Topological Engineering in $Pr_2Ir_2O_7$

Gang Chen
Fudan University

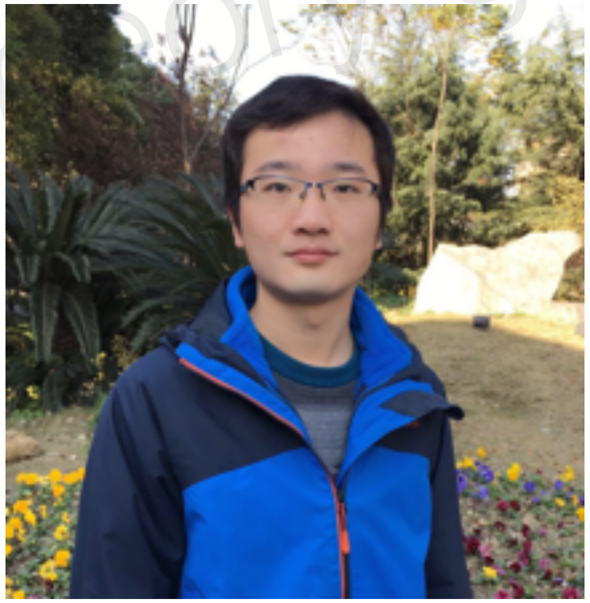
Outline

1. Microscopics of $Pr_2Ir_2O_7$: 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



Xu-Ping Yao

(Fudan)

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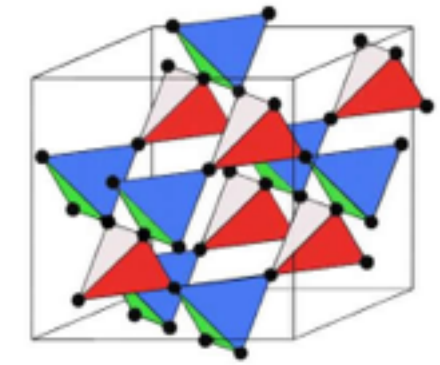
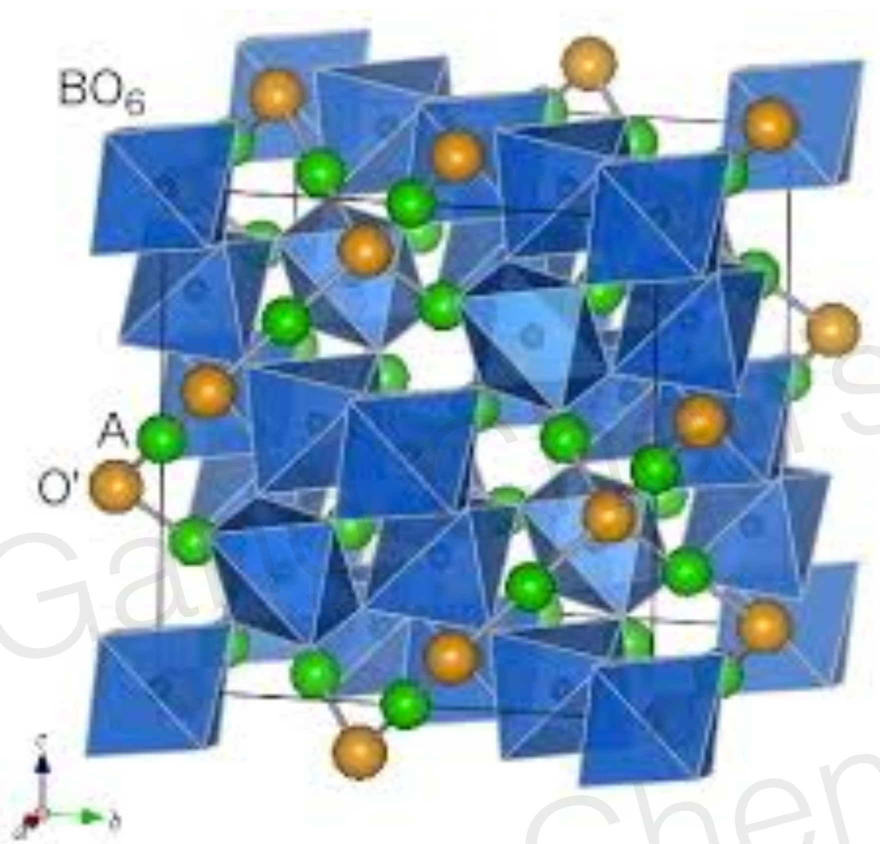
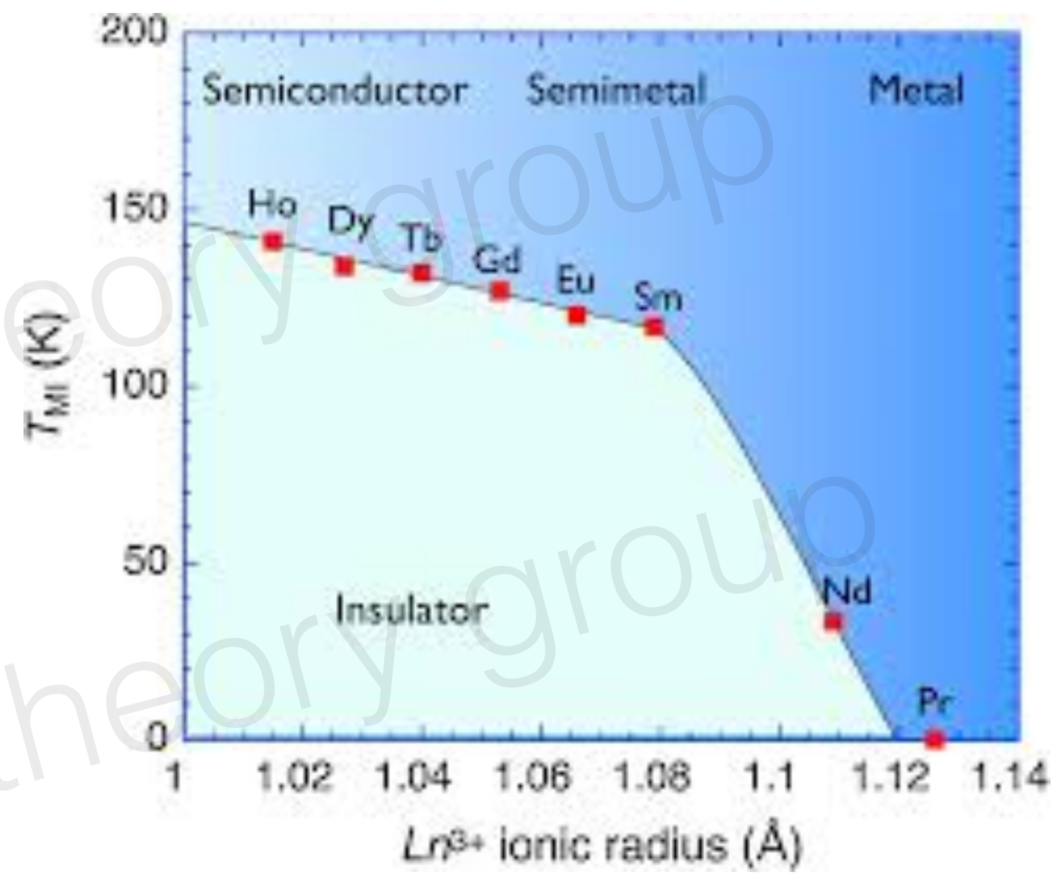


Pyrochlore iridates



$R_2Ir_2O_7$



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

$Pr_2Ir_2O_7$ remains metallic and disordered !

Early motivation: correlation physics in spin-orbit (to

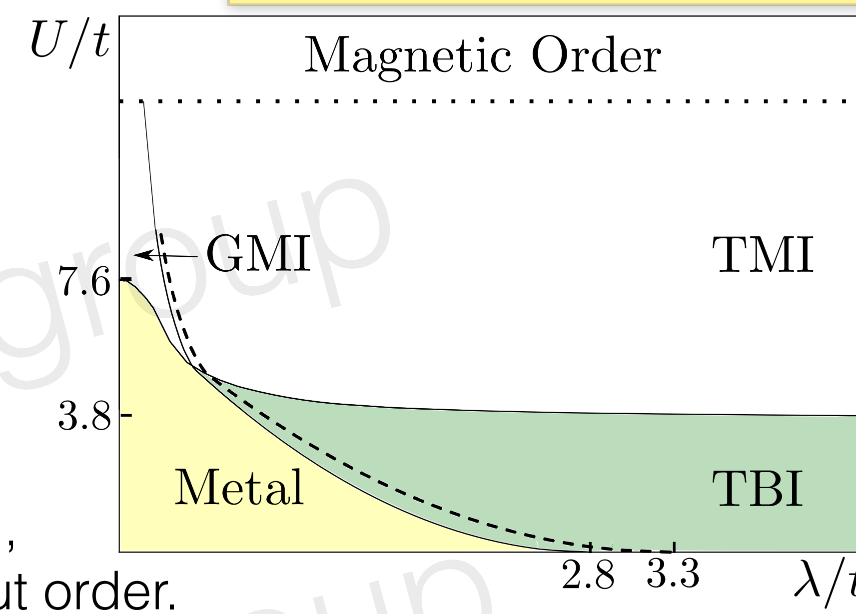
iridate provides such a setting, has interaction a
strong spin-orbit coupling

Leon knows a lot of solid state physics, Mott transition, density of state is suppressed, the longer range part of interaction becomes impor
and could induce exciton magnetism.

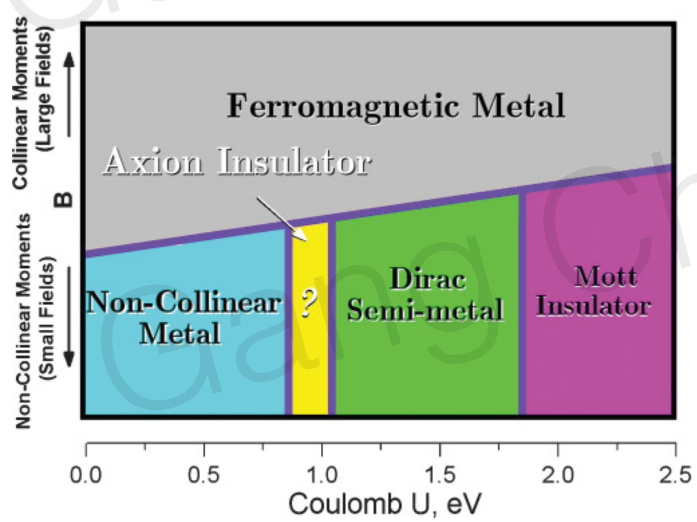
Halperin 1960s.

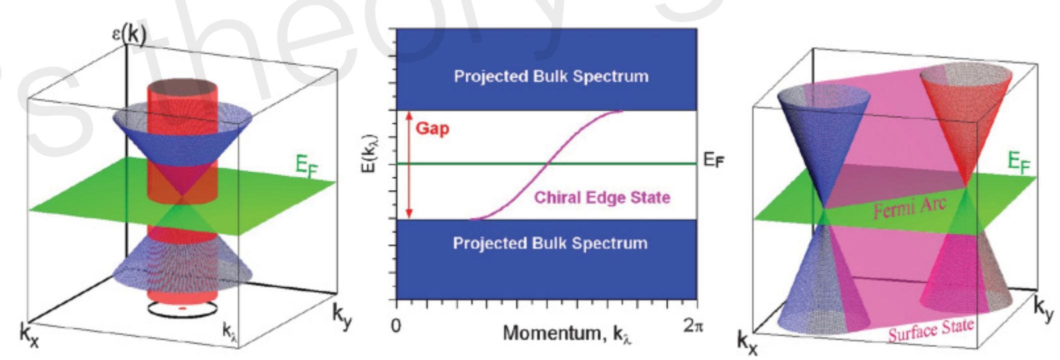
D Pesin, L Balents, NatPhys 2010, Topological Mott insulator
(or A 3D U(1) quantum spin liquid)

$$H = \sum_{Ri\alpha} (\varepsilon_\alpha - \mu) d^\dagger_{Ri\alpha} d_{Ri\alpha} + t \sum_{\substack{\langle Ri,R'i' \rangle \\ \alpha\alpha'}} T^{ii'}_{\alpha\alpha'} d^\dagger_{Ri\alpha} d_{R'i'\alpha'} + \frac{U}{2} \sum_{Ri} \left(\sum_\alpha d^\dagger_{Ri\alpha} d_{Ri\alpha} - n_d \right)^2$$



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





Weyl semimetal and surface Fermi arcs

Later on, many interesting works about Iridium physics
(YB Kim, L Savary, L Fu, Xi Dai, Imada, BJ Yang, EG Moon, Nagaosa, etc)

