Persistent currents and spin torque caused by percolated quantum spin Hall state

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Motivated by recent experiments, we investigate the quantum spin Hall state in 2D topological insulator/ferromagnetic metal planar junctions by means of a tight-binding model and linear response theory. We demonstrate that whether the edge state Dirac cone is submerging into the ferromagnetic subbands and the direction of the magnetization dramatically affect how the edge state percolates into the ferromagnet. Despite the percolation, spin-momentum locking of the edge state remains robust in the topological insulator region. In addition, laminar flows of room temperature persistent charge and spin currents near the interface are uncovered, and the current-induced spin torque is found to be entirely field-like due to the real wave functions of the percolated edge state and the quantum well state of the ferromagnet.

I. INTRODUCTION

The quantum spin Hall effect (QSHE) represents one of the important properties of two-dimensional (2D) time-reversal (TR) invariant topological insulators (TIs). Owing to the existence of edge states, the defining feature of QSHE is the spin current circulating the edge of the system, which motivates a variety of edge state based topological spintronic devices. To exploit the edge spin current, the TI is often made in conjunction with a ferromagnetic metal (FMM), for instance in three-dimensional (3D) TI/FMM heterostructures, such that the magnetization can be used to affect the edge spin transport or vice versa. On the theoretical side, a significant amount of work has been dedicated to understanding the complicated spintronic mechanisms in such a hybrid structure. However, to delineate an adequate theoretical description, it is crucial to understand how the QSH state is altered when the TI is made in conjunction with a metallic material, especially given that the boundary condition of the edge state wave function is modified.

In this article, we show that the modification of QSH state in a 2D TI/FMM planar junction depends significantly on whether the edge state Dirac cone submerges into the FMM subbands, as well as on the direction of the magnetization. These factors strongly influence the percolation of the edge state into the FMM, which nevertheless remains a symmetry eigenstate in the TI region. We uncover a number of peculiar dissipationless responses, including the existence of room temperature persistent charge and spin currents that manifest as laminar flows. Moreover, we elaborate that the real wave function of the percolated edge state is crucial to the direction and magnitude of the current-induced spin torque.

The structure of the article is organized in the following manner. In Sec. II A, we detail the lattice model for the 2D TI/FMM junction, and delineate two different types of band structures and the corresponding percolation of topological edge states in Sec. II B. We proceed to demonstrate that the asymmetric band structure yields a laminar flow of persistent charge current, as well as elaborating the proximity induced persistent spin current in the system in Sec. II C. The current-induced spin torque is investigated by means of a linear response theory in Sec. II D, where we emphasize the field-like nature of the spin torque due to the real wave functions of the percolated edge state and the quantum well state of the FMM. Section III summarizes the results.

II. BHZ/FMM PLANAR JUNCTION

A. Lattice model

To properly address the percolation of the edge state, we employ a tight-binding model approach similar to that used for 3D TIs. For concreteness, we consider a strip of 2D Bernevig-Hughes-Zhang (BHZ) model of width $N_{y,TI}$ in conjunction with a strip of 2D FMM of width $N_{y,FMM}$, as indicated in Fig. 1(a). Periodic boundary condition (PBC) in the longitudinal $x$ direction and open boundary condition (OBC) in the transverse direction $y$ are imposed, i.e., a closed BHZ/FMM ribbon. The BHZ region is composed of the spinful $s$ and $p$ orbitals $\psi = (s \uparrow, p \uparrow, s \downarrow, p \downarrow)^T$, with the Dirac matrices $\gamma_i = \{\sigma^x \otimes \sigma^x, I \otimes s^y, I \otimes s^z, \sigma^y \otimes \sigma^x, \sigma^z \otimes s^x, \sigma^x \otimes \sigma^z\}$ and the TR operator $T = -i\sigma^y \otimes IK$, where $\sigma^b$ and $s^b$ are Pauli matrices in the spin and orbital spaces, respectively. The continuum model reads

$$H(k) = \sum_{i=1}^{3} \epsilon_i(k) \gamma_i = A \sin k_x \gamma_1 + A \sin k_y \gamma_2 + (M - 4B + 2B \cos k_x + 2B \cos k_y) \gamma_3. \quad (1)$$

where $A$ and $B$ are kinetic parameters, and $M < 0$ is the topologically nontrivial phase that hosts the edge state. We now detail the lattice model of the BHZ/FMM ribbon. Due to the proximity to the TI, the conduction band of the FMM is assumed to be split into $s$-like and $p$-like orbitals, both are subject to the magnetization $\mathbf{S}$ of the FMM through an exchange coupling. The model is described by

