Emergent magnetic order from weak-crystal field, Octupolar quantum spin ice, Hole doped Sr_2IrO_4

as usual psychology, one is more excited about the new work. today i will present some preliminary results of these new problems.

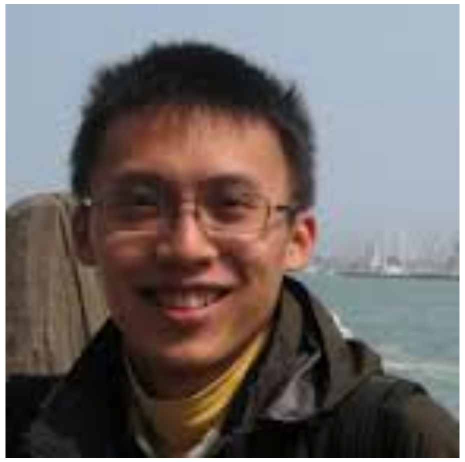
Gang Chen

June 11, 2016

復旦大學 FUDAN UNIVERSITY

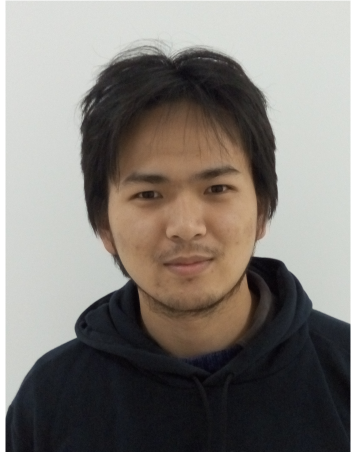
Outline

- Emergent magnetic order due to "weak" crystal field gap.



Yi-Ping Huang
(Univ of Colorado, Boulder)

- Field driven Anderson-Higgs' transition in octupolar quantum spin ice.

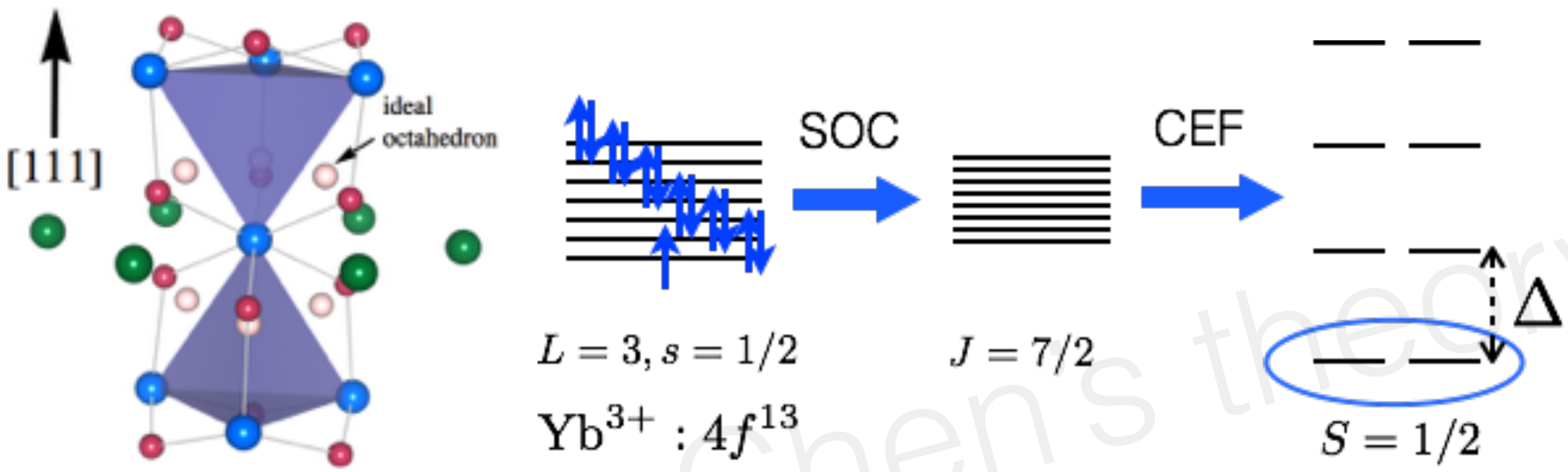


Yao-Dong Li
(Dept of computer sciences, Fudan)

- Hole doped Sr_2IrO_4: the difference from cuprates ! (by myself)

if I am asked, I will talk about it.

Crystal field energy levels



e.g. YbMgGaO4, Yao-dong Li, XQ Wang, GC, 2016

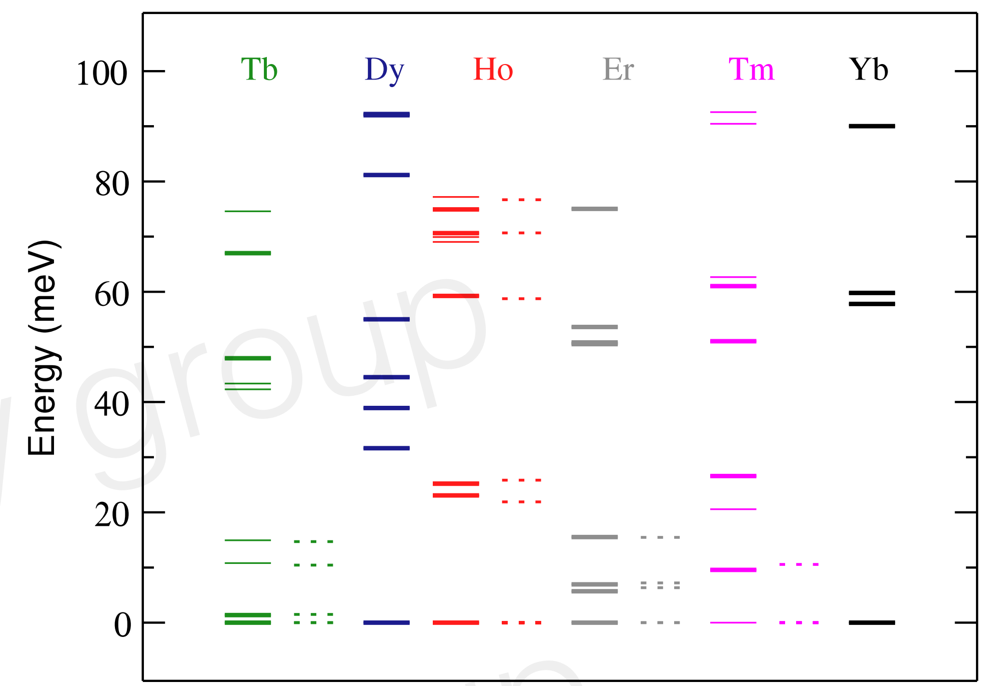
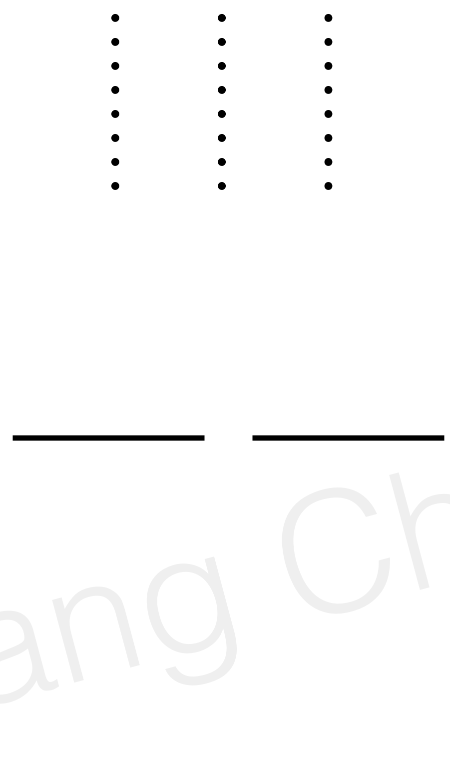


