Predominance of the Kitaev interaction in a three-dimensional honeycomb iridate: From ab initio to spin model

Heung-Sik Kim¹, Eric Kin-Ho Lee¹ and Yong Baek Kim¹,²

¹ Department of Physics and Center for Quantum Materials, University of Toronto - 60 St. George St., Toronto, Ontario, M5S 1A7, Canada
² Canadian Institute for Advanced Research / Quantum Materials Program - Toronto, Ontario MSG 1Z8, Canada

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Abstract – The recently discovered three-dimensional hyperhoneycomb iridate, β-Li₂IrO₃, has raised hopes for the realization of the dominant Kitaev interaction between spin-orbit entangled local moments due to its near-ideal lattice structure. If true, this material may lie close to the sought-after quantum spin-liquid phase in three dimensions. Utilizing ab initio electronic structure calculations, we first show that the spin-orbit entangled basis, j_eff = 1/2, correctly captures the low-energy electronic structure. The effective spin model derived in the strong-coupling limit supplemented by the ab initio results is shown to be dominated by the Kitaev interaction. We demonstrated that the possible range of parameters is consistent with a non-coplanar spiral magnetic order found in a recent experiment. All of these analyses suggest that β-Li₂IrO₃ may be the closest among known materials to the Kitaev spin-liquid regime.

Introduction. – Kitaev’s exact solution of a quantum spin liquid on a spin-1/2 honeycomb model has spurred considerable interest in the search for a material realization [1,2]. Of particular focus is the family of quasi–two-dimensional (2D) honeycomb iridate materials α-A₂IrO₃ (A = Na, Li, hereafter αAIO), where iridium (Ir) ions form decoupled layers of honeycomb lattices [3,4] and have been argued to host spin-orbital entangled j_eff = 1/2 degrees of freedom [5–7]. Due to the interplay of strong atomic spin-orbit coupling (SOC) and correlation effects, these j_eff = 1/2 moments in the ideal αAIO structure interact in the highly anisotropic manner described by the Kitaev model [8]. In addition to these Kitaev-type exchanges, the symmetries of the ideal structure also permit additional exchanges that generate a plethora of interesting phases of matter [9]. In reality, however, these materials possess sizeable monoclinic distortions that deform the octahedral oxygen cages surrounding Ir ions [4,10]. These distortions lower the symmetry of the system and therefore complicate the description of these materials. Thus far, a consensus on the minimal model required to describe this family of 2D honeycomb iridates has not been reached yet; a distortion-free analog of these honeycomb iridates may offer a more direct path towards the realization of Kitaev physics.

The timely discovery and synthesis [11,12] of the hyperhoneycomb β-Li₂IrO₃ (hereafter βLIO) may present such an exciting opportunity. Much like its 2D counterpart, the Kitaev model on the ideal 3D hyperhoneycomb lattice supports an exact spin-liquid ground state [13–16]. In addition, the distortion-free, classical pseudospin-1/2 model on the hyperhoneycomb lattice also supports a myriad of complex magnetic phases [17]. Moreover, interesting topological phases have been predicted on this lattice [18]. These previous results illustrate the possibilities that the Kitaev model may be realizable in βLIO; however, they rely on the use of the j_eff = 1/2 degrees of freedom in the low-energy description of βLIO, which has not been justified microscopically. Furthermore, whether the near-ideal structure of βLIO can give rise to a simple minimal pseudospin model dominated by the Kitaev exchange has so far not been validated. Also, with the recent experimental observation of a magnetic spiral order in βLIO, any minimal model and its accompanying parameters must also be capable of predicting the observed order: this provides a stringent test of feasibility for any model describing βLIO.
In this letter, we tackle these issues by combining results of our ab initio electronic structure calculations and a strong-coupling theory to arrive at a $j_{\text{eff}} = 1/2$ model to describe $\beta$LIO. From our ab initio band structure results, we find that the low-energy states can be described in terms of localized $j_{\text{eff}} = 1/2$ states because of the large atomic SOC present in Ir. In fact, the magnitude of SOC in the paramagnetic state is enhanced by the electron interactions in Ir $d$ orbitals, which is consistent with recent observations in several 4$d$ and 5$d$ transition metal compounds [19–21]. To go beyond the limitation of ab initio calculations in treating electron interactions, we employ the strong-coupling expansion recently proposed in [9] to arrive at a minimal pseudospin-1/2 model. Due to the near-ideal structure of $\beta$LIO, we discover that the resulting pseudospin model is near-isotropic while both distortion-induced and further neighbor interactions are small. Remarkably, the estimated exchange interactions place the model near the ferromagnetic Kitaev limit and within a region where the classical ground state agrees well with the experimentally observed spiral phase [11]. Our results are summarized in fig. 1 and elaborated in the rest of this work.

