Dissipative Edge Transport in Disordered Axion Insulator Films

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We investigate the role of disorder in the edge transport of axion insulator films. We predict by first-principles calculations that even-number-layer MnBi2Te4 have gapped helical edge states. The random potential will dramatically modify the edge spectral function to become gapless. However, such gapless helical state here is fundamentally different from that in quantum spin Hall insulator or topological Anderson insulator. We further study the edge transport in this system by Landauer-Büttiker formalism, and find such gapless edge state is dissipative and not immune to backscattering, which would explain the dissipative nonlocal transport in the axion insulator state observed in six septuple layer MnBi2Te4 experimentally. Several transport experiments are proposed to verify our theory on the dissipative helical edge channels. In particular, the longitudinal resistance can be greatly reduced by adding an extra floating probe even if it is not used. These results will facilitate the observation of long-sought topological magnetoelectric effect in axion insulators.

Topological phenomena have been one of the central topics in condensed matter physics [1–4]. The interplay between band topology and magnetism gives rise to a variety of exotic quantum states [4–6]. A prime example is the quantum anomalous Hall (QAH) effect discovered in magnetic topological insulator (TI) films [7–14], where the spin-orbit coupling and ferromagnetic (FM) ordering combine to give rise to a topologically nontrivial phase characterized by a finite Chern number and gapless chiral edge states [5, 15–17]. Another interesting example is axion insulator, which is three-dimensional magnetic TI with a nonzero quantized Chern-Simons magnetoelectric coupling (axion θ = π) protected by inversion symmetry I instead of time-reversal symmetry Θ [5, 18–23]. Such axion coupling leads to the prediction of topological magnetoelectric (TME) effect [5], which is the hallmark of axion insulator but remains unexplored due to difficulties in realizing the axion insulator state.

The simplest scenario for axion insulator state is obtained in bulk TI with a surface gap induced by a hedgehog magnetization while preserving the bulk gap [5, 24–26]. In the thin-film geometry, the above condition of hedgehog magnetization is simply fulfilled with an antiparallel magnetization on top and bottom surfaces, where the absence of all surface state transport leads to a zero Hall plateau σxy = 0, σxx → 0, and ρxy = 0, ρxx → ∞ [25, 27]. Such peculiar charge transports have been observed in FM-TI-FM heterostructure [28–31] and even layer MnBi2Te4 antiferromagnetic (AFM) TI [32], which were predicted to be axion insulator state [25, 33–35]. Theoretically, the low-energy physics in two different systems are similar and generate topological θ response which is nonquantized due to finite-size effect [25, 26, 36]. However, recent transport and microwave imaging experiments find quite different behaviors in these two systems, where gapless edge states do not exist in the former [28, 37] but do exist in the latter [38, 39]. Especially, the edge transport in MnBi2Te4 even layer is shown to be dissipative [38]. Thus, it is important to trace where such dissipative gapless edge states come from and understand the origin of the discrepancy in these two systems.

Here we study the role of disorder in the edge transport of axion insulator films. By combining first-principles calculations and analytic models, we show that six septuple layers (SL) of MnBi2Te4 studied in experiments [38, 39] have gapped helical edge states. A random potential will modify the edge spectral function to become gapless. Such gapless edge state is dissipative and not immune to backscattering, which would explain dissipative transport of the recent transport and image experiments [38, 39].

Materials.— We carry out first-principles calculations on MnBi2Te4 films. The material consists of Van der Waals coupled SL and develops A-type AFM order with an out-of-plane easy axis below Néel temperature, which is FM within each SL but AFM between adjacent SL along z axis. The bulk state is an AFM TI with nontrivial Z2 index protected by S = Θτ1/2 [40], where τ1/2 is the half translation operator along z axis. The odd SL with a net magnetization breaks TΘ and shows QAH effect [14, 33–35]. While even SL with full compensated magnetic layers conserves TΘ and exhibits zero-plateau QAH [32]. We study the edge band structure of even SL along edge ΓM direction. As shown in Fig. 1, the 2D band structure has an inverted band gap at the Γ point, and there indeed exists gapped helical edge state Λ in the insulating bulk. As we show below, it originates from helical edge states of the quantum spin Hall (QSH) effect but with Θ-breaking due to magnetic ordering, where the gap is opened at Dirac point.