$$H(k) = \sum_{i=1}^{3} \epsilon_i(k) \gamma_i = ...$$
In order to maintain the bulk gap and demonstrate the edge states on the two opposite edges overlap. For this reason we reduce the artifact of using a lattice model to simulate the continuous monoplicics will wash out the bulk gap. This is obviously an artifact of using a lattice model if we take the value of $t = 1.7\text{eV}$ as energy unit). However, we find that in the lattice model, if we take the value $t = 1.7\text{eV}$ as energy unit throughout the article (that is, we take 1.7eV as energy unit). Hence we reduce the artifact of using a lattice model to simulate the continuous HgTe quantum well. For this reason we reduce the energy unit. The magnetization of the FMM is denoted by $S = S(\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$. To make connection with the real HgTe quantum well parameters, the hopping parameters are

$$A = 2t \approx -3.4\text{eV}, \quad B = -t' \approx -17\text{eV} = 10t. \quad (3)$$

We will treat the hopping $t = A/2 = -1.7\text{eV} \equiv -1$ as the energy unit throughout the article (and we will treat the hopping $t = -1.7\text{eV} \equiv -1$ as the energy unit throughout the article). However, we find that in the lattice model, if we take the value $t = -10t = 10$, then the energy spectrum does not clearly show a gap. This is obviously because the higher order term in the $d_0$ component. If we simulate it with $4t' - 2t' \cos k_x - a - 2t' \cos k_y a$ with a large hopping amplitude $t'$, then this large harmonics will wash out the bulk gap. This is obviously an artifact of using a lattice model to simulate the continuous HgTe quantum well. For this reason we reduce the hopping $t = -10t = 10$ to $t' \approx -1$ in our lattice model in order to maintain the bulk gap and demonstrate the edge state.

The other approximation we will use is about the mass term $M$. In reality, $A/M = 2t/M$ gives the decay length of the edge state. Because we will simulate the system on a lattice size of the order of $10 \times 10$ sites, this means the decay length cannot exceed few lattice sites, otherwise the edge states on the two opposite edges overlap. Therefore for our simulation we choose the mass term to be $M = -1$, which is quite different from real HgTe quantum wells. The calculations of persistent currents and the magnetoelectric susceptibility (see below) are performed at room temperature $k_B T = 0.03$. Finally, the interface hopping, assumed to be between the same orbital and spin species, is fixed at $t_B = 0.8$ for concreteness. In summary, we use the parameters

$$-t = t' = -M = t_F = 1, \quad \mu = 0, \quad \mu_F = 0.5 \text{ (pristine)}$$

$$\mu_F = -0.5 \text{ (submerged)}, \quad t_B = 0.8, \quad J_{ex} = 0.1, \quad k_B T = 0.03$$

We emphasize that the statements made in the present
work are fairly robust against the change of these parameters.

FIG. 2. The band structures of the BHZ/FMM ribbon with directions of the magnetization along \( S \parallel \hat{x} \) or \( S \parallel \hat{y} \), for either the pristine \( \mu_F = 0.5 \) or the submerged \( \mu_F = -0.5 \) type. The edge state wave function and spin polarization of the corresponding states in the dispersion are shown in the same colors.

B. Band structure and percolation of the edge state

The band structure \( E(n, k_x) \) can be solved by a partial Fourier transform

\[
c_i I \sigma = c_{x_0 y_0} = \sum_k c_{k x} e^{i k x} c_{k y} y_0 \sigma,
\]

where \( c_i I \sigma \) is the electron annihilation operator of orbital \( I = \{s, p\} \) and spin \( \sigma = \{\uparrow, \downarrow\} \) at site \( i = \{x, y\} \). For comparison, in Fig. 1(b) we show the band structure when the BHZ and the FMM are uncoupled \( t_B = 0 \), in which the edge state Dirac cone and the quadratic FMM bands are clearly distinguishable. The FMM wave functions are confined quantum well states since the FMM is sandwiched between the TI and the vacuum. Figure 1(c) shows what we call the pristine type of band structure for the coupled BHZ/FMM strip simulated by \( \mu_F = 0.5 \) and interface hopping \( t_B = 0.8 \), and the corresponding percolations of the edge state, with magnetization pointing along the spin polarization of the edge state \( S \parallel \hat{z} \). The Dirac cone remains gapless, and at larger momenta gradually merges with the FMM subbands of the same spin polarization. As going from small to large momentum, the edge state wave function

