Octupolar quantum spin ice:

Controlling spinons in a U(1) quantum spin liquid

Gang Chen (陈 钢)
Fudan University

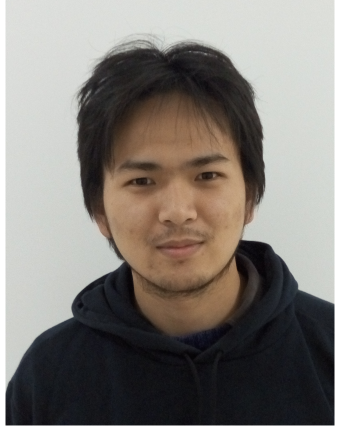
Opportunity for students and postdocs

- My group is looking for graduate students and postdocs
- Our **postdocs and visiting professors** are generously funded.
  Postdoc: ~230K RMB/year + other benefits
  Visiting Prof: ~500 RMB/day + hotel + travel

Outline

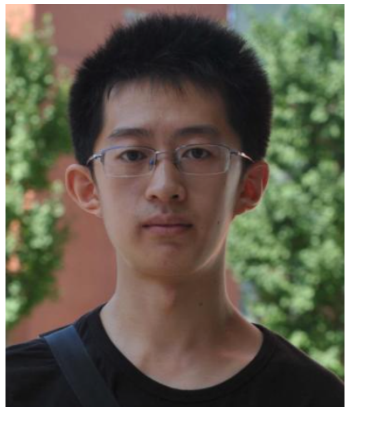
- Symmetry enriched U(1) topological order:
  dipolar and octupolar U(1) quantum spin liquids

- Control spinons in a U(1) quantum spin liquid



Yao-Dong Li
(Fudan)

- Quantum order by disorder, Weyl magnon, Kitaev-Heisenberg model in rare-earth double perovskites



Fei-Ye Li
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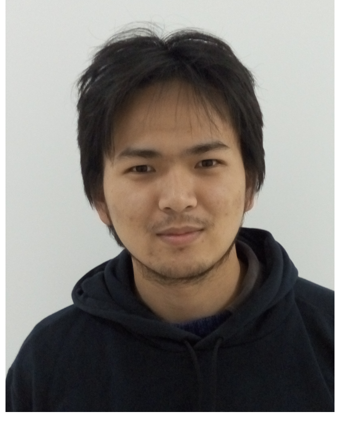

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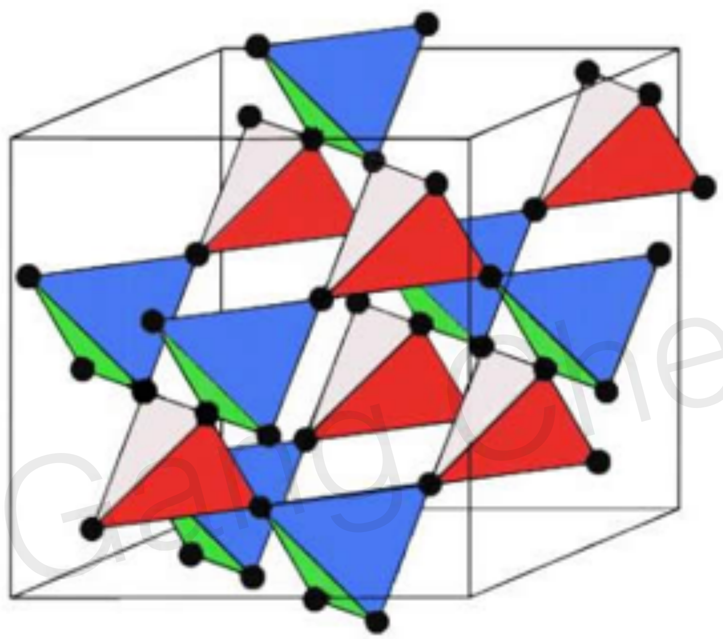
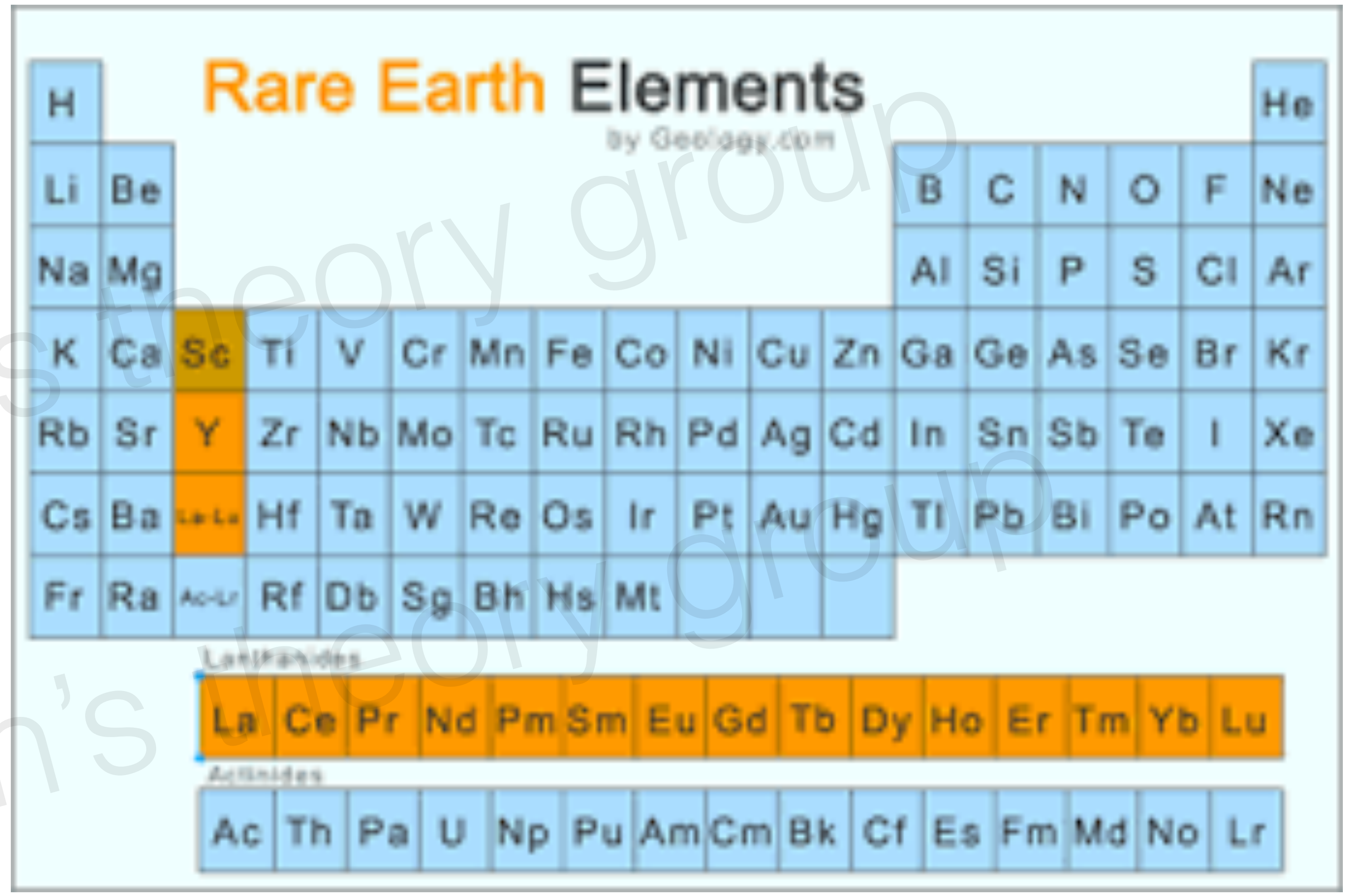
- Octupolar U(1) quantum spin liquid of quantum spin ice