Model.— The effective model for the low energy physics of even SL can be written down near the Γ point. We start from 3D Hamiltonian H_{3d}(k) for AFM MnBi2Te4, which is the same as that for Θ-invariant TI due to con-
served $S$ [33]. For even SL, $S$ is broken and a term $H_{ex}$
describing the spatial alternating exchange field enters into $H_{3d}(k)$.
The confinement in $z$ direction quantizes $k_z$ and leads to 2D subbands labeled by the subband index $n$. The 2D subbands have band inversion for film thickness $\geq 4$ SL [33], and without $H_{ex}$, the system is QSH with the low energy physics determined by Dirac surface states on top and bottom surfaces [41, 42].

The effect of $H_{ex}$ is to introduce opposite Zeeman terms on these two surfaces. Thus the effective model for even SL described by the massive Dirac surface states is given by [25, 43, 44]

$$H_0(k) = \epsilon_0(k) + v(k_y\sigma_x - k_x\sigma_y)\tau_z + m(k)\tau_x + \Delta_0\sigma_z\tau_z,$$  

(1)

with the basis of $|t\uparrow\rangle, |t\downarrow\rangle, |b\uparrow\rangle$ and $|b\downarrow\rangle$, where $t, b$ denote top and bottom surfaces and $\uparrow, \downarrow$ represent spin up and down states, respectively. The particle-hole asymmetry $\epsilon_0(k)$ is neglected for simplicity. $\sigma_i$ and $\tau_i$ ($i = x, y, z$) are Pauli matrices acting on the spin and layer, respectively. $v$ is the Dirac velocity, $m(k) = m_0 + m_1(k_x^2 + k_y^2)$ describes the tunneling effect between $t$ and $b$ surface states, $\Delta$ is the exchange field along $z$ axis introduced by the opposite magnetic ordering on $t$ and $b$.

Equ. (1) correctly characterizes the gapped helical edge state shown in Fig. 1. The energy gap for 2D bulk is

$$2\sqrt{m_0^2 + \Delta^2}$$

at $\Gamma$ point. If $\Delta = 0$, this model is similar to Bernevig-Hughes-Zhang model for HgTe quantum wells [45] describing QSH with $m_0m_1 < 0$, where there exists gapless helical edge state. Then $\Delta$ further induces a gap to the edge state. The effective model for 1D gapped helical edge state is obtained analytically as $H_{1d} = vk_x\xi_x + \Delta_0\xi_x$, where $\xi_x$ are Pauli matrices denoting pseudo-spin. The edge state gap $2\Delta$ is less than that of 2D bulk, consistent with Fig. 1. It is worth mentioning there also exist other gapped helical edge states with higher energy than $\Lambda$ in 2D bulk gap as shown in Fig. 1(d), which are from the band inversion of extra 2D subbands with $n > 1$ in thick film [46]. In the following we investigate the edge transport determined by $\Lambda$ in the presence of disorder. Take 6 SL for a concrete example, we fit the parameters $v = 3.2$ eV·Å, $m_0 = -0.014$ eV, $m_1 = 9.4$ eV·Å$^2$ and $\Delta_z = 5$ meV.

In general, the disorder will generate spatially random perturbations to the pure Hamiltonian $H_0$. Specifically, the system mainly has random scalar potential $H_U = U(\mathbf{r})$ induced by impurities in the materials. There also exists random exchange field along $z$ axis induced by the inhomogenous AFM order potential $U$ in Eq. (1) and will not affect the edge transport essentially. Therefore we only need to consider $H_U$, which is nonuniform and random in space but constant in time.

**Analysis of disorder.** Now we will show that disorder will renormalize Eq. (1). We extract the renormalized topological mass $m_0$, and the renormalized exchange field $\Delta$, from the self-energy $\Sigma$ of the disorder-averaged effective medium. In numerical simulations, we discretize $H_0(k)$ on a square lattice and take a random on-site disorder potential $U(\mathbf{r})$, uniformly distributed in the interval $(-U_0, U_0)$. We denote $H_0(k)$ as the lattice Hamiltonian for Eq. (1).