\[
|\psi|^2 = \sum_{I \sigma} |\psi_{I \sigma}|^2
\]

gradually evolves from that highly localized at the edge to a profile that merges with the FMM quantum well state of the first harmonic. The other type of band structure simulated by \( \mu_F = -0.5 \) is what we call the submerged type where the Dirac point overlaps with the FMM subbands, as shown in Fig. 1(d). In this case the Dirac cone is highly distorted due to the coupling to the FMM subbands. Tracking the states originating from the Dirac cone shows that the Dirac cone splits into different branches, each branch hybridizes with the FMM quantum well state of a different harmonic, such as the second harmonic shown by the \( |\psi|^2 \) in Fig. 1(d). The percolation in both situations also increase with the interface hopping \( t_B \), as expected (not shown). Finally, whether the Dirac point submerges into the FMM subbands also depends on the number of the FMM subbands, which is given by the width \( N_{y,FM} \) of the FMM. For either the pristine or submerged situation, the edge state at the vacuum/BHZ interface at \( y = 1 \) is unaffected by the contact to the FMM at \( y = N_{y,TI} \) interface, and the Dirac cone therein remains undistorted.

The simulations for the two other magnetization directions \( S \parallel \hat{x} \) and \( S \parallel \hat{y} \) that are orthogonal to the spin polarization of the edge state are shown in Fig. 2. The results reveal a remarkable feature, namely despite the percolation and merging with the quantum well states, the spin polarization of the edge state wave function in the BHZ region remains quantized along \( \hat{z} \) regardless of the magnetization direction, meaning that it remains as the symmetry eigenstate of \( \sigma_z \). In other words, the spin-momentum locking is strictly preserved in the TI region. In contrast, the wave function in the FMM region is quantized in the plane spanned by \( S \) and \( \hat{z} \), so the spin-momentum locking is distorted in this region. For instance, for either the pristine or the submerged type of band structure, the spin polarization in the \( S \parallel \hat{x} \) case entirely lies in the \( xz \)-plane. As we shall see in Sec. II D, such a peculiar spin texture eventually yields a current-induced spin torque that is entirely field-like.
C. Laminar charge and spin currents

The dispersion for either the pristine or submerged situation becomes asymmetric between $+k_x$ and $-k_x$ when the magnetization has a component along the spin polarization of the edge state $S_z$, as shown in Fig. 3(b). This is because such a component makes one branch of the Dirac cone more energetically favorable than the other, similar to what occurs in 2D magnetized Rashba systems. Although this asymmetry motivates us to speculate the existence of a persistent charge current, one should keep in mind that an asymmetric dispersion does not yield a nonzero net current. This can be seen by noticing that the expectation value of the velocity operator $v_x$ for the eigenstate $|u_{n,k_x}\rangle$ is simply the group velocity

$$\langle u_{n,k_x}|v_x|u_{n,k_x}\rangle = \langle u_{n,k_x}|\frac{1}{\hbar}\frac{\partial H}{\partial k_x}|u_{n,k_x}\rangle = \frac{\partial E(n,k_x)}{\hbar \partial k_x}. \quad (5)$$

The expectation value of the current operator integrated over momentum vanishes identically

$$\langle v_x \rangle = \sum_n \int \frac{dk_x}{2\pi} \frac{\partial E(n,k_x)}{\hbar \partial k_x} f(E(n,k_x)) = 0, \quad (6)$$

where $f(E(n,k_x)) = 1 / (e^{E(n,k_x)/k_B T} + 1)$ is the Fermi function, and hence there is no net current.

$$\langle J^x \rangle = \sum_n \int \frac{dk_x}{2\pi} \frac{\partial E(n,k_x)}{\hbar \partial k_x} f(E(n,k_x)),$$

where $f(E(n,k_x)) = 1 / (e^{E(n,k_x)/k_B T} + 1)$ is the Fermi function, and hence there is no net current.

