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Electromagnetic Response of Three-dimensional Topological Crystalline Insulators

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Topological crystalline insulators (TCI) are a new class of materials which have metallic surface states on select surfaces due to point group crystalline symmetries. In this letter, we consider a model for a three-dimensional (3D) topological crystalline insulator with Dirac nodes occurring on a surface that are protected by the mirror and time reversal symmetry. We demonstrate that the electromagnetic response for such a system is characterized by a 1-form \( b \), which can be inferred from the locations of the surface Dirac nodes in energy-momentum space. From both the effective action and analytical band structure calculations, we show that the vortex core of \( b \) or a domain wall of a component of \( b \) can trap surface charges.

Topological phases of matter have been at the forefront of condensed matter physics for the past decade. One reason for the excitement is that topological phases can exhibit electromagnetic responses that display their topological nature. The integer quantum Hall (IQH) effect was the first such system, and its quantized Hall conductance is characterized by a topological integer \([1]\) multiplying the conductance quantum \( e^2/h \). In recent years, the ten-fold, periodic table classification of electronic topological insulators and superconductors with time-reversal (TR) \( T \), particle-hole (PH) \( C \), and/or chiral symmetry \( S \) was completed in Refs. [2–4], and ushered in the concept of a symmetry protected topological (SPT) phase. The electromagnetic (EM) response theories of many of the topological insulator (TI) phases were developed in Ref. [3], and extended from what was known about the IQH to all fermionic SPTs. For example, the 3D \( T \)-invariant topological insulator has an odd number of Dirac cones on each surface, and harbors a half quantum Hall effect when \( T \) is broken on the surface. An odd number of Dirac cones, and the corresponding Hall effect, can never occur in a purely 2D system with the same symmetries without interactions. Indeed, the surface quantum Hall effect is actually a signature of a bulk EM response: the topological magneto-electric effect [3, 5, 6] with a response coefficient determined by a \( \mathbb{Z}_2 \) topological invariant [3].

After the periodic table was complete, and after many exciting materials predictions and discoveries [7–14], the classification of topological crystalline phases (TCIs) with point/group-symmetry symmetries, such as reflection and discrete rotation, was initiated and continues to be an active area of research [15–31]. One highlight of this line of research was the prediction and experimental confirmation of a 3D TCI phase in PbSnTe [32–35]. The topological properties of this system are protected by mirror symmetry, and it exhibits an insulating bulk with an even number of symmetry-protected Dirac-cone surface states on mirror-symmetric surfaces. The goal of this article is to predict a characteristic electromagnetic response property that can be observed in PbSnTe and similar 3D TCIs protected by mirror symmetry (mTCIs).

Three-dimensional mTCIs are characterized by integer invariants: the mirror Chern numbers \( C_M [16] \). To define and illustrate the consequences of the \( C_M \) let us consider a system with mirror symmetry \( M_z \) in the \( z \)-direction with \( M_z^2 = -1 \). We can label eigenstates in the \( k_z = 0 \) and \( k_z = \pi \) planes of the Brillouin zone (BZ) with the eigenvalues \( \pm i \) of \( M_z \), and this allows one to define mirror Chern numbers \( C_M(\Lambda) = \frac{C_M(\Lambda) - C_{-M}(\Lambda)}{2} \), where \( C_{\pm i}(\Lambda) \) is the usual Chern number of each mirror sector in the plane \( \Lambda = 0, \pi \). When a \( C_M \) is non-vanishing, then, on mirror-invariant surfaces, say one normal to \( \hat{x} \), there will be Dirac cones protected by the mirror symmetry. Furthermore, these cones lie in mirror invariant lines in the surface BZ projected from the corresponding \( \Lambda \) planes. The number of stable Dirac cones on each mirror line is given by \( C_M(\Lambda) [16] \). If we allow for broken translation symmetry, then the total number of stable surface cones is \( C_M = C_M(\Lambda_1) + C_M(\Lambda_2) \). We illustrate the case with \( C_M(0) = 2, C_M(\pi) = 0 \) in Fig. 1 where we have two stable Dirac nodes on the surface perpendicular to \( \hat{x} \) on the \( k_z = 0 \) plane.

