Magnetic states and quantum spin ices from dipole-octupole doublets on pyrochlore lattice

thanks very much for coming to my talk

Gang Chen

Fudan University, Shanghai, China

Currently on a visit at Perimeter Institute, Waterloo, Canada

Job opening

- **Postdocs** are generously funded and will have tremendous freedom.
- **Freedom**: 1. can apply for his/her own research grant
  2. can invite visitors/collaborators, propose and organize workshops
  3. get access to the frontier experiments both in Shanghai and the rest of China.

I am looking for postdocs. Our postdocs are generously supported and will have tremendous freedom.

top notch experimentalist in the world.

I don’t care about money.

i don’t look so great by comparison.

it is time to explore this modern city in this ancient nation !

Shanghai, Ch

Take-home message

1. We propose a **generic "XYZ" model** for "dipole-octupole" doublet on pyrochlores.

2. This model has both nontrivial ordered phases and distinct **symmetry-enriched U(1) QSL ground states**. Moreover, it does not have **a sign problem** for quantum Monte Carlo simulation in a large parameter space.

3. We discuss the relevance to real materials such as Dy_2Ti_2
   $Nd_2Ir_2O_7$, $Nd_2Sn_2O_7$,$CdEr_2Se_4$, $CdYb_2S_4$ and $Ce_2Sn_2O_7$

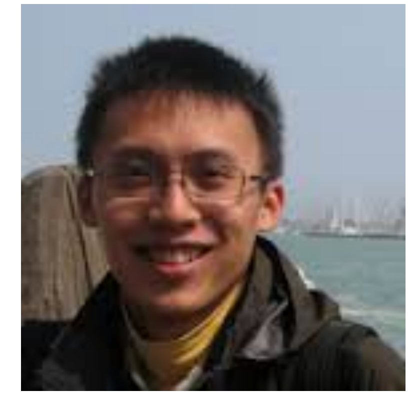
this word is very popular among fundamental theorists !

distinct by symmetry

how to bridge/realize the abstract fundamental with the realistic material.

this word is most important problem among numerical orientated theorists. I will also bridge the numerics with the realistic materials.

Outline



Yi-Ping Huang

Mike Hermele

1. Frustrated magnetism in rare-earth pyrochlores
2. Dipole-octupole doublets
3. Realistic XYZ model and symmetry enriched quantum spin ices (U(1) quantum spin liquids)
4. Related materials

i will explain that the model support both exotic order and a highly nontrivial symmetry enrihed quantum spin liuqid.

finally, i list some of the relevant materials

Collaborators: Yi-Ping Huang, Mike Hermele, CU Boulder
Ref: arXiv 1311.1231, **Phys. Rev. Lett**.112,167203 (2014)

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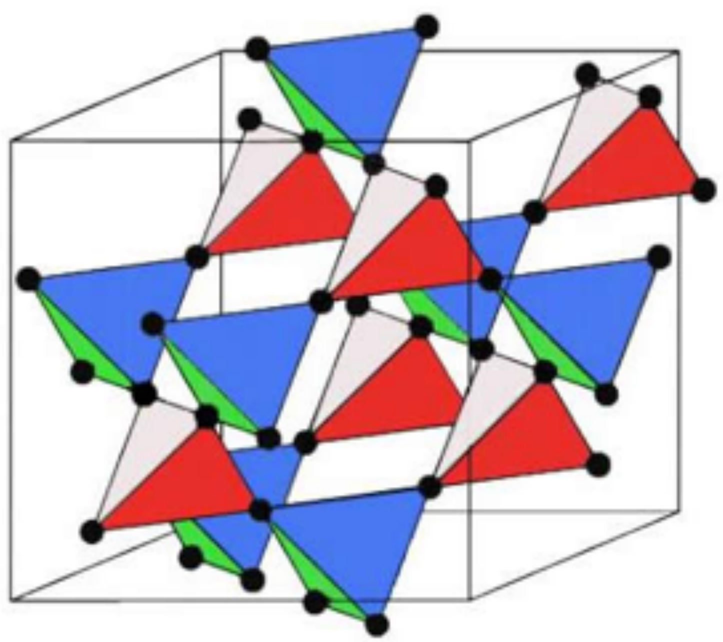
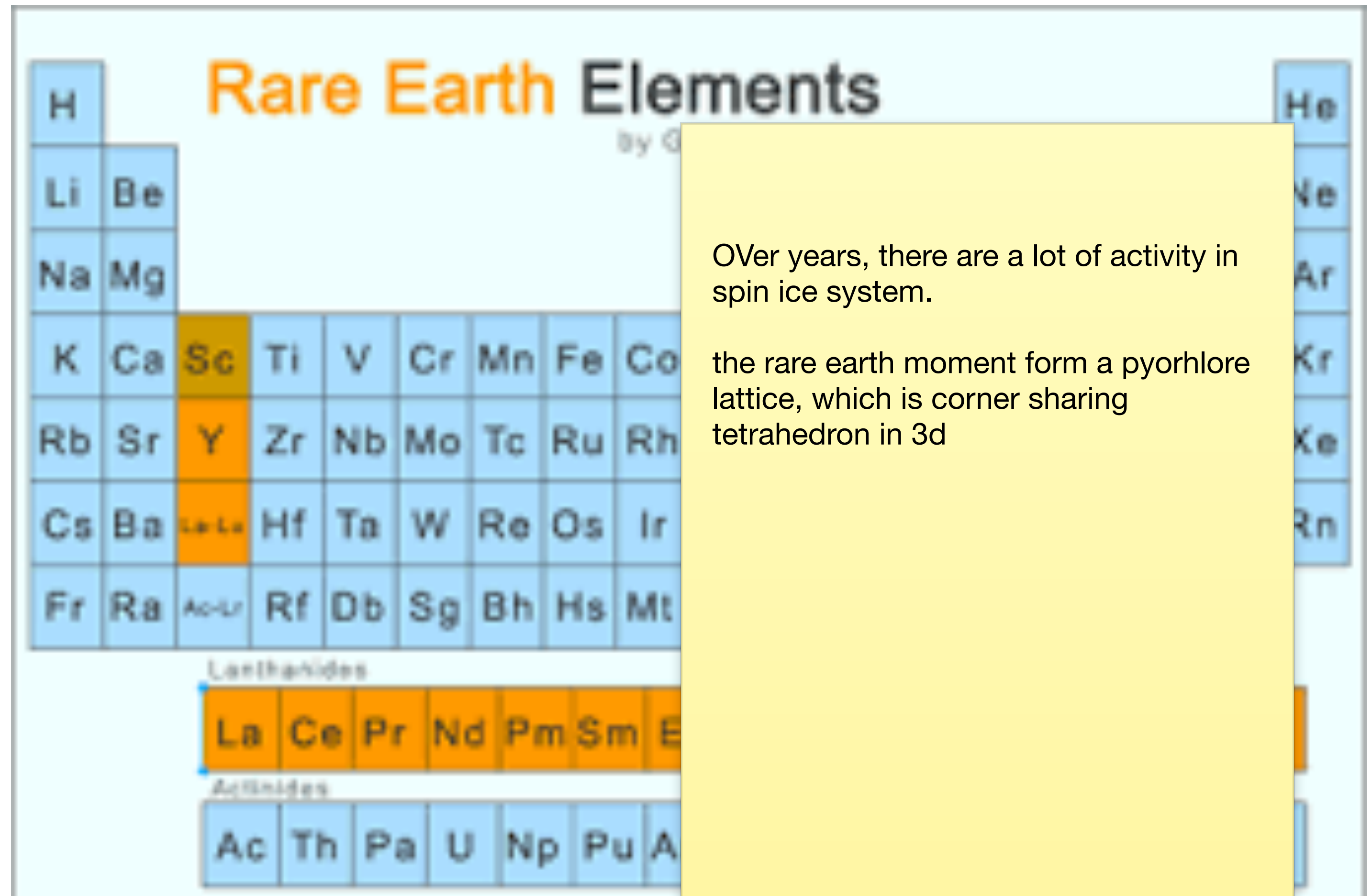
Rare-earth pyrochlores



