Dipolar quantum spin Hall insulator phase in extended Haldane model

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The higher-order corner modes for quantum anomalous Hall insulator in C3 symmetry broken honeycomb lattice have been engineered recently. Here we consider an extended Haldane model in presence of inversion symmetry breaking sub-lattice mass, time reversal symmetry breaking Zeeman field and spin-orbit coupling interaction where we find that only the quantum spin Hall insulator can host the second-order dipolar phase while the remaining two first-order topological phases do not morph into the latter. Remarkably, four-fold degeneracy of zero-energy dipolar states can be reduced to two-fold under the application (withdrawn) of sub-lattice mass (Zeeman field) term when the spin-orbit coupling is already present. On the other hand, the sub-lattice mass and Zeeman field terms compete with each other to pin down the two mid-gap states at zero-energy in absence or presence of spin-orbit coupling. Interestingly, the bulk-polarization can topologically characterize the dipolar phase irrespective of the energy of the mid-gap states as long as inversion symmetry is preserved. The effective gap criterion can qualitatively mimic the extent of SOT phase originated by the interplay between finite Zeeman exchange field, sub-lattice mass, and SOC interaction.

I. INTRODUCTION

The higher-order topological (HOT) phases [1, 2] have drawn a considerable research endeavour in the field of topological systems [3–11] due to their intriguing bulk-boundary correspondence. A d-dimensional nth-order HOT [first-order topological (FOT)] insulator is associated with (d – n) [(d – 1)]-dimensional boundary modes where 1 < n ≤ d. There exist various symmetries such as, reflection, inversion, rotational and time-reversal symmetries which are becoming instrumental in engineering the HOT phases [12–16]. For example, the second-order topological (SOT) phase in two-dimensional (2D) quantum spin-Hall insulator and topological superconductor host 0-dimensional (0D) electronic and Majorana corner modes, respectively, which are characterized by various topological invariant such as, quantized quadrupole moment, edge and bulk polarizations [17–25]. Importantly, HOT phases have been theoretically predicted and experimentally realized in honeycomb [26–31] and Kagome [32–37] lattices extending their presence beyond the realm of square or cubic lattices [21, 38–53]. Interestingly, the C3 symmetry broken modified Haldane model is shown to harbour corner modes in quantum anomalous Hall insulator (QAH) phase under an appropriate lattice termination [54].

Interestingly, by making use of pseudospin degree of freedom and anisotropic hopping strength, the honeycomb lattice can host helical edge state in a HOT phase even without spin-orbit coupling (SOC) interaction [27]. Such modulation in hopping for the honeycomb lattice can in principle lead to a mismatch between the Wannier centers (WCs), defined by the expectation value of the position operator in the unit cell of a crystal, and the lattice sites [1, 12, 26, 55]. The WC, being related to d-dimensional polarization, is located at a high-symmetry point with respect to the mirror symmetries and remains quantized for the SOT phase [56, 57]. Notice that the spin-Chern number [58–60] and Z2 invariant [6], defining the FOT phase, vanishes in the SOT phases being the primary criteria to look for the SOT phase.

The time-reversal symmetry (TRS) broken quantum spin Hall insulator (QSHI) [61–64], based on graphene, is vastly unexplored so far in the context of SOT phases. Given the fact that inversion symmetry (IS) protected HO-QAHI can be generated only in absence of sub-lattice mass [54], we here seek the answers for the following question: Can we engineer mid-gap zero-energy HOT states using the interplay of sub-lattice mass, Zeeman exchange field and SOC interaction? To be precise, the HO analogue of QAHI, QSHI and quantum anomalous spin Hall insulator (QASHI) phases, as already observed in the extended Haldane model [65], is the main focus of the present work.