**Structure and ab initio calculations.** — $\beta$LIO is a member of the generic three-dimensional (3D) harmonic honeycomb iridate series [22], which are structural variants of 2D-honeycomb iridates $\alpha$AIO. The hyperhoneycomb lattice is composed of a tri-coordinated network of edge-shared IrO$_6$ octahedra as shown in fig. 2(a). There are two types of nearest-neighbor (NN) bonds in this network: we denote these bonds as X and Z. Despite being symmetry-inequivalent, these two bonds are almost identical owing to their similar local crystal structures as revealed by recent structural analyses [11,12].

The crystal structure refinement also revealed nearly ideal IrO$_6$ octahedra compared to those from $\alpha$LIO: standard deviations of the Ir-O bond length and O-Ir-O bond angles in $\beta$LIO (0.002 Å and 2.77°) are much smaller than those in $\alpha$LIO (0.050 Å and 4.56°) [10]. Since finite standard deviations in O-Ir-O bond angles are a result of trigonal distortion in the IrO$_6$ octahedra, the small value present in $\beta$LIO indicates that trigonal distortions are indeed small in this compound (the directions of trigonal distortion are shown as colored arrows in the figure). The nearly ideal IrO$_6$ octahedra in $\beta$LIO suggest that local crystal fields are principally cubic in symmetry, therefore the spin-orbital entangled $j_{\text{eff}} = 1/2$ states would be a good basis to construct a low-energy description of this material in the presence of strong SOC.

![Fig. 1: (Color online) Phase diagram of the $J$-$K$-$\Gamma$ model reproduced from ref. [17], overlaid with density distributions of exchange interaction parameters estimated from ab initio calculations in treating electron interactions, we employ the strong-coupling expansion recently proposed in [9] to arrive at a minimal pseudospin-1/2 model. Due to the near-ideal structure of $\beta$LIO, we discover that the resulting pseudospin model is near-isotropic while both distortion-induced and further neighbor interactions are small. Remarkably, the estimated exchange interactions place the model near the ferromagnetic Kitaev limit and within a region where the classical ground state agrees well with the experimentally observed spiral phase [11]. Our results are summarized in fig. 1 and elaborated in the rest of this work.](Image 1)

![Fig. 2: (Color online) (a) Network of IrO$_6$ octahedra in the hyperhoneycomb lattice. The two distinct nearest-neighbor (NN) bonds, X and Z, are depicted as solid green and red lines, respectively. X and $X'$ bonds are symmetry equivalent, whereas Z bonds are distinct. Emerging from the octahedra, the red and blue arrows point in the direction of the trigonal distortions for red and blue IrO$_6$ octahedra, respectively. The trigonal distortion, which consists of the compression and rotations of the opposing oxygen triangles, is illustrated in the figure and in the inset. (b) shows the band structure with the presence of spin-orbit coupling (SOC). Solid red and dashed grey curves are the band structure of the experimental and ideal structures, respectively.](Image 2)
To validate the use of $j_{\text{eff}} = 1/2$ states in the low-energy description of $\beta$LIO, we turn to ab initio electronic-structure calculations\(^1\). The band dispersions of the ideal and experimental structures with SOC can be seen in fig. 2(b). The dispersions from the experimental structure (red solid curves) and those from the ideal one (dashed grey curves) share a similar overall shape, especially near the chemical potential. The separation between the upper eight bands and the lower sixteen bands (including Kramers degeneracies) can be clearly seen in the figure, suggesting the formation of $j_{\text{eff}} = 1/2$ and $j_{\text{eff}} = 3/2$ bands\(^2\).

In fig. 3(a), we show the $j_{\text{eff}}$-projected band dispersions and density of state (PDOS) in the presence of SOC based on the experimental structure. The projection is done by taking inner products between the atomic $j_{\text{eff}}$ states and the Bloch state represented in terms of the local pseudatomic orbital basis. Weights of the $j_{\text{eff}} = 1/2$ and $3/2$ components within each Bloch state are depicted as the size of red and blue circles, respectively, in the band plots. The large $j_{\text{eff}} = 1/2$ PDOS weight in the upper eight bands—the closest bands to the Fermi level—indicates the development of $j_{\text{eff}} = 1/2$ bands and confirms that the basis states relevant to the low-energy description of $\beta$LIO possess mostly $j_{\text{eff}} = 1/2$ character. The effect of electron correlations inherent to Ir $t_{2g}$ orbital further enhances the $j_{\text{eff}} = 1/2$ character as shown in fig. 3(b), where the effective on-site Coulomb interaction $U_{\text{eff}} \equiv U - J_{H}$ is included within the DFT+$U$ formalism ($J_{H}$ is Hund’s coupling; for details see sect. A in Supplementary Material).