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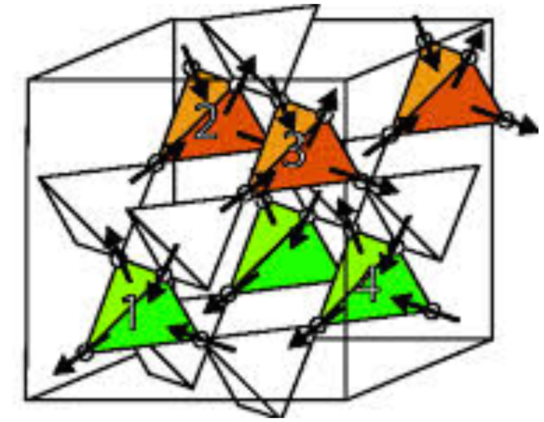
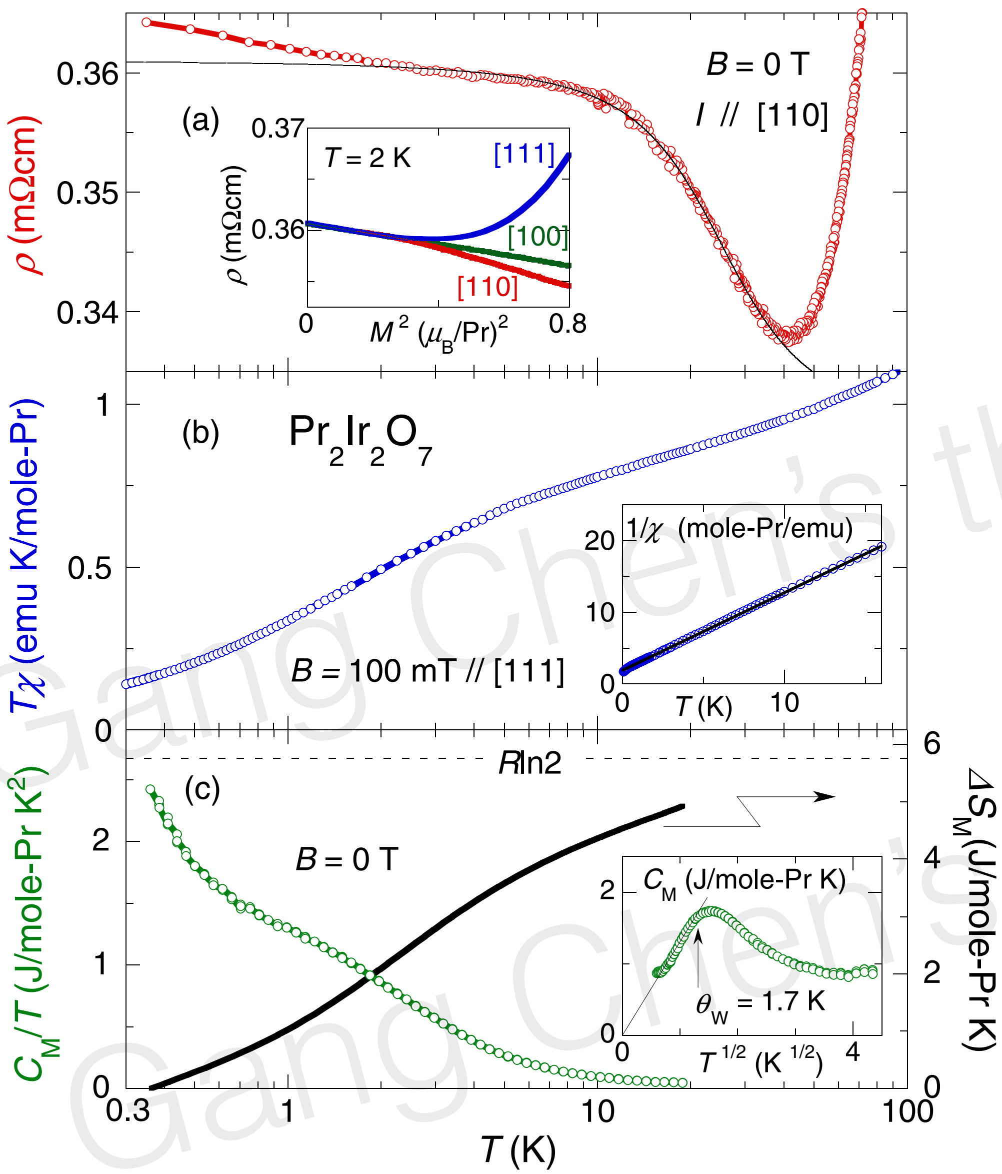
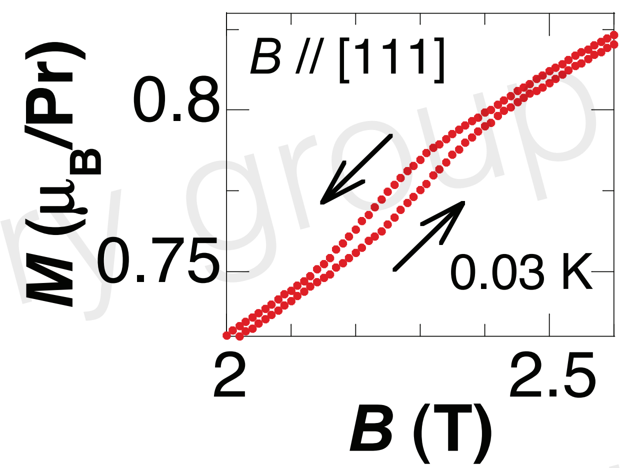
Peculiar one: $Pr_2Ir_2O_7$



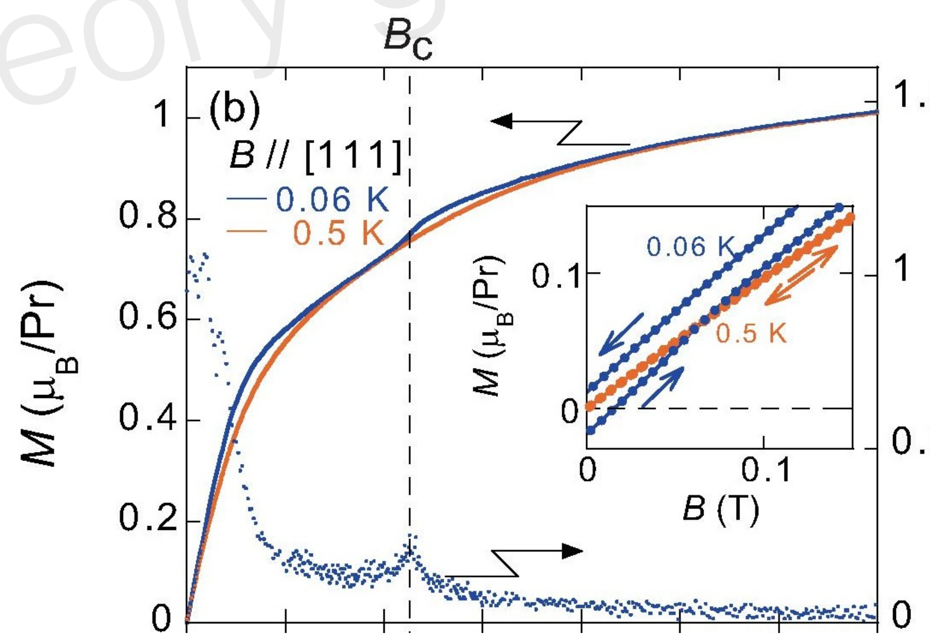


Nakatsuji, etc

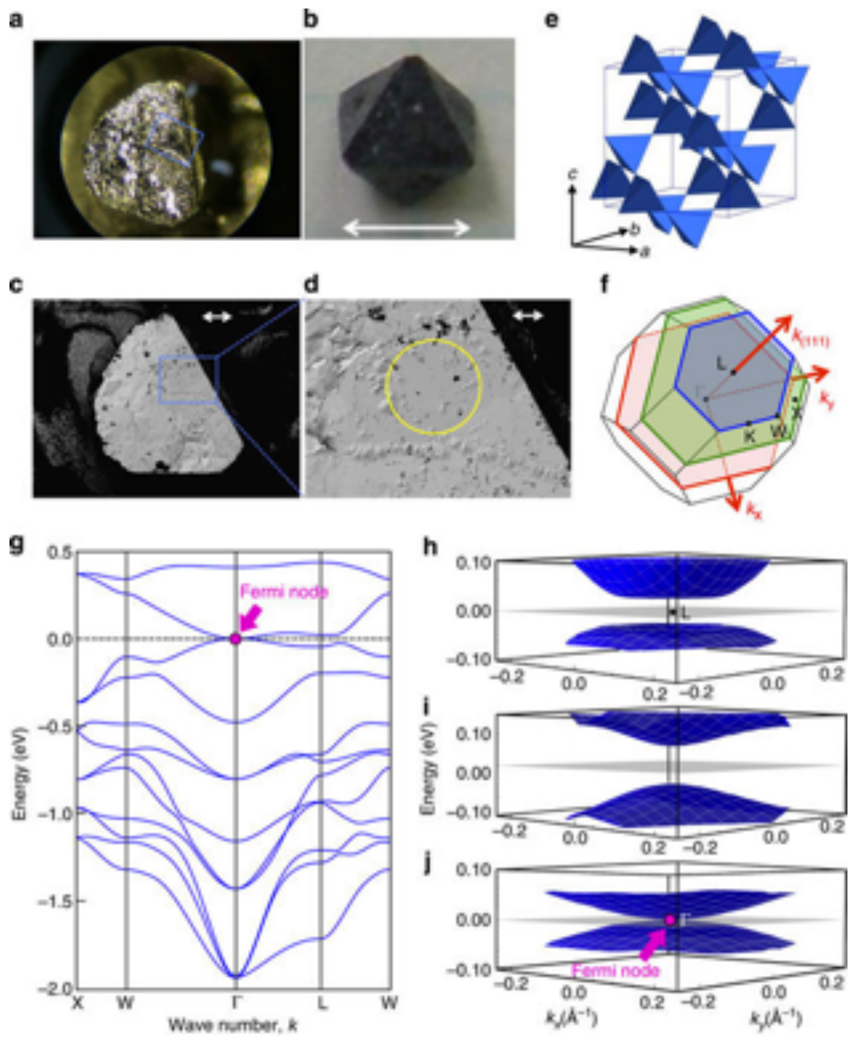
PRL **96,** 087204 (2006)

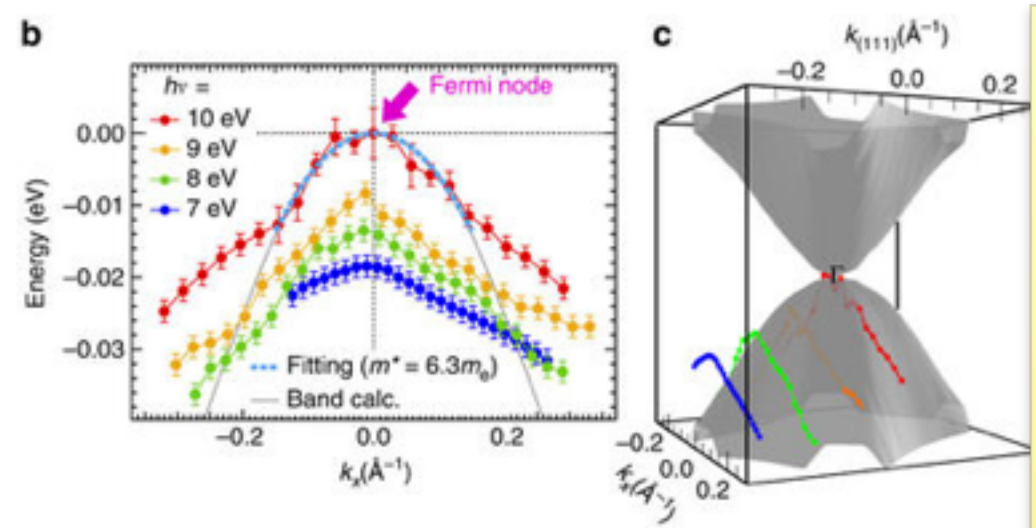


metamagnetic transition



Ir conduction electron: Luttinger semimetal





vanishing DOS, p
the coulomb inte

ARPES: Quadratic band

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 $Pr_2Ir_2O_7$ sample does order magnetically

Unstable Spin-Ice Order in the Stuffed Metallic Pyrochlore $Pr_{2+x}Ir_{2-x}O_{7-\delta}$

D. E. MacLaughlin,[1,2,*] O. O. Bernal,[3] Lei Shu,[1,4,5] Jun Ishikawa,[2] Yosuke Matsumoto,[2]
J.-J. Wen,[6,†] M. Mourigal,[6,‡] C. Stock,[6,7,§] G. Ehlers,[8] C. L. Broholm,[6,7,8,9] Yo Machida,[2,¶]
Kenta Kimura,[2] Satoru Nakatsuji,[2,10,**] Yasuyuki Shimura,[2] and Toshiro Sakakibara[2]

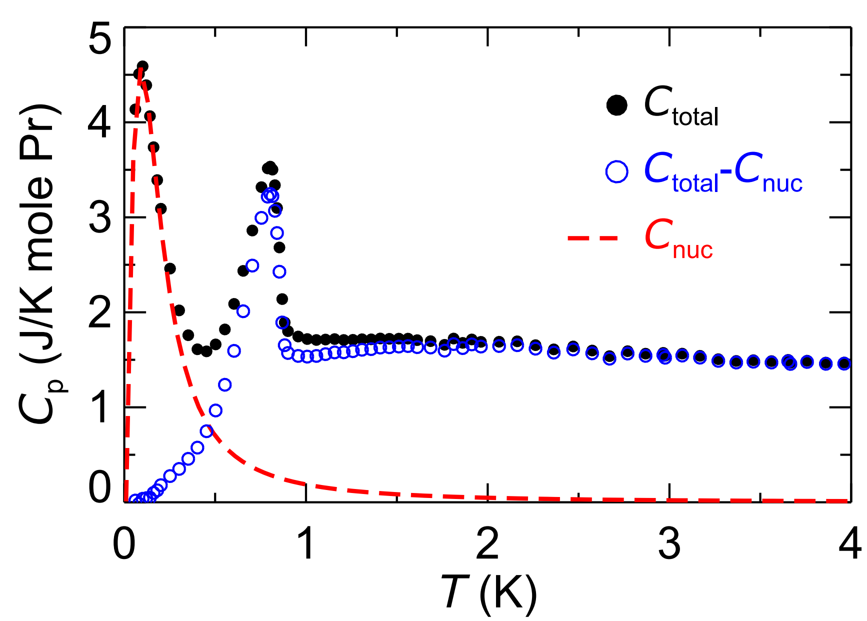


FIG. 1. (color online) Temperature dependence of the specific heat of $Pr_{2+x}Ir_{2-x}O_{7-\delta}$ in zero field. Filled circles: experimental total specific heat. Dashed curve: calculated specific

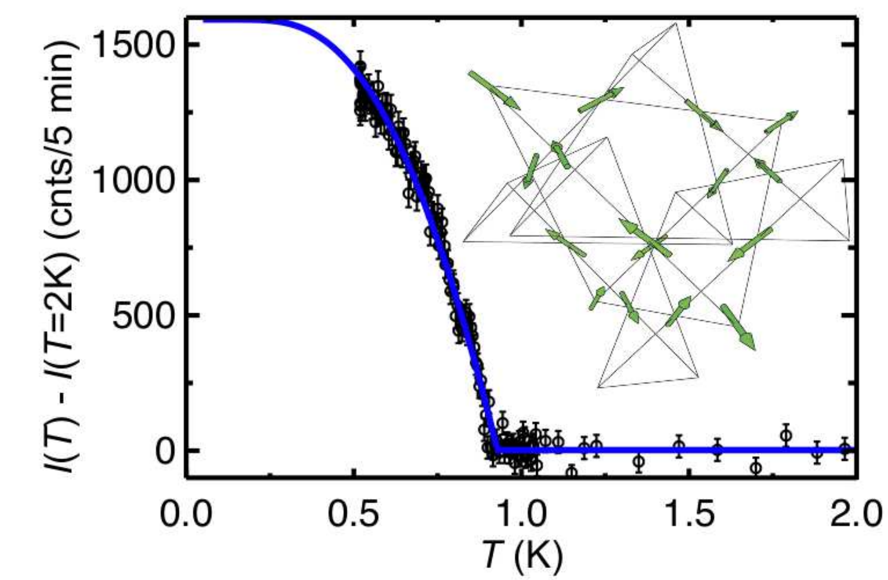


FIG. 2. (color online) Temperature dependence of elastic neutron scattering intensity of $Pr_{2+x}Ir_{2-x}O_{7-\delta}$ at the position of the $\mathbf{q}_m = (100)$ reflection. The intensity measured at $T = 2$ K

actually “Melko-Hertog-Gingras" spin state
(obtained numerically for a **different and classical** system)

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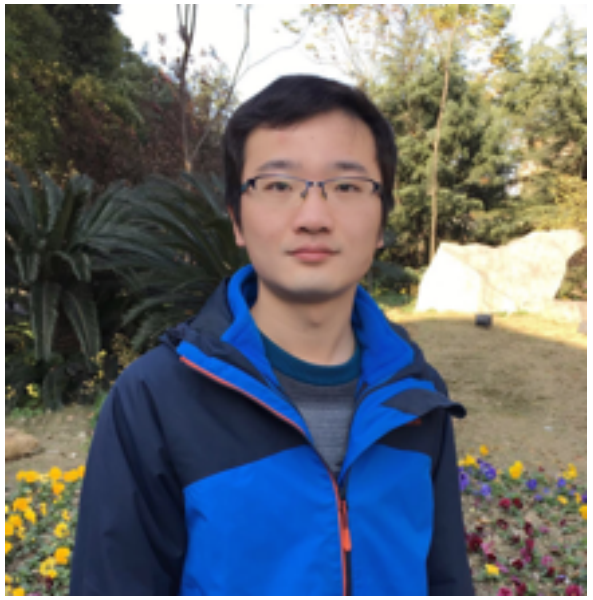
2. Pr-magnetism induced Weyl nodes and symmetry protected Dirac band touching

Here we focus on the ordered side/sample.



