Symmetry enriched quantum spin ices

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Many thanks to Prof Zhou Yi and Prof Fuchun Zhang

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Symmetry enriched quantum spin ices

- Present a **realistic model** on pyrochlore lattice: XYZ model

- This model does not have a sign problem for quantum Monte Carlo simulation.

In fact, **no sign problem** on any lattice !

- This model supports **two distinct** (or **symmetry enriched**) **quantum spin ice** (or U(1) spin liquid) phases.

Collaborators

- Yi-Ping Huang (graduate student at Univ of Colorado Boulder)
- Prof. Michael Hermele (Univ of Colorado Boulder)
- Ref: **Phys. Rev. Lett. 112, 167203, 2014** (contain much more stuff)

work done in Univ of Colorado, Boulder

$$$ DOE

Outline

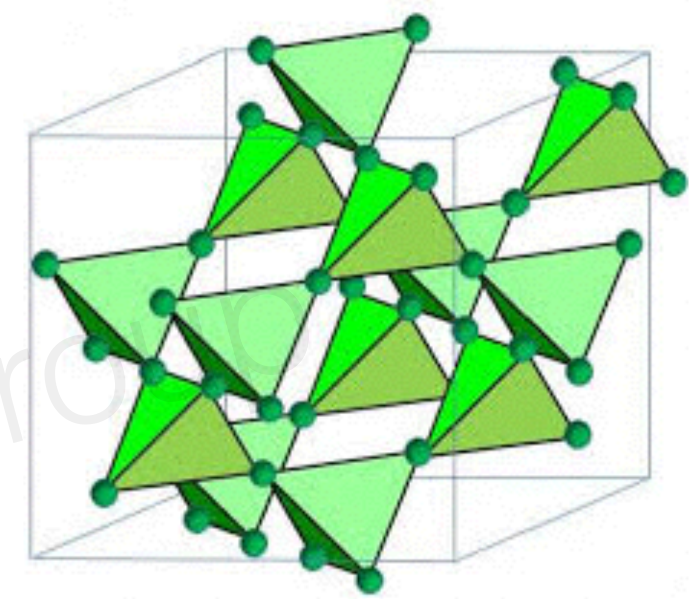
- Introduction to classical spin ice and quantum spin ice
- Realistic XYZ model from **octupole-dipole** moment on pyrochlore lattice
- Symmetry enriched quantum spin ice ground states and material survey.

Classical spin ice in pyrochlores

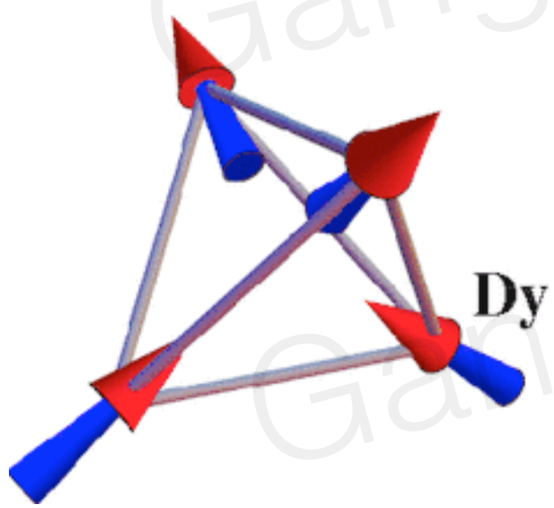
- $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$: Ising local moment from spin-orbit coupling + crystal electric field

- AFM Ising interaction in

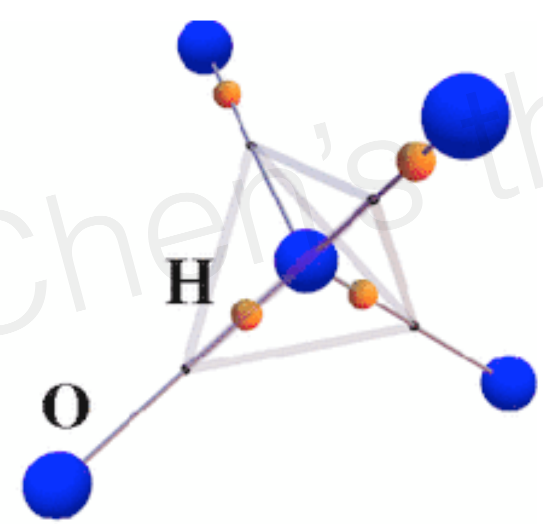
$$H = \sum_{\langle ij \rangle} J \, S_i^z S_j^z = \frac{J}{2} \sum_{tet} \Big(\sum_{i \in tet} S_i^z \Big)^2 + const$$



pyrochlore lattice



two-in two-out ice rule in spin ice



ice rule in water ice

Extensive classical ground state degeneracy

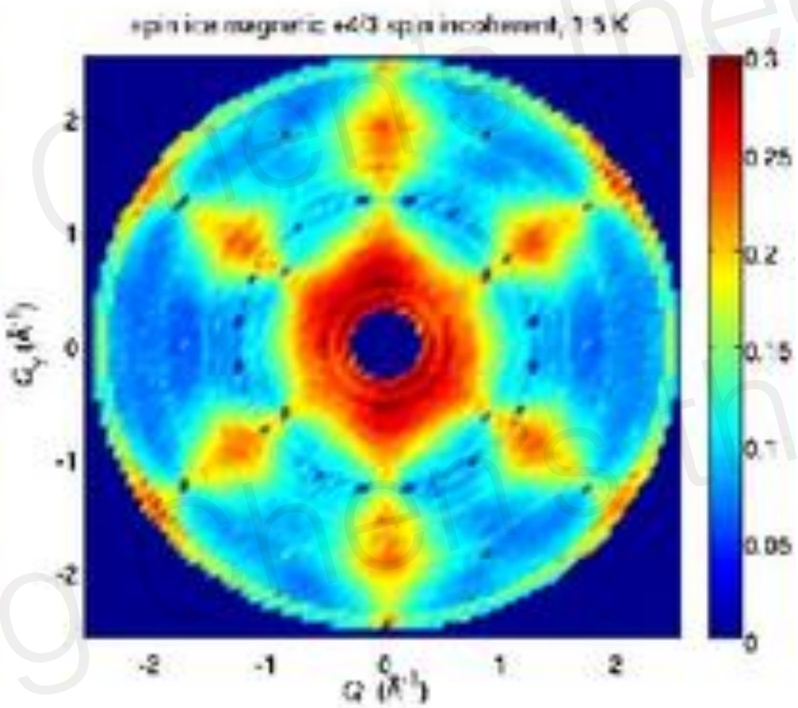
(also see Chapter 5, **Phase transition and critical phenomena** Prof Yu Lu & Hao Bolin)