In order to capture the role of electron correlations in the low-energy $j_{\text{eff}} = 1/2$-dominated states, we adopt the coordinate system such that $t_{2}$ is negative for both Z and X bonds. By symmetry, $t_{2}$ is positive for the X’ bonds.

Table 1: Magnitude of SOC within the Ir $t_{2g}$ states and $t_{2g}$ hopping terms from Wannier orbital calculations in the presence of $U_{\text{eff}}$. We adopt the coordinate system such that $t_{2}$ is negative for both Z and X bonds. By symmetry, $t_{2}$ is positive for the X’ bonds.

| $U_{\text{eff}}$ (eV) | 0.0 | 1.5 | 3.0 |
|---------------------|-----|-----|-----|
| $\lambda_{t_{2g}}$  | 0.401 | 0.482 | 0.516 |
| $t_{1}$             | +0.085 | +0.077 | +0.064 |
| X                   | +0.083 | +0.074 | +0.058 |
| $|t_{2}|$            | 0.238 | 0.255 | 0.270 |
| X                   | 0.260 | 0.276 | 0.289 |
| $t_{3}$             | −0.162 | −0.119 | −0.060 |
| X                   | −0.153 | −0.110 | −0.055 |

Fig. 3: (Color online) (a), (b) Band structure and density of states (DOS) projected onto the $j_{\text{eff}}$ states in the presence of SOC (a) without and (b) with the on-site Coulomb interaction $U_{\text{eff}} = 3.0$ eV. (c) shows the schematic shape of the $j_{\text{eff}} = 1/2$-like Wannier orbital constructed from the $j_{\text{eff}} = 1/2$-dominated bands near the Fermi level. Dashed and solid circles depict the Wannier orbitals from calculations without and with finite $U_{\text{eff}}$, respectively. Weights of the central $j_{\text{eff}} = 1/2$ and nearest-neighboring $j_{\text{eff}} = 3/2$ tail in the orbital are shown in (d) as a function of $U_{\text{eff}}$.

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\(^1\)See sect. A in the Supplementary Material posted in the author’s personal web page [https://sites.google.com/site/heungskim/home/temporary-files] for details.

\(^2\)We comment that, due to the loss of chiral symmetry and the mixing of the $j_{\text{eff}} = 3/2$ states in the $j_{\text{eff}} = 1/2$ subspace, the nodal Fermi ring mentioned in the previous tight-binding analysis is absent in both of the ideal and experimental structures.

\(^3\)In order to capture the role of electron correlations in the band structure only, we do not consider any magnetism in our DFT+$U$ calculations in this work.
octahedra (as supported by the small amount of trigonal distortion of less than 100 meV), the Wannier orbitals consist of pure 1/2 state on the center Ir site, while it has 3/2 tails on the NN sites. Similar features have been reported in αNIO and αLIO [23,24], which mirror the remnant molecular orbital character originating from the t_{2g} hopping [25]. As \( U_{\text{eff}} \) is included and \( \lambda_{2g} \) is enhanced, the \( j_{\text{eff}} = 1/2 \) character becomes more dominant while \( j_{\text{eff}} = 3/2 \) component on the NN sites decreases as shown in fig. 3(c) and (d). The \( j_{\text{eff}} = 1/2 \)-like Wannier orbital is more localized accordingly, which makes the low-energy description of \( \beta \text{LIO} \) in terms of the localized \( j_{\text{eff}} = 1/2 \) states more feasible in the strong-coupling limit.

