Quantized Electromagnetic Response of Three Dimensional Chiral Topological Insulators

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Protected by the chiral symmetry, three dimensional chiral topological insulators are characterized by an integer-valued topological invariant. How this invariant could emerge in physical observables is an important question. Here we show that the magneto-electric polarization can identify the integer-valued invariant if we gap the system without a quantum Hall layer on the surface. The quantized response is demonstrated to be robust against weak perturbations. We also study the topological properties by adiabatically coupling two nontrivial phases, and find that gapless states appear and are localized at the boundary region.

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The periodic table of topological insulators (TIs) and superconductors classifies topological phases of free fermions according to the system symmetry and spatial dimensions [1, 2]. Notable examples include integer quantum Hall insulators breaking all those classification symmetries and the time-reversal-invariant TIs protected by the time-reversal symmetry [3, 4]. Mathematically, these exotic states can be characterized by various topological invariants. An interesting question is how to relate these invariants to physical observables. For integer quantum Hall insulators, the Chern number (Z invariant) corresponds to the quantized Hall conductance [5], while for the time-reversal-invariant TIs, the Z_2 invariant is associated with a quantized magneto-electric effect in three dimensions (3D) [6, 7].

The 3D chiral TIs protected by the chiral symmetry [8, 9] are of particular interest as they are 3D TIs characterized by a Z (instead of Z_2) invariant and may be realized in ultracold atomic gases with engineered spin-orbital coupling [10]. An experimental scheme was recently proposed to implement a three-band chiral TI in an optical lattice [11]. For such 3D chiral TIs, it is known that the topological magneto-electric effect should also arise, but in theory it captures only the Z_2 part of the Z invariant due to the gauge dependence of the polarization in translationally invariant systems [8]. It is thus an important question to find out how the Z character could manifest itself in experiments. It was proposed in Ref. [12] that the Z effect may become visible in certain carefully engineered heterostructures, but the implementation of such a heterostructure is experimentally challenging.

In this paper, we study the nontrivial Z character of the chiral TI by exploring the adiabatic transition between two nontrivial phases and by numerically simulating the magneto-electric effect. We show that not only the Z_2 response but the Z character can be observed by gapping the system without adding a quantum Hall layer on the surface, i.e., the ambiguity resulting from different terminations appears to be avoidable in practice. Also, the quantized polarization is demonstrated to be robust against small perturbations even in the absence of a perfect chiral symmetry. This observation is important for experimental realization, because in a real system the chiral symmetry is typically an approximate instead of exact symmetry. We briefly discuss detection of such an effect in the context of cold atom systems, which have the possibility to measure such integrally quantized responses.

First, we introduce a minimal lattice tight-binding model for chiral topological insulators with the Hamiltonian in the momentum space given by $H_1 = \sum_{k} \Psi_k^\dagger H_1(k) \Psi_k$, where $\Psi_k = (a_{k\uparrow}, a_{k\downarrow}, b_{k\uparrow}, b_{k\downarrow})^T$ denotes fermionic annihilation operators with spins $\uparrow, \downarrow$ on sublattices or orbitals $a, b$. In cold atom systems, the pseudospins and sublattices can be represented by different atomic internal states. The $4 \times 4$ Hamiltonian is

$$
H_1(k) = \begin{pmatrix}
0 & 0 & -iq_0 + q_3 & q_1 - iq_2 \\
0 & 0 & q_1 + iq_2 & -iq_0 - q_3 \\
(iq_0 + q_3 & q_1 + iq_2 & 0 & 0) \\
(q_1 - iq_2 & iq_0 - q_3 & 0 & 0)
\end{pmatrix}
$$

where $q_0 = h + \cos k_x + \cos k_y + \cos k_z, q_1 = \sin k_x + \delta, q_2 = \sin k_y, q_3 = \sin k_z$, with $h, \delta$ being control parameters. The lattice constant and tunneling energy are set to unity. In real space, this Hamiltonian represents onsite and nearest neighbor hoppings and spin-flip hoppings between two orbitals. These hoppings can be realized by two-photon Raman transitions in cold atoms [11, 12]. The energy spectrum for this Hamiltonian is $E_{\pm}(k) = \pm((\sin k_x + \delta)^2 + \sin^2 k_y + \sin^2 k_z + (\cos k_x + \cos k_y + \cos k_z + h)^2)^{1/2}$, with two-fold degeneracy at each $k$. For $\delta = 0$, the system acquires time-reversal symmetry $T$, particle-hole symmetry $C$, and chiral symmetry...
FIG. 1. The winding number $\Gamma$ as a function of the parameter $h$. The Hamiltonians are $H_1(k)$ in (a) and $H_2(k)$ in (b) respectively. $\delta = 0.5$ for both panels.

