Interaction correction to the magnetoelectric polarizability of $Z_{\{2\}}$ topological insulators

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Interaction Correction to the Magneto-Electric Polarizability of $Z_2$ Topological Insulators

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When time-reversal symmetry is weakly broken and interactions are neglected, the surface of a $Z_2$ topological insulator supports a half-quantized Hall conductivity $\sigma_S = e^2/(2h)$. A surface Hall conductivity in an insulator is equivalent to a bulk magneto-electric polarizability, i.e. to a magnetic field dependent charge polarization. By performing an explicit calculation for the case in which the surface is approximated by a two-dimensional massive Dirac model and time-reversal symmetry is broken by weak ferromagnetism in the bulk, we demonstrate that there is a non-universal interaction correction to $\sigma_S$. Our prediction can be tested by measuring the capacitance of magnetized thin films in which the anomalous quantum Hall effect is absent.

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I. INTRODUCTION

The quantum Hall effect\(^1\) stands alone among transport phenomena because it is characterized by a non-zero transport coefficient whose value is universal, dependent only on fundamental constants of nature and not at all on crystal imperfections and other peculiarities of individual samples. The accuracy of the quantum Hall effect is now established to better than eight figures\(^2\) and has no established limitation. This surprising property can be traced to its identification with a topological index\(^3\) of electronic structure, one that can be non-trivial only in systems with broken time-reversal symmetry. For many years quantum Hall states endured as the only known example of topologically non-trivial electronic structure. In recent years, however, the topological classification\(^5\,^6\) of electronic states has broadened considerably. The $Z_2$ classification\(^7\,^8\,^9\,^{10}\,^{11}\) of what are seemingly the most innocent of states—time-reversal invariant insulators—has particularly broad experimental implications. Only in the original quantum Hall case, however, is the topological index a readily measured macroscopic observable.

Non-trivial electronic topology is most commonly revealed by the presence of protected boundary states at surfaces and heterojunctions.\(^12\,^{13}\) The topological character of a three-dimensional insulator, for example, can be revealed by examining its surface states\(^14\) to determine whether the number of Dirac points (linear band crossings) is even or odd. The observable that is most closely related to the non-trivial $Z_2$ topological index of time-reversal invariant insulators is its magneto-electric polarizability,\(^15\,^{16}\,^{17}\,^{18}\,^{19}\) or equivalently its surface-state Hall conductivity. Because a finite Hall conductivity requires broken time-reversal symmetry, the association of magneto-electric polarizability with a time-reversal invariant state is puzzling. The accepted resolution\(^20\) of this conundrum, briefly, is that the bulk magneto-electric polarizability is observable only when time-reversal invariance is weakly broken at the surface and the Fermi level lies in the resulting surface-state gap. When these conditions are satisfied, it is commonly argued that the surface Hall conductivity of a non-interacting $Z_2$ topological insulator (TI) must be quantized at a half-odd-integer multiple of $e^2/h$ because i) it must change sign under time reversal, and ii) it can change only by integer multiples of $e^2/h$ under time-reversal or under any other change in the Hamiltonian. This magneto-electric response of a TI has been referred to as its Chern-Simons polarizability. In this article we show that, in contrast to the case of the quantum Hall effect, weak interactions quite generally yield a correction to this observable.

Our conclusions are based on an explicit calculation for the case of a TI surface with a single Dirac cone, and time-reversal symmetry that is broken by weak bulk ferromagnetism (see Fig. 1). The model we consider provides a good description of the thin-film diluted-moment ferromagnets based on (Bi,Sb)$_2$Te$_3$ TIs in which the quantized anomalous Hall effect (QAHE)\(^21\,^{22}\,^{23}\,^{24}\,^{25}\) has recently been observed. Chromium or vanadium doping in these materials introduces local moments that order at low temperatures, breaking time-reversal symmetry and opening a gap in the surface-state spectrum. The discovery\(^21\) of a QAHE in this material was inspired by
earlier theoretical work which predicted that thin films of the tetradymite semiconductors $\text{Bi}_2\text{Te}_3$, $\text{Bi}_2\text{Se}_3$, and $\text{Sb}_2\text{Te}_3$ would reveal a quantized Hall effect when doped with transition metal elements.