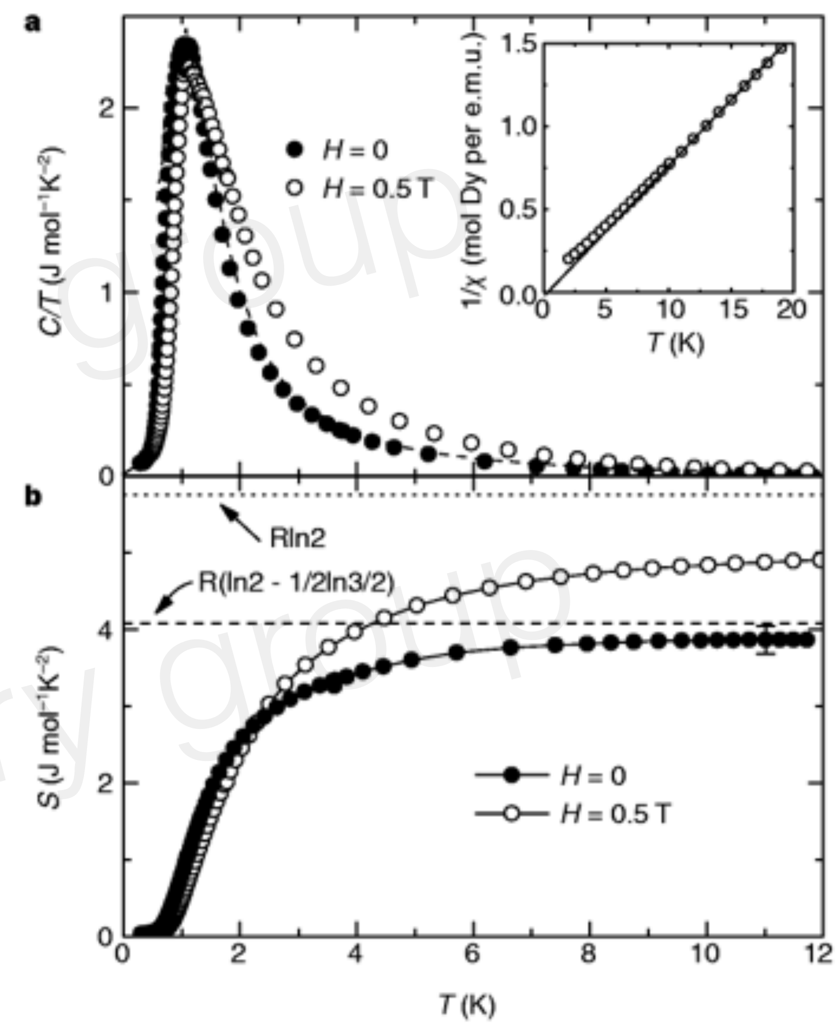
Ramirez, Bramwell, Gingras,etc 2000s, Castelnovo, Moessner, Sondhi etc 2000s, CL Henley

Experimental consequences of spin ice rules

- T < J, the spins are thermally fluctuating within classical ground state manifold that is demanded by spin ice rule

1. Pauling entropy: missing entropy due to the extensive ground state degeneracy





A Ramirez, etc, Nature 1997

- 2. Pinch points in neutron scattering: dipolar like spin correlation is a consequence of spin ice constraint

a signature of dipolar like spin-spin correlation

$$\left(\delta_{\mu\nu} - \frac{k_\mu k_\nu}{|\mathbf{k}|^2}\right)$$

Classical spin ice is certainly very interesting, but it is not a new phase of matter.

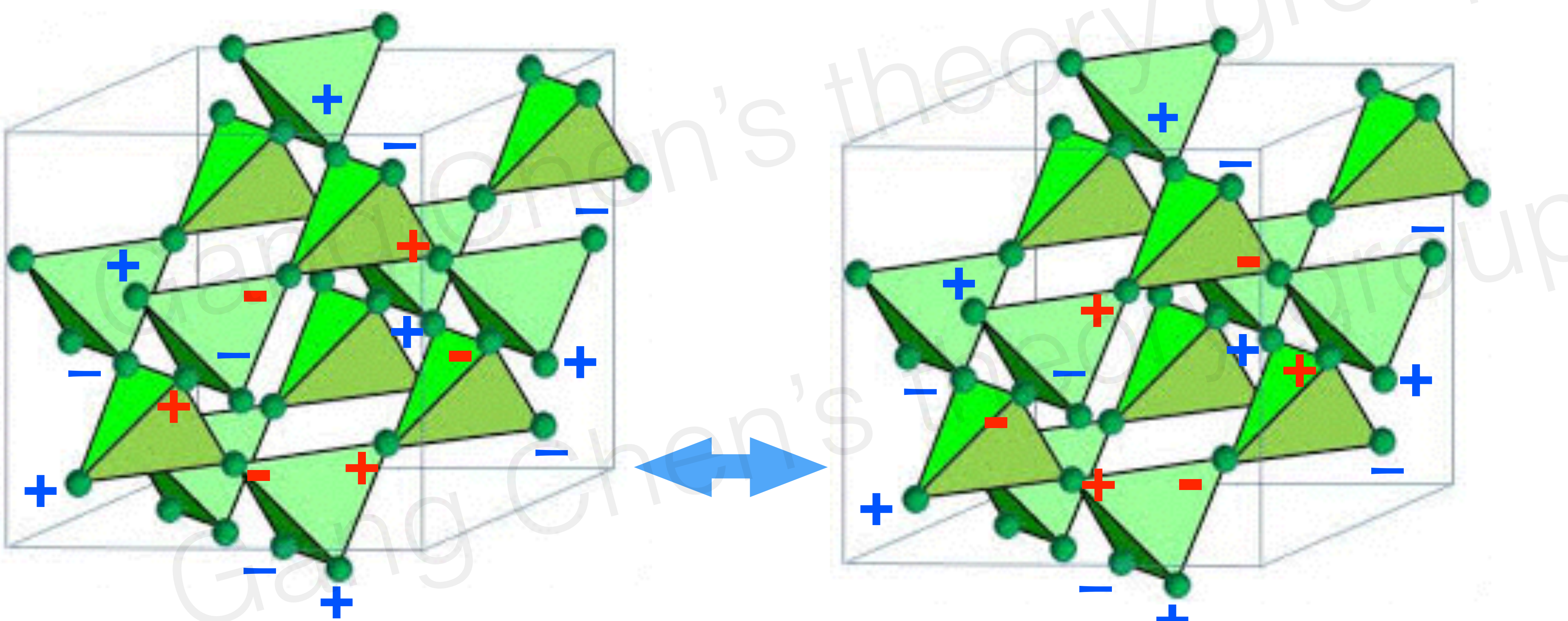
It is smoothly connected to the high temperature paramagnet phase.

In contrast, **quantum spin ice** is a new quantum phase of matter.

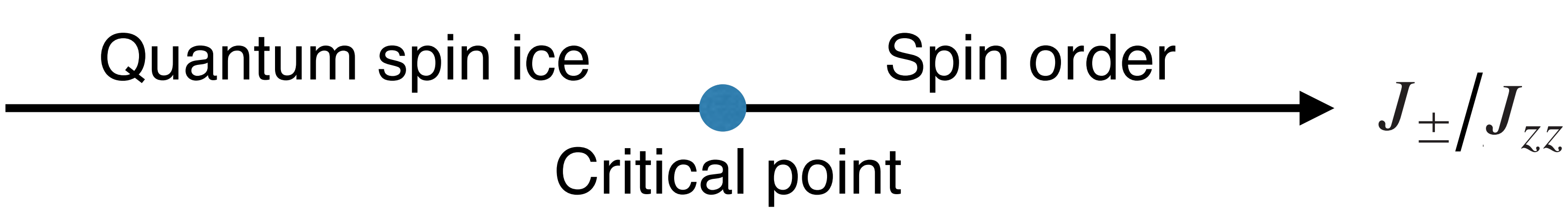
Quantum spin ice: early theory work with toy models

- A toy "XXZ" model: introduce **quantum tunneling** within the classical ground state manifold

$$H = \sum_{\langle ij \rangle} \{ J_{zz} \mathsf{S}_i^z \mathsf{S}_j^z - J_{\pm} (\mathsf{S}_i^+ \mathsf{S}_j^- + \mathsf{S}_i^- \mathsf{S}_j^+) $$



+ : in
− : out

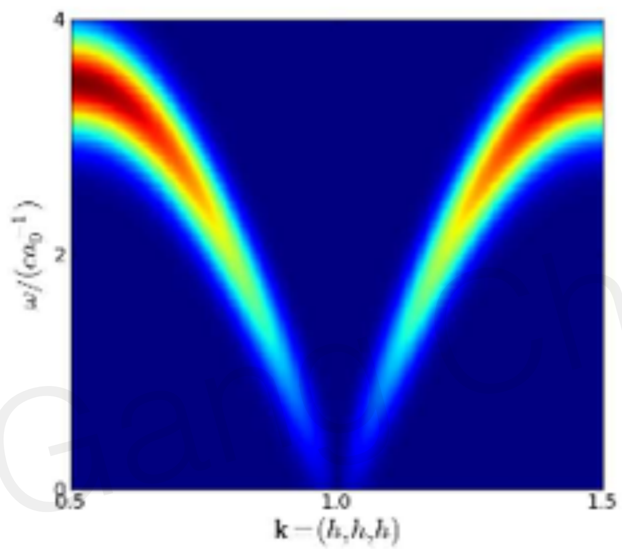


Hermele, Fisher, Balents, PRB 2004
Isakov, etc, PRL 2008
Shannon, etc, PRB 2012
Onoda, etc, ArXiv 2014