Figure 1. The computed CEF energy scheme drawn for the R ions in the $R_2Ti_2O_7$ pyrochlore series and comparison with experimental values when available, as extracted from inelastic neutron scattering measurements. Energy levels are given in units of millielectronvolts.

We often think that the ground state doublet controls the low temperature magnetic properties.

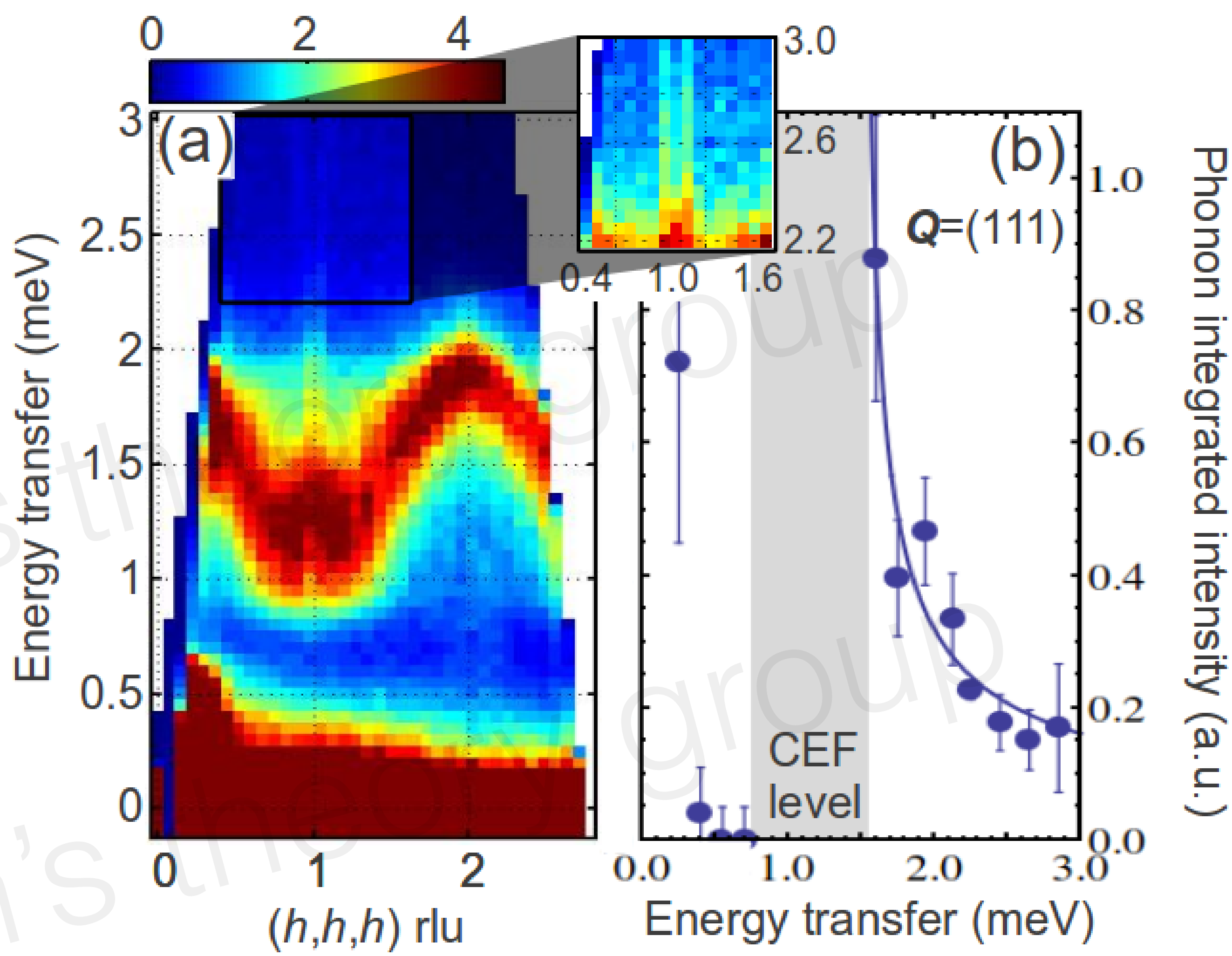
This happens when the crystal field gap is much larger than the temperature and exchange interaction scales.

