Topological Engineering in Pr$_2$Ir$_2$O$_7$

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Outline

1. Microscopics of Pr$_2$Ir$_2$O$_7$: conduction elections and local moments

2. Pr-magnetism induced Weyl nodes and symmetry protected Dirac band touching

3. Proximate phase transition out of U(1) quantum spin liquid

Refs:
GC, PRB 94, 205107, (2016)
GC, PRB 96, 195127, (2017)
X-P Yao, GC, arXiv:1712.06534
Pyrochlore iridates

\[ \text{Pr}_2\text{Ir}_2\text{O}_7 \]

K Matsuhira, M Wakeshima, Y Hinatsu, S. Takagi
JPSJ, 2011

Pr\(_2\)Ir\(_2\)O\(_7\) remains metallic and disordered!
Early motivation: correlation physics in spin-orbit (to)

D Pesin, L Balents, NatPhys 2010, Topological Mott insulator
(or A 3D U(1) quantum spin liquid)

\[
H = \sum_{R} (\varepsilon_{\alpha} - \mu) d_{R}^{\dagger} d_{R} + t \sum_{\alpha \neq \alpha'} \langle R \rangle \langle \langle R' \rangle \rangle \mathbb{T} \mathbb{T}^{\dagger} d_{R}^{\dagger} d_{R'}^{\dagger} + U/2 \sum_{R} \left( \sum_{\alpha} d_{R}^{\dagger} d_{R} - n_{d} \right)^{2}
\]

Xiangang Wan, Turner, Vishwanath, Savrasov, PhysRevB 2011,
Magnetic Weyl semimetal from the Ir correlation driven all-in all-out order.

Later on, many interesting works about Iridium physics
(YB Kim, L Savary, L Fu, Xi Dai, Imada, BJ Yang, EG Moon, Nagaosa, etc)
Peculiar one: Pr$_2$Ir$_2$O$_7$

Nakatsuji, etc

PRL 96, 087204 (2006)
Ir conduction electron: Luttinger semimetal

T Kondo, …Ru Chen, …, Nakatsuji, Balents, Shin
Nature Comm, 2015

P Amitage’s optical measurement 2017

Correlation effect: EG Moon, L Savary, YB Kim, Cenke Xu, L Balents

Partial screening of long range Coulomb interaction
Some Pr$_2$Ir$_2$O$_7$ sample does order magnetically

Unstable Spin-Ice Order in the Stuffed Metallic Pyrochlore Pr$_{2+x}$Ir$_{2-x}$O$_{7−δ}$


FIG. 1. (color online) Temperature dependence of the specific heat of Pr$_{2.4}$Ir$_2$O$_{7−δ}$ in zero field. Filled circles: experimental total specific heat. Dashed curve: calculated specific heat.

FIG. 2. (color online) Temperature dependence of elastic neutron scattering intensity of Pr$_{2.4}$Ir$_2$O$_{7−δ}$ at the position of the $\mathbf{q}_m = (100)$ reflection. The intensity measured at $T = 2$ K actually "Melko-Hertog-Gingras" spin state (obtained numerically for a different and classical system)
2. Pr-magnetism induced Weyl nodes and symmetry protected Dirac band touching

Here we focus on the ordered side/sample.

Xu-Ping Yao, GC, 1712.06534
What is the impact of the Pr magnetism on Ir conduction electrons?

Ir Luttinger semimetal + Pr magnetism = ????

When electron behaves as electron, when spin behaves as spin!
Quantum Anomalous Hall Effect

1. One understanding: TI -> Dirac cone
   ferromagnetism -> gapped Dirac fermion -> QAHE

2. Our understand: QAHE is an example of interplay between conduction electron and local moments. Here in QAHE, itinerant electron band topology is modulated by magnetism, and magnetism is rather simple.

Here, we study the system with both local moments and itinerant electrons, trying to understand their interplay and interactions. How local moments influence conduction electrons, and ice versa.
Microscopics: Ir conduction electron + Pr local moment

Ir 5d electron: hopping, SOC, interaction

~<1eV

Pr-Ir interaction: f-d exchange

~

~10K

Pr 4f electron: exchange interaction

Energy Scale

GC, Hermele, PRB 2012
X-P Yao, GC, 1712.06534
Ir 5d electron: SOC, hopping and correlation

\[ e_g : x^2 - y^2, 3z^2 - r^2 \]

Ir\(^{4+} : 5d^5\)

IrO\(_6\) octahedron

Crystal electric field

Spin-orbit coupling

\[ j = 1/2 \]

\[ j = 3/2 \]

Besides Ir electron hopping via intermediate oxygens, there is also direct electron hopping

For Pr\(_2\)Ir\(_2\)O\(_7\), correlation renormalizes the band width.
Pr local moments: non-Kramers doublets

\[ 4f^2 \]

\[ L = 5, \quad S = 1, \quad J = 4 \]

\[ \Pr^{3+} \]

