Projective Symmetry Group Classification of Chiral Spin Liquids
New Kagome Materials and farther-neighbor Spin Models

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Abstract

Frustrated low-dimensional quantum spin systems – such as the kagome antiferromagnet – can exhibit highly unusual physical properties at low temperature. In recent years, materials science has managed to create new spin $S = 1/2$ kagome quantum magnets with farther-neighbor exchange interactions. From a theoretical perspective, this is interesting since – at the classical level – it can lead to non-planar spin orders, and spontaneous breaking of time-reversal symmetry. In the quantum limit, exotic chiral spin liquids may emerge in such systems.

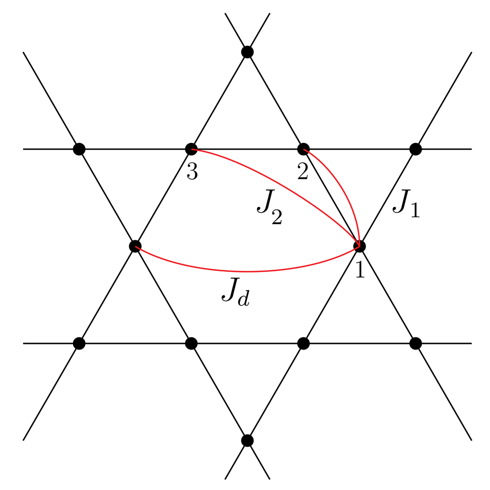
Motivated by these developments, we perform an exhaustive projective symmetry group (PSG) classification of chiral $\mathbb{Z}_2$ quantum spin liquids (QSLs) with fermionic spinons on kagome and triangular lattices. We use variational Monte Carlo to investigate the energetic competitiveness of the subset of U(1) phases in extended kagome Heisenberg models, and we identify some of the classified spin liquids as ground state candidates. Our theoretical results are relevant to recent experiments.

Motivation and Experiments

Recently investigated model compounds for spin $S = 1/2$ quantum magnetism on the kagome lattice:

- *Herbertsmithite* ($ZnCu_3(OH)_6Cl_2$) [4, 5]: Strong first-neighbor $J_1 \simeq 200$ K + potentially weak perturbations (DM, J_2, etc). Clearly a QSL, but of controversial nature [gapped $\mathbb{Z}_2$, gapless U(1)], both experimentally and numerically [6, 7].
- *Kapellasite* (polymorph) [8, 9]: No ordering observed (unbroken spin rot.) down to low temp, but $\Theta_{CW} = +10$ K (!); gapless triplet excitations. Dominant anti-ferro exchange across the hexagon diagonals ($J_d = 16$, $J_1 = -12$; $J_2 = -4$ K).
- *Haydeeite* (Zn↦Mg) [3]: Ordering $T_C = 4$, $J_d = 11$, $J_1 = -38$ K; $J_2 \simeq 0$. Kagome ferromagnet with DM $\simeq 0$.
- others: Vanadite, Vesignieite, ...

Heisenberg model describing magnetism in these spin-1/2 materials:



$$H = \sum_{i,j} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \qquad (1)$$

Figure 1: Farther-neighbor exchange interactions on the kagome lattice

Phase diagram of classical spin model with interactions of Fig. 1:

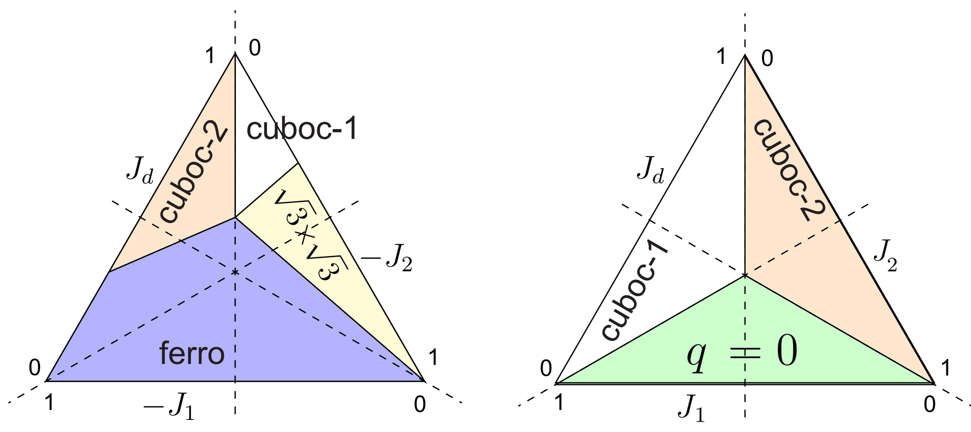


Figure 2: Ternary phase diagrams of classical kagome Heisenberg model within *regular magnetic orders* [10]; $J_d + |J_1| + |J_2| = 1$. Left: $J_1, J_2 \leq 0$, $J_d \geq 0$ (J_1, J_2 ferro); Right: $J_1, J_2, J_d \geq 0$ (all anti-ferro).