Dispersion of the excited doublets



crystal field levels of Tb^{3+}

at one site



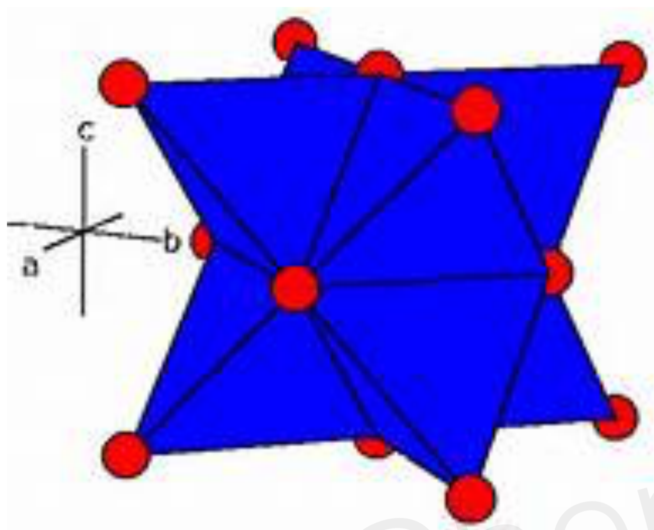
S. Guitteny, et al, arXiv: 1305.6363

Question: how if the crystal field gap is "weak"?

or equivalently, the exchange is strong.

intuition.

Model Calculation



FCC lattice

$$\vdots \quad \vdots \quad \vdots$$

$S^z = 1$ $\quad$ $S^z = -1$

$S^z = 0$

$$\tau^z = \frac{1}{2} s^z$$

$$\tau_i^{\pm} = \frac{1}{2} \left(s_i^{\pm}\right)^2$$

$$H_{ex} = \frac{1}{2} \sum_{\langle ij \rangle} J_{zz} \tau_i^z \tau_j^z - J_{\pm} \left(\tau_i^{+} \tau_j^{-} + h.c. \right)$$

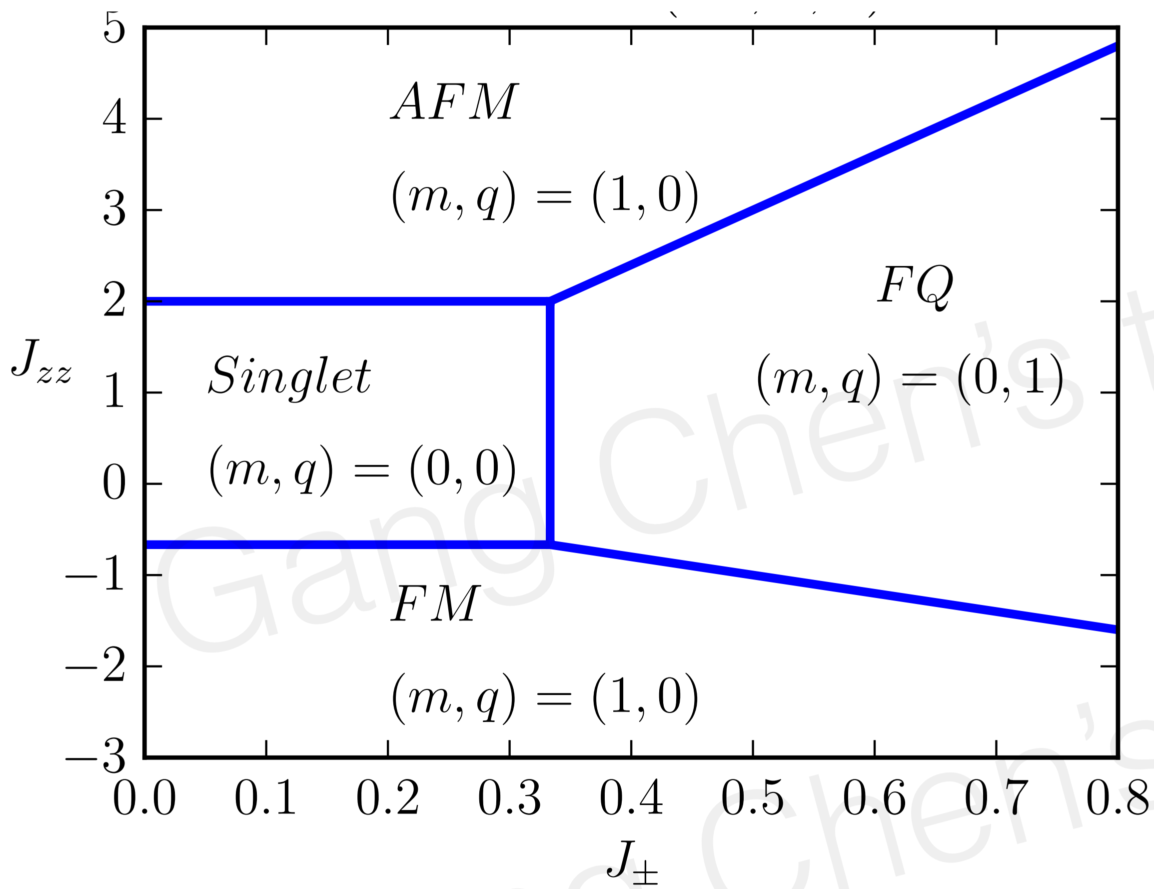
$H = $ …

H_{CEF} …

Since this observation is general, we can actually demonstrate this physics can happen in any other lattice.

Our formalism here can be easily adapted to more general situations.

