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

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We study the band structure topology and engineering from the interplay between local moments and itinerant electrons in the context of pyrochlore iridates. For the metallic iridate Pr$_2$Ir$_2$O$_7$, the Ir 5$d$ conduction electrons interact with the Pr 4$f$ local moments via the f-d exchange. While the Ir electrons form a Luttinger semimetal, the Pr moments can be tuned into an ordered spin ice with a finite ordering wavevector, dubbed “Melko-Hertog-Gingras” state, by varying Ir and O contents. We point out that the ordered spin ice of the Pr local moments generates an internal magnetic field that reconstructs the band structure of the Luttinger semimetal. Besides the broad existence of Weyl nodes, we predict that the magnetic translation of the “Melko-Hertog-Gingras” state for the Pr moments protects the Dirac band touching at certain time reversal invariant momenta for the Ir conduction electrons. We propose the magnetic fields to control the Pr magnetic structure and thereby indirectly influence the topological and other properties of the Ir electrons. Our prediction may be immediately tested in the ordered Pr$_2$Ir$_2$O$_7$ samples.

**I. INTRODUCTION**

The study of the electron band structure topology has attracted a significant attention since the proposal and discovery of topological insulators\cite{1,2}. The fundamental aspect between the topological protection and the band structure has been well understood. More practically, there is a growing effort that proposes experimental schemes such as the strain or magnetic dopings to control or engineer the band structure topology. Along this line, a great success was achieved in the discovery of quantum anomalous Hall effect in the magnetically doped Bi$_2$Se$_3$ material\cite{3,4}. Quantum materials, that contain extra degrees of freedom besides the nearly free electrons, would be ideal for the practical purpose to control the band structure properties. In this paper, we illustrate this general idea and specifically study the Pr-based pyrochlore iridate. We show that the 4$f$ local moment of the Pr ions and their impacts on the Ir conduction electrons provide a natural setup to explore the band structure engineering via the coupling between these two degrees of freedom.

Pyrochlore iridates, R$_2$Ir$_2$O$_7$, have received a considerable attention in recent years partly because the 5$d$ electrons of the Ir pyrochlore system provide an interesting arena to explore the correlation effects in the strong spin-orbit-coupled matter\cite{5,6,7,8,9,10}. Aligned with this original motivation, many interesting phases and phenomena, including topological Mott insulator, axion insulator, Weyl semimetal, Luttinger-Abrikosov-Beneslavskii non-Fermi liquid, et al, have been proposed\cite{11,12}. Despite the fruitful achievements since the original motivation\cite{22,23}, the role of the rare-earth local moments in this system has not been extensively studied except few works\cite{15,16,17,18}. Recent experiments\cite{19,20} in Nd$_2$Ir$_2$O$_7$ and Pr$_2$Ir$_2$O$_7$ do suggest the importance of the local moments and the coupling between the local moments and the Ir conduction electrons.

Our work is mainly inspired by the experiments on Pr$_2$Ir$_2$O$_7$. Depending on the stoichiometry, the Pr$_2$Ir$_2$O$_7$ samples show rather distinct behaviors. While the early samples remain metallic and paramagnetic down to the lowest temperature\cite{24,25}, recent samples with different iridium and oxygen contents develop an antiferromagnetic Ising order in the Pr subsystem with a 2$\pi$(001) ordering wavevector\cite{26}. This particular order is a state within the spin ice manifold and coincides with the classical Ising order in the Pr subsystem with a 2$\pi$(001) ordering wavevector\cite{36}. In Ref. 36, we refer this Ising order as “Melko-Hertog-Gingras” state or order. Since the Pr local moment was argued to fluctuate within the “2-in 2-out” spin ice manifold in the paramagnetic samples and the “Melko-Hertog-Gingras” state of the ordered samples is a particular antiferromagnetic state within the spin ice manifold, it was proposed by one of us that, the Pr subsystem is proximate to a quantum phase transition from the $U(1)$ quantum spin liquid to the “Melko-Hertog-Gingras” order via a confinement transition by proliferating the “magnetic monopoles”\cite{36}.

Besides the interesting aspects of the Pr local moments, the Ir conduction electron was shown to display interesting phenomena. Recent works have identified the presence of a quadratic band touching at the $\Gamma$ point for the Ir 5$d$ electrons\cite{35,36}. Theoretical works have con-
sidered the long-range Coulomb interaction for the Luttinger semimetal phase of the Ir subsystem. These efforts surely fall into the original motivation of searching for correlation physics in strong spin-orbit-coupled materials and provide an important understanding of the rich physics in this material. The purpose of this work is to deviate from the intense efforts on the correlation physics of the Ir subsystems, and is instead to understand the interplay between the Ir conduction electrons and the Pr local moments. As is already pointed out in Ref. [37] the large and finite ordering wavevector of the Pr local moments and the quadratic band touching of the Ir 5d electrons suppress the Yukawa coupling between the Pr magnetic order and the Ir particle-hole excitation near the (small) Fermi surface or Γ point. Therefore, the Ir electron near the Fermi surface does not modify the critical and long-distance properties of the Pr local moments at the lowest order, though it is thought that the phase transition of the Pr local moment was induced by the modified Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction mediated by the Ir electrons. The opposite, however, is not true. The Luttinger semimetal with a quadratic band touching is a parent state of various topological phases such as Weyl semimetal and topological insulators. The coupling to the Pr local moment naturally provides such a perturbation to the parabolic semimetal. In this work, we focus on the Ising ordered phase and explain the effect of the Pr magnetism on the Ir conduction electrons.