Regular $q = 0$ and $\sqrt{3} \times \sqrt{3}$ are *coplanar* spin orders; "cuboc-1" and "cuboc-2" are *non-coplanar* with 12-site cell, $\chi = \boldsymbol{S}_1 \cdot (\boldsymbol{S}_2 \times \boldsymbol{S}_3) \neq 0$.

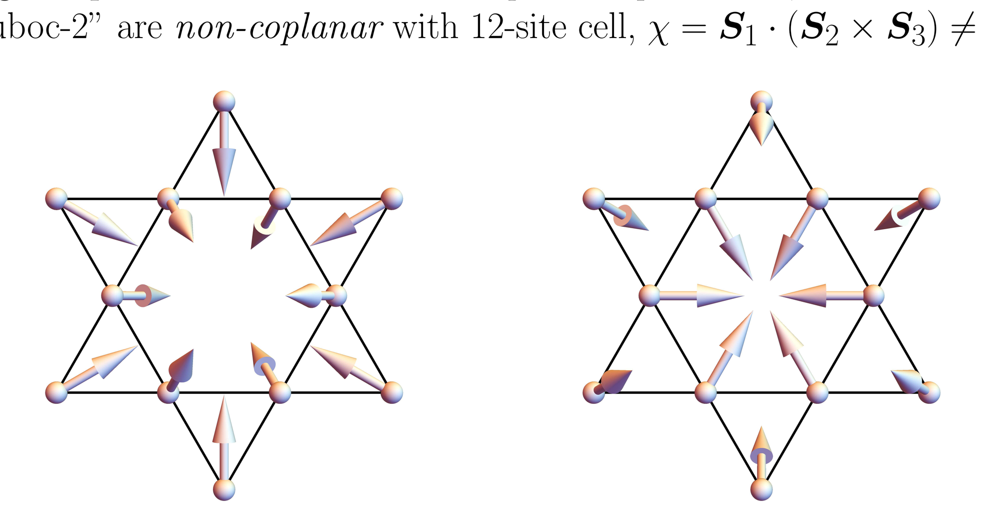


Figure 3: Classical spin ordering of type cuboc-1 (left) and cuboc-2 (right).

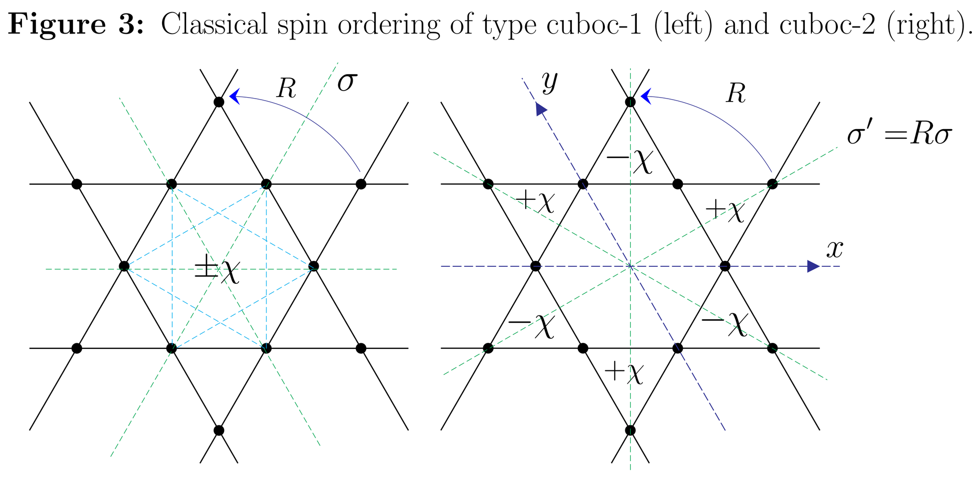


Figure 4: Scalar chirality in cuboc-1 (left) and cuboc-2 (right).