Phase diagram



m is the magnetic dipolar order
q is the magnetic quadrupolar order

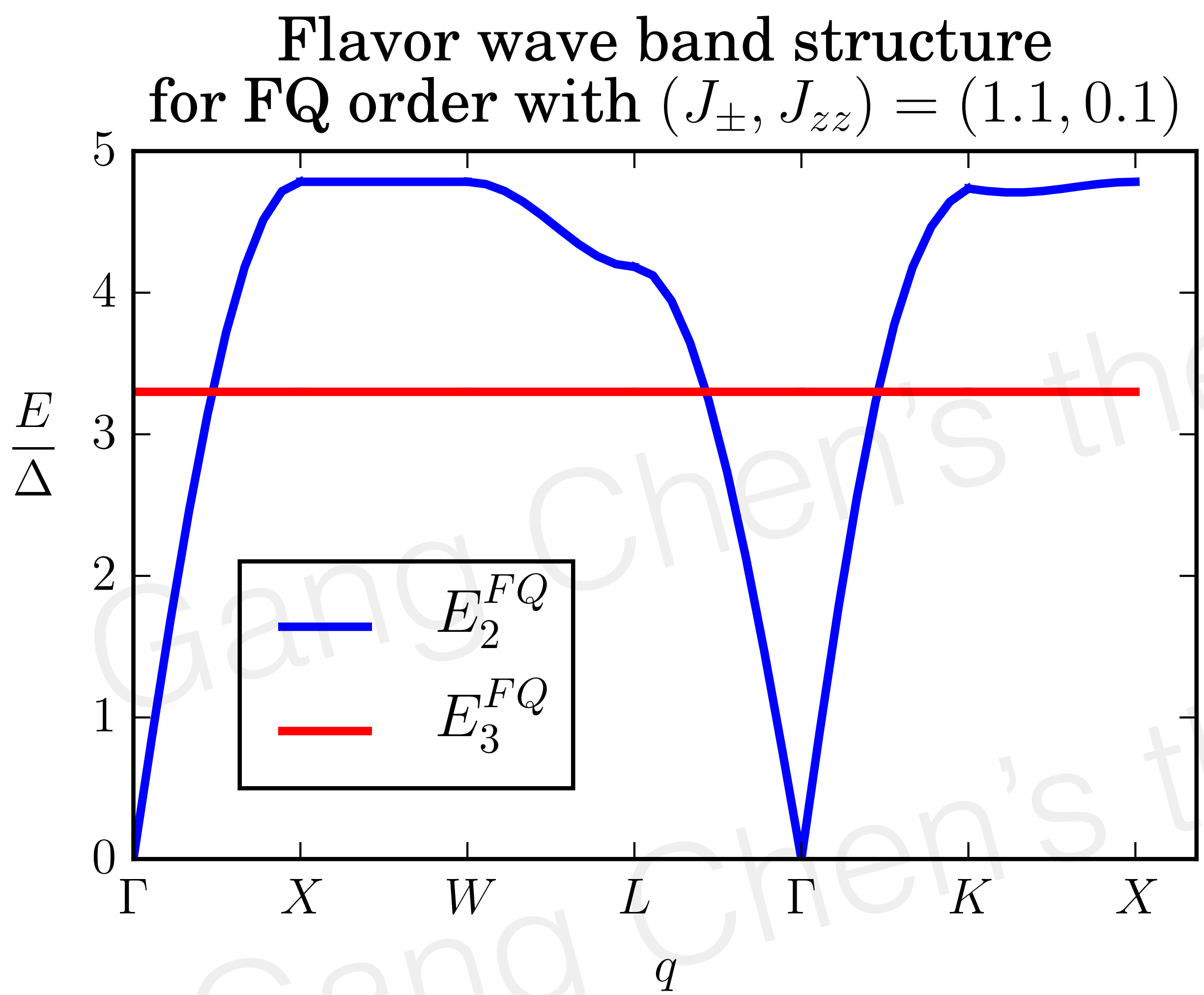
FQ = Ferroquadrupolar order
or Ferro-Spin-Nematic order

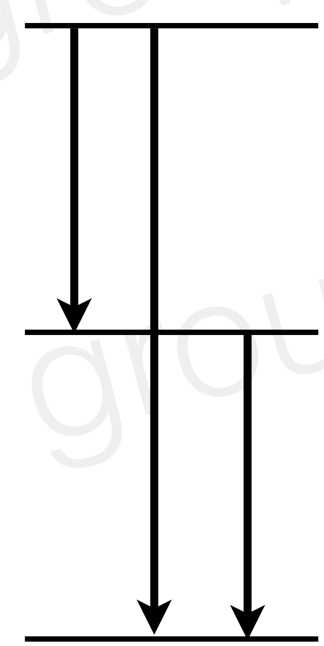
$$\langle (s_i^+)^2 \rangle \neq 0$$

Δ is set as the energy unit

two spins are condensed,
one spin is not condensed.

Excitation spectrum





excitation of the ferroquadrupolar phase

$$-J_\pm \left[(s_i^+)^2 (s_j^-)^2 + h.c. \right]$$

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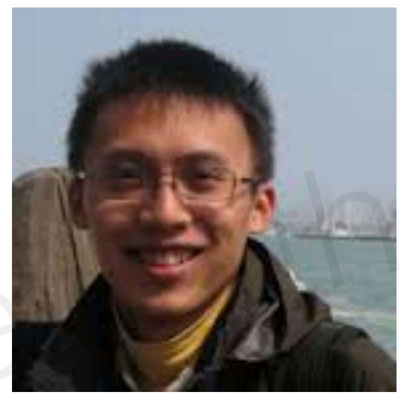

Yi-Ping Huang
(CU-Boulder)

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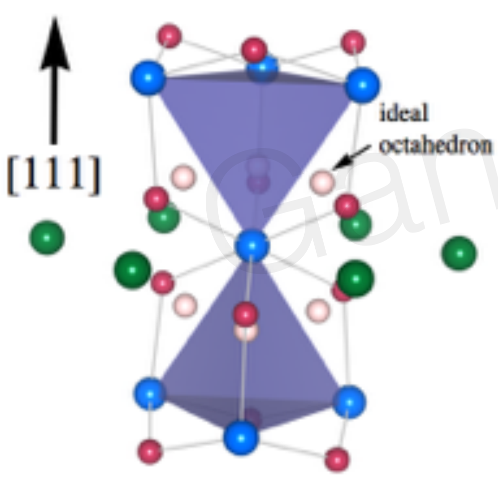
Yao-Dong Li
(Fudan)

- Hole doped Sr_2IrO_4: the difference from cuprates !

Dipole-octupole doublet

- 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 ea
other under the point group
transfomation.

simple algebar

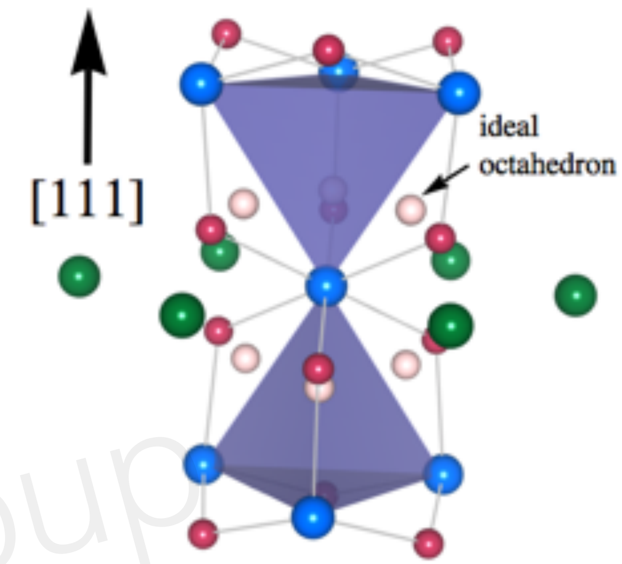
this is very different from 2-dim irep
where these two states of the doub
are mixed.

