The Bulk-Hinge Correspondence and Three-Dimensional Quantum Anomalous Hall Effect in Second Order Topological Insulators

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The chiral hinge modes are the key feature of a second order topological insulator in three dimensions. Here we propose a quadrupole index in combination of a slab Chern number in the bulk to characterize the flowing pattern of chiral hinge modes along the hinges at the intersection of the surfaces of a sample. We further utilize the topological field theory to demonstrate the correspondent connection of the chiral hinge modes to the quadrupole index and the slab Chern number, and present a picture of three-dimensional quantum anomalous Hall effect as a consequence of chiral hinge modes. The two bulk topological invariants can be measured in electric transport and magneto-optical experiments. In this way we establish the bulk-hinge correspondence in a three-dimensional second order topological insulator.

Figure 1. Illustration of selected patterns of chiral hinge modes and their projection in a second order topological insulator in three dimensions. (a) A double-loop pattern with the quadrupole indices \( \Delta_{xy} = -\Delta_{xx} = 1 \) and \( \Delta_{yz} = 0 \) and the slab Chern number \( n_x = n_y = n_z = 0 \). (b) A single-loop pattern with \( \Delta_{xy} = 1 \) and \( \Delta_{yz} = \Delta_{xz} = 0 \) and \( n_x = n_y = 0 \) and \( n_z = -1 \). (c) A single-loop pattern with \( \Delta_{xy} = \Delta_{yz} = \Delta_{xz} = 0 \) and \( n_x = n_y = -n_z = 1 \).

demonstrate the correspondent connection of the CHMs to the quadrupole index and the slab Chern number by means of topological field theory. Finally we propose to utilize magneto-optical Faraday and Kerr effects to detect these topological invariants.

Model Hamiltonian and symmetry analysis We start with a minimal four-band Hamiltonian, \( \mathcal{H} = \mathcal{H}_0 + \sum_{i=1}^{3} V_i \), which consists of four parts. The first part is

\[
\mathcal{H}_0 = \hbar \sigma_z [v_1 (k_x s_x + k_y^2) s_y + v_2 k_z s_z] + [m_0 + m_1 (k_x^2 + k_y^2) + m_2 k_z^2] \sigma_z s_0
\]

(1)

where \( k_x, k_y, k_z \) are the wave vectors, \( m_i \) and \( v_i \) are model parameters. \( \sigma \) and \( \sigma \) are the Pauli matrices acting in spin and orbital space, respectively. \( \mathcal{H}_0 \) possesses the time reversal symmetry \( T \) \( (T^2 = -1) \) and belongs to the symplectic symmetry class AII. Here we focus on the case of both \( m_0 m_2 < 0 \) and \( m_0 k_z = 0 \) such that \( \mathcal{H}_0 \) describes a 3D strong topological insulator with gapless Dirac cone of the surface states at all surfaces \( \mathcal{H} \). \( \mathcal{H}_0 \) also respects the global chiral symmetry \( C = \sigma_y s_0 \), \( \{ C, \mathcal{H}_0 \} = 0 \). Including the crystalline symmetries, the total point symmetry group is \( G_0 = D_{sh} \times \{ 1, T, P, C \} \) with the particle-hole symmetry \( P \equiv CT^{-1} \). As shown below all the terms in \( \mathcal{H} \) preserve \( P \), it is more

