The honeycomb lattice with multi-orbital structure: topological and quantum anomalous Hall insulators with large gaps

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We construct a minimal four-band model for the 2D topological insulators and quantum anomalous Hall insulators based on the $p_z$ and $p_y$-orbital bands in the honeycomb lattice. The multi-orbital structure allows the atomic spin-orbit coupling which lifts the degeneracy between two sets of onsite Kramers doublets $j_z = \pm \frac{1}{2}$ and $j_z = \pm \frac{3}{2}$. Non-trivial band topology is generated without band inversion. Because of the orbital angular momentum structure of Bloch-wave states at $\Gamma$ and $K(K')$ points, topological gaps are equal to the atomic spin-orbit coupling strength, which are much larger than those from the usual band inversion mechanism. The energy spectra and eigen-wavefunctions are solved analytically based on Clifford algebra. The competition among spin-orbit coupling, lattice asymmetry and the Neel exchange field results in band crossings at $\Gamma$ and $K(K')$ points which lead to various topological band structure transitions. Flat bands also naturally arise which allow a local construction of eigenstates. The above mechanism is related to several classes of solid state semiconducting materials.

PACS numbers: 73.22.-f, 73.43.-f, 71.70.Ej, 73.43.Nq, 85.75.-d

I. INTRODUCTION

The 2D quantum Hall effect[19] is among the early examples of topological states of matter whose magnetic band structure is characterized by the first Chern number[20,21]. Later on quantum anomalous Hall (QAH) insulators were proposed with regular Bloch band structure[22]. Insulators with non-trivial band topology were also generalized into time-reversal (TR) invariant systems termed topological insulators (TIs) in both 2D and 3D, which have become a major research focus in contemporary condensed matter physics[23-25]. The topological index for TR invariant TIs is no longer an integer but $\mathbb{Z}_2$-valued in both 2D and 3D[26,27], while in 4D it is the integer-valued second Chern number[28]. Various 2D and 3D TI materials are predicted theoretically and observed experimentally[29-31,32]. They exhibit gapless helical 1D edge modes and 2D surface modes through transport and spectroscopic measurements.

Solid state materials with the honeycomb lattice structure (e.g. graphene) are another important topic of condensed matter physics[22,23]. The celebrated 2D Kane-Mele model was originally proposed in the context of graphene-like systems with the $p_z$-band as a TR invariant doublet of Haldane’s QAH model[28,29]. However, the atomic level spin-orbit (SO) coupling in graphene does not directly contribute to opening the topological band gap[28]. Due to the lattice symmetry, the band structure SO coupling is at the level of the second order perturbation theory and thus is tiny.

Recently, the $p_x$ and $p_y$-orbital physics in the honeycomb lattice has been systematically investigated in the context of ultra-cold atom optical lattice[33-35]. The optical potential around each lattice potential minimum is locally harmonic. The $s$ and $p$-orbital bands are separated by a large band gap, and thus the hybridization between them is very small. The $p_z$-orbital band can also be tuned to high energy by imposing strong laser beams along the $z$-direction. Consequently, we can have an ideal $p_x$ and $p_y$-orbital system in the artificial honeycomb optical lattice.

Such an orbital active system provides a great opportunity to investigate the interplay between non-trivial band topology and strong correlations that are fundamentally different from graphene[23-25]. Its band structure includes not only Dirac cones but also two additional narrow bands which are exactly flat in the limit of vanishing $\pi$-bonding. Inside the flat bands, due to the vanishing kinetic energy scale, non-perturbative strong correlation effects appear such as the Wigner crystallization of spinless fermions[36,37] and ferromagnetism[38] of spinful fermions as exact solutions. The band structure can be further augmented topologically non-trivial by imposing the experimentally available technique of the onsite rotation method[39,40]. This provides a natural way to realize the QAH effect as proposed in Refs. [30] and [33], and the topological gaps are just the rotation angular velocity[30,33]. In the Mott-insulating states, the frustrated orbital exchange described by a novel quantum 120° model[23], whose classic ground states map to all the possible loop configurations in the honeycomb lattice. The $p_x$ and $p_y$-orbital structure also enables unconventional $f$-wave Cooper pairing even with conventional interactions exhibiting flat bands of zero energy Majorana edge modes along boundaries parallel to gap nodal direction[43].

The $p_x$ and $p_y$-orbital structures have also been studied very recently in several classes of solid state semiconducting materials including fluoridated tin film[44-47], functionalized germanene systems[48], BiX/SeX (X=H,F,Cl,Br) systems[49-51], and in organic materials[51,52]. All these materials share the common feature of the active $p_x$ and $p_y$-orbitals in the honeycomb lattice, enabling a variety of rich structures of topological band physics. The most...
striking property is the prediction of the large topological band gap which can even exceed room temperature.

In this article, we construct a minimal four-band model to analyze the topological properties based on the $p_x$ and $p_y$-orbital structure in the honeycomb lattice. The eigen energy spectra and wavefunctions can be analytically solved with the help of Clifford $\Gamma$-matrices. The atomic SO coupling lifts the degeneracy between two on-site Kramers pairs with $j_z = \pm \frac{3}{2}$ and $j_z = \pm \frac{1}{2}$. And this atomic level SO coupling directly contributes to topological band gap openings at both $\Gamma$ and $K$ ($K'$) points. The lattice asymmetry and the SO coupling provide two different gap opening mechanisms, and their competition leads to a variety of topological band structures. With introducing both the sublattice anisotropy and the Néel exchange field, the system can become a large gap QAH insulator.

The article is organized as follows. The four-band model for the $p_x$ and $p_y$-orbital system in the honeycomb lattice is constructed in Sect. II. The symmetry analysis is presented in Sect. III. In Sect. VI the analytic solutions of energy spectra and eigen-wavefunctions are presented. The study of band topology and band crossing is presented in Sect. VII. Effective two-band models are constructed around high symmetry points near band crossings in Sect. VII. We add the Néel exchange field term in Sect. VIII and investigate how to get a large gap QAH insulator. Conclusions are made in Sect. IX.

