Large Chern Number Quantum Anomalous Hall Effect In Thin-film Topological Crystalline Insulators

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Quantum anomalous Hall (QAH) insulators are two-dimensional (2D) insulating states exhibiting properties similar to those of quantum Hall states but without external magnetic field. They have quantized Hall conductance $\sigma_H = Ce^2/h$, where integer $C$ is called the Chern number, and represents the number of gapless edge modes. Recent experiments demonstrated that chromium doped thin-film $(\text{Bi,Sb})_2\text{Te}_3$ is a QAH insulator with Chern number $C = \pm 1$. Here we theoretically predict that thin-film topological crystalline insulators (TCI) can host various QAH phases, when doped by ferromagnetically ordered dopants. Any Chern number between $\pm 4$ can, in principle, be reached as a result of the interplay between (a) the induced Zeeman field, depending on the magnetic doping concentration, (b) the structural distortion, either intrinsic or induced by a piezoelectric material through proximity effect and (c) the thickness of the thin film. The tunable Chern numbers found in TCI possess significant potential for ultra-low power information processing applications.

A quantum anomalous Hall state is a 2D topological insulating state that has quantized Hall conductance in the form of $Ce^2/h$ where $C$ is an integer, and possesses $|C|$ gapless edge modes along any 1D edge. These properties are shared by the well-known quantum Hall states. Nevertheless, there is no external magnetic field in a QAH state, which makes it ‘anomalous’. Hence, the nontrivial topology in QAH does not come from the topology of the Landau levels, but rises from the band structure of electrons coherently coupled to certain magnetic orders, e.g., spin orders and orbital current orders. The first theoretical model that shows this phase is given in Ref. [2], which is followed by other models and experimental proposals in various systems [3, 4]. Very recently, experimentalists have adapted one of the proposals and realized a QAH state with $|C| = 1$ in chromium doped thin-film $(\text{Bi,Sb})_2\text{Te}_3$, which is a 3D topological insulator (TI) [5].

We first recapitulate the basic idea underlying the realization of QAH insulators with $|C| = 1$ in a thin-film 3D topological insulator [6–7]. Each surface of a 3D TI is a gapless 2D Dirac spin-split semi-metal [10, 11], as opposed to spin-degenerate Dirac semi-metals such as graphene. The surface is spin-split except at the Dirac point where double-degeneracy is protected by time-reversal symmetry, and spectral flow into the bulk conduction and valence bands occurs away from the Dirac point. Upon the application of a Zeeman field along the perpendicular direction, induced by ferromagnetic dopants, a gap is opened at the Dirac point, giving rise to a massive Dirac cone. Such a massive Dirac cone has been well known to contribute Hall conductance of $\pm e^2/2h$ or, a Chern number of $\pm 1/2$. Moreover, since a thin film has two surfaces (top and bottom), the total Chern number is $\pm 1$. An identical effect would take place in bulk samples - thin films are being used here only because they allow tuning of the Fermi level in the gap by gating. Here we use a symmetry-based analysis to show that the topological crystalline insulators [13–21] such as $(\text{Pb,Sn})(\text{Te,Se})$ are much richer compounds to explore QAH physics. As thin films of $(\text{Pb,Sn})(\text{Te,Se})$ have already been grown [22–24] and various magnetic dopants have been successfully doped [25–27], we believe our proposal is experimentally realizable. The existence of such a widely tunable topological phase transition in the TCI class of materials may form the basis for new types of information processing devices which consume much less power compared to current technology.