However, the local current is nonzero. This can be seen by evaluating the charge and spin currents directly from the lattice model according to the following procedure. First, the BHZ model does not commute with $\sigma^x$ and $\sigma^y$, so we only investigate the longitudinal charge current and the spin current polarized along $\sigma^z$, and consider the charge/spin polarization operator

$$P^a = \sum_{iI\eta\lambda} x_i c_{iI\sigma}^\dagger \sigma^a_{\eta\lambda} c_{iI\lambda} = \sum_{I\eta\lambda} P^a_{I\eta\lambda}, \quad (7)$$

where $x_i$ is the longitudinal coordinate of site $i$, and $\sigma^a = \{\sigma^0, \sigma^z\} = \{I, \sigma^z\}$. The current operators are then $J^a = P^a = \frac{1}{\hbar} [H, P^a]$, as calculated explicitly in Appendix A. The ground state expectation value of the current operator gives the local current

$$\langle J^a \rangle = \sum_n \langle n|J^a|n \rangle f(E_n), \quad (8)$$

where $|n\rangle$ is the eigenstate with eigenenergy $E_n$ of the BHZ/FMM lattice model, and one may separate $\langle J^a \rangle$ into contributions from each bond connecting site $i$ and $i + a$ to investigate the local current.

The longitudinal charge current as a function of transverse coordinate $\langle J^0(y) \rangle$ is shown in Fig. 3, which features a laminar current whose direction of flow depends on $y$. The net current vanishes up to numerical precision, in accordance with Eq. (5). The local current is finite only when the magnetization has an out-of-plane component $S_z$, a feature inherited from the asymmetric band structure. A close inspection reveals that both the charge and spin currents arise from contributions not only from the edge states, but from all the subbands. This makes the currents easily persist up to room temperature, which is an advantage over that induced at the topological superconductor/FMM interface. For our choice of parameters, the magnitude of the current is of the order of $\langle J^0(y) \rangle \sim 10^{-5} e \tau /h \sim 10^{-7}$ A, and the flow direction alternates between $+\hat{x}$ and $-\hat{x}$ at the length scale of lattice constant $\sim$ nm. The Ampere’s circuital law $B = \mu_0 (\langle J^0(y) \rangle) /2\pi r$ then indicates that at a distance $r \sim$ nm above the surface, the laminar current produces a magnetic field $\sim 10$ Oe that points along $\hat{y}$ and alternates at the length scale of nm. Thus although the laminar current is not expected to manifest in the transport properties, the alternating magnetic field it produces should in principle be measurable.

Concerning the spin current, we first remark that the BHZ model alone does not produce a net edge spin current if the Dirac point locates at the chemical potential. This is because the spin current caused by the edge state is canceled out by the contribution from the BHZ bulk bands that are also spin polarized. As shown in Fig. 4 (a), the dispersion of the BHZ ribbon displays the well

FIG. 3. The laminar charge current $\langle J^0(y) \rangle$ and spin current $\langle J^z(y) \rangle$ as a function of transverse coordinate $y$, at different magnetization directions $S \parallel \{\hat{x}, \hat{y}, \hat{z}\}$ and for either the pristine or submerged type of band structure. The charge current is nonzero only when the magnetization has a $\hat{z}$ component.

FIG. 4. (a) The dispersion of BHZ ribbon of width $N_y = 10$, with Dirac point located at chemical potential, and (b) the resulting persistent spin current versus transverse coordinate $\langle J^z(y) \rangle_{cut}$ calculated by summing only the states within an energy window $|E(n,k_x)| < E_{cut}$. The $E_{cut} = 1$ case includes only the Dirac cone contribution, whereas the $E_{cut} = 8$ case sums over the entire band structure.
known edge state Dirac cone with spin polarized along \( \hat{z} \), and the Dirac point is located at zero energy. The persistent charge current \( \langle J^0(y) \rangle \) is zero everywhere. Quite surprisingly, the spin current \( \langle J^z(y) \rangle \) at either the edge \( y = 1 \) or the edge \( y = N_y/T_I \) also vanishes even though the Dirac cones consist of counter propagating spins at both edges. To understand this, we calculate the spin current in the lattice model by summing the states within an energy window \( E_{\text{cut}} \) around the chemical potential

\[
\langle J^z \rangle_{\text{cut}} = \sum_n \langle n | J^z | n \rangle f(E_n) \theta(E_{\text{cut}} - |E_n|).
\]

As shown in Fig. 4(b), the \( E_{\text{cut}} = 1 \) case that includes only the Dirac cone contribution has a finite spin current, but the \( E_{\text{cut}} = 8 \) case that sums over the entire band structure gives a zero spin current. In other words, the contribution from the bulk bands cancels out that from the edge state Dirac cone to yield a zero spin current. A finite spin current occurs only when the Dirac point is shifted away from the chemical potential. On the other hand, when the BHZ model is made in conjunction with an FMM, a persistent spin current is produced for both the pristine and the submerged cases, and is a laminar flow that percolates into the FMM, as shown in Fig. 3. Such a laminar spin current appears regardless of the direction of the magnetization and the energy of the Dirac point.