II. THE $p_x$ AND $p_y$ BAND HAMILTONIAN

The two sublattices of the honeycomb lattice are denoted as $A$ and $B$, respectively. The bonding part of the Hamiltonian is

$$H_0 = t_\parallel \sum_{\vec{r} \in A,s} \{ p^\dagger_{i,s}(\vec{r}) p_{i,s}(\vec{r} + a\hat{e}_i) + h.c. \} - t_\perp \sum_{\vec{r} \in A,s} \{ p^\dagger_{i,s}(\vec{r}) p^\dagger_{i,s}(\vec{r} + a\hat{e}_i) + h.c. \},$$

(1)

where $s = \uparrow, \downarrow$ represents two eigenstates of spin $s_z$; $\hat{e}_{1,2} = \pm \sqrt{\frac{3}{2}} \hat{e}_x + \frac{1}{2} \hat{e}_y$ and $\hat{e}_3 = -\hat{e}_y$ are three unit vectors from one $A$-site to its three neighboring $B$-sites; $a$ is the nearest neighbor bond length; $p_i \equiv (p_x \hat{e}_x + p_y \hat{e}_y) \cdot \hat{e}_i$ and $p^\dagger_i \equiv (-p_x \hat{e}_x + p_y \hat{e}_y) \cdot \hat{e}_i$ are the projections of the $p$-orbitals parallel and perpendicular to the bond direction $\hat{e}_i$ for $i = 1 \sim 3$, respectively; $t_\parallel$ and $t_\perp$ are the corresponding $\sigma$ and $\pi$-bonding strengths, respectively. Typically speaking, $t_\perp$ is much smaller than $t_\parallel$. The signs of the $\sigma$ and $\pi$-bonding terms are opposite to each other because of the odd parity of $p$-orbitals. The $p_z$-orbital is inactive because it forms $\sigma$-bonding with halogen atoms or the hydrogen atom.

There exists the atomic SO coupling $\vec{s} \cdot \hat{L}$ on each site. However, under the projection into the $p_x$ and $p_y$-orbital states, there are only four onsite single-particle states. They can be classified into two sets of Kramers doublets: $p^\dagger_{i,\uparrow}(0)$ and $p^\dagger_{i,\downarrow}(0)$ with $j_z = \pm \frac{3}{2}$ and $p^\dagger_{i,\uparrow}(0)$ and $p^\dagger_{i,\downarrow}(0)$ with $j_z = \pm \frac{1}{2}$ where $p^\dagger_{i,\pm} = \frac{1}{2}(p^\dagger_{i,s} \pm ip^\dagger_{i,s}')$ are the orbital angular momentum $L_z$ eigenstates and $j_z$ is the $z$-component of total angular momentum. These four states cannot be mixed under $j_z$ conservation, and thus only $s_zL_z$-term survives which splits the degeneracy between the two sets of Kramers doublets. The SO coupling is modeled as

$$H_{so} = -\lambda \sum_{\vec{r},\sigma,s} (-)^\sigma \gamma p^\dagger_{\sigma,s}(\vec{r}) p_{\sigma,s}(\vec{r}),$$

(2)

where $\sigma = \pm$ refers to the orbital angular momentum number $L_z$, $s = \pm$ corresponds to the eigenvalues of $s_z = \uparrow, \downarrow$, and $\lambda$ is the SO coupling strength. For completeness, we also add the sublattice asymmetry term

$$H_m = m \left\{ \sum_{\vec{r} \in A,\sigma,s} p^\dagger_{\sigma,s}(\vec{r}) p_{\sigma,s}(\vec{r}) - \sum_{\vec{r} \in B,\sigma,s} p^\dagger_{\sigma,s}(\vec{r}) p_{\sigma,s}(\vec{r}) \right\}.$$  

(3)

In Sect. VIII we will consider the QAHE state based on this system by adding the following time-reversal (TR) symmetry breaking Néel exchange term

$$H_n = n \left\{ \sum_{\vec{r} \in A,\sigma,s} s p^\dagger_{\sigma,s}(\vec{r}) p_{\sigma,s}(\vec{r}) - \sum_{\vec{r} \in B,\sigma,s} s p^\dagger_{\sigma,s}(\vec{r}) p_{\sigma,s}(\vec{r}) \right\}.$$  

(4)

where $n$ is the Néel exchange field strength. Before Sect. VIII we only consider the Hamiltonian $H_0 + H_{so} + H_m$ without the Néel exchange term.

III. SYMMETRY PROPERTIES

One key observation is that electron spin $s_z$ is conserved for the total Hamiltonian $H_0 + H_{so} + H_m$. We will analyze the band structure in the sector with $s = \uparrow$, and that with $s = \downarrow$ can be obtained by performing time-reversal (TR) transformation. $H_0 + H_{so}$ is a TR doubled version of the QAH model proposed in ultra-cold fermion systems in honeycomb optical lattice. In the sector with $s = \uparrow$, we introduce the 4-component spinor representation in momentum space defined as

$$\psi_{\sigma, \vec{k}} = (\psi_{\uparrow, \vec{k}}, \psi_{\downarrow, \vec{k}})^T,$$

$$\psi_{\uparrow, \vec{k}} = (\psi_{\uparrow, A, +}(\vec{k}), \psi_{\uparrow, B, +}(\vec{k})), \psi_{\downarrow, A, -(\vec{k}), \psi_{\downarrow, B, -(\vec{k})})^T,$$

(5)

where two sublattice components are denoted as $A$ and $B$, respectively. The doublet of orbital angular momentum and that of the sublattice structure are considered as two independent pseudo-spin degrees of freedom, which are denoted by two sets of Pauli matrices as $\sigma_{1,2,3}$ and $\tau_{1,2,3}$, respectively. Unlike $s_z$, these two pseudospins are...
not conserved. The nearest neighbor hopping connects A-B sublattices, which does not conserve the orbital angular momentum moments due to orbital anisotropy in lattice systems.