In Eu₂Ir₂O₇ and other pyrochlore iridates, the Ir subsystem experiences a metal-insulator transition by developing an all-in all-out magnetic order with the ordering wavevector \( Q = 0 \), and it is believed that the magnetic order is driven by the correlation of the Ir 5d electrons. For Pr₂Ir₂O₇, the magnetic unit cell of Pr₂Ir₂O₇ is twice the size of the crystal unit cell, and it is the Pr local moment that develops the magnetic order. The exchange field, that is experienced by the Ir conduction electron and generated by the “Melko-Hertog-Gingras” order of Pr moments, is thus very different from other pyrochlore iridates. Therefore, we construct a minimal model to incorporate the coupling and interactions of the relevant microscopic degrees of freedom. This model, as we introduce in Sec. [II], naturally captures the physics that we describe above. We find that, the exchange field enlarges the unit cell of the Ir subsystems, and couples the electrons/holes near the Γ point with the electrons/holes near the ordering wavevector \( Q = 2\pi(001) \). The combination of the time reversal operation and the elementary lattice translation by \((1/2, 0, 1/2)\) or \((0, 1/2, 1/2)\) remains to be an (anti-unitary) symmetry of the “Melko-Hertog-Gingras” state. Using this symmetry, we demonstrate that there exist Dirac band touchings at the high symmetry momenta. Our explicit calculation with the realistic model confirms these band touchings. In addition, we find the existence of Weyl nodes in the Ir band structure due to the breaking of the time reversal by the Pr magnetic order. Unlike the symmetry protected Dirac band touchings, the Weyl nodes are not symmetry protected and are instead topologically stable.

Apart from the immediate effect on the Ir conduction electron from the Pr Ising magnetic order, we further explore the role of the external magnetic field. It is noticed that, the external magnetic field primarily couples to the Pr local moments rather than to the conduction electron. This is because every Pr local moment couples to the external magnetic field, while for the Ir conduction electrons only small amount of electrons on the Fermi surface couple to the magnetic field, not to say, there is a vanishing density of states right at the Γ point of the quadratic band touching. The Zeeman coupling to the Pr local moment would simply favor a \( Q = 0 \) state and thus competes with the exchange interaction of the Pr subsystem. The combination of the magnetic field and the Pr exchange coupling generates several different magnetic states for the Pr local moments. These magnetic orders create distinct exchange fields on the Ir conduction electrons and thereby gives new reconstructions of the conduction electron band structure. From the symmetry point of view, the Dirac band touchings at the time reversal invariant momenta are no longer present in the magnetic field. We further find that the Weyl nodes exist broadly when the magnetic field is applied to the system. This provides a feasible experimental scheme to engineer the band structure properties of the Ir itinerant electrons.

The following part of the paper is organized as follows. In Sec. [II] we introduce the microscopic Hamiltonian for the Ir subsystem and the \( f-d \) exchange between the Ir subsystem and the Pr subsystem. In Sec. [III] we include the antiferromagnetic Ising order of the Pr local moments and study the reconstruction of the Ir band structure under this magnetic order. In Sec. [IV] we further explore the interplay between the Zeeman coupling, the Pr exchange coupling and the Ir band structure, and point out that the external field can be used to engineer the topological band structure. Finally in Sec. [V] we conclude with a discussion and propose various experiments to confirm our prediction.

\[ H = H_{tb} + H_{ex} + H_{fd} + H_{Zeeman}. \]

where \( H_{tb} \) is the tight-binding model of the Ir conduction electron, \( H_{ex} \) is the interaction between the Pr local moments and originates from the superexchange process and the dipolar interaction, \( H_{fd} \) is the coupling between

\[ H_{Zeeman} = \epsilon_0 \sum\limits_{\sigma} \sum\limits_{\mathbf{r}} \mathbf{S}_\mathbf{r} \cdot \mathbf{M}_\mathbf{r}, \]

where \( \mathbf{S}_\mathbf{r} \) is the local spin at site \( \mathbf{r} \) and \( \mathbf{M}_\mathbf{r} \) is the magnetic field at site \( \mathbf{r} \).
the Pr local moment with the spin density of the Ir conduction electrons, and the $H_{\text{Zeeman}}$ defines the Zeeman coupling of the Pr local moment to the external magnetic field.