I. RESULTS

A. Unperturbed Hamiltonian on the (001)-surface

Consider the symmetries of such a thin film, $(\text{Pb,Sn})(\text{Te,Se})$ crystalizes into a face-centered-cubic lattice with point group $O_h$. Below a critical temperature, depending on composition, the cubic symmetry spontaneously breaks into either rhombohedral or orthorhombic symmetries, resulting in a small lattice distortion. Here we assume that the lattice has cubic symmetry and treat the small distortion as perturbative strain. The thin-film sample is terminated on the (001)-plane, where $O_h$ reduces to 2D point group $C_{4v}$. The bulk system also has time-reversal symmetry and inversion symmetry, which relates the top and the bottom surfaces in the absence of asymmetric surface terminations. The in-plane translational symmetry allows the definition of the surface Brillouin zone (SBZ), which is centered at $\Gamma$ and bounded by $X$ along the [110]-direction and $Y$ along [110]-direction [Figure 1(a)]. Four Dirac points close to the Fermi energy have been observed in experiments [15–17]. Two Dirac points, denoted by $D_{1\pm}$, are located along $\Gamma X$, close to and symmetric about $X$; two others, denoted by $D_{1\perp}$, are located along $\Gamma Y$, close to and symmetric about $Y$. 


to gap-opening perturbations. The minimal model for each Dirac cone \( h_{i=1,2,1',2'}(\mathbf{q}) \), where \( \mathbf{q} = \mathbf{k} - \mathbf{D}_i \), is a two-band \( k \cdot p \) model, due to the double-degeneracy at \( \mathbf{D}_i \). The form of \( h_i \) is determined by how the doublet at \( \mathbf{D}_i \) transforms under the little group at \( \mathbf{D}_i \), i.e., a subgroup of the full symmetry group which leaves \( \mathbf{D}_i \) invariant. For example, consider \( \mathbf{D}_1 \): the little group is generated by the mirror reflection about the \([1\bar{1}0]\)-plane, denoted by \( M_{1\bar{1}0} \) and a combined operation of a 180-degree rotation about the \([001]\)-direction followed by time-reversal, denoted by \( C_{2T} \). This little group has only one 2D irreducible representation (see Sec.III A): \( M_{1\bar{1}0} = i\sigma_y \) and \( C_{2T} = K\sigma_x \), where \( K \) means complex conjugation, and \( \sigma_{x,y,z} \) are Pauli matrices. It restricts \( h_1(\mathbf{q}) \) to the form

$$h_1(\mathbf{q}) = v_0q_1 I_{2 \times 2} + v_1q_1\sigma_y + v_2q_2\sigma_x$$  \hspace{1cm} (1)$$

up to the first order of \( |\mathbf{q}| \). \( \mathbf{q} \) decomposes into two components \( q_1 = \mathbf{q} \cdot \hat{e}_{1\bar{1}0} \) and \( q_2 = \mathbf{q} \cdot \hat{e}_{10} \), where \( \hat{e}_{mnl} \) is the unit vector along the \([mnl]\)-direction. The parameters \( v_{0,1,2} \) can be fixed by matching the dispersion of equation (1), \( E(\mathbf{q}) = v_0q_1 \pm \sqrt{v_1^2 q_1^2 + v_2^2 q_2^2} \) to the measured Fermi velocities along \([110]\)- and \([1\bar{1}0]\)-directions \((v_0, |v_1|, |v_2|) \sim (0, 1.1, 2.8)\text{eVÅ})\). The Dirac cones centered at \( D_{2,1',2'} \) can be related to the cone centered at \( D_1 \) by \( C_4 \) symmetry. This automatically gives the effective theories of the other Dirac cones: \( h_2(q_1, q_2) = h_1(-q_1, -q_2) \), \( h_{1'}(q_1, q_2) = h_1(-q_2, q_1) \) and \( h_{2'}(q_1, q_2) = h_1(q_2, -q_1) \) (see Sec.III B for a formal proof).

B. The effect of induced Zeeman field

We assume a Zeeman field in the sample along \([001]\)-direction, induced by ferromagnetically ordered dopants. In order to couple this field to the electrons in the \( k \cdot p \) models, we add an additional term \( \delta H^Z \) to \( h_{i=1,2,3,4}(\mathbf{q}) \) and note the following facts: (i) magnetization along \([001]\)-direction changes sign under both \( M_{1\bar{1}0} \) and \( C_{2T} \) and (ii) it is invariant under 90-degree rotations about \([001]\)-direction. Using these facts, we have:

$$\delta H^Z = \Delta Z \sigma_z + O(|\mathbf{q}|),$$

where \( |\Delta Z| \) is the field strength of the Zeeman field, which is proportional to the Curie temperature, \( T_c \), of the ferromagnetism. The sign of \( \Delta Z \) depends on the direction of the magnetization. The Hamiltonian for each cone with the induced Zeeman field is \( h_i(\mathbf{q}) + \delta H^Z \), which has a gap of size \( |\Delta Z| \) at each Dirac point (see Figure 2 [b]).