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convenient to rewrite $\mathcal{G}_0$ as $\mathcal{G}_0 = s_{\mathbf{t}}0 \times \{1, \mathcal{P}\}$ with the magnetic group $\mathcal{G}_0 = D_{4h} \times \{1, \mathcal{T}\} = D_{4h} \oplus \mathcal{T}D_{4h}$ (or $4/mnm\). \mathcal{V}_1 = c(k^2 - y^2)\sigma_{x} \sigma_{y}$ breaks the time reversal symmetry $\mathcal{T}$. The presence of $\mathcal{V}_1$ reduces magnetic group to $\mathcal{G}' = D_{2d} \oplus \mathcal{T}(D_{4h} - D_{2d})$. The term proportional to $c$ opens an gap with opposite sign for the surface states on the neighboring surfaces parallel to $z$ axis and the CHMs may be localized at their intersections. The CHMs are protected by the combination of four fold rotational symmetries and time-reversal symmetry $\mathcal{R}^2 \mathcal{T}$. The surface states on the bottom (001) and top (001) surface remain gapless. $\mathcal{V}_2 = \mathcal{d}s_{y} \sigma_{x}$ and $\mathcal{V}_3 = \sum_{i=x,y,z} b_{i}s_{i}$ is the magnetic Zeeman interaction. The two terms $\mathcal{d}s_{y} \sigma_{x}$ and $b_{i}s_{i}$ anticommute with the linear terms $h\nu_{z}(k_x \sigma_{x} s_{y} + k_y \sigma_{y} s_{y})$ along $x$ and $y$ directions. Thus they act as the mass terms and gap out the surface states on (001) and (001) while being projected onto the x-y surface. Since both of them commute with the mass term $\mathcal{s}_{y} \sigma_{x}$, so they only modifies the mass term for the surface states parallel with the $z$-axis and have no influences on the four hinge states along the $z$ direction. When all the surface states are gapped out and the Fermi level is located in the surface band gap, the electrons can only propagate unidirectionally along the hinges shared by adjacent side surfaces due to time reversal symmetry breaking. However, with different parameters, the chiral hinge modes can exhibit distinctly different patterns. The presence of both $\mathcal{V}_{1}$ and $\mathcal{V}_{3}$ reduces the magnetic group to $\mathcal{G} = D_{2d} \oplus \mathcal{T}(D_{2h} - D_{2d})$. The term proportional to $d$ breaks both the time reversal $\mathcal{T}$ and inversion symmetry $\mathcal{I}$, respectively, but respects the antiunitary combination $\mathcal{IT}$ which means the fact that if one CHMs propagates along any hinge there must be another hinge state propagating in the same direction on its spatial inversion. Thus the CHMs may form two closed loops on the surfaces (100) and (100) as shown in Fig. 1(a). The relative sign between $c$ in $\mathcal{V}_{1}$ and $d$ in $\mathcal{V}_{3}$ will determine which surface the two hinge mode loops locate around.

The presence of both $\mathcal{V}_{1}$ and $\mathcal{V}_{3}$ with magnetic field in $z$ direction reduces the magnetic group to $\mathcal{G} = S_{4} \oplus \mathcal{T}(D_{2d} - S_{4})$. The term breaks the $\mathcal{IT}$ symmetry while preserving the $S_{4}$ symmetry which protects a single-loop CHMs wriggling around the bulk as shown in Fig. 1(b). The relative sign between $b$ and $c$ determines the wriggling way of the single-loop CHMs. Only in the presence of $\mathcal{V}_{3} = b \sum_{i=x,y,z} s_{i}$ that magnetic field points to (111) direction, the magnetic point group is $\mathcal{G} = C_{i} \oplus \mathcal{T}(C_{2h} - C_{i})$. Due to the presence of the inversion symmetry $\mathcal{I}$, the CHMs at the inversion symmetric hinges are propagating in the opposite directions, and form a closed loop as shown in Fig. 1(c). A detailed symmetry analysis can be found in Ref. [39].

**Quadrupole index and slab Chern number** In order to characterize the topological hinge modes, we introduce two topological invariants: the quadrupole index and slab Chern number. There are the CHMs along four hinges in the $z$ direction in the case of Figs. (a) and (b). The energy dispersions of the four hinge modes connect the conduction and valence bands, and cross at $k_z = 0$ (see Fig.S1 in [39]). For a specific $k_z$, $\mathcal{H}(k_z)$ can be viewed as a 2D system in the $x$-$y$ plane and there are four corner states. The existence of corner states can be characterized by the quadrupole moment $\mathbf{Q}$, which protects the corner charges. Thus we can introduce a quadrupole index,

$$ q_{xy}(k_z) = \frac{1}{2\pi} \text{Im} \log \left[ \text{Det}[U_{k_z}^\dagger Q_{xy} U_{k_z}] \right] \sqrt{\text{Det}Q_{xy}^\dagger} $$