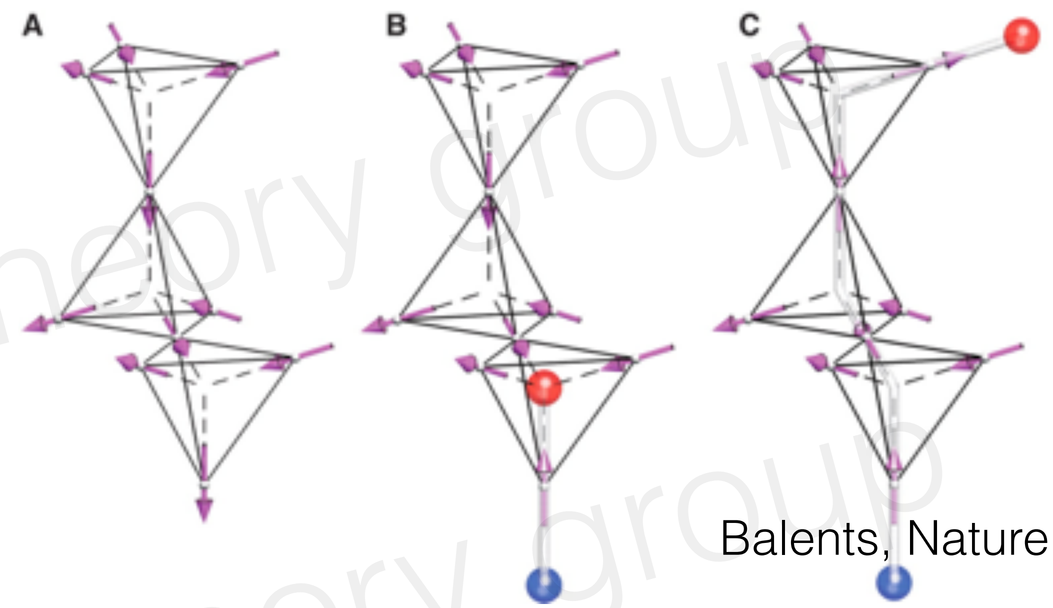
Properties of quantum spin ice

- Quantum spin ice does not have any conventional spin ordering.

- It is a **new quantum phase of matter** that is characterized by emergent **gapless** U(1) gauge photon and fractionalized excitations.

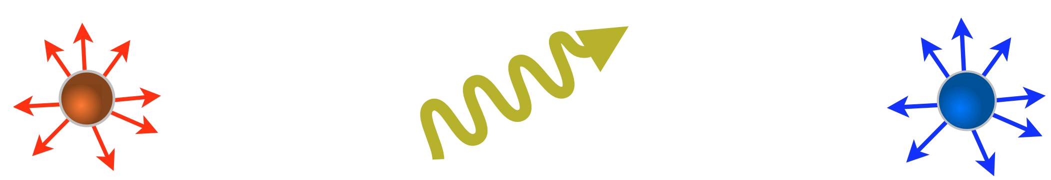


Emergent "**light**"



Balents, Nature 2010

Deconfined "spinons" (also called monopoles): only cost a **finite energy** to separate them apart



Compact QED: gapless U(1) gauge photon mediates the long-range interaction between the spinons (monopoles).

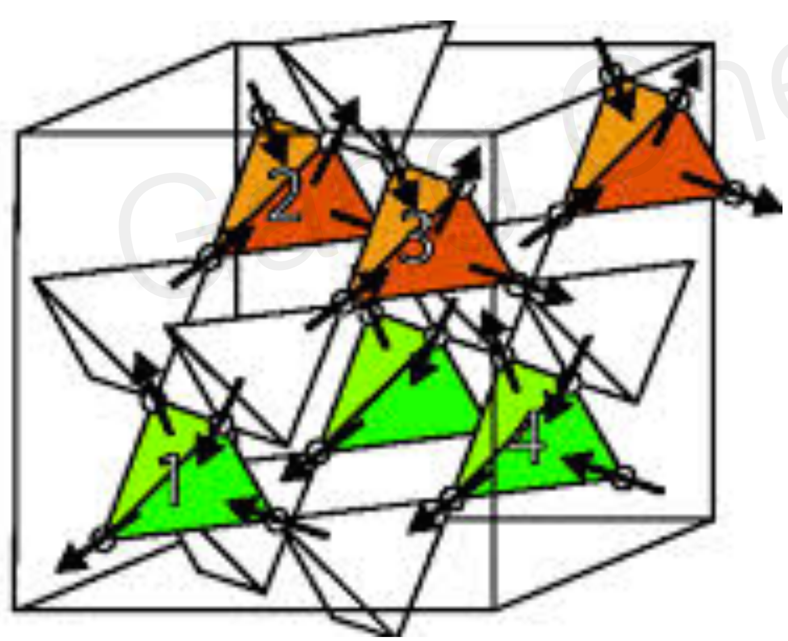
Theory is very elegant. How about reality? Any materials?

Jung Hoon Han's talk

1. rare-earth pyrochlores: $Ho_2Ti_2O_7$, $Dy_2Ti_2O_7$, $Ho_2Sn_2O_7$, $Dy_2Sn_2O_7$, Er_2Ti_2O7, $Yb_2Ti_2O_7$, $Tb_2Ti_2O_7$, $Er_2Sn_2O_7$, $Tb_2Sn_2O_7$, $Pr_2Sn_2O_7$, $Nd_2Sn_2O_7$, $Gd_2Sn_2O_7$, …….

2. rare-earth B-site spinel: $CdEr_2S_4$,$CdEr_2Se_4$, $CdYb_2S_4$, $CdYb_2Se_4$, $MgYb_2S_4$, $MgYb_2S_4$, $MnYb_2S_4$, $MnYb_2Se_4$, $FeYb_2S_4$, $CdTm_2S_4$ $CdHo_2S_4$, $FeLu_2S_4$, $MnLu_2S_4$, $MnLu_2Se_4$, ….

some courtesy from L Savary



$HgCr_2Se_4$ (double WSM)

Xu, Weng, Wang, Dai, Fang, PRL 2011

There are many pyrochlore materials !
Some of them are actually quantum .

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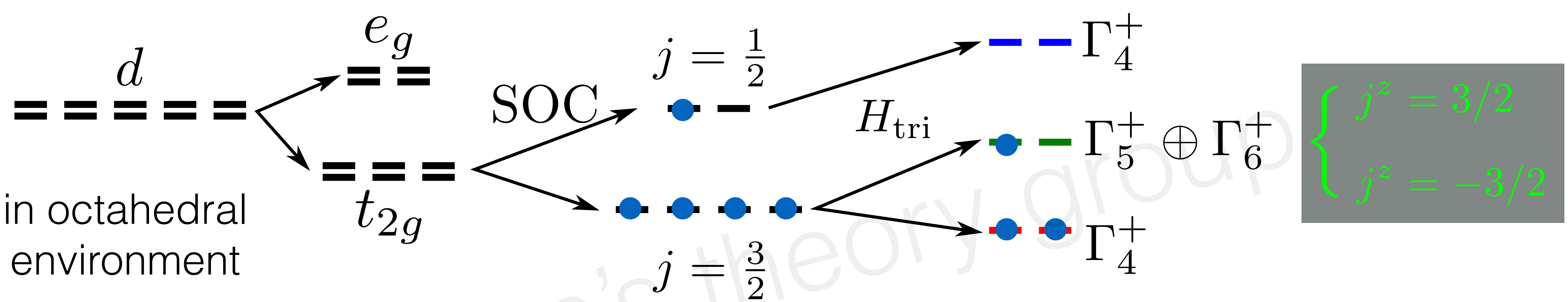
Dipole-octupole doublet: local physics

