Projective Symmetry Group Classification of Z_2 Spin Liquids in a Pyrochlore Lattice

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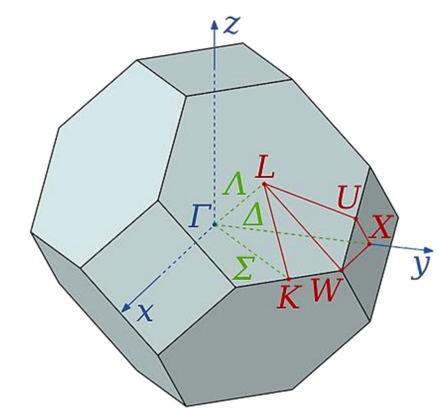
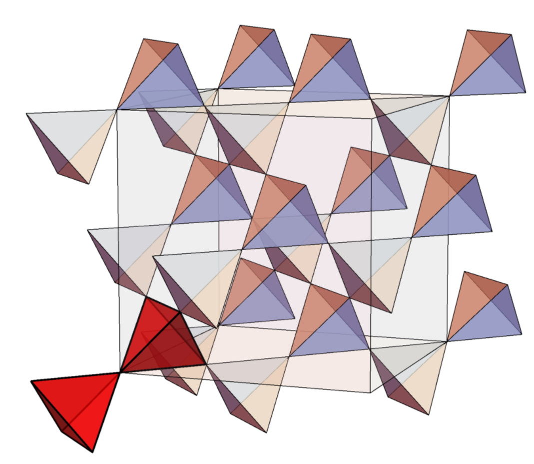
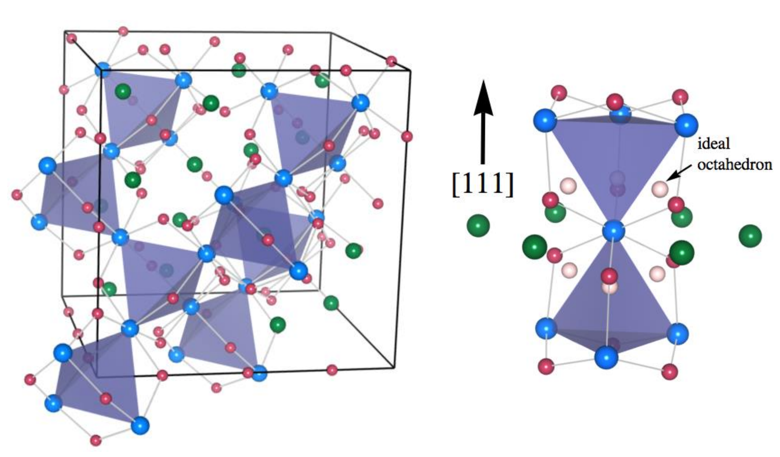
1. Introduction

Question: is there a parent spin liquid phase as a result of the competition of different ordered phases?

- Rare-earth pyrochlores are a family of material that support diverse physics. There are the ordered family of ferromagnet and antiferromagnet; the spin-glass family and the spin-ice family; What's more, some materials are possibly in the quantum spin-liquid regime.
- Given the diversity of physics in the pyrochlore family, a natural question to ask is the connection between these phases. A good guess is that the competition of different orders at phase boundaries may result in a parent spin liquid state.







$T_1, T_2, T_3, \overline{C}_6, S$

- Space group of R-atoms: $Fd\bar{3}m$
- Point group of R-atoms: O_h
- Strong spin-orbit coupling[1]:

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

- Time reversal symmetry $\mathcal{T}$

- $Tb_2Sn_2O_7$; $Gd_2Ti_2O_7$, $Gd_2Sn_2O_7$, $Er_2Ti_2O_7$, $R_2Ru_2O_7$
- $Y_2Mo_2O_7$, $Tb_2Mo_2O_7$...
- $Dy_2Ti_2O_7$, $Ho_2Ti_2O_7$, $R_2Sn_2O_7$ (R=Pr,Dy,Ho)...
- $Tb_2Ti_2O_7$, $Yb_2Ti_2O_7$, $Er_2Sn_2O_7$, $Pr_2Ir_2O_7$...

$$H = \sum_{\langle ij\rangle}\left[J_z S_i^z S_j^z - J_\pm(S_i^+S_j^- + S_i^-S_j^+) + J_{\pm\pm}(\gamma_{ij}S_i^+S_j^+ + \gamma_{ij}^*S_i^-S_j^-) + J_{z\pm}\left(S_i^z(\zeta_{ij}S_j^+ + \zeta_{ij}^*S_j^-) + i\leftrightarrow j\right)\right]$$

[1]Ross, Savary *et. al.*, 2011

2. Projective Symmetry Group: classification of spin liquids

Spin liquids: highly entangled ground state (which usually breaks no lattice symmetry); spinon excitation coupled to gauge field!