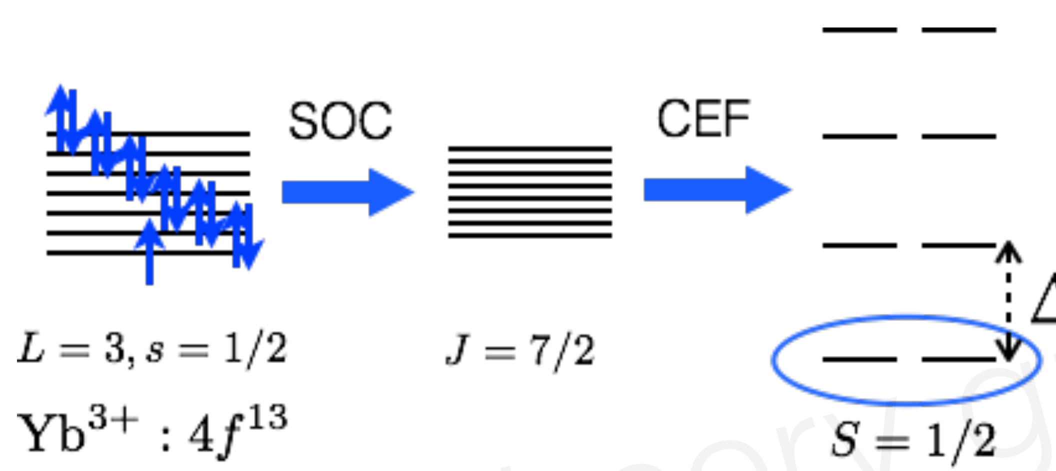
$RE_2M_2O_7$



OVer years, there are a lot of activity in spin ice system.

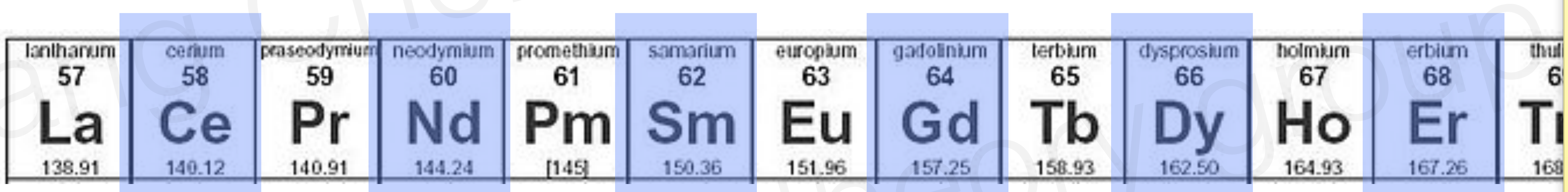
the rare earth moment form a pyorhlore lattice, which is corner sharing tetrahedron in 3d

Rare-earth local moments: a **crude** classification

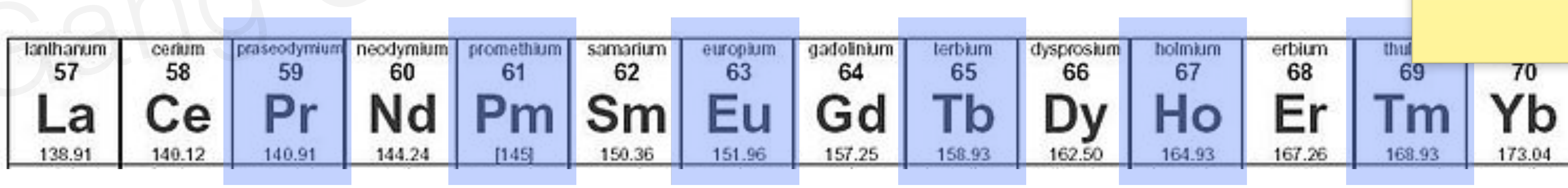


SOC+CEF

Kramers' doublet: R^{3+} with **odd** number of electrons



Non-Kramers' doublet / singlet: R^{3+} with **even** number of electrons



in a rare earth ion site, the c
form a spin-orbit entangled
moment J, and then CEF s
multiple doublet, or singlets
lexcited state is much high
than the energy scale of the
one can simply foucs on th
state doublet, which is mod
effective spin-1/2 DOF.

Crudely speaking, the rare
moments can be classified
doublet and non-kramer do
rare earth ions with odd nu
electorn form krme, even f

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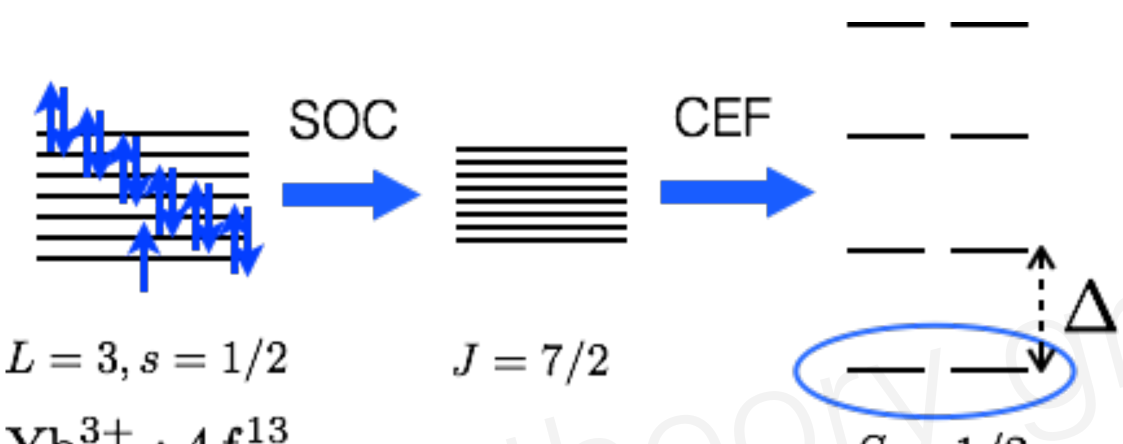
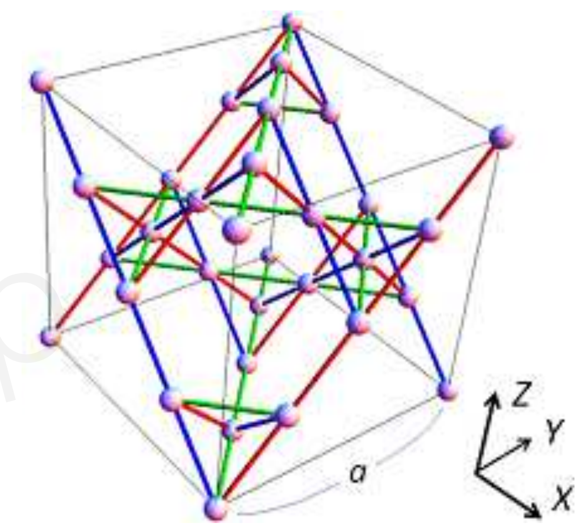
A generic model that describe the interaction between local effective spin-1/2 moments is given by this complicated form,

because of the intrinsic spin-orbit entanglement, the spin interaction is anisotropy both in position space and spin space. This is manifested i the bond dependent phase factors.

the locking between the spin interaction and bond orientioan

A generic spin Hamiltonian





Curnoe, 2008
Onoda, etc 2009

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

$$+ J_{\pm\pm} (\gamma_{ij} \mathsf{S}_i^+ \mathsf{S}_j^+ + \gamma_{ij}^* \mathsf{S}_i^- \mathsf{S}_j^-)$$

$$+ J_{z\pm} [\mathsf{S}_i^z (\zeta_{ij} \mathsf{S}_j^+ + \zeta_{ij}^* \mathsf{S}_j^-) + i \leftrightarrow j] \},$$

$\gamma_{ij} = 1, e^{i2\pi/3}, e^{-i2\pi/3}$

$\zeta = -\gamma^*$ for different bond orientations.