Indication:
1. Only \( z \) (or Ising) component couples to external magnetic field.
2. Magnetic order necessarily implies \( z \) (or Ising) component ordering.
3. Only \( z \) (or Ising) component couples to the Ir electron spin density.
Pr's 4f local moments: exchange interaction

\[ \mathcal{H}_{\text{ex}} = \sum_{i,j} J_{z,ij} \tau_i^z \tau_j^z + \sum_{i,j} J_{\perp,ij} \sum_{\mu,\nu=x,y} \tau_i^{\mu} \tau_j^{\nu}, \]

\[ \mathcal{H}_{\text{ex}} \approx \sum_{\langle i,j \rangle} J_{1z} \tau_i^z \tau_j^z + \sum_{\langle\langle i,j \rangle\rangle} J_{3z} \tau_i^z \tau_j^z, \]
Pr-Ir interaction: 4f-5d exchange

\[
\mathcal{H}_{fd} = \left[ c_1 \tau_4^z - c_2 (\tau_2^z + \tau_3^z) \right] j_1^x + \left[ c_1 \tau_3^z - c_2 (\tau_2^z + \tau_4^z) \right] j_1^y \\
+ \left[ c_1 \tau_2^z - c_2 (\tau_3^z + \tau_4^z) \right] j_1^z + [2 \leftrightarrow 2', 3 \leftrightarrow 3', 4 \leftrightarrow 4'],
\]
evaluate the Ir band structure in the magnetic Brillouin zone after the band reconstruction. A remarkable band structure property of the Ir subsystem is determined by the presence of the Weyl nodes in the reconstructed Ir band structure in Fig. 3. The reconstructed Ir band structure in Fig. 3 is immediately modified. Before we present the reconstruction symmetries, and each band of the Ir electrons remains to be a symmetry of the system after the development of the Pr magnetic order. As we show in Fig. 3, the system has both time reversal and in-plane exchange, \( T \) and \( d \) exchange, \( f \) exchange terms show different Ir and O contents from the old ones.

\[ \tilde{T} \equiv T \circ t \]

FIG. 2. (a) The Brillouin zone of the original pyrochlore lattice. (b) Under the Neel state on square lattice. Like the pure time reversal for the antiferromagnetic Néel state on square lattice. (c) The staggered time reversal for the antiferromagnetic Neel state on square lattice. (d) The folded energy band without exchange, \( |k_1, k_2, k_3| = 2 \) for the momentum points at \( \tilde{T} \) points.

Neel state on square lattice

3D analogue of the magnetic translation for Neel state
Symmetry protected Dirac band touching

\[ \bar{T}^2 = -1 \text{ at } \bar{T} \text{ point} \]

in addition, there are Weyl nodes whose existence does not require symmetry

Pr magnetic order transfers its time reversal symmetry breaking to Ir Luttinger semimetal.
1. Magnetic field primarily couples to Pr moments, modifies Pr spin state, thereby indirectly influence the Ir band structure, 
2. Field immediately removes the Dirac band touching, 
3. Field induces Weyl nodes on the Ir band structure as well, anomalous Hall effect
Quantum control under magnetic field

The Pr magnetic state under different direction magnetic field

Gang Chen’s theory group

Gang Chen’s theory group
111 magnetic field, Ir band structure

We predict that external magnetic field destroy the symmetry protected Dirac band touching, and Weyl nodes still persist and give to anomalous Hall effect.

Xu-Ping Yao, Gang Chen, arXiv 1712.06534
3. Proximate phase transition out of U(1) quantum spin liquid
Some \( \text{Pr}_2\text{Ir}_2\text{O}_7 \) sample does order magnetically

Unstable Spin-Ice Order in the Stuffed Metallic Pyrochlore \( \text{Pr}_{2+x}\text{Ir}_{2-x}\text{O}_{7-\delta} \)

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FIG. 1. (color online) Temperature dependence of the specific heat of \( \text{Pr}_{2.8}\text{Ir}_{2.2}\text{O}_{7.5} \) in zero field. Filled circles: experimental total specific heat. Dashed curve: calculated specific heat of \( \text{Pr}_2\text{Ir}_2\text{O}_7 \) from Gang Chen’s theory group.

FIG. 2. (color online) Temperature dependence of elastic neutron scattering intensity of \( \text{Pr}_{2.8}\text{Ir}_{2.2}\text{O}_{7.5} \) at the position of the \( \mathbf{q}_m = (100) \) reflection. The intensity measured at \( T = 2 \) K actually “Melko-Hertog-Gingras” spin state (obtained numerically for a different and classical system)
Our suggestion

The Pr subsystem is proximate to a quantum phase transition from pyrochlore ice U(1) QSL to Ising magnetic order.