### A. Ir subsystem

We start with the tight-binding model for the Ir conduction electrons. The $\text{Ir}^{4+}$ ion has a $5d^5$ electron configuration, and these five electrons occupy the $t_{2g}$ orbitals. The atomic spin-orbit coupling splits the sixfold degenerate spin and orbital states in the $t_{2g}$ manifold into the lower $j = 3/2$ quadruplets and the upper $j = 1/2$ doublets. Due to the lattice geometry of the pyrochlore system, the $t_{2g}$ orbitals and the effective spin $\mathbf{J}$ are defined in the local coordinate system of the IrO$_6$ octahedron. For the Ir$^{4+}$ ion, the lower $j = 3/2$ quadruplets are fully filled, and the upper $j = 1/2$ doublets are half-filled.$^{34,35}$ It was shown that, the pyrochlore iridate band structure near the Fermi level is well approximated by a tight-binding model based on the $j = 1/2$ doublets.$^{34,35}$ The model is given as

$$H_{tb} = \sum_{i,j \in \text{Ir}} \sum_{\alpha \beta} t_{ij,\alpha \beta} d_{i \alpha}^\dagger d_{j \beta},$$

where $d_{i \alpha}^\dagger$ ($d_{i \alpha}$) creates (annihilates) an electron with an effective spin $\alpha$ in the $j = 1/2$ doublet. The hopping $t_{ij,\alpha \beta}$ includes both the direct electron hoppings ($t_\sigma$ and $t_x$) between the nearest-neighbor Ir ions and the indirect electron hopping ($t_{id}$) through the intermediate oxygen. It has been shown$^{34}$ that in the regime $-1.67t_{id} < t_\sigma < -0.67t_{id}$ and $t_\sigma = -2t_x/3$, the system becomes a Luttinger semimetal with a quadratic band touching at the $\Gamma$ point. This quadratic band touching is protected by the cubic lattice symmetry.$^{12,34,35}$ The Ir conduction electron of Pr$_2$Ir$_2$O$_7$ is described by the Luttinger semimetal of this tight binding model.

Since all the pyrochlore iridates except Pr$_2$Ir$_2$O$_7$ experience a metal-insulator transition via the development of magnetic orders, a Hubbard-$U$ interaction is then introduced to capture this correlation driven Mott transition. As for Pr$_2$Ir$_2$O$_7$ that remains metallic, it is expected that the Hubbard-$U$ interaction merely renormalizes the bands but does not change the nature of the Luttinger semimetal. Without losing any generality, we set $t_\sigma = -2t_x/3$, $t_{id} = -t_\sigma$ throughout this work.

Prior theoretical works, that focused on the Ir subsystem, have invoked the $k.p$ theory and the Luttinger model as the starting point to analyze the correlation effect of the electrons.$^{34,36}$ In our case, the “Melko-Hertog-Gingras” state of the Pr local moments has a large and finite ordering wavevector and necessarily connect the Ir bands near the $\Gamma$ point with the bands near the ordering wavevector, so the lattice effects cannot be ignored. As a result, we cannot start with the $k.p$ theory of the $\Gamma$ point at low energies, and instead, we should begin with the tight-binding model on the Ir pyrochlore lattice.

### B. Pr subsystem

The Pr$^{3+}$ ion has a $4f^2$ electron configuration, and the $4f$ electron is well localized. The combination of the atomic spin-orbit coupling and the crystal electric field creates a two-fold degenerate ground state for the Pr$^{3+}$ ion. This two-fold ground state degeneracy defines the non-Kramers doublet nature of the Pr local moment, and a pseudospin-1/2 operator, $\tau_i$, is introduced to operate on the two-fold degenerate ground states. The non-Kramers doublet has a peculiar property under the time reversal symmetry, i.e.

$$\mathcal{T} : \tau_z^i \to -\tau_z^i,$$

$$\mathcal{T} : \tau_x^i \to +\tau_x^i,$$

$$\mathcal{T} : \tau_y^i \to +\tau_y^i,$$

where the $z$ direction is defined locally on each sublattice and is given as the local (111) lattice direction of the pyrochlore system. Here, the magnetic dipolar moment is purely from the $\tau_z$ component, and the transverse components are known to be the quadrupolar moments.