Spinons: elementary excitations of spin liquids (in the deconfined phase):

$$\vec{S} = \frac{1}{2}c^\dagger\vec{\sigma}c \qquad (c = b \text{ or } f)$$

$$H_{\text{spin}} \xrightarrow{\text{mean field}} H_{\text{MF}}$$

- Mean field theory H_{MF} describes spinon coupled to gauge field
- $H_{\text{MF}} \leftrightarrow H_{\text{spin}}$ is multiple $\leftrightarrow$ one!
- The symmetry of H_{MF}: gauge symmetry $\rtimes$ lattice symmetry
  symmetries are realized projectively!

Projective Symmetry Group: classify all possible projective symmetries of H_{MF}, and use them to write down all possible H_{MF}

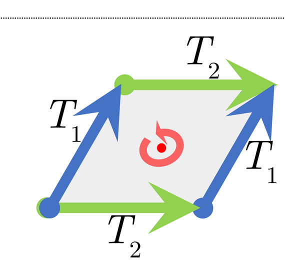
In our study, we use Schwinger boson decomposition of spin, and the gauge group is $\mathbb{Z}_2$

$$\begin{aligned}
U_g^\dagger G_g^\dagger[g(\vec{r}_\mu)]u_{\vec{r}_\mu,\vec{r}'_\nu}G_g[g(\vec{r}'_\nu)]U_g &= u_{g(\vec{r}_\mu),g(\vec{r}'_\nu)}\\
U_g^T G_g^T[g(\vec{r}_\mu)]v_{\vec{r}_\mu,\vec{r}'_\nu}G_g[g(\vec{r}'_\nu)]U_g &= v_{g(\vec{r}_\mu),g(\vec{r}'_\nu)}\\
U_\mathcal{T}^\dagger G_\mathcal{T}^\dagger(\vec{r}_\mu)u^*_{\vec{r}_\mu,\vec{r}'_\nu}G_\mathcal{T}(\vec{r}'_\nu)U_\mathcal{T} &= u_{\vec{r}_\mu,\vec{r}'_\nu}\\
U_\mathcal{T}^T G_\mathcal{T}^T(\vec{r}_\mu)v^*_{\vec{r}_\mu,\vec{r}'_\nu}G_\mathcal{T}(\vec{r}'_\nu)U_\mathcal{T} &= v_{\vec{r}_\mu,\vec{r}'_\nu}.
\end{aligned}$$

$$\begin{aligned}
(G_{T_i}T_i)(G_{T_j}T_j)(G_{T_i}T_i)^{-1}(G_{T_j}T_j)^{-1} &\in \mathbb{Z}_2,\\
(G_{\overline{C}_6}\overline{C}_6)^6 &\in \mathbb{Z}_2,\\
(G_S S)^2(G_{T_3}T_3)^{-1} &\in \mathbb{Z}_2,\\
(G_{\overline{C}_6}\overline{C}_6)(G_{T_i}T_i)(G_{\overline{C}_6}\overline{C}_6)^{-1}(G_{T_{i+1}}T_{i+1}) &\in \mathbb{Z}_2,\\
(G_S S)(G_{T_i}T_i)(G_S S)^{-1}(G_{T_3}T_3)^{-1}(G_{T_i}T_i) &\in \mathbb{Z}_2,\\
(G_S S)(G_{T_3}T_3)(G_S S)^{-1}(G_{T_3}T_3)^{-1} &\in \mathbb{Z}_2,\\
[(G_{\overline{C}_6}\overline{C}_6)(G_S S)]^4 &\in \mathbb{Z}_2,
\end{aligned}$$