**D. Current-induced spin torque**

The components \( b = \{x, y, z\} \) of the spin polarization induced by a longitudinal electric field \( E(i,t)\hat{x} \)

\[
\sigma^b(i,t) = \chi^b(i,\omega)E(i,t).
\]

in our lattice model can be formulated within a linear response theory, where the real part of the DC magnetoelectric susceptibility is calculated by

\[
\lim_{\omega \to 0} \text{Re} \chi^b(i,\omega) = - \sum_j \sum_{m,n} \langle n | \sigma^b(i) | m \rangle \langle m | J^0(j) | n \rangle \tilde{F}(E_n, E_m),
\]

as detailed in Appendix B. The function \( \tilde{F}(E_n, E_m) \) is highly peaked at \( E_n \approx E_m \approx 0 \), meaning that the states at the Fermi surface contribute the most to the response, as expected, which include both the Dirac cone-like bands and the FMM-like subbands according to Fig. 1(c) and (d). We focus on the DC magnetoelectric susceptibility

\[
\lim_{\omega \to 0} \text{Re} \chi^b(i,\omega) \equiv \chi^b(y)
\]

as a function of transverse coordinate \( y \). The simulation for the BHZ model alone yields a nonzero \( \chi^x(y) \) component at the two edges, as shown by the orange line in Fig. 5(a). This indicates the Edelstein effect, i.e., current induced spin polarization, caused by the edge state, analogous to that occurs in 3D TIs. Assuming a constant mean free time \( \tau \approx 5 \times 10^{-14}s \), at a typical experimental electric field strength \( E \sim 10^4\text{kgm/Cs} \) the induced spin polarization at the edge is of the order of \( 10^{-7} \) (in units of \( \mu_B \)). In contrast, when the BHZ model is made in conjunction with the FMM, the magnitude of \( \chi^b(y) \) is dramatically enhanced by one to two orders of magnitude even at a very small interface hopping \( t_B = 0.2 \), and the spatial profile of \( \chi^b(y) \) extends into the FMM for both the pristine and the submerged situations, as shown in Fig. 5. The band structures in Fig. 1(c) and (d) naturally explain this enhancement: Compared to an isolated BHZ model, the BHZ/FMM junction has many additional FMM states at the chemical potential \( \{n \rangle \) and \( \{m \rangle \) in Eq. (11) \) that participate in the particle-hole excitation process of the magnetoelectric response. Moreover, the FMM wave functions and the edge state wave functions have a significant overlap due to percolation of the edge state, yielding nonzero matrix elements \( \langle n | \tilde{O} | m \rangle \) in Eq. (11). Notice that the an isolated FMM does not exhibit Edelstein effect, so the nonzero \( \chi^b(y) \) in the FMM region \( y \in FM \) entirely originates from the proximity to the BHZ model.

The average magnetoelectric susceptibility in the FMM region \( \chi_F^E \equiv \sum_{y \in FM} \chi^E(y)/N_y,F_M \) is what yields the spin torque on the magnetization \( \mathbf{S} \). Since the current-induced spin polarization is polarized along \( \hat{z} \) at the edge of an isolated BHZ model, it is customary to define the field-like torque in the FMM to be along \( \hat{S} \times \hat{z} \) and the damping-like torque to be along \( \hat{S} \times (\hat{S} \times \hat{z}) \), as in the usual metallic thin film spin-transfer torque (STT) devices. We find that the components of the magnetoelectric susceptibility \( \chi_F^E \equiv \{\chi_F^x, \chi_F^y, \chi_F^z\} \) entirely lie...
on the plane spanned by $S$ and $\hat{z}$, indicating the spin torque is entirely field-like. If the magnetization lies in the $xy$-plane, then only the $\chi^b_F$ component is nonzero. This is very different from the STT in usual metallic heterostructures\cite{32,33} or that induced by the spin Hall effect\cite{34,35} where the propagation of plane waves can accumulate a phase difference between spin up and down components that eventually contributes to a damping-like torque. In contrast, the percolated edge state and the quantum well state, with a magnitude greatly enhanced by the presence of the FMM, the current-induced spin torque is found to be entirely field-like due to the real wave function of the FMM quantum well state wave functions are completely real and hence do not support such a spin-dependent phase, rendering an entirely field-like torque (we neglect other complications such as spin-orbit torques\cite{36,37} and spin relaxation). At a typical external electric current $j_e \sim 10^{11}$ A/m$^2$, the spin polarization obtained from Eq. (10) yields a spin torque according to the Landau-Lifshitz dynamics

$$\frac{dS}{dt} = \frac{J_{ex}}{\hbar} S \times \left[ \frac{1}{N_{y,FM}} \sum_{i \in FM} \sum_{\sigma} \delta(i) \right]. \quad (12)$$

which is basically the numerical values of $\chi^b_F$ multiplied by GHz, as demonstrated in Appendix A\cite{6}. This magnitude is close to that observed in 3D TI/FMM by films\cite{6}.