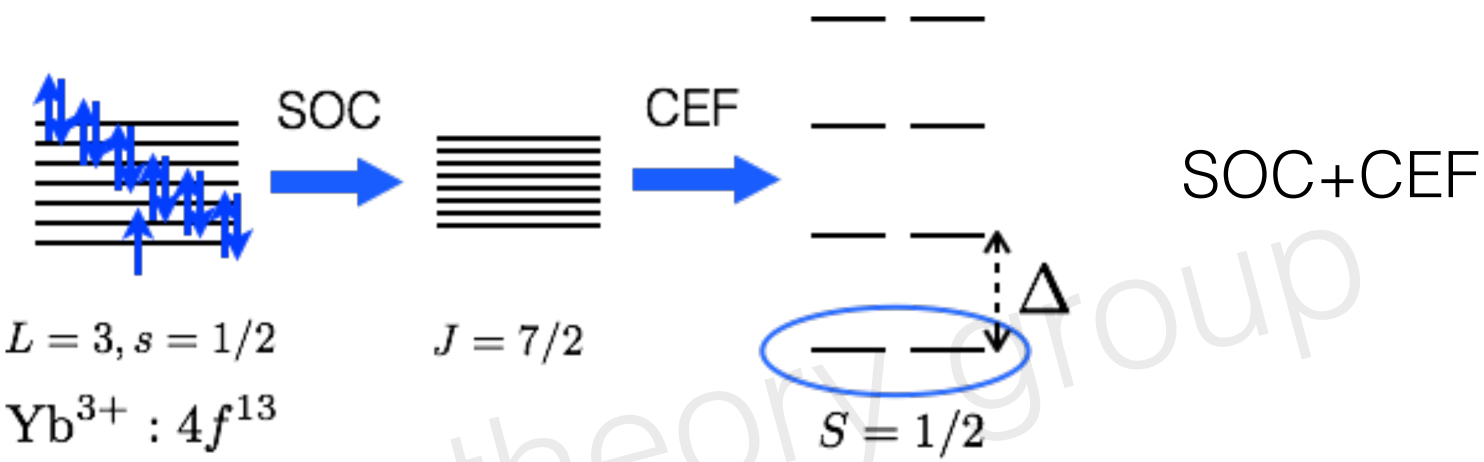
Rare-earth pyrochlores



$RE_2M_2O_7$



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



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

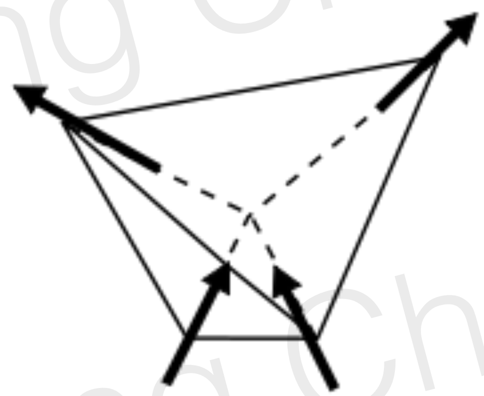
lanthanum	cerium	praseodymium	neodymium	promethium	samarium	europium	gadolinium	terbium	dysprosium	holmium	erbium	thulium	ytterbium
57	58	59	60	61	62	63	64	65	66	67	68	69	70
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
138.91	140.12	140.91	144.24	[145]	150.36	151.96	157.25	158.93	162.50	164.93	167.26	168.93	173.04

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

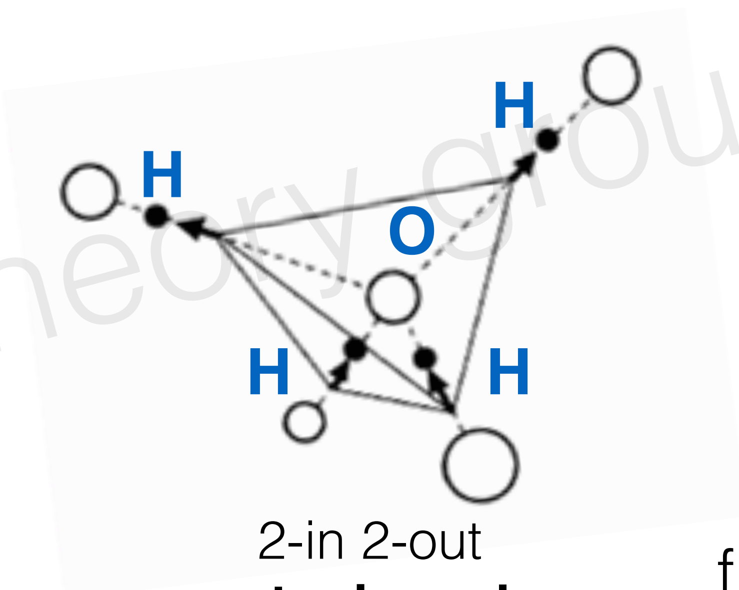
lanthanum	cerium	praseodymium	neodymium	promethium	samarium	europium	gadolinium	terbium	dysprosium	holmium	erbium	thulium	ytterbium
57	58	59	60	61	62	63	64	65	66	67	68	69	70
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
138.91	140.12	140.91	144.24	[145]	150.36	151.96	157.25	158.93	162.50	164.93	167.26	168.93	173.04