$$\begin{aligned}
\phi_{T_1}(r_1,r_2,r_3)_\mu &= 0,\\
\phi_{T_2}(r_1,r_2,r_3)_\mu &= n_1\pi r_1,\\
\phi_{T_3}(r_1,r_2,r_3)_\mu &= n_1\pi(r_1+r_2),\\
\phi_{\overline{C}_6}(r_1,r_2,r_3)_\mu &= \phi_{\overline{C}_6}(\vec{0})_\mu + n_1\delta_{\mu=2,3}\pi r_1 + n_1\delta_{\mu=2}\pi r_3 + n_1(r_1r_2 + r_1r_3),\\
\phi_S(r_1,r_2,r_3)_\mu &= \phi_S(\vec{0})_\mu + (n_1\delta_{\mu=1,2} - n_{13})\pi r_1 + (n_1\delta_{\mu=2} - n_{13})\pi r_2\\
&\quad + n_1\delta_{\mu=1,2}\pi r_3 - \frac{1}{2}n_1\pi(r_1+r_2)(r_1+r_2+1),\\
\phi_\mathcal{T}(r_1,r_2,r_3)_\mu &= 0,\\
\phi_{\overline{C}_6}(\vec{0})_\mu &= \left(\frac{n_{\overline{C}_6}}{2} + m\delta_{\mu=1,2,3}\right)\pi,\\
\phi_S(\vec{0})_\mu &= \left((-)^{\delta_{\mu=1,2,3}}\frac{n_{13}+n_1}{2} + m_\mu\delta_{\mu=1,2}\right)\pi,\\
n_{\overline{C}_6}, m, m_1, m_2, n_1, n_{13} &\in \mathbb{Z}_2.
\end{aligned}$$

64 gauge inequivalent $\mathbb{Z}_2$ spin liquids!



As an example, the translation along two directions gives a closed loop around one plaquete. It gives rise to a group relation here, and in our calculation, we promote this equation to a gauge equation, and it is the gauge, those G's, that we want to solve. Physically, the $\mathbb{Z}_2$ number here means that the flux of the plaquete can be either zero or π. They distinguish two types of mean field Hamiltonian: the zero-flux type and the π-flux type.

$$T_1T_2T_1^{-1}T_2^{-1} = 1 \Rightarrow (G_{T_1}T_1)(G_{T_2}T_2)(G_{T_1}T_1)^{-1}(G_{T_2}T_2)^{-1} \in \mathbb{Z}_2$$

3. Six NN zero flux Hamiltonian classes

$$H = H_{\text{onsite}} + H_{\text{hopping}} + H_{\text{pairing}} = \sum_{\vec{k}}\left(\sum_\mu a_\mu b^\dagger_{\mu\vec{k}}b_{\mu\vec{k}} + \sum_{\mu\neq\nu}2b^\dagger_{\mu\vec{k}}\widetilde{u}_{\mu,\nu}b_{\nu\vec{k}} + b_{\mu,-\vec{k}}\widetilde{v}_{\mu,\nu}b_{\nu,\vec{k}} + b^\dagger_{\mu,\vec{k}}\widetilde{v}^\dagger_{\nu,\mu}b^\dagger_{\nu,-\vec{k}}\right)$$

