Frustrated metal Pr$_2$Ir$_2$O$_7$: when Luttinger semimetal meets with ordered spin ice

Gang Chen
Fudan University
When Luttinger semimetal meets Melko-Hertog-Gingras spin ice state in Pr2Ir2O7

Ir Luttinger semimetal

MHG spin ice state

Xu-Ping Yao, GC, 1712.06534
Pyrochlore iridates

\( \text{R}_2\text{Ir}_2\text{O}_7 \)

Pr\(_2\)Ir\(_2\)O\(_7\) remains metallic and disordered, all rest have metal-insulator transition with Ir magnetism

Early/pioneering theories: Leon Balents, Dima Pesin, Lucile Savary, Sungbin Lee, Yong Baek Kim, et al
Peculiar one: Pr$_2$Ir$_2$O$_7$

\begin{figure}
\centering
\includegraphics[width=\textwidth]{pr2ir2o7.png}
\caption{Field dependence of the magnetization along the [100], [110], and [111] directions.}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{pr2ir2o7_magnetic.png}
\caption{Magnetic properties of Pr$_2$Ir$_2$O$_7$.}
\end{figure}

Nakatsuji, etc
PRL 96, 087204 (2006)
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$_{7-\delta}$


FIG. 1. (color online) Temperature dependence of the specific heat of Pr$_{2+x}$Ir$_{2-x}$O$_{7-\delta}$ in zero field. Filled circles: experimental total specific heat. Dashed curve: calculated specific heat due to a reduced nuclear Schottky anomaly (see text).

FIG. 2. (color online) Temperature dependence of elastic neutron scattering intensity of Pr$_{2+x}$Ir$_{2-x}$O$_{7-\delta}$ at the position of the $q_m = (100)$ reflection. The intensity measured at $T = 2$ K actually "Melko-Hertog-Gingras" spin state (obtained numerically for a different and classical system)
Our proposal for Pr subsystem

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.

Gang Chen, PRB 94, 205107 (2016)
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

ARPES: Quadratic band touching
Partial screening of long range Coulomb interaction
What is the impact of Pr magnetism on Ir conduction electrons in the ordered regime?

Ir Luttinger semimetal + MHG spin ice state = ????

Ir Luttinger semimetal
MHG spin ice state

T Kondo, etc, 2015
C Broholm, etc, 2015

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

Qikun Xue’s group

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 vice versa.
Microscopics: Ir conduction electron + Pr local moments

For each Ir ion, six nearest Pr ions form a hexagon with the Ir ion in the hexagon center. Under the nearest-neighbor Kondo-like coupling, the Ir conduction electrons were found to be driven by the short-ranged and most of the time restricted to the nearest neighbors. The long-range or extended RKKY interaction is quite different from the usual rare-earth description.

D. Zeeman coupling

Finally, we introduce the Zeeman coupling. Because the external Zeeman coupling competes with the exchange Hamiltonian, the ground state is antiferromagnetically ordered with an ordering wavevector $Q^\parallel$ for Pr $(001)$ and other marks are used to distinguish Ir (pink), Pr (white).

C. Pr-Ir coupling

The Pr subsystem.

E. Energy scales

Ir 5d electron: hopping, SOC, interaction

$\sim<1\text{eV}$

Pr-Ir interaction: f-d exchange

$\sim$ $\sim10K$

Pr 4f electron: exchange interaction

Energy Scale

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

IrO$_6$ octahedron

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

$t_2g$: $xy, xz, yz$

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

Crystal electric field

Spin-orbit coupling

Besides Ir electron hopping via intermediate oxygens, there is direct electron hopping (Yong Baek Kim)

For Pr$_2$Ir$_2$O$_7$, correlation renormalizes the overall band width.