The Hall conductivity on both top and bottom surfaces of a dilute-moment TI ferromagnet is expected to be half-quantized, provided that time-reversal-symmetry breaking energy scales are small compared to the bulk energy gap. When electronic properties of the system are evaluated using mean-field theory, this expectation is corroborated in the small surface-state-gap limit by calculations based on a Dirac model with an energy gap due to exchange interactions between surface-state quasiparticles and the bulk magnetic condensate. We show below that the surface Hall effect is no longer exactly half-quantized when interactions between surface-state quasiparticles and quantum fluctuations of the bulk magnetization, described as magnons, are included. The total Hall effect obtained by summing over the top and bottom surfaces of a thin film remains quantized however, in agreement with experiment.

II. SURFACE-STATE HAMILTONIAN

We consider two-dimensional (2D) surface-state model Hamiltonians with a single Dirac cone, exchange interactions, and spin-dependent disorder or interaction terms:

$$ H = H_{qp} + H_{pert}, $$

where $H_{qp}$ is a mean-field-theory quasiparticle Hamiltonian for a gapped Dirac system, and $H_{pert}$ is a perturbation. The mean-field Hamiltonian can quite generally be expressed in the form

$$ H_{qp} = \sum_k \Psi_k^\dagger H_{qp}(k) \Psi_k, $$

where $\Psi_k$ is an annihilation operator spinor, and $H_{qp}(k)$ is expanded in a Pauli matrix basis:

$$ H_{qp}(k) = d_0(k)\sigma_0 + d(k) \cdot \sigma. $$

This Hamiltonian has a gap separating low-energy valence-band surface states, which are occupied in the case of interest, from high-energy conduction-band surface states:

$$ \xi_{\pm}(k) = d_0(k) \pm |d(k)|. $$

When the surface-state Hamiltonian is time-reversal invariant, $d$ and hence the gap must vanish at $k = 0$. In order to clearly explain the origin of the surface-state Hall conductivity correction, we specialize below to the case of the 2D massive Dirac model which is simplified by isotropic energy bands:

$$ H_{qp}^{MD}(k) = \hbar v \hat{z} \cdot (k \times \sigma) \pm \hbar m_\sigma \sigma_z = d_{\pm}^{MD}(k) \cdot \sigma, $$

where we have chosen the zero of energy at the Dirac point, $v$ is the Fermi velocity of the surface-state Dirac fermions, $\Delta = 2\hbar|m|$ is the surface-state gap, and the sign in Eq. (5) depends on the direction of the thin-film magnetization relative to the surface normal. The $\sigma_z$ term in this Hamiltonian is the mean-field exchange interaction between the surface-state spins and perpendicular anisotropy bulk magnetization.

We describe our Hall conductivity calculation in detail for the case in which the surface normal and the exchange field on the surface are parallel and in the $\hat{z}$ direction. This choice corresponds to spin-$\downarrow$ occupied surface states and, if the interaction between the surface state quasiparticle and the bulk magnetization is ferromagnetic, to a spin-$\downarrow$ bulk spin orientation. The gapped surface-state conduction- and valence-band energies are given by:

$$ \xi_{\pm}^{MD}(k) = \pm \hbar \sqrt{v^2|k|^2 + m^2}. $$

We distinguish two types of perturbative corrections to the massive Dirac model: i) static perturbations in which the Hamiltonian is changed but the Hilbert space is not, and ii) dynamic perturbations in which the surface-state quasiparticle are coupled to external bosonic degrees of freedom like phonons or magnons. In the first case, we consider the Hamiltonian $H_{pert}^{st} = g_0\sigma_0 + g \cdot \sigma$, where $g_0$ and $g$ are charge and spin disorder potentials that depend randomly on position. Since in this article our goal is simply to establish that the interaction corrections to the Hall conductivity do not vanish, we calculate corrections only to leading order in perturbation theory. Because the leading order response can be written as a sum over contributions from different Fourier components $p$ of $g_0$ and $g$, we can consider one component at a time. It is therefore sufficient to assume that these functions vary sinusoidally with position with arbitrary wavevector $p$.

In the dynamic perturbation case, $H_{pert}^{dy} = H_b + H_{qp-b}$, we add to the Hamiltonian both a bare boson contribution $H_b$ and an interaction $H_{qp-b}$ between quasiparticles and bosons:

$$ H_b = \sum_p \hbar \omega_p a_p^\dagger a_p, $$

$$ H_{qp-b} = A^{-1/2} \sum_k \langle \Psi_k^\dagger p a_{-p}^\dagger M \Psi_k + h.c. \rangle. $$

Here, $a_p^\dagger (a_p)$ creates (annihilates) bosons with momentum $p$, $\omega_p$ specifies the boson dispersion, $A$ is the surface area, and $M$ is a quasiparticle-boson interaction coupling matrix which can be spin-dependent. In the zero temperature limit, we can, in calculating the leading-order quasiparticle-boson interaction correction, truncate the boson Hilbert space both to a single boson momentum $p$ and to the $n = 0$ and $n = 1$ occupation numbers. These simplifications allow the dressed eigenstates to be obtained by diagonalizing $4 \times 4$ matrices for each $k$.

