Pr$_2$Ir$_2$O$_7$: when Luttinger semimetal meets with Melko-Hertog-Gingras spin ice state

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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
References


Xu-Ping Yao, Gang Chen, arXiv:1712.06534 PRX

Xu-Ping Yao
(Fudan)
Pyrochlore iridates

$R_2Ir_2O_7$

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)

\[ H = \sum_{R_i \alpha} (\varepsilon_\alpha - \mu) d_{R_i \alpha}^\dagger d_{R_i \alpha} + t \sum_{\langle R_i, R_i' \rangle} T_{\alpha \alpha'}^{i i'} d_{R_i \alpha}^\dagger d_{R_i' \alpha'} + \frac{U}{2} \sum_{R_i} \left( \sum_{\alpha} d_{R_i \alpha}^\dagger d_{R_i \alpha} - n_d \right)^2 \]


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, C Xu, L Balents

Partial screening of long range Coulomb interaction
**Pr local moments: non-Kramers doublets**

- **Pr**$^{3+}$
- $L = 5$
- $S = 1$
- $J = 4$
- $\tau = 1/2$

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.
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$_{7-δ}$

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FIG. 1. (color online) Temperature dependence of the specific heat of Pr$_{2+x}$Ir$_{2-x}$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$_{2+x}$Ir$_{2-x}$O$_{7-δ}$ at the position of the $q_m = (100)$ reflection. The intensity measured at $T = 2\,\text{K}$ 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)**
Microscopics: Ir conduction electron + Pr local moment

Ir 5d electron: hopping, SOC, interaction

~1eV

Pr-Ir interaction: f-d exchange

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Pr 4f electron: exchange interaction

~10K

Energy Scale

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

Ir$^{4+}$: 5$d^5$

IrO$_6$ octahedron

$e_g: x^2 - y^2, 3z^2 - r^2$

t$_{2g}$: xy, xz, yz

Crystal electric field

Spin-orbit coupling

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-Ir interaction: 4f-5d exchange

\[ \mathcal{H}_{fd} = \left[ c_1 \tau_4^z - c_2 (\tau_2^z + \tau_3^z) \right] j_1^x + \left[ c_1 \tau_3^z - c_2 (\tau_2^z + \tau_4^z) \right] j_1^y + \left[ c_1 \tau_2^z - c_2 (\tau_3^z + \tau_4^z) \right] j_1^z + [2 \leftrightarrow 2', 3 \leftrightarrow 3', 4 \leftrightarrow 4'] \]
the electrons is governed by the Ir tight binding model and after the band reconstruction. remarkable band structure property of the Ir subsystem tain lattice translations remains to be a symmetry of the structure, the combination of the time reversal and cer-tal unit cell. Due to this interesting magnetic ordering reversal and the lattice translation by doubling the crys-

The “Melko-Hertog-Gingras” spin state breaks the time reversal and the lattice translation by doubling the crys-ples with di-Ir. We here study the band structure reconstruction of the sal symmetry breaking is transmitted to the Luttinger tor and Weyl semimetal. The Pr Ising magnetic order of various topological phases such as topological insula-

lines are defined in (b) as red lines. (d) The folded energy band without quadratic touching at (1/2,1/2,1/2). High symmetry momentum point results from the cubic symmetry. As we show in Fig. 3, the explicit calculation of the Ir band structure in the presence of the Pr magnetic order. These two symmetries development of the Pr magnetic order. These two symmetries and involve the lattice translations, sal, and Néel state on a square lattice. Like the pure time rever-

3D analogue of the magnetic translation for Neel state

\[ \tilde{T} \equiv T \circ t \]
Symmetry protected Dirac band touching

In the absence of the Pr magnetic order and give a conduction electron bands form a Luttinger semimetal. Pr Ising magnetic order. As we depict in Fig. 2, the Ir zone corresponding to the doubled unit cell due to the presence of the Weyl nodes in the reconstructed Ir band touchings at the Pr magnetic order transfers its time reversal sal symmetry breaking is transmitted to the Luttinger and Weyl semimetal. The Pr Ising magnetic order of various topological phases such as topological insulator lines are defined in (b) as red lines.

It is a 2-in 2-out spin wave with a finite ordering wavevector. After the band reconstruction.

The "Melko-Hertog-Gingras" spin state breaks the time symmetry breaking is transmitted to the Luttinger symmetry protected Dirac band touching (d) The folded energy band without quadratic touching at (b) The Brillouin zone of the original pyrochlore lattice. (b) Under the presence of the Pr Ising magnetic order transfers its time reversal symmetry breaking to the antiferromagnetic 

Besides the emergent and symmetry protected Dirac quadratic band touching at the \( \tilde{\Gamma} \) point. High symmetry momentum \( \tilde{\Gamma} \) is immediately modified. Before we present the reconstructed band structure in details, we first understand the band structure properties from the symmetry point of view. For our choice of the propagating wavevector, the "Melko-Hertog-Gingras" spin state of the Pr moments to have a propagating wavevector \( \tilde{\Gamma} \) and \( \tilde{\Gamma} \), and \( \tilde{\Gamma} \) for the momentum points at \( \tilde{\Gamma} \) and \( \tilde{\Gamma} \), respectively. It turns out that, the presence of the Weyl nodes in the reconstructed Ir band touchings at the Pr magnetic order transfers its time reversal symmetry breaking to Ir Luttinger semimetal.

Pr magnetic order transfers its time reversal symmetry breaking to Ir Luttinger semimetal.
Band engineering by external magnetic field

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

Magnetic field modifies the Pr magnetic structure, thereby modifies the 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.
Conclusion

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.

Some prediction has been confirmed by Nakatsuji’s experiments.