The phase factors depend on the bond orientations:

"Locking" of the spin interaction and bond orientation.

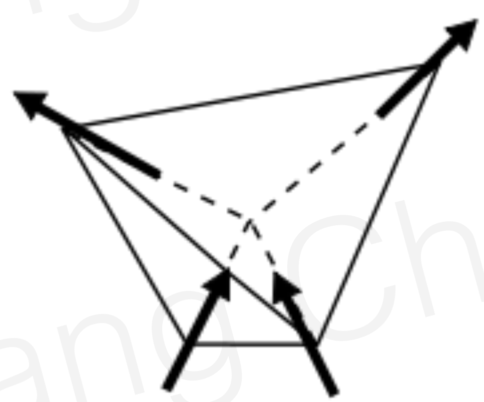
This is the **key property** of strong spin-orbit coupled magnets.

Witczak-Krempa, **GC**, YB Kim, Balents, Annual Review of CMP 2014 if one google search, one can find a lot of nice work by these distinguished theoretical physicists.

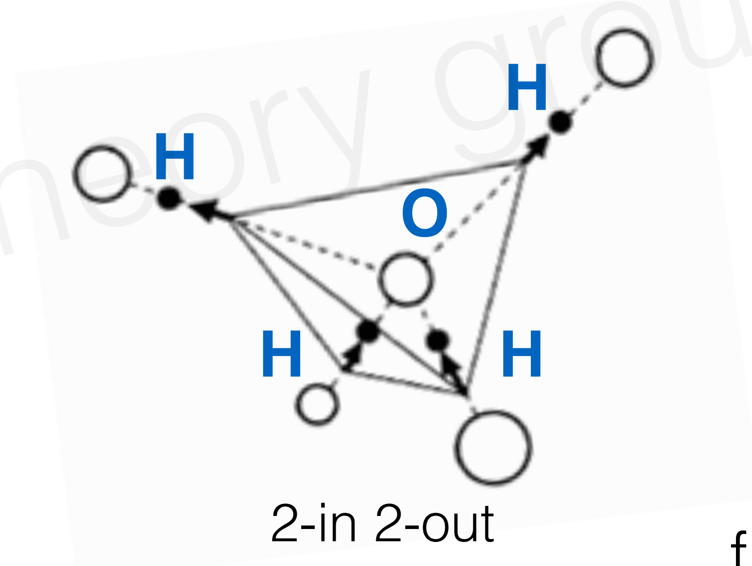
Spin ice (Ising) limit

$$H = J_{zz} \sum_{\langle i,j \rangle} S_i^z S_j^z + \ldots\ldots$$

Ref: Gingras, Moessner, Tchernyshyov, Castelnovo, Sondhi, Schiffer, Penc, Hermele, Balents, Fisher, Savary…….



2-in 2-out
spin ice rule



2-in 2-out
water ice rule

from wiki

Over years, there are a lot of activity in spin ice system.

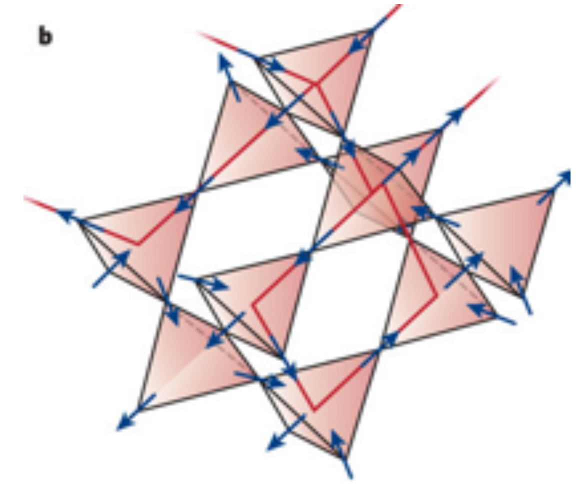
spin ice is realized in rare earth pyrochlore systems, when the ising part of the exchange is AFM and dominant.

if one google search, one can find a lot of nice work by these distinguished theoretical physicists.

The interaction between the ising is AFM, it favor 2 spin in 2 spin out of the tetrahedra. This is the 2-in 2-out spin ice rule.

Beucase of the analog relation with H position in water ice, each O has 4 H near it, 2 are close, 2 are further.

Classical spin ice



- The “2-in 2-out” states are extensively degenerate.
- At temperature T < Jzz, the system thermally fluctuates within the ice manifold, leading to classical spin ice and interesting experimental discoveries.

Pinch points in spin correlation

1. the 2-in 2-out spin ic
extensively degenera
tetrahedron, one car
the other 2-out.

2. at T << Jzz, the syste
fluctuating within the ic
classical spin ice and in
consequences. Many o
in nature and science.

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Dipole-octupole doublet

The early classification of local moments is a bit crude !

One should carefully examine the wavefunction of the local doublet.

what is dipole-octupole doublet, the early classicialcation is a bit curde, one should carefully examine the wavefuction of the local doublet .

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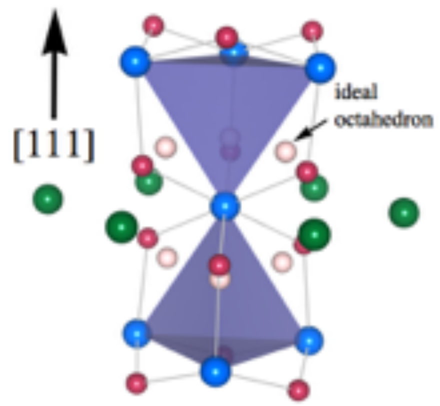
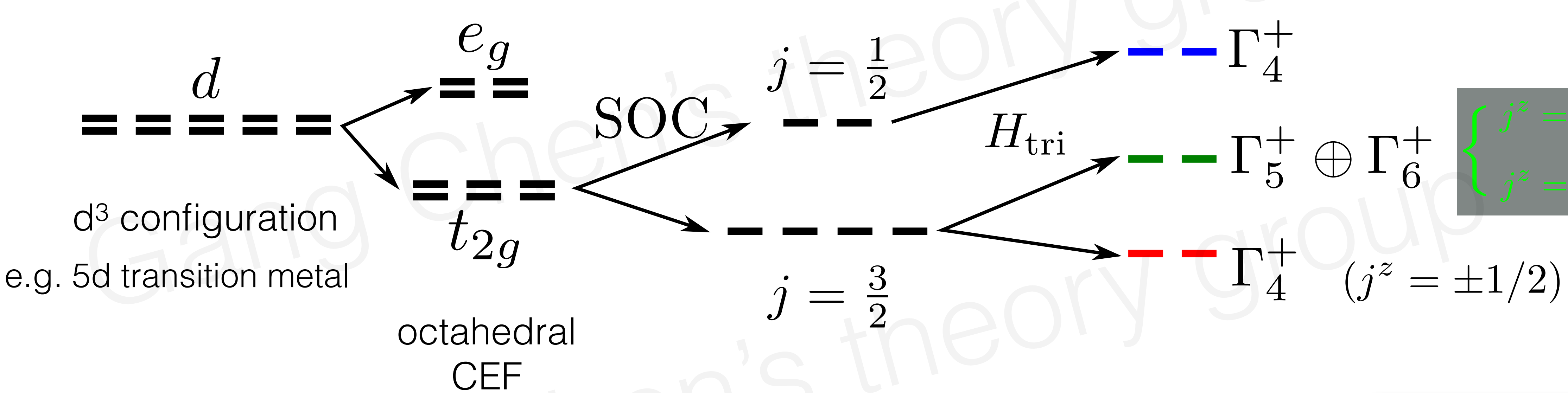
Local physics: start with t_{2g} electrons