Due to the spin-orbit-entangled nature of the Pr local moment, the effective interaction between the Pr local moments is anisotropic in the pseudospin space and also depends on the bond orientation. The general form of the interaction$^{12,13,36}$

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

where the interaction between the Ising component $\tau_z$ and the transverse component $\tau_{x,y}$ is strictly forbidden by time reversal symmetry. Here, $\hat{H}_{ex}$ differs from $H_{ex}$ in Eq. (1). $\hat{H}_{ex}$ contains all sources of interactions between the local moments, and is obtained by integrating out the Ir conduction electrons. $\hat{H}_{ex}$ would contain both the RKKY interaction and $H_{ex}$. Since the Pr local moment is in the spin ice manifold, we thus expect the nearest-neighbor Ising interaction $J_{z,ij}$ is positive and dominant. The interaction between the transverse components creates the quantum fluctuation so that the system fluctuates quantum mechanically within the spin ice manifold. Clearly, the nearest-neighbor interaction alone cannot generate the finite momentum Ising order of the Pr system whose magnetic cell is twice the size of the crystal cell. Further neighbor interactions are required. We here introduce the third neighbor antiferromagnetic Ising interaction and approximate $\hat{H}_{ex}$ as

$$\hat{H}_{ex} \approx \sum_{(ij)} J_{1z,ij} \tau_i^z \tau_j^z + \sum_{((ij))} J_{3z,ij} \tau_i^z \tau_j^z.$$

where the interaction between the transverse components has been abandoned in this approximation. In our previous work that focuses on the quantum phase transition of the Pr subsystem, this quantum fluctuation is an important ingredient to understand the nature of the phase transition and the nearby phases. In contrast, our purpose in this paper is to understand the feedback effect
on the Ir electron structure from the Pr Ising magnetic order, so the quantum dynamics of the Pr local moment is irrelevant for this purpose. In Sec. [III] of the paper, we would simply regard the Ising magnetic order that is observed in Pr$_2$Ir$_2$O$_7$ as a given condition, and this exchange Hamiltonian is not invoked until in Sec. [IV] where the external Zeeman coupling is not invoked until in Sec. [IV] where the external Zeeman coupling competes with the exchange and modifies the Pr magnetic order.

The extended interaction for the Pr local moments in Pr$_2$Ir$_2$O$_7$ is expected because the RKKY interaction that is mediated by the Ir conduction electrons is not short-ranged. This is quite different from the usual rare-earth magnets where the exchange interaction is often short-ranged and mostly restricted to the nearest neighbors. The long-range or extended RKKY interaction is the reason that we point out the Ir conduction drives the quantum phase transition of the Pr moments.

Due to the Ising nature of the moment in the approximate exchange model, the ground state is antiferromagnetically ordered with an ordering wavevector $Q = 2\pi(001)$ for $J_{3z} > 0$. Clearly, the approximate model captures the observed magnetic order in Pr$_2$Ir$_2$O$_7$.

C. Pr-Ir coupling

Precisely because of the non-Kramers doublet nature of the Pr local moment, it was pointed out in Ref. [16] based on the space group symmetry analysis that, the $\tau^z$ component couples to the spin density of the Ir conduction electron while the transverse component would couple to the electron density. The transverse component may also couple to the spin current that is even under time reversal. The general expression for the $f$-$d$ exchange between the Pr local moment and the Ir spin density has been obtained in the previous work. The coupling between the transverse component $\tau^{x,y}$ and the Ir electron density was worked out in Ref. [17]. Again, since it is the Ising component $\tau^z$ of the Pr local moment that develops the magnetic order in Pr$_2$Ir$_2$O$_7$, the leading order effect on the Ir conduction electron originates from the coupling between the Ir spin density and the Pr Ising component. Therefore, we consider the following $f$-$d$ exchange between the Pr Ising moment and the Ir spin density:

$$H_{fd} = \sum_{(ij)} \sum_{i \in \text{Pr}, j \in \text{Ir}} \tau^z_i \left[ \langle d^\dagger_{j\alpha} \sigma_{\alpha\beta} d_{j\beta} \rangle \cdot \mathbf{v}_{ij} \right], \quad (8)$$

where $\mathbf{v}_{ij}$ is a vector that defines the coupling between the Ir spin density and the Pr local moments. For each Pr ion, there are six Ir ions nearby, and these six Ir ions form a hexagon with the Pr ion in the hexagon center (see Fig. [1]). Under the nearest-neighbor Kondo-like coupling approximation, the standard symmetry analysis gives for example

$$v_{11} = (0, 0, 0), \quad (9)$$

$$v_{12} = (c_1, c_2, c_2), \quad (10)$$

D. Zeeman coupling

Finally, we introduce the Zeeman coupling. Because only the $\tau^z$ is odd under time reversal, we have the Zeeman coupling

$$H_{\text{Zeeman}} = -g\mu_B B \sum_{i \in \text{Pr}} \tau^z_i (\hat{z}_i \cdot \hat{n}) \equiv -\hbar \sum_{i \in \text{Pr}} \tau^z_i (\hat{z}_i \cdot \hat{n}), \quad (13)$$

where $\hat{n}$ is the direction of the external magnetic field. The $\hat{z}_i$ direction is defined locally for each sublattice of the Pr subsystem.

E. Energy scales

Clearly, the largest energy scale in the model is the bandwidth and interaction of the Ir conduction interaction. The second largest energy scale is the $f$-$d$ exchange coupling. The lowest ones would be the exchange coupling between the Pr moments and the Zeeman coupling. Since the Zeeman coupling can be tuned experimentally, the magnetic state of the Pr local moments can thus be manipulated by the external magnetic field.