### III. CONCLUSIONS

In summary, we address the percolation of QSHE into an adjacent FMM by means of a lattice model. The band structure displays a pristine/submerged dichotomy due to the difference in work functions, which strongly influences the percolation of the edge state. Moreover, despite the percolation and merging with the quantum well state of the FMM, the spin momentum-locking of the edge state in the TI region remains unaltered. A laminar flow of persistent charge current owing to the asymmetry of the band structure is uncovered, and the edge spin current also turns into a laminar flow that percolate into the FMM. The current-induced spin torque is found to be entirely field-like due to the real wave function of the percolated edge state and the quantum well state, with a magnitude greatly enhanced by the presence of the FMM subbands. Finally, although we restrict our discussions to 2D, we anticipate that these features can also manifest in the contact between TI and FMM in other dimensions, which await to be clarified.

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### Appendix A: The current operators

The charge and spin current operator of this lattice model can be calculated conveniently in the following manner. Firstly, the system is translationally invariant along $\hat{x}$, so we only calculate the currents flowing along $\hat{x}$. In the calculation of the current operator from the polarization operator $J^a = P^a = \frac{i}{\hbar} [H, P^a]$, one may simplify the tedious commutator $[H, P^a]$ from the following general consideration. Since only hopping terms in Eq. (2) contribute to the current operator, we focus on these terms that generally take the form

$$H^\delta_{LaM\beta} = \sum_j T^\delta_{LaM\beta} \sigma_j^1 L\alpha c_j + \delta M\beta c_j L\alpha,$$

(A1)

which describes the hopping of electron between site/orbital/spin $j L\alpha$ and $j + \delta M\beta$ along the planar directions $\delta = \{a, b\}$, with $T^\delta_{LaM\beta}$ the hopping amplitude. Using the fact that the hopping part of the total Hamiltonian is the summation of $H_t = \sum_\delta \sum_{LaM\beta} H^\delta_{LaM\beta}$, we obtain that a specific orbital/spin species $I\eta \lambda$ contributes to the charge current ($a = 0$) and the spin current ($a = z$) by following the definition in Eq. (7).

$$J_{I\eta \lambda}^a = \frac{i}{\hbar} \sum_\delta \sum_{LaM\beta} \{H^\delta_{LaM\beta}, P^a_{I\eta \lambda}\}$$

$$= \frac{i}{\hbar} \sum_\delta \sum_{LaM\beta} \left\{ \sum_{M\beta} [-x_i T^\delta_{LaM\beta}] c_i^\dagger \sigma_{\eta \lambda}^{\sigma} c_{i+aM\beta} + \sum_{M\beta} \left[ (x_i + a) T^\delta_{LaI\lambda} \right] c_i^\dagger \sigma_{\eta \lambda}^{\sigma} c_{i+aI\lambda} + \sum_{M\beta} \left[ (x_i - a) T^{\delta^*}_{LaI\lambda} \right] c_i^\dagger \sigma_{\eta \lambda}^{\sigma} c_{i+1aI\lambda} \right. + \sum_{M\beta} \left[ x_i T^{\delta^*}_{I\eta M\beta} \right] c_i^\dagger \sigma_{\eta \lambda}^{\sigma} c_{i+1aM\beta} \right\}. \quad (A2)$$

We then put in all the nonzero hopping amplitudes $T^\delta_{LaM\beta}$ and $T^{\delta^*}_{LaM\beta}$ according to Eq. (2), and sum over all the $I\eta \lambda$ species. The resulting charge current operator reads
where \( \eta = 1, \eta_l = -1, \) and \( i \in T I, i \in F M \) and \( i \in B D \) indicate that the sites \( i \) and \( i + a \) belong to the BHZ model part, the FMM part, and the interface bonds. Likewise, the operator for spin current polarized along \( z \) is