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

YP Huang, GC*, Hermele, **Phys. Rev. Lett**.112,167203 (2014)

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 $Dy_2Ti_2O_7$

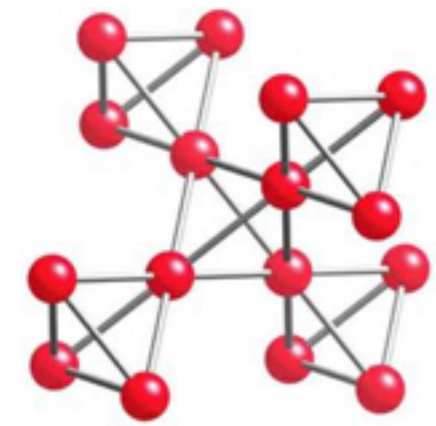
$$|\phi_0^{\pm}\rangle = 0.981|\pm\tfrac{15}{2}\rangle \pm 0.190|\pm\tfrac{9}{2}\rangle - 0.022|\pm\tfrac{3}{2}\rangle \mp 0.037|\mp\tfrac{3}{2}\rangle + 0.005|\mp\tfrac{9}{2}\rangle \pm 0.001|\mp\tfrac{15}{2}\rangle$$

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: **$Ce_2Sn_2O_7$**



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

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

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.

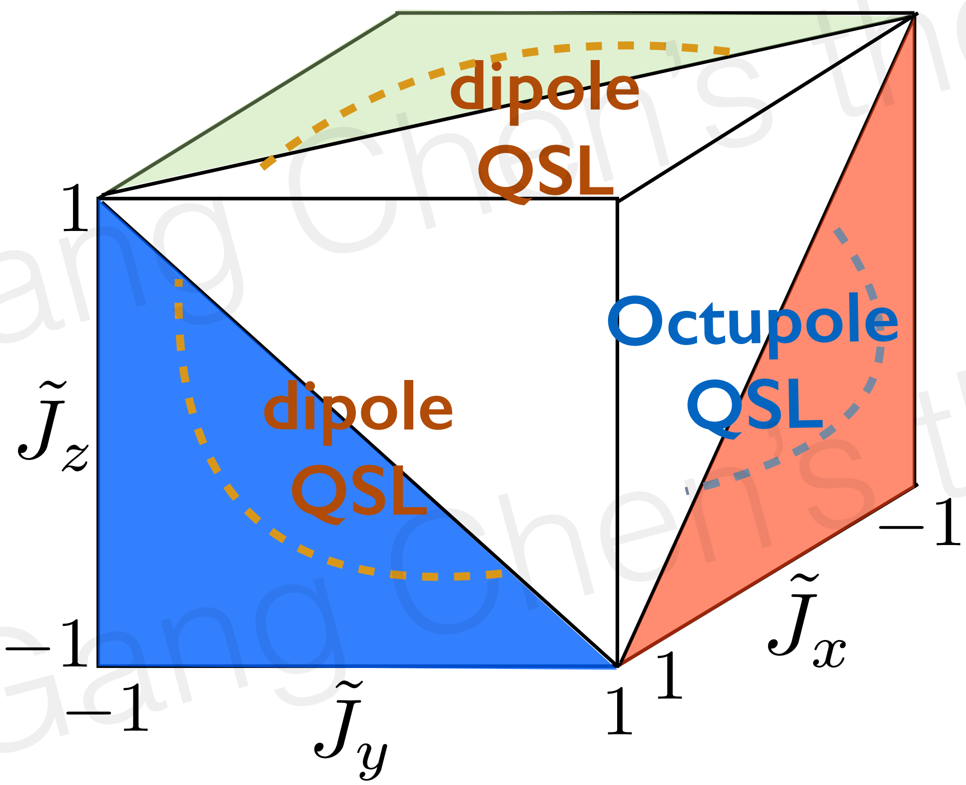
experimentalists of this paper do not know what they really talk about.

But this sentence means a lot to us. It means that gs doublet is a DO doublet, and the model is described by XX