Projective Symmetry Group (PSG)

Spin fractionalization, using "parton construction" [11] for spin-1/2,

$$2S_a = \boldsymbol{f}^\dagger \sigma_a \boldsymbol{f}\,, \qquad (2)$$

$\boldsymbol{f} = (f_\uparrow, f_\downarrow)^T$ fermionic (Abrikosov) spinon operators, σ_a are Pauli matrices. Enlarged local Hilbert space: $\{\uparrow, \downarrow\} \to \{0, \uparrow, \downarrow, \uparrow\downarrow\}$, constraint

$$2G_a = \boldsymbol{\psi}^\dagger \sigma_a \boldsymbol{\psi} \equiv 0\,, \qquad (3)$$

where $\boldsymbol{\psi} = (f_\uparrow, f_\downarrow^\dagger)^T$ is a "gauge doublet". E.g., $G_z = n_\uparrow + n_\downarrow - 1 \equiv 0$.

Fractionalization entails emergent SU(2) gauge symmetry in the enlarged spinon Hilbert space,

$$\boldsymbol{\psi} \mapsto g\boldsymbol{\psi}\,, \qquad (4)$$

with $g \in$ SU(2), leaves the spin $\boldsymbol{S}$ invariant, while $\boldsymbol{G}$ transforms as a vector. Similarly, $\boldsymbol{f} \mapsto U\boldsymbol{f}$ rotates the spin, leaving $\boldsymbol{G}$ invariant (singlet).

Substituting Eq. (2) into a spin model (1), one still needs to decouple quartic terms, e.g., by path integral/Hubbard-Stratonovich. Saddle points are quadratic spinon Hamiltonians,

$$H_0 = \sum_{i,j} \boldsymbol{\psi}_i^\dagger u_{ij} \boldsymbol{\psi}_j + \text{H.c.} + \sum_j \lambda_j^a \boldsymbol{\psi}_j^\dagger \sigma_a \boldsymbol{\psi}_j\,, \qquad (5)$$

with $\boldsymbol{\lambda}_j$ Lagrange multipliers, matrices $u_{ij} = u_{ij}^\mu \tau_\mu$, $(\tau_\mu) = (i\mathbb{1}_2, \sigma_a)$, and $u_{ij}^\mu \in \mathbb{R}$ for singlet spin liquids ($u_{ij}^\mu \in i\mathbb{R}$ for triplets), and $u_{ij} = u_{ji}^\dagger$. The *ansatz* $u = [u_{ij}; \boldsymbol{\lambda}_j]$ transforms as

$$u_{ij} \mapsto g_i u_{ij} g_j^\dagger \qquad (6)$$

under local SU(2) (gauge) transformations $g = \otimes_j g_j \in \mathcal{G}$.

To impose symmetry (e.g., lattice translation, reflection, etc) on the effective spinon theory (5), the symmetry group SG must be *represented* in the enlarged spinon space. The representation $Q_x = (g_x, x) \in \mathcal{G} \rtimes$ SG acts on the ansatz as $u_{ij} \mapsto [Q_x(u)]_{ij} = g_x(i) u_{x^{-1}(ij)} g_x(j)^\dagger$. It must respect the group multiplication law *up to a subgroup of* $\mathcal{G}$, called the *invariant gauge group* (IGG):

$$Q_x Q_y = (g_x x g_y x^{-1}, xy) = g_e Q_{xy}\,, \qquad (7)$$

with $g_e = (g, e) \in$ IGG, $e =$ id in SG. Global signs IGG $= \mathbb{Z}_2$ are always possible (and are used here), while larger subgroups constrain the spinon theory.

Two representations $Q^{(1)}$ and $Q^{(2)}$ of SG are equivalent, if there is a pure gauge $g_e = (g, e)$ relating them:

$$Q^{(1)} \sim Q^{(2)} \Leftrightarrow \exists\, g_e \text{ s.t. } Q^{(1)} = g_e\, Q^{(2)} g_e^\dagger\,. \qquad (8)$$

The number of inequivalent gauge representations of a lattice space group (translation + point group) is finite and discrete. These representation classes constitute a *classification* of fractionalized quantum spin liquids. They are called *algebraic PSG*.

In *chiral spin liquids* (CSLs), we want to impose lattice symmetries *up to time-reversal*. That is, SG (e.g., for kagome lattice) is generated by

$$\text{SG} = \{T_{\hat{x}}, T_{\hat{y}}, \sigma\Theta^{\tau_\sigma}, R\Theta^{\tau_R}\}\,, \qquad (9)$$

where $T_{\hat{x},\hat{y}}$ are translations, and the point group generators R and σ are defined in Fig. 4. The time-reversal signatures $\tau_\sigma, \tau_R = 0, 1$ specify broken generators. $\tau_\sigma, \tau_R = 0$ corresponds to fully *symmetric* QSLs; $\tau_\sigma = 1, \tau_R = 0$ breaks all reflections (i.e., *Kalmayer-Laughlin* CSLs); The cases $\tau_R = 1$ have the symmetry of the two cuboc states shown in Figs. 3 and 4, leading to *staggered flux* CSL phases.