Xu-Ping Yao, GC, 1712.06534

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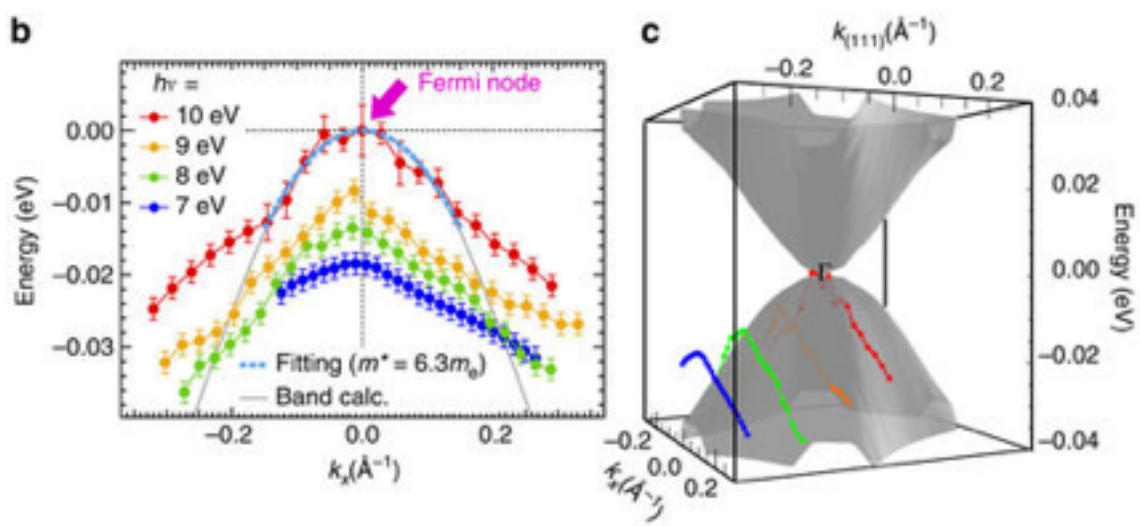
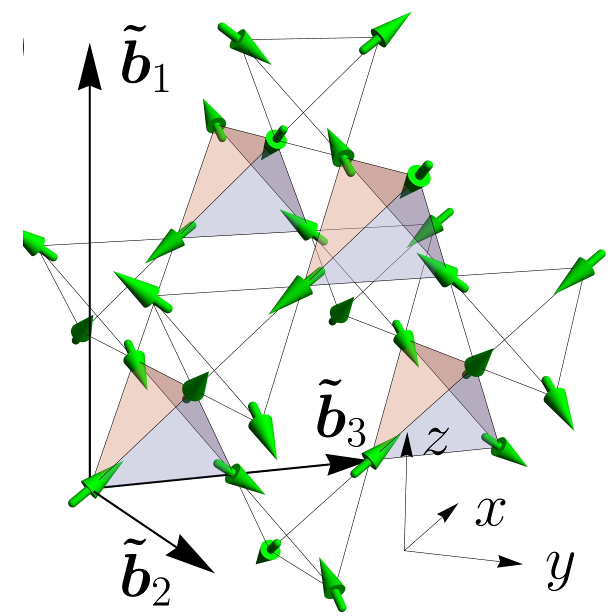
What is the impact of the Pr magnetism on Ir conduction electrons?



Ir Luttinger semimetal

+



Pr magnetism

= ????

When electron behaves as electron,
when spin behaves as spin !

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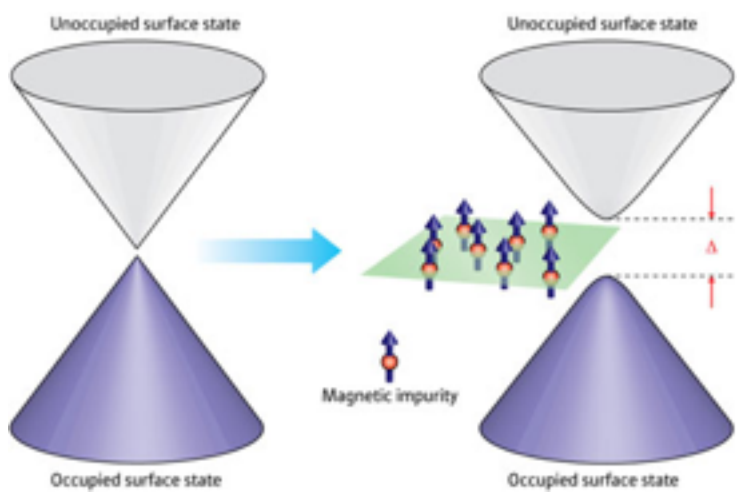
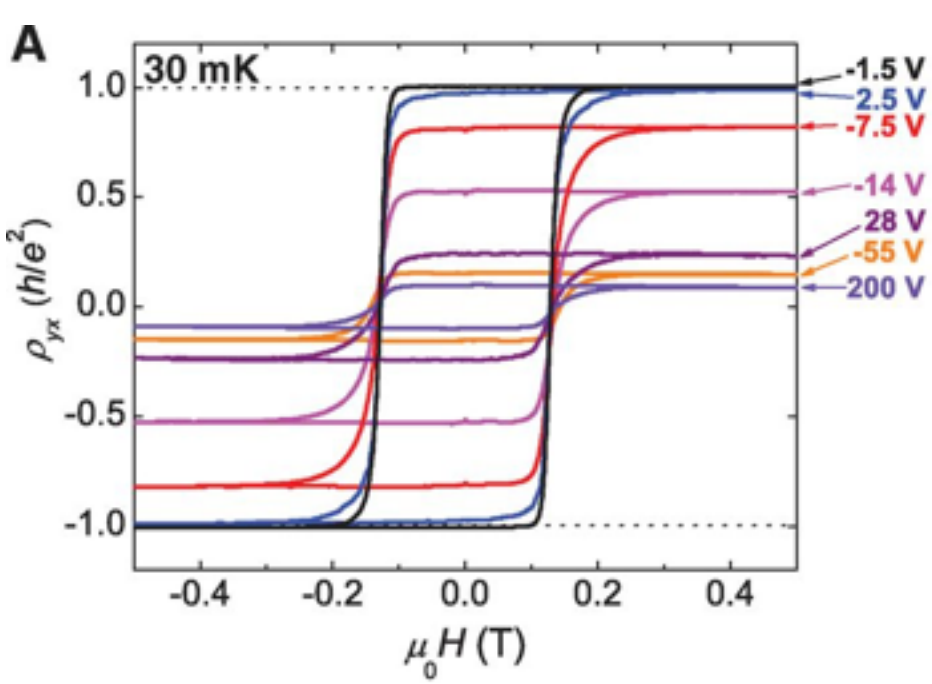
Xue's group





Quantum Anomalous Hall Effect

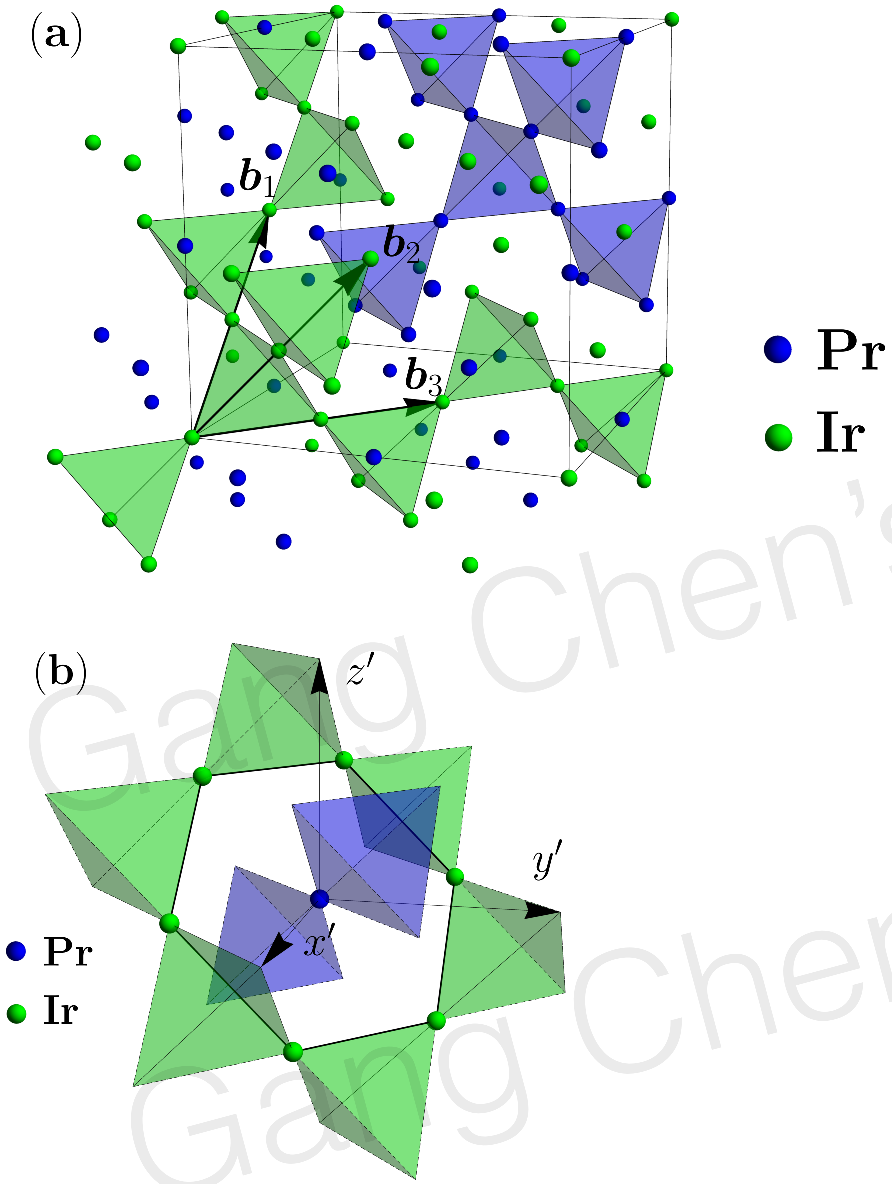
1. One understanding: TI -> Dirac cone ferromagnetism -> gapped Dirac fermion -> QAHE

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

interact with
interact with
very comple
system



GC, Hermele, PRB 2012
X-P Yao, GC, 1712.06534

Energy Scale

~<1eV — Ir 5d electron: hopping, SOC, interaction

~ — **Pr-Ir interaction: f-d exchange**

~10K — Pr 4f electron: exchange interaction

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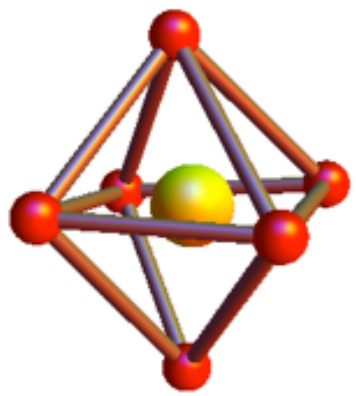
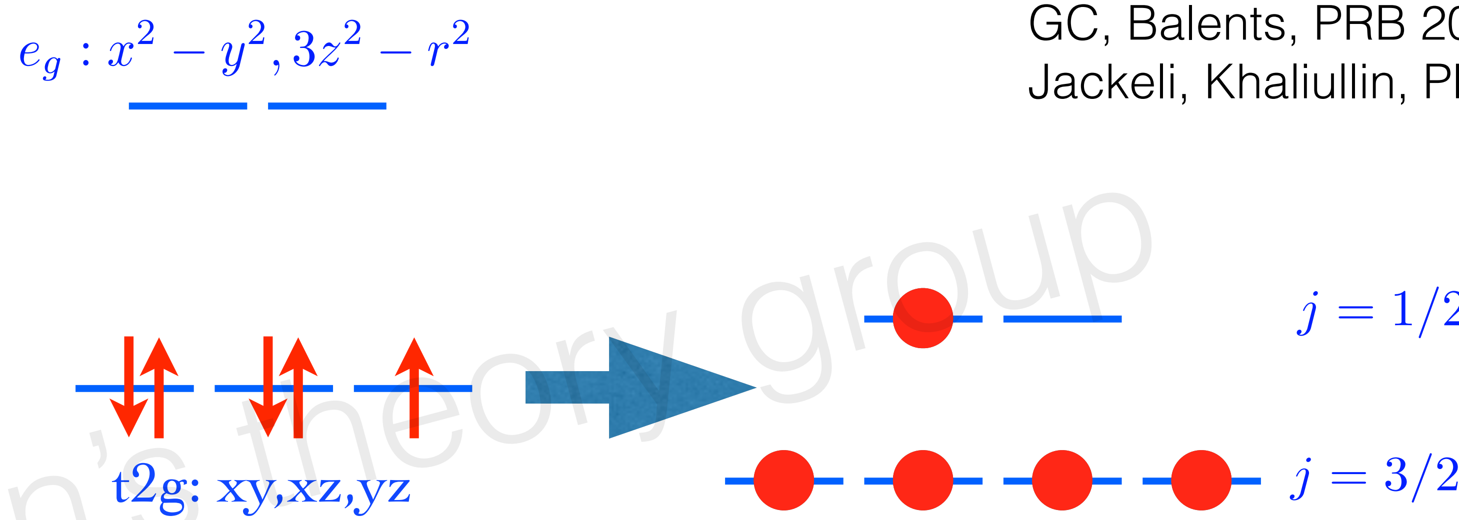
Ir 5d electron: SOC, hopping and correlation