Spin ice (Ising) limit

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

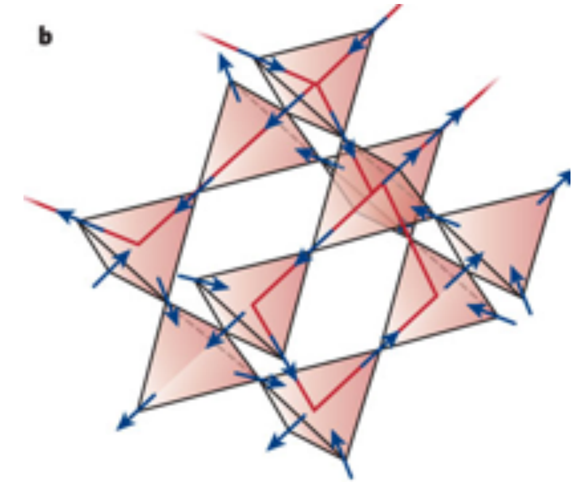


2-in 2-out
spin ice rule



2-in 2-out
water ice rule

from wiki



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.

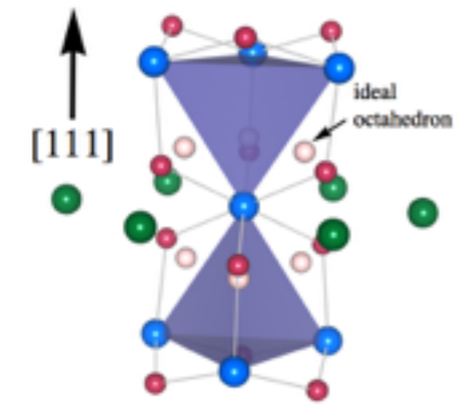
Pinch points in spin correlation

Dipole-octupole doublet

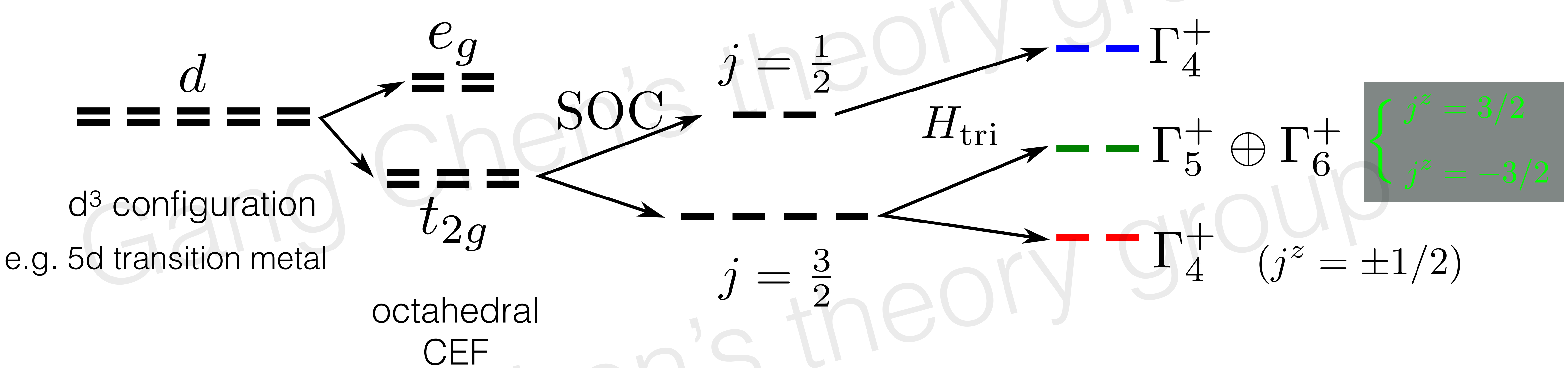
The early classification of local moments is a bit crude !

One should carefully examine the wavefunction of the local doublet.

Local physics: start with t_{2g} electrons



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



d electrons under D_{3d}
point group crystal field

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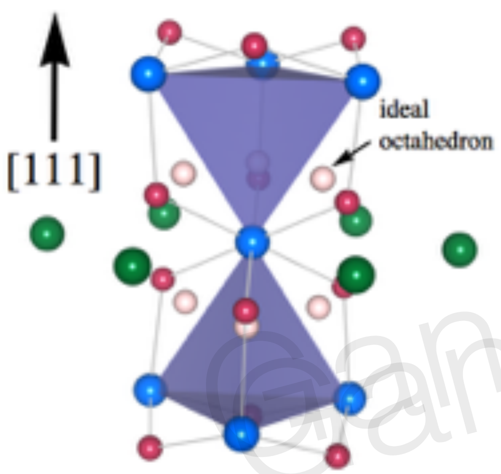
- Why is this Kramers doublet so special ?

ONE-dimensional representations of the point group !