- Local moments on pyrochlore lattice: effective spin-1/2



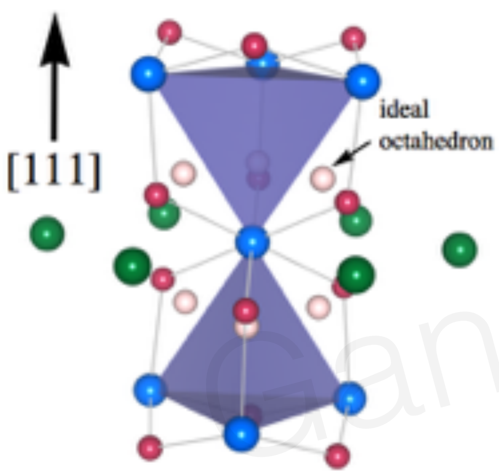
d electrons under D3d
point group crystal field

for my convenience, let me start with t2g electrons. Let 's consider 5d electron in octahedral environment.

add Jz=\pm 1/2

- Why is this Kramers doublet so special ?

ONE-dimensional representations of the point gro



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

$$R(2\pi/3) \equiv e^{-i\frac{2\pi}{3}J^z} = e^{-i\frac{2\pi}{3}\times(\pm\frac{3}{2})} = e^{\mp i\pi} = -1$$

$$|J^z = +3/2\rangle \xrightarrow{\text{time reversal}} |J^z = -3/2\rangle$$

why special,

they are one dimensional rep of po
group.

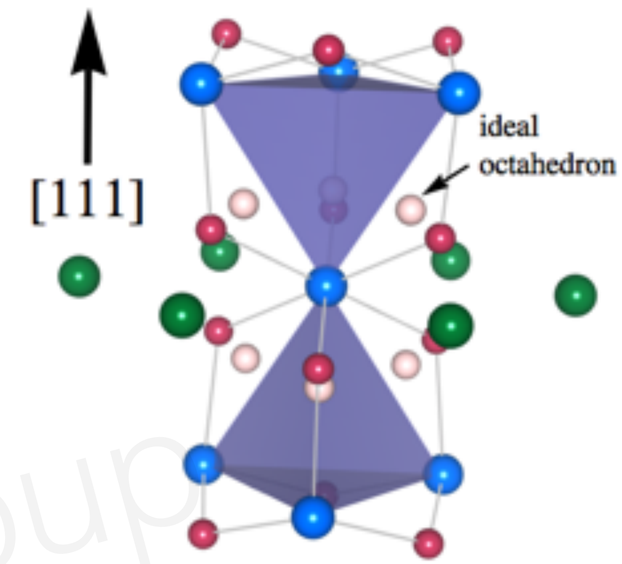
in particular, if you look at the 3-fol
rotation operation, under this rotati
ech state stay invariant, except a m
sign. they do not transform into eac
other under the point group
transformation.

simple algebar

this is very different from 2-dim irep
where these two states of the doub
are mixed.

These two state are dgenerate und
time reversal, deg proctected by ti
reversal.

More generally, …



- Also applies to 4*f* electron moments on pyrochlore

$$J = \frac{3}{2}, \frac{9}{2}, \frac{15}{2}, \cdots$$

with the local crystal field Hamiltonian

$$H_{\rm cf} \; = 3B_2^0 (J^z)^2 + \cdots \quad \text{if } B_2^0 < 0$$

more generially, it applies to xxxx.
if the local crystal field hamiltnian is
easy axis like.

e.g. local doublet wavefunction of Dy^{3+} $(J = \frac{15}{2})$ in $Dy_2Ti_2O_7$

$$|\phi_0^{\pm}\rangle = 0.981|\pm\tfrac{15}{2}\rangle \pm 0.190|\pm\tfrac{9}{2}\rangle - 0.022|\pm\tfrac{3}{2}\rangle \mp 0.037|\mp\tfrac{3}{2}\rangle + 0.005|\mp\tfrac{9}{2}\rangle \pm 0.001|\mp\tfrac{15}{2}\rangle$$

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

Emphasis: what matters is the wavefunction, not the spin value !

- may generally apply to any Kramers' doublets with J > 1/2 !

e.g, Ce: **$Ce_2Sn_2O_7$**

Candidate Quantum Spin Liquid in the Ce^{3+} Pyrochlore Stannate $Ce_2Sn_2O_7$

Romain Sibille,[1,*] Elsa Lhotel,[2] Vladimir Pomjakushin,[3] Chris Baines,[4] Tom Fennell,[3,†] and Michel Kenzelmann[1]

$4f^1$ ion in D_{3d} local symmetry to the susceptibility was realized between $T = 1.8$ and 370 K, and the resulting calculation of the single ion magnetic moment is shown in Fig. 2(c). The wave functions of the ground state Kramers doublet correspond to a linear combination of $m_J = \pm 3/2$ states. The fitted coefficients result in energy levels at 50 ±

Ce^{3+} $(4f^1, {}^2F$

$$J = \frac{5}{2}$$

the wavefucntion shou
of states with odd inte
3/2.

this really because of t
they are one-dimensio
even in the YbTiO, suc
the excited doublets.

Realistic **XYZ model**

and

Symmetry Enriched U(1) quantum spin liquids

next i will introduce the realistic XYZ model that describe the interaction between these peculiar doublet, and discuss the remarkable physical properties.