Considering C3 symmetry and TRS broken extended Haldane model, we find that an interior part of QSHI phase can only host mid-gap corner states while the entire QAHI and QASHI phases do not support any SOT insulator (SOTI) phase (see Fig. 1). The SOT dipolar insulator is characterized by the bulk-dipole moment only when IS is preserved in the absence of sub-lattice mass term (see Fig. 2). In the presence (absence) of SOC interaction (Zeeman field), the four-fold degeneracy of zero-energy dipolar states can be reduced to two-fold degeneracy when the IS is broken by a finite sub-lattice mass even though the bulk-polarization fails to detect the latter phase (see Fig. 3). In the absence of SOC interaction, the sub-lattice mass and Zeeman field terms compete each
other to pin down two of the four mid-gap states at zero-energy (see Fig. 4). Interestingly, the interplay between finite Zeeman exchange field, sub-lattice mass, and SOC interaction can further enrich the tunability of the mid-gap dipolar modes within the SOT phase that can be qualitatively understood from the effective gap criterion (see Fig. 5).

II. MODEL HAMILTONIAN

We start with the $C_{4}$ symmetry broken extended Haldane model as follows [3, 5, 46, 65]

$$H = -\sum_{(ij)} t_{ij}^{1} c_{i}^{\dagger} c_{j} + \sum_{(ij)} t_{ij}^{2} e^{i\phi_{ij}} c_{i}^{\dagger} c_{j} + M \sum_{i} c_{i}^{\dagger} \sigma_{z} c_{i}$$

$$+ \frac{\nu_{SO}}{\sqrt{3}} \sum_{(ij)} e^{i\phi_{ij}} \nu_{ij} c_{i}^{\dagger} \sigma_{x} c_{j} + g \sum_{i} c_{i}^{\dagger} \tau_{z} c_{i}$$  \hspace{1cm} (1)

where $c_{i}(c_{i}^{\dagger})$ indicates the creation (annihilation) operator with $\sigma \in (A, B)$ and $\tau \in (\uparrow, \downarrow)$ representing the orbital and spin degrees of freedoms. The spin-independent nearest neighbour (NN) [next nearest neighbour (NNN)] anisotropic hopping are represented by $t_{1} = (\eta_{1}, \eta_{f1}, t_{1})$ $[t_{2} = (t_{2}, t_{2}, \eta_{t2})]$ along $\delta_{1} = (-1/2, 1/2, \sqrt{3})$, $\delta_{2} = (1/2, 1/2\sqrt{3})$, and $\delta_{3} = (0, -1/\sqrt{3})$ $[a_{1} = (-1/2, \sqrt{3}/2)$, $a_{2} = (1/2, \sqrt{3}/2)$, and $a_{3} = (1, 0)]$. The factor $|\eta| \neq 1$ (with $|\eta| < 1$) is responsible for the breaking of $C_{4}$ symmetry allowing strong and weak bonds of strengths $t_{1,2}$ and $t_{3,4}$, respectively. The SOC interaction of strength $\nu_{SO}$ corresponds to the spin-dependent NNN hopping. The phase factor $e^{i\phi_{ij}}$ designates the staggered magnetic flux. Notice that we consider uniform strength of SOC interaction for simplicity. $M \langle g \rangle$ is the IS breaking sub-lattice mass term (TRS breaking magnetic field acting on spin-degrees of freedom). The factor $\nu_{ij} = (d_{ij}^{1} \times d_{ij}^{2})_{z}$ contains unit vectors $d_{ij}^{1,2}$ along the two bonds the electron traverses going from site $j$ to $i$ [5, 65].