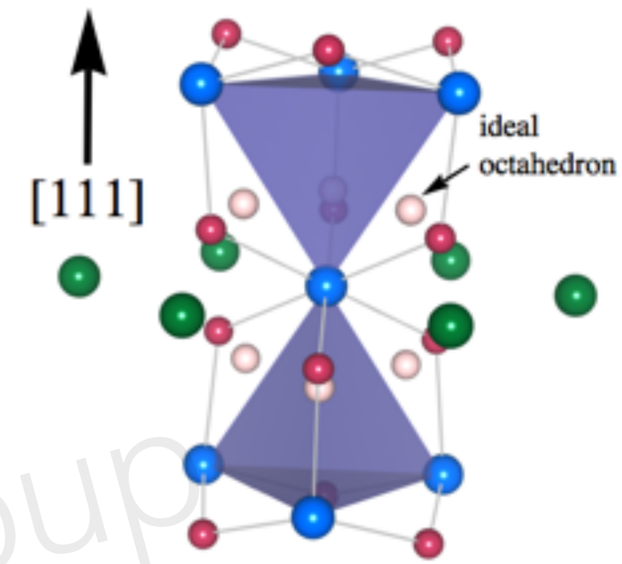


$$R(2\pi/3)|J^z = \pm 3/2\rangle = -|J^z = \pm 3/2\rangle$$

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

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

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

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

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: **$Ce_2Sn_2O_7$**

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

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

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+} $(4f^1, {}^2F_{5/2})$.

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

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Realistic **XYZ model**

and

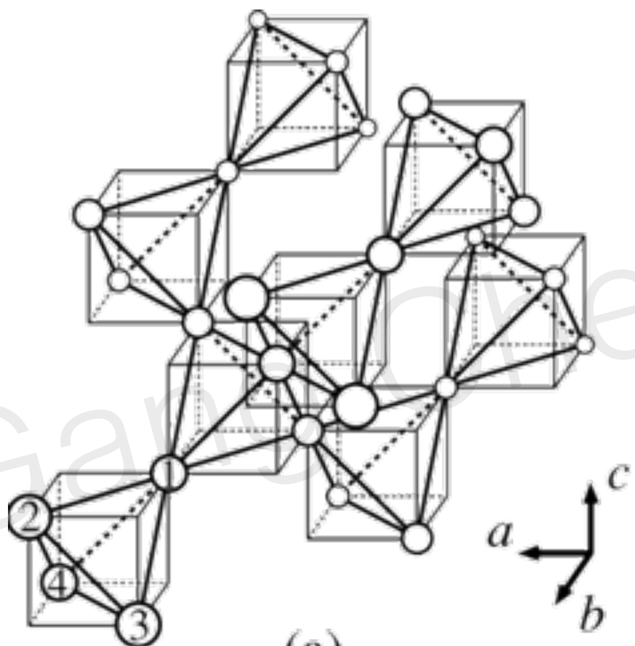
Symmetry Enriched U(1) topological order

Symmetry properties

- Effective spin-1/2 under lattice symmetry

Tetrahedral Group

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



(a)

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

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

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

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

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

Generic model: XYZ model

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

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 !