Because the exchange interaction between a magnetic quasiparticle and a ferromagnetic condensate is (at least approximately) invariant under simultaneous rotation of
the magnetic order parameter and the quasiparticle spin, magnon creation (which raises spin for the ↓ condensate spin direction considered here) is accompanied by quasiparticle spin-flip from ↑ to ↓ and magnon annihilation by quasiparticle spin-flip from ↓ to ↑. We therefore write $M_{\text{sw}} = \gamma_{\text{sw}}(\sigma_x - i \sigma_y)/2$. We show below that this interaction vertex implies a correction to the surface Hall conductivity.

III. MAGNETO-ELECTRIC POLARIZABILITY

Using linear-response theory (see Sec. I of the supplemental material), the surface-state Hall conductivity can be expressed in terms of current-operator matrix elements between momentum-dependent ground $|0\rangle$ and excited states $|n\rangle$:

$$\sigma_{xy} = -\frac{\hbar}{2\pi^2} \int_{\text{DP}} d^2k \sum_{n \neq 0} \frac{\text{Im}(\langle 0 | j_x | n \rangle \langle n | j_y | 0 \rangle)}{(E_n - E_0)^2}/\hbar^2 \tag{8a}$$

$$= \frac{e^2}{2\pi \hbar} \int_{\text{DP}} d^2k \Omega_{xy}(k) \tag{8b}$$

$$= \frac{e^2}{2\pi \hbar} \int_{\text{DP}} dk \cdot A(k). \tag{8c}$$

In Eq. (8) the integrals over momentum are taken over the Dirac point region DP, bounded by $\partial\text{DP}$, defined as the region in which the surface states lie inside the bulk gap. Eqs. (8b) and (8c) rely on the observation that the continuum model current operator expression, $j_\mu = -(e/\hbar)(\partial H/\partial k_\mu)$, remains valid when quasiparticle-boson coupling is included. When the boson momentum is restricted to $p$ and the boson Hilbert space is truncated to $n = 0, 1$, the eigenstates in Eq. (8) are linear combinations of $n = 0$ band electron states with momentum $k$, and $n = 1$ band states with momentum $k - p$. The Berry curvature is given by:

$$\Omega_{xy}(k) = i \sum_{n \neq 0} \frac{\langle 0 | \frac{\partial H}{\partial x} | n \rangle \langle n | \frac{\partial H}{\partial y} | 0 \rangle - (x \leftrightarrow y)}{(E_n - E_0)^2}$$

$$= \partial_{k_x} A_y(k) - \partial_{k_y} A_x(k), \tag{9}$$

where the Berry connection $A_\mu(k) = i \langle 0 | \partial_{k_\mu} | 0 \rangle$. When applying Eq. (8c) we must choose a gauge in which the ground state is a smooth function of wavevector inside the region DP.

In the absence of interactions and disorder (i.e. for $H_{\text{pert}} = 0$), Eq. (8a) reduces to

$$\sigma_{xy} = -\frac{\hbar}{2\pi^2} \int_{\text{DP}} d^2k \frac{\text{Im}(\langle 0 | j_x | 1 \rangle | 1 \rangle j_y | 0 \rangle)}{(E_1 - E_0)^2}/\hbar^2, \tag{10}$$

where $|0\rangle$ now represents a valence band and $|1\rangle$ a conduction band single-particle state. Performing the wavevector integration recovers the half-integer QAHE obtained in independent-particle theories:16,31

$$\sigma_{xy} = \text{sign}(Y) \text{sign}(m) \frac{e^2}{2\hbar} \tag{11}$$

where by $Y$ we denote the sense of the vorticity of the momentum-space valence-band-spinor texture in the absence of a gap. The same result for the Hall conductivity can be obtained by using the Berry connection expression. For the massive Dirac model the line integral in Eq. (8c) is around a circle with radius $\Lambda$ such that $\nu \Lambda \gg m$. Eq. (8c) then simplifies to

$$\sigma_{xy} = \frac{e^2}{2\pi \hbar} \int_0^{2\pi} d\phi i \langle 0 | \frac{\partial}{\partial \phi} | 0 \rangle|_{k=\Lambda}. \tag{12}$$

where $\phi$ is the momentum orientation angle. We use this expression below to calculate the correction to the surface state Hall conductivity when electron-magnon interactions are included.