Microscopics: different samples have different Fermi energy, induces different RKKY interaction between Pr local moments.

GC, PRB 94, 205107 (2016)
Pyrochlore ice U(1) spin liquid

Hermele, Fisher, Balents, 2004

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

\[ \tau^z \sim E \]
\[ \tau^\pm \sim e^{\pm iA} \]

emergent electric field
emergent vector gauge potential

It is an example of XG Wen's string-net condensed phase.
Fluctuating closed string-> lights/photon, ends of open strings-> particles (spinon,..)
It is like topological order.

Gang Chen's theory group
Electromagnetic duality and monopole condensation

\[ \mathcal{T} : \tau^z \rightarrow -\tau^z \]
\[ \mathcal{T} : \tau^{x,y} \rightarrow +\tau^{x,y} \]

Magnetic transition of non-Kramers doublet implies confinement transition.

Confinement transition is obtained by magnetic monopole condensation.

“Fictitious” string now has a finite tension.
Electric field gets a static value.
Spinons are confined.

Motrunich Senthil 2005,
DL Bergman, G Fiete, Balents 2005
GC PRB 94, 205107 (2016)
Monopole condensation and magnetic order

\[ H_{\text{dual}} = \sum_{\square^*_d} \frac{U}{2} \left( \text{curl} \ a - \bar{E} \right)^2 - \sum_{r,r'} K \cos B_{rr'} - \sum_{(r,r')} t e^{-i2\pi \bar{a}_{rr'}} \Phi^\dagger_r \Phi^\dagger_{r'} - \mu \sum_r \Phi^\dagger_r \Phi_r, \]

This theory gives the same magnetic order in Pr2Ir2O7, the magnetic order has to break translation symmetry.

GC, PRB 94, 205107 (2016)
Where to see Dirac’s magnetic monopoles?

Let’s forget Pr$_2$Ir$_2$O$_7$. Now given a U(1) QSL, what should we measure?

\[ \tau^z \sim E \text{ (emergent electric field)} \]

\[ \text{Im} [E^\alpha_{-\mathbf{k},-\omega} E^\beta_{\mathbf{k},\omega}] \propto \left[ \delta_{\alpha\beta} - \frac{k_\alpha k_\beta}{k^2} \right] \omega \delta(\omega - v|\mathbf{k}|), \]

Low energy theory (Savary, Balents)

**Electromagnetic duality**

Electric loop current $\rightarrow$ Magnetic field

Magnetic loop current $\rightarrow$ Electric field

at higher energy, detect monopole continuum

**GC, PRB 96, 195127 (2017)**
we carry out the mean-field approximation for the and demonstrate the spectral periodicity enhancement, with a fold Brillouin zone is a strong indication of the is very different from the conventional case where the I sublattice of the dual diamond lattice, and two arise from the gauge link that is present in the “monopole” current correlation. Here we are interested in the spectral structure of the upper excitation edges of the “monopole” continuum. For both figures, we set the dual gauge potential as

\[ q \equiv \bar{q} \equiv (1, 0, 0), (0, 1, 0), (0, 0, 1), (1, 1, 1) \]

Upper excitation edge of monopole continuum

Lower excitation edge of monopole continuum

Projective realization of translation symmetry for monopoles leads to enhanced spectral periodicity of monopole continuum.

Monopole continuum in Pr$_2$Hf$_2$O$_7$?

In fact, continuum has been observed in Pr$_2$Hf$_2$O$_7$

Further suggestions for experiments 1

For **non-Kramers doublets** such as Pr ion in Pr$_2$Zr$_2$O$_7$ and Tb ion in Tb$_2$Ti$_2$O$_7$

Visible in thermal transport

Visible in inelastic neutron scattering

GC, PRB 96, 195127 (2017)
Thermal transport in spin ice, Yuji Matsuda, 2016
Further suggestions for experiments 2

\[ H_{\text{Zeeman}} = \vec{B} \cdot \sum_i \vec{z}_i \vec{z}_i \]

The weak magnetic field polarizes tau^z slightly, and thus modifies the background electric field distribution. This further modulates monopole band structure, creating “Hofstadter” monopole band, which may be detectable in inelastic neutron.

GC, PRB 96, 195127 (2017)
Summary

1. We point out the Pr local moment is proximate to a quantum phase transition from U(1) QSL to the Ising magnetic order in Pr$_2$Ir$_2$O$_7$.

2. We point out the presence of monopole continuum in inelastic neutron scattering, and predict the enhanced spectral periodicity.

3. We predict the band structure reconstruction of the Ir conduction electrons by the Pr magnetic order. We predict symmetry protected Dirac band touching and topologically protected Weyl nodes.

4. This work points out the interesting interplay of conduction electron and local moments in hybrid quantum materials.