A small transformation into XYZ model

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

Rotation around the y axis
in the effective spin space

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

XYZ model

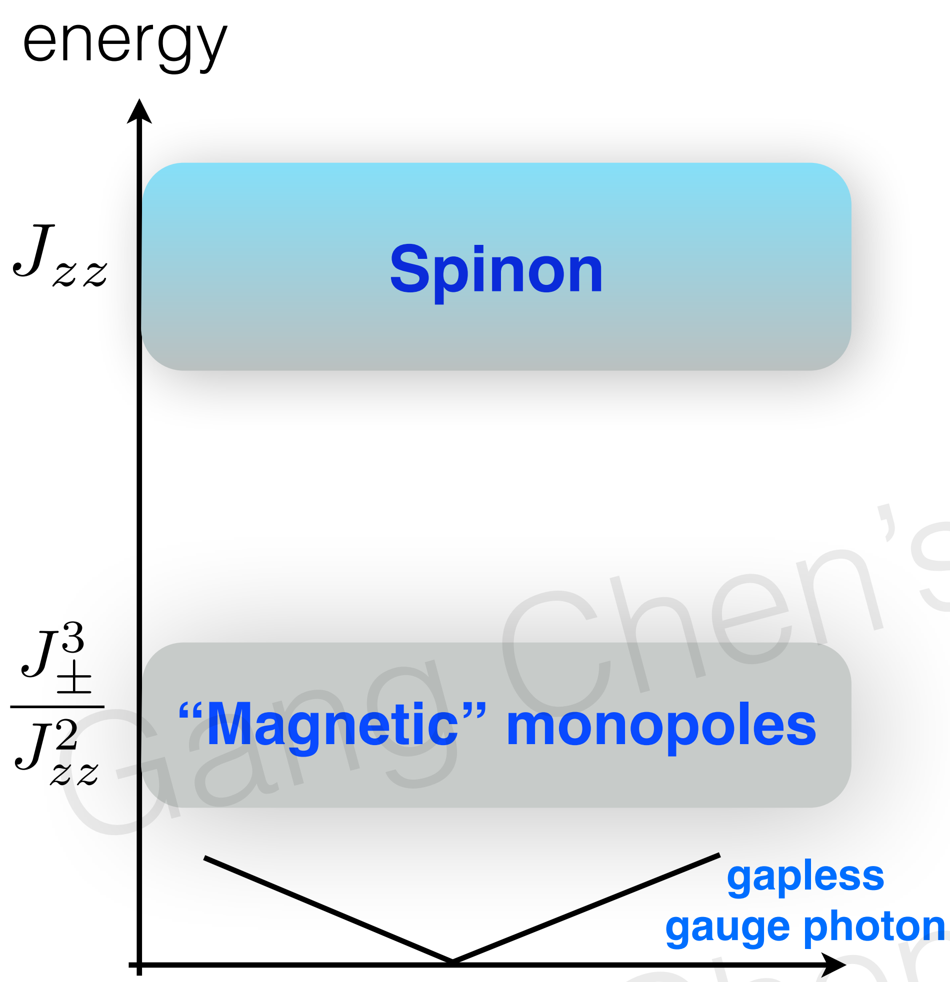
XXZ model can lead to U(1) QSL

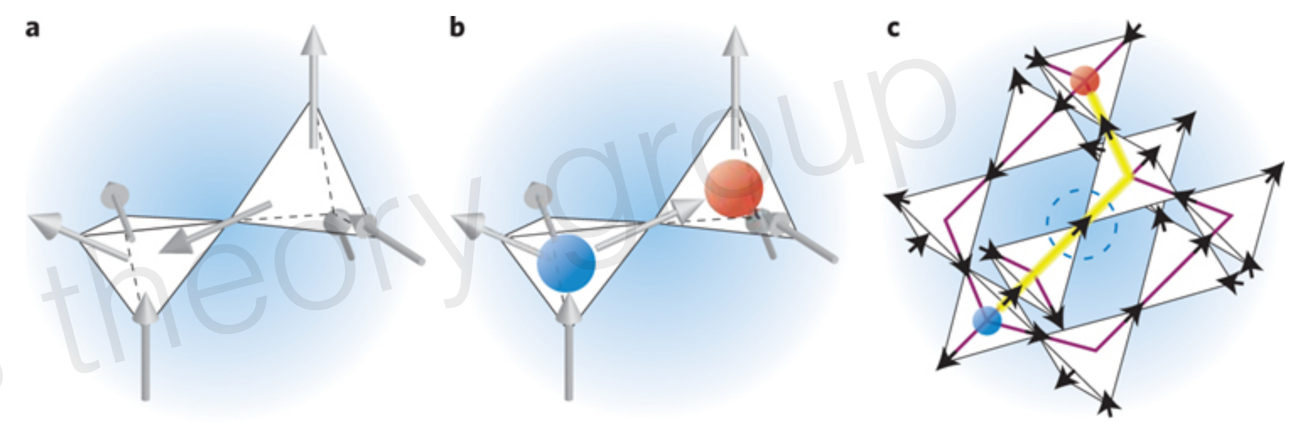
$$H = J_{zz} \sum_{\langle i,j \rangle} S_i^z S_j^z - J_{\pm} \sum_{\langle i,j \rangle} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + \cdots\cdots$$

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

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

Emergent Quantum Electrodynamics





Figs from Moessner&Schiffer,2009

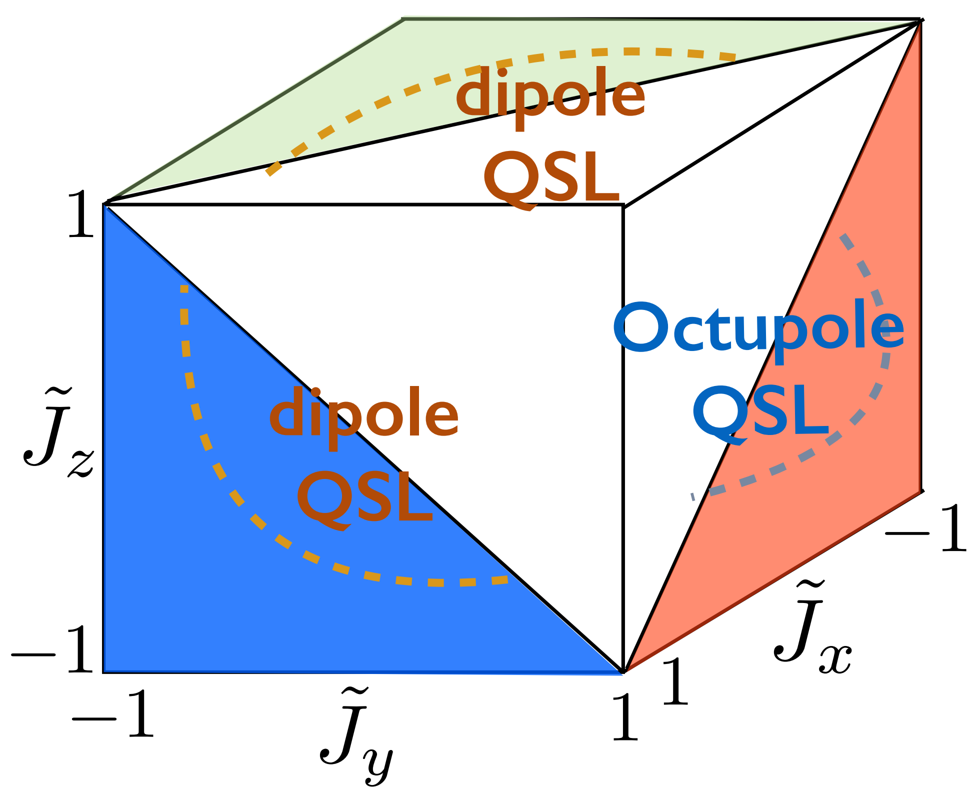
Spinon deconfinement

Emergent electric field $S^z \sim E$

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

XYZ model is the generic model that describes the interaction between DO doublets.

$$H_{\mathrm{XYZ}} = \sum_{\langle ij \rangle} \mathcal{J}_x \tau_i^z \tau_j^z + \mathcal{J}_y \tau_i^y \tau_j^y + \mathcal{J}_z \tau_i^z \tau_j^z$$



3D phase diagram

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

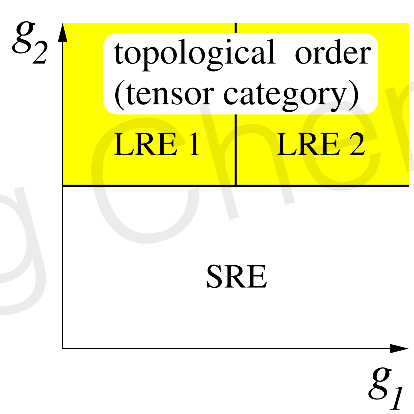
Study phase on a cube: $-1 \leq \tilde{J}_{x,y,z} \leq 1$.