The momentum space Hamiltonian, obtained from Eq. (1), in the basis $(e_{A1}, e_{A1'}, e_{B1}, e_{B1'})$ is given by $H(k, \eta) = \sum_{i=0}^{5} n_{i} \Gamma_{i}$ with $\Gamma_{i} = \sigma_{i} \otimes \tau_{0}$ for $i = 1, 2, 3$, $\Gamma_{4} = \sigma_{3} \otimes \tau_{3}$, $\Gamma_{5} = \sigma_{0} \otimes \tau_{3}$ and $\Gamma_{6} = \sigma_{0} \otimes \tau_{0}$. The components $n_{i}$ are given by: $n_{0} = 2 t_{2} f(k, \eta) \cos \phi$, $n_{1} = -t_{1}(1 + 2 b f(k, \eta))$, $n_{2} = -2 n_{1} \sin \frac{\sqrt{3}k_{y}}{2} \cos \frac{k_{x}}{2}$, $n_{3} = -2 t_{2} g(k, \eta) \sin f(k, \eta)$, $n_{4} = \frac{\nu_{SO}}{\sqrt{3}} g(k, \eta) \cos \phi$, $n_{5} = 2 t_{2} |f(k, \eta)| \sin \phi$, $n_{6} = 2 t_{2} |f(k, \eta)| \cos \phi$, $n_{7} = \eta \cos k_{x}, n_{8} = 2 \cos \frac{\sqrt{3}k_{y}}{2} \sin \frac{k_{x}}{2} + \eta \sin k_{x}$, $h(k, \eta) = \eta \cos \frac{\sqrt{3}k_{y}}{2} \cos \frac{k_{x}}{2}$.

To this end, we consider $\eta = 1$ to investigate various FOT phases before exploring their second-order counterparts. The Zeeman field $g$ destroys the $\phi \rightarrow -\phi$ symmetry by shrinking or expanding different phases as compared to $g = 0$ case where the eight-fold FOT phases can symmetrically appear under $\phi \rightarrow -\phi$ [65]. The size of QSFI (QAHI) phases increases (reduces) referring to fact that magnetic field stabilizes QSFI phases (see Fig. 1 (a)). For IS case with $M = 0$, QASHI and QAH phases are completely suppressed (see Fig. 1 (b)). The red tick marks suggest that only QSFI allows the SOT to appear.

The gap vanishes at the Dirac points over the boundaries between two FOT phases or non-topological and FOT phases. For $0.5 < |\eta| < 1$, two Dirac points appear at $K_{\pm} = (\pm 2\theta, -2\sqrt{3}\theta)$ with $\theta = \arctan(\sqrt{4\eta^{2} - 1})$. The phase boundaries can be obtained when the gap vanishes for $H(K_{\pm}, \eta)$ whose eigenvalues are given by $\lambda_{1}^{\pm} = n_{3}^{\pm} - n_{4}^{\pm} - n_{5}^{\pm}$, $\lambda_{2}^{\pm} = n_{3}^{\pm} - n_{4}^{\pm} - n_{5}^{\pm}$, $\lambda_{3}^{\pm} = n_{6}^{\pm} - n_{4}^{\pm} + n_{5}^{\pm}$, and $\lambda_{4}^{\pm} = n_{6}^{\pm} + n_{4}^{\pm} + n_{5}^{\pm}$.

FIG. 1. We show the FOT phase diagram in $M \phi$ and $g \phi$ planes in (a) with $g = -0.33$ and in (b) with $M = 0$. For $M = 0$, the QSFI and QAHI phases are completely suppressed. Red tick marks indicate that QSFI phase can only host SOT phase unlike the QAHI and QASHI phases.

The stripped (shaded) region designates SOT phase with $p_{y} = 0.5$ (critical phase with vanishing spin-gap). We consider $t_{1} = 1.0$, $t_{2} = 0.2$, $\eta = 1$ (0.25) for SOTI (SOTI), and $\nu_{SO} = 2.5$.