As explained previously, the half-quantized surface state Hall conductivity is expected to be invariant under weak perturbations. In Sec. II of the supplemental material we demonstrate explicitly that this expectation is confirmed when the massive Dirac single-particle Hamiltonian is perturbed by a weak spin-dependent disorder term. However, as we now show, corrections are finite when the Dirac surface-state quasiparticle interact with quantum fluctuations of the ordered state responsible for time-reversal symmetry breaking.

The origin of the interaction effect is schematically summarized in Fig. 2 where we illustrate (panels a-c) the surface-state band structure of the massless Dirac model, the massive Dirac model, and the Dirac model coupled to a bosonic mode. The band eigenstates can be viewed (panels d and e) as momentum-dependent spin-1/2 coherent states. When electron-magnon coupling is neglected the massive Dirac model spin has spin↓ orientation at the Dirac point $k = 0$, and an in-plane orientation at large $|k|$ with a finite vorticity, forming a meron. The $k = 0$ spin orientation fixes the gauge choice for the unperturbed spin-coherent states. Because of the large splitting between conduction- and valence-band states at large $|k|$ used to evaluate the Berry connection, electron-magnon scattering coherently mixes primarily $n = 0$ and $n = 1$ magnon states, leaving the electronic state in the valence band. The Hall conductivity correction is due in part to the reduced weight of the $n = 0$ valence-band state responsible for the non-interacting Hall effect, and in part due to the momentum-orientation coherence between $n = 0$ and $n = 1$ states which changes the sign of the $n = 1$ Berry connection contribution. In panel f of Fig. 2 we plot the Berry connection integral of Eq. (12), calculated as a function of $|k|$ both neglecting and including electron-magnon interactions. For large $|k|$ the interacting model does not converge to the quantized value of 1/2 but obtains an interaction correction. The calculation is described in greater detail below.

At leading order in perturbation theory, corrections are obtained by summing over contributions from distinct boson modes, and the boson Hilbert space can be truncated to occupation numbers 0 and 1. To bring out the physics of the interaction correction as simply as possible we focus first on the contribution from interactions...
FIG. 2. (Color online) Band structure for a) a pure \((\hbar v = 1, m/v = 0)\) Dirac model, b) a massive \((m/v = 1)\) Dirac model, and c) a massive Dirac model interacting with momentum \(p = 0\) magnons restricted to occupation numbers 0 and 1 \((A^{-1/2}M_{21} \Omega/v = 1/3, \omega/v = 1/2)\). Panel d) shows the momentum space spin texture of the ground state of the pure Dirac model in which spins projections lie in the \(xy\) plane and rotate along with the momentum direction. Panel e) shows the spin texture of the massive Dirac model with a momentum-space vortex centered at \(k = 0\). The spin is in the \(-\hat{z}\) direction at \(k = 0\). (The color code denotes the \(z\) component of the spins.) Panel f) shows the result of Eq. (12) in units of \(e^2/(2\hbar)\) as a function of \(|k|\) in the non-interacting and the electron-spinwave-interacting 2D massive Dirac model. For large \(|k|\) the interacting model does not converge to the quantized value of \(e^2/(2\hbar)\) but obtains a correction given by \([-\Omega/\omega^2/2] \times e^2/(2\hbar)\).
of the mass $m$ and/or the vorticity of momentum-space spin texture. ($\chi = \text{sign}(\nabla)(\phi + \pi/2)$.)

Because the valence-band states on $\partial DP$ vary with momentum on the scale of $\Lambda$, the magnon-mode Hall conductivity correction calculation at finite $p$ is unchanged relative to $p=0$ provided that the momentum magnitude $|p|$ is much smaller than $\Lambda$. An expression for the Hall conductivity correction valid for arbitrary quasiparticle-boson interaction vertex and arbitrary surface-state band-structure model requires a lengthy and detailed calculation, and is provided in Sec. 1B of the supplemental material. Note that the general expression for the interaction correction to the Hall conductivity is odd, as required, under time-reversal.