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

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

unlike XXZ model, XYZ model is r
richer

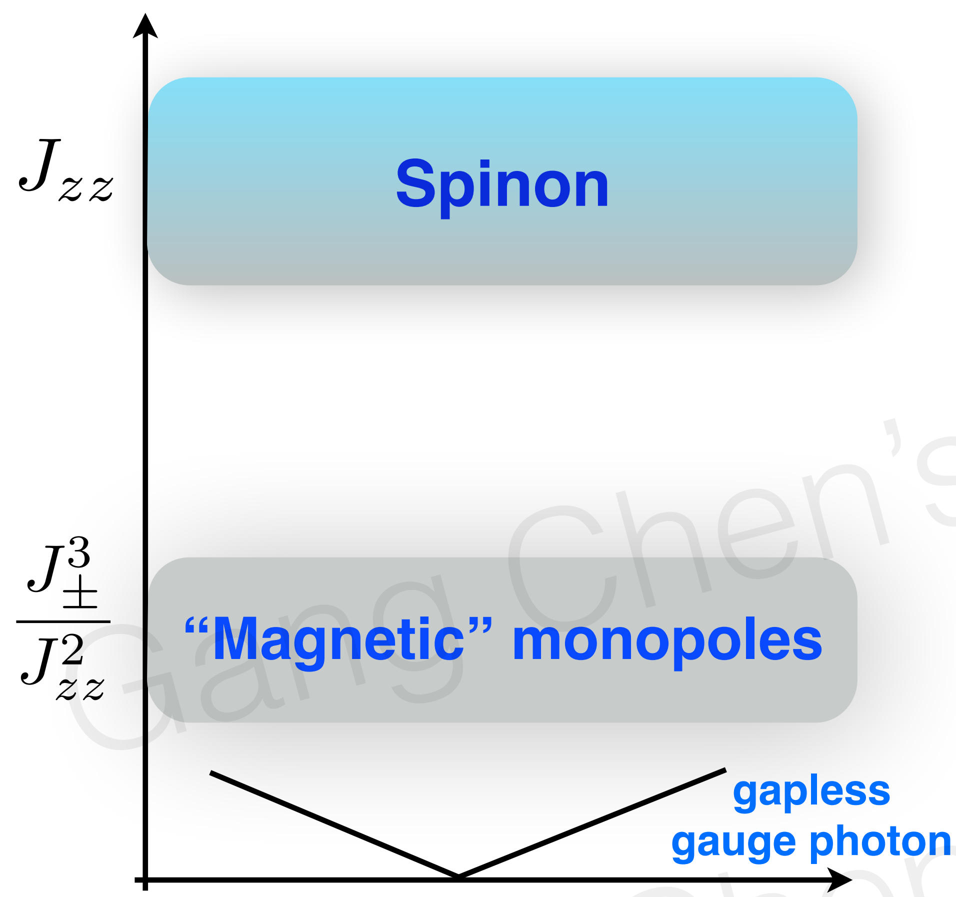


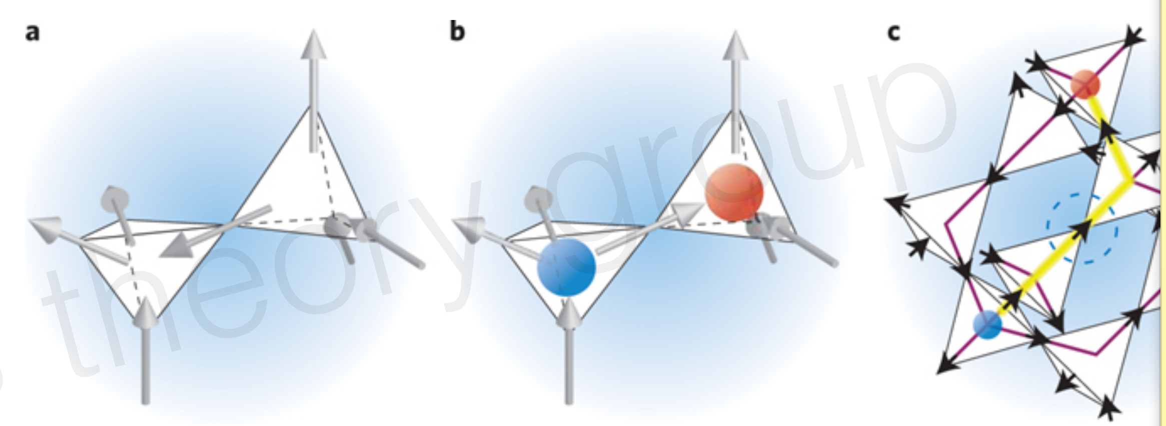
3D phase diagram

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

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

Emergent Quantum Electrodynamics of U(1) QSL





Figs from Moessn

Spinon deconfinement

as quantum spin ice i
there is no long range
a new phase of matte
in the landau's paradi

the right description c
fractionalization and e

there are 3 elementary
gauge photon,
it is not goldstone bos
breaking, there is no s
of emergent gauge st

there are deconfined s
create 2 spinons,
you can flip the furthe
arbitrary distance, it is
image there is a string
spin is strongly fluting
spinon are decofined

the 3rd is magnetic m
defect of the emergen

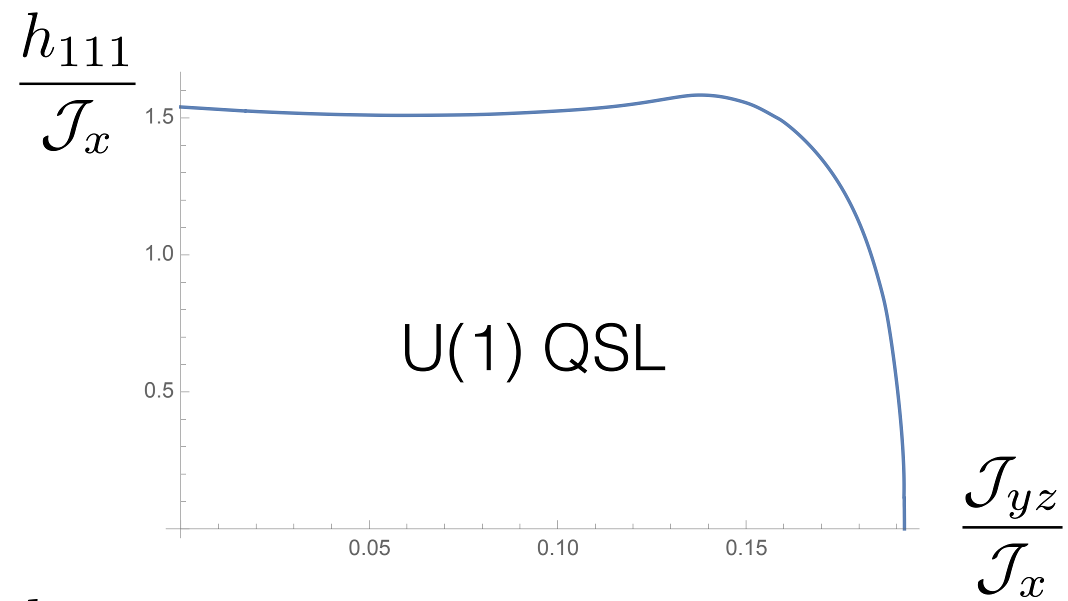
It is exotic phase of m
propertes as too orde