where the matrix $U_{k_z}$ is constructed by the occupied lowest energy states, $Q_{xy} = e^{\pm i\pi \nu_{x} r_{y}/L_{x} L_{y}}$, $r_{y}$ are the position operators, and $L_{x}$ are the lengths of the system in the $x$ direction. Any anti-symmetry $\mathcal{O}_{a}$ leaves $xy$ plane invariant $\mathcal{O}_{a} \mathcal{H}(k_{z}) \mathcal{O}_{a}^{-1} = -\mathcal{H}(-k_{z})$ will put a constraint on the quadrupole moment $q_{xy}(k_{z})$: $q_{xy}(k_{z}) + q_{xy}(-k_{z}) = 0 \text{ or } 1$. At two high symmetry points $k_{z} = 0 \text{ or } \pi$, the symmetry is restored, $\mathcal{O}_{a} \mathcal{H}(k_{z}) \mathcal{O}_{a}^{-1} = -\mathcal{H}(k_{z})$, and $q_{xy}(k_{z})$ must be quantized to 0 or $\frac{1}{2}$ (see Ref. [39]). Non-zero quantized $q_{xy}(k_{z})$ indicates the system topologically nontrivial and the existence of four zero-energy corner states in the reduced 2D subspace. For example, if $q_{xy}(k_{z} = 0) = 1/2$, then $q_{xy}(\pm \pi) = 0 \text{ or } 1$. In this case, there exist CHMs which compensate for the difference of the corner charges. Thus we can introduce a quadrupole index,

$$ \Delta_{xy} = \int_{0}^{2\pi} dk_{z} \partial_{k_{z}} q_{xy}(k_{z}) \tag{2} $$

to characterize the existence and the flowing direction of four CHMs. For the double-loop case in Fig. (a), we have $\Delta_{xy} = -\Delta_{yx} = 1$ and $\Delta_{yz} = 0$, which are protected by the combination of chiral symmetry and the mirror symmetry $\mathcal{C} \mathcal{M}_{a}$ and the combination of chiral symmetry and the time reversal symmetry $\mathcal{C} \mathcal{T}$. For the single-loop case in Fig. (b), we have $\Delta_{xy} = 1$ and $\Delta_{yz} = \Delta_{xz} = 0$. The quadrupole index along the $z$ direction is protected only by $\mathcal{C} \mathcal{T}$ and along the $x \text{ (y)}$ direction is protected by both $\mathcal{C} \mathcal{M}_{a}$ and $\mathcal{C} \mathcal{T}$. For the case in Fig. (c), $\Delta_{xy} = \Delta_{yz} = \Delta_{xz} = 0$.

The slab Chern number is another topological invariant as the quadrupole index alone are not enough to characterize the diversity of the flowing pattern of the CHMs. Consider a slab geometry of the sample with a finite thickness $L_{z}$ with the periodic boundary condition along the $x$ and $y$ direction. Denote the Bloch eigenstates by $|u_{n}(k_{\perp}, z)\rangle$ are the Bloch eigenstates, $\mathcal{H}(k_{\perp}, z)|u_{n}(k_{\perp}, z)\rangle = \varepsilon_{n}(k_{\perp})|u_{n}(k_{\perp}, z)\rangle$ with $k_{\perp} = (k_{x}, k_{y})$ and the index $n$ for the bands. The space-resolved Berry connection is given by $\mathcal{A}_{m,n}(k_{\perp}, z) = -i \langle u_{n}(k_{\perp}, z)|\partial_{z}|u_{m}(k_{\perp}, z)\rangle$ for the two occupied bands $n, m$. In this way we define the slab Hall conductance and its relation to a slab Chern number $n_{z}$ [33].