The contribution of a single magnon mode to the Hall conductivity interaction correction is inversely proportional to the surface area of the system. However, the correction to the Hall conductivity varies slowly with magnon momentum $p$ provided $p$ is close to the Dirac point. Summing over magnons with momenta inside DP we predict an overall correction proportional to $(A_{DP}/M_0)(m/\omega)^2$, where $A_{DP}$ is the area in momentum space of the Dirac point region DP. Since the gap in the magnon spectrum, due either to weak external fields used to saturate the magnetization or to the perpendicular magnetic anisotropy of magnetically doped TI thin films, is typically smaller than the gap produced in the surface-state quasiparticle spectrum, the interaction correction can be large even when $m \ll v\Lambda$. A large interaction correction to the magneto-electric coefficients of TI thin films is present even when time-reversal symmetry breaking is weak when measured by the size of the surface-state gap it produces. This result, which may seem surprising, is in fact natural because of the strong spin-orbit coupling inevitably present in TIs. A magnetic order parameter in a magnetically doped TI will never be a good quantum number. Quantum fluctuations of the magnetic condensate interact with surface-state quasiparticles and cause the system’s broken time-reversal symmetry to be manifested even in quasiparticles that are far from the Dirac point.

#### IV. MAGNETO-ELECTRIC COUPLING MEASUREMENTS

Magneto-electric coupling is most easily detected by examining the magnetic field dependence of dielectric properties. These measurements require that the sample under study is a reasonable good insulator. For a diluted-moment magnetically ordered TI thin film, the quasiparticle mass and the quasiparticle vorticity are both opposite in sign on top and bottom surfaces. It follows that, although the Hall conductivities of the top and bottom surfaces both have corrections, they differ in sign. The total Hall conductivity of the thin film is not altered by the interaction corrections we have calculated. Verification of our prediction requires a direct measurement of magneto-electric coupling in TI thin films. A TI differs from an ordinary insulator mainly via its protected surface states, and these complicate the task of measuring the magneto-electric effects discussed here. In particular, electrical measurements of a magnetic field dependent film polarization are not possible when the system has a non-zero total Hall conductivity, because this is necessarily associated with edge states which are localized on side walls and short the top and bottom surfaces of the film. A magnetized TI thin film is truly insulating at sufficiently low temperature if a domain wall is present between top and bottom surfaces. Even though the domain wall energies of TI-based diluted magnetic semiconductors are not known and may be quite small, this scenario seems difficult to achieve. As recently discussed in Ref. 35, however, electrical measurements should be feasible when the top half of the thin film is doped with Cr ions and the bottom half with Mn ions. These atoms have exchange interactions with surface-state electrons that have opposite sign. When they are aligned by a weak magnetic field, the sign of the effective exchange field on top and bottom surface Dirac cones is opposite. In terms of the massive Dirac models we have studied in this paper, this circumstance implies that there are no side wall states and that while the signs of the momentum-space vorticities on the top and bottom surfaces are opposite, the masses have the same sign. Because the total Hall conductivity is zero in this case, there should be an energy range over which there are no side wall states. The individual surface Hall conductivities are non-zero however, and they can be measured electrically by detecting current flow between top and bottom surfaces as magnetic field strength is varied. We predict that this measurement will identify an interaction correction to the surface state Hall conductivity. Similar interaction corrections which contribute to the valley Hall effect but cancel out in the total anomalous Hall effect occur in honeycomb lattice Dirac systems when the quasiparticle-boson interaction is sublattice dependent.

#### V. CONCLUSIONS

The surface Hall conductivity of an insulator is proportional to its magneto-electric polarizability, i.e. to the coefficient which describes how the polarization of a film depends on magnetic field strength. By explicitly evaluating the surface Hall conductivity of surface states described by a massive Dirac model, we have shown that there is a non-universal interaction correction to the quantized magneto-electric coefficient of thin films formed from TIs. Corrections to the top and bottom surface Hall conductivities cancel, however, implying that there is no correction to the quantized anomalous Hall effect in magnetically doped TIs. The interaction correction to the magneto-electric polarizability can be measured electrically only when the total Hall conduc-
tivity of top and bottom surfaces is made to vanish, for example by aligning local moments with opposite signs of exchange coupling to the Dirac surface states, for example in a setup where the top half and bottom half of the TI are doped by aligned local moments with opposite signs of exchange coupling to the Dirac surface states.

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nomic system with a finite number of magnon modes at each 2D wavevector. To demonstrate that interactions with magnons correct the surface Hall conductivity, it is sufficient to consider only the lowest energy magnon branch in which the magnetization orientation does not fluctuate as a function of position within the film. The surface-state-magnon interaction strength can be related to the quasiparticle energy gap and the thin film magnetization per unit area by general arguments. See A. H. MacDonald, T. Jungwirth, and M. Kasner, “Temperature Dependence of Itinerant Electron Junction Magnetoresistance,” Phys. Rev. Lett. 81, 705 (1998).

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