$S = TC$, which can be explicitly seen as [9]:

$$
T : \quad \langle \sigma_x \otimes \sigma_y \rangle [H_1(k)]^* \langle \sigma_x \otimes \sigma_y \rangle = H_1(-k)
$$

(1)

$$
C : \quad \langle \sigma_y \otimes \sigma_y \rangle [H_1(k)]^* \langle \sigma_y \otimes \sigma_y \rangle = -H_1(-k)
$$

(2)

$$
S : \quad \langle \sigma_z \otimes I_2 \rangle [H_1(k)] \langle \sigma_z \otimes I_2 \rangle = -H_1(k)
$$

(3)

with $\sigma_i$ as Pauli matrices, and $I_2$ as the $2 \times 2$ identity matrix. When $\delta \neq 0$, time-reversal and particle-hole symmetries are explicitly broken, but the chiral symmetry survives.

With the Hamiltonian $H_1(k)$, one can define the $Q$ matrix, $Q(k) = 1 - 2P(k)$, where $P(k) = \sum_j \langle u_f(k) | u_j(k) \rangle | u_f(k) \rangle$ is the projector onto the filled Bloch bands with wavevectors $|u_f(k)\rangle$. The $Q$ matrix can be brought into the block off-diagonal form $Q(k) = \begin{pmatrix} 0 & b(k) \\ b(k)' & 0 \end{pmatrix}$ with the chiral symmetry. The topological property of the Hamiltonian can thus be characterized by the winding number [1, 9]:

$$
\Gamma = \frac{1}{24\pi^2} \int_{BZ} \mathbf{k} \epsilon^{\mu \rho \lambda} \text{Tr}[(b^{-1} \partial_{\mu} b)(b^{-1} \partial_{\rho} b)(b^{-1} \partial_{\lambda} b)],
$$

where $\epsilon^{\mu \rho \lambda}$ is the antisymmetric Levi-Civita symbol and $\partial_{\mu} b \equiv \partial_{\mu} b(k)$. The Hamiltonian $H_1(k)$ supports topological phases with $\Gamma = 1, -2$. To obtain chiral TIs with arbitrary integer topological invariants, one can use the quaternion construction proposed in Ref. [14]. By considering $q = q_0 + q_1 i + q_2 j + q_3 k$ as a quaternion and raising to a power, all Z topological phases can be realized by the family of tight-binding Hamiltonians. By taking the quaternion square for example, one obtains $q^2 = q_0^2 - q_1^2 - q_2^2 - q_3^2 + 2q_0 q_1 i + 2q_0 q_2 j + 2q_0 q_3 k$, and we can therefore acquire another tight-binding Hamiltonian $H_2 = \sum_k \Psi_k^\dagger H_2(k) \Psi_k$ with each component of $q^2$ replacing the respective components $q_0, q_1, q_2, q_3$ in $H_1(k)$. This second Hamiltonian $H_2(k)$ contains next-nearest-neighbor hopping terms. The winding number $\Gamma$ can be calculated numerically, which is shown in Fig. 1 for both $H_1(k)$ and $H_2(k)$.

By imposing an open boundary condition along the $z$ direction, and keeping the $x$ and $y$ directions in momentum space, surface Dirac cones are formed for nontrivial topological phases. We find that the winding number coincides with the total number of Dirac cones counted for all inequivalent surface states (i.e. not counting the 2-fold degeneracy for each band), which confirms explicitly the bulk-edge correspondence [15]. A distinctive difference from the time-reversal invariant TI is that any number of Dirac cones on the surface is protected by the chiral symmetry [8].