The Hamiltonian \( H_f(\vec{k}) \) can be conveniently represented as

\[
H_f(\vec{k}) = h_{03} 1_\tau \otimes \sigma_3 + h_{30} \tau_3 \otimes 1_\sigma + h_{10}(\vec{k}) \tau_1 \otimes 1_\sigma + h_{20}(\vec{k}) \tau_3 \otimes 1_\sigma + h_{11}(\vec{k}) \tau_1 \otimes \sigma_1 + h_{22}(\vec{k}) \tau_2 \otimes \sigma_2 + h_{21}(\vec{k}) \tau_2 \otimes \sigma_1 + h_{12}(\vec{k}) \tau_1 \otimes \sigma_2, \quad (6)
\]

with the expressions of

\[
h_{03} = -\lambda, \quad h_{30} = m, \\
h_{10} = t_1 \sum_{i=1}^3 \cos(\vec{k} \cdot \hat{e}_i), \\
h_{20} = -t_1 \sum_{i=1}^3 \sin(\vec{k} \cdot \hat{e}_i), \\
h_{11} = t_2 \sum_{i=1}^3 \cos(\vec{k} \cdot \hat{e}_i) \cos 2\theta_i, \\
h_{22} = -t_2 \sum_{i=1}^3 \sin(\vec{k} \cdot \hat{e}_i) \sin 2\theta_i, \\
h_{21} = -t_2 \sum_{i=1}^3 \sin(\vec{k} \cdot \hat{e}_i) \cos 2\theta_i, \\
h_{12} = t_2 \sum_{i=1}^3 \cos(\vec{k} \cdot \hat{e}_i) \sin 2\theta_i, \quad (7)
\]

where \( t_{1,2} = \frac{1}{2}(t\parallel \pm t\perp) \) and \( \theta_i = \frac{1}{6}\pi, \frac{5}{6}\pi, \frac{2}{3}\pi \) are the azimuthal angles of the bond orientation \( \hat{e}_i \) for \( i = 1, 2 \) and 3, respectively.

For the sector with \( s = \downarrow \), the four-component spinor \( \psi' \) are constructed as \( \psi'_{1\tau\sigma}(\vec{k}) = (\psi_{1A,+}(\vec{k}), \psi_{1B,+}(\vec{k}), \psi_{1A,-}(\vec{k}), \psi_{1B,-}(\vec{k}))^T \).

Under this basis, \( H_f(\vec{k}) \) has the same matrix form as that of \( H_f(\vec{k}) \) except flipping the sign of \( \lambda \) in the \( h_{03} \)-term.

Next we discuss the symmetry properties of \( H_f(\vec{k}) \). We first consider the case of \( m = 0 \), i.e., in the absence of the lattice asymmetry. \( H_f(\vec{k}) \) satisfies the parity symmetry defined as

\[
PH_f(\vec{k})P^{-1} = H_f(-\vec{k}), \quad (8)
\]

with \( P = \tau_1 \otimes 1_\sigma \). \( H_f(\vec{k}) \) also possesses the particle-hole symmetry

\[
C' H_f(\vec{k}) (C')^{-1} = -H_f^\dagger(-\vec{k}), \quad (9)
\]

where \( C' = \tau_3 \otimes \sigma_1 \) satisfying \((C')^2 = 1\) and \( \dagger \) represents complex conjugation. \( C' \) is the operation of \( p_{\tau,A,\sigma} \rightarrow p_{\tau,A,\sigma} \) and \( p_{\tau,B,\sigma} \rightarrow -p_{\tau,B,\sigma} \) combined with switching eigenstates of \( L_z \).

Furthermore, when combining two sectors of \( s = \uparrow \) and \( \downarrow \) together, the system satisfies the TR symmetry defined as \( T = i\tau_2 \otimes 1_\tau \otimes 1_\sigma \otimes K \) with \( T^2 = -1 \), where \( K \) is the complex conjugation. Due to the above symmetry proprieties, our system is in the DIII class in the absence of lattice asymmetry. However, in the presence of lattice asymmetry, the particle-hole symmetry \( C' \) is broken, only the TR symmetry exists. In that case, the system in the in sympletic class AII. In both cases, the topological index is \( \mathbb{Z}_2 \).

Nevertheless, in the presence of sublattice asymmetry \( m \), the product of parity and particle-hole transformations remains a valid symmetry as

\[
CH_f(\vec{k})C^{-1} = -H_f^\dagger(\vec{k}), \quad (10)
\]

where \( C = i\tau_2 \otimes 1_\tau \) satisfying \( C^2 = -1 \). This symmetry ensures the energy levels, for each \( \vec{k} \), appear symmetrically with respect to the zero energy.

Without loss of generality, we choose the convention that \( m > 0 \) and \( \lambda > 0 \) throughout the rest part of this article. The case of \( m < 0 \) can be obtained through a parity transformation that flips the A and B sublattices as

\[
H_{m<0}(\vec{k}) = (\tau_1 \otimes 1_\sigma)H_{m>0}(-\vec{k})(\tau_1 \otimes 1_\sigma)^{-1}. \quad (11)
\]

And the case of \( \lambda < 0 \) can be obtained through a partial TR transformation only within each spin sector but without flipping electron spin

\[
H_{\lambda<0}(\vec{k}) = (1_\tau \otimes \sigma_1)H_{\lambda>0}^\dagger(-\vec{k})(1_\tau \otimes \sigma_1)^{-1}. \quad (12)
\]

IV. ENERGY SPECTRA AND EIGENFUNCTIONS

In this section, we provide solutions to the Hamiltonian of \( p_x \) and \( p_y \) orbital bands in honeycomb lattices. Based on the properties of \( \Gamma \)-matrices, most results can be expressed analytically.

A. Analytic solution to eigen-energies

Due to Eq. (10), the spectra of \( H_f(\vec{k}) \) are symmetric with respect to the zero energy. Consequently, they can be analytically solved as follows. The square of \( H_f(\vec{k}) \) can be represented in the standard \( \Gamma \)-matrix representation as

\[
H^2(\vec{k}) = g_0(\vec{k}) + 2 \sum_{i=1}^5 g_i(\vec{k}) \Gamma_i, \quad (13)
\]

with the expressions of \( g_i \)'s expressed as
where $\vec{b}_1 = \vec{e}_2 - \vec{e}_3$, $\vec{b}_2 = \vec{e}_3 - \vec{e}_1$, and $\vec{b}_3 = \vec{e}_1 - \vec{e}_2$.