III. DIRAC BAND TOUCHINGS AND WEYL NODES OF THE IRIDIUM SUBSYSTEM

For Pr$_2$Ir$_2$O$_7$, the Ir conduction electrons were found to develop a Luttinger semimetallic band structure that
is similar to the bulk HgTe. It is well-known that the Luttinger semimetal is a parent state of various topological phases such as topological insulator and Weyl semimeta. The Pr Ising order breaks the time reversal symmetry, and the time reversal symmetry breaking is transmitted to the Luttinger semimetal of the Ir subsystem through the $f$-$d$ exchange. We here study the band structure reconstruction of the Ir 5$d$ electrons through the above mechanism.

### A. Emergent Dirac band touchings

The Pr local moments were found to develop the “Melko-Hertog-Gingras” spin ice state in the recent samples with different Ir and O contents from the old ones. The “Melko-Hertog-Gingras” spin state breaks the time reversal and the lattice translation by doubling the crystal unit cell. Due to this interesting magnetic ordering structure, the combination of the time reversal and certain lattice translations remains to be a symmetry of the system. As we show below, this symmetry leads to a remarkable band structure property of the Ir subsystem after the band reconstruction.

The reconstructed band structure of the Ir conduction electrons is governed by the Ir tight binding model and the $f$-$d$ exchange, $H_{fb} + H_{fd}$. As a comparison, we first evaluate the Ir band structure in the magnetic Brillouin zone corresponding to the doubled unit cell due to the Pr Ising magnetic order. As we depict in Fig. 2, the Ir conduction electron bands form a Luttinger semimetal in the absence of the Pr magnetic order and give a quadratic band touching at the $\Gamma$ point. Without losing any generality, in Fig. 2 we choose the “Melko-Hertog-Gingras” spin state of the Pr moments to have a propagating wavevector $Q = 2\pi(001)$ and the band structure in Fig. 2(d) is plotted in the magnetic Brillouin zone of Fig. 2(b). Before the appearance of the Pr Ising order, the system has both time reversal ($T$) and inversion ($I$) symmetries, and each band of the Ir electrons has a two-fold Kramers degeneracy at the $\Gamma$ point. The quadratic band touching at the $\Gamma$ point results from the cubic symmetry. As the Pr magnetic order appears, the Ir band structure 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 breaks the lattice translations, $t_1$ and $t_2$. Here, $t_1$ and $t_2$ translate the system by the lattice basis vector $b_1 \equiv (0, 1/2, 1/2)$ and $b_2 \equiv (1/2, 0, 1/2)$, respectively. It turns out that, the combination of time reversal and $t_1$ or $t_2$, i.e.,

$$\tilde{T}_1 \equiv t_1 \circ T, \quad \tilde{T}_2 \equiv t_2 \circ T,$$

remains to be a symmetry of the system after the development of the Pr magnetic order. These two symmetries of the “Melko-Hertog-Gingras” spin state are analogous to the staggered time reversal of the antiferromagnetic Néel state on a square lattice. Like the pure time reversal, $\tilde{T}_1$ and $\tilde{T}_2$ are anti-unitary operations. Similar anti-unitary symmetry has been considered in the proposal of antiferromagnetic topological insulator by Mong, Essin and Moore. Due to the involvement of the lattice translations, $\tilde{T}_1$ and $\tilde{T}_2$ do not lead to the Kramers degeneracy for all the time reversal invariant momenta in the magnetic Brillouin zone. It is ready to confirm that,

\[
\tilde{T}_1 |\tilde{\Gamma}, \uparrow\rangle = i|\tilde{\Gamma}, \downarrow\rangle, \quad \tilde{T}_2 |\tilde{\Gamma}, \uparrow\rangle = i|\tilde{\Gamma}, \downarrow\rangle,
\]

\[
\tilde{T}_1 |\tilde{M}, \uparrow\rangle = i|\tilde{M}, \downarrow\rangle, \quad \tilde{T}_2 |\tilde{M}, \uparrow\rangle = -i|\tilde{M}, \downarrow\rangle,
\]

\[
\tilde{T}_1 |\tilde{R}, \uparrow\rangle = -i|\tilde{R}, \downarrow\rangle, \quad \tilde{T}_2 |\tilde{R}, \uparrow\rangle = -i|\tilde{R}, \downarrow\rangle,
\]