$$ \sigma_{xy}^{\text{slab}} = \int_{0}^{L_{z}} dz \varepsilon_{xy}(z) = n_{z} \frac{e^{2}}{h} \tag{3} $$
where \( \sigma_{xy}(z) = \frac{e^2}{2\pi^2} \int d^2k \text{Tr}[\mathcal{F}_{xy}(k_z, z)] \) and \( \mathcal{F}_{xy}(k_z, z) \) is the non-Abelian Berry curvature in terms of \( A_{\sigma_n n'}(k_z, z) \). Because of the periodicity of the Berry connection in the first Brillouin zone, it can be proved that the slab Chern number \( n_z \) is quantized if the filled bands has a band gap to the excited states for a band insulator. According to the bulk-boundary correspondence [5], each non-zero Chern number is associated with the closed loop of chiral edge state. In Fig. 1(a), \( n_x = n_y = n_z = 0 \), while two quadrupole indices are not vanishing \( \Delta_{xy} = -\Delta_{zx} = 1 \). The system in a slab geometry (the open boundary condition is imposed in the \( z \) direction) is analogue to the quantum spin Hall insulator except the the two counter-propagating hinges modes are localized on the opposite sides. Experimentally, the quantized anomalous Hall effect can be measured by using the surface-sensitive method [43]. In Fig. 1(b), \( n_z = -1 \) and \( n_x = n_y = 0 \). There is a closed loop of chiral edge mode around the \( z \) axis. Combined with the non-zero quadrupole index \( \Delta_{xy} = 1 \), there are four CHMs along the four hinges along the \( z \) axis, the two indices can determine that a single-loop of CHMs that wriggles around the bulk. QAHE can be detected through a global quantum Hall measurement probing the whole sample due to the nonzero \( n_z \). In Fig. 1(c), \( n_x = n_y = -n_z = 1 \). There is a single loop of chiral edge mode around each axis. Because of the zero quadrupole indices around the three axis, there is no four CHMs along one direction. It exhibits a single CHM traversing half of its hinges, which can be projected out a single closed loop in the direction of \( x, y \) and \( z \). The QAHE can be observed for three directions due to the non vanishing slab Chern numbers.

3D QAHE The CHMs can be further understood in the framework of topological field theory with an effective action [44],

\[
S = \int d^3r dt \left[ \frac{1}{8\pi} \left( \epsilon E^2 - \frac{1}{\mu} B^2 \right) + \frac{\theta(r, t) e^2}{4\pi^2 \hbar c} \mathbf{E} \cdot \mathbf{B} \right],
\]

where \( \mathbf{E} \) and \( \mathbf{B} \) are the electromagnetic fields, \( \epsilon \) and \( \mu \) are the dielectric constant and magnetic permeability, respectively. \( \theta(r, t) \) is known as the axion angle [45]. The product \( \mathbf{E} \cdot \mathbf{B} \) is odd under the time reversal or spatial inversion, \( \theta \) has to be 0 (modulo \( 2\pi \)) for a trivial insulator and the vacuum and \( \pi \) for a topological insulator with respect to the symmetries [43, 46, 47]. In the quadratic order of electric and magnetic fields, besides the Maxwell term, the \( \theta \) term may give rise to the topologically magnetoelectric effect that an electric field can induce a magnetic field and vice versa [48, 50, 52]. By taking the functional derivative of \( \theta \) term with respect to a gauge field, the induced electric current density depends on the spatial and temporal gradients of the \( \theta \)-field [44, 45],

\[
j_\theta(r, t) = \frac{e^2}{2\pi \hbar} \left[ \partial_t \theta(r, t) \mathbf{B} - \nabla \theta(r, t) \times \mathbf{E} \right].
\]

The first term depends on the temporal gradient of the \( \theta \)-field and is proportional to magnetic field, i.e., the so-called chiral magnetic field, and vanishes in a static limit. The second term depends spatial gradient of the \( \theta \)-field and is perpendicular to the electric field, i.e., the anomalous Hall effect. Thus there will be surface anomalous Hall effect at the interface between two regions with different \( \theta \) values and no Hall response will exist in the bulk as \( \theta \) takes a constant value \( \theta_b \) [53, 54]. The value of \( \theta_b \) is given by the three-dimensional integration of the Chern-Simons 3-form over momentum space [53, 56]. In addition to the inversion or time-reversal symmetry, \( \theta_b \) will be quantized with improper rotation symmetries or a combination of time-reversal symmetry and proper rotation symmetries [39, 57]. From Eq. (4), the layer-resolved Hall conductivities in the \( xy \) plane is associated with the gradient of \( \theta \), \( \sigma_{xy}(z) = \frac{e^2}{\pi \hbar} \partial_z \theta(z) \). Thus the slab Hall conductance [49] is given by the difference of the \( \theta \) values of bottom and top vacuum \( \sigma_{xy}^{\text{slab}} = \frac{2}{\pi \hbar} [\theta_b - \theta_b(0)] \), which is integer-quantized independent of the \( \theta \) value of the bulk.