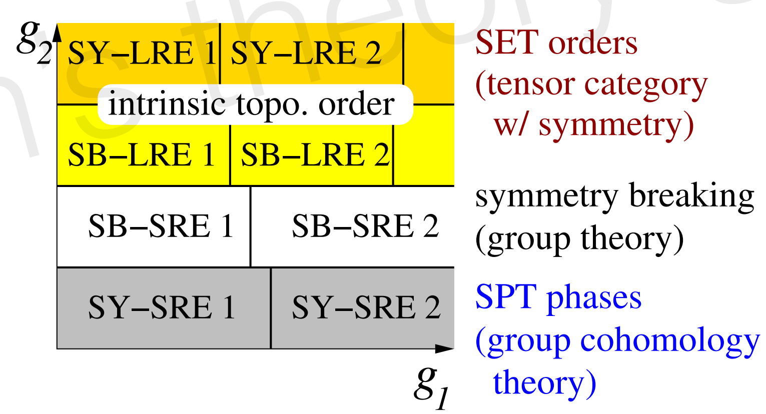
Xiaogang Wen

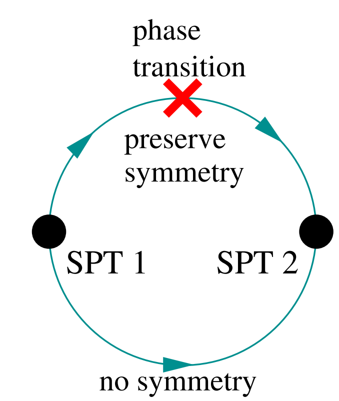
Gapped phases w/ symmetry → SET and SPT phases

- there are LRE symmetric states → Symm. Enriched Topo. phases
  - 100s symm. spin liquid through the PSG of topo. excit. Wen 02
  - 8 trans. symm. enriched Z_2 topo. order in 2D, 256 in 3D Kou-Wen 09
  - $1000,000$s symm. Z_2 spin liquid through $[\mathcal{H}^2(SG, Z_2)]^2\times$ Hermele 12
  - Classify SET phases through $\mathcal{H}^3[SG \times GG, U(1)]$ Ran 12
- there are SRE symmetric states → many different phases

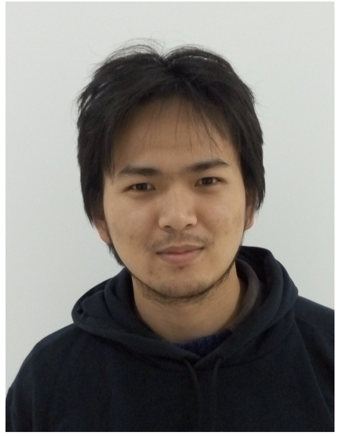
We may call them **symmetry protected** **trivial** **(SPT)** phase







- Control spinons in a quantum spin ice U(1) quantum spin liquid



Yao-Dong Li
(Fudan)

arxiv yesterday

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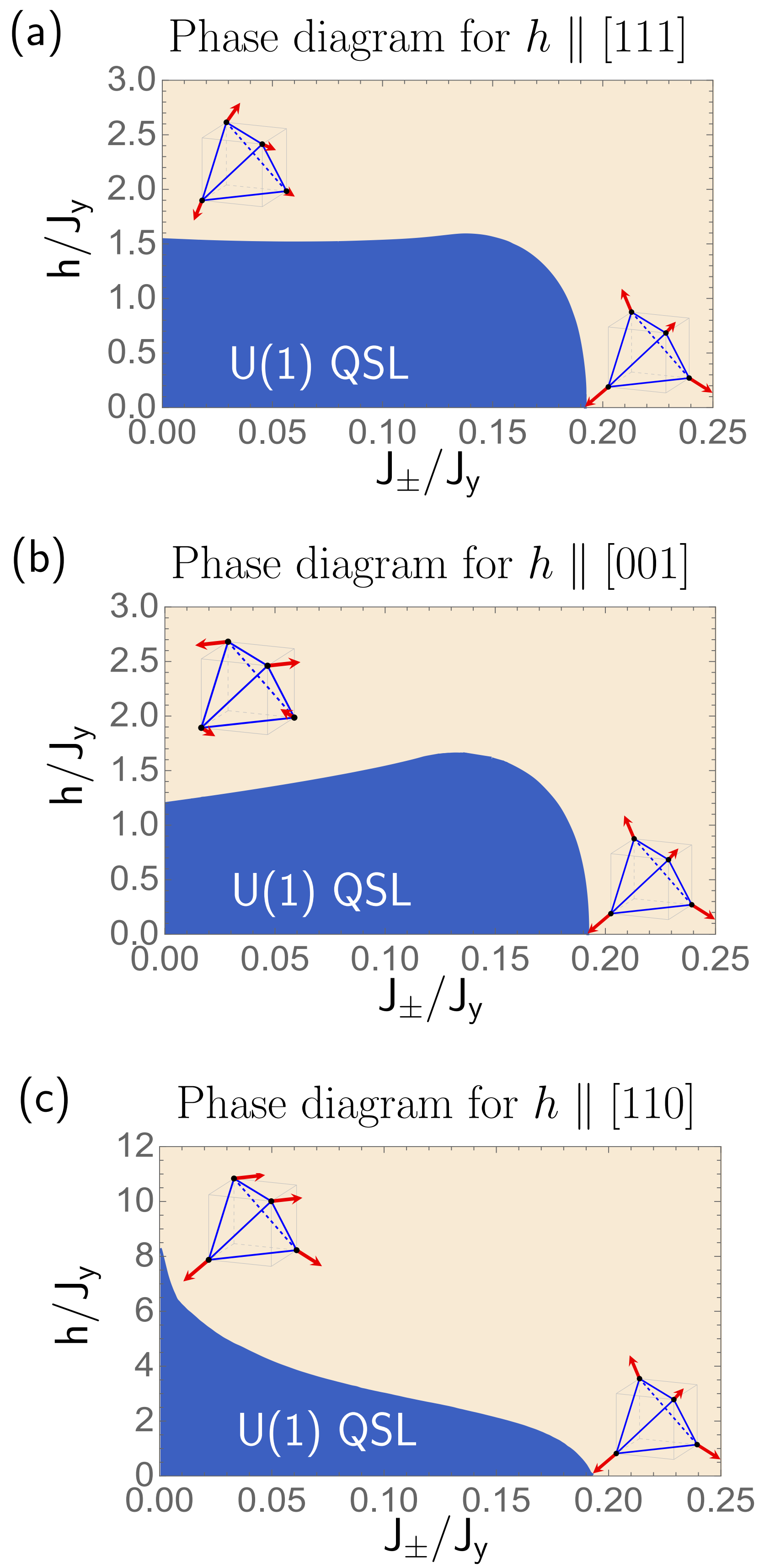
Field-driven Higgs transition for octupolar U(1) QSL



How to tell if Ce2Sn2O7 is an octupolar U(1) QSL or not ?