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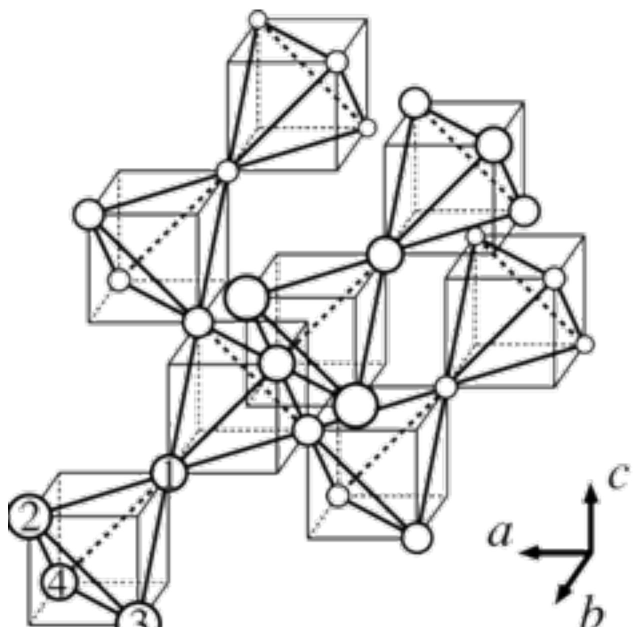
Symmetry properties

- Effective spin-1/2 under lattice symmetry

Tetra

$T_d \times \mathcal{I} \times translations$ and $T_d =$



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

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

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

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

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

just like what we do for any two-fold degree doublet, one can introduce an effective spin-1/2 to describe this doublet.

because of the peculiar property, the symmetry transformation of the effective spin components are rather interesting.

to simplify my notation, i use j =3/2 he

Generic model: XYZ model

with the symmetries, one can write down the generic symmetry allowed Hamiltonian.

even though the local moment results from strong spin-obit coupling, remarkable, the coupling is uniform spatially.

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

Uniform Spatially !

VS

$$H = \sum_{\langle ij \rangle} \{ J_{zz} \mathsf{S}_i^z \mathsf{S}_j^z - J_{\pm} (\mathsf{S}_i^+ \mathsf{S}_j^- + \mathsf{S}_i^- \mathsf{S}_j^+) + J_{\pm\pm} (\gamma_{ij} \mathsf{S}_i^+ \mathsf{S}_j^+ + \gamma_{ij}^* \mathsf{S}_i^- \mathsf{S}_j^-) + J_{z\pm} [\mathsf{S}_i^z (\zeta_{ij} \mathsf{S}_j^+ + \zeta_{ij}^* \mathsf{S}_j^-) + i \leftrightarrow j] \},$$

Anisotropic Spatially !

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A small transformation into XYZ model

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

this does not look like XYZ,

just because of the spatial uniformity, one can do a rotation in spin space without effecting real space,

Rotation around the y axis
in the effective spin space

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

XYZ model

Unfrustrated regime: ordered phase

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 by symmetry.

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

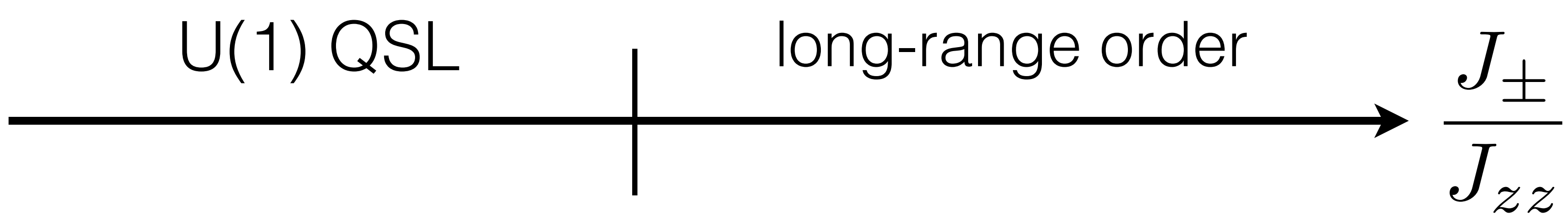
   This state is **rather distinct** from the above two states !
   It has an **antiferro-octupolar** order but **NO** dipolar order.

Symmetry-Enriched
U(1) quantum spin liquid

XXZ model can lead to U(1) QSL

$$H = J_{zz} \sum_{\langle i,j \rangle} S_i^z S_j^z - J_{\pm} \sum_{\langle i,j \rangle} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + \cdots\cdots$$

Hermele, Fisher, Balents, Moessner, Isakov, YB Kim….



- Pretty much one can add any term to create **quantum** tunneling, as not too large to induce magnetic order, the **ground state** is a U(1) Q

1. But classical spin ice is purely classical and is not a new phase matter. It is smoothly connected high temperature paramagnetic

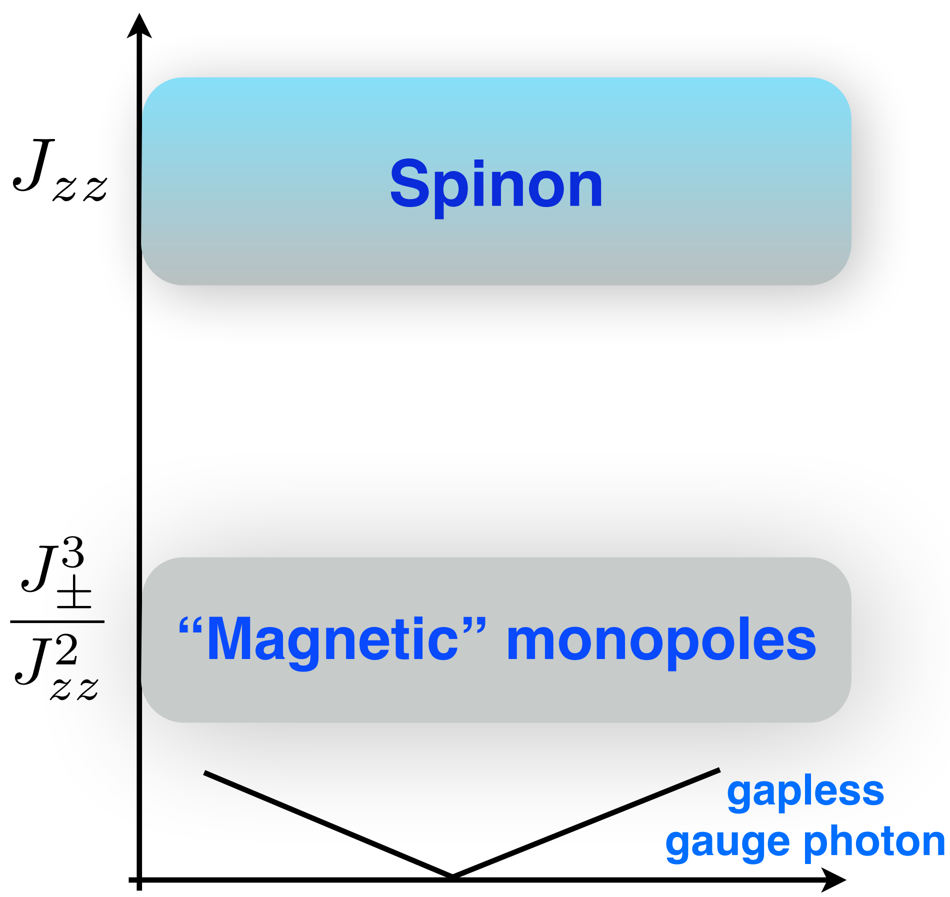
2. In contrast, quantum spin ice new quantum phase of matter.