BJ Kim, etc 2008,
GC, Balents, PRB 2008
Jackeli, Khaliullin, PRL 2009
Pr local moments: non-Kramers doublet

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-Ir interaction: 4f-5d exchange

\[
\mathcal{H}_{\text{fd}} = \left[ c_1 \tau_4^z - c_2 (\tau_2^z + \tau_3^z) \right] j_1^x + \left[ c_1 \tau_3^z - c_2 (\tau_2^z + \tau_4^z) \right] j_1^y + \left[ c_1 \tau_2^z - c_2 (\tau_3^z + \tau_4^z) \right] j_1^z + [2 \leftrightarrow 2', 3 \leftrightarrow 3', 4 \leftrightarrow 4'],
\]

GC, Hermele, PRB 2012
Magnetic translation of MHG spin ice state

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

3D analogue of the magnetic translation for Neel state

Neel state on square lattice
Symmetry protected Dirac band touching

Pr magnetic order transfers its time reversal symmetry breaking to Ir Luttinger semimetal.

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

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

(b) \( c_1 = 0.05, c_2 = 0.30 \)

\[ Q = 2\pi(001), 2I2O \]
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

- **Fig. 5.** Phase diagram of the Pr local moments under the external magnetic field.

- **Fig. 4.** Phase diagram for the Ir band structure in the parameter space of the Hamiltonian.

- For the Pr subsystem, we consider the following Hamiltonian,

  \[ H = \sum_{\langle ij \rangle} J_{ij} S_i \cdot S_j + h \cdot \mathbf{S} \]

  where the exchange part includes both the first neighbor exchange and the Ir tight-binding exchange couplings. The bold dots represent the effective hoppings of the Ir electrons, so the realistic case for the ordered Pr spin configurations from the phase diagram in Fig. 5(a).

  For specific choices of the parameters, in Fig. 6, we depict theIr band structures for the magnetic state on the Ir conduction electrons. Besides the modification can be small. This would allow us to create a finite polarization for the Pr local moment and the magnetic field would primarily couple to the Pr local moments. A uniform external magnetic field to the system is expected to occur in the semimetallic regime of Fig. 4.

- The occurrence of the Weyl nodes. Indeed, as we show in Sec. II under this approximation, this should be the case for large parameter regime in the phase diagram.

- In reality, the magnetic field would cave the approximation of the Pr local moment as an Ising spin that ignores the quantum nature of the system. We refer to the four parameter choices in Fig. 3.

- Like the previous section where the Ir band structure is controlled by the symmetries of the ordered Pr on the Pr local moments, and thus breaks the degeneracy/band touching that is protected by the symmetry operations of magnetic fields are considered.
Ir band property under 111 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.

Xu-Ping Yao, Gang Chen, arXiv 1712.06534
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 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.

3. This work points out the interesting interplay of conduction electron and local moments in hybrid quantum materials.
Discovery of intertwined multipolar order in TmMgGaO4

(to appear soon)

Changle Liu (Fudan)
Yao Shen (Fudan)
Jun Zhao (Fudan)
approximately thought as non-Kramers doublets
The presence of well-defined spin wave indicates the presence of the hidden order!
Comparison with theory

Figure 3. Observed and calculated spin wave dispersion in TmMgGaO$_4$ at $T = 0.05$ K. a, Intensity of the spin-excitation spectra as a function of momentum and energy transfer along the high-symmetry directions illustrated by the black solid lines in d with $E_i = 4.8$ meV. The strong signal around the zero energy transfer comes from the elastic incoherent scattering. b, The spectral intensity calculated by LSW with $J_{zz1} = 0.57$ meV, $J_{zz2} = 0.026$ meV and $\hbar = 0.776$ meV [15]. The calculated result is convoluted with Gaussian distribution with width of 0.25 meV. c, Energy-momentum ($E - k$) slice along high-symmetry points illustrated by the grey lines in d with $E_i = 1.7$ meV. The white dashed lines stand for the high-symmetry points. d, Sketch of the reciprocal space. Black dashed lines indicate the Brillouin zone boundaries.

Changle Liu

Gang Chen's theory group
Summary