Frustrated metal Pr$_2$Ir$_2$O$_7$
and
Spin liquid candidate YbMgGaO$_4$

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Part 1

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
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$_7$

![Diagram of Pr$_2$Ir$_2$O$_7$ structure]

The field dependence of the magnetization along the [100], [110], and [111] axes shows a metamagnetic transition and “2-in, 2-out” correlation.

Inset: inverse susceptibility

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$_{7-\delta}$

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FIG. 1. (color online) Temperature dependence of the specific heat of Pr$_{2+\delta}$Ir$_{2-\delta}$O$_{7-\delta}$ in zero field. Filled circles: experimental total specific heat. Dashed curve: calculated specific heat of Pr$_{2+\delta}$Ir$_{2-\delta}$O$_{7-\delta}$. 

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 $\mathbf{q}_m = (100)$ reflection. The intensity measured at $T = 2$ K actually “Melko-Hertog-Gingras” spin state (obtained numerically for a different and classical system)
Our 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

Partial screening of long range Coulomb interaction

ARPES: Quadratic band touching
What is the impact of Pr magnetism on Ir conduction electrons in the ordered regime?

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!
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 moments

FIG. 1. The pyrochlore lattice structure for Pr$_2$Ir$_2$O$_7$.

(a) Different marks are used to distinguish Ir (pink triangle) and Pr (green triangle). Diagonal faces solid edges) and Pr (white faces and dashed edges).

(b) $a'$'s can be obtained by simple lattice symmetry. This is the direction of the external magnetic field. Since the Zeeman coupling can be tuned experimentally, one can play with the coupling between the Pr moments and the Zeeman coupling.

Clearly, the largest energy scale in the model is the exchange coupling. The lowest ones would be the exchange coupling between the Pr moments and the Zeeman coupling. The highest one would be the non-local 3d exchange and modifies the Pr magnetic order. So the quantum dynamics of the Pr local moment that develops the magnetic order, so the quantum dynamics of the Pr local moment can thus be manipulated by the external magnetic field. Finally, we introduce the Zeeman coupling. Because the magnetic state of the Pr local moments can thus be manipulated by the external magnetic field. Since the Zeeman coupling can be tuned experimentally, one can play with the coupling between the Pr moments and the Zeeman coupling.

The 3d exchange between the Pr moments is odd under time reversal, we have the Zee-Man coupling. The lowest ones would be the exchange coupling. The highest one would be the non-local 3d exchange and modifies the Pr magnetic order. So the quantum dynamics of the Pr local moment can thus be manipulated by the external magnetic field. Finally, we introduce the Zeeman coupling. Because the magnetic state of the Pr local moments can thus be manipulated by the external magnetic field. Since the Zeeman coupling can be tuned experimentally, one can play with the coupling between the Pr moments and the Zeeman coupling.

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

IrO\(_6\) octahedron

Crystal electric field

Spin-orbit coupling

\[ j = 1/2 \]

\[ j = 3/2 \]

Besides Ir electron hopping via intermediate oxygens, there is 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

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

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
Symmetry protected Dirac band touching

(b) \( c_1 = 0.05, \ c_2 = 0.30 \)
\( Q = 2\pi(001), 2I2O \)

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

**Figure 5.** Phase diagram of the Pr local moments under the external magnetic fields along different directions. The magnetic field is applied along high symmetry directions. The reduced lattice symmetry of the system if the field is applied along a random direction. Here the choice of a random direction. As we have explained in Sec. I, the external magnetic field first modifies the Pr magnetic state and then indirectly influences the Ir band structure through the exchange couplings. The bold dots refer to the four parameter choices in Fig. 3.
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
Part 2

Fractionalization in a spin liquid candidate YbMgGaO$_4$: a weak-field regime

Yaodong Li (now at UCSB)

Yao Shen (Fudan)

Jun Zhao (Fudan)
Rare-earth triangular lattice magnets: spin liquid

with Yuesheng Li, Qingming Zhang, Jun Zhao, Yao Shen, Yaodong Li
Proposal of spinon Fermi surface U(1) QSL

The proposed spinon particle-hole continuum of a spinon Fermi surface is consistent with the experimental results.