C. The effect of intrinsic and applied strain

Now we consider the effect of intrinsic and external strains. Depending on Sn and Se concentration, the cubic lattice can have spontaneous distortions into either rhombohedral or the rhombohedral symmetries. One may also
cap the top surface of the film with a piezoelectric material such as BaTiO$_3$, to control the strain on the top surface. A general strain tensor is given by a symmetric matrix $\varepsilon_{ij}$ where $i,j = 1,2,3$, written in the frame spanned by $(\hat{e}_{110}, \hat{e}_{110}, \hat{e}_{001})$. In order to represent couplings to the strain tensor in the $k \cdot p$ models, we need to determine the transform of each component under the symmetry group $C_4v$ and time-reversal (Table I). Using these relations, we obtain the following strain induced terms for the four Dirac cones, to the zeroth order of $|q|$:  

$$
\delta H_{1/2}^S = (\lambda_{11} \varepsilon_{11} + \lambda_{22} \varepsilon_{22} + \lambda_{33} \varepsilon_{33}) \sigma_y + \lambda_{12} \varepsilon_{12} \sigma_x \pm \lambda_{23} \varepsilon_{23} \sigma_z,
$$

$$
\delta H_{1/2}^{S'} = (\lambda_{11} \varepsilon_{11} + \lambda_{22} \varepsilon_{22} + \lambda_{33} \varepsilon_{33}) \sigma_y - \lambda_{12} \varepsilon_{12} \sigma_x \pm \lambda_{32} \varepsilon_{32} \sigma_z,
$$

where $\lambda_{ij}$ are electro-phonon couplings.

Consider the full Hamiltonian for each Dirac cone under both Zeeman field and strain, $H_t = H_i + \delta H_{i/2}^S + \delta H_{i/2}^{S'}$. In $H_i$, only terms proportional to $\sigma_z$ open gaps in the spectrum while others move the position of the Dirac point $D_i$. The gap at each $D_i$, i.e., the coefficient before the $\sigma_z$ term in the Hamiltonians, denoted below by $\Delta_i$, is:

$$
\Delta_{1,2} = \Delta_Z \pm \Delta_{23},
$$

$$
\Delta_{1',2'} = \Delta_Z \pm \Delta_{13},
$$

where we have defined $\Delta_{13/23} = \lambda_{23/13} \varepsilon_{23/13}$. Each gapped Dirac cone contributes

$$
\sigma_i^H = -\text{sign}(v_1 v_2) \Delta_i e^2 / (2h)
$$

to the Hall conductance (see Sec. III C for formal proof).

### D. The effect of finite thickness

We have so far assumed that the top and the bottom surfaces are isolated from each other, and hence the total Hall conductance is

$$
\sigma_i^H = \sum_{i=1,2} \frac{\sigma_i^{H,t} + \sigma_i^{H,b}}{2},
$$

where superscript $t/b$ denotes the top/bottom surface. When the thickness is comparable to the decay length of the surface states, the hybridization gap between the two surfaces, denoted by $\Delta_H$, becomes significant, and the total Hall conductance is generically not given by equation (3). Diagonalizing each $k \cdot p$ Hamiltonian with

![FIG. 2: (a) The schematic of a thin-film Pb$_{0.5}$Sn$_{0.5}$Te grown on a substrate, capped by a piezoelectric. (b-d) The schematic dispersions of the gapped Dirac cones on the top surface in the presence of uniform Zeeman field and strains, corresponding to the parameters $\Delta_Z > |\Delta_{13}| = |\Delta_{23}| = 0$, $|\Delta_{13}| > \Delta_Z > |\Delta_{23}| = 0$, and $0 < \Delta_Z < |\Delta_{13}| = |\Delta_{23}|$, respectively. (e) The Chern number of the system in the thick limit (sample thickness $> 20$nm) plotted against the transverse electric fields applied on the piezoelectric. (f) The Chern number of the system with thickness of 5 ~ 10nm.](image)
hybridization (see Sec. II D for the explicit forms of the band dispersion)