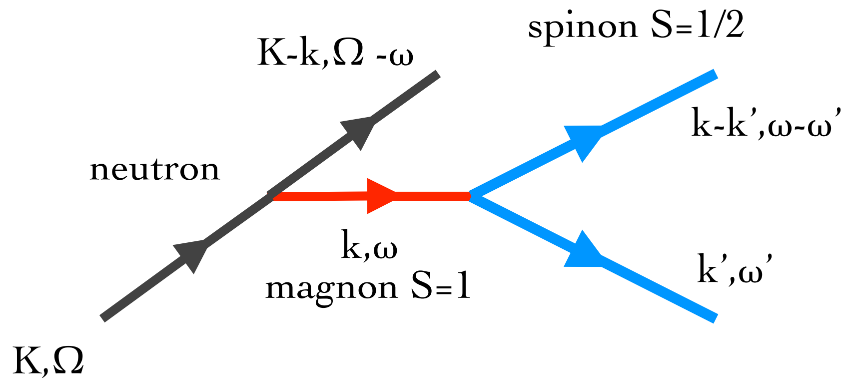
The idea to use a little knob that could simply lead to some clear experimental consequence, very much like the isotope effect of BCS superconductors.

Here we apply external magnetic field, and expect a field-driven Higgs transition to magnetic ordering as the field only couples to the matter field (spinons).

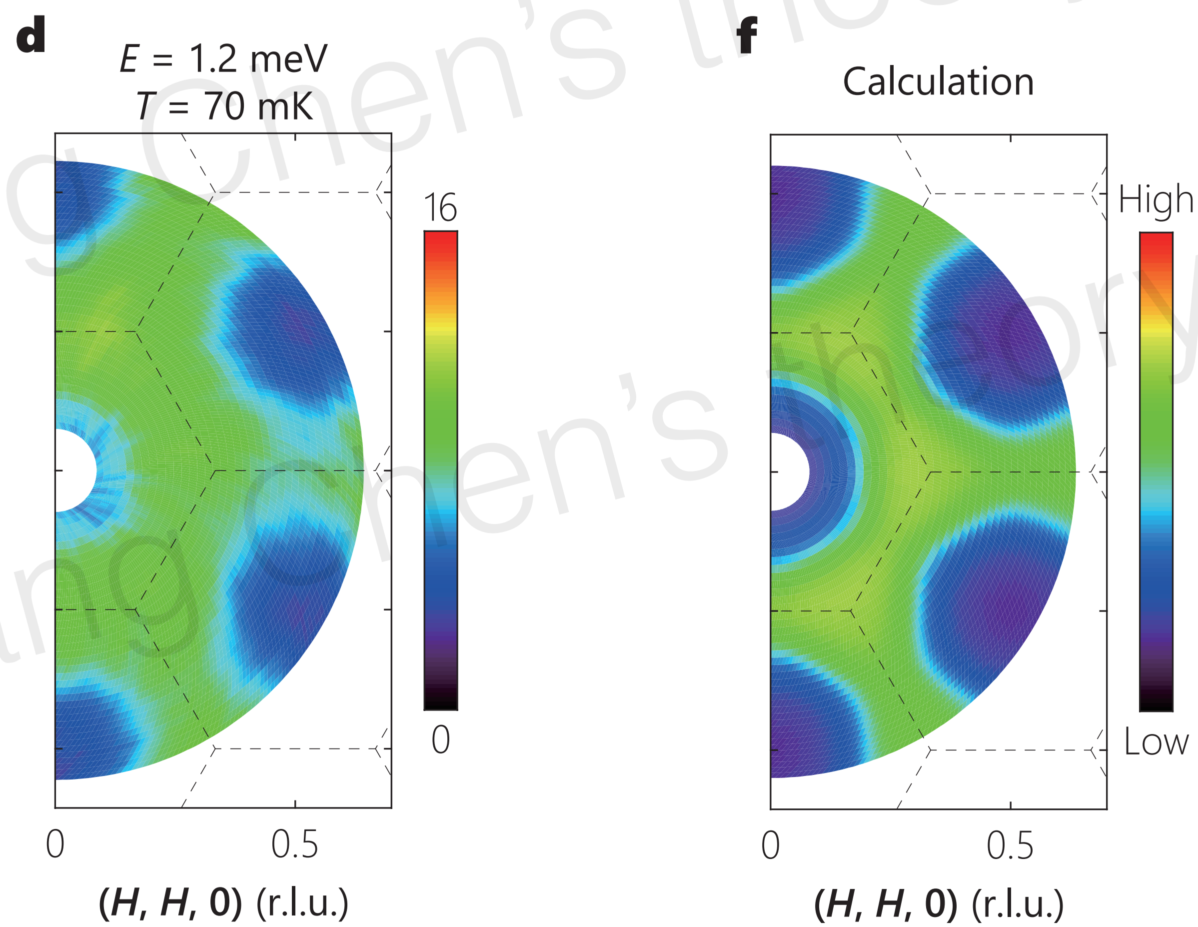
$$H_{\rm sim} = \sum_{\langle ij \rangle} J_y \tau_i^y \tau_j^y - J_\pm (\tau_i^+ \tau_j^- + h.c.) - \sum_i h\,(\hat{n} \cdot \hat{z}_i)\, \tau_i^z,$$