BJ Kim, etc 2008,
GC, Balents, PRB 2008
Jackeli, Khaliullin, PRL 2009



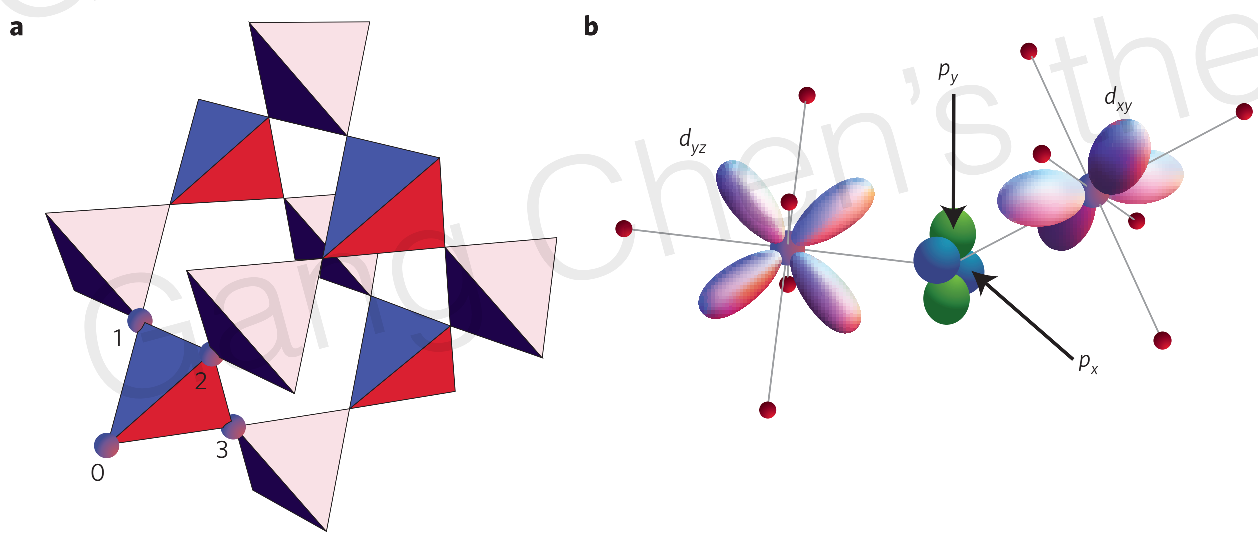
IrO6 octahedron

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



Crystal electric field

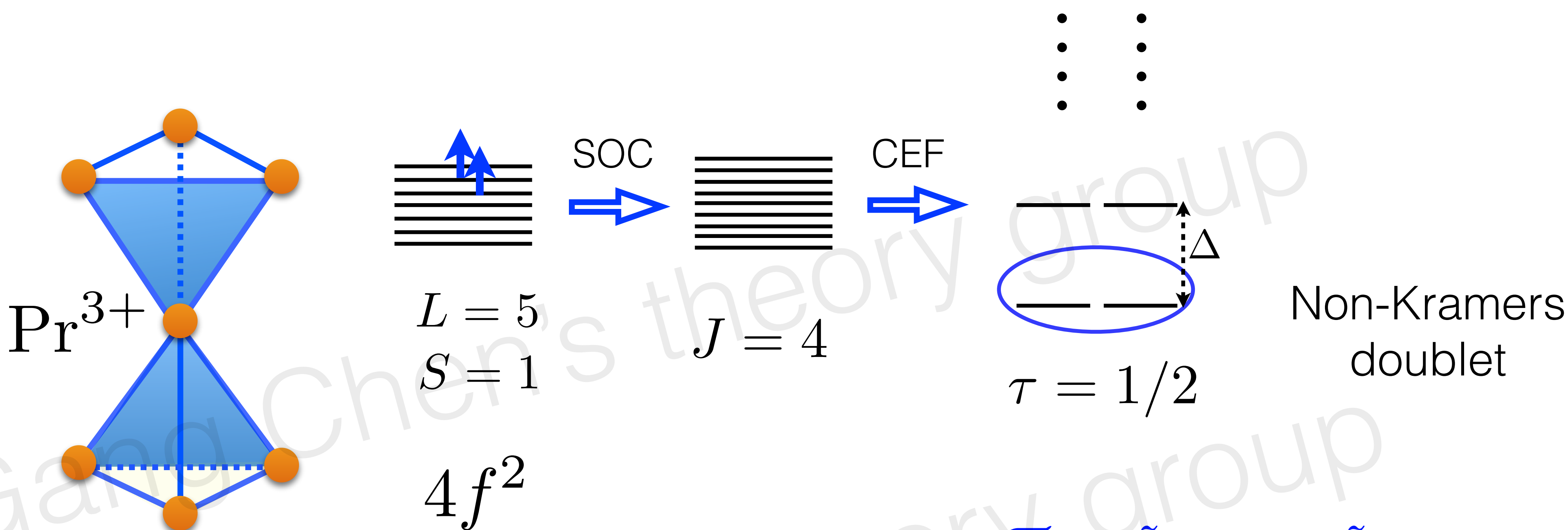
Spin-orbit coupling



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

For $Pr_2Ir_2O_7$, correlation renormalizes the band width.

Pr local moments: non-Kramers doublets



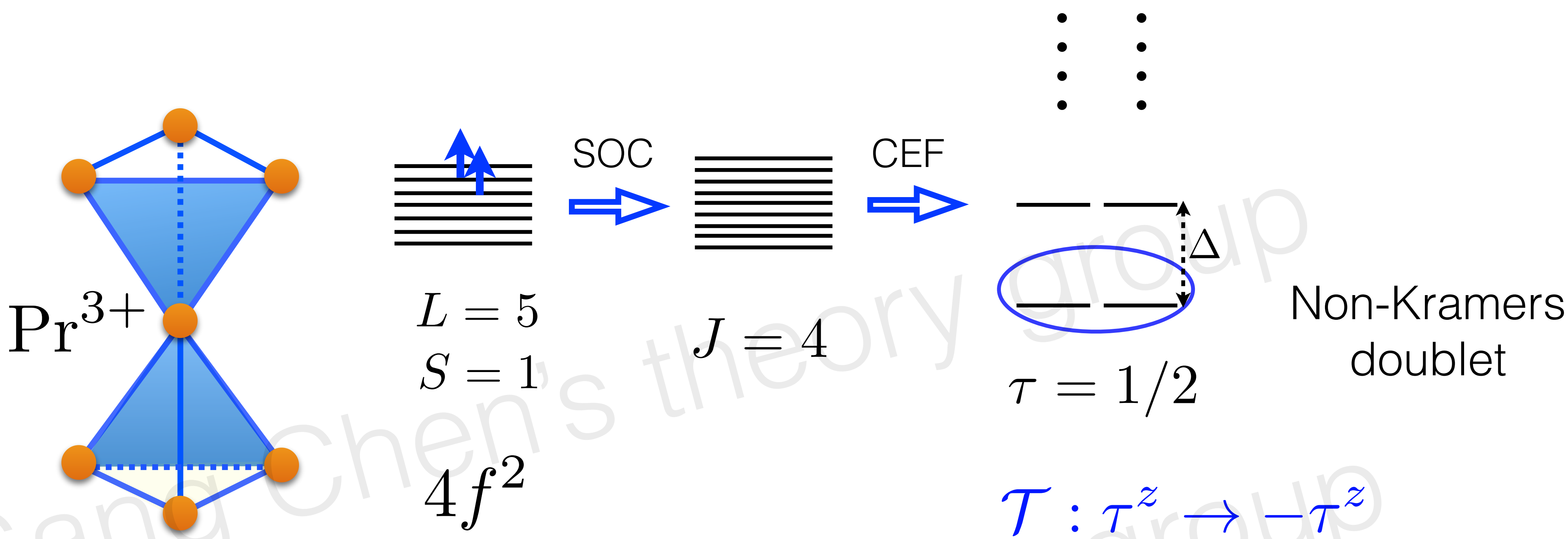
$$\mathcal{T} : \tau^z \rightarrow -\tau^z$$

$$\mathcal{T} : \tau^{x,y} \rightarrow +\tau^{x,y}$$

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



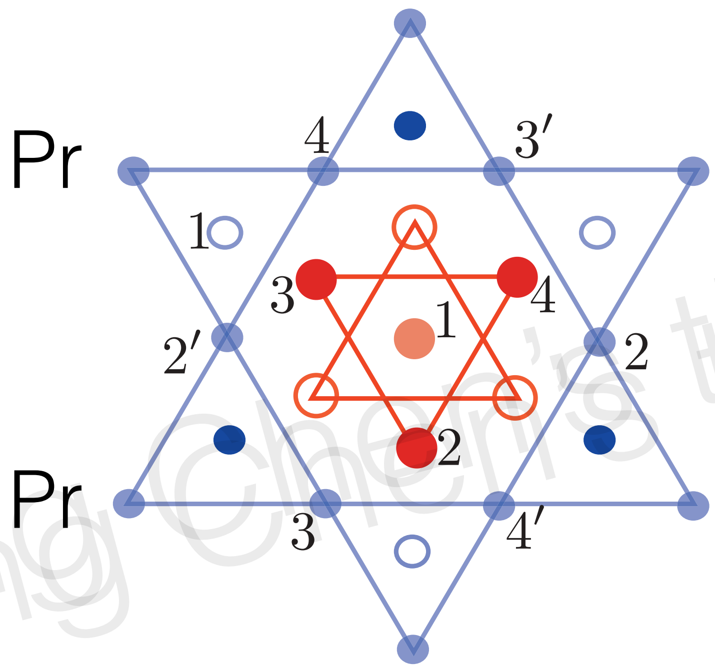
$$\mathcal{T} : \tau^z \rightarrow -\tau^z$$

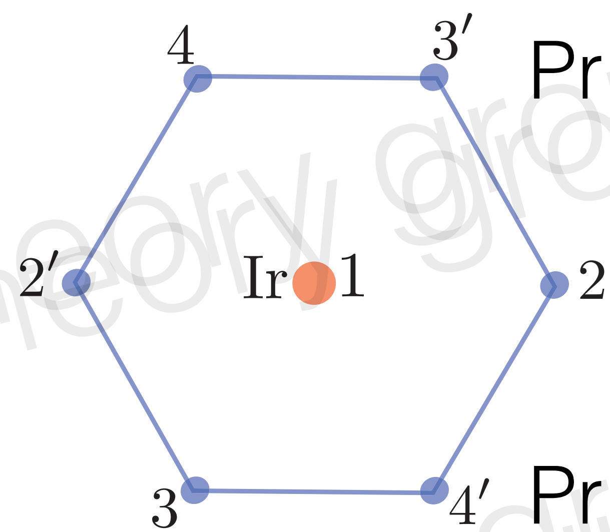
$$\mathcal{T} : \tau^{x,y} \rightarrow +\tau^{x,y}$$

$$\tilde{H}_{ex} = \sum_{ij} J_{z,ij} \tau_i^z \tau_j^z + \sum_{ij} J_{\perp,ij} \sum_{\mu,\nu=x,y} \tau_i^\mu \tau_j^\nu ,$$

$$\tilde{H}_{ex} \simeq \sum_{\langle ij \rangle} J_{1z} \tau_i^z \tau_j^z + \sum_{\langle\langle\langle ij \rangle\rangle\rangle} J_{3z} \tau_i^z \tau_j^z ,$$

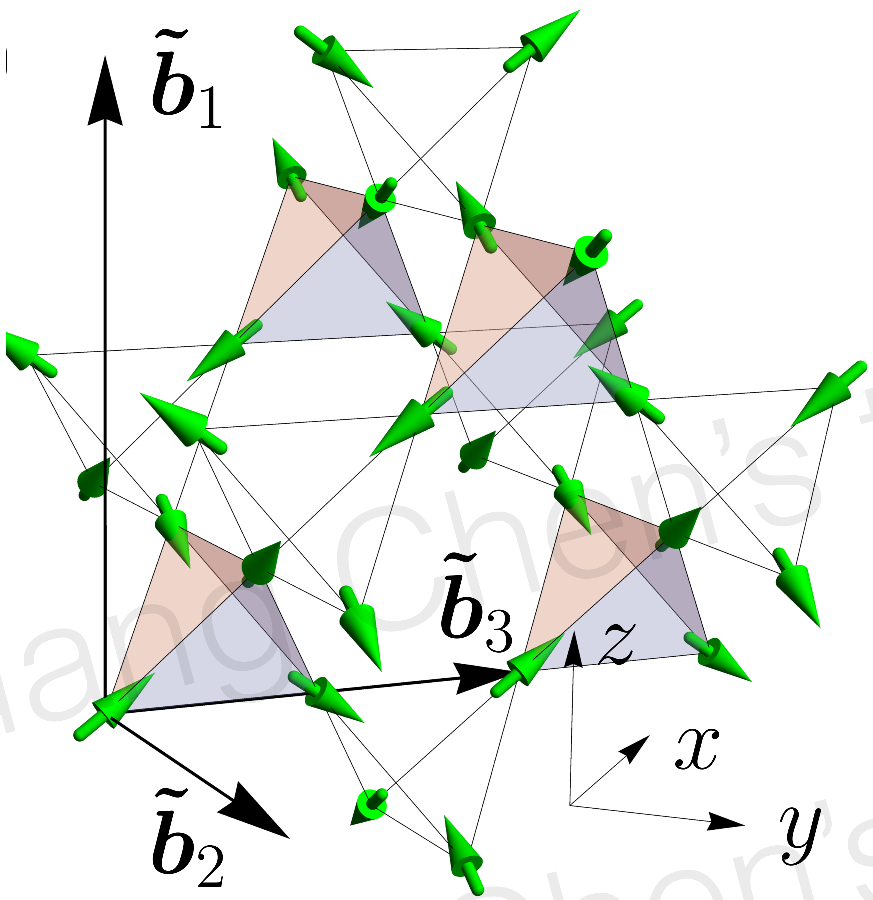
Pr-Ir interaction: 4f-5d exchange



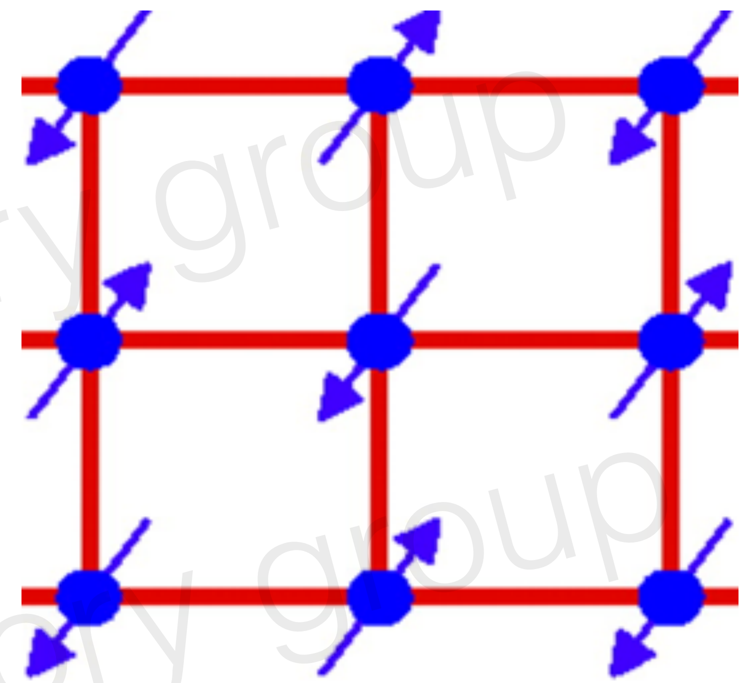


$$\mathcal{H}_{\rm fd} = \big[c_1\tau_4^z - c_2\big(\tau_2^z + \tau_3^z\big)\big] j_1^x + \big[c_1\tau_3^z - c_2\big(\tau_2^z + \tau_4^z\big)\big] j_1^y + \big[c_1\tau_2^z - c_2\big(\tau_3^z + \tau_4^z\big)\big] j_1^z + [2 \leftrightarrow 2', 3 \leftrightarrow 3', 4 \leftrightarrow 4'],$$

