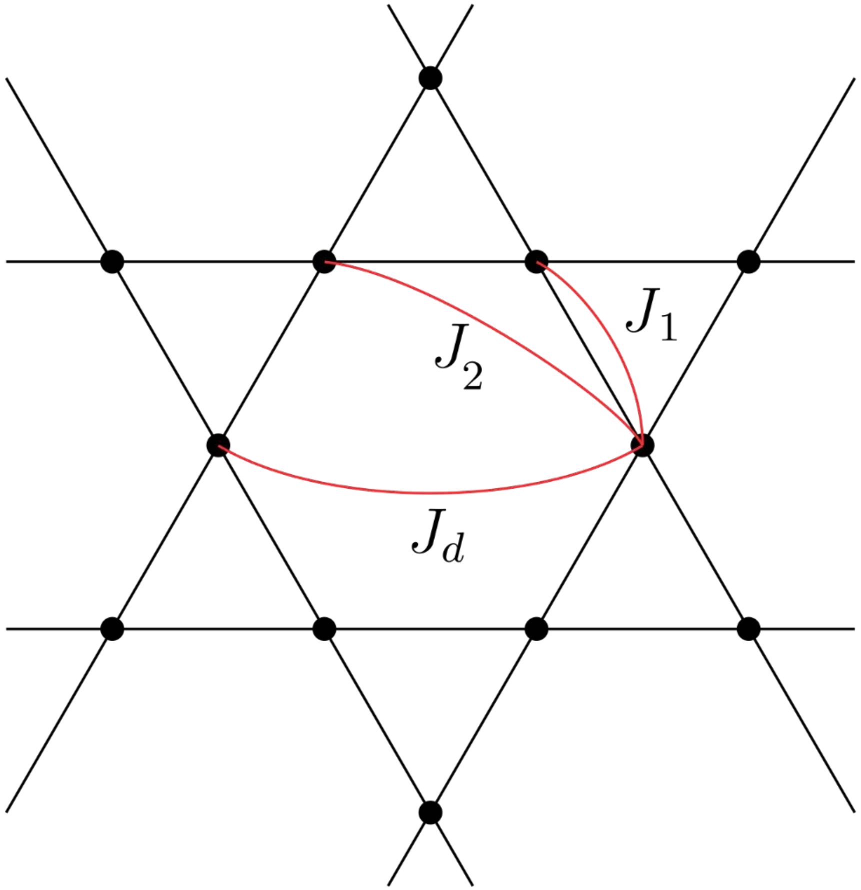


$$H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_d \sum_{\langle i,j \rangle_d} \mathbf{S}_i \cdot \mathbf{S}_j$$

