Emergent magnetic order from weak-crystal field,
Octupolar quantum spin ice,
Hole doped Sr$_2$IrO$_4$

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Outline

• Emergent magnetic order due to “weak” crystal field gap.

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

• Hole doped Sr$_2$IrO$_4$: the difference from cuprates! (by myself)
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.

Crystal field energy levels

Figure 1. The computed CEF energy scheme drawn for the R ions in the R$_2$Ti$_2$O$_7$ pyrochlore series and comparison with experimental values when available, as extracted from inelastic neutron scattering measurements. Energy levels are given in units of millielectronvolts.
Dispersion of the excited doublets

The data have been taken at 1.5 K but similar results are observable at 10 K. The crossing of the acoustic phonon dispersion. (b) Simultaneously, the intensity scale (from 0 to 1) to highlight the two branches of the acoustic phonon mode and the dispersing CEF occurs close to Q=(111). The inset has been plotted using a different energy transfer scale.

crystal field levels of $Tb^{3+}$ at one site


Question: how if the crystal field gap is “weak”? or equivalently, the exchange is strong.
Model Calculation

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

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.
The first step is to identify the eigenstates. For the ferromagnetic case, the ground state is given by the representation of interacting eigenstates giving the basis to construct flavor wave theory.

If we define $\text{SU}(3)$ symmetry, we can still use HP transformation for the $z$ component of spin. The non-interacting eigenstates are $|s\rangle$.

**Figure 3. Phase diagram for $J_{zz}$**

The phase diagram shows the following:

- **AFM** $(m, q) = (1, 0)$
- **Singlet** $(m, q) = (0, 0)$
- **FM** $(m, q) = (1, 0)$
- **FQ** $(m, q) = (0, 1)$

$m$ is the magnetic dipolar order, and $q$ is the magnetic quadrupolar order. The magnetic quadrupolar order is $\langle (S_i^+)^2 \rangle \neq 0$.

FQ = Ferroquadrupolar order or Ferro-Spin-Nematic order

$\Delta$ is set as the energy unit. Two spins are condensed, one spin is not condensed.
Thus, we expect relaxing the constrain not changing the low energy physics in a significant way.

We can thus construct the imaginary time path integral representation.

The flavor wave theory for the ferro quadrupolar order is also, notice as $\mathbf{Y}_h$.

FIG. 6. The band structure for FQ phase.

Excitation spectrum

Flavor wave band structure for FQ order with $(J_{\pm}, J_{zz}) = (1.1, 0.1)$

excitation of the ferroquadrupolar phase

$-J_{\pm} \left[ (s_i^+)^2(s_j^-)^2 + h.c. \right]$
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Dipole-octupole doublet

- Why is this Kramers doublet so special?

**ONE**-dimensional representations of the point group

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

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

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

More generally, …

- Also applies to 4f electron moments on pyrochlore

\[ J = \frac{3}{2}, \frac{9}{2}, \frac{15}{2}, \ldots \]

with the local crystal field Hamiltonian

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

e.g. local doublet wavefunction of Dy\(^{3+}\) \( (J = \frac{15}{2}) \) in Dy\(_2\)Ti\(_2\)O\(_7\)

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

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$_2$Sn$_2$O$_7$

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Candidate Quantum Spin Liquid in the Ce$^{3+}$ Pyrochlore Stannate Ce$_2$Sn$_2$O$_7$
Romain Sibille, Elsa Lhotel, Vladimir Pomjakushin, Chris Baines, Tom Fennell, and Michel Kenzelmann

4$f^1$ 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 ± 250 K. The wavefunction should explain the excited doublets.

The 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.

\[ H_{\text{XYZ}} = \sum_{\langle ij \rangle} J_x \tau^z_i \tau^z_j + J_y \tau^y_i \tau^y_j + J_z \tau^z_i \tau^z_j \]

Study phase on a cube: \(-1 \leq \tilde{J}_{x,y,z} \leq 1\).
Emergent Quantum Electrodynamics of U(1) QSL

Emergent electric field

Emergent vector potential

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

energy

\[ J_{zz} \]

Spinon

“Magnetic” monopoles

\[ \frac{J_3}{J_{zz}^2} \]

gapless gauge photon

Spinon deconfinement

Figs from Moessner & Schiffer, 2009

S. Curnoe, 2008

S. Onoda, 2010

as quantum spin ice is a disordered state, there is no long range order, no symmetry breaking, it is a new phase of matter, cannot be understood in the Landau’s paradigm of symmetry breaking theory. the right description of quantum spin ice is in terms of fractionalization and emergent gauge structure.

there are 3 elementary excitations: emergent gapless gauge photon, it is not a Goldstone boson, which is due to symmetry breaking, there is no symmetry breaking. it is a consequence of emergent gauge structure.

there are deconfined spinons: you can create 2 spinons, you can flip the further spins and separate them by arbitrary distance, it is only cost fine energy. one can image there is a string connecting 2 spinons, because the spin is strongly fluctuating the spinons are deconfined.

the 3rd is magnetic monopoles, which are topological defects of the emergent U(1) gauge field. It is exotic phase of matter, like FQHE and share similar properties as topological order.
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).

\[
H = \sum_{\langle ij \rangle} \mathcal{J}_x \tau_i^x \tau_j^x - \mathcal{J}_{yz} (\tau_i^y \tau_j^y + \tau_i^z \tau_j^z) - \hbar \sum_i \tau_i^z (\hat{n}_i)
\]

without losing generality

Higgs transition is very much like Meisner effect in superconductor.
Lower excitation edge

Brioullin zone of FCC lattice

FCC path: $\Gamma$-X-W-K-\Gamma-L-U-W-L-K|U-X

\[ h_{111} = J_x \]

\[ h_{111} = 1.5J_x \]
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 continuum.

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!