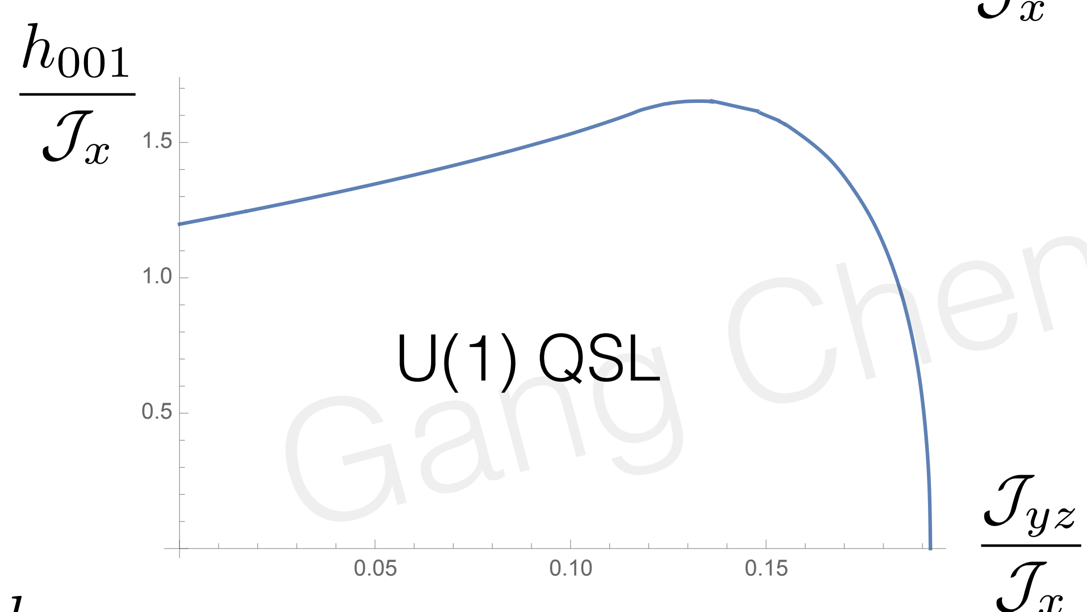
Emergent electric field $S^z \sim E$

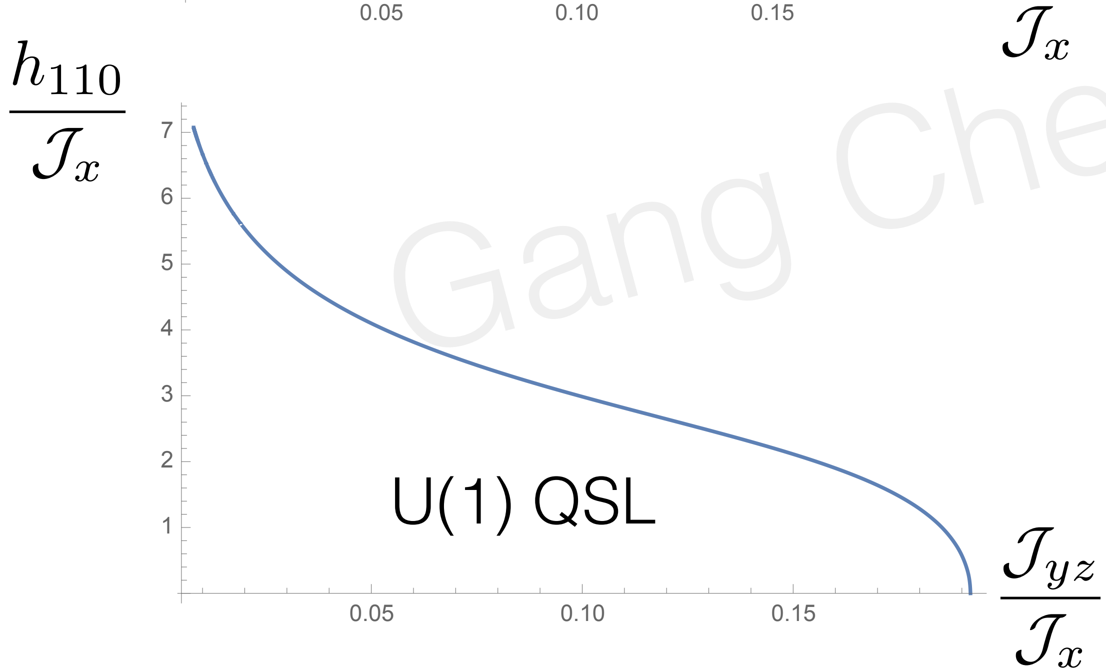
Emergent vector potential $S^{\pm} \sim e^{\pm iA}$

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

Field-driven Higgs transition







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 supercond.

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).

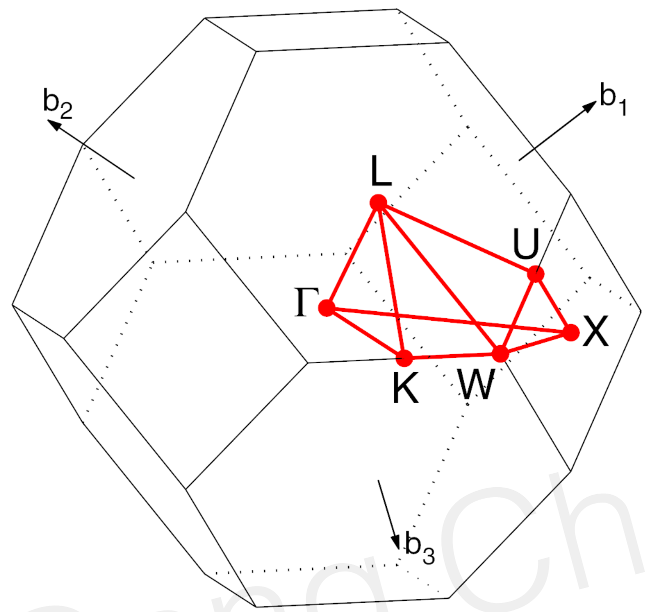
$$H = \sum_{\langle ij \rangle} \mathcal{J}_x \tau_i^x \tau_j^x - \mathcal{J}_{yz} (\tau_i^y \tau_j^y + \tau$$