Magnetic translation of Pr magnetic state

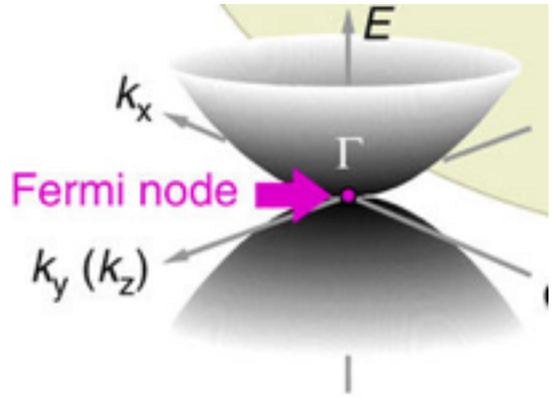


$$\tilde{\mathcal{T}} \equiv \mathcal{T} \circ t$$

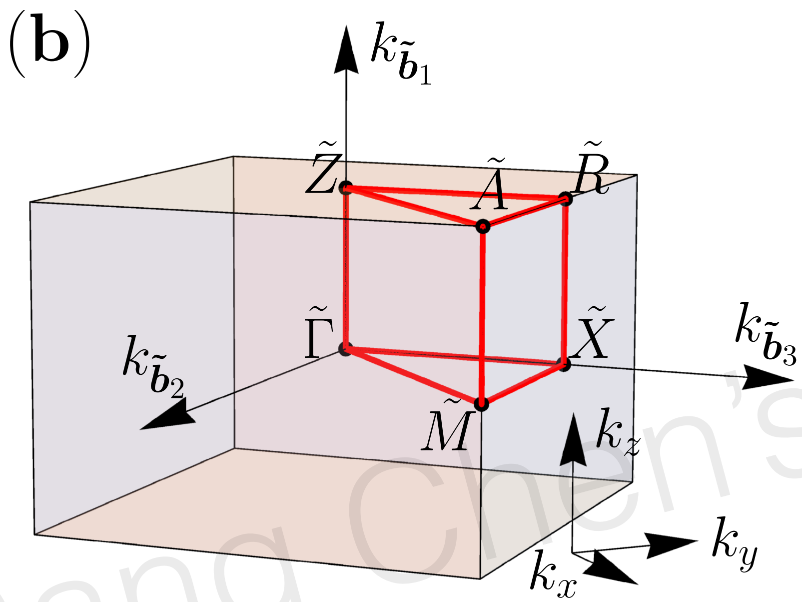


Neel state on square lattice

3D analogue of the magnetic translation for Neel state

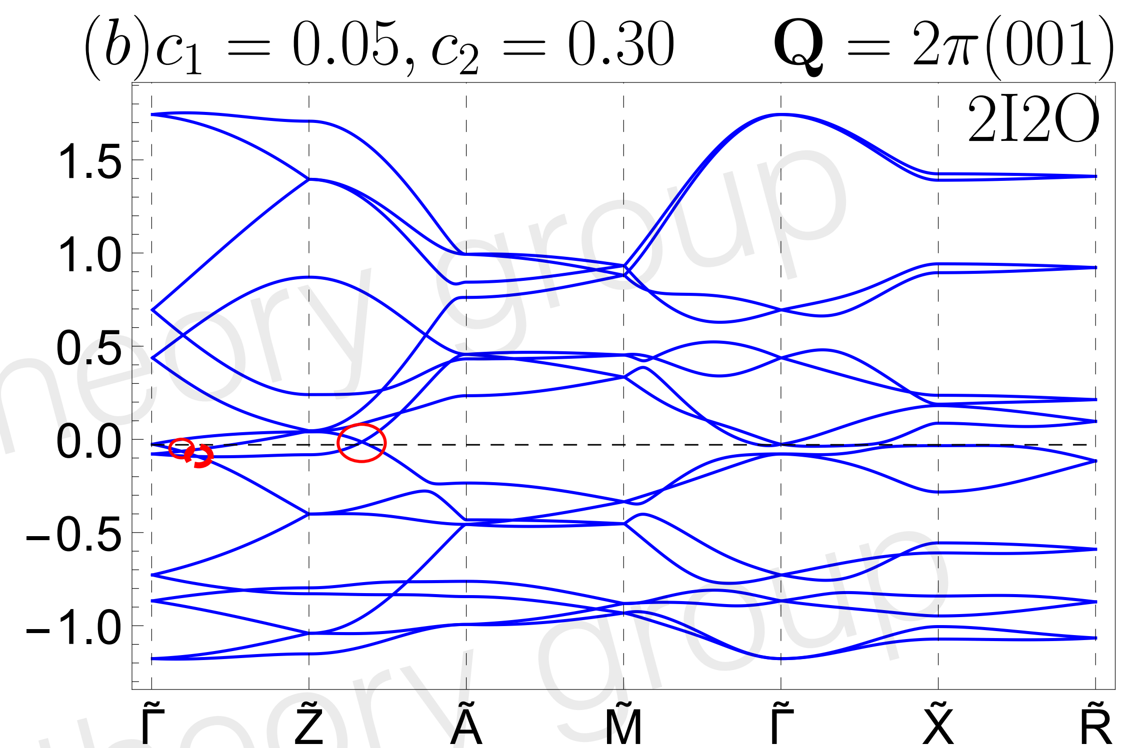


Symmetry protected Dirac band touching



magnetic Brillouin zone

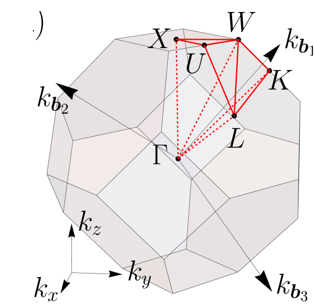
$\tilde{\mathcal{T}}^2 = -1$ at $\tilde{\Gamma}$ point

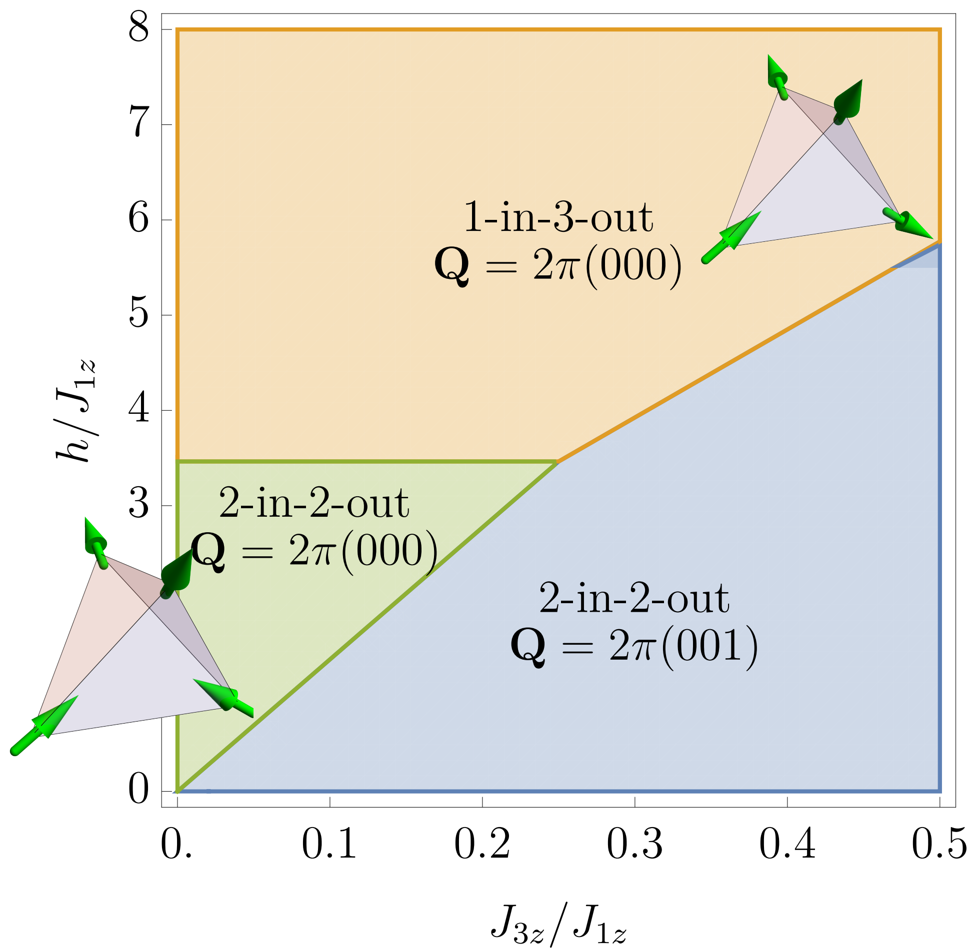


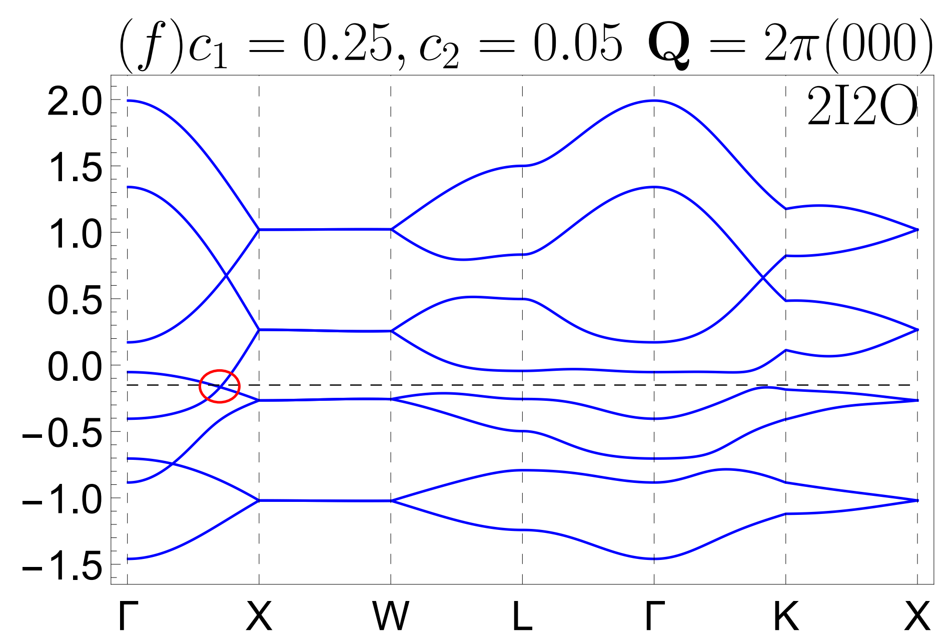
in addition, there are Weyl nodes
whose existence does not require symmetry

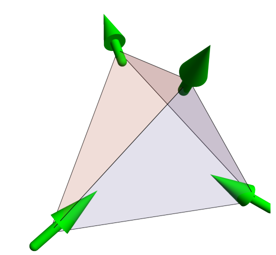
Pr magnetic order transfers its time reversal
symmetry breaking to Ir Luttinger semimetal.