$$\tilde{H}_i = \left( \begin{array}{cc} H^t_i & \Delta_H \sqrt{I_2 \times 2} \\ \Delta_H \sqrt{I_2 \times 2} & H^b_i \end{array} \right),$$

we have two scenarios. (i) If $\text{sign}(\Delta^t_i) = \text{sign}(\Delta^b_i)$ (where $\Delta^t/b$ denotes the gap at top/bottom surface), as $\Delta_H$ increases, the gap at $D_i$ closes at $|\Delta_H| = \Delta_{i,H,a} \equiv \sqrt{|\Delta^t_i|}$ and reverses [see Figure 3] and at $|\Delta_H| > \Delta_{i,H,a}$, the total contribution to $\sigma^H$ vanishes; (ii) if $\text{sign}(\Delta^t_i) = -\text{sign}(\Delta^b_i)$, there is no quantum phase transition as $\Delta_H$ increases, and the total contribution to Hall conductance stays at zero. The complete expression for the Hall conductance is therefore

$$\sigma^H = \sum_{i=1,2} (\sigma^H_{i,t} + \sigma^H_{i,b}) \theta(\Delta_{i,H,a} - |\Delta_H|),$$

where $\theta(x)$ is the Heaviside step function.

E. Proposals of materials and experiments

Depending on the parameter set of $\{\Delta_Z, \Delta^t/b, \Delta_H\}$, the Chern number of the system takes each integer from $-4$ to $+4$. In a realistic system, however, not all parameters are easily tunable, so the range of the Chern number is generically restricted. We propose a system shown in Figure 2(a): a thin-film Pb$_{0.5}$Sn$_{0.5}$Te doped with Mn or Cr, grown on a substrate, e.g., NaCl or KCl, with its top surface deposited with piezoelectric crystal such as BaTiO$_3$. Below $T \sim 10K$, the (Cr,Mn) moments develop ferromagnetism, inducing a small Zeeman gap $\Delta_Z \sim 1 meV$ in the sample. The external strain on the top surface may be tuned by the piezoelectric. Assuming that the strain in BaTiO$_3$ be completely transferred to the top surface of the film, we estimate that $\Delta^t_{13} = 2 \times 10^{-6} E_{110} \text{meV-m-V}^{-1}$ and $|\Delta^b_{13}| = 2 \times 10^{-6} E_{110} \text{meV-m-V}^{-1}$. Since the sample with such composition has zero or negligible intrinsic distortion at low temperatures, $\Delta^b_{13} = 0$. In the thick limit ($d > 20 nm$), $\Delta_H \ll 1 meV$ and is negligible. From equation 2, the bottom surface always contributes $C = 2$. There are three possible scenarios for the top surface, resulting in $\sigma^H = 1/2, 0, 1$ respectively: (i) $|\Delta_{13,23}| < |\Delta_Z|$, (ii) $|\Delta_{23}| < |\Delta_Z| < |\Delta_{13}|$ and (iii) $|\Delta_Z| < |\Delta_{13,23}|$, where we have assumed $|\Delta_{13,23}| > |\Delta_{23}|$ without loss of generality. The dispersion of the four gapped cones for the three scenarios are plotted in Figure 2(b-d). The total Chern number can thus be tuned between 2, 3 and 4, plotted against $E_{110}$ and $E_{110}$ in Figure 2(e). In a thiner film with thickness $d = 5 \sim 10 nm$, the hybridization gap is $|\Delta_H| = 5 \sim 15 \text{meV}$, from which we take $\Delta_H = 10 \text{meV}$ as a typical value and we plot the Chern number against $E_{110}$ and $E_{110}$ in Figure 2(f). From this Figure, we see that around the critical field strength $|E_{110}| = |E_{110}| = 5 \times 10^5 \text{V m}^{-1}$, the Chern number can be electrically tuned to $0, 1$ or $2$. If the length and width of the sample are both $100 nm$, this means that the Chern number can be tuned by varying $V_{110,110}$ within $10 mV$. The ability to tune the topological phase transition with such a small electric field offers hope that such a logic devices based on piezoelectric deformation of a TCI could possess on/off ratios and sub-threshold slopes which far exceed current logic device technologies.