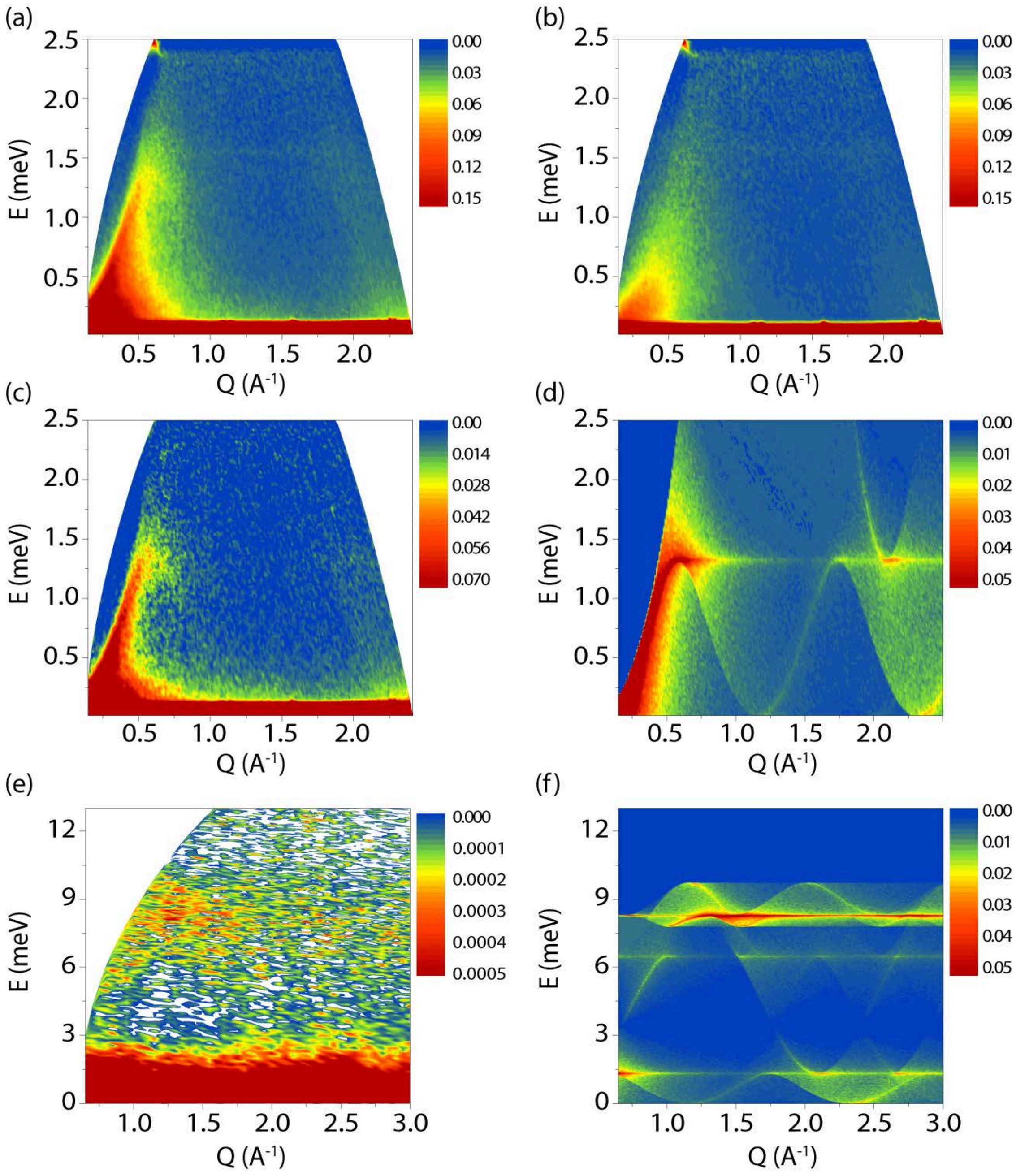
High-T series expansion, and fits to C_v and χ:

B. Fak et al, PRL 109, 037208 (2012).
B. Bernu et al, PRB 87, 155107 (2013).

$$J_1 \simeq -12K$$
$$J_2 \simeq -4K$$
$$J_d \simeq +16K$$

Haydeeite

neutron scattering



Projective symmetry group (PSG)

local SU(2) symmetry in $H_0 = \sum_{ij} \psi_i^\dagger u_{ij} \psi_j + \mathrm{h.c.}$ or $|\{u_{ij}\}\rangle$

gauge doublet: $\psi = (f_\downarrow, f_\uparrow^\dagger)^T$

gauge transformation: $\psi \mapsto g\psi,\ g \in \mathrm{SU}(2)$

1. Representation of a symmetry X in spinon Hilbert space: $X\colon \Psi(\boldsymbol{r}) \mapsto g_X \Psi(X\boldsymbol{r})$
(time reversal, lattice translation, -rotation, -reflections)

Algebraic relations must be respected up to IGG, e.g.: $\sigma^2 = 1 \Longrightarrow g_\sigma(\boldsymbol{r}) g_\sigma(\sigma\boldsymbol{r}) \in \mathrm{IGG}\ \{\pm 1\}$

Algebraic PSGs $\{g_X\}$ are classes of symmetry representations (equiv. under gauge transformations)

2. Invariant PSG - quadratic phases H_0 respecting symmetries in given representation: $X(H_0) = H_0$

Here: modulo time reversal Θ for the point group:
➔ spin rotation, lattice translation, reflection $\sigma\Theta^{\tau_\sigma}$, rotation $R\Theta^{\tau_R}$, $\tau_\sigma, \tau_R \in \{0,1\}$

$\Longrightarrow$ Exhaustive classification of chiral spin liquids
(with fermionic fractionalization)

Analog "Schwinger boson" construction: Messio et al, PRB 87, 125127 (2013); Wang et al, PRB 74, 174423 (2006).

spin rotation: $\boldsymbol{f} \mapsto U\boldsymbol{f},\ U \in \mathrm{SU}(2)$: leaves G_a invariant (singlet)