The self-energy defined by $(E_F - H_0 - \Sigma)^{-1} = ((E_F - H)^{-1})$, with (...) the disorder average, is a $4 \times 4$ matrix which we decompose into $\Gamma$ matrices: $\Sigma = \Sigma_0 + \Sigma_1\sigma_x\tau_z + \Sigma_2\sigma_y\tau_z + \Sigma_4\tau_x + \Sigma_5\sigma_z\tau_z$. Then the renormalized $\tilde{m}_0$ and $\Delta$ are given by

$$\tilde{m}_0 = m_0 + Re\Sigma_4, \quad \tilde{\Delta} = \Delta + Re\Sigma_5.$$  

(2)

The self-consistent Born approximation (SCBA) is employed to capture the main feature of disorder [47], where $\Sigma$ is given by the self-consistent equation,

$$\Sigma = \frac{U_0^2}{3} \left(\frac{a}{2\pi}\right)^2 \int_{BZ} d^2k \frac{1}{\omega - H_0(k) - \Sigma(\omega) + i\delta}. $$  

(3)

The self-energy is momentum independent, so there is no renormalization to $v$ and $m_1$. The corrections to $m_0$ and $\Delta$ are obtained approximately as

$$\tilde{m}_0 - m_0 = -\frac{U_0^2a^2}{12\pi} m_1 \ln \left| \frac{m_1^2\Pi}{m_0^2 + \Delta^2 - E_F^2} \right|,$$

(4a)

$$\tilde{\Delta} - \Delta = \frac{U_0^2a^2}{6\pi} \frac{\Delta \tanh^{-1} \left| \mathcal{Z}(k) \right|}{\sqrt{v^4 + 4v^2m_0m_1 + 4m_1^2(E_F^2 - m_0^2)}},$$

(4b)

$$\mathcal{Z}(k) = \sqrt{v^4 + 4v^2m_0m_1 + 4m_1^2(E_F^2 - m_0^2)}.$$  

(4c)

FIG. 1. (a) & (c) Band structure for 4 SL and 6 SL MnBi$_2$Te$_4$. The dashed line shows the Fermi level. The inset of (a) shows 2D Brillouin zone with high-symmetry $k$ points $\Gamma(0,0), K(\pi,\pi)$ and $M(\pi,0)$ labelled. The energy dispersion of the semi-infinite film along edge $\Gamma M$ is plotted for (b) 4 SL and (d) 6 SL, respectively. The gapped edge states are clearly seen around $\Gamma$ point as red lines dispersing in the 2D bulk gap.
essentially the gapless edge state here in the spectral function is microwave impedance microscopy [39]. We point out that sides at the sample boundary in Fig. 2(b). This explains order broadens the quasiparticle spectral weight and rest of disorder strength.

FIG. 2. (a) DOS of 2D bulk for typical $U_0$. (b) The real space distribution for state at $E = 0$ in (c) and (d). (c,d) The edge spectral function $A(k,\omega)$ within SCBA of disorder strength $U_0 = 0.06$ eV and $U_0 = 0.1$ eV, respectively. A cylinder geometry is adopted with periodic boundary condition along $x$-axis and open boundary condition in $y$-axis with width $L_y = 100a$. The lattice constant of the discretization $a = 2$ nm.

where $\Pi = \pi/a$ is ultraviolet cutoff in momentum. Here we only keep the most logarithmically divergent term in Eq. (4a). The sign of $\bar{m}_0$ and $m_0$ remains the same, as the the correction to $m_0$ has opposite sign to $m_1$. Then the system is always in the inverted region [48]. Similarly, the renormalized $\bar{\Delta}$ only decreases slightly. Therefore, the topological property of 2D bulk remains unchanged due to disorder, which is evidenced in the density-of-state (DOS) calculation in Fig. 2(a).

To get information about the edge excitations in the disordered system, we further calculate the edge spectral function $A(k,\omega)$ within SCBA in a cylinder geometry. The self-energy is $\Sigma(\omega) = (U_0^2/3)(a/2\pi) \int dk_x G(\omega,k_x;y,y)$, with $G(\omega,k_x;y,y)$ be the Green’s function on cylinder, and the Dyson equation is $G(k_x;y_1,y_0) = \int dy G_0(k_x;y_1,y) \Sigma(y) G(k_x;y,y_0) + G_0(k_x;y_1,y_0)$. In a lattice $\int dy \to a \sum_{y'}$ we have $G(k_x) = G_0(k_x) - \Sigma$. The spectral function $A(k_x,\omega) = (1/\pi) \text{Im} G^R(k_x,\omega)$ is plotted in Fig. 2 for different disorder strength $U_0$. We can see that the disorder broadens the quasiparticle spectral weight and reduces the edge gap when $U_0$ is relatively small. While $U_0$ exceeds a critical value $U_c$, the edge spectrum is gapless as shown in Fig. 2(d), and such gapless state indeed resides at the sample boundary in Fig. 2(b). This explains the gapless edge state observed in this system by microwave impedance microscopy [39]. We point out that the gapless edge state here in the spectral function is essentially different from that in topological Anderson insulator (TAI) [48–50]. In TAI, the gapless helical edge state is induced by disorder driven band inversion, which is dissipationless and immune from backscattering as protected by $\Theta$. Here in disordered axion insulator film, the edge state is dissipative because $\Theta$-breaking $\Delta$ induces backscattering. This is the main result of this paper.