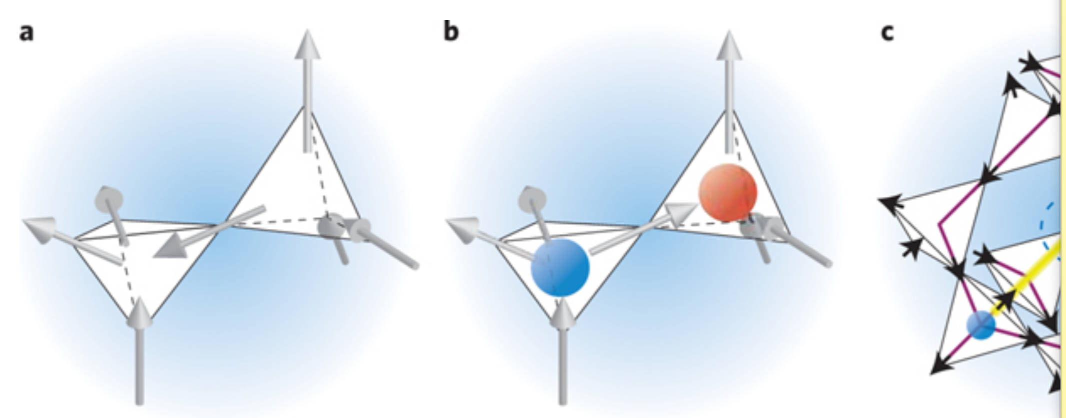
3. To obtain quantum spin ice, o simply add quantum spin flip ter the ising hamiltonian.

4. the quantum term allows the to tunnel from one spin ice state other.

5. As long as the term is not too the system is disordered, and th ground sate is quantum spin ice.

Emergent Quantum Electrodynamics





Figs from Mo

Spinon deconfinement

as quantum spin ice is a dis
there is no long range order,
a new phase of matter and c
in the landau’s paradigm of

the right description of quan
fractionalization and emerge

there are 3 elementary excita
gauge photon,
it is not goldstone boson, w
breaking, there is no sym br
of emergent gauge structure

there are deconfined spinon
create 2 spinons,
you can flip the further spins
arbitrary distance, it is only c
image there is a string conne
spin is strongly fluting, the s
spinon are decofnined.

the 3rd is magnetic monopo
defect of the emergent U(1)

It is exotic phase of matter, l
propertes as too order.

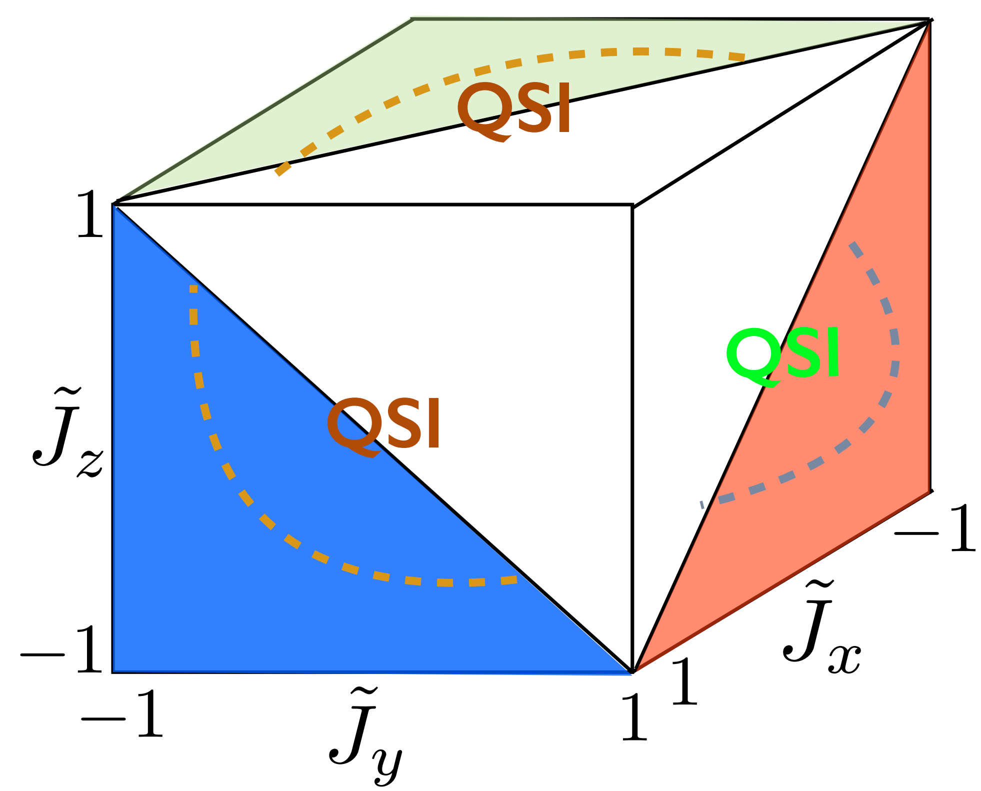
Emergent electric field $S^z \sim E$

Emergent vector potential $S^{\pm} \sim e^{\pm iA}$

XYZ model is **much richer** !

unlike XXZ model, XYZ model is r
richer

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



3D phase diagram

Each component (not just Sz) can be emergent electric field, depending on the parameters !

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

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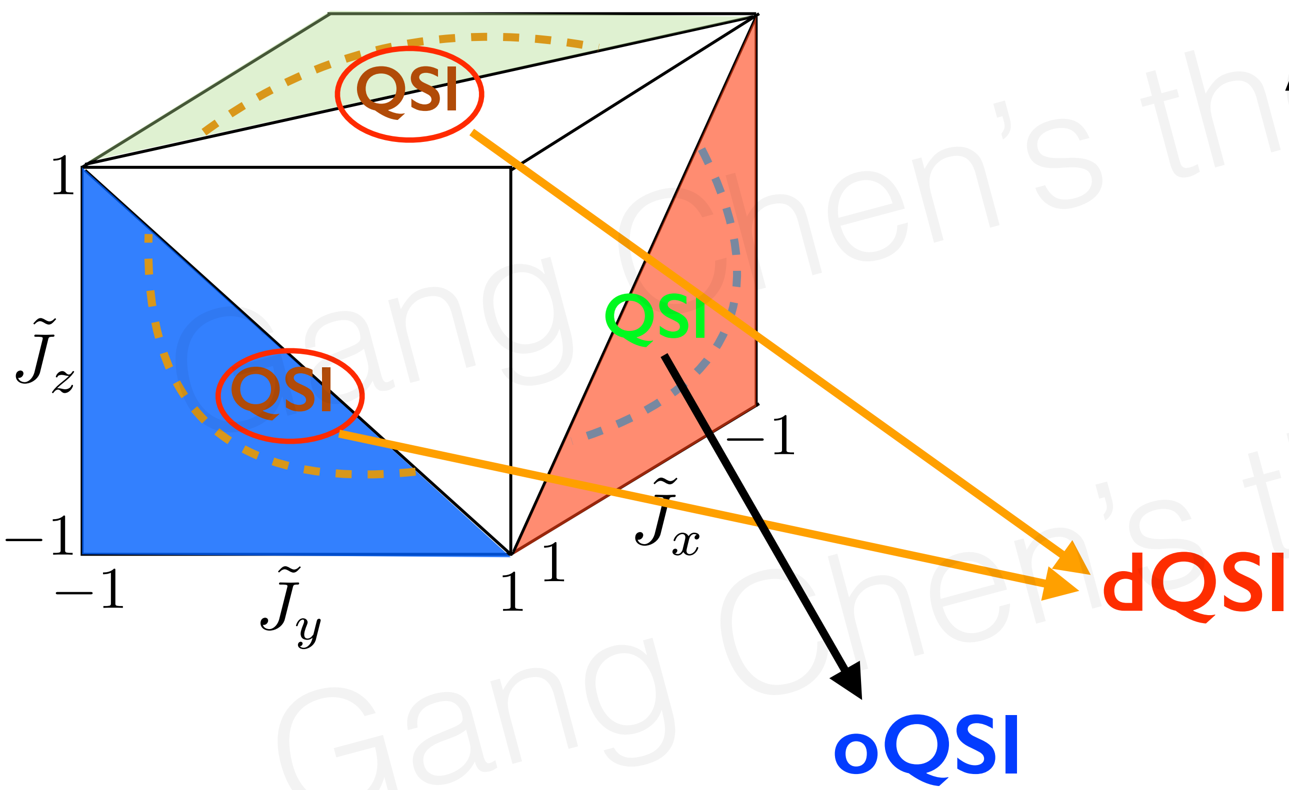
Realistic Symmetry Enrichment

Xiao-Gang Wen
Symmetry Enriched Topological order (**SET**)

Are they different?