\( t_{2g} \) Wannier orbital hopping amplitudes. — For a detailed understanding of how the near-ideal structure of \( \beta \text{LIO} \) is manifested in the electronic-band structure, we calculated the Ir \( t_{2g} \) hopping amplitudes from the Wannier orbitals in the experimental structure. Table 1 shows the magnitude of the three largest hopping terms \(-t_1, t_2, \) and \( t_3 \)— as the value of \( U_{\text{eff}} \) changes (\( U_{\text{eff}} = 0.0 \text{ eV}, 1.5 \text{ eV}, \) and 3.0 eV, and SOC is included in the calculation); see sect. B and fig. S1(a) in the Supplementary Material in footnote \(^1 \) and ref. [26] for illustration of these hopping processes. Since the Ir-Ir bond lengths and Ir-O-Ir bond angles are similar on the two inequivalent bonds of \( \beta \text{LIO} \) (X and Z bonds), the values of their respective hopping amplitudes are expected to be similar. Indeed, by comparing the hopping amplitudes between the two inequivalent NN bonds, we observe small anisotropies between the X and Z bonds (<10\%), which reflects the close-to-ideal structure of \( \beta \text{LIO} \).

The evolution of the NN hopping amplitudes as we include on-site Coulomb interactions can be seen in table 1. As \( U_{\text{eff}} \) increases, \( |t_2| \) increases while \( t_1 \) and \( t_3 \) decrease. Such behavior is understood in terms of the enhanced hybridization between the Ir \( t_{2g} \) and oxygen \( p \) states in the presence of \( U_{\text{eff}} \). The inclusion of \( U_{\text{eff}} \) pushes the \( j_{\text{eff}} = 3/2 \) states down energetically so that they become closer to the oxygen \( p \) states. This leads to increased hybridization between the Ir \( t_{2g} \) and oxygen \( p \) states, which yields the enhancement of oxygen-mediated \( t_2 \) (and the reduction of \( t_1 \) and \( t_3 \)).

**Strong-coupling minimal model and experimental spiral phase.** — Having validated the use of the \( j_{\text{eff}} = 1/2 \) basis and the similarity of hopping amplitudes between inequivalent bonds, we can now construct an effective model to describe the low-energy properties of \( \beta \text{LIO} \) in the large-\( U \) limit. Following the derivation in ref. [9], we start with localized \( j_{\text{eff}} = 1/2 \) states then perform a strong-coupling expansion using NN \( t_{2g} \) hopping amplitudes\(^5 \). In the presence of Hund’s coupling \( J_H \), we arrive at a NN, \( j_{\text{eff}} = 1/2 \) model with highly anisotropic pseudospin exchanges

\[
H = \sum_{\langle ij \rangle \in \alpha \beta \gamma} J^\alpha S_i \cdot S_j + K^\alpha S_i^z S_j^z + \Gamma^\alpha (S_i^\gamma S_j^\gamma + S_i^{\gamma^\dagger} S_j^{\gamma^\dagger}),
\]

where \( S_i \) is the \( j_{\text{eff}} = 1/2 \) pseudospin on site \( i \), \( \alpha \) labels the NN \( \langle ij \rangle \) bond by its Kitaev component, and \( \beta \) and \( \gamma \) denote the two non-Kitaev components of the \( \langle ij \rangle \) bond. The exchanges \( J, K, \) and \( \Gamma \) are functions of the hopping amplitudes \( t_1-t_3 \), strength of Hund’s coupling \( J_H \), SOC \( \lambda \), and the on-site Coulomb interaction \( U \). The relations between these quantities are given in sect. D in the Supplementary Material in footnote \(^1 \).

To establish the region in the parameter space that best models \( \beta \text{LIO} \), the following statistical analysis was employed. First, the hopping amplitudes and SOC values in table 1 were interpolated as a function of \( U_{\text{eff}} \). Next, \( U_{\text{eff}} \) and \( J_H \) were treated as independent variables with choices of ranges 1.5 < \( U_{\text{eff}} < 3.0 \) eV and \( |t_2| < J_H < \lambda_{2g} \), that is the largest hopping term\(^6 \), due to the difficulty in determining specific values of \( U_{\text{eff}} \) and \( J_H \). In order to present the phase evolution as a function of \( U_{\text{eff}} \), we chose six \( U_{\text{eff}} \) intervals centered at 1.5, 1.8, 2.1, 2.4, 2.7, and 3.0 eV with ranges \( \Delta U_{\text{eff}} = \pm 0.1 \) eV. From these parameters, six possible ranges of the exchange parameters were estimated as shown in the inset of fig. 1\(^7 \). We found that the mean anisotropies between X and Z bonds in \( J, K, \) and \( \Gamma \) are 3\%, 15\%, and <1\%, respectively, relative to the largest energy scale, which is the Kitaev exchange. As a first approximation, we treated all exchanges as isotropic between the X and Z bonds, which yields the NN Hamiltonian studied in the classical limit in ref. [17]. Lastly, we overlaid the density distributions of the exchange parameters on top of the relevant portion of the classical phase diagram reproduced from ref. [17], thereby yielding fig. 1.