In this article we will show that mTCIs have a robust electromagnetic (EM) response that is determined by both a topological property (the existence of stable surface states determined by \( C_M \)), and a geometrical property (the momentum and energy locations of the surface nodes). To show this, we first provide a lattice model for a mTCI built from two copies of a 3D time-reversal invariant TI on a cubic lattice. By itself, this system has a trivial topological magnetoelectric effect, but when coupled to a field \( b_\mu \) which preserves the mirror symmetry, yet splits the surface Dirac nodes in energy-momentum space, an additional EM response is generated. In this article we only consider systems which also retain \( T \) symmetry since the experimentally realized mTCIs have \( T \)-symmetry, and it will simplify some discussions.

For the simplest case with \( C_M = 2 \), and with \( T \)-symmetry, we can obtain a response theory of the mTCI via analogy with the 3D TI. In the continuum limit, the field \( b_\mu \) in which we are interested couples to the theory...
precisely as a valley gauge field for the two species of surface Dirac cones/valleys. By performing a diagrammatic calculation in the continuum limit, we find that the effective response action is given by:

$$S_{TCI}[A, b] = \frac{e}{8\pi} \int d^4x \epsilon^{\mu\nu\rho\sigma} \Theta f_{\mu\nu} F_{\rho\sigma},$$

(1)

where $$\Theta = \pi$$ inside the bulk of the mTCI, and $$f_{\mu\nu}, F_{\mu\nu}$$ are the field-strengths of $$b_\mu$$ and $$A_\mu$$. The surface of the mTCI, can be thought of as a domain wall of $$\Theta$$ from $$\pi$$ to 0, and Eq. (1) implies a surface response $$S_{2D}[A, b] = \frac{e}{4\pi} \int_{\text{surf}} d^3x \epsilon^{\mu\nu\rho\sigma} b_\mu \partial_\nu A_\rho$$ bound to the $$\Theta$$ domain wall. This surface response matches an EM response of a 2D Dirac semi-metal (DSM). However, we find precisely half the coefficient that would occur in a 2D DSM with mirror and $$T$$ ($$T^2 = -1$$) symmetries, which makes it anomalous. Ultimately, the EM response of the mTCI implies localized charge and/or current density bound at defects in the $$b_\mu$$ field on the surface. To verify the validity of the result Eq. (1) obtained in the continuum limit, we explicitly calculate the microscopic origin of the response from a lattice model bound state calculation. Finally, we discuss experimental proposals and predictions.

**Lattice Model for TCI.**— Let us begin with the lattice Hamiltonian for a single copy of TI given by[3]:

$$H_{TI} = \sin k_x \Gamma^x + \sin k_y \Gamma^y + \sin k_z \Gamma^z - m(k_x, k_y, k_z)\Gamma^0,$$

(2)

where $$m(k_x, k_y, k_z) = m + \cos k_x + \cos k_y + \cos k_z$$ and $$m$$ controls the bulk gap, and hence the topological phase. The matrices $$\Gamma^\mu$$ satisfy a Clifford algebra, and are given by $$\Gamma^0 = \tau^z s^0$$, $$\Gamma^z = \tau^z s^z$$, $$\Gamma^y = \sigma^y$$, and $$\Gamma^x = \tau^x s^y$$, with the zeroth components $$\tau^0$$ and $$s^0$$ are identity matrices. We can take $$\tau$$ to be an orbital degree of freedom and $$s$$ is spin; hence the time-reversal operator is $$T = is^y K$$ where $$K$$ is complex conjugation. Further, this model has mirror symmetries along the i-th directions with $$M_i = \Gamma^5$$ where $$i = x, y, z$$, and importantly $$M_i^2 = -1$$. For example, we have $$M_x H_{TI}(k_x, k_y, k_z) M_x^{-1} = H_{TI}(k_x, k_y, -k_z)$$.

To introduce a lattice model of the TCI, let us strictly enforce $$M_x$$, and add an additional flavor degree of freedom $$\sigma^0$$ to the TI model (2). With the help of the time-reversal operator, we consider a case where $$-3 < m < -1$$: in this case there are two Dirac nodes (one for each copy) centered at the $$k$$-point on any surface (see Supplementary Material (SM) Sec. IIIA). $$T$$-symmetry enforces $$C_{M}(\Lambda) = -C_{x}(\Lambda)$$, and this model has $$C_M(0) = 2, C_M(\pi) = 0$$, and $$C_M = 2$$.