II. DISCUSSION

In the derivation of the main results, we have ignored physical parameters of (i) the impurities and (ii) the electron-electron interaction. The mirror Chern number of a TCI is only well defined in the presence of mirror planes. In a system with a random impurity configuration, mirror symmetries are broken and the mirror Chern number is not a good quantum number, and consistently, the gapless modes at the Dirac points are gapped by impurity scattering. This mirror symmetry breaking by impurity has, however, no effect on the Chern number in a ferromagnetically doped system, as long as the intensity of the random potential is much smaller compared with the Zeeman gap. This is because the Chern number, unlike the mirror Chern number, does not presume any symmetry, as long as the surface is gapped. Weak interactions smaller than the Zeeman gap do not have any effect on the quantized Hall conductance either, because the Chern number is also a good quantum number of an interacting gapped 2D system.

It is also interesting to discuss other surface terminations besides the (001)-surface. On the (110)-surface of SnTe, first principles calculation shows that there are two Dirac cones centered at two Dirac points that are close to and symmetric about $X$ along $\Gamma \cdot X$ in the surface BZ. The two Dirac points are protected by the (110) mirror plane and have equal energy due to the (001) mirror plane. A Zeeman field along $[110]$ gaps both Dirac
points and results in a QAH phase with Chern number of ±2. A strain along [111]-direction breaks both the (110) and the (001) mirror planes, opening two gaps of opposite signs at the two Dirac points. When both the strain and the Zeeman field are present, a discussion similar to the one given in Sec.IC shows that the Chern number is generated by \(M\) and the little group along with the symmetry constraints de-

\[C\] causes the Zeeman gap is generically much smaller than 40meV. Therefore, an insulator with quantized Hall con-
ductance on the (111)-surface is not possible using the current scheme.

### III. METHODS

#### A. Derivation of \(h_1(q)\) using the little group at \(D_1\)

The full symmetry group of the thin film in the absence of applied fields is \(D_{4h} \otimes T\). The little group at a Dirac point \(D_1\) is the subgroup of all operations that leave \(D_1\) invariant. The little group therefore consists of a mirror plane that passes \(\bar{\Gamma}\) and \(M\) and the (001) mirror planes, opening two gaps of opposite signs and results in a QAH phase with Chern number of ±2. A strain along [111]-direction breaks both the (110) and the (001) mirror planes, opening two gaps of opposite signs at the two Dirac points. When both the strain and the Zeeman field are present, a discussion similar to the one given in Sec.IC shows that the Chern number is generated by \(M\) and the little group along with the symmetry constraints de-

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#### B. Relating the four Dirac cones by \(C_4\) symmetry

In the main text, we mention that by 90-degree ro-
tations the effective theories for the four cones can be related. This is an intuitive statement yet to be made precise. In fact, \(k \cdot p\) theories are always written with respect to a chosen basis, which is our case is furnished by (the periodic part of) the two Bloch states that are degenerate at the Dirac point. Due to the degener-

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ductance on the (111)-surface is not possible using the current scheme.
C. Calculation of the Chern number of the top/bottom surface