The dissipative nature could be understood from effective theory for edge state with action

$$S = \int dt dx \psi^\dagger (\partial_t - i v \partial_x + \Delta \partial_x + \mu(x)) \psi,$$

where $\mu(x)$ is the edge disorder potential with a zero mean. Via a nonlocal transformation $\psi(x) = Q(x) \tilde{\psi}$ where $Q(x) = P \exp(-it \int_{-\infty}^{\infty} dx' \mu(x')/v)$, one can rewrite the action as

$$S = \int dt dx \tilde{\psi}^\dagger (\partial_t - i v \partial_x + \Delta \partial_x + \mu(x)) \tilde{\psi}$$

where $P$ stands for path ordering. The last term in Eq. (6) has long range correlation from the random string phase factor $Q$, which is a relevant perturbation and describes backscattering. This term is absent in the quantum Hall chiral edge states with $\nu = 2$ filling due to $SU(2)$ symmetry [51, 52]. Now we can see that the transformed action describes a gapless helical edge state with a backscattering term from random disorder.

Numerics. The above analytic results can be corroborated numerically by using the package Kwant [53]. The resistance is calculated by the Landauer-Büttiker formalism with disorder-averaged transmission amplitude. The device geometry with standard Hall bar is illustrated in Fig. 3(a). The two terminal conductance $G$ as a function of Fermi energy $E_F$ is shown in Fig. 3(b). In the clean limit, $G$ vanishes when $E_F$ is in the edge gap and is finite exhibiting oscillating behaviour when $E_F$ is in the $\Lambda$ band, where the transmission resonance $G = 2e^2/h$ is consistent with the gapped helical edge state. For finite disorder, $G$ is finite when $E_F$ is in the edge gap (of the clean limit) and gradually grows as $E_F$ increases. The disappearance of conductance oscillation and $G < 2e^2/h$ when $E_F$ is in the conducting edge band are the manifestation of dissipative nature of edge state. $G$ as a function of disorder strength $U_0$ at $E_F = 0$ is plotted in Fig. 3(d). We can see $G$ is finite only with moderate $U_0$. When $U_0 < U_c$, $G = 0$ due to finite edge gap in the spectral function in Fig. 2, while $G$ vanishes for strong $U_0$ is from the Anderson localization. Furthermore, the dissipative edge transport leads to monotonically decreasing $G$ versus increasing device length $L_x$ in Fig. 3(c).

The dissipative transport measured in the two terminals does not allow us to distinguish experimentally between helical edge channels and residual bulk conduction channels in a convincing manner. An unambiguous way to reveal the existence of dissipative helical edge state transport in the system is to use nonlocal electrical measurements. The edge states necessarily lead to nonlocal
transport, and such nonlocal transport provides definitive evidence for the existence of chiral edge states in the quantum Hall effect [54, 55]. The nonlocal resistance $R_{ij,kl}$ is plotted in Fig. 3(e) and 3(f), which is defined as voltage between electrode $k$ and $l$ divided by the current flowing through electrode $i$ and $j$, i.e., $R_{ij,kl} = V_{kl}/I_{ij}$. All of the nonlocal resistances are greater than the corresponding quantized value for dissipationless gapless helical edge state in QSH, which further demonstrates the edge transport is dissipative here. The nonlocal resistances decreases and finally vanishes when $E_F$ further goes into bulk. Moreover, one interesting feature in Fig. 3(f) is that $R_{15,23} \approx 4R_{45,kl}$, which agrees with the recent transport experiment qualitatively [38]. We emphasize the transmission amplitude and resistance in numerical simulation depend on system size and position of electrodes, which is the key feature for dissipative edge transport in this system.