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



$C_3 : S$

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

$\mathcal{I} : S$

there is a hugh theoretical activity in SET, there are a lot of classification of SET with fancy mathematics such as group cohomology

dQSI vs oQSI

Transformation of continuum E/B field under Oh point group

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

since the lowenrgy field theory is identical , both phyase have identical theromonydmica properties

- Both phases have identical thermodynami
  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 nearest-neighbor Z2xZ2 symmetry, decay exponentially.

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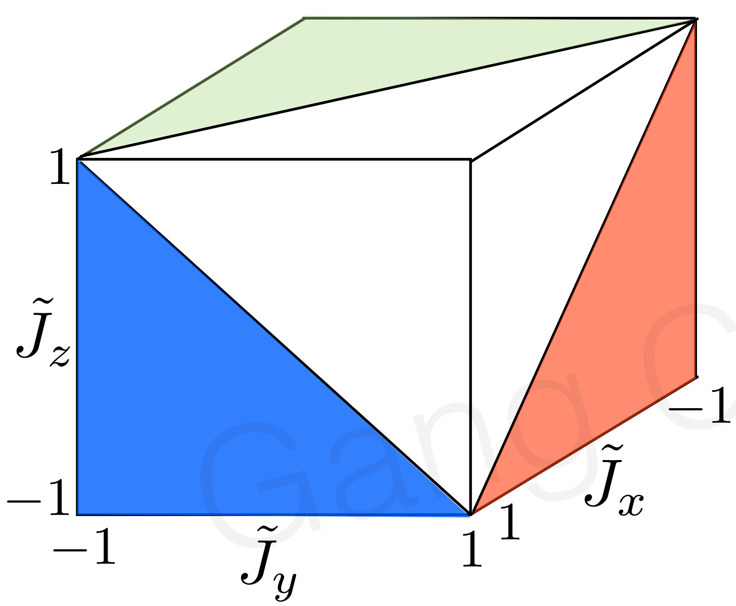
Sign problem free for QMC



no sign problem
in the shaded parts

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

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

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

- Realistic (and nontrivial) model for QMC.
- Actually no sign problem on any lattice !
- Possibility of Z2 liquid?

"*Classification of Kagame Z2 liquid*", Feiye Li, A Essin, **GC**, 2016 (appear soon)
"*Classification of Kagame Z2 liquid*", YP Huang, Hermele, 2016 (see Huang's talk)

Kagome lattice, Carrasquilla, Hao, Melko, 2015
Triangular lattice, Y-B Yang, **GC**, etc (in preparation)
Pyrochlore lattice, ZY Meng, **GC**, etc (in preparation)
FCC lattice, J. Lou, **GC**, etc (in preparation)
Checkerboard lattice R Yu, **GC**, etc (in preparation)

Materials

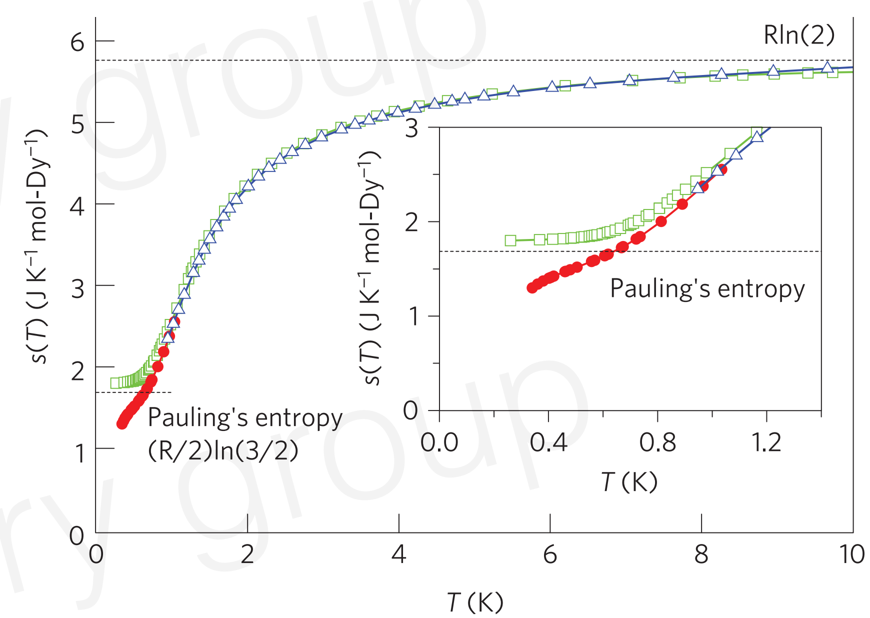
Material survey

Our doublet can potentially be realized for any Kramers spin moment with J>1/2.

Two well-known systems:

- Pyrochlores $A_2B_2O_7$,

  e.g. ,
  $Nd_2Ir_2O_7$, $Nd_2Sn_2O_7$, $Nd_2Zr_2O_7$, etc
  $Dy_2Ti_2O_7$,
  $Cd_2Os_2O_7$, etc
  $Ce_2Sn_2O_7$,



Prof Gaulin's group, Dy2Ti2O7, Nat Phys, 2013

- Spinels AB_2X_4, B=lanthanide?