We use bulk-dipole moment $p_{\alpha} = -(1/2\pi)^{2} \int d^{2}k \text{Tr}[A_{\alpha}]$ $(\alpha = x, y)$ with non-Abelian Berry connection $[A_{\alpha}]^{nm} = -i \langle n| \partial_{\eta}\langle m| k \rangle^{2}$ to characterize the topological nature of the SOT phases where...
the integration is over the Brillouin zone (BZ) and $|u_k^\alpha\rangle$ represents $n$-th occupied band associated with the Hamiltonian [26, 32, 55]. Employing the concept of Wannier centers, the polarization for one-dimensional crystal can take the form $p_\alpha(k_\beta) = -i \log \det |W_{\alpha,k}|/2\pi$ with the Wilson loop $W_{\alpha,k} = F_{k+(N_\alpha-1)\Delta k_\alpha}\cdots F_{k+\Delta k_\alpha}F_k$. Here, $[F_k]^{mn} = \langle u_{k+\Delta k_\alpha}^m|u_k^n\rangle$, and $\Delta k_\alpha = 2\pi/N_\alpha$ ($N_\alpha$ being the number of discrete points considered inside the BZ along $k_\alpha$). Now the total polarization along $\alpha$ in a two-dimensional crystal i.e., the bulk-dipole moment can be found as $p_\alpha = \sum_{k_\beta} p_\alpha(k_\beta)/N_\beta$. The dipolar QAHI phase in modified Haldane model with IS i.e., without sub-lattice mass $M = 0$, is characterized by $p_y = 0.5$ and $p_x \neq 0.5$ (modulo unity) [54]. The SOT phase is depicted by the stripped region in Fig. 1 (b) where IS protects the half-integer quantization of $p_y$. Under IS breaking $M \neq 0$, the quantization of $p_y$ is expected to deviate from the half-integer value that we encounter below for various parameter regimes while investigating the SOT phases (see Fig. 1 (a)). We consider $\eta = 0.25$ henceforth.

III. EFFECT OF DIFFERENT PARAMETERS

A. $M = 0$ case

We investigate the mid-gap modes, residing inside the SOT phase as depicted in Fig. 1 (b), in the presence (absence) of infinitesimal Zeeman field and substantial SOC interaction (sub-lattice mass). For the cut over the weak [strong] bonds, referred to as cut 2 [cut 1], helical edge modes cease [continue] to exist even when $|\eta| < 0.5$ that is depicted in Fig. 2 (a) [(b)] under zigzag ribbon geometries [54]. One hence finds SOTI, hosting the localized mid-gap modes between the bulk gap, for cut 2 as shown in Fig. 2 (c) where the energy spectrum of a nano-disc with cut 2 is demonstrated. The four zero-energy states inhabit only in two corners at $(i,j) = (0, \pm L_y)$ while the remaining two corners at $(i,j) = (\pm L_x, 0)$ are left unoccupied (see lower inset of Fig. 2 (c)). The four-fold degeneracy of the mid-gap states can be reduced to two-fold by tuning $g$ (see upper inset of Fig. 2 (c)). Such a dipolar insulator is characterized by $p_y$ which is found to be 0.5 everywhere in $\phi$ except for $\phi = 0, \pm \pi$ (see Fig. 2 (d)). This refers to the fact that the WC lies at the middle of strong bond protecting the dipolar insulator in cut 2 under IS.

The $C_3$ symmetry breaking with $|\eta| < 0.5$ can gap out the edge states lying on the boundary of the nano-disc in cut 2 except at $(i,j) = (0, \pm L_y)$. In this geometry, the domain-wall only forms at corner $(i,j) = (0, \pm L_y)$ where the two neighbouring cuts over the weak bonds meet precisely at a strong bond [54]. The entire QSHI phase, as shown in Fig. 1 (a) and (b), does not morph into the dipolar phase rather an interior part only can incubate SOT phase. This is in stark contrast to the square lattice case where the entire QSHI phase becomes quadrupolar insulator under $C_4$ symmetry and TRS breaking [2, 16, 39]. Further notice that $p_y$ can exhibit half-integer quantization, being consistent with Fig. 1 (b), even when the four mid-gap dipolar states with two-fold degeneracy are at finite energy. Interestingly, it is found that the QASHI [QAHI] evolve into the trivial insulator [semi-metallic] phase, bearing no analogue of SOT phase, while energy dispersion is studied for the nano-disc under cut 2 configuration.