$$\tau_i^\pm = \tau_i^z \pm i \tau_i^x$$

Inelastic neutron scattering and spinon continuum



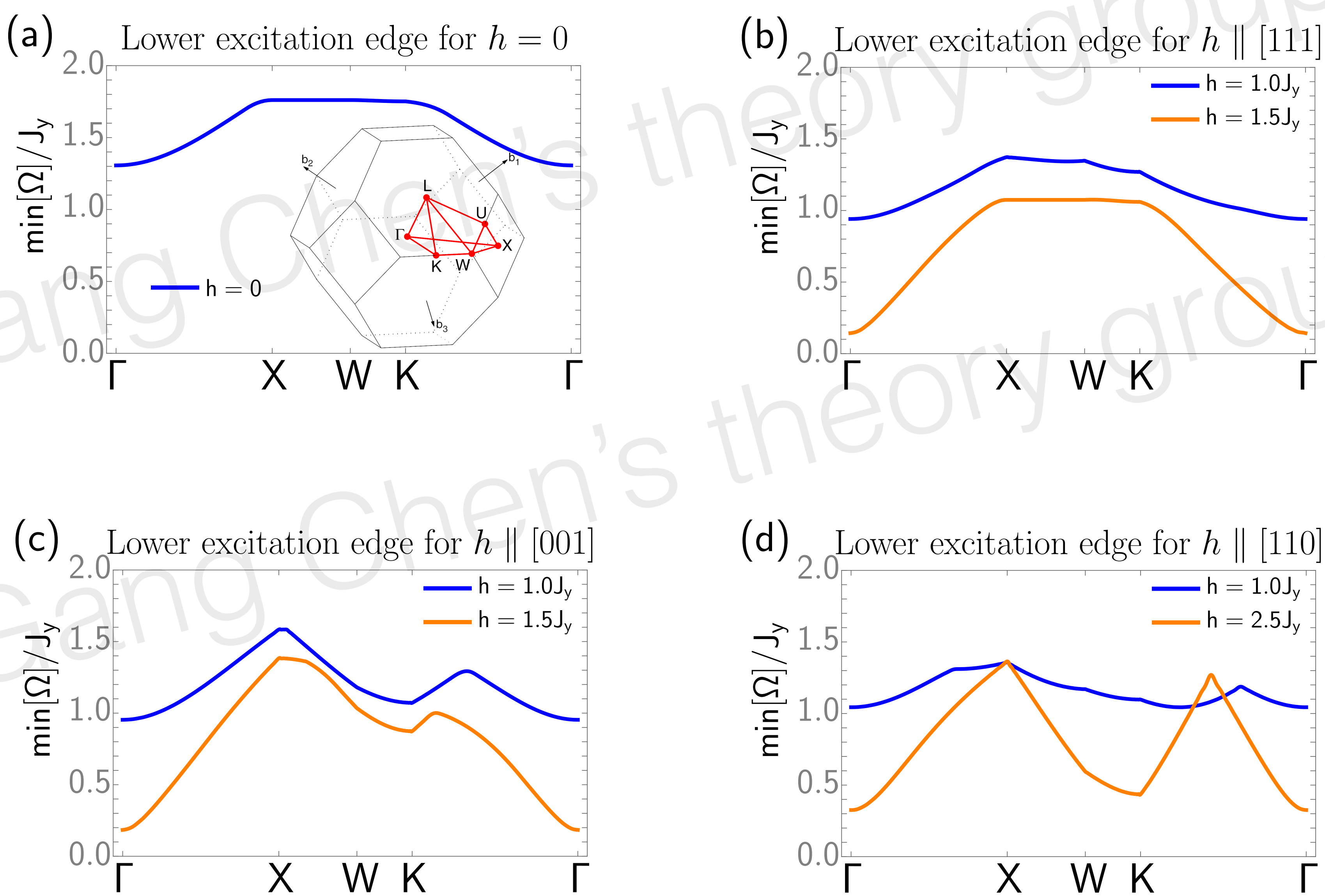
broad peak with
ω=ε(k’)+ε(k-k’)



Spinon continuum
in $YbMgGaO_4$
(today’s arXiv)

Lower excitation edge

$$\mathbf{q} = \mathbf{k}_1 + \mathbf{k}_2,$$
$$\Omega(\mathbf{q}) = \omega_i(\mathbf{k}_1) + \omega_j(\mathbf{k}_2),$$



Neutron scattering and thermal transport

Different U(1) QSLs	Heat capacity	Inelastic neutron scattering measurement
Octupolar U(1) QSL for DO doublets	$C_v \sim T^3$	Gapped spinon continuum
Dipolar U(1) QSL for DO doublets	$C_v \sim T^3$	Both gapless gauge photon and gapped spinon continuum
Dipolar U(1) QSL for non-Kramers' doublets	$C_v \sim T^3$	Gapless gauge photon
Dipolar U(1) QSL for usual Kramers' doublets	$C_v \sim T^3$	Both gapless gauge photon and gapped spinon continuum

Thermal transport

see both contribution, but there is a big separation of energy scales in spinon and gapless photons.

Material survey: other DO doublet systems

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

Two well-known systems:

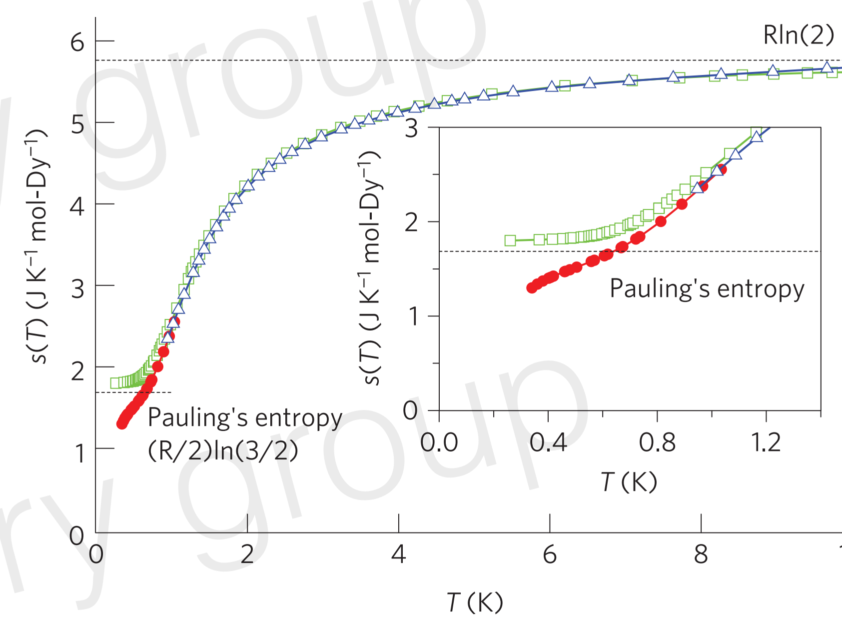
- Pyrochlores $A_2B_2O_7$,

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

- Spinels AB_2X_4, B=lanthanide?

  e.g. $CdEr_2Se_4$

  $CdYb_2S_4$



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

Conclusion

- 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. We propose a way to detect the consequence of symmetry enrichment.