Band engineering by external magnetic field









example: double Weyl nodes

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

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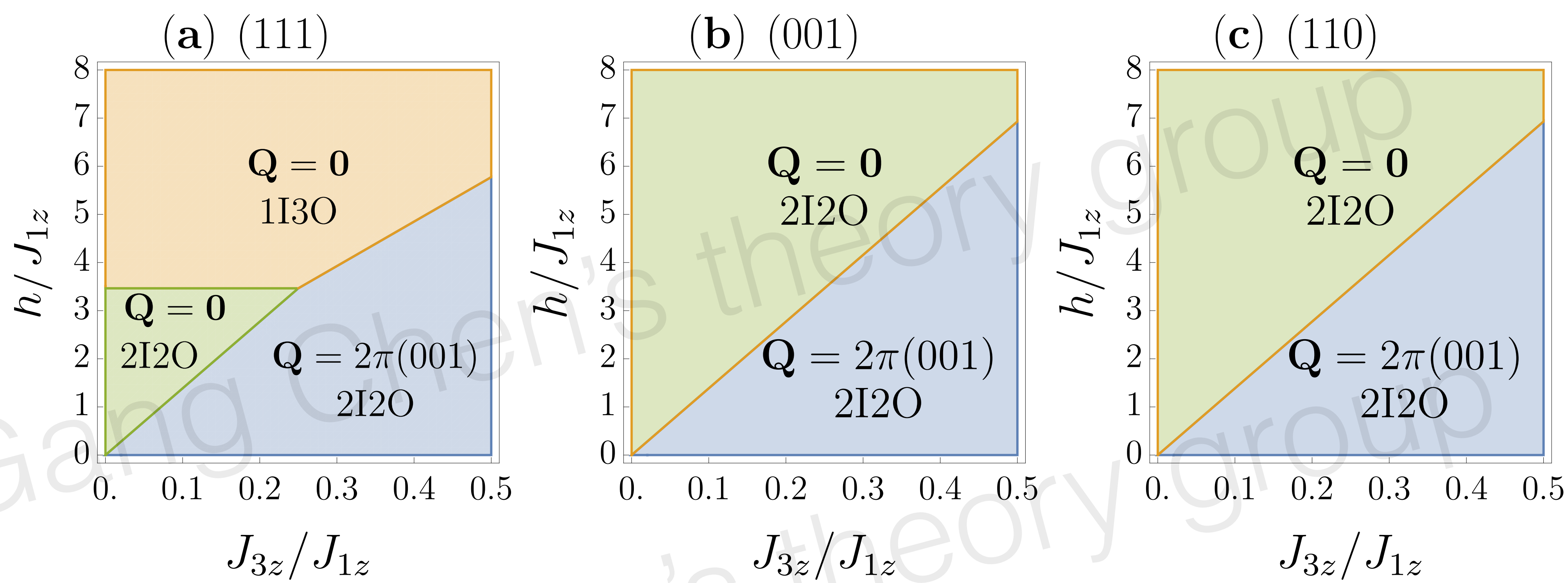
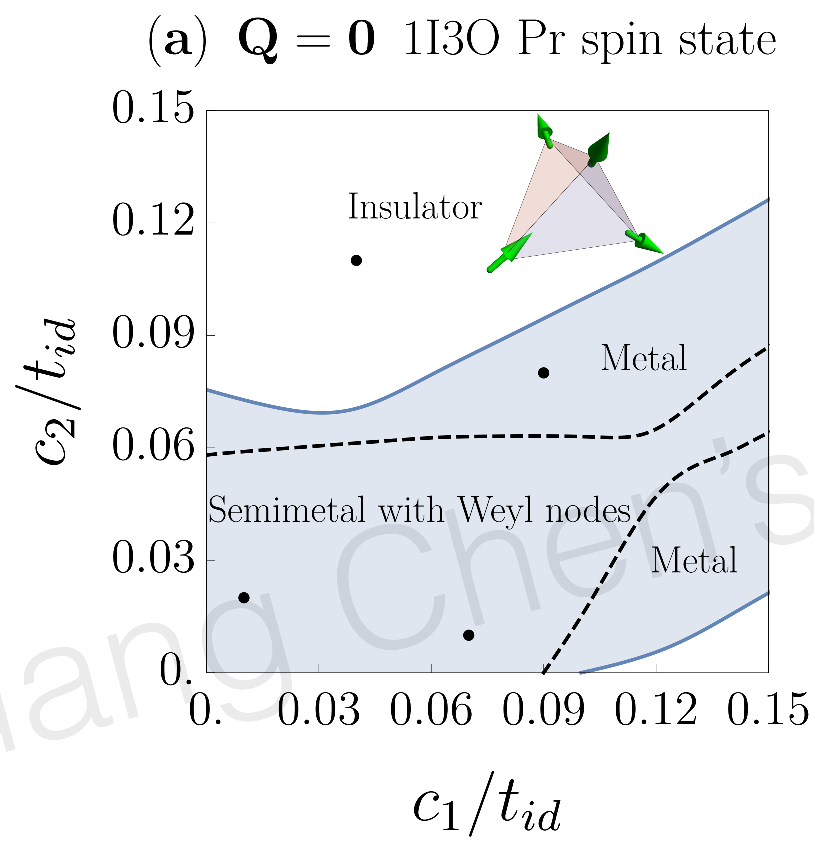
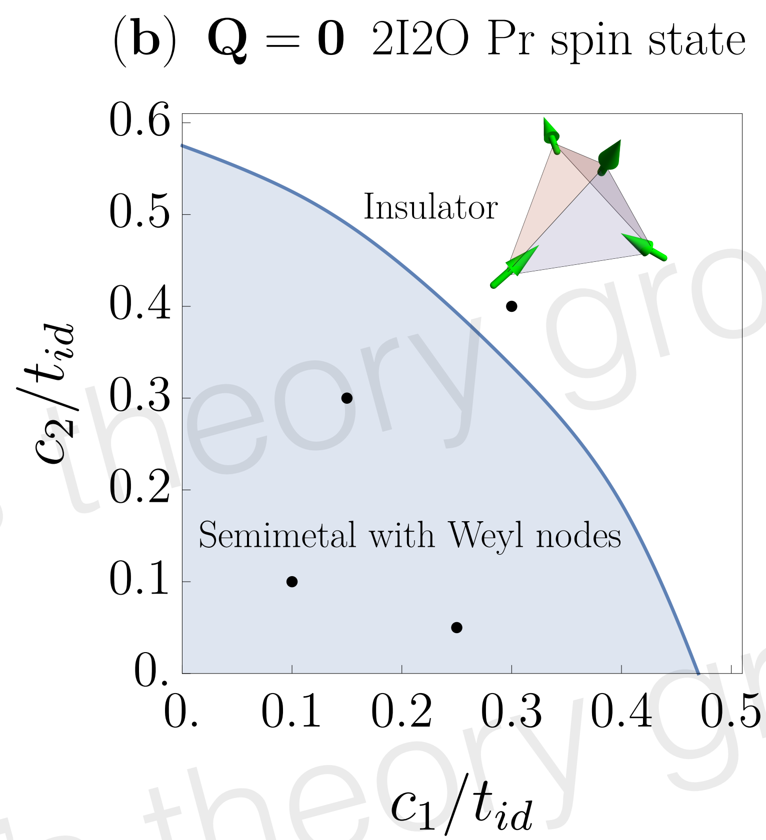
Quantum control under magnetic field



The Pr magnetic state under
different direction magnetic field

111 magnetic field, Ir band structure





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

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

Some $Pr_2Ir_2O_7$ 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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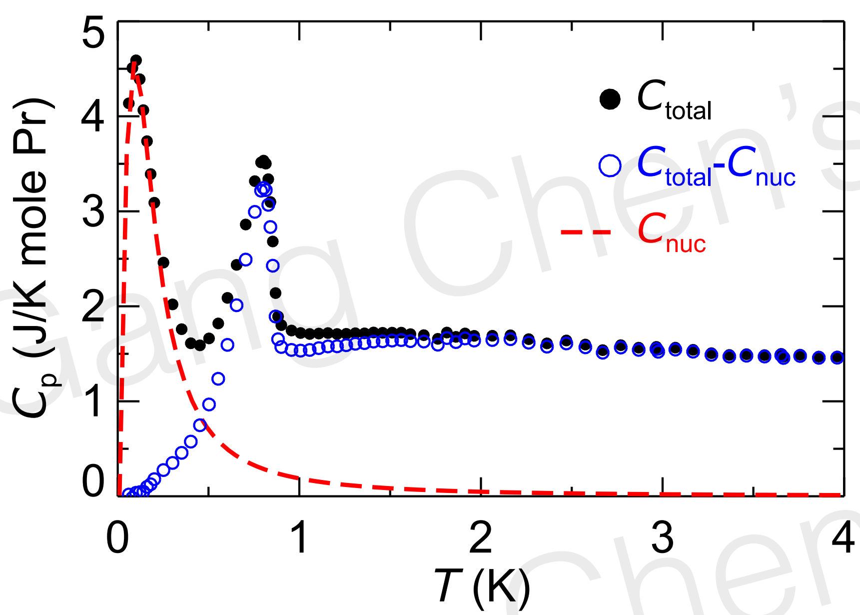


FIG. 1. (color online) Temperature dependence of the specific heat of $Pr_{2+x}Ir_{2-x}O_{7-\delta}$ in zero field. Filled circles: experimental total specific heat. Dashed curve: calculated specific

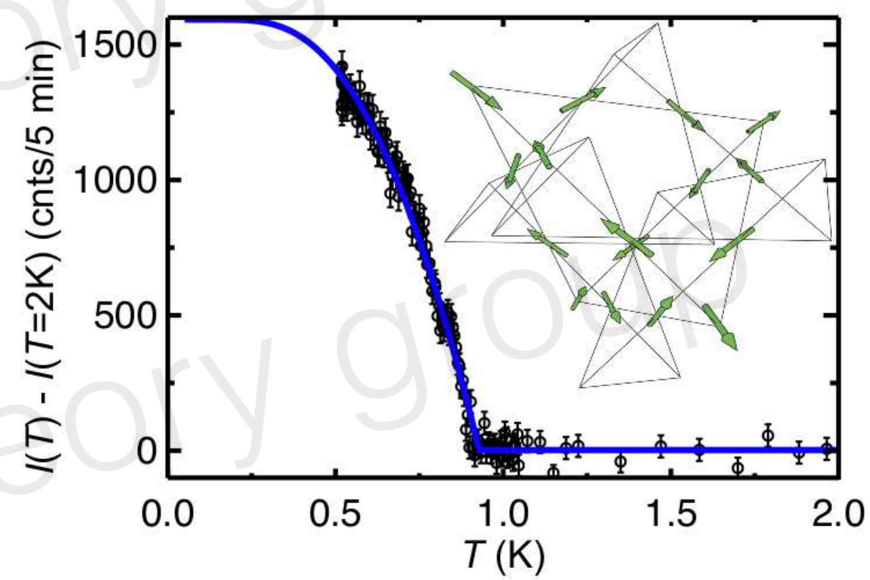
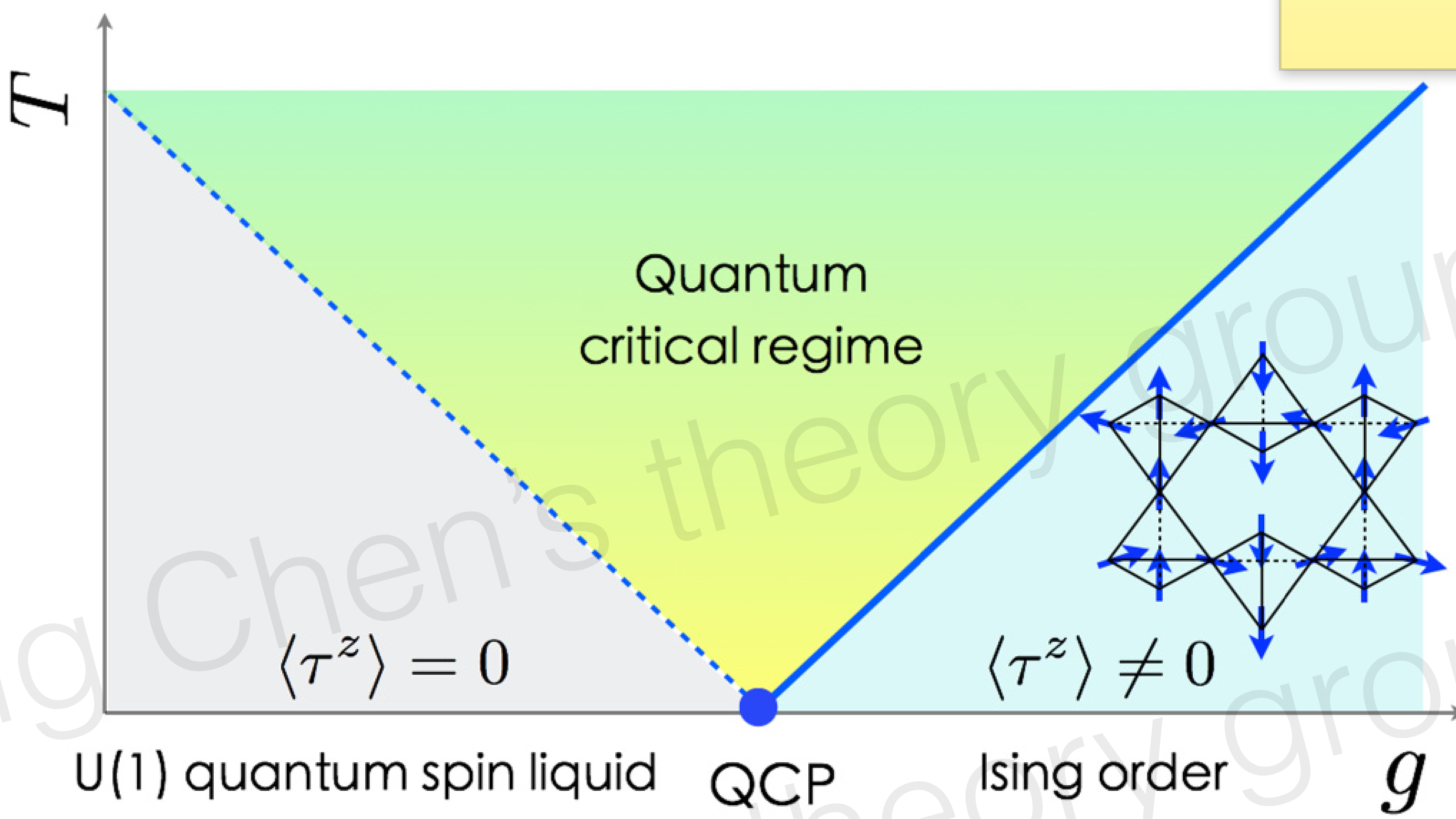


FIG. 2. (color online) Temperature dependence of elastic neutron scattering intensity of $Pr_{2+x}Ir_{2-x}O_{7-\delta}$ at the position of the $\mathbf{q}_m = (100)$ reflection. The intensity measured at $T = 2$ K

actually "Melko-Hertog-Gingras" spin state
(obtained numerically for a **different and classical** system)

there may be some jump in logic

Our suggestion

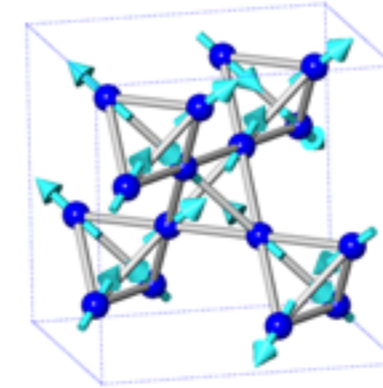


The Pr subsystem is proximate to a quantum phase transition from pyrochlore ice U(1) QSL to Ising magnetic order.