and $\tilde{T}_1^2 = \tilde{T}_2^2 = -1$ for the momentum points at $\tilde{\Gamma}$, $\tilde{M}$ and $\tilde{R}$; and $\tilde{T}_1^2 = \tilde{T}_2^2 = +1$ for the momentum points at $\tilde{X}$, $\tilde{Z}$ and $\tilde{A}$. Note that $\tilde{\Gamma}$, $\tilde{M}$ and $\tilde{R}$ are also time reversal invariant momenta for the crystal Brillouin zone while $\tilde{X}$, $\tilde{Z}$ and $\tilde{A}$ are not. It immediately indicates that there are two-fold Kramers degeneracy at the $\tilde{\Gamma}$, $\tilde{M}$ and $\tilde{R}$ points, but not for the $\tilde{X}$, $\tilde{Z}$ and $\tilde{A}$ points. To confirm the above prediction, we carry out the explicit calculation of the Ir band structure in the presence of the Pr magnetic order. As we show in Fig. 3 for four specific choices of the $f$-$d$ exchange couplings, there exist emergent two-fold Kramers degeneracies with Dirac band touchings at the $\tilde{\Gamma}$, $\tilde{M}$ and $\tilde{R}$ points.

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**FIG. 2.** (a) The Brillouin zone of the original pyrochlore lattice. (b) Under the $Q = 2\pi(001)$ “Melko-Hertog-Gingras” spin ice state, the unit cell is enlarged. The plot is the magnetic Brillouin zone corresponding to the enlarged unit cell. (c) The spin configuration of the “Melko-Hertog-Gingras” spin ice state. It is a 2-in 2-out spin wave with $Q = 2\pi(001)$ ordering wavevector. (d) The folded energy band of the Ir conduction electrons without $f$-$d$ exchange term develops a quadratic touching at $\Gamma$ point. High symmetry momentum lines are defined in (b) as red lines.
FIG. 3. Evolution of the Ir band structure as a function of f-d exchange parameters $c_1$ and $c_2$. The dashed (solid) circle marks the usual (double) Weyl node. Here, usual Weyl node has linear dispersions along all three momentum directions while the double Weyl node has quadratic dispersions along two momentum direction and linear along one momentum direction.[22] For sufficiently large parameters (d), the Weyl nodes disappear and a band gap is opened. Here, “2120” refers to the “2-in 2-out” spin configuration. The energy unit in the plots is $t_{id}$. The dashed line refers to the Fermi energy.

B. Magnetic Weyl nodes

Besides the emergent and symmetry protected Dirac band touchings at the $\Gamma$, $\bar{M}$ and $\bar{R}$ points, we discover the presence of the Weyl nodes in the reconstructed Ir band structure in Fig. 3. The reconstructed Ir band structure is determined by the f-d exchange couplings. The actual couplings of the f-d exchange in the material Pr$_2$Ir$_2$O$_7$ are unknown to us. To proceed, we fix the tight-binding part of the Ir hopping Hamiltonian and study the band structure phase diagram of Ir electrons by varying the f-d exchange couplings. This approach is not designed to be self-consistent, but is phenomenological. The Pr Ising order, that is observed experimentally, is used as the input information to the Ir band structure calculation in this section. We expect, the realistic case for Pr$_2$Ir$_2$O$_7$ would be located at one specific parameter point in the phase diagram. It is possible that the pressure could vary the exchange couplings and allow the system to access different parameters of the phase diagram.

In Fig. 4, we depict our phase diagram according to the exchange couplings. For small exchange couplings, a semimetal is always obtained. The name “semimetal” here not only refers to the Dirac band touching or dispersion at some time reversal invariant momenta, but also refers to the (topologically protected) Weyl nodes in the magnetic Brillouin zone. In fact, Weyl semimetal with the surface Fermi arcs was first predicted for pyrochlore iridates with the all-in all-out magnetic order, and the magnetic order is suggested to be driven by the Ir electron correlation[13]. In our result here, the magnetic order comes from the Pr Ising order, and the time reversal symmetry breaking is then transmitted to the Ir conduction electron via the f-d exchange. The magnetic order is not the simple all-in all-out magnetic order. It was also suggested that the correlation-driven Weyl semimetal for pyrochlore iridates appears in a rather narrow parameter regime[13]. The f-d exchange, however, could significantly enlarge the parameter regime for Weyl semimetal. Indeed, in Fig. 4, the semimetal region does support several Weyl nodes near the Fermi level, and thus, we expect the usual properties for Weyl semimetal[12] to hold in this regime. Moreover, since the f-d exchange coupling is much smaller than the effective hoppings of the Ir electrons, so the realistic case for the ordered Pr$_2$Ir$_2$O$_7$ is expected to occur in the semimetallic phase of Fig. 4.

IV. ROLE OF EXTERNAL MAGNETIC FIELDS

To further control the property of the system, we suggest to apply an (uniform) external magnetic field to the system. As we have explained in Sec. I, the magnetic field would primarily couple to the Pr local moments. A uniform magnetic field induces a finite magnetic polarization on the Pr local moments, and thus breaks the $T_1$ and $T_2$ symmetries of the ordered Pr$_2$Ir$_2$O$_7$. As a consequence, the emergent Dirac band touchings at the $\Gamma$, $\bar{M}$ and $\bar{R}$ points, that are protected by the $T_1$ and $T_2$ symmetries, should disappear immediately in a generic magnetic field along a random direction. Here the choice of a random direction for the magnetic field simply avoids the accidental degeneracy/band touching that is protected by the reduced lattice symmetry of the system if the field is applied along high symmetry directions.