Anti-unitary *time reversal* Θ is chosen to act in spinon space as $\Theta: \boldsymbol{\psi} \mapsto \boldsymbol{\psi}^*$. For the ansatz, we therefore have $\Theta: u \mapsto -u$ (additional gauge rep. g_Θ is irrelevant in the case of chiral spin liquids).

Imposing symmetry on an ansatz u within an algebraic PSG representation Q translates to

$$u = (-)^{\tau_x} Q_x(u)\,, \qquad (10)$$

for all generators x in SG. For symmetries x leaving lattice links invariant (reflections), Eq. (10) is a constraint on u. Otherwise (e.g., for translations or rotations), it can be used to propagate u_{ij} on a given link to the entire lattice. Q and τ therefore provide a systematic and exhaustive construction of spinon theories H_0 that conserve lattice symmetries up to time reversal. They are called *invariant PSG*.

From a spinon theory Eq. (5), microscopic (chiral) spin liquid wave function are constructed by Gutzwiller projection,

$$|\psi\rangle = \prod_j (n_{j\uparrow} - n_{j\downarrow})^2 |\psi_0(u)\rangle\,, \qquad (11)$$

where $|\psi_0(u)\rangle$ is the ground state of H_0. Properties of $|\psi\rangle$ (e.g., energies) can be computed on large lattice clusters using variational Monte Carlo [12]. Optimized QSL energies are compared with those of ordered Huse-Elser states [13].

Results

We find *10* algebraic PSG representation classes for *kagome*, and *14* for *triangular* lattice: $g_{\hat{x}}(x,y) = \mathbb{1}_2$, $g_{\hat{y}}(x,y) = (\varepsilon)^x \mathbb{1}_2$, $g_\sigma(x,y) = (\varepsilon)^{xy} g_\sigma$, $g_R(x,y) = (\varepsilon)^{xy + y(y+1)/2} g_R$, with $\varepsilon = \pm 1$ (cell doubling) and g_σ, g_R given in Tables 1 and 2.

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	$i\sigma_2$	$i\sigma_3$	−	−	−	$\mathbb{Z}_2$

Table 1: Point group PSG representations for kagome and triangular lattice.

No.	g_σ	g_R	ϵ_σ	$\epsilon_{R\sigma}$	ϵ_R	sym
6	$i\sigma_2$	a	−	−	+	$\mathbb{Z}_2$
7	$i\sigma_2$	b	−	−	−	$\mathbb{Z}_2$

Table 2: Additional PSG representations for triangular lattice. $a = \exp(i\sigma_3\pi/3)$ and $b = \exp(i\sigma_3\pi/6)$.

For the algebraic PSG in Tables 1 and 2, and all signatures τ in (9), we construct corresponding chiral spinon theories and ansätze for first three neighbors. (details in [2])

The spin model (1) on the kagome lattice is investigated, using variational U(1) CSL, and correlated Néel states.

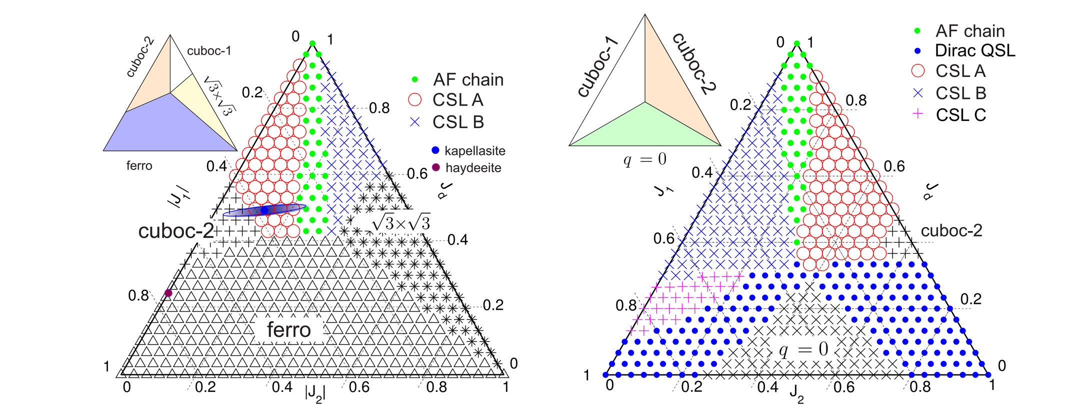


Figure 5: Ternary phase diagrams of quantum kagome Heisenberg model within Gutzwiller projected symmetric and chiral spin liquids; $J_d + |J_1| + |J_2| = 1$. Left: $J_1, J_2 \leq 0$, $J_d \geq 0$ (J_1, J_2 ferro); Right: $J_1, J_2, J_d \geq 0$ (all anti-ferro).