![Fig. 2. The band structure $E$ vs $k_x$ of anisotropic extended Haldane model (Eq. (1)) with $\eta = 0.25$ under ribbon geometry along cut 2 i.e., cut over strong bonds [cut 1 i.e., cut over weak bonds] is demonstrated in (a) [(b)] indicating the absence [presence] of helical edge modes. The gapless edge states are observed for $\eta = 0.75$ in the insets of (a) and (b) that suggest the FOT phase, hosting edge modes, remains stable when $0.5 \leq |\eta| \leq 1$. (c) The energy dispersion $E$ vs $N$ for cut 2 nano-disc geometry depicts the four mid-gap states being pinned down at (away from) zero-energy for $g = -0.023$ ($g = -0.01, \text{upper inset}$). The lower inset shows the localization of mid-gap states at the corners $(0, \pm L_y)$ for the above geometry where the origin $(0,0)$ is at the centre of the nanodisc. (d) The variation of the bulk-dipole moment components $p_y$ (solid-circle) and $p_x$ (empty-circle) as a function of $\phi$ clearly indicate the SOT phase in stripped-region depicted in Fig. 1 (b) with $g = -0.023$. The inset in (d) shows the robustness of SOT phases with $V_{SO}$. We consider $M = 0, \phi = 0.1, \text{and } V_{SO} = 2.5$ accordingly.]

B. $g = 0$ case

We consider here, $M \neq 0, V_{SO} \neq 0$, and $g = 0$ case where we find that the degeneracy of the mid-gap states at non-zero energy is lifted due to the finite sub-lattice mass while the bulk gap is controlled by $V_{SO}$. With changing $M$, two out of four mid-gap states can be brought to zero-energy and the remaining two move further away from zero-energy, towards the bulk levels. This
refers to the fact that four-fold degeneracy of the dipolar states at zero-energy reduces to two-fold. The four non-degenerate mid-gap states are depicted in Fig. 3 (a). Figure 3 (c) demonstrates another instance where the QSHI hosts doubly degenerate zero-energy modes along with two finite-energy non-degenerate dipolar states. The band dispersion for the above situation in cut 2 ribbon geometry clearly shows a gap as evident from Fig. 3 (b). One can find that for positive (negative) values of $M$, $p_y$ remains close to unity (zero) [Fig. 3 (d)].

**FIG. 3.** (a) The four non-degenerate mid-gap states at finite energies are observed in $E$ vs $N$ for nano-disc with $M = -0.01$. The gapped band structure [energy dispersion with two-fold degenerate zero energy and two non-degenerate finite energy mid-gap dipolar states], considering ribbon [nano-disc] geometry for cut 2, is shown in (b) [(c)] where $M = -0.037$. The gapless helical edge states exist for cut 1 as shown in the inset of (b). (d) The bulk-polarization $p_y$ deviates from 0.5 for $|M| \neq 0$ even though zero-energy dipolar states are present. We considered $\phi = 0.1$, $V_{SO} = 2.5$, and $g = 0.0$.

**C. $V_{SO} = 0$ case**

We will now study the interplay between $M$ and $g$ only with keeping $V_{SO}$ fixed at zero. Such a competition between the above two parameters, depending on the relative signs, can push two mid-gap states towards zero energy while the remaining two mid-gap states move into the bulk bands rapidly as compared to the earlier case with $g = 0$. The evolution of mid-gap states are demonstrated in Figs. 4 (a), (b), (c) and (d) by varying $g$, keeping $M$ fixed at 0.5. Interestingly, for $M = -g$, we find that two mid-gap states out of four mid-gap states can be constrained at zero energy. Importantly, the bulk-gap around zero energy reduces with increasing $|g|$ unlike the above two cases where $V_{SO}$ mostly determines the bulk-gap. The continuous bulk bands, observed for $|g| < M$, become gapped out at finite energies within which the mid-gap dipolar state can be present for $|g| > M$. The individual [combined] localization for the mid-gap states are depicted in the four insets of Figs. 4 (a) [upper insets of Figs. 4 (b) and (c)]. This is characteristically different from the quadrupolar insulator where each of the mid-gap states populate more than a single corner of a 2D square lattice [39]. The ribbon geometry clearly indicates the gapped band structure in Figs. 4 (b) and (d). The polarization $p_y$ changes with $M$ demonstrating the breakdown of topological characterization for IS broken case (see the insets in Fig. 4 (d)).