Refs:

YD Li, XQ Wang, GC*, PRB 94, 035107 (2016)
YD Li, XQ Wang, GC*, PRB 94, 201114 (2016)
YD Li, Y Shen, YS Li, J Zhao, GC*, PRB 97, 125105 (2018)
YD Li, YM Lu, GC*, PRB 96, 054445 (2017)
YD Li, GC*, PRB 96, 075105 (2017)

Y Shen, YD Li, .., GC*, J Zhao*, arXiv 1708.06655

Probably most important question is whether the continuum represents the fractionalized spinon excitation.
A new idea: explore the weak field regime

Continuing the recent proposal of the spinon Fermi surface U(1) spin liquid state for YbMgGaO$_4$ in Yao-Dong Li, et al, arXiv:1612.03447 and Yao Shen, et al, Nature 2016, we explore the experimental consequences of the external magnetic fields on this exotic state. Specifically, we focus on the weak field regime where the spin liquid state is preserved and the fractionalized spinon excitations remain to be a good description of the magnetic excitations. From the spin-1/2 nature of the spinon excitation, we predict the unique features of spinon continuum when the magnetic field is applied to the system. Due to the small energy scale of the rare-earth magnets, our proposal for the spectral weight shifts in the magnetic fields can be immediately tested by inelastic neutron scattering experiments. Several other experimental aspects about the spinon Fermi surface and spinon excitations are discussed and proposed. Our work provides a new way to examine the fractionalized spinon excitation and the candidate spin liquid states in the rare-earth magnets like YbMgGaO$_4$.

Realizable and Predictable.

Yao-Dong Li, GC, PRB 96, 075105 (2017)
Strong Mott regime: only Zeeman coupling

\[ H_{\text{MFT}} = -t \sum_{\langle ij \rangle, \alpha} f_{ij}^\dagger f_{ji} - \mu \sum_i f_{i\alpha}^\dagger f_{i\alpha} - g_\text{\mu_B} H \sum_i f_{i\alpha}^\dagger \frac{\sigma^z_{\alpha \beta}}{2} f_{i\beta} \]

The combined dynamic spin structure experiment at 2.5T
Use new materials to support materials

<table>
<thead>
<tr>
<th>Compound</th>
<th>Magnetic ion</th>
<th>Space group</th>
<th>Local moment</th>
<th>$\Theta_{cw}$ (K)</th>
<th>Magnetic transition</th>
<th>Frustration para. $f$</th>
<th>Refs.</th>
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<td>YbMgGaO$_4$</td>
<td>Yb$^{3+}$($4f^{13}$)</td>
<td>R$3m$</td>
<td>Kramers doublet</td>
<td>$-4$</td>
<td>PM down to 60 mK</td>
<td>$f &gt; 66$</td>
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<td>CeCd$_3$P$_3$</td>
<td>Ce$^{3+}$($4f^1$)</td>
<td>P$6_3/mmc$</td>
<td>Kramers doublet</td>
<td>$-60$</td>
<td>PM down to 0.48 K</td>
<td>$f &gt; 200$</td>
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<td>P$6_3/mmc$</td>
<td>Kramers doublet</td>
<td>$-6.6$</td>
<td>AFM order at 0.8 K</td>
<td>$f = 8.2$</td>
<td>[7]</td>
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<td>Unknown</td>
<td>[8]</td>
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</table>

YD Li, XQ Wang, GC*, PRB 94, 035107 (2016)

Magnetism in the KBaRE(BO$_3$)$_2$ (RE=Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu) series: materials with a triangular rare earth lattice

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many ternary chalcogenides NaRES$_2$, NaRESe$_2$, KRES$_2$, KRESe$_2$, KRET$_2$, RbRES$_2$, RbRESe$_2$, RbRET$_2$, CsRES$_2$, CsRESe$_2$, etc.)

Lots of isostructural materials
Summary

1. 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. We point out the interesting interplay of conduction electron and local moments in hybrid quantum materials.

2. We propose the weak field regime to detect the signatures of fractionalization. Such a regime can be realized in current laboratory settings. It has already been performed and observed by Jun Zhao’s group.

Further directions: how to detect spinon-gauge coupling? how to detect gauge field? any other material with similar properties?