- Local moments with d electrons on pyrochlores: effective spin-1/2



Iridates: $Ir^{4+}(5d^5)$, five d electron in t_{2g} manifold.
What about d^1 and d^3 ? e.g. Os^{5+} in $Cd_2Os_2O_7$

$$\mathcal{P}_{t_{2g}} \boldsymbol{L} \mathcal{P}_{t_{2g}} = -\boldsymbol{\ell} \qquad \boldsymbol{j}_{\rm eff} = \boldsymbol{\ell} + \boldsymbol{S}$$

$$H_{t_{2g}} = -\lambda \boldsymbol{\ell} \cdot \boldsymbol{S} + H_{\rm tri} + H_{\rm int}$$

Local Hamiltonian allowed by point group symmetry (D_{3d})

SOC + trigonal distortion + onsite interaction

Gang Chen, Balents, PRB 2008
Jackeli, Khaliullin, PRL 2009,
Witczak-Krempa, **Gang Chen**, YB Kim, Balents, Annual Review of CMP, 2014

Dipole-octupole doublet

- Why is this Kramers doublet so special?

  1-dimensional representations of the point group!

$$R(2\pi/3)|J^z = \pm 3/2\rangle = -|J^z = \pm 3/2\rangle$$

- Symmetry demands that **1d irrep** should also occur for f electron moments

$$j = 3/2, 9/2, 15/2, \cdots$$

j = odd integer X 3/2

e.g. Dy2Ti2O7 (j=15/2) local Kramers doublet wavefunction

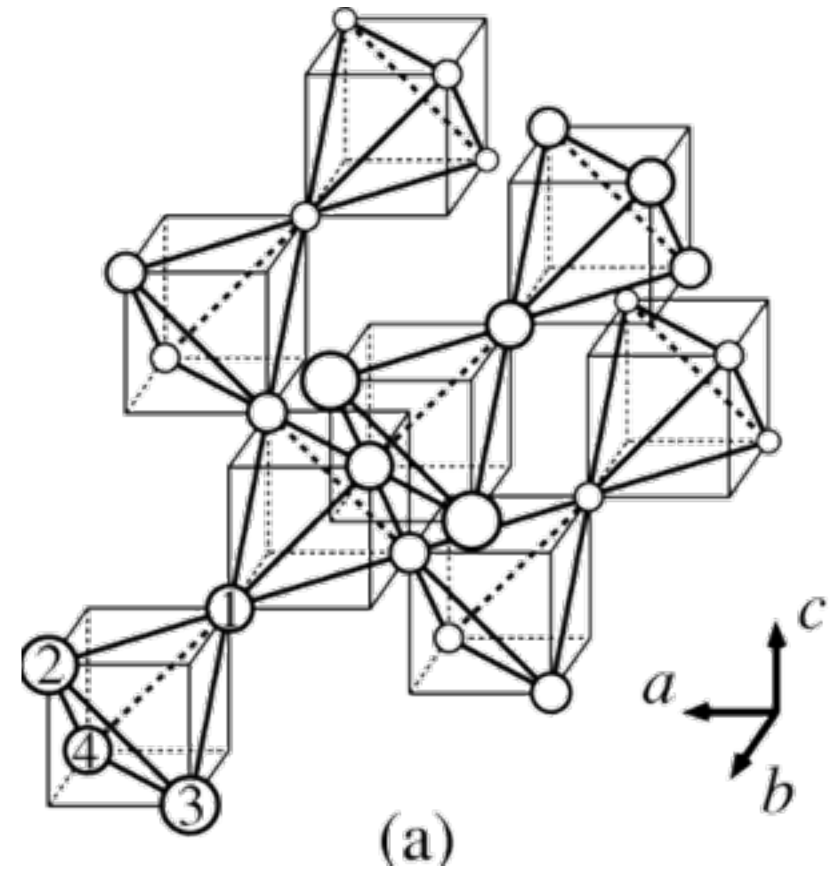
$$0.981|\pm\tfrac{15}{2}\rangle \pm 0.190|\pm\tfrac{9}{2}\rangle - 0.022|\pm\tfrac{3}{2}\rangle \mp 0.037|\mp\tfrac{3}{2}\rangle + 0.005|\mp\tfrac{9}{2}\rangle \pm 0.001|\mp\tfrac{15}{2}\rangle$$

Bertin, etc, J. Phys: cond.mat 2012

Symmetry properties

Define
spin operator

$$\begin{cases} S^z = \frac{1}{2}|\frac{3}{2}\rangle\langle\frac{3}{2}| - \frac{1}{2}|-\frac{3}{2}\rangle\langle-\frac{3}{2}| \\ S^+ = |\frac{3}{2}\rangle\langle-\frac{3}{2}|,\ S^- = |-\frac{3}{2}\rangle\langle\frac{3}{2}| \end{cases}$$



- Space group symmetry $Fd\bar{3}m$

$T_d \times \mathcal{I} \times translations$ and $T_d = \{C_3, M\}$

$$C_3 : S^\mu \to S^\mu$$

$$\boxed{M : S^{x,z} \to -S^{x,z},\ S^y \to S^y}$$

$$\mathcal{I} : S^\mu \to S^\mu$$

Important: S^x and S^z transform identically (as a **dipole**), while S^y transforms as an **octupole** moment under M.

XYZ model: a realistic model beyond Heisenberg

- Nearest neighbour exchange from symmetry $Fd\bar{3}m$

$$H = \sum_{\langle ij \rangle} J_z S_i^z S_j^z + J_x S_i^x S_j^x + J_y S_i^y S_j^y + J_{xz}(S_i^x S_j^z + S_i^z S_j^x)$$

Same on every bond !

Apply a global rotation around y axis in the effective spin space and obtain XYZ model

$$H = \sum_{\langle ij \rangle} \tilde{J}_z \tilde{S}_i^z \tilde{S}_j^z + \tilde{J}_x \tilde{S}_i^x \tilde{S}_j^x + \tilde{J}_y \tilde{S}_i^y \tilde{S}_j^y$$

"TOY" XXZ model → **"Realistic" XYZ model**

also **realistic** is Savary-Balents' model for dipolar doublets.
Curnoe PRB 2008 Savary & Balents PRL 2011; SB Lee & Balents PRB 2012

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Unfrustrated regime: Magnetic order

1. $\tilde{J}_z < 0$ and $|\tilde{J}_z| \gg \tilde{J}_{x,y}$, then $\langle \tilde{S}_i^z \rangle \neq 0$.

   This is an "all-in all-out" AFM state with magnetic dipolar order.

2. $\tilde{J}_x < 0$ and $|\tilde{J}_x| \gg \tilde{J}_{y,z}$, then $\langle \tilde{S}_i^x \rangle \neq 0$.