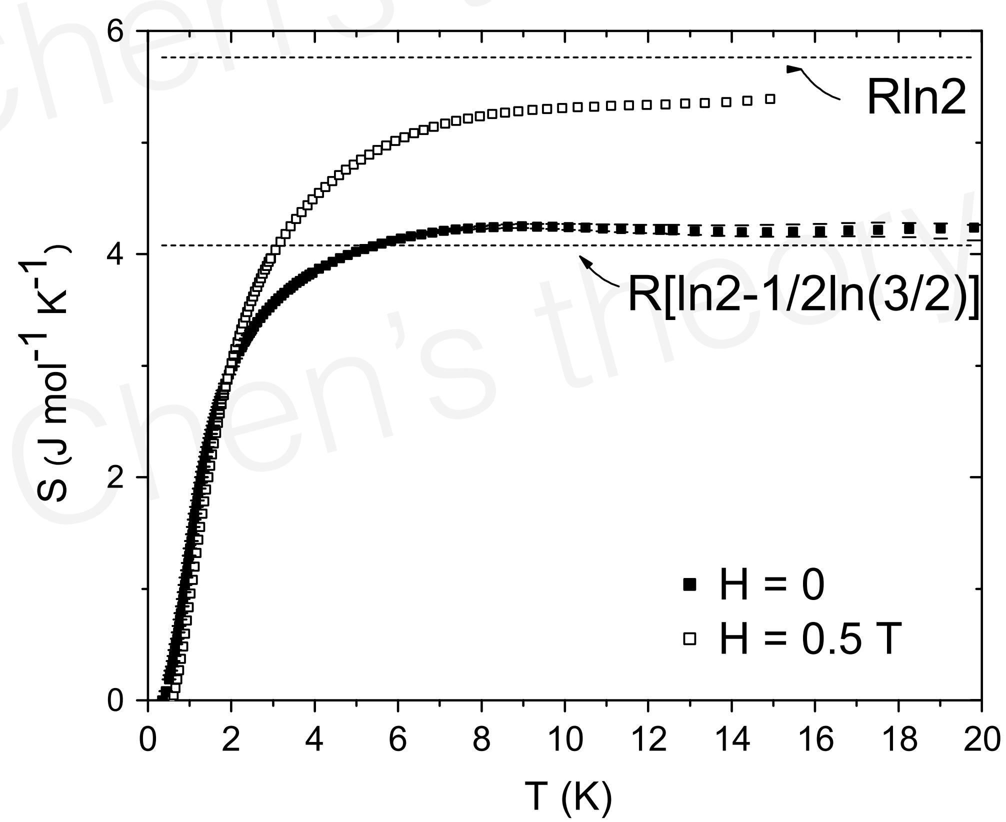
  e.g. $CdEr_2Se_4$

  $CdYb_2S_4$

$CdEr_2Se_4$: A New Erbium Spin Ice System in a Spinel Structure

J. Lago,[1,*] I. Živković,[2,3] B. Z. Malkin,[4] J. Rodriguez Fernandez,[5] P. Ghigna,[6] P. Dalmas de Réotier,[7]
A. Yaouanc,[7] and T. Rojo[1,†]

the ground state Kramers doublet are $|\pm\rangle = 0.8792|\pm 15/2\rangle \mp 0.4418|\pm 9/2\rangle + 0.1571|\pm 3/2\rangle \pm 0.0843|\mp 3/2\rangle$, where $|J_z\rangle = |^4I_{15/2}, J_z\rangle$ are the eigenfunctions of the z component of the angular moment with z being the easy magnetization axis $\langle 111\rangle$. The values of



Pauling entropy in $CdEr_2Se_4$

PRL 115, 097202 (2015) PHYSICAL REVIEW LETTERS week ending 28 AUGUST 2015

Candidate Quantum Spin Liquid in the Ce^{3+} Pyrochlore Stannate $Ce_2Sn_2O_7$

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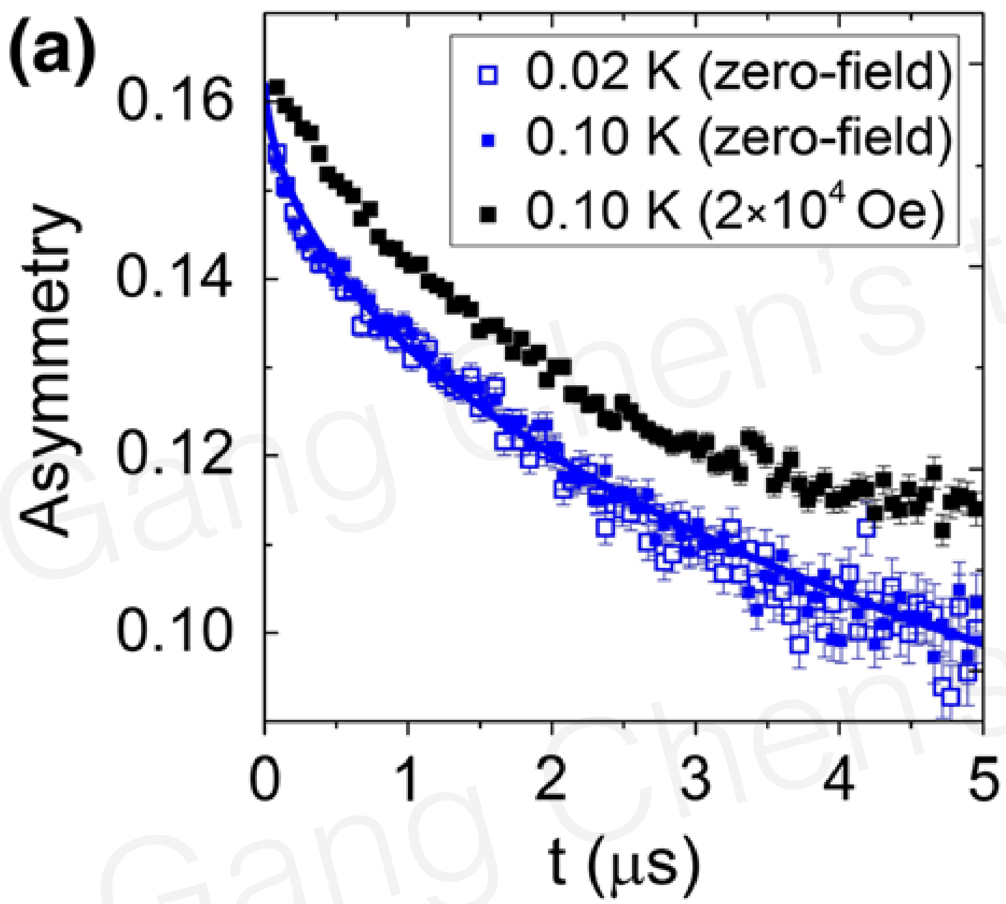

muSR

- No sign of ordering down to 0.02K
- Is it dipole-QSI, or, octupole-QSI?

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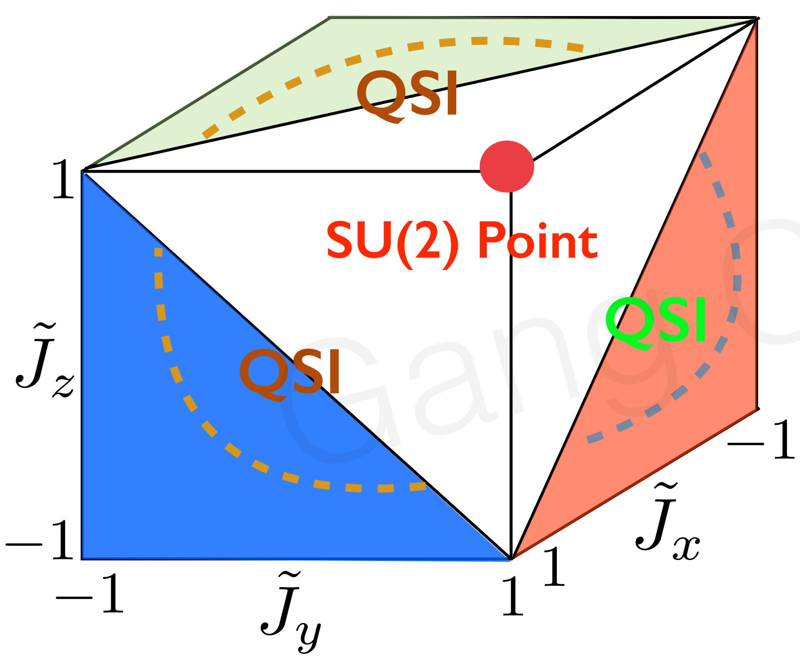
Summary

- We propose a new doublet dubbed "dipole-octupole" doublet.
- We propose a generic XYZ model for our new doublet.
- This XYZ model supports both exotic (octupolar) order and symmetry enriched U(1) quantum spin liquid (quantum spin ice) ground states.
- There exist a large class of materials (not just pyrochlore, **any other lattices with the same point group**) that can support such doublets.
- The remarkable properties of the doublet allows a direct comparison between numerics and experiments.

OPEN 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