The $\Gamma$-matrices satisfy the anti-commutation relation as \( \{ \Gamma_i, \Gamma_j \} = 2\delta_{ij} \). They are defined here as
\[
\Gamma_1 = 1_{\tau} \otimes \sigma_1, \quad \Gamma_{2,3,4} = \tau_{1,2,3} \otimes \sigma_3, \quad \Gamma_5 = 1_{\tau} \otimes \sigma_2. \tag{15}
\]

The spectra are solved as \( E^2(\vec{k}) = g_0 \pm 2(\sum_{i=1}^5 g_i^2)^{1/2} \).

In the case of neglecting the $\pi$-bonding, i.e., $t_1 = t_2 = \frac{1}{2} t_{1,2}$, the spectra can be expressed as
\[
E_{1,4}(\vec{k}) = \pm \sqrt{f_1(\vec{k}) + f_2(\vec{k})},
\]
\[
E_{2,3}(\vec{k}) = \pm \sqrt{f_1(\vec{k}) - f_2(\vec{k})}, \tag{16}
\]

where
\[
f_1(\vec{k}) = \lambda^2 + m^2 + \frac{3}{2} t_{1,2}^2 + \frac{1}{4} t_{1,2}^4 \eta_c(\vec{k}),
\]
\[
f_2(\vec{k}) = \left\{ \frac{t_{1,2}^2}{4} [3 - \eta_c(\vec{k})] - 4\lambda^2 \right\}^2
\]
\[
+ \lambda^2 \left[ 9t_{1,2}^2 - 16\lambda^2 + 4m^2 \right] - \frac{\sqrt{3}}{4} t_{1,2}^2 m \lambda \eta_s(\vec{k}), \tag{17}
\]

and the expressions for $\eta_c, \eta_s$ are defined as
\[
\eta_c(\vec{k}) = \sum_{j=1}^3 \cos \vec{k} \cdot \vec{b}_j, \quad \eta_s(\vec{k}) = \sum_{j=1}^3 \sin \vec{k} \cdot \vec{b}_j. \tag{18}
\]

### B. Solution to eigen-wavefunctions

Eigen-wavefunctions $\psi_i(\vec{k})$ for the band index $i = 1 \sim 4$ can be obtained by applying two steps of projection operators successively. The first projection is based on $H^2(\vec{k})$ which separates the subspace spanned by $\psi_{1,4}(\vec{k})$ from that by $\psi_{2,3}(\vec{k})$. We define
\[
P_{14}(\vec{k}) = \frac{1}{2} \left[ 1 + \sum_{i=1}^5 g_i^2(\vec{k}) \Gamma_i \right],
\]
\[
P_{23}(\vec{k}) = \frac{1}{2} \left[ 1 - \sum_{i=1}^5 g_i^2(\vec{k}) \Gamma_i \right]. \tag{19}
\]

where $g_i^2$ is normalized according to $g_i^2(\vec{k}) = g_i(\vec{k})/\sqrt{f_2(\vec{k})}$ such that $\sum_i g_i^2 = 1$. In each subspace, we can further distinguish the positive and negative energy states by applying
\[
P_i(\vec{k}) = \frac{1}{2} \left\{ 1 + \frac{1}{E_i} H_i(\vec{k}) \right\}. \tag{20}
\]

for each band $i = 1 \sim 4$. In other words, starting from an arbitrary state vector $\psi(\vec{k})$, we can decompose it into $\psi(\vec{k}) = \sum_{i=1}^4 \phi_i(\vec{k})$ according to
\[
\phi_{1,4}(\vec{k}) = P_{1,4}(\vec{k}) P_{1,4}(\vec{k}) \psi,
\]
\[
\phi_{2,3}(\vec{k}) = P_{2,3}(\vec{k}) P_{2,3}(\vec{k}) \psi. \tag{21}
\]

which satisfy $H \phi_i(\vec{k}) = E_i \phi_i(\vec{k})$. Nevertheless, the concrete expressions of eigen-wavefunctions $\psi_i(i = 1 \sim 4)$ after normalization are rather complicated and thus we will not present their detailed forms.

### C. A new set of bases

Below we present a simplified case in the absence of SO coupling, i.e., $\lambda = 0$, in which the two-step diagonalizations can be constructed explicitly. This also serves as a set of convenient bases for further studying the band topology after turning on SO coupling. We introduce a new set of orthonormal bases denoted as
\[
|A_1(\vec{k})\rangle = \frac{1}{\sqrt{2N_k}} \begin{pmatrix}
\gamma^+_1(\vec{k}) \\
0 \\
\gamma^-_1(\vec{k}) \\
0
\end{pmatrix},
\]
\[
|B_1(\vec{k})\rangle = \frac{1}{\sqrt{2N_k}} \begin{pmatrix}
0 \\
\gamma^-_1(\vec{k}) \\
0 \\
\gamma^+_1(\vec{k})
\end{pmatrix}. \tag{22}
\]
where \( \alpha \) are expressed as

\[
|A_2(\vec{k})| = \frac{1}{\sqrt{2N_k}} \begin{pmatrix}
\gamma_{2-}(\vec{k}) & 0 \\
0 & \gamma_{2+}(\vec{k})
\end{pmatrix},
\]

\[
|B_2(\vec{k})| = \frac{1}{\sqrt{2N_k}} \begin{pmatrix}
\gamma_{2+}(\vec{k}) & 0 \\
0 & \gamma_{2-}(\vec{k})
\end{pmatrix}.
\tag{23}
\]

where

\[
\gamma_{1\pm}(\vec{k}) = \sum_{i=1}^{3} e^{i\vec{k} \cdot \vec{e}_i \pm 2i\theta_i}, \quad \gamma_{2\mp}(\vec{k}) = \sum_{i=1}^{3} e^{i\vec{k} \cdot \vec{e}_i \pm i\theta_i},
\]

\[
N(\vec{k}) = 3 - \eta_c(\vec{k}). \tag{24}
\]