To produce our phenomena of interest various $$M_x$$ preserving perturbations should be added to $$H_{TCI}^{(0)}$$.[38] Including some such perturbations we can write down a more generic lattice model for the TCI:

$$H_{TCI} = \sin k_x \sigma^0 \Gamma^x + (\sin k_y \sigma^0 + b_0 \sigma^y) \Gamma^y + \sin k_z \sigma^0 \Gamma^z - (m + \cos k_x + \cos k_y + \cos k_z) \sigma^0 \Gamma^0 + b_0 \sigma^y,$$

(3)

where tensor products are implicit, and we will omit $$\sigma^0$$ from now on for compactness. One can verify that the Hamiltonian (3) is invariant under $$M_x$$ and $$T$$ (when $$b_0 = 0$$). One can also introduce $$b_x$$ and $$b_z$$ terms that couple to the Hamiltonian in a similar fashion to $$b_y$$, and will fill out the entire $$b_\mu = (b_0, b_x, b_y, b_z)$$ field. Specific mirror symmetries will enforce some entries to be zero, for example $$M_z$$ enforces $$b_z = 0$$. We have left out a non-zero $$b_z$$, and some other possible $$M_x$$ and $$T$$-invariant terms since we will usually specialize to a particular surface ($$\hat{n} = \hat{x}$$) for convenience, and these additional terms, when small, will not impact our analysis. We note that $$b_0$$ breaks time reversal, but not mirror, and we include it in the Hamiltonian because it leads to an interesting EM response contribution. We show in the SM Sec. IIIA that $$b_0$$ and $$b_y$$ move the zero-energy Dirac nodes in the surface BZ from the $$\Gamma$$-point to $$(E, k_y, k_z) = (\pm b_0, \pm b_y, 0)$$, which, from Eq. (1), is exactly what we need to generate a non-vanishing EM response.

**Electromagnetic response.**— For our choice of $$m$$ the TCI Hamiltonian (3) is naturally expanded in the continuum limit around the $$\Gamma$$-point. For $$b_0 = b_y = 0$$, the continuum Hamiltonian has two identical copies, each with eigenvalue $$\sigma^y = \pm 1$$[39] given by

$$H^{(a)} = k_x \Gamma^x + k_y \Gamma^y + k_z \Gamma^z + m' \cos \theta^{(a)} \Gamma^0 + m' \sin \theta^{(a)} \Gamma^5,$$

(4)
where \( n' > 0 \), \( a = 1, 2 \) corresponds to the two TI sectors with \( \sigma^z = \pm 1 \), and we have introduced a new angle parameter \( \theta^{(a)} \) for each TI block. Under mirror symmetry \( M_z = \Gamma^T \Gamma^5 \), the Hamiltonian satisfies: \( M_z H^{(a)}(k_x, k_y, k_z, \theta^{(a)}) M_z^{-1} = H^{(a)}(k_x, k_y, -k_z, -\theta^{(a)}) \). Thus, mirror symmetry enforces \( \theta^{(a)} = \pi \) to take quantized values of 0 or \( \pi \). Indeed, our lattice model (3) maintains \( \theta^{(a)} = \pi \) throughout the mTCI phase with \( C_M = 2 \).

The topological magnetoelectric response [3, 5, 6] of such a system, which is obtained by gapping the surface Dirac nodes with a \( T \)-breaking mass, is trivial since we have two copies of the usual TI. However, we now show that there is a response characteristic of a mTCI, once a \( M_z \)-breaking mass term is added instead. To calculate the response in the continuum limit we couple each of the continuum Hamiltonians to its own gauge field \( A^{(a)} \) via \( k \to k + A^{(a)} \). A diagrammatic calculation similar to those in Refs. 3 and 40 shows that
\[
S[A^{(a)}] = \frac{1}{32\pi^2} \int d^4 x \theta^{(a)}(x) e^{\mu
u\rho\sigma} F^{(a)}_{\mu\nu} F^{(a)}_{\rho\sigma}
\]
where \( F^{(a)}_{\mu\nu} = \partial_\mu A^{(a)}_\nu - \partial_\nu A^{(a)}_\mu \) is the curvature associated with the gauge field \( A^{(a)}_\mu \). The symmetric combination of the gauge fields \( A^{(1)}_\mu \) and \( A^{(2)}_\mu \) represents the usual EM field \( A_\mu \), while the antisymmetric combination generates the energy-momentum separation of the Dirac nodes \( b_\mu \), i.e., \( e_{A_\mu} = \frac{1}{2}(A^{(1)}_\mu + A^{(2)}_\mu), b_\mu = \frac{1}{2}(A^{(1)}_\mu - A^{(2)}_\mu) \). Thus, the total effective response action is given by:
\[
S[A, b] = \frac{1}{32\pi^2} \int d^4 x \left( e^{\mu
u\rho\sigma} [\epsilon_2(\theta^{(1)} + \theta^{(2)}) F^{(1)}_{\mu\nu} F^{(2)}_{\rho\sigma} + 2e(\theta^{(1)} - \theta^{(2)}) f_{\mu\nu} F_{\rho\sigma} + (\theta^{(1)} + \theta^{(2)}) f_{\mu\nu} f_{\rho\sigma}] \right)
\]
where \( f_{\mu\nu} = \partial_\mu b_\nu - \partial_\nu b_\mu \) is the curvature of the \( b_\mu \). The first (topological magnetoelectric effect) and second terms (the mTCI response of interest) both generate EM responses add and do not cancel. The defect structure that generates this response is illustrated for this case in Fig. 2. At the end we discuss the physical setup needed to experimentally probe this response.