Unlike the previous section where the Ir band structure is controlled by the f-d exchange and the Ir tight-binding model, the Ir band structure in the magnetic field requires the knowledge of the Pr magnetic state that is modified by the external magnetic field. 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 \( f-d \) exchange interaction. For the Pr subsystem, we consider the following Hamiltonian,

\[
H_{\text{Pr}} = H_{\text{ex}} + H_{\text{Zeeman}},
\]

where the exchange part includes both the first neighbor and third neighbor Ising exchange interactions. Since here the Pr local moment is set to be an Ising degree of freedom, it is ready to obtain the magnetic phase diagram of the Pr moments by comparing energies of candidate ground states. The magnetic phase diagram for the Pr moments is depicted in Fig. 5 where three different directions of magnetic fields are considered.

Here we focus on one specific field orientation, \( \hat{n} \equiv (1/3, 1/3, 1/3) \), and evaluate the feedback of the Pr magnetic state on the Ir conduction electrons. Besides the original “Melko-Hertog-Gingras” spin state, two additional spin states are obtained. While the Ir band structure in the presence of “Melko-Hertog-Gingras” spin state stays the same as the ones in Sec. III under this approximation, this should be the caveat of the approximation of the Pr moment as the Ising spin that ignores the quantum nature of the Pr moments. In reality, the magnetic field would create a finite polarization for the Pr local moment and modifies the Ir band structure immediately, even though the modification can be small. This would allow us to move the positions of the Weyl nodes in the momentum space. The other two spin configurations of the Pr moments, that result from strong magnetic field, have an ordering wavevector \( Q = 0 \) and restores the lattice translation symmetry. Hence, we expect two different Ir band structures for these spin configurations. In Fig. 6 we depict the Ir band structures for specific choices of the \( f-d \) exchanges with two \( Q = 0 \) spin configurations from the phase diagram in Fig. 5(a). Our explicit calculation of the Ir band structure in Fig. 6 shows that the Dirac band touchings at the \( \Gamma (\equiv \Gamma) \), \( R (\equiv L) \) points are absent in the magnetic field, and now the magnetic unit cell is now identical to the crystal unit cell. Moreover, although the time reversal symmetry breaking is transmitted by the Pr spin configuration due to the external magnetic field, the overall effect is that one applies the time reversal symmetry breaking to the Ir Luttinger semimetal. Since Luttinger semimetal can be regarded as the parent state of the Weyl semimetal, it seems natural to expect the occurrence of the Weyl nodes. Indeed, as we show in Fig. 7 we obtain the Weyl semimetal (or Weyl metal) for a large parameter regime in the phase diagram.

With large magnetic fields along (001) and (110) directions, the \( Q = 0 \) state is obtained for the Pr moments under this approximation (see Fig. 5(b) and (c)). This Pr spin state is the same as one of the spin states when the field is applied along (111) direction, and there it does not bring different Ir band structures under this approximation.

FIG. 5. Phase diagram of the Pr local moments under the external magnetic fields along different directions. Here “I13O” refers to “1-in 3-out” spin configuration.

FIG. 6. Evolution of the Ir band structure as a function of \( f-d \) exchange parameters for (a-d) “1-in 3-out” and (e-h) “2-in 2-out” Pr magnetic states with \( Q = 0 \) from Fig. 5(a). The dashed (solid) circle marks the usual (double) Weyl node. In (a) and (b), one band from \( L \) to \( \Gamma \) is flat. This is accidental for the nearest-neighbor hopping model and could be dispersive if further neighbor hoppings are included. In (g), the Weyl nodes are actually at different energies. The energy unit in the plots is \( t_{ud} \). The dashed line refers to the Fermi energy.
emission spectroscopy (ARPES). The optical measure-
field) would be best detected by the angle-resolved photo-
both in the ordered Pr$_2$Ir$_2$O$_7$ Hertog-Gingras" spin state for the Pr subsystem. More-
from the magnetic translation symmetry of the "Melko-
invariant momenta and the symmetry protection comes
theoretical framework, and study the band reconstruc-
tion electrons in the presence of the
local moments, as the input information for our
results, such as the Luttinger semimetal of the Ir conduc-
structure after the reconstruction from the Pr magnetic
U
Hertog-Gingras" spin state, would immedi-
band touchings at some of the time reversal invariant mo-
ments, that are protected by the magnetic translation of the “Melko-Hertog-Gingras” spin state, would immedi-
this field-driven metal-insulator transition. Although it
the "Melko-Hertog-Gingras" spin state, would immedi-
due to the breaking of the cubic symmetry, the Weyl
semimetal that is induced by the external magnetic field
show anomalous Hall effect. Finally, we point out the
field-driven metal-insulator transition. Although it
was not emphasized in Sec. IV, the large portion of the
semi-metal region in the phase diagram of Fig. 4 is con-
verted into the insulating region in the phase diagram
of Fig. 7(a). From the experience in Nd$_2$Ir$_2$O$_7$ with
the dipole-octupole Nd$^{3+}$ magnetic ion, this field-
transport measurement.