In terms of this set of new bases, \( H_{\uparrow}(\vec{k}) \) is represented as

\[
H_{\uparrow}(\vec{k}) = \begin{bmatrix}
m - n(\vec{k}) & -\frac{3}{2}t_\parallel & h(\vec{k}) & 0 \\
-\frac{3}{2}t_\parallel & -m + n(\vec{k}) & 0 & h(\vec{k}) \\
h^*(\vec{k}) & 0 & m - n(\vec{k}) & -\frac{1}{2}t_\parallel l(\vec{k}) \\
0 & h^*(-\vec{k}) & -\frac{1}{2}t_\parallel l^*(\vec{k}) & -m - n(\vec{k})
\end{bmatrix}.
\tag{25}
\]

The spectrum is the same as that in graphene at \( m = 0 \). The eigen-wavefunctions are enriched by orbital structures which can be solved as

\[
\begin{bmatrix}
|\phi_2(\vec{k})| \\
|\phi_3(\vec{k})|
\end{bmatrix} = \begin{bmatrix}
\sin \frac{\beta}{2} & \cos \frac{\beta}{2} e^{i\phi} \\
\cos \frac{\beta}{2} e^{-i\phi} & -\sin \frac{\beta}{2}
\end{bmatrix} \begin{bmatrix}
|A_2(\vec{k})| \\
|B_2(\vec{k})|
\end{bmatrix}.
\tag{30}
\]

where \( \beta(\vec{k}) = \arctan\left[\frac{1}{2m_\parallel} l(\vec{k})\right] \) and \( \phi(\vec{k}) = \arg l(\vec{k}) \).

### D. Appearance of flat bands

According to the analytical solution of spectra Eq. \(16 \)

flat bands appear in two different situations: (1) In the absence of SO coupling such that the bottom and top bands are flat with the eigen energies described by Eq. \(27 \)

(2) In the presence of SO coupling, at \( \lambda = \frac{3}{4}t_\parallel \), the two middle bands are flat with the energies \( E_{2,3}(\vec{k}) = \pm \frac{3}{4}t_\parallel \).

In both cases, the band flatness implies that we can construct eigenstates localized in a single hexagon plaquette. The localized eigenstates for the case of \( \lambda = 0 \) is constructed in Ref. \(27 \), and those for the case of \( \lambda = \frac{3}{4}t_\parallel \) was presented in Ref. \(33 \). Since the kinetic energy is suppressed in the flat bands, interaction effects are non-perturbative. Wigner crystallization \(27 \) and ferromagnetism \(11 \) have been studied in the flat band at \( \lambda = 0 \).
V. BAND TOPOLOGY AND BAND CROSSINGS

In this section, we study the topology of band structures after SO coupling is turned on. Due to the $s_z$ conservation, the $Z_2$ topological class is augmented to the spin Chern class. Without loss of generality, we only use the pattern of Chern numbers of the sector $s = \uparrow$ to characterize the band topology, and that of the $s = \downarrow$ sector is just with an opposite sign. The Berry curvature for the $i$-th band is defined as

$$F_i(\vec{k}) = \partial_{k_x} A_y(\vec{k}) - \partial_{k_y} A_x(\vec{k})$$

in which the Berry connection is defined as $\vec{A}_i(\vec{k}) = -i(\phi_i(\vec{k})|\nabla_k|\phi_i(\vec{k}))$. The spin Chern number of band $i$ can be obtained through the integral over the entire first Brillouin zone as

$$C_{s,i} = \frac{1}{2\pi} \int_{F\text{BZ}} dk_x dk_y F_i(\vec{k}_x, \vec{k}_y).$$

A. Band crossings at $\Gamma$, $K$ and $K'$

We have performed the numerical integration for spin Chern numbers ($C_{s,1}, C_{s,2}, C_{s,3}, C_{s,4}$) for $H_1(\vec{k})$ as presented in Fig. 1 based on Eq. 32. The phase boundary lines $L_{1,2,3}$ are associated with band touching, which occur at high symmetry points $\Gamma$, $K$ and $K'$, respectively. The momenta of these points are defined as $(0,0)$,
\[ E_{2,3}(\Gamma) = \pm \left( \lambda - \sqrt{m^2 + \left( \frac{3}{2} t_{\parallel} \right)^2} \right). \]  

The level crossing can only occur at zero energy with the following hyperbolic condition
\[ \lambda^2 = m^2 + \left( \frac{3}{2} t_{\parallel} \right)^2, \]
which corresponds to line \( L_1 \) in Fig. 1.

The sublattice asymmetry parameter \( m \) and SO coupling \( \lambda \) are different mass generation mechanisms. The former breaks parity and contributes equally at \( K \) and \( K' \), while the latter exhibits opposite signs. Their total effects superpose constructively, or, destructively at \( K \) and \( K' \), respectively, as shown in the spectra of the two lower energy levels at \( K \) and \( K' \). At \( K' = (-\frac{4\sqrt{3}}{3}, 0) \), they are
\[ E_{2,3}(K') = \pm (\lambda - m), \]
and those at \( K = (\frac{4\sqrt{3}}{3}, 0) \) are
\[ E_{1,4}(K) = \mp \sqrt{(m-\lambda)^2 + \left( \frac{3}{2} t_{\parallel} \right)^2}, \]
\[ E_{2,3}(K) = \mp (m+\lambda). \]

Thus the level crossing at \( K' \) occurs at zero energy with the relation
\[ \lambda = m, \]
which is line \( L_2 \) in Fig. 1. Similarly, the level crossing at \( K \) occurs when \( E_2(K) = E_1(K) \) leading to the condition
\[ \lambda m = \left( \frac{3}{4} t_{\parallel} \right)^2, \]
which is line \( L_3 \) in Fig. 1.

B. Evolution of the topological band structures

The lattice asymmetry term \( m \) by itself can open a gap at \( K \) and \( K' \) in the absence of SO coupling. In this case, the gap value is \( m \) at both \( K \) and \( K' \). The lower two bands remain touched at the \( \Gamma \) point with quadratic band touching. Nevertheless, the overall band structure remains non-topological.