\[
J^z = \frac{1}{\hbar} \sum_{i \in T I} \sum_{\sigma} \left\{ t c^\dagger_{i \sigma} c_{i + a \sigma} + t c^\dagger_{i + a \sigma} c_{i \sigma} + t c^\dagger_{i \sigma} c_{i + a \sigma} + t c^\dagger_{i + a \sigma} c_{i \sigma} \right\} \\
+ \frac{1}{\hbar} \sum_{i \in T I} \sum_{\sigma} \left\{ -it' c^\dagger_{i \sigma} c_{i + a \sigma} + it' c^\dagger_{i + a \sigma} c_{i \sigma} + it' c^\dagger_{i \sigma} c_{i + a \sigma} - it' c^\dagger_{i + a \sigma} c_{i \sigma} \right\} \\
+ \frac{1}{\hbar} \sum_{i \in F M} \sum_{\sigma} \left\{ -it_F c^\dagger_{i \sigma} c_{i + a \sigma} + it_F c^\dagger_{i + a \sigma} c_{i \sigma} - it_F c^\dagger_{i \sigma} c_{i + a \sigma} + it_F c^\dagger_{i + a \sigma} c_{i \sigma} \right\} ,
\]

(A3)

which is essentially the same as \( J^x \) except the spin up and down channel have an additional minus sign difference, as expected.

**Appendix B: Linear response theory for the magnetoelectric susceptibility**

To calculate the spin accumulation induced by a charge current, we employ the linear response theory for the local spin accumulation \( \sigma^b(i, t) \) in the presence of a perturbation \( H'(t') \) in the Hamiltonian

\[
\sigma^b(i, t) = -i \int_{-\infty}^{t} dt' \langle [\sigma^b(i, t), H'(t')] \rangle ,
\]

(B1)

where \( \sigma^b(i, t) = \sum_{\beta \gamma} \gamma^\dagger \beta \gamma c_{i \beta}(t) \beta \gamma c_{i \gamma}(t) \) is the \( b = \{ x, y, z \} \) component of the spin operator at position \( i \), and the fermion operators \( c_{i \gamma}(t) \) are defined in the Heisenberg picture. The perturbation comes from the longitudinal component of the vector field \( A(j, t) \) that induces the electric field and the current, and hence

\[
H'(t') = -\sum_{j} J^b(j, t') A(j, t') ,
\]

(B2)

where the vector field \( A(i, t) = A(i) e^{-i \omega t} \)

\[
E = -\partial_\beta V - \frac{\partial A}{\partial t} = \frac{\partial A}{\partial t} = i \omega A .
\]

(B3)

As a result, the commutator in Eq. (B1) reads

\[
[\sigma^b(i, t), H'(t')] = \frac{i}{\omega} \sum_{j} e^{i \omega(t - t')} E(j, t) [\sigma^b(i, t), J^b(j, t')] ,
\]

(B4)

since the electric field has a single wave length and frequency \( E(i, t) = E^0 e^{i q \cdot r - i \omega t} \). Consequently, the local spin accumulation in Eq. (B1) becomes

\[
\sigma^b(r, t) = \sum_{j} \int_{-\infty}^{t} dt' e^{i \omega(t - t')} \frac{1}{\omega} \theta(t - t') \times \langle [\sigma^b(i, t), J^b(j, t')] \rangle E(j, t) \\
= \sum_{j} \int_{-\infty}^{t} dt' e^{i \omega(t - t')} \frac{\pi^b(i, j, t - t')}{\omega} E(j, t) \\
= \sum_{j} \frac{i \pi^b(i, j, \omega)}{\omega} E(j, t) = \sum_{j} \chi^b(i, j, \omega) E(j, t) .
\]

(B5)

Here \( \chi^b(i, j, \omega) \) is the response coefficient for the contribution to the \( \sigma^b(i, t) \) at site \( i \) due to the longitudinal electric field \( E(j, t) \) applied at site \( j \). We will further assume that the electric field is constant everywhere, i.e., \( q \to 0 \) such that \( E(i, t) = E(j, t) = E^0 e^{-i \omega t} \). In this case,

\[
\sigma^b(i, t) = \left\{ \sum_{j} \chi^b(i, j, \omega) \right\} E(i, t) = \chi^b(i, \omega) E(i, t) ,
\]

(B6)

We aim to calculate the real part of the DC magnetoelectric susceptibility

\[
\lim_{\omega \to 0} \Re \chi^b(i, \omega) = \lim_{\omega \to 0} \Re \left\{ \frac{i}{\omega} \sum_{j} \pi^b(i, j, \omega) \right\} ,
\]

(B7)