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



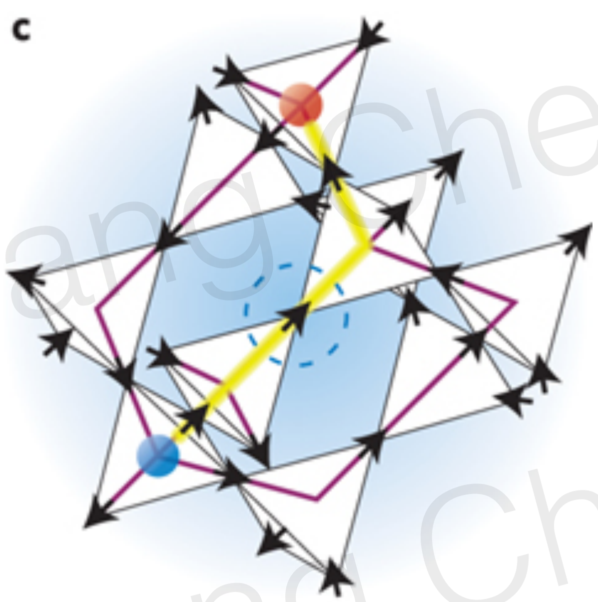
spin ice

Hermele, Fisher, Balents, 2004

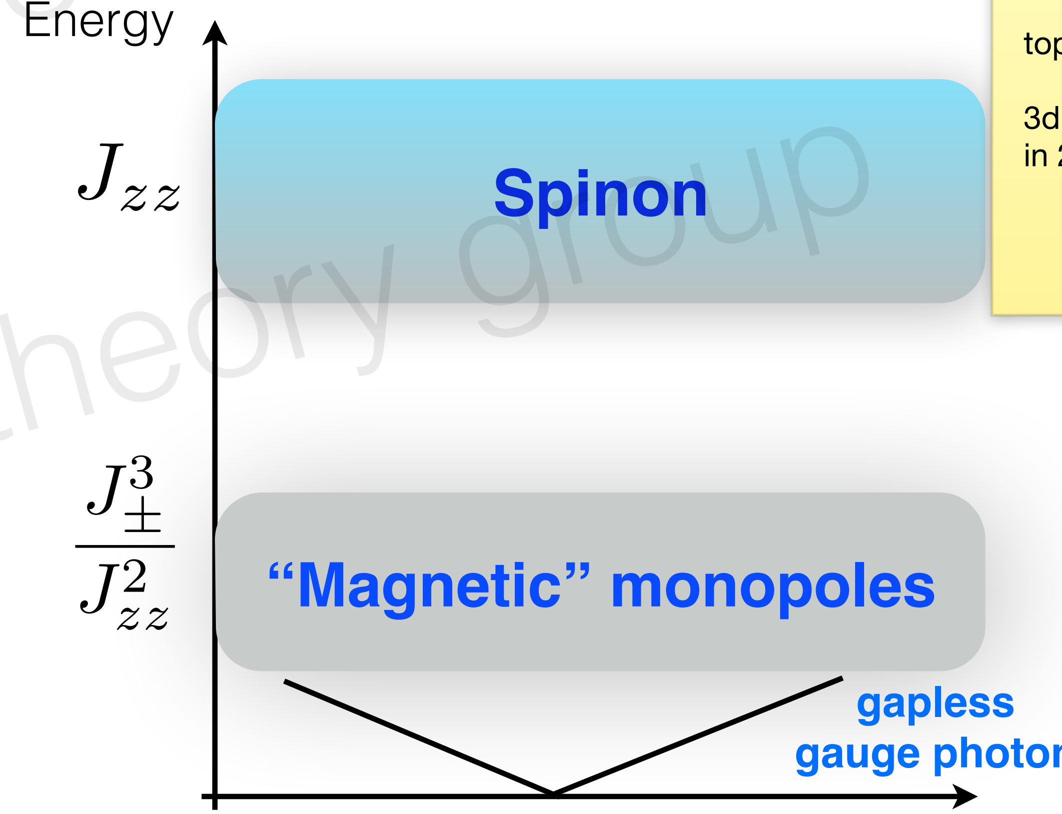
$$H = \sum_{\langle ij \rangle} J_{zz} \tau_i^z \tau_j^z - J_{\pm}(\tau_i^+ \tau_j^- + h.c.)$$

$\tau^z \sim E$ emergent electric field

$\tau^{\pm} \sim e^{\pm iA}$ emergent vector gauge potential



Balents, Savary, Gingras, SB Lee,
Moessner, Onoda, Shannon…….



it is like topological
topogical defect of v
3d analogue of visor
in 2d z2 spin liquid.

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.

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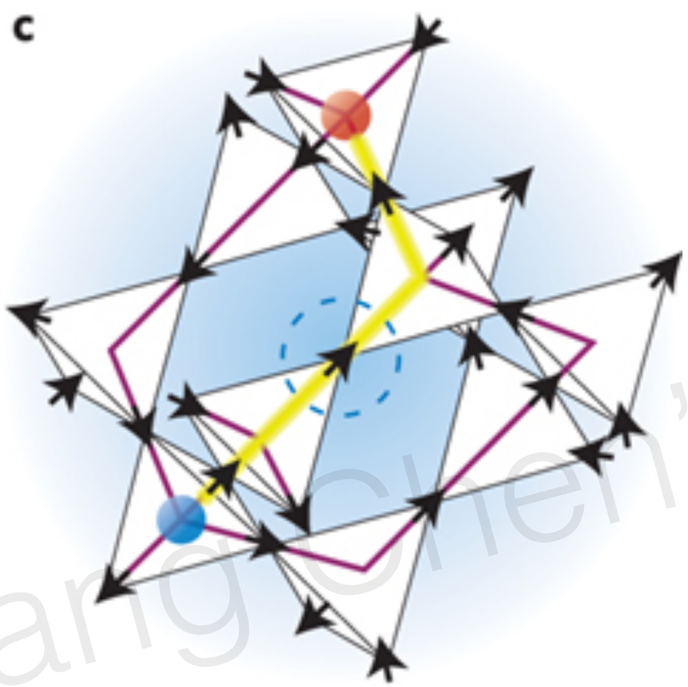
Electromagnetic duality and monopole condensation



$$\mathcal{T}: \tau^z \rightarrow -\tau^z$$

$$\mathcal{T}: \tau^{x,y} \rightarrow +\tau^{x,y}$$

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.

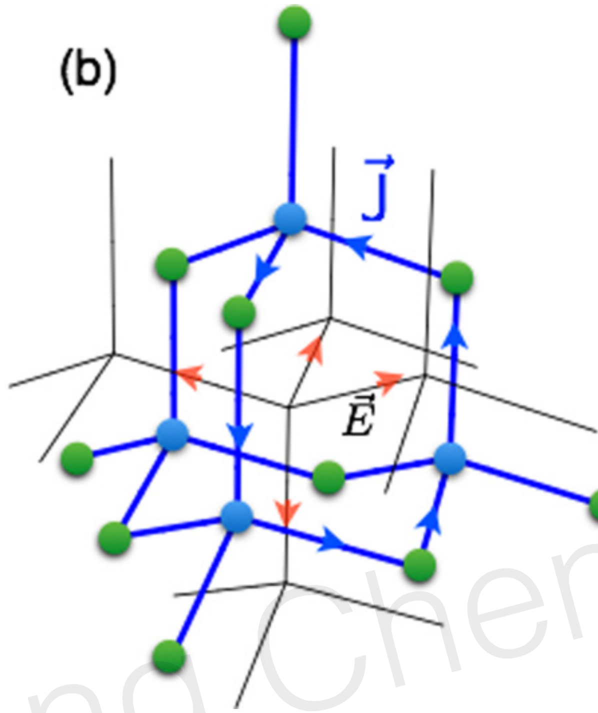
Motrunich Senthil 2005,
DL Bergman, G Fiete, Balents 2005
GC PRB 94, 205107 (2016)

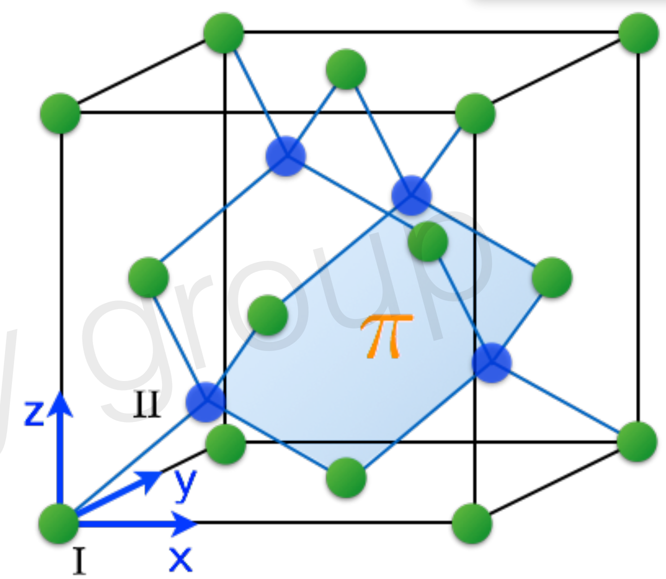
quark confinement

Monopole condensation and magnetic or

like Ginzburg Landau,

except the gauge is internal and emergent





$$H_{\rm dual} = \sum_{\hexagon_d^*} \frac{U}{2}(\mathrm{curl}\, a - \bar{E})^2 - \sum_{\mathbf{r},\mathbf{r}'} K \cos B_{\mathbf{rr}'} - \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} t\, e^{-i2\pi \bar{a}_{\mathbf{rr}'}} \Phi_{\mathbf{r}}^\dagger \Phi_{\mathbf{r}'} - \mu \sum_{\mathbf{r}} \Phi_{\mathbf{r}}^\dagger \Phi_{\mathbf{r}},$$

Electromagnetic duality
and right-hand rule

$$\tau_i^z \sim E_{\boldsymbol{rr}'} \sim \sum_{\mathbf{rr}' \in \hexagon_d^*}^{\circlearrowleft} \mathbf{J}_{\mathbf{rr}'},$$

This theory gives the same magnetic order in $Pr_2Ir_2O_7$,
the magnetic order has to break translation symmetry.

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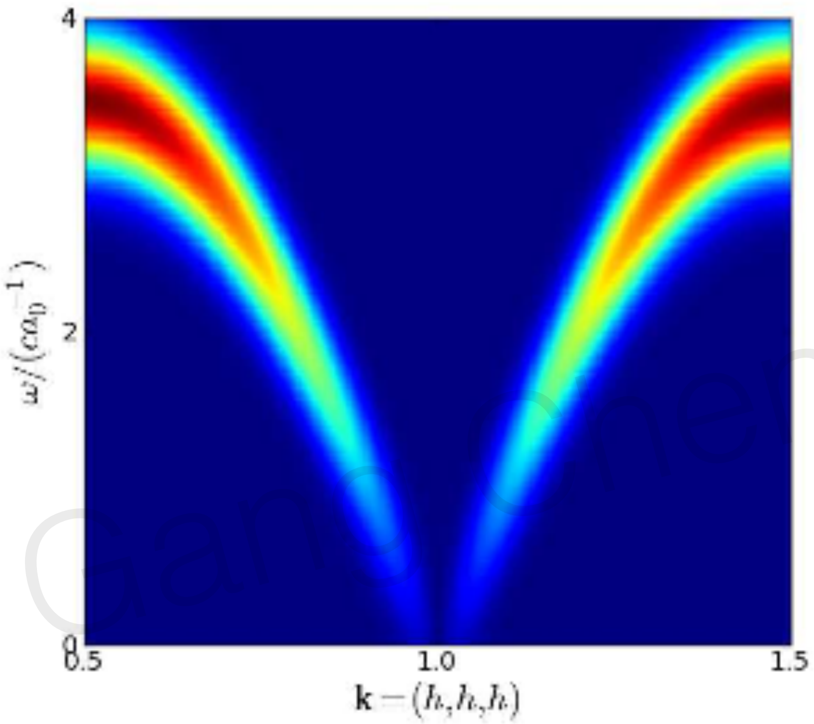
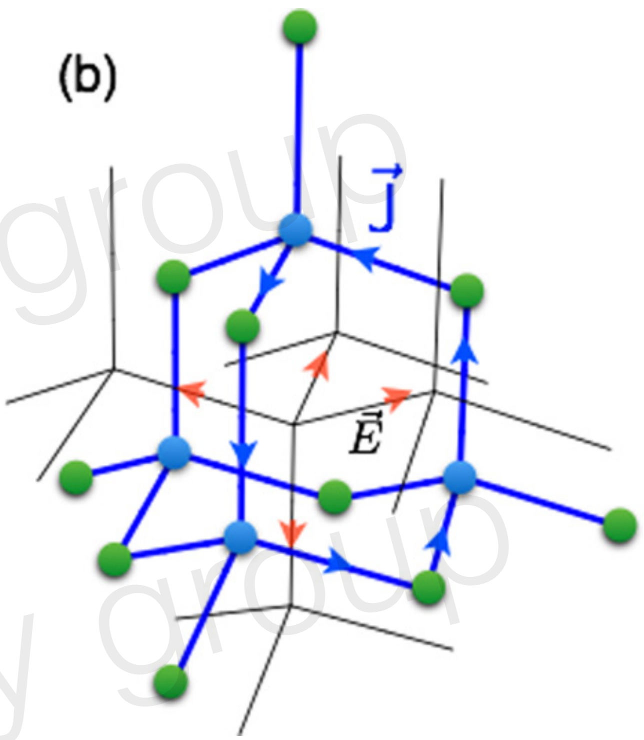
Where to see Dirac's magnetic monopoles?

Let's forget $Pr_2Ir_2O_7$. Now given a U(1) QSL, what should we measure?