The SO coupling \( \lambda \) brings non-trivial band topology. Its competition with the lattice asymmetry results in a rich structure of band structure topology presented in Fig. 1, which are characterized by their pattern of spin Chern numbers. There are two phases characterized by the same spin Chern number pattern \((1, -1, 1-1)\) marked as \( A_1 \) and \( A_2 \), respectively; two phases characterized by \((1, 0, 0, -1)\) marked as \( B_1 \) and \( B_2 \); two trivial phases denoted as \( C_1 \) and \( C_2 \) \((0, 0, 0, 0)\).

Even an infinitesimal value of \( \lambda \) removes the quadratic band touching between the band 1 and 2, and brings non-trivial band topology. The line of \( m = 0 \) corresponds to the situation investigated in the QAH insulator based on the \( p_x \) and \( p_y \) orbital bands in the honeycomb lattice.\( ^{[30,33]} \) The current situation is a 2D topological insulator with \( s_z \) conserved which is just a double copy of the previous QAH model. At small values of \( \lambda \), the system is in the \( B_1 \) phase. It enters the \( A_2 \)-phase after crossing the line \( L_1 \) at \( \lambda = \frac{3}{2} t_{\parallel} \).

If the system begins with a non-zero lattice asymmetry parameter \( m \), it first enters the \( A_1 \). If we increase SO coupling strength \( \lambda \) by fixing \( m \) at different values, different band topology transitions appear. To further clarify these transitions, we plot the spectra evolutions as increasing \( \lambda \) while fixing \( m = 0.3, 0.5, \) and 1 in Fig. 2, Fig. 3, and Fig. 4 respectively. Only the spectra along the line cut from \( K' \) to \( \Gamma \) to \( K \) in Brillouin zone are plotted. At small values of \( m \) as shown in Fig. 2, the gap first closes at \( K' \), then at \( \Gamma \), and finally at \( K \) as increasing \( \lambda \). The sequence of phase transitions is \( A_1 \rightarrow B_1 \rightarrow A_2 \rightarrow C_1 \). At intermediate values of \( m \) shown in Fig. 3, the gap first closes at \( K' \), then at \( K \), and finally at \( \Gamma \) leading to a sequence of phase transitions as \( A_1 \rightarrow B_1 \rightarrow B_2 \rightarrow C_1 \). At large values of \( m \) as shown in Fig. 4, the gap first closes at \( K' \), then at \( K \), and finally...
VI. REDUCED TWO-BAND MODELS AROUND BAND CROSSINGS

In order to further clarify topological band transitions, we derive the effective two-band Hamiltonians around the gap closing points (Γ, K, and K') respectively in this section.

Since the crossing at Γ-point occurs at zero energy, we consider the middle two states. We construct the two bases as

\[
\phi_2(\vec{k}) = \cos \frac{\alpha}{2} |\psi_{A,+}(\vec{k})\rangle + \sin \frac{\alpha}{2} |\psi_{B,+}(\vec{k})\rangle
\]
\[
\phi_3(\vec{k}) = -\sin \frac{\alpha}{2} |\psi_{A,-}(\vec{k})\rangle + \cos \frac{\alpha}{2} |\psi_{B,-}(\vec{k})\rangle,
\]

where \(\alpha = \arctan \frac{3t_1}{2m}\). Right at the Γ-point, these two bases are the eigenvectors of the middle two bands with energies \(E_{2,3}(\Gamma) = \mp(\sqrt{m^2 + (\frac{3}{2}t_1)^2} - \lambda)\), respectively. As \(\lambda \to \sqrt{m^2 + (\frac{3}{2}t_1)^2}\), we construct the low energy Hamiltonian for \(\vec{k}\) around the Γ point by using \(\phi_{2,3}(\vec{k})\) as bases as

\[
\begin{pmatrix}
\langle \phi_2 | H | \phi_2 \rangle & \langle \phi_2 | H | \phi_3 \rangle \\
\langle \phi_3 | H | \phi_2 \rangle & \langle \phi_3 | H | \phi_3 \rangle
\end{pmatrix}
= \begin{pmatrix}
-\lambda + \sqrt{m^2 + (\frac{3}{2}t_1)^2} & \frac{3}{4}t_1(k_x + ik_y) \\
\frac{3}{4}t_1(k_x - ik_y) & \lambda - \sqrt{m^2 + (\frac{3}{2}t_1)^2}
\end{pmatrix}.
\]

(40)

which describes the band crossing of line 1 in Fig. 1. The two-band effective model for the crossing at the K' point is just what we have constructed in Eq. (40). It describes the crossing at zero energy represented by line \(L_3\) in Fig. 1.

As for the band crossing at the K point, it occurs between band 1 and 2, and between 3 and 4 symmetrically with respect to zero energy \((B_2, C_1, \text{ and } C_2)\) phases. For simplicity, we only consider the effective two-band model at small values of \(m\). In this case, the band crossing is described by line \(L_3\) in Fig. 1 occurs at large values of \(\lambda \gg m\). The onsite energy level splitting between the states of \((p_+, \uparrow)\) and \((p_-, \uparrow)\) is larger than the hopping integral \(t_1\), and each of them will develop a single band in a honeycomb lattice. The bands of \(p_{\pm}\)-orbitals lie symmetrically with respect to zero energy. Nevertheless, as shown in Refs. [30] and [31], the inter-band coupling at the second order perturbation level effectively generates the complex valued next-nearest-neighbor hopping as in Hal-dane’s QAH model[3]. Our current situation is a TR double copy and thus it gives rise to the Kame-Mele model.