Fig. 5 shows that dominant J_d quickly favors a quasi-one-dimensional phase when $J_1 \sim J_2$. Otherwise, we find gapless CSLs A and B in this region (spinon Fermi surfaces). Fig. 6 displays the corresponding static spin structure factors, $S(\boldsymbol{k}) = \sum_{ij} \langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{ij}}$.

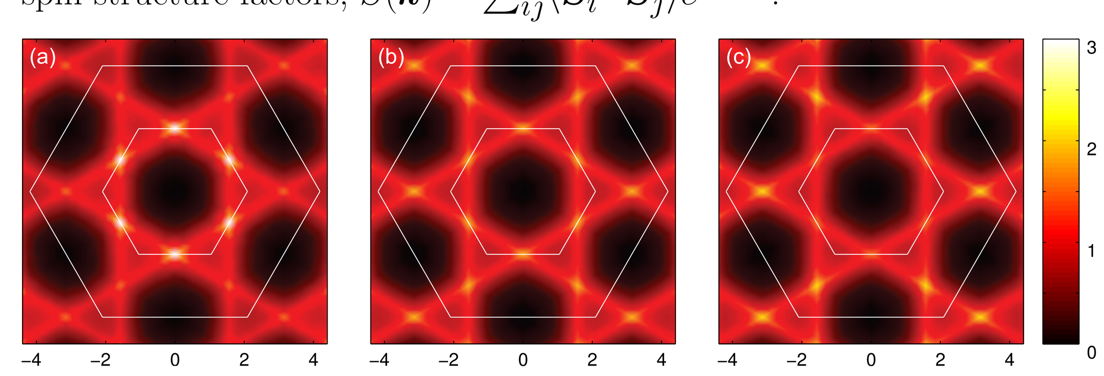


Figure 6: Spin structure factors in (a) CSL A, (b) quasi-1D phase, and (c) CSL B on the kagome lattice.

Kapellasite [9] lies in the parameter region of gapless CSL A in Fig. 5, inelastic neutron data on powder samples [8] is consistent with $S(\boldsymbol{k})$ in Fig. 6(a). Haydeeite is in the ferro region [3].

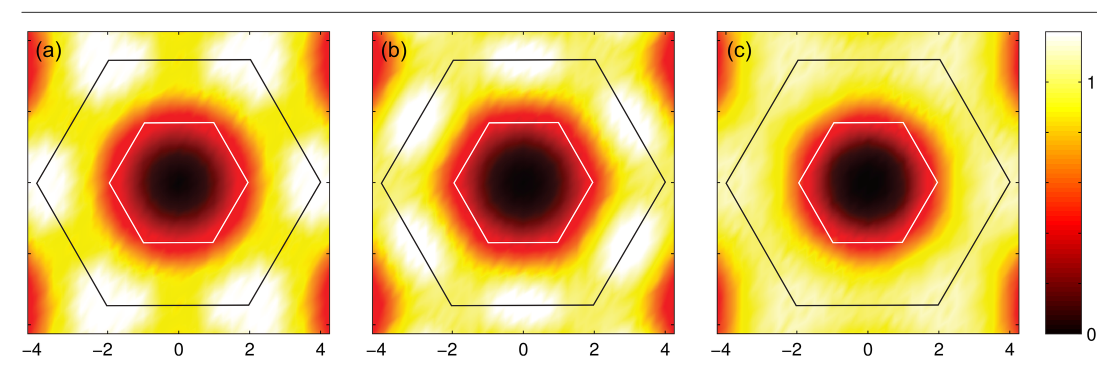


Figure 7: Spin structure factors in (a) FS QSL (No. 1 in Tab. 1, $\varepsilon = +1$, $\tau = 0$), (b) Dirac QSL (No. 1 in Tab. 1, $\varepsilon = -1$, $\tau = 0$), and (c) CSL C (No. 1 in Tab. 1, $\varepsilon = -1$, $\tau_\sigma = 1, \tau_R = 0$), first-neighbor ansätze.

Conclusion

Motivated by non-planar magnetic orders in classical Heisenberg models on extended triangular and kagome lattices, we systematically classify chiral spin liquids within the fermionic parton construction. The projective symmetry group is discussed in detail, and we extend it to chiral spin liquids. Variational quantum phase diagrams for the kagome lattice are calculated, and physical properties such as spectral functions are discussed. Our theoretical results can explain the exotic magnetism in Kapellasite, and the kagome ferromagnet Haydeeite.

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