Let us illustrate the physical consequences of Eq. 7. The surface of the mTCI can be thought of as a domain wall of \( \Theta = \Theta(x) \) where \( \Theta \) changes from \( \pi \) to 0 traversing from the mTCI to vacuum. The effective action now reduces to a response localized at the \( \Theta \) domain wall: \( S_{\text{TCI}} = e \sgn(m_A)/(4\pi) \int_{\text{surf}} d^2 x \epsilon^{\mu
u\rho\sigma} f_{\mu\nu} A_\rho \). Taking a derivative of the effective action with respect to \( A_\mu \), i.e., \( j_\mu = \delta S/\delta A_\mu \), we obtain the responses:
\[
j^0_{\text{surf}} = -\frac{e \sgn(m_A)}{2\pi} \partial_x b_y, \quad j^z_{\text{surf}} = -\frac{e \sgn(m_A)}{2\pi} \partial_y b_x,
\]
These equations are analogs of the Streda formula and Ohm’s law for a Hall current, where \( \partial_x b_y, \partial_y b_x \), and \( \partial_z b_0 \) are the “magnetic field” and “electric field” of the 1-form \( b_\mu \). The first equation of (8) indicates that additional charge density is bound at a flux/vortex core of \( \vec{b} \). For a domain wall \( b_y = |b_y| \sgn(z) \) on the \( yz \)-surface of the TCI, which has a “magnetic flux” of \( \vec{b} \), Eq. (8) predicts that there exists a charge density of \( j^0 = e|b_y| \sgn(m_A)/\pi \) trapped at the center of the domain wall. Macroscopically these responses arise from the half quantum Hall effect of each surface Dirac cone. They effectively see opposite electric and magnetic fields, but have opposite masses from the mirror-breaking \( m_A \). Hence, their responses add and do not cancel. The defect structure that generates this response is illustrated for this case in Fig. 2. At the end we discuss the physical setup needed to experimentally probe this response.

These results are based on the particular lattice model (3). However, they hold for any model with \( C_M = C_M(0) + C_M(\pi) = 2 \). We show in the SM Sec. II that for a system with \( M_z \) and \( T \) (or even with weakly broken \( T \), \( C_M = 2 \) necessarily gives rise to two stable Dirac cones, and thus, upon the introduction of proper mirror-breaking mass terms, the response is described by Eq. (8).
(see Ref. 41 for a discussion of the usual magneto-electric response for $C_M = 2$ systems).

For higher $C_M = N$, there exist $N$ stable surface Dirac nodes, and in principle more complex TCI responses can be obtained, but we leave discussion of those for future work (see Ref. 36 for some related examples in 2D DSMs). For cases with $C_M = 0$, the surface Dirac cones can be gapped without breaking $M_z$. However, if the bulk band inversions are at different $k$-points, then on certain surfaces the two Dirac cones can be located at different locations in the surface BZ. In this case gapping the Dirac cones, when mirror is preserved, requires breaking translational symmetry. By analogy with a weak TI [42, 43], we dub the system with surface Dirac nodes protected by $M_z$ and translational symmetry a weak mTCI. When translation symmetry is intact, a weak mTCI can have a response (8) on certain surfaces with mirror symmetry, but not necessarily all of them.

**Microscopic origin of the response.**— Eq. (8) is obtained from the continuum limit. However, from Eq. (3) we see $b_y \sigma^y$ couples to the system like a gauge field only in the continuum limit, i.e., when $b_y$ is small. To obtain a complete picture, it is useful to verify the response from a microscopic lattice calculation.