With an integer number of nontrivial phases, it is intriguing to study the topological phase transition between two different phases. A simple way to explore this is to adiabatically vary $h$ from one end to the other end of the sample. The parameter $h$ concerns the onsite tunneling strength between opposite orbitals ($a_i^\dagger b_j$ and $a_j^\dagger b_i$ terms). This hopping can be realized by a two-photon Raman process, and the strength $h$ can be controlled by the laser intensity [11]. Numerically, we vary $h$ in the form of $h = 1 + \tan h(z - L_z/2)$, where $z$ denotes the $z$th layer and $L_z$ the total number of slabs along the $z$ direction. This form ensures that $h$ changes adiabatically from 0 on one end to 2 on the other end of the sample, so that it effectively couples two nontrivial phases. For the Hamiltonian $H_1$, it couples two topological phases with winding numbers $\Gamma = -2$ and $\Gamma = 1$. Similar to the interface between a topological insulator and the trivial vacuum, a surface state should appear at the interface. As shown in Fig. 2, three Dirac cones are formed inside the band gap. In addition to the surface states observed on both ends of the sample, a localized state is formed at the interface between two topologically distinct regions. These interface states are always present regardless of the detailed structure of the interface. Even for sharp boundaries, the interface states remain. The Dirac cone structure may be probed through Bragg spectroscopy in cold atom experiments [16].
A remarkable manifestation of the bulk non-trivial topology is the magneto-electric effect. The linear response of a TI to an electromagnetic field can be described by the magneto-electric polarizability tensor as

\[
\alpha_{ij} = \frac{\partial P_i}{\partial B_j} \bigg|_{E=0} = \frac{\partial M_j}{\partial E_i} \bigg|_{B=0},
\]

where \(E\) and \(B\) are the electric and magnetic field, \(P\) and \(M\) are the polarization and magnetization [7]. Unique to topological insulators is a diagonal contribution to the tensor with \(\alpha_{ij} = \theta \frac{e^2}{2\pi \hbar} \delta_{ij}\). This is a peculiar phenomenon as an electric polarization is induced when a magnetic field is applied along the same direction [6]. This effect can be described by a low-energy effective field theory in the Lagrangian as \((c=1)\)

\[
\Delta \mathcal{L} = \theta \frac{e^2}{2\pi \hbar} \mathbf{B} \cdot \mathbf{E}
\]

known as the “axion electrodynamics” term [7]. For time-reversal invariant TIs, an equivalent understanding will be a surface Hall conductivity induced by the bulk magneto-electric coupling. When the time-reversal symmetry is broken on the surface generating an insulator, a quantized surface Hall conductance will be produced:

\[
\sigma_H = \frac{\theta \frac{e^2}{2\pi \hbar}}{2}\]

where \(\theta\) is quantized to be 0 or \(\pi\) to preserve the time-reversal invariance [6]. \(\theta = \pi\) corresponds to the non-trivial time-reversal invariant TI with a fractional quantum Hall conductivity. The electric polarization can be understood with Laughlin’s flux insertion argument [17].

A changing magnetic field through the insulator induces an electric field (by Faraday’s law), which together with the quantized Hall conductivity will produce a transverse current and accumulate charge around the magnetic flux tube at a rate proportional to \(\sigma_H\) as \(Q = \sigma_H \Phi\) [18].

Theoretically, chiral TIs are also predicted to have this topological magneto-electric effect [8, 9]. The field theory only captures the \(Z_2\) part of the integer winding number due to the \(2\pi\) periodicity of \(\theta\) associated with a gauge freedom in transitionally invariant systems. However, we numerically show that the \(Z\) character can actually be observed by gapping the system without adding a strong surface orbital magnetic field. Apparently, this corresponds to a particular gauge such that the \(Z\) character can be distilled from the polarization. More concretely, we consider the chiral TI represented by both Hamiltonians \(\mathcal{H}_1(\mathbf{k})\) and \(\mathcal{H}_2(\mathbf{k})\). A uniform magnetic field is inserted through the chiral TI sample via the Landau gauge \(\mathbf{A} = Bx\hat{y}\) with a minimal coupling by replacing \(k_y\) with \(k_y - \frac{e}{\hbar} Bx\). We keep \(x\) and \(y\) directions in momentum space, and the \(z\) direction in real space with open boundaries and \(L_z\) slabs. By taking a magnetic unit cell with \(N\) sites along the \(x\) direction, the Hamiltonian can be partially Fourier transformed to be a \(4L_z \times N\) matrix for each \(k_x\) and \(k_y\), with 4 taking into account of spins \(\uparrow, \downarrow\) and orbitals \(a, b\). For a unit magnetic cell with \(N\) lattice cells, the total magnetic flux through the unit cell is quantized to be integer multiples of a full flux quantum \(\Phi = n\Phi_0 = n\frac{\hbar}{e}\) due to the periodic boundary condition along the \(x\) direction, so the flux through a single lattice plaquette is quantized to be \(\Phi/N\). In the weak magnetic field limit, one needs to take a large \(N\). Besides the bulk Hamiltonian \(\mathcal{H}_1(\mathbf{k})\) or \(\mathcal{H}_2(\mathbf{k})\), we also add a surface term to break the chiral symmetry and open a gap on the surface,