In the text we refer to the Chern number contributed by one massive Dirac cone, which is not mathematically well-defined. In fact, the integrated Berry’s curvature of a gapped Dirac cone is non-quantized in any finite k-space, hence possesses no well-defined Chern number. The Chern number of a whole 2D surface (top surface for example) is, however, a well-defined quantity (if periodic boundary is taken for the other two directions), which may be calculated. Suppose we are interested in the Chern number, $C$, at some Zeeman field $\Delta_Z = \Delta_0 > 0$. Then since time-reversal reverses the Chern number, we know for $\Delta_Z = -\Delta_0$, the Chern number must be $-C$. Consider a 3D space spanned by $q_1$ and $\Delta_Z$, then from Gauss’s law, the Chern number change from $\Delta_Z = -\Delta_0$ to $\Delta_0$ equals the total monopole charge between these two planes in the 3D parameter space. The monopole, or gap closing point, is always at $(q_1, q_2, \Delta_Z) = 0$, around which the Hamiltonian is that of 3D Weyl fermions: $h(q_1, q_2, q_3) = \sum_{i,j=1,2,3} A_{ij} \sigma_i q_j$, where $q_3 = \Delta_Z$. The charge of such a monopole is $\text{sign} \det(A)$, and since there are in total four such monopoles between $\Delta_Z = \pm \Delta_0$, we have the difference in Chern number $C - (-C) = 4\text{sign} \det(A)$, or $C = 2\text{sign} \det(A)$. All Chern numbers obtained in the text are derived using this method.

D. Diagonalizing the Hamiltonian in equation (11)

A Hamiltonian that describes isolated top and surface states around $D_i$ is

$$
\tilde{H}_i = \begin{pmatrix} H^t_{i} & 0 \\ 0 & H^b_{i} \end{pmatrix},
$$

and hybridization is equivalent to adding an off-diagonal block term, resulting in, to the lowest order in $|q|$, 

$$
\tilde{H}_i = \begin{pmatrix} H^t_{i} & \Delta_H I_{2 \times 2} \\ \Delta_H I_{2 \times 2} & H^b_{i} \end{pmatrix}.
$$

Diagonalizing $\tilde{H}_1$ directly, we obtain four bands:

$$
E_1(q) = v_0 q_1 + \sqrt{\Delta_1^2 + \Delta_1^2 + 2\Delta_1^2 q_1^2 + 2q_1^2 v_1^2 + 2q_2^2 v_2^2 + \sqrt{(\Delta_1^2 - \Delta_1^2)^2 + 4[(\Delta_1^2 + \Delta_1^2)^2 + 4v_1^2 q_1^2 + 4v_2^2 q_2^2]}},
$$

$$
E_2(q) = v_0 q_1 + \sqrt{\Delta_1^2 + \Delta_1^2 + 2\Delta_1^2 q_1^2 + 2q_1^2 v_1^2 + 2q_2^2 v_2^2 - \sqrt{(\Delta_1^2 - \Delta_1^2)^2 + 4[(\Delta_1^2 + \Delta_1^2)^2 + 4v_1^2 q_1^2 + 4v_2^2 q_2^2]}},
$$

$$
E_3(q) = v_0 q_1 - \sqrt{\Delta_1^2 + \Delta_1^2 + 2\Delta_1^2 q_1^2 + 2q_1^2 v_1^2 + 2q_2^2 v_2^2 - \sqrt{(\Delta_1^2 - \Delta_1^2)^2 + 4[(\Delta_1^2 + \Delta_1^2)^2 + 4v_1^2 q_1^2 + 4v_2^2 q_2^2]}},
$$

$$
E_4(q) = v_0 q_1 - \sqrt{\Delta_1^2 + \Delta_1^2 + 2\Delta_1^2 q_1^2 + 2q_1^2 v_1^2 + 2q_2^2 v_2^2 + \sqrt{(\Delta_1^2 - \Delta_1^2)^2 + 4[(\Delta_1^2 + \Delta_1^2)^2 + 4v_1^2 q_1^2 + 4v_2^2 q_2^2]}},
$$

Straightforward algebraic work shows that the only solution for $E_2(q) = E_3(q)$, i.e., a gap-closing point, exists at $q_1 = q_2 = 0$ when $|\Delta_H| = \sqrt{\Delta_1^2 \Delta_1^2}$.

Parallel discussion for $D_{2,1',2'}$ proceeds and we conclude that a topological phase transition happens when

$$
|\Delta_H| = \sqrt{\Delta_1^2 \Delta_1^2},
$$

whereas the Chern number contributed by the cone at $D_i$ changes from $\pm 1$, depending on the sign of $\Delta_1^2 \Delta_1^2$, to zero. Mark that on the right hand side of equation (13), if $\Delta_1^2 \Delta_1^2 < 0$, the transition cannot happen at any $\Delta_H$.

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