V. DISCUSSION

We here summarize our understanding of the rich
physics in Pr$_2$Ir$_2$O$_7$ and suggest future experiments to
further reveal its physics. In the previous field the-
ory work by one of the authors, we pointed out that
the Pr subsystem of Pr$_2$Ir$_2$O$_7$ is proximate to a quan-
tum phase transition from the U(1) quantum spin liquid
to the magnetic order. The proximate magnetic order,
that is obtained from the condensation of the “magnetic
monopolies” in the U(1) quantum spin liquid, breaks the
lattice translation and is precisely the one that is ob-
served in the neutron scattering experiments. This the-
oretical work indicates that the paramagnetic state of
the magnetic order of Pr$_2$Ir$_2$O$_7$ sample is a U(1) quantum spin liquid.
In the current paper, we focus on the magnetically
ordered Pr$_2$Ir$_2$O$_7$ sample. We have developed a system-
atic modelling to understand the interplay between the
Ir conduction electrons and the Pr local moments for the
material Pr$_2$Ir$_2$O$_7$. We use the existing experimental
results, such as the Luttinger semimetal of the Ir conduc-
tion electrons and the “Melko-Hertog-Gingras” spin state
of the Pr local moments, as the input information for our
theoretical framework, and study the band reconstruc-
tion of the Ir conduction electrons in the presence of the
Pr magnetic order. We predict that the symmetry pro-
tected Dirac cones emerge at part of the time reversal invariant momenta and the symmetry protection comes
from the magnetic translation symmetry of the “Melko-
Hertog-Gingras” spin state for the Pr subsystem. More-
over, there generically exist Weyl nodes of different kinds
both in the ordered Pr$_2$Ir$_2$O$_7$ samples and Pr$_2$Ir$_2$O$_7$ in
the external magnetic fields.

Based on our prediction about the non-trivial Ir band
structure after the reconstruction from the Pr magnetic
state, we here propose the future experiments. Cer-
tainly, the non-trivial features of the Ir band structure
in the ordered Pr$_2$Ir$_2$O$_7$ sample (without the magnetic field) would be best detected by the angle-resolved photo-
emission spectroscopy (ARPES). The optical measure-
ments can also be useful for the inter-band particle-hole
transition near the band touching points. The Dirac
band touchings at some of the time reversal invariant mo-
ments that are protected by the magnetic translation of the “Melko-Hertog-Gingras” spin state, would immediately disappear when the magnetic field is applied. This prediction may be a sharp feature for the experimen-
tal confirmation. Besides the direct band structure mea-
surement, the magneto-transport can be a useful probe.

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Appendix A: Sublattices and crystal momenta for
Pr$_2$Ir$_2$O$_7$

In Pr$_2$Ir$_2$O$_7$, both Ir and Pr pyrochlore lattices are
composed of linked tetrahedra and can be viewed as FCC
lattice with primitive lattice vectors

\[ b_1 = (0, \frac{1}{2}, \frac{1}{2}) \]  
\[ b_2 = (\frac{1}{2}, 0, \frac{1}{2}) \]  
\[ b_3 = (\frac{1}{2}, \frac{1}{2}, 0) \]  

After choosing one of the Ir site as reference point, the
reference positions of four Ir sublattices can be set to be

\[ \text{Ir}_1 = (0, 0, 0), \quad \text{Ir}_2 = (0, \frac{1}{4}, \frac{1}{4}) \]  

FIG. 7. Phase diagram for the Ir band structure in the pa-
parameter space of the f-d exchange couplings for different Pr
magnetic states from Fig. 5(a). The bold dots in the plots are
the parameter choices for Fig. 6.
Likewise, for the Pr subsystem we have the reference positions of four Pr sublattices as

\[ \text{Pr}_1 = (0, \frac{1}{2}, 0), \quad \text{Pr}_2 = (0, 0, \frac{3}{4}), \quad \text{Pr}_3 = (\frac{1}{4}, 0, \frac{1}{4}), \quad \text{Pr}_4 = (\frac{1}{4}, 0, \frac{3}{4}). \]  

(A5)

The crystal momenta in Fig. 2 are

\[ \hat{\Gamma} = (0, 0, 0), \quad \hat{M} = (2\pi, 0, 0), \quad \hat{R} = (\pi, \pi, \pi), \quad \hat{X} = (\pi, \pi, 0), \quad \hat{Z} = (0, 0, \pi), \quad \hat{A} = (2\pi, 0, 0). \]  

(A8)

(A9)

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