Let \( |n \rangle \) be the eigenstate with eigenenergy \( E_n \) after diagonalizing the BHZ/FMM junction described by Eq. (2),
the retarded $\pi^b(i, j, \omega)$ operator is given by

$$
\pi^b(i, j, \omega) = \sum_{m, n} \langle n|\sigma^b(i)|m\rangle \langle m|J^0(j)|n\rangle J^0(j)|n\rangle \frac{f(E_n) - f(E_m)}{\omega + E_n - E_m + i\eta},
$$

(B8)

where $\eta$ is a small artificial broadening. Using $\eta/(x^2 + \eta^2) = \pi\delta(x)$, the limit in Eq. (B7) reads

\[-\lim_{\omega \to 0} \text{Re} \left\{ \frac{i}{\omega} \sum_j \pi^b(i, j, \omega) \right\} = \lim_{\omega \to 0} \left\{ \sum_{m, n} \langle n|\sigma^b(i)|m\rangle \langle m|J^0(j)|n\rangle \frac{f(E_n) - f(E_m)}{\omega + E_n - E_m + i\eta} \right\} = \lim_{\omega \to 0} \left\{ \sum_{m, n} \langle n|\sigma^b(i)|m\rangle \langle m|J^0(j)|n\rangle \frac{f(E_n) - f(E_m + \omega)}{\omega} \delta(\omega + E_n - E_m) \right\} \]

$$
= \sum_{m, n} \langle n|\sigma^b(i)|m\rangle \langle m|J^0(j)|n\rangle \left( \pi \frac{\partial f(E_n)}{\partial E_n} \right) \delta(\omega + E_n - E_m) = \sum_{m, n} \langle n|\sigma^b(i)|m\rangle \langle m|J^0(j)|n\rangle \tilde{F}(E_n, E_m),
$$

(B9)

where we have used the fact that $\langle m|\sum_j J^0(j)|n\rangle$ is real and even in $(n, m)$, Re $[\langle n|\sigma^b(i)|m\rangle]$ is even but Im $[\langle n|\sigma^b(i)|m\rangle]$ is odd in $(n, m)$, and the real part of $(1/\omega)(f(E_n) - f(E_m))/\omega + E_n - E_m + i\eta$ in the $\eta \to 0$ and $\omega \to 0$ limit is even in $(n, m)$ to eliminate several terms in the $\sum_{nm}$ summation. The function $\tilde{F}(E_n, E_m)$ can be further approximated by

$$
\tilde{F}(E_n, E_m) = \left( \pi \frac{\partial f(E_n)}{\partial E_n} \right) \delta(\omega - E_n - E_m) = \int d\omega \delta(\omega - E_n) \left( \pi \frac{\partial f(\omega)}{\partial \omega} \right) \delta(\omega - E_m) \approx \int d\omega \frac{\eta}{(\omega - E_n)^2 + \eta^2} \frac{1}{\pi} \frac{\partial f(\omega)}{\partial \omega} \frac{\eta}{(\omega - E_m)^2 + \eta^2}.
$$

(B10)

To summarize, we calculate the magnetoelectric susceptibility numerically by

$$
\lim_{\omega \to 0} \text{Re} \chi^b(i, \omega) = -\sum_j \sum_{m, n} \langle n|\sigma^b(i)|m\rangle \langle m|J^0(j)|n\rangle \tilde{F}(E_n, E_m),
$$

$$
\tilde{F}(E_n, E_m) = \int d\omega \frac{\eta}{(\omega - E_n)^2 + \eta^2} \left( \pi \frac{\partial f(\omega)}{\partial \omega} \right) \frac{\eta}{(\omega - E_m)^2 + \eta^2}.
$$

(B11)

The numerical values of $\chi^b(i)$ increases with the scattering rate $\eta = \hbar/\tau$, as expected. Using a typical value $\eta = 0.05t$ (mean free time $\tau \sim 5 \times 10^{-14}$s), we obtain a numerical value of $\chi^b$ of the order of $\mathcal{O}(1) \times ac/e \sim 10^{-9}$mC/J. Given the typical external charge current in experiment $j_c \sim 10^{11}$A/m$^2$ and the electrical conductiv-

The correspondence field is $E \sim 10^4$km/C$^2$, which yields a spin polarization $\sigma^b(i) \sim 10^{-5}$. Using $J_{ex} = 0.1$eV, the spin torque at this typical current density is essentially the numerical values of $\chi^b(i)$ averaged over the FMM sites and then multiplied by GHz.

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