Relation between the \( \theta \) term and the chiral hinge modes

The current carried by the CHMs can be evaluated from the spatial dependent \( \theta \), and each chiral hinge channel carries one conductance quantum \((e^2/h)\). We calculate the current through a 2D section disk \((D)\) encircling a
hinge normal to the plane as illustrated in Fig. 2(a), \( \int d\mathbf{S} \cdot \mathbf{j}_\mathbf{p} \). The electric field is determined by the gradient of a scalar potential, \( \mathbf{E} = -\nabla \Phi(\mathbf{r}) \), and we choose the boundary of the disk as an equipotential line \( \Phi_0 \).

By utilizing Stokes theorem, \( \int = \frac{e^2}{2\pi} \int \mathbf{C} \cdot \nabla \theta(\mathbf{r}) \Phi(\mathbf{r}) \).

Thus there is no current or equivalently gapless conducting channel on the hinge when \( \theta(\mathbf{r}) \) in the two vacuum areas takes the same value \( n_1 = n_2 \). If they are different \( n_1 \neq n_2 \), there will be a branch cut separating the two vacuums where \( \theta(\mathbf{r}) \) is singular. In this situation, the contour integral gives the number of the conducting channels \( I/(\Delta \Phi e^2/h) = n_2 - n_1 \) which is the winding number of the field \( \theta(\mathbf{r}) \). \( \Delta \Phi = \Phi_e - \Phi_{in} \) denotes the potential difference between the outer contour \( C_{out} \) and the inner contour \( C_{int} \). In other words, the gapless hinge modes track the singularity of the \( \theta \) term and vice versa.

We also want to emphasize that, even when \( \theta \) in the bulk is not quantized, the above argument for the gapless chiral hinge channel is still valid.

As shown in Fig. 2 (c-f), we plot the layer-resolved Hall responses \( \sigma_{\alpha\beta}(r_\gamma) \) (\( \epsilon_{\alpha\beta\gamma} = 1 \)) and the integrated value for \( \theta(r_\gamma) \) as a function of the layer index for three directions. In numerical evaluation, we consider a slab geometry with the periodic boundary in the \( \alpha \beta \) plane and open boundary condition in \( r_\gamma \) direction. The layer resolved Hall response only distributes near the slab surfaces where \( \theta \) changes and quickly drops to zero as the position moves into the bulk where \( \theta \) takes constant value. For the double-loop case in Fig. 2 (c) and (e), the magnetic point group \( \mathcal{G}_1 \) put a constraint on the Hall response that the layer-resolved Hall conductivity takes the opposite values for the slab center. Thus the slab Chern numbers vanish for three directions. Due to the presence of the mass term \( \delta \), the axion angle will deviate from \( \pi \), for example, \( \theta/2\pi \approx -0.59 \) in Fig. 2 (e). It is also consistent with the symmetry analysis that there is no such symmetry to guarantee the quantization \( \theta_\theta \) in \( \mathcal{G}_1 \). As a consequence, the surface Hall conductance \( \sigma_{xy}^p = \frac{e^2}{2\pi} (n_2^B - n_2^B) \) for the bottom interface and \( \sigma_{xy}^T = \frac{e^2}{2\pi} (n_2^T - n_2^T) \) for the top interface are not half quantized in sharp contrast to the axion insulators. However, the summation of the surface Hall conductance of the adjacent surface must be quantized since \( \sigma_{ix}^T + \sigma_{iy}^y = \frac{e^2}{2\pi} (n_3^T - n_3^T) \) with \( i, j = T, B \), indicates whether the hinge mode at the intersection of two surfaces exists or not.