\[
H_S = \Delta_S \sum_{k_x, k_y} \sum_{j \in \text{surf}} \mathbf{\hat{S}} \cdot \mathbf{\hat{z}} \left( \psi^\dagger_{j,k_x,k_y} (I_2 \otimes \sigma_z) \psi_{j,k_x,k_y} \right),
\]
where \( \mathbf{\hat{S}} \) represents the unit vector perpendicular to the surface along \( z \) direction, so \( \mathbf{\hat{S}} \cdot \mathbf{\hat{z}} = 1 \) for the upper surface, and \( \mathbf{\hat{S}} \cdot \mathbf{\hat{z}} = -1 \) for the lower surface. This term represents a surface magnetization with a Zeeman coupling, creating a different chemical potential for spins \( \uparrow \) and \( \downarrow \). It can be directly verified that this surface term breaks the chiral symmetry \( S \) in Eqn. (3).

As the surface becomes gapped, at half filling, an increasing uniform magnetic field accumulates charges on the surface via the magneto-electric coupling. In the weak magnetic field limit, the charge accumulated on the surface is proportional to \( \sigma_H \) as

\[
Q = \sigma_H \Phi = \frac{\theta}{2\pi} n e. \tag{8}
\]

A priori, \( \theta \) needs not be quantized. However, analogous to the role played by time-reversal symmetry, chiral symmetry pins down \( \theta \) to be \( m\pi \) with an integer value \( m \) \([9]\). Conventionally, \( \theta \) should be periodic in \( 2\pi \). An intuitive picture is that the \( 2\pi m \) ambiguity results from the freedom to coat an integer quantum Hall layer on the surface, or equivalently to change the chemical potential and hence the Landau level occupancy of the surface in an orbital magnetic field. So the integer part depends on the details of the surface \([6, 7, 19]\). However, once a fixed surface Hamiltonian is defined, the adiabatic change in polarization associated with the increase in magnetic flux does have a physical meaning. This ambiguity can be avoided in cold atom systems, where the precise Hamiltonian can be engineered, allowing a direct link between the winding number \( \Gamma \) and the charge accumulation rate \( \theta/2\pi \).

Numerical results in Fig. 3 show that \( \Gamma = \theta/\pi \), which reveals that the magneto-electric polarization is a direct indication of the non-trivial bulk topological phase characterized by the integer winding number. To gain some intuition for why in our Hamiltonian the value \( \Gamma = \theta/\pi \) is observed, consider how a Zeeman term and an orbital magnetic term produce different quantum Hall effects for a Dirac fermion: the latter leads to Landau levels with a different chemical potential for spins \( \uparrow \) and \( \downarrow \). It can be seen from the phase of laser beams \([11, 13]\). The accumulated charge can be obtained from the atomic density measurements \([20]\).

In summary, we study the \( \mathbb{Z} \) character of chiral topological insulators by probing the topological phase transition between non-trivial phases and by simulating the quantized magneto-electric effect. We show that the \( \mathbb{Z} \) character, not only the \( \mathbb{Z}_2 \) part, can be observed through magneto-electric polarization by gapping the system without adding an integer quantum Hall layer. This demonstrates explicitly how the topological invariant appears in physical observables for chiral TIs and will be important for experimental characterization.

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**SUPPLEMENTAL MATERIAL: QUANTIZED ELECTROMAGNETIC RESPONSE OF THREE DIMENSIONAL CHIRAL TOPOLOGICAL INSULATORS**

In this supplemental material, we numerically establish the correspondence between the bulk topological index and the number of Dirac cones on the surface, and also investigate the effect of a strong surface orbital field to the quantized magneto-electric polarization.

### Bulk-edge correspondence

The bulk edge correspondence tells us that the bulk topological index should have a surface manifestation, typically through the number of gapless Dirac cones on the surface. This is generally verified for lower topological index, such as 1 or 2. By imposing an open boundary condition along the $z$ direction for chiral topological insulators of different index, we find that the winding number corresponds to the total number of Dirac cones counted for all inequivalent surface states (i.e. not counting degeneracies).