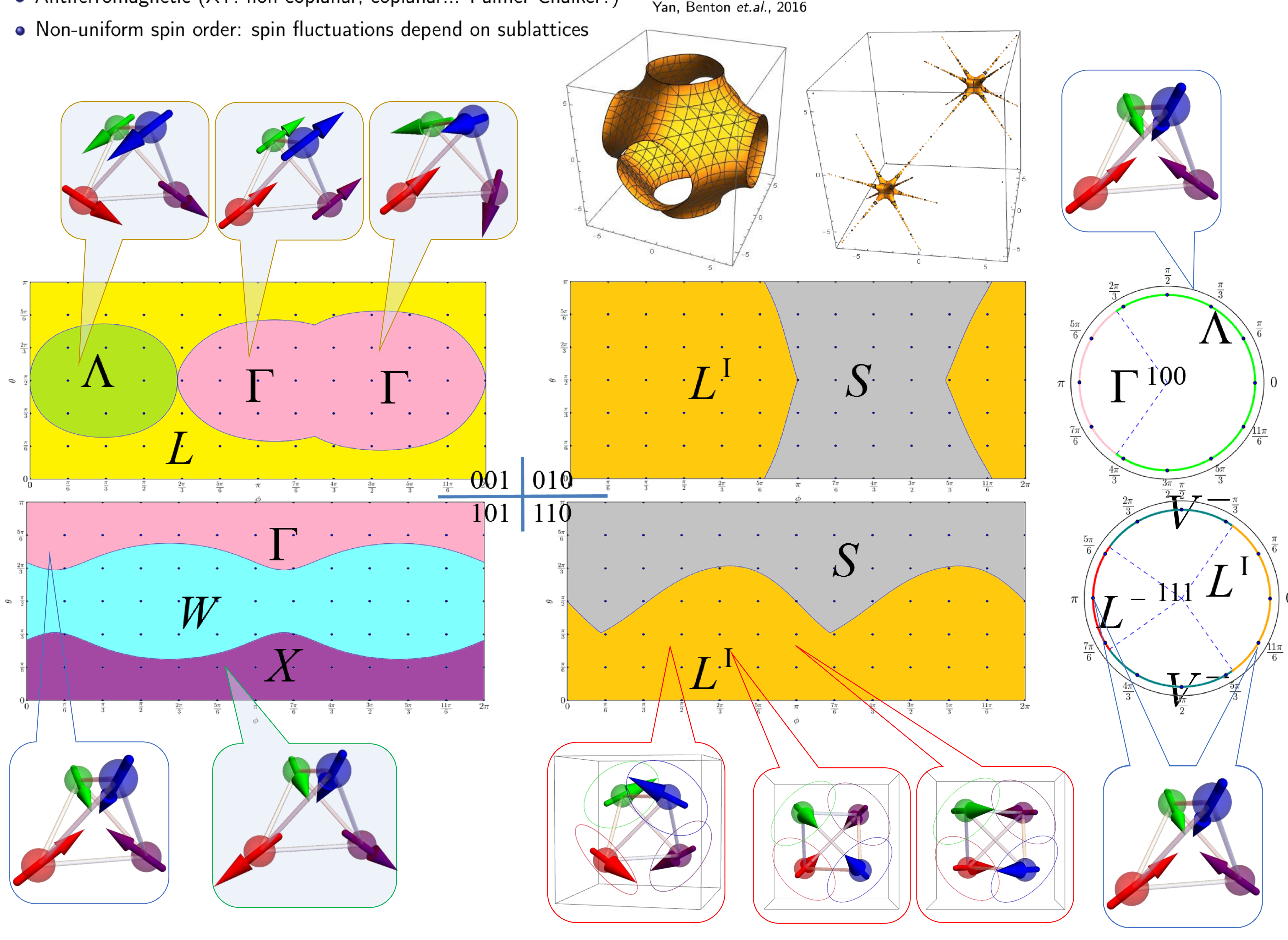
- Time reversal symmetry $\mathcal{T}$: $U_\mathcal{T}\mathcal{H}^*(\vec{k})U_\mathcal{T}^{-1} = \mathcal{H}(-\vec{k})$
- "Particle-hole symmetry" $\mathcal{C}$: $U_\mathcal{C}\mathcal{H}^*(\vec{k})U_\mathcal{C}^{-1} = \mathcal{H}(-\vec{k})$
- Inversion symmetry $\mathcal{I}$: $U_\mathcal{I}\mathcal{H}(\vec{k})U_\mathcal{I}^{-1} = \mathcal{H}(-\vec{k})$

Spin configurations: recovery of classical orders at $\mathbf{q} = 0$

- Ferromagnetic (maximal, two-in-two-out...)
- Antiferromagnetic (XY: non-coplanar, coplanar... Palmer Chalker?)
- Non-uniform spin order: spin fluctuations depend on sublattices