To describe the above physics, we only keep the \(p_\pm\)-orbitals on each site in the case of large values of \(\lambda\). Then the terms of \(h_{11}, h_{22}, h_{12}\) and \(h_{12}\) in Eq. (41) become perturbations. By the second order perturbation theory, we derive the low energy Hamiltonian of \((p_{A,+}(\vec{k}), p_{B,+}(\vec{k})\) bands as

\[
\begin{pmatrix}
|\psi_{A+}| H |\psi_{A+}\rangle & |\psi_{A+}| H |\psi_{B+}\rangle \\
|\psi_{B+}| H |\psi_{A+}\rangle & |\psi_{B+}| H |\psi_{B+}\rangle
\end{pmatrix} = \begin{pmatrix}
m + m_H(\vec{k}) & -\frac{t_1}{2}t_0(\vec{k}) \\
\frac{t_1}{2}t_0(\vec{k}) & -m - m_H(\vec{k})
\end{pmatrix},
\]

where

\[
m_H(\vec{k}) = \frac{\sqrt{3}}{8} \frac{t_1^2}{\lambda} \sin \eta_{\vec{k}}(\vec{k}).
\]

(41)

Around K'-point, \(m + m_H(\vec{k}) = \frac{9}{16} \frac{t_1^2}{\lambda}\). The band crossing occurs when \(m + m_H(\vec{k})\) switches the sign which gives rise to line \(L_3\) in Fig. 1.

The topological gap opens at K' point between band 2 and 3. According to Eq. (22) we only need to keep the right-bottom block for the construction of the low energy two-band model. By expanding around the K' point, we have

\[
\begin{pmatrix}
|A_2\rangle |H| A_2\rangle & |A_2\rangle |H| B_2\rangle \\
|B_2\rangle |H| A_2\rangle & |B_2\rangle |H| B_2\rangle
\end{pmatrix}
= \begin{pmatrix}
m - \lambda & -\frac{3}{4}t_1(\delta k_x + i\delta k_y) \\
-\frac{3}{4}t_1(\delta k_x - i\delta k_y) & -m + \lambda
\end{pmatrix},
\]

(42)

where \(\delta k = \vec{k} - \vec{k}'\), and thus the mass term is controlled by \(m - \lambda\). For completeness, we also derive the effective two-band Hamiltonian for band 2 and 3 around K point similarly, which yields the gap value \(m + \lambda\). In the absence of lattice asymmetry, the gap values at K and K' are both the SO coupling strength.

Now let us look more carefully at the eigenfunctions of the effective two-band Hamiltonian for band 2 and 3 at K' and K points and check their orbital angular momenta. The eigenstates are just \(|A_2(K')\rangle\), and \(|B_2(K')\rangle\) at K', and \(|A_2(K)\rangle\), and \(|B_2(K)\rangle\) at K point. In the bases of Eq. (5), we express

\[
|A_2(K')\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |B_2(K')\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix},
\]
\[
|A_2(K)\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad |B_2(K)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.
\]

(43)

All of them are the orbital angular momentum eigenstates with \(L_z = \pm 1\). Considering this is the sector with \(s = \uparrow\), the gap is just the atomic SO coupling strength \(\lambda\) in the absence of the lattice asymmetry term \(m\).

VII. LARGE TOPOLOGICAL BAND GAPS

The most striking feature of the these \(p_x-p_y\) system is the large topological band gap at K', K, and Γ points.
In this section, we analyze the origin of large topological band gaps at these \( k \)-points in the \( B_1 \) phase (QSH phase, \( \lambda > m \)). For the case of a single component fermion QAH model studied in Ref. 30, it has been analyzed that the gap values at the \( \Gamma, K \) and \( K' \) points are just the onsite rotation angular velocity \( \Omega \) in the absence of the lattice asymmetry term. The situation in this paper is a TR invariant double copy of the previously single component case, and thus the role of \( \Omega \) is replaced by the onsite atomic SO coupling strength \( \lambda \).

At the \( K' \) point, according to Eq. [43] the eigenstates for the band 2,3 are orbital angular momentum eigenstates with \( L_z = \pm 1 \). The energy and corresponding eigenstates for band 2 and 3 are

\[
E_2(K') = m - \lambda, \quad |\phi_2(K')\rangle = |\psi_{A,+}(K')\rangle.
\]
\[
E_3(K') = \lambda - m, \quad |\phi_3(K')\rangle = |\psi_{B,-}(K')\rangle.
\]
\[
\Delta_{K'} = 2(\lambda - m).
\] (44)

As shown in Fig. [3] the eigenstate for band 2 has \( L_z = +1 \) with the energy \( m - \lambda \), which is of \( p_x + ip_y \) type, and its wavefunction is totally on the \( A \) sublattice. In contrast, the eigenstate for band 3 has \( L_z = -1 \) with the energy \( \lambda - m \). It is of the \( p_x - ip_y \) type whose wavefunction completely distributes on the \( B \) sublattice. The topological band gap is thus \( 2(\lambda - m) \). If the sublattice asymmetry term vanishes, i.e., \( m = 0 \), the band gap is just \( 2\lambda \).

Obviously, the atomic on-site SO coupling strength \( \lambda \) directly contributes to the topological band gap, leading to a large band splitting. It is because at \( K' \) point, the eigenstates of the system are also \( L_z \) eigenstates, which means the topological band gap is the eigenenergy difference between the SO coupling term \( s_z L_z \) for \( L_z = \pm 1 \). It is easy to generalize the analysis to the \( K \) point similarly.

At the \( \Gamma \) point, the Hamiltonian \( H(\vec{k}) \) preserves all the rotation symmetries of the system, and thus the SO coupling term \( s_z L_z \) commutes with \( H(\vec{k}) \). The eigenstates simultaneously diagonalize the SO coupling term and \( H(\vec{k}) \). The energy and corresponding eigenstates for bands 1 and 2 at the \( \Gamma \) point are

\[
E_1(\Gamma) = -\lambda - \sqrt{m^2 + (\frac{3}{2} t_1^2)},
\]
\[
|\phi_1(\Gamma)\rangle = \sin \frac{\alpha}{2} |\psi_{A,-}(\Gamma)\rangle + \cos \frac{\alpha}{2} |\psi_{B,+}(\Gamma)\rangle.
\]
\[
E_2(\Gamma) = \lambda - \sqrt{m^2 + (\frac{3}{2} t_1^2)},
\]
\[
|\phi_2(\Gamma)\rangle = \cos \frac{\alpha}{2} |\psi_{A,+}(\Gamma)\rangle + \sin \frac{\alpha}{2} |\psi_{B,-}(\Gamma)\rangle.
\]
\[
\Delta_{\Gamma} = 2\lambda.
\] (45)

The eigenstates for band 1,2 are the superpositions of wavefunctions on both the \( A \) and \( B \) sublattices. However, for band 1, the eigenstate is an \( L_z = -1 \) eigenstate, and the eigenstate for band 2 is an \( L_z = 1 \) eigenstate (See Fig. [5]). As a result, the topological band gap \( \Delta_{\Gamma} \) is the energy difference of the SO coupling term \( s_z L_z \), which is \( 2\lambda \).