The phase diagram is the quarter of a polar plot near the ferromagnetic Kitaev limit: The angular coordinate \( \phi \) shows the ratio between \( J \) and \( K \) —tan(\( \phi \)) = \( J/K \). Meanwhile, the radial coordinate depicts the strength of \( \Gamma - \theta \in (\pi/2, \pi) \), tan(\( \theta \)) = \( \sqrt{T^2 + K^2}/\Gamma \). The bottom boundary of the half-ring (\( \theta = \pi/2, \phi = 3\pi/2 \)) is the Heisenberg-Kitaev limit (\( \Gamma = 0 \)) and the origin (\( \theta = \pi \)) is the pure \( \Gamma \) limit. As seen in the figure, the NN exchanges in \( \beta \text{LIO} \) are likely dominated by a large, ferromagnetic Kitaev exchange, perturbed by small \( |J| \) and \( |\Gamma| \). Note that, higher \( U_{\text{eff}} \) and \( J_H \) prefer smaller \( \theta \) (larger \( K \)) and smaller \( \phi \), respectively.

We find that, when \( U_{\text{eff}} \geq 2.4 \) eV, the corresponding phases lie within area of the spiral phase \( \text{SP}_{\alpha -} \). Remarkably, this non-coplanar spiral magnetic phase possesses

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\(^5\) Such ab initio based perturbative approach applied to Na\(_2\)IrO\(_3\) [27] yielded consistent results with the state-of-the-art quantum chemistry calculation performed in ref. [28].

\(^6\) The ranges of \( U_{\text{eff}} \) and \( J_H \) used in this work are consistent with recent constrained RPA calculations of both parameters in the Ir 5d orbitals [27,29].

\(^7\) For \( U_{\text{eff}} \) and \( J_H \), we chose the triangular and uniform distributions, respectively, for the stated ranges. The qualitative features of the resulting exchange parameters’ density distribution are not dependent on the precise distribution used but only on the mean and range of the distribution.
the same symmetries as the experimentally determined magnetic order [11,17]. In other words, using the \textit{ab initio} hopping and SOC parameters, the resulting exchange parameters in the isotropic $J$-$K$-$\Gamma$ pseudospin model results in a classical ground state that agrees with the experimental magnetic order.

Discussion and conclusion. – Although we have shown that the $j_{\text{eff}} = 1/2$ states form a valid basis as a consequence of the small amount of distortions present, the difference between the dispersions of the ideal and experimental structures away from the Fermi level are due to these distortions and the resulting bond anisotropies. However, in the context of the effective pseudospin model, we have shown that these non-idealities are negligible for the $J$ and $\Gamma$ exchanges. The Kitaev exchange, on the other hand, is more anisotropic between the X and Z bonds, but the experimental magnetic order.

In addition to distortions and bond anisotropies, an accurate description of the electronic structure also requires hopping amplitudes beyond the NN level (see sect. C in the Supplementary Material in footnote \textsuperscript{1} for details). These terms would generate further neighbor exchange interactions in the strong-coupling theory. However, these exchanges are no more than 10\% of those at the NN level. Since we expect that such small further-neighbor interactions do not change our conclusions, we focused on the NN exchange interactions in our manuscript.

To enhance the Kitaev exchange relative to other interactions and to approach the spin-liquid regime of the Kitaev model, strengthening the oxygen-mediated-type hopping ($t_2$) is a viable option. Increasing the on-site Coulomb interaction can further localize the $t_{2g}$ orbitals, which reduces the amplitudes for direct hopping channels like $t_1$ and $t_3$ while oxygen-mediated hopping channels like $t_2$ are comparatively less affected. In addition, increasing $U$ has the effect of driving the system deeper into the Mott insulating regime and reducing the strength of further neighbor interactions. Therefore, a 4$d$ variant of the $\beta$LIO may offer the right ingredients to enhance the Kitaev exchange.

Indeed, the isoelectronic, 2D honeycomb $\alpha$-Li$_2$RhO$_3$ has been synthesized and argued to be a relativistic Mott insulator driven by electronic correlations and SOC [30]. Furthermore, this material does not magnetically order down to 0.5 K, which is an indication of magnetic frustration [30]. We speculate that the hypothetical 3D polymorph —hyperhoneycomb $\beta$-Li$_2$RhO$_3$ — may be a less distorted version of $\alpha$-Li$_2$RhO$_3$ that has all the right properties to further approach the Kitaev region, in analogy to $\beta$LIO.

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