$$-h \sum_i \tau_i^z (\hat{n}$$

without losing generality

Higgs trnasiton is very much like meisner effect in superconductor

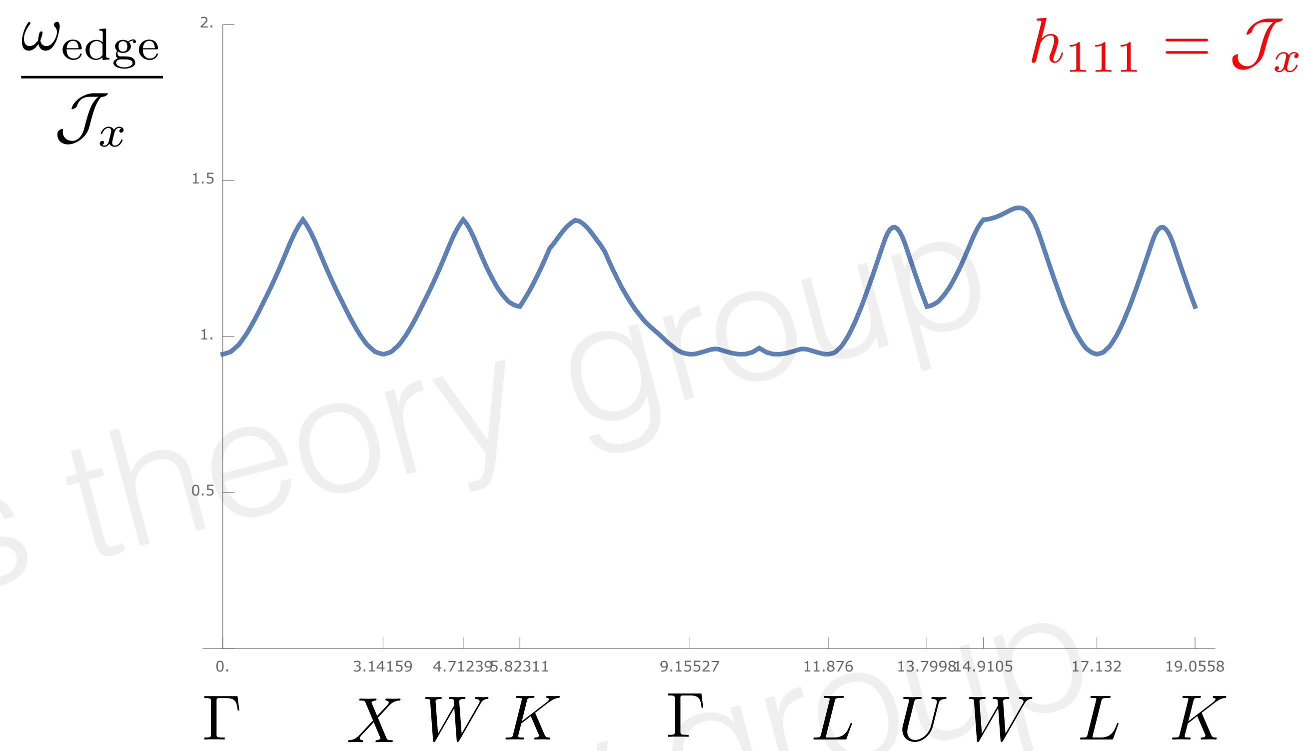
Lower excitation edge

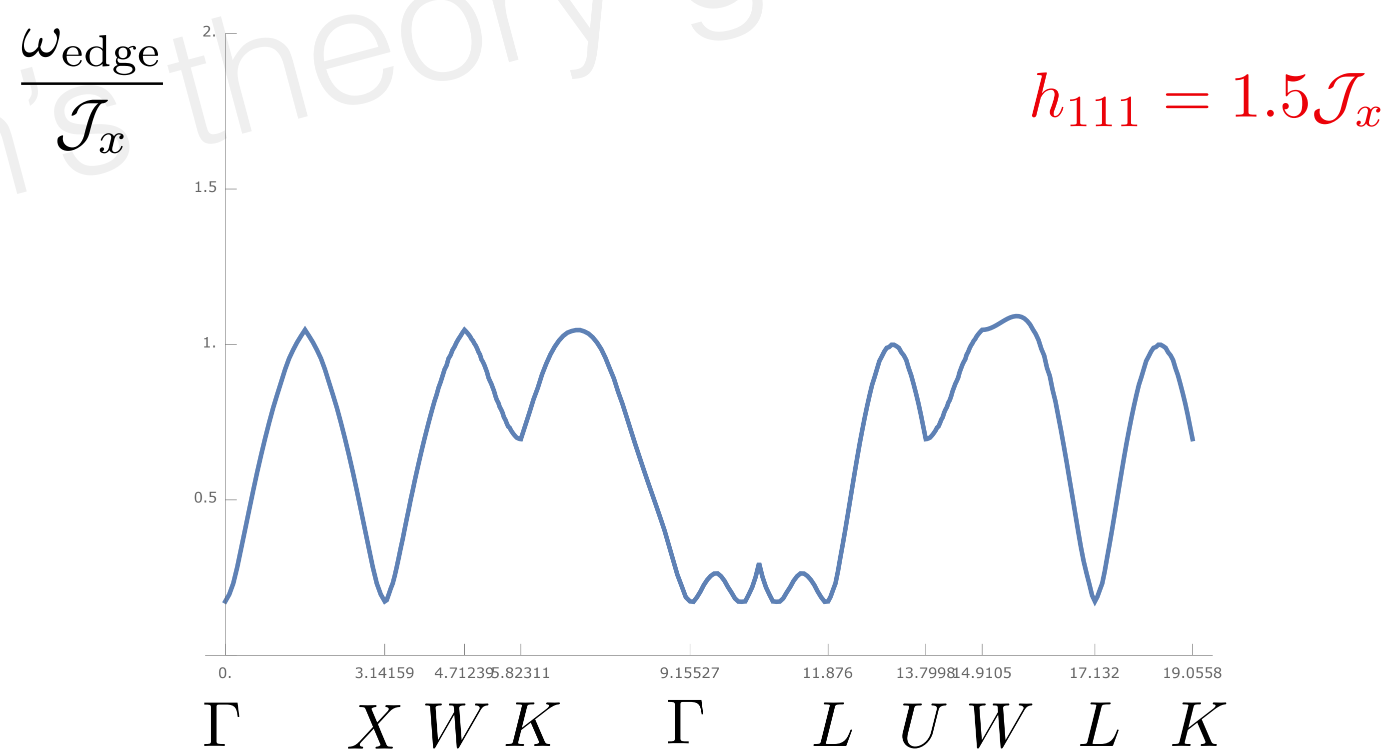


FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

Brioullin zone of
FCC lattice





Neutron scattering and thermal transport

Dipolar-U(1) QSL

neutron spin couples to both gauge field and matter field, observe both gapless gauge photon and gapped spinon continnum

Octupolar-U(1) QSL

neutron spin only couples to the matter field (spinons), observes only the gapped spinon continuum. External magnetic field can manipulate the spinon continuum, which can be confirmed by neutron scattering.

Thermal transport

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

It can be beneficial to observe the low temperature peak in the thermal transport.

Summary

We propose a general mechanism due to “weak” crystal electric field for the emergent magnetic order.

We propose a field-driven Anderson-Higgs’ transition as a simple knob to identify the octupolar U(1) quantum spin liquid.

Thank you !