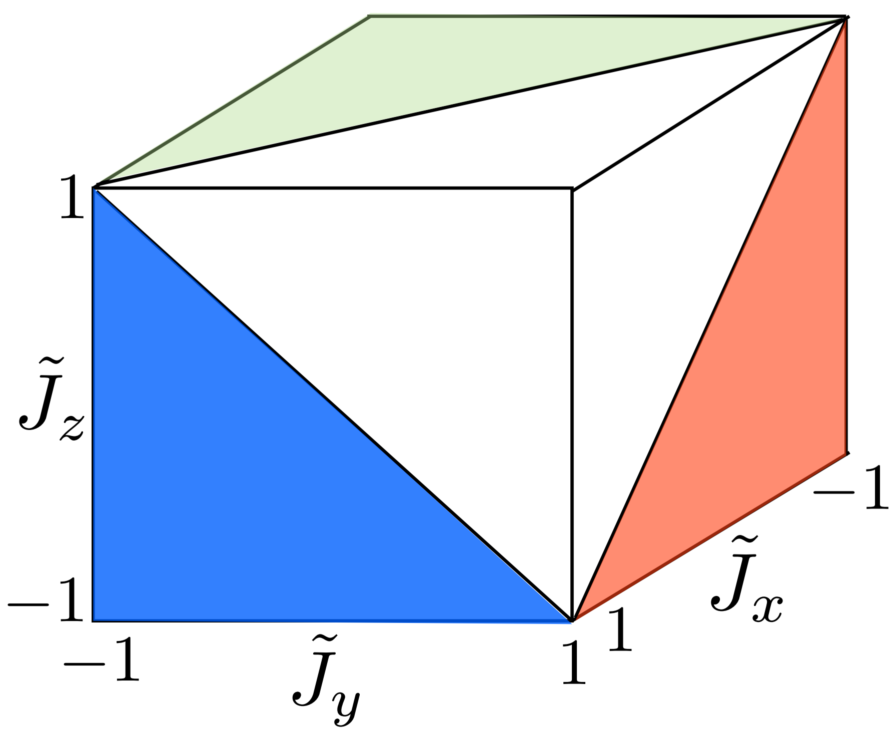
   This state is **not distinct** from the first state on symmetry grounds.

3. $\tilde{J}_y < 0$ and $|\tilde{J}_y| \gg \tilde{J}_{x,z}$, then $\langle \tilde{S}_i^y \rangle \neq 0$.

   This state is **distinct** from the above two states!
   It has an AFM-octupolar order but no dipolar order.

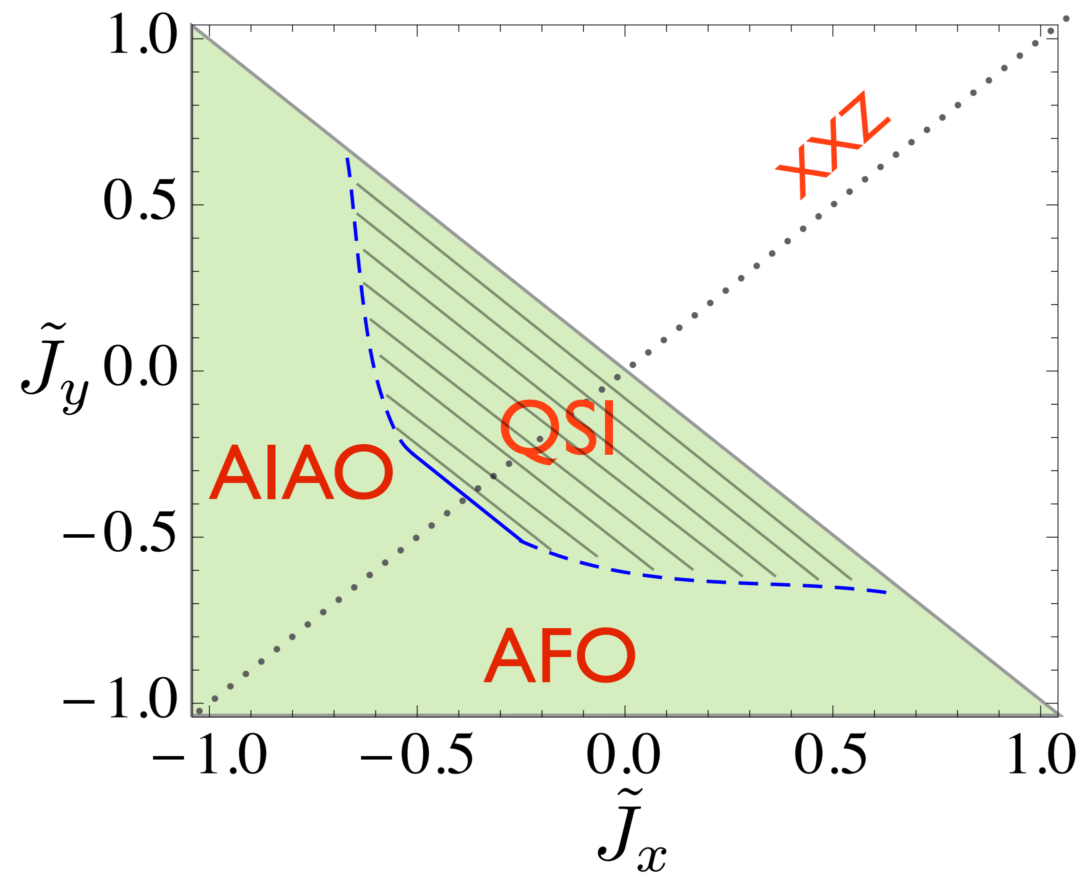
Quantum spin ice and phase diagram

Study phase on a cube: $-1 \leq \tilde{J}_{x,y,z} \leq 1.$



three dimensional phase diagram

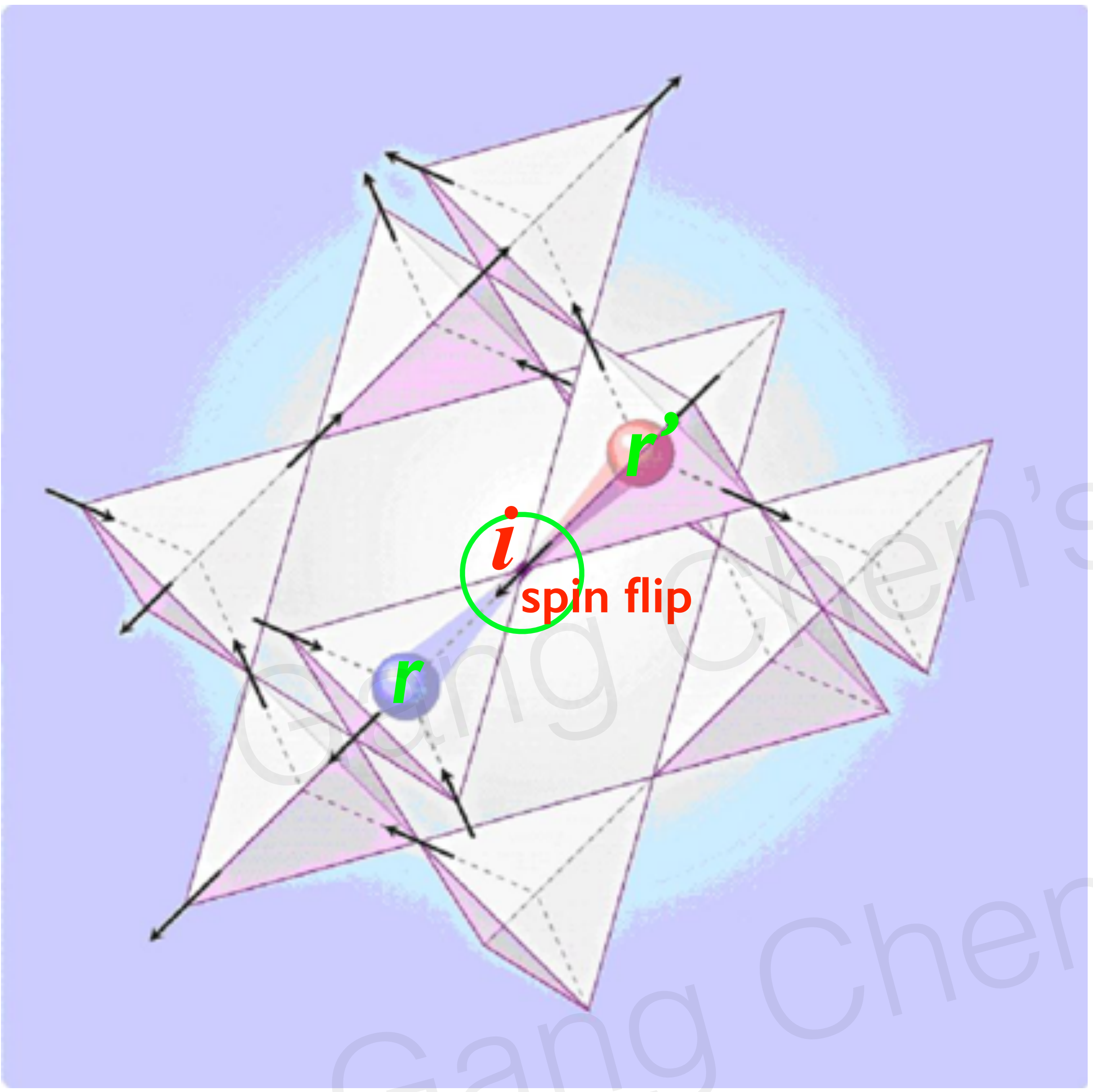
$\tilde{J}_z = 1$:



Phase diagram by gauge mean field theory.