From the TCI lattice model Eq. (3), we first solve for the surface Dirac states on the boundary of a mTCI ($x < 0$) with the vacuum ($x > 0$). The surface Dirac cones at $x = 0$ are given by

$$H_{2D} = - (\sin k_y + b_y \sigma^y) s^x - \sin(k_z) s^z - m_A s^x \sigma^y,$$

where $m_A$ is the mirror symmetry breaking mass, and the momentum range over which $H_{2D}$ is valid is given by (see SM Sec. IIIIB) $|m - 1 + \cos k_y + \cos k_z| < 1$. In the continuum limit where $|b_y|$ is small, we can drop the sine in Eq. (9) and neglect the upper cutoff for $k_y, z$. Next, for the non-uniform $b_y$ with a domain wall $b_y(z) = |b_y| \, \text{sgn } z$, the solution of Eq. (9) is given by

$$\Psi(x = 0, k_y, z) = \exp \left\{ -\int_0^z [k_y \sigma^y + b_y(z')] dz' \right\},$$

where $\Psi_0(k_y)$ satisfies $s^y \sigma^y \Psi_0(k_y) = -1$. Eq. (10) describes two bound states at each $k_y$, corresponding to the two eigenvalues of $\sigma^y$, both localized in the $z$-direction at the zero of the integrand of the exponent. Since $b_y$ ranges from $-|b_y|$ to $|b_y|$, only states for which $|k_y| < |b_y|$ have bound state solutions. Therefore, the total number of bound states is $2 \times 2 |b_y|/(2\pi/L_y)$. For a finite system, the surface $x = 0$ will also have an opposite domain wall with $b_y(z) = -|b_y| \, \text{sgn } z$. There exist the same number of bound states at the opposite domain wall with $s^y \sigma^y = 1$. With a small but finite $m_A$, the states localized at opposite domain walls are split away from zero energy and can be unambiguously filled (all states on one domain wall are filled). Due to the usual arguments [44], each state generates a localized charge $-\frac{1}{2} \text{sgn } m_A$. Therefore we find that the bound state charge density is $j^0 = -e |b_y| \text{sgn}(m_A)/\pi$, and is in agreement with Eq. (8). We note that to see this response, we only need to break mirror symmetry with an infinitesimal mass term, while time reversal symmetry is intact.

For a larger magnitude of the domain wall $|b_y|$, the charge response can deviate from the prediction from Eq. (8) and become non-universal, but this happens only with a gap closing transition in the bulk. To this end, for a sufficiently small $|b_y|$, the Dirac nodes given by Eq. (9) simply get shifted. However, depending on the momentum range of validity of $H_{2D}$, a larger value of $|b_y|$ can either eliminate the Dirac nodes or introduce additional Dirac nodes that can gap out each original one. In both cases, there is a gap closing in the bulk which indicates a transition from a mTCI to a trivial insulator. We show in the SM Sec. III that, as long as the bulk gap does not close, the response (8) from the continuum model remains exact even in the lattice model. However for the cases when a large $b_y$ eliminates or cancels the original Dirac nodes on the two sides of the domain wall, the charge density bound at the domain wall becomes non-universal.

**Implication for experiments.**— As discussed above, the universal bulk contribution to the topological magneto-electric effect [3, 5, 6] is absent in a TCI; the Faraday effect and Kerr angles are non-universal when TR is explicitly and infinitesimally broken. However, our predicted response in Eq. (8) can be directly detected in other experiments, which requires engineering a domain wall or time gradient of the $b_y$ field, i.e., the momentum/energy displacement of the Dirac nodes. The surface Dirac nodes of a TCI can be moved in $k$-space via compression or dilation strains [46]. For SnTe, the surface Dirac nodes perpendicular to the (001) direction arise at $\pm k_1, \pm k_2$ and are protected by mirror symmetry along (110) and (1\bar{1}0) axes, and are related by a $C_4$ rotation. With Isotropic compression or dilation, $b_y$’s for both pairs of Dirac nodes increase or decrease. With uniaxial compression or stretching that breaks the $C_4$ symmetry, $b_{1,2}$ increases while $b_{1,2}$ decreases, or vice versa. A spatially inhomogeneous compression/dilation can thus generate the domain wall structure. A temporal gradient of $b$ can be generated by surface acoustic waves produced by electromagnetically stimulating a piezo-electric layer deposited on the surface. The mass terms of the surface Dirac fermions can be generated [32, 47] through structural distortions where the atoms are displaced. After setting up the spatially-varying or time-dependent $b_y$, the localized charges can be detected by Scanning Tunneling Microscopy (STM) [48, 49] or the Scanning Single Electron Transistor Microscopy (SSETM) [50], while surface currents can be observed by a SQUID magnetometer.
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