order parameter	definition in terms of spin components	associated ordered phases
m_{A_2}	$\frac{1}{2\sqrt{3}}(S_0^x+S_0^y+S_0^z+S_1^x-S_1^y-S_1^z-S_2^x+S_2^y-S_2^z-S_3^x-S_3^y+S_3^z)$	"all in-all out"
$\mathbf{m}_E$	$\begin{pmatrix}\frac{1}{2\sqrt{6}}(-2S_0^x+S_0^y+S_0^z-2S_1^x-S_1^y-S_1^z+2S_2^x+S_2^y-S_2^z+2S_3^x-S_3^y+S_3^z)\\ \frac{1}{2\sqrt{2}}(-S_0^y+S_0^z+S_1^y-S_1^z-S_2^y-S_2^z+S_3^y+S_3^z)\end{pmatrix}$	Ψ_2 and Ψ_3
$\mathbf{m}_{T_{1,A}}$	$\begin{pmatrix}\frac{1}{2}(S_0^x+S_1^x+S_2^x+S_3^x)\\ \frac{1}{2}(S_0^y+S_1^y+S_2^y+S_3^y)\\ \frac{1}{2}(S_0^z+S_1^z+S_2^z+S_3^z)\end{pmatrix}$	collinear FM
$\mathbf{m}_{T_{1,B}}$	$\begin{pmatrix}\frac{-1}{2\sqrt{2}}(S_0^y+S_0^z-S_1^y-S_1^z-S_2^y+S_2^z+S_3^y-S_3^z)\\ \frac{-1}{2\sqrt{2}}(S_0^x+S_0^z-S_1^x+S_1^z-S_2^x-S_2^z+S_3^x-S_3^z)\\ \frac{-1}{2\sqrt{2}}(S_0^x+S_0^y-S_1^x+S_1^y+S_2^x-S_2^y-S_3^x-S_3^y)\end{pmatrix}$	non-collinear FM
$\mathbf{m}_{T_2}$	$\begin{pmatrix}\frac{1}{2\sqrt{2}}(-S_0^y+S_0^z+S_1^y-S_1^z+S_2^y+S_2^z-S_3^y-S_3^z)\\ \frac{1}{2\sqrt{2}}(S_0^x-S_0^z-S_1^x-S_1^z-S_2^x+S_2^z+S_3^x+S_3^z)\\ \frac{1}{2\sqrt{2}}(-S_0^x+S_0^y+S_1^x+S_1^y-S_2^x-S_2^y+S_3^x-S_3^y)\end{pmatrix}$	Palmer–Chalker (Ψ_4)

Yan, Benton *et.al.*, 2016

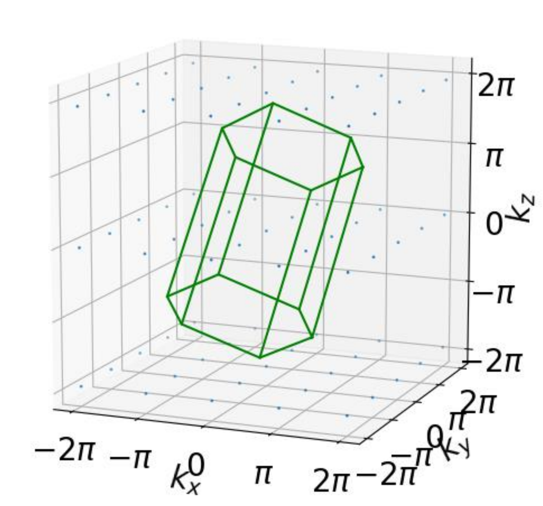


$L^- = L\backslash\{(\pi,\pi,\pi), -(\pi,\pi,\pi)\} = \{\pi(1,1,-1), \pi(1,-1,1), \pi(-1,1,1), \pi(-1,-1,1), \pi(-1,1,-1), \pi(1,-1,-1)\}$

$V^- = \{\pi(1,-1,0), \pi(-1,1,0), \pi(1,0,-1), \pi(-1,0,1), \pi(0,1,-1), \pi(0,-1,1)\}$

4. Six NN π-flux Hamiltonian classes

- On the parton level, the π-flux Hamiltonians have enlarged unit cell (4 times larger). This reduces the size of BZ and is in principle observable to neutron scattering experiments.
- So far experiments have not seen any evidence of π-flux spin liquid.



5. Work in progress

- We are systematically looking at all possible ordered spin configurations using representation theory.
- We are studying the ordered spin configurations with nonzero momentum, which exhibit even richer patterns.
- We are computing the structure factor for all six zero flux classes.
- What's more, we are studying the π-flux nearest neighbor mean field Hamiltonian, which is also expected to give interesting ordered spin states.
- Furthermore we will study the energetics of different states.

6. Conclusions

- We give a complete classification of $\mathbb{Z}_2$ spin liquid states using Schwinger boson PSG.
- We find six zero-flux classes + six π-flux classes on NN level.
- Classical ordered states are recovered and abundant phases are found through PSG.
- These serve as very good guidance for experiments as to where to look for spin liquids in rare-earth pyrochlores.