No sign problem for quantum Monte Carlo in the shaded region !

Non-perturbative parton construction



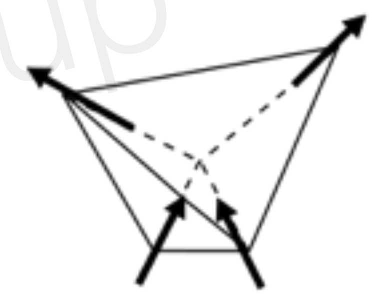
here treating Sz as **gauge electric field**

Spin flip creates spinon-antispinon pair on neighboring diamond sites.

$$S_i^{\pm} = \Phi_{\boldsymbol{r}}^{\dagger} \Phi_{\boldsymbol{r}'} s_{\boldsymbol{rr}'}^{\pm}$$

where $s_{\boldsymbol{rr}'}^{\pm} = e^{\pm i A_{\boldsymbol{rr}'}}$ is the gauge field.

and gauge charge is defined as



$$Q_{\boldsymbol{r}} = (-1)^{\boldsymbol{r}} \sum_{i \in \boldsymbol{r}} S_i^z$$

invariant under local U(1) gauge transformation

$$\Phi_{\boldsymbol{r}} \to \Phi_{\boldsymbol{r}} e^{i\chi_{\boldsymbol{r}}}$$

$$s_{\boldsymbol{rr}'}^{\pm} \to s_{\boldsymbol{rr}'}^{\pm} e^{i\chi_{\boldsymbol{r}} - i\chi_{\boldsymbol{r}'}}$$

* Framework is developed by Balents in L Savary, Balents, 2012, SB Lee, S Onoda, Balents 2012

Apply to XYZ

Rewrite the XYZ model to manifest the gauge structure

$$
\begin{aligned}
H_{\mathrm{XYZ}} &= \sum_{\langle ij \rangle} \tilde{J}_z \tilde{S}_i^z \tilde{S}_j^z + \tilde{J}_y \tilde{S}_i^x \tilde{S}_j^x + \tilde{J}_x \tilde{S}_i^y \tilde{S}_j^y \\
&\boxed{= \sum_{\langle ij \rangle} J_{zz} \tilde{S}_i^z \tilde{S}_j^z - J_{\pm} (\tilde{S}_i^+ \tilde{S}_j^- + h.c.)} + J_{\pm\pm} (\tilde{S}_i^+ \tilde{S}_j^+ + \tilde{S}_i^- \tilde{S}_j^-)
\end{aligned}
$$

with $J_{zz} = \tilde{J}_z$, $J_{\pm} = -\frac{1}{4}(\tilde{J}_x + \tilde{J}_y)$ and $J_{\pm\pm} = \frac{1}{4}(\tilde{J}_x - \tilde{J}_y)$.

Show the spinon-gauge coupling explicitly

Spinon hopping

$$
\begin{aligned}
H_{\mathrm{XYZ}} = \frac{J_{zz}}{2} \sum_{\mathbf{r}} Q_{\mathbf{r}}^2 &- J_{\pm} \sum_{\mathbf{r}} \sum_{i \neq j} \Phi_{\mathbf{r}+\eta_{\mathbf{r}}\mathbf{e}_i}^{\dagger} \Phi_{\mathbf{r}+\eta_{\mathbf{r}}\mathbf{e}_j} s_{\mathbf{r},\mathbf{r}+\eta_{\mathbf{r}}\mathbf{e}_i}^{-\eta_{\mathbf{r}}} s_{\mathbf{r},\mathbf{r}+\eta_{\mathbf{r}}\mathbf{e}_j}^{+\eta_{\mathbf{r}}} \\
&+ \frac{J_{\pm\pm}}{2} \sum_{\mathbf{r}} \sum_{i \neq j} \left(\Phi_{\mathbf{r}}^{\dagger} \Phi_{\mathbf{r}}^{\dagger} \Phi_{\mathbf{r}+\eta_{\mathbf{r}}\mathbf{e}_i} \Phi_{\mathbf{r}+\eta_{\mathbf{r}}\mathbf{e}_j} s_{\mathbf{r},\mathbf{r}+\eta_{\mathbf{r}}\mathbf{e}_i}^{\eta_{\mathbf{r}}} s_{\mathbf{r},\mathbf{r}+\eta_{\mathbf{r}}\mathbf{e}_j}^{\eta_{\mathbf{r}}} + h.c. \right)
\end{aligned}
$$

Spinon interaction

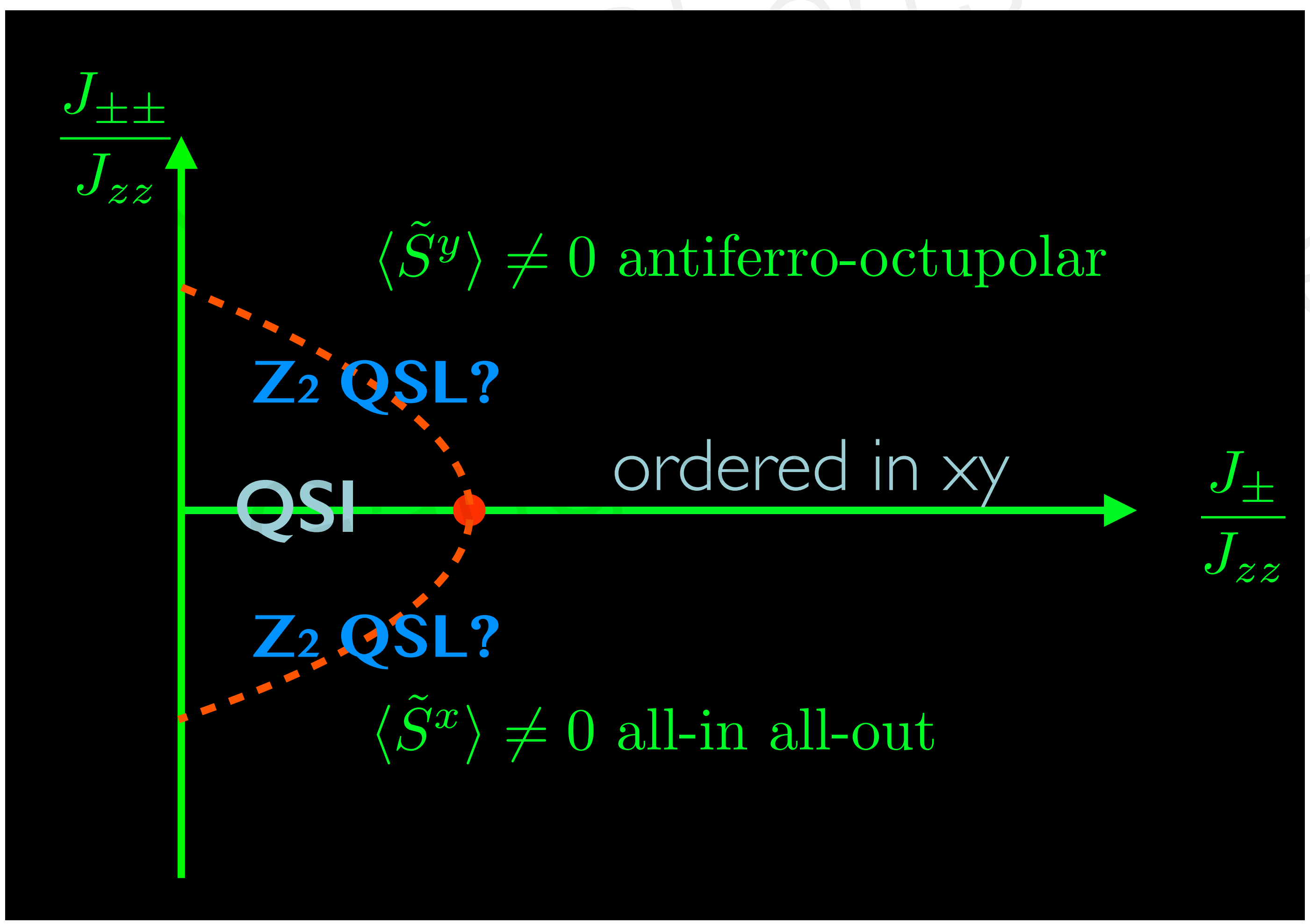
Bosonic spinons minimally coupled with U(1) lattice gauge field