For the single-loop case, the symmetry \( \mathcal{G}_2 \) constrains that the layer-resolved Hall conductivities for \( z \) direction are symmetric about the slab center, while for \( x \) and \( y \) directions are antisymmetric about the slab center. The layer-resolved Hall conductivities in \( xx \) plane and \( yz \) plane are also related to each other by the \( S_4 \) symmetry. Furthermore, \( \theta_\theta \) will be quantized due to the presence of improper rotation symmetry \( S_4 \) and a combination of time-reversal and the diagonal mirror symmetry \( \mathcal{T} \mathcal{M}^{x+y} \). As a result, the surface Hall conductance are half-quantized for three directions. In this way, we establish the relation between the the CHMs and the two physical invariants, \( \sigma_{\alpha\beta} = \frac{e^2}{2\pi} (n_1^T - n_1^T) \) and \( \Delta_{\alpha\beta} = \delta_{n_1^T} n_2^B \delta_{n_2^B} (n_3^T - n_3^T) \) with \( \epsilon_{\alpha\beta\gamma} = 1 \).

**Magneto-optical effect as a detection of topological invariants**

Consider a normally incident linearly polarized light with frequency \( \omega \) propagating along the \( z \) direction through the sample \( E_{\text{in}} = E_{\text{in}} \exp[i(k_{0z}z - \omega t)] \) with \( k_0 = \omega/c \). \( E_r \) and \( E_i \) are the reflected and transmitted electric field, respectively. Their values at the interface between two materials are related to the incident field \( E_{\text{in}} \) by the \( 2 \times 2 \) reflection and transmission tensors, and can be solved by matching the electrodynamic boundary conditions. The Kerr and Faraday angles are defined by the \( \tan \theta_F = -E_r^T/E_r^T \) and \( \tan \theta_K = E_r^T/E_i^T \), respectively [48, 49]. When the chemical potential is located within the surface gap \( E_g \) and \( \hbar \omega \ll E_g \), the magnetic fields at the interface of the two materials are discontinuous due to the presence of surface Hall current. The reflection and transmission tensors for a slab can be obtained by composing the single-interface scattering matrices for top and bottom surfaces. For simplicity, we only consider a free-standing sample, the influence of a substrate do not change our conclusion qualitatively. The reflectivity \( R = |E_r|^2/|E_i|^2 \) will depend on the relative magnitude of the slab thickness and the wavelength \( \lambda_0 = \frac{2\pi}{\omega \sqrt{\mu_0}} \) inside the bulk. When the slab thickness contains an integer multiple of half wavelength \( L_z = N\lambda_0/2 \) with an integer \( N \) (the resonance condition), \( R \) reaches the minima. At the resonance, the Faraday \( \theta_F \) and Kerr \( \theta_K \) rotations have the same universal quantized value [48, 50]. \( \tan \theta_F = \cot \theta_K = \alpha (n_1^B - n_1^T) \), where \( \alpha = \frac{\pi}{2\sqrt{\mu_0c}} \) the fine structure constant. At the resonance, the difference of \( \theta \) values between the top and bottom vacuum can be obtained irrespective of the specific value of \( \theta_0 \). In order to determine \( n_1^T - n_1^T \) and \( n_1^B - n_1^B \) for top and bottom surface, we also need to use the results at reflectivity maxima when \( L_z = (N + \frac{1}{2})\lambda_0/2 \). The measured Faraday angle \( \theta_F \) and Kerr angle \( \theta_K \) give a relation...
\[ \tan(\theta_K^* + \theta_K^0) \left( 1 - \frac{\tan \theta_K^0}{\tan \theta_K^*} \right) = \alpha(n_z^T + n_z^B - \theta_k) \pi. \]

Using the two relations, we can determine the values of the quadrupole indices and the slab Chern numbers. In short, the quadrupole index in combination with the slab Chern number can determine the flowing pattern of the quadrupole indices and the slab Chern numbers.

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