**FIG. 4.** We depict the energy dispersion under nano-disc geometry with cut 2 for $g = -0.06, -0.11, -0.5,$ and $-0.6$ in (a), (b), (c) and (d), respectively, with $M = 0.5, \phi = 0.1,$ and $V_{SO} = 0.0$. The two mid-gap states can be pinned down at zero energy when $|M| = |g|$ and the other two states are pushed towards the bulk bands when $|g|$ increases. Insets of (a) display that the two mid-gap states are localized at $(0, +L_y)$ while the remaining two at $(0, -L_y)$. Upper insets in (b) [(c)] indicate the combined localization for the two mid-gap at finite-energy [zero-energy] states in nano-disc geometry with cut 2. The band structures for ribbon geometry with above cut are shown in lower insets of (b), (c), and (d). Upper inset in (d) illustrates the variation of $p_x$ and $p_y$ as a function of $M$ with $|M| = |g|$.
D. $M \neq 0$, $g \neq 0$, and $V_{SO} \neq 0$ case

Now we investigate the most complex situation, with all the tuning parameters being finite, in Figs. 5 (a) and (b) to show the emergence and disappearance of the mid-gap modes, respectively. It is thus evident that the SOT dipolar phase is not embedded on the entire QSHI phase rather an interior part of it for $M, g \ll V_{SO}, \phi < \pi/4$ as qualitatively estimated from the effective band-gaps for $|\eta| < 0.5$. The determination of exact phase boundary for the SOT phase in $M - \phi - g - V_{SO}$ parameter space is beyond the scope of the present study as the appropriate topological invariant is yet to be determined for IS broken case.

![Figure 5](image)

**FIG. 5.** We consider $(M, g, V_{SO}, \phi) = (0.5, -0.33, 2.5, 0.1)$ and $(1.0, -0.33, 2.5, 0.5)$ from interior and exterior of QSHI in Fig. 1 (a) to show the zero-energy dipolar modes and gapped dispersion in (a) and (b), respectively. Lower insets in (a) and (b) demonstrate the band dispersion in ribbon geometry with cut 2. Upper inset in (b) shows semi-metallic energy dispersion inside the QSHI phase where $p_y \neq 0.5$ in Fig. 1 (b).

IV. CONCLUSIONS

Having motivated by the HOT phases in $C_3$ symmetry broken graphene-like system [26, 29, 54], here we analyze the evolution of eight-fold phases [65] for extended Haldane model in the anisotropic limit. We extensively explore the interplay between the IS breaking sub-lattice mass, TRS breaking Zeeman field and SOC interaction in engendering the corner modes for the dipolar phase. We find that the above SOTI can only emerge out of the underlying QSHI phase while the remaining QAHI and QASHI phases do not have any SOTI analogue (see Fig. 1). In the absence of sub-lattice mass (Zeeman exchange field), the finite energy mid-gap state can be two-fold degenerate (non-degenerate) while SOC interaction remains finite. The SOTI is characterized by the bulk-dipole moment only for IS case where the dipolar mid-gap states can be four-fold degenerate at zero-energy with finite Zeeman field (see Fig. 2). Interestingly, zero-energy states become two-fold degenerate under the application (withdrawn) of sub-lattice mass (Zeeman field) [see Fig. 3]; however, the SOTI is not characterized by the bulk-dipole moment. Remarkably, two mid-gap dipolar states are constrained to reside at zero energy by appropriately tuning the sub-lattice mass and Zeeman field without the SOC interaction (see Fig. 4). The interplay between finite Zeeman exchange field, sub-lattice mass, and SOC interaction can further manipulate the mid-gap states from which one can estimate the boundary for the SOT phase; the effective band-gap relation might be useful in predicting such boundaries (see Fig. 5). The FOT phases are found to be preserved by effective TRS and dressed particle-hole symmetry that can be instrumental in preserving the dipolar modes in the presence of the above three tuning parameters [54]. The experimental realization of SOC interaction [66–68] and Haldane model [69, 70] allow our model to become experimentally viable. The disordered and Floquet extension of these phases can be the open future directions.

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