Condense spinons

$$H_{\mathrm{XYZ}} = \sum_{\langle ij \rangle} \tilde{J}_z \tilde{S}_i^z \tilde{S}_j^z + \tilde{J}_y \tilde{S}_i^x \tilde{S}_j^x + \tilde{J}_x \tilde{S}_i^y \tilde{S}_j^y$$

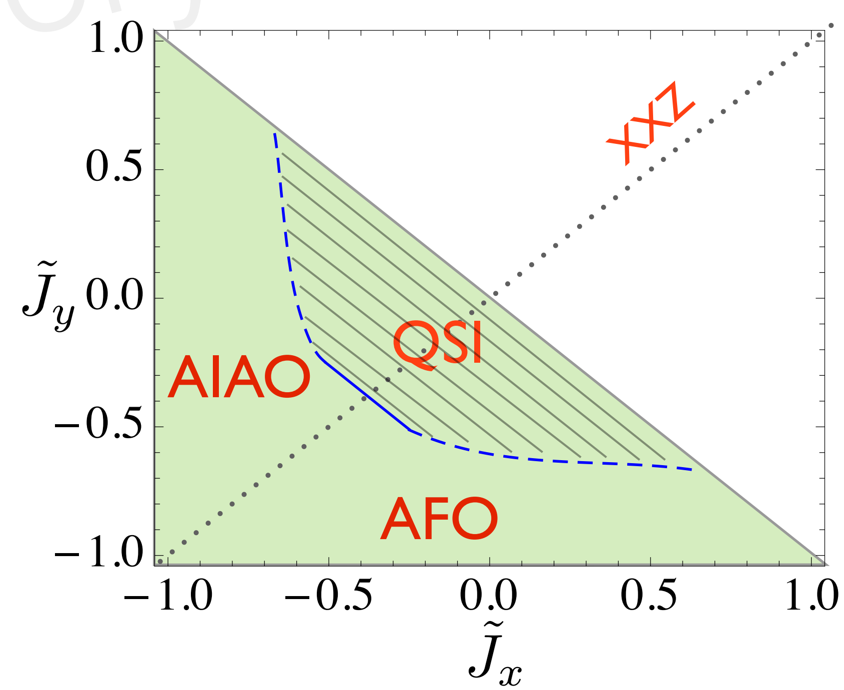
$$= \sum_{\langle ij \rangle} J_{zz} \tilde{S}_i^z \tilde{S}_j^z - J_{\pm}(\tilde{S}_i^+ \tilde{S}_j^- + h.c.) + J_{\pm\pm} \underline{(\tilde{S}_i^+ \tilde{S}_j^+ + \tilde{S}_i^- \tilde{S}_j^-)}$$

$$= 2(\tilde{S}_i^x \tilde{S}_j^x - \tilde{S}_i^y \tilde{S}_j^y)$$



Z2 QSL: $\langle \Phi \rangle = 0$ but $\langle \Phi\Phi \rangle \neq 0$

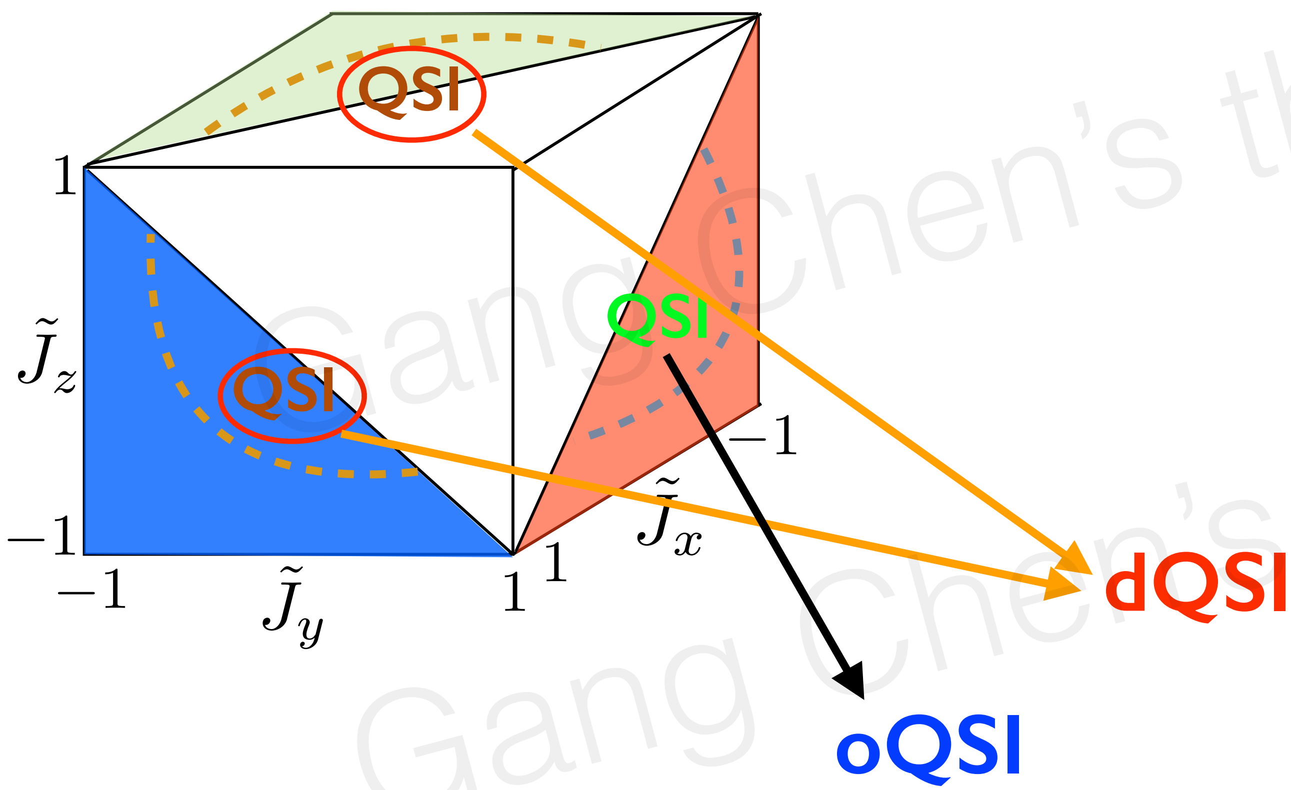
not found in the gauge MFT



$\tilde{J}_z = 1$

Symmetry enrichment by space group

$$H = \sum_{\langle ij \rangle} \tilde{J}_z \tilde{S}_i^z \tilde{S}_j^z + \tilde{J}_x \tilde{S}_i^x \tilde{S}_j^x + \tilde{J}_y \tilde{S}_i^y \tilde{S}_j^y$$



Are they different?