![Spectrum for the surface states showing the number of Dirac cones](image)

**FIG. 4.** Spectrum for the surface states showing the number of Dirac cones. The upper panels in (a) and (b) show the lowest conduction and highest valence band. The lower panels show the next two bands closest to the Fermi energy. (a) For $H_1(k)$, $h = 2, \delta = 0.5$ with winding number $\Gamma = 1$ and 1 Dirac cone. (b) For $H_2(k)$, $h = 0, \delta = 0$ with winding number $\Gamma = 4$ and 4 Dirac cones in total. The $\Gamma$ point is displaced from the center for better display of the Dirac cones.

Following Ref. [14] to take a quaternion power $n$, we can generalize the Hamiltonians in the main text from $H_1(k)$ and $H_2(k)$ to $H_n(k)$. For the Hamiltonian $H_1(k)$ (i.e. $n = 1$), when $h = 2$, the winding number $\Gamma = 1$ guarantees the existence of 1 Dirac cone [Fig. 4(a)]. For the Hamiltonian $H_2(k)$ (i.e. $n = 2$), when $h = 0$, the winding number is $\Gamma = 4$. So there are two inequivalent surface states on each surface with two Dirac cones each [Fig. 4(b)]. In general, we have

\[ n = m, 1 < |h| < 3, \Gamma = m \implies m \text{ inequivalent surface states with 1 Dirac cone each} \]

\[ n = m, -1 < h < 1, \Gamma = 2m \implies m \text{ inequivalent surface states with 2 Dirac cones each} . \]

These have been explicitly verified up to $n = 3$. Hence, the winding number $\Gamma$ does correspond to the total number of Dirac cones for all inequivalent surface states.
Surface orbital field and integer quantum Hall layers

The $2\pi$ periodicity of the $\theta$ term is mathematically related to the gauge freedom in the low-energy effective field theory. Physically, it is associated with the freedom to coat an integer quantum Hall layer on the surface, or equivalently to change the chemical potential and hence the Landau level occupancy of the surface in an orbital magnetic field. Here, we numerically verify this physical intuition. To do that, we consider a single layer of the Hamiltonian $\mathcal{H}_1(k)$, so the $z$ component drops out. A strong uniform orbital field is added to the layer via Peierls substitution with the Landau gauge $A = B x \hat{y}$, $B a^2 = \frac{1}{3} \Phi_0$, where $a$ is the lattice constant, and $\Phi_0$ is the flux quantum. For Hofstadter Hamiltonian, this strong orbital field will produce three gapped Landau levels. Here, a similar structure is developed as shown in Fig. 5(a). There are six bands with the middle two bands gapless. The extra number of bands are due to the spin and orbital degrees of freedom. On top of the strong uniform magnetic field, an additional weak flux tube is inserted through the center lattice. By Laughlin’s flux insertion argument, the charge accumulated around the flux tube should be $Q/e = C \Phi/\Phi_0$, where $C$ is the Chern number being an integer. Figure (b) and (c) [(d) and (e)] show the charge polarization at a chemical potential $\mu_1$ [$\mu_2$]. From the slope, we infer that the first band has a Chern number $C = 2$ and the second band has a Chern number $C = -4$. So by changing the surface chemical potential, we could modify the charge accumulation rate by an integer. Alternatively, in the absence of this strong orbital magnetic field, with a surface gapping term $H_S$ in Eqn. (7) of the main text, there is only one gap and no such integer quantum Hall layers. Therefore, the $\mathbb{Z}$ character of the winding number can be observed through such integrally quantized magneto-electric polarization measurements.

FIG. 5. (a) Energy spectrum for the one-layer Hamiltonian $\mathcal{H}_1(k)$ with a strong uniform magnetic field and unit cell flux as $\frac{1}{3} \Phi_0$. An additional weak flux tube is inserted through the center lattice cell of the layer, with flux up to $\Phi/\Phi_0 = 0.1$. (b) and (c) [(d) and (e)] corresponds to the charge polarization with respect to the increasing flux tube at a chemical potential $\mu_1$ [$\mu_2$]. Charge is accumulated around the flux tube, and by changing the chemical potential and hence the Landau level occupancy, the charge accumulation rate can be modified by an integer.