A common mechanism to generate topological band gap in the literature is band inversion. In such a case, the onsite atomic SO coupling strength determines the
energy level splitting at the Π points. However, this splitting is not the topological gap. The topological gap occurs at finite values of $\bar{k}$ due to the s-p hybridization, and thus is much smaller. In the single band systems in the honeycomb lattice such as graphene, the effect from the atomic level SO coupling to the band structure is not direct but through the second-order perturbation theory.

In contrast, our case is markedly different from the band inversion mechanism. The atomic SO coupling $\lambda$ completely contributes to band gap. Since the atomic SO coupling can be very large, the topological band gap can even reach the level 0.3 eV according to the estimation in Ref. [38].

VIII. QUANTUM ANOMALOUS HALL STATE

In this section, we add the Néel antiferromagnetic exchange field term (Eq. 2) to the Hamiltonian. This term gives rise to another mass generation mechanism. Together with the atomic SO coupling term of $L_{\sigma} \sigma_z$, and the sublattice asymmetry term (Eq. 3) discussed before, we can drive the system to a QAH state. Similar mechanism was also presented in the single-orbital honeycomb lattice[33], and here we generalize it to the $p_x$-$p_y$-orbital systems.

We consider the gap opening at the $\bar{k}$ and $\bar{k}'$ points, and assume that the band 1 and 2 are filled. In the absence of the Néel term (Eq. 2), the system is in the trivially gapped phase $A_1$ at $m > \lambda$, and in the QSH phase $B_1$ at $\lambda > m$.

Let us start with the QSH phase $B_1$ with $\lambda > m > 0$, and gradually turn on the Néel exchange magnitude $n > 0$. The energy levels for different spin sectors at the $K'$ and $K$ points for the middle two bands are

$$
E_{2,3,\uparrow}(K') = \mp(\lambda - m - n), \\
E_{2,3,\downarrow}(K') = \mp(\lambda + m - n), \\
E_{2,3,\uparrow}(K) = \mp(\lambda + m + n), \\
E_{2,3,\downarrow}(K) = \mp(\lambda - m + n).
$$

(46)

The gap will not close for both spin-$\uparrow$ and $\downarrow$ sectors at the $K$-point as increasing $n$, and thus we focus on the band crossing at the $K'$ point. At this point, the first band crossing occurs in the spin-$\uparrow$ sector at $n = \lambda - m$, which changes the spin-$\uparrow$ sector into the topologically trivial regime. Meanwhile, the spin-$\downarrow$ sector remains topologically non-trivial, and thus the system becomes a QAH state. If we further increase $n$, the second band crossing occurs in the spin-$\downarrow$ sector at $n = \lambda + m$, at which the spin-$\downarrow$ sector also becomes topologically trivial. In this case, the entire system is a trivial band insulator. The QAH state can be realized for $\lambda - m < n < \lambda + m$. The band crossing diagrams are shown in Fig. 6(a).

Similarly, if we start from $A_1$ trivially gapped phase ($0 < \lambda < m$), and gradually turn on the Néel exchange field $n$. The middle two energy levels for both spin sectors

$$
E_{2,3,\uparrow}(K') = \mp(m - \lambda + n), \\
E_{2,3,\downarrow}(K') = \mp(m + \lambda - n), \\
E_{2,3,\uparrow}(K) = \mp(m + \lambda + n), \\
E_{2,3,\downarrow}(K) = \mp(m - \lambda - n).
$$

(47)

In this case, the spin-$\uparrow$ sector remains in the trivially gapped phase as increasing $n$, since there is no band inversion in this sector (see Fig. 6(b)). The first band crossing occurs in the spin-$\downarrow$ sector at the $K'$ point when $n = m - \lambda$, rendering this sector topologically nontrivial, and then the whole system goes into a QAH phase. The second band inversion occurs at the $K'$ point also in the spin-$\downarrow$ sector at $n = \lambda + m$. Now the spin-$\downarrow$ sector is back into a topologically trivial phase, and the whole system is a trivial band insulator for $n > \lambda + m$. Similarly to the previous case, the QAH phase is realized at $\lambda - m < n < \lambda + m$.

IX. CONCLUSIONS AND OUTLOOKS

In summary, we have presented a minimal model to describe the 2D topological insulator states in the honeycomb lattice which have been recently proposed in literature. The $p_x$ and $p_y$-orbitals are the key, and thus their properties are dramatically different from those in graphene. The atomic level SO coupling directly contributes to the topological gap opening, and thus the gap can be large. Due to the conservation of $s_z$, the band structures are a TR invariant doublet of the previously investigated QAHE based on $p$-orbital in the honeycomb lattice. The band topology is described by the spin Chern numbers. Both sublattice asymmetry and the on-site SO coupling can open the gap, and their competition leads...
to a rich structure of topological band insulating phases. Due to the underlying structure of Clifford algebra, the energy spectra and eigen-wavefunctions can be obtained analytically. Also, the transition lines among different topological insulator are also analytically obtained. Low energy two-band models are constructed around band crossings. Furthermore, with the help of Néel antiferromagnetic exchange field, the model can enter into a QAH phase. This work provides a useful platform for further exploring interaction and topological properties in such systems.

ACKNOWLEDGMENTS

G. F. Z. and C. W. are supported by the NSF DMR-1105945 and AFOSR FA9550-11-1-0067(YIP). YL thanks the Inamori Fellowship and the support at the Princeton Center for Theoretical Science. C.W. acknowledges the financial support from the National Natural Science Foundation of China (11328403, J1210061).

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Note added Near the completion of this work, we became aware of the work Ref. [39] in which the low energy effective model of the 2D topological insulators on honeycomb lattice are also constructed.
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