**Edge transport.** We further propose a theory for the dissipative edge transport within the general Landauer-Büttiker formalism [54, 55], where the current-voltage relationship is expressed as $I_i = (e^2/h) \sum_j (T_{ij}V_i - T_{ij}V_j)$, where $V_i$ is the voltage on the $i$th electrode, $I_i$ is the current flowing out of the $i$th electrode into the sample, and $T_{ij}$ is the transmission probability from the $i$th to the $j$th electrode. There is no net current ($I_j = 0$) on a voltage lead or floating probe $j$, and the total current is conserved, namely $\sum_i I_i = 0$. The current is zero when all the potentials are equal, implying the sum rules $\sum_i T_{ij} = \sum_i T_{ij}$. For a standard Hall bar with $N$ current and voltage leads [such as Fig. 3(a) with $N = 8$], the transmission matrix elements for the dissipative helical state are given by $T_{i+1,i} = T_{i,i+1} = \kappa_i$ (from the disorder-averaged $\mathcal{I}\Theta$ symmetry) and others $0$ (Here we identify $i = N + 1$ with $i = 1$). These states are not protected from backscattering and the transmission from one electrode to the next is not perfect, implying $\kappa_i < 1$ [56], which is different from dissipationless helical edge states in QSH where $\kappa_i = 1$ [57]. In general, $\kappa_i$ become zero for infinitely large sample, because dissipation occurs once the phase coherence is destroyed in the metallic leads or the momentum is relaxed $\kappa_i \sim e^{-L/l_m}$, where $L$ is the size between adjacent leads, $l_m$ is the mean free path which is $1/2$ of the localization length for 1D state [58]. For simplicity, we have assumed $T_{ij}$ to be translation invariant, namely $T_{i+1,i} = \kappa$ is $i$ independent. The edge theory leads to the two terminal conductance $G \sim \kappa e^2/h \propto e^{-L_c/l_m}$, which agrees with Fig. 3(c) quantitatively. Considering again the nonlocal transport as in Fig. 3(f), one finds that $R_{15,23} = h/2ke^2$, $R_{45,kl} = h/8ke^2$, and the relation $R_{15,23} = 4R_{45,kl}$.

The effect of decoherence between two real leads can be modeled as an extra floating lead, in which dissipative gapless helical states interact with infinitely many low-energy degrees of freedom, completely losing their phase coherence [57]. $\kappa$ is length dependent for the dissipative helical state in axion insulator film, while it is length independent ($\kappa = 1$) for dissipationless helical state in QSH. This leads to quite different transport signatures between these two helical states. For example, if we put extra pairs of floating probes ($2'$ and $8'$ in Fig. 3(a)) in the standard two terminal device with $L \gg l_m$, we can see the longitudinal conductance increases (but not necessarily monotonically) as the number of floating leads increases.
for dissipative helical state in Fig. 4(a) [46], which is just the opposite for QSH in Fig. 4(b). This is a rather sharp feature which is easy to implement in experiments.

**Discussion.**—The dissipative gapless helical edge state from disorder in MnBi$_2$Te$_4$ films and its transport properties well explain the recent transport and image experiments [38, 39]. The nonlocal resistance $R_{37.21}$ is greater than $R_{37.45}$, $R_{37.56}$, and $R_{37.18}$ in experiment [38], since $\kappa$ is length dependent, one possible explanation is that the position of the electrodes are neither equally spaced nor perfectly aligned, which is common in experiments. Moreover, Eq. (1) also describes the low energy physics in FM-TI-FM heterostructure with $m_0 \approx 0$ [28], the disorder will induce band inversion with a negative renormalized $m_0$. However, the disorder strength is expected to be small and the exchange field is large in such a modulated doping system [12], thus the system should not have any gapless edge states. Finally, high magnetic field drives MnBi$_2$Te$_4$ even layer into Chern insulator state with a full magnetization. The helical edge state evolves into gapless chiral edge state, while other higher-energy helical states become quasi-helical states with a larger gap due to stronger exchange field, and the transport is only determined by the dissipationless chiral edge channel.

In summary, disorder with moderate strength will dramatically modify the edge transport in axion insulator films, which is a generic phenomenon. Thinner films of axion insulator such as SL MnBi$_2$Te$_4$ has a larger edge gap as shown in Fig. 1(b), such gapped state may persist even in the presence of disorder, and one can realize the long-sought TME effect in axion insulator without any gapless states.

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