Yes. They are distinct by symmetry, i.e. they are symmetry enriched QSIs

$$C_3 : S^\mu \rightarrow S^\mu$$

$$\boxed{M : S^{x,z} \rightarrow -S^{x,z},\ S^y \rightarrow S^y}$$

$$\mathcal{I} : S^\mu \rightarrow S^\mu$$

In fact, white region (Pi-flux state) is also also example of symmetry enrichment. This is similar as the 3 symmetry enriched Z_2 QSLs in Kitaev's toric code model.

dQSI vs oQSI

Transformation of continuum E/B field under O_h point group

	dQSI	oQSI
E-field	T_1^+ (pseudovector)	T_2^+
B-field	T_1^- (vector)	T_2^-

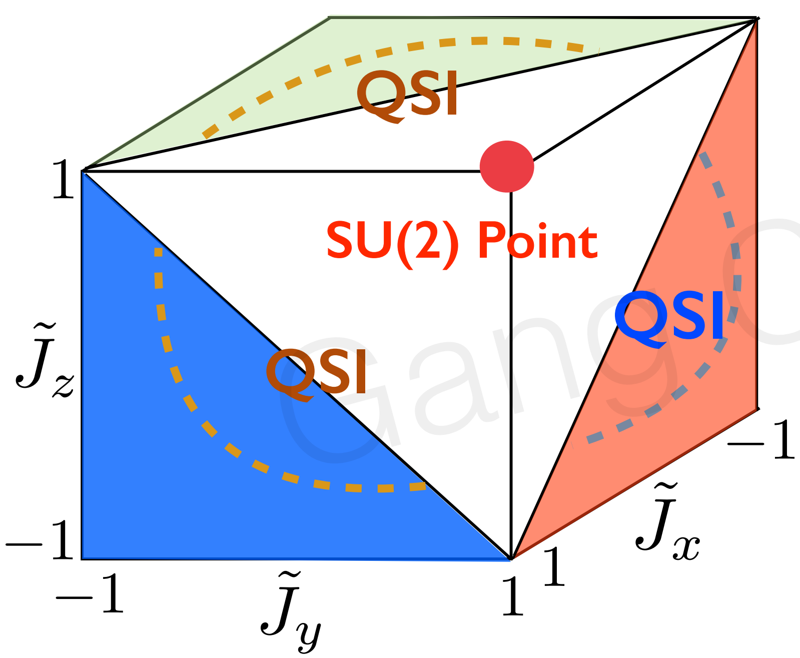
- Both phases have identical thermodynamical properties, e.g. T^3 heat capacity
- Different dipolar static spin correlation:

  dQSI: $< S_z(0)\, S_z(r) > \sim 1/r^4$.

  oQSI: $< S_z(0)\, S_z(r) > \sim 1/r^8$,

  with $Z_2 x Z_2$ symmetry, decay exponentially.

Open theory question



It is expected that, QSIs are more stable in the (frustrated) white region. But how are the QSIs connected with each other?

What is the ground state of SU(2) Heisenberg model on the pyrochlore lattice?

My conjecture: multicritical point or critical region with emergent non-Abelian gauge structure,
i.e. SU(2) quantum spin liquid ?

Material survey

Two well-known systems:

- Pyrochlores $A_2B_2O_7$,

  A = Nd, Er, Dy, … ?

  e.g. ,

  $Nd_2Ir_2O_7$, $Nd_2Sn_2O_7$, $Nd_2Zr_2O_7$, etc

  $Dy_2Ti_2O_7$,

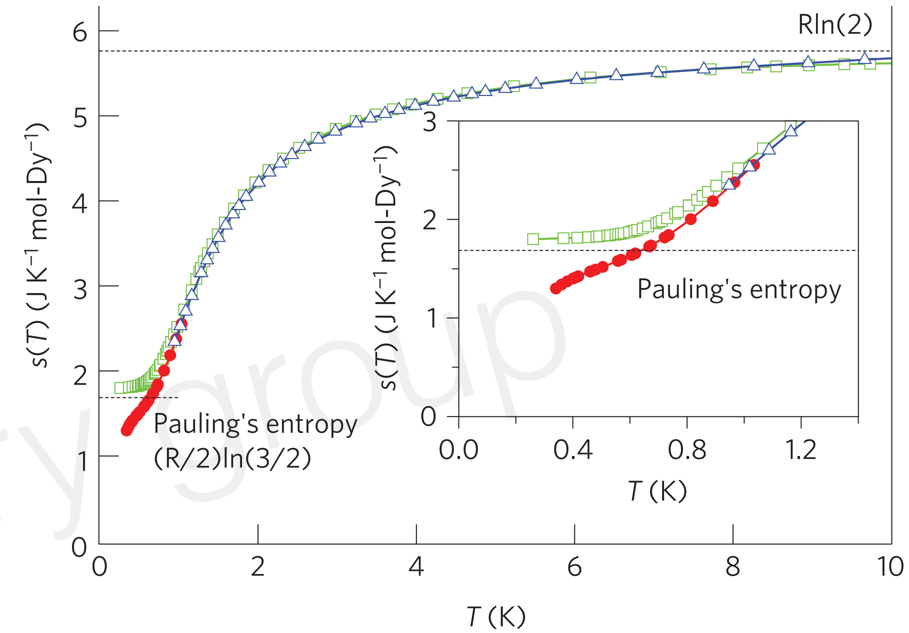
  $Cd_2Os_2O_7$, etc

- Spinels AB_2X_4, B = lanthanide?

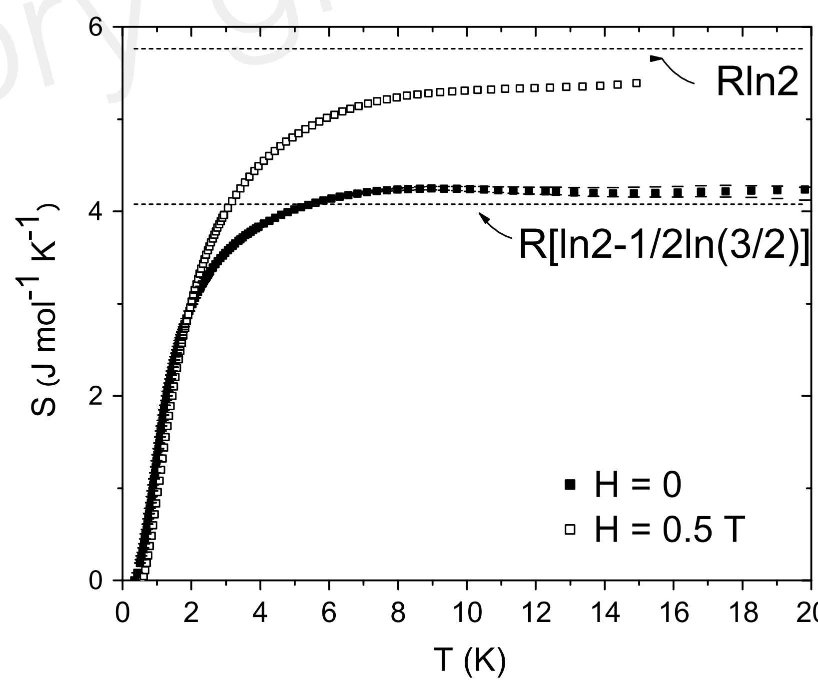
  e.g. $CdEr_2Se_4$

Some experiments may need to invoke the spin exchange beyond Ising like.

Bogdanov, etc, PRL 2013,
Watahiki, etc, 2011,
Bertin, etc, 2012.



Dy2Ti2O7: Bruce Gaulin's group, Nat Phys, 2013



CdEr2Se4, J Lago, etc, PRL 2010

Summary

- We propose a realistic XYZ model based on a octupole-dipole doublet on the pyrochlore lattice.
- This realistic model supports two distinct symmetry enriched quantum spin ice phases.
- This model should be well understood by quantum Monte Carlo simulation.

Thank you for your attention !