$\tau^z \sim E$ (emergent electric field)

$$\mathrm{Im}[E^{\alpha}_{-\mathbf{k},-\omega} E^{\beta}_{\mathbf{k},\omega}] \propto [\delta_{\alpha\beta} - \frac{k_\alpha k_\beta}{\mathbf{k}^2}]\,\omega\,\delta(\omega - v|\mathbf{k}|),$$

Low energy theory (Savary, Balents)

Electromagnetic duality

Electric loop current -> Magnetic field
Magnetic loop current -> Electric field

at higher energy, detect monopole continuum

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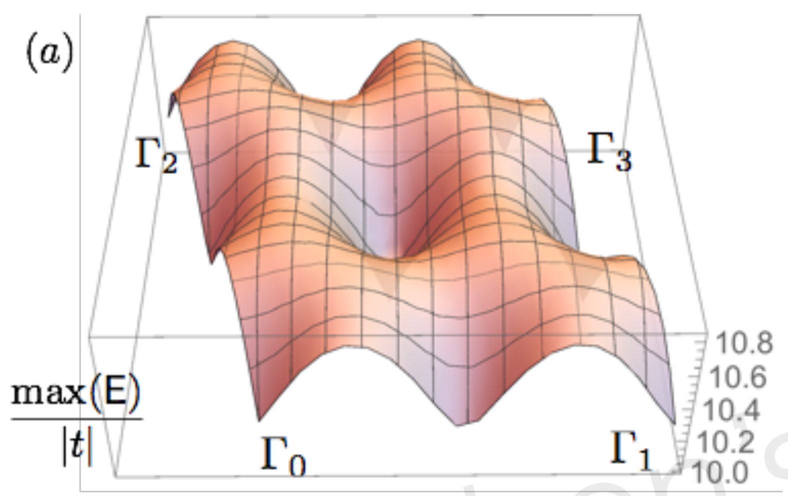
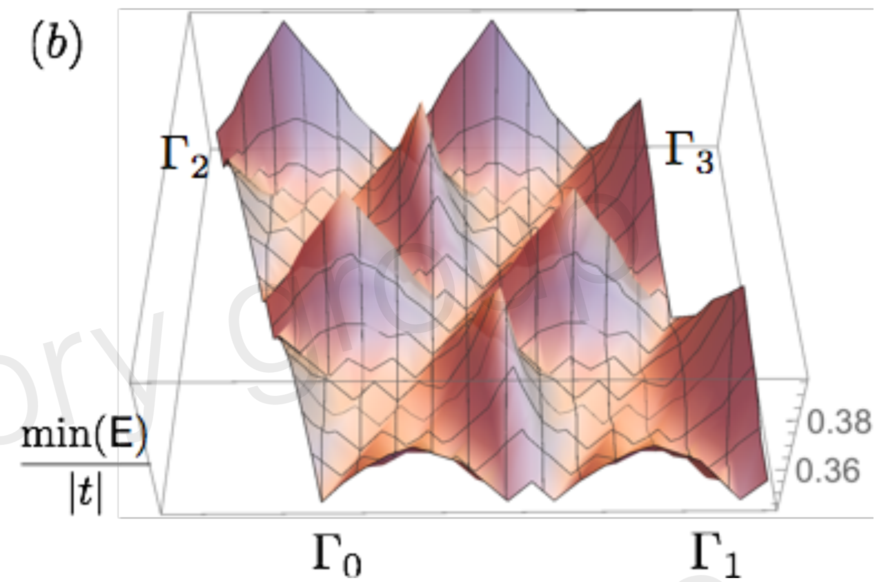
Spectral periodicity of monopole continuum



Upper excitation edge of monopole continuum



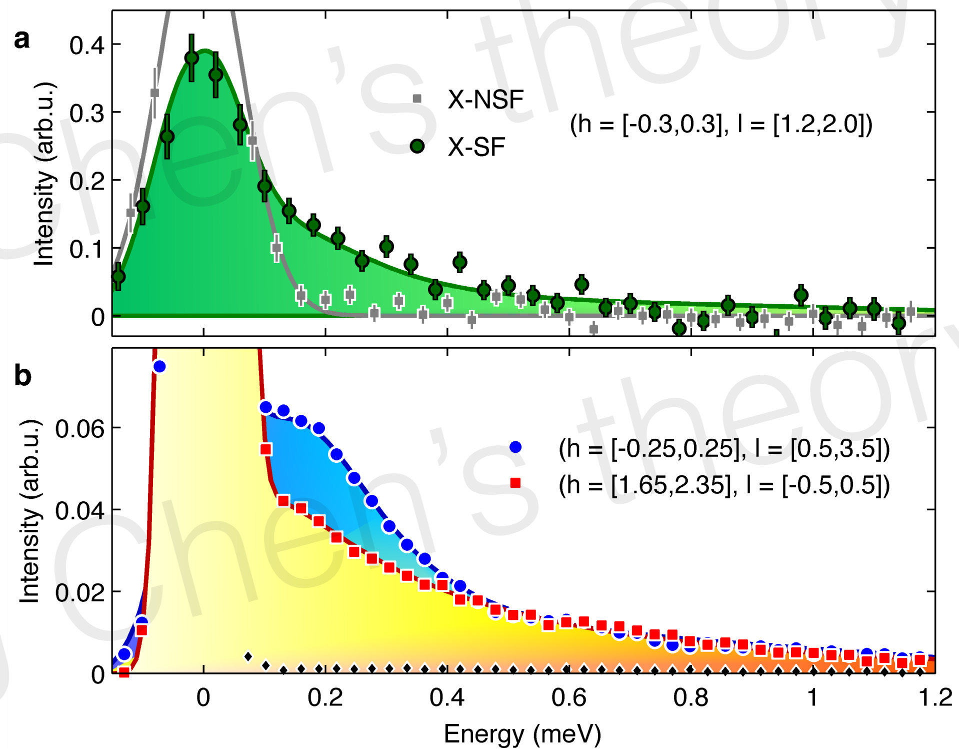
Lower excitation edge of monopole continuum

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

General connection was first understood by Xiao-Gang Wen 2001,2002.
Essin, Hermele, 2015, GC PRB 96, 195127 (2017)

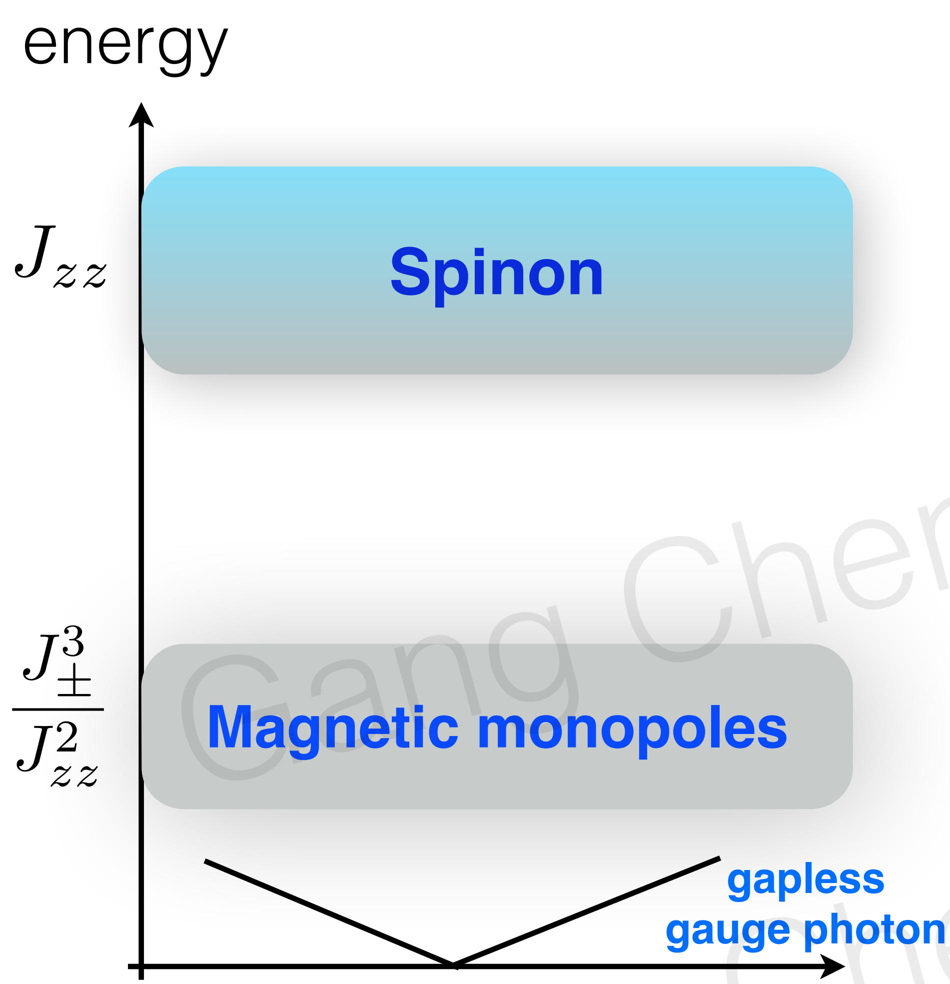
Monopole continuum in $Pr_2Hf_2O_7$?

In fact, continuum has been observed in $Pr_2Hf_2O_7$

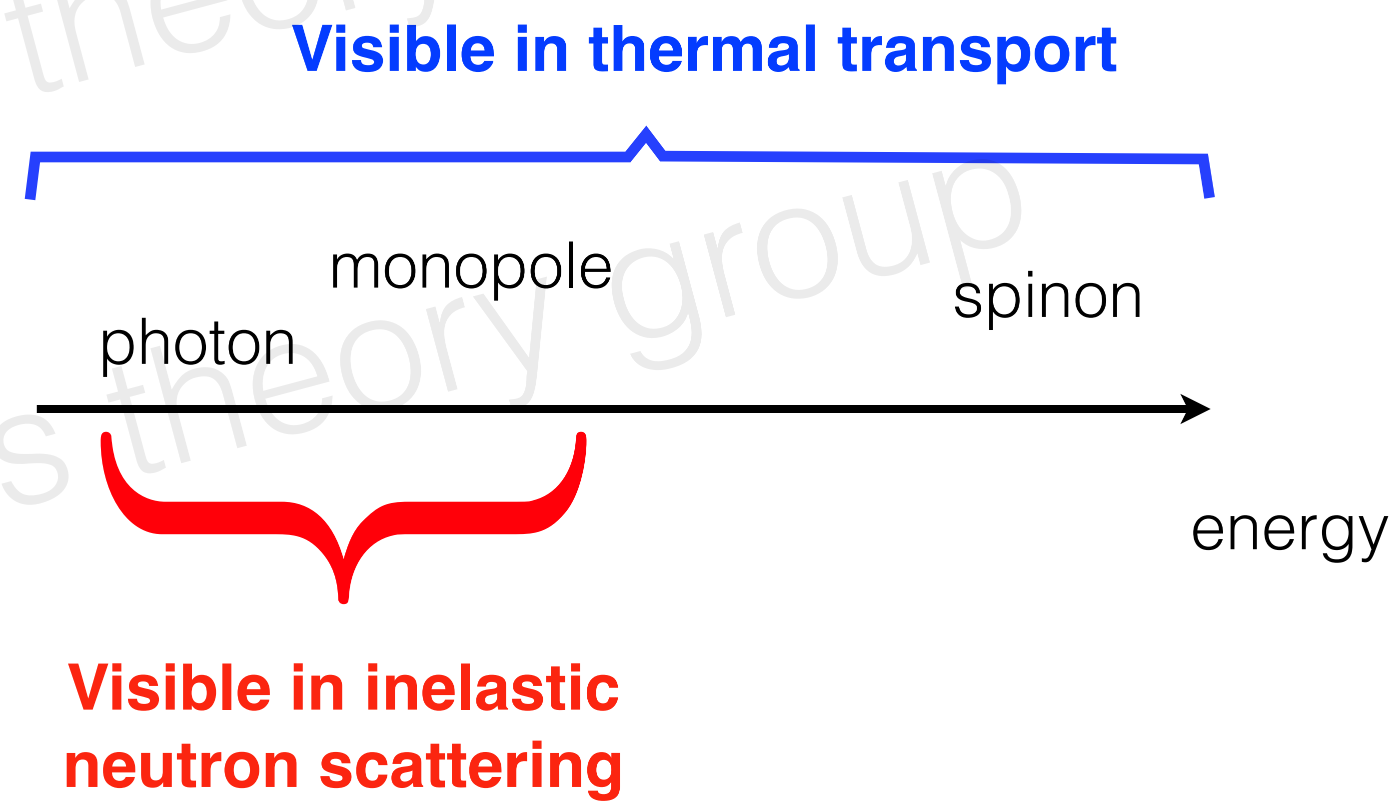


(R. Sibille, et al, arXiv 1706.03604).

Further suggestions for experiments 1



For **non-Kramers doublets** such as Pr ion in $Pr_2Zr_2O_7$ and Tb ion in $Tb_2Ti_2O_7$



GC, PRB 96, 195127 (2017)
Thermal transport in spin ice, Yuji Matsuda, 2016

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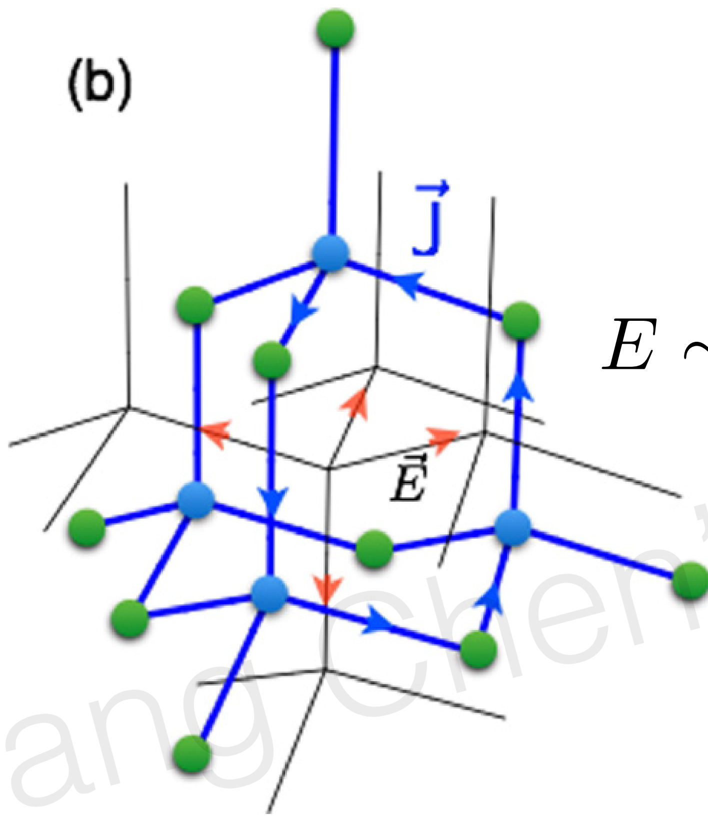
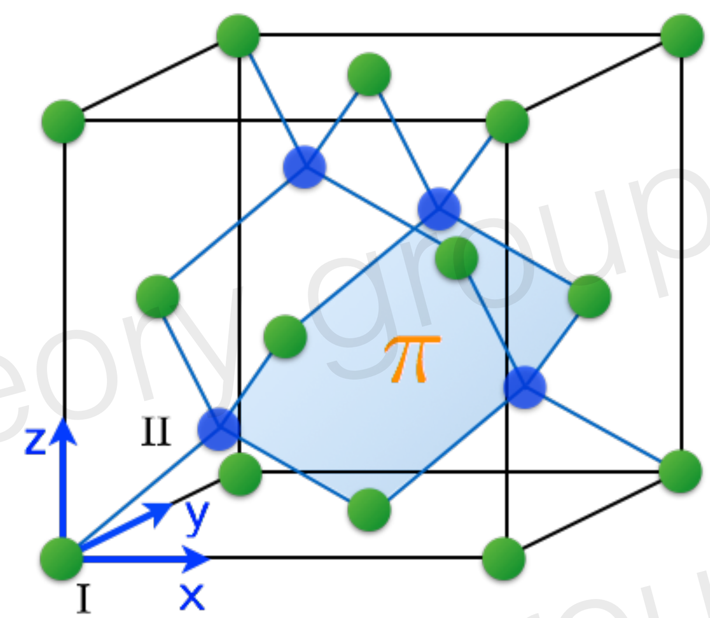
Further suggestions for experiments 2



$E \sim \tau^z$



$$H_{\text{Zeeman}} = \vec{B} \cdot \sum_i \tau_i^z \hat{z}_i$$

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.

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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 $Pr_2Ir_2O_7$.

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**.