Reflectionless Transport of Surface Dirac Fermions on Topological Insulators with Induced Ferromagnetic Domain Walls

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Three dimensional strong topological insulators (3D-STI) are a recently discovered class of materials, with a prominent example being Bi$_2$Se$_3$ [1]. Contrary to ordinary insulators, they exhibit topologically protected surface states with characteristic spin-momentum coupling, a result of strong spin-orbit interactions [2]. To exploit the full potential of these materials and for possible applications, a combination of the surface states with more conventional materials like ferromagnets or superconductors in proximity structure are desired. E.g., induced superconductivity gives rise to Majorana Fermions [3-6] and induced magnetization textures exhibit a quantized magneto-electric effect [7,8]. Ref. [9] is a recent review covering topological states of matter.

Proximity induced ferromagnetism, where the order parameter can in general be inhomogeneous and time-dependent gives rise to phenomena interesting for spintronics and magnetotransport [10-13]. Due to the spin-momentum locking, electrical current flow leads to a significant contribution to the spin-torque acting on the magnetization dynamics [11,13]. Magnetically doped 3D-STI could be used as a condensed matter realization of axion-electrodynamics [14]. The transport of Dirac-Fermions through DWs has been also studied in graphene [15].

In this Letter, we consider a transport configuration in which a single static domain wall (DW) is located between two contacts as illustrated in Fig. 1. We calculate the ballistic conductance for in-plane (IP) and out-of-plane (OOP) wall configurations. As our main result, the ballistic conductance for in-plane (IP) and out-of-plane (OOP) DW.

The general setup we study is illustrated in Fig. 1 and described by the effective Hamiltonian for the two-dimensional surface electrons

\[ H = i\hbar v \cdot (\hat{e}_z \times \nabla) - M \mathbf{m}(r) \cdot \mathbf{\sigma}. \quad (1) \]

Here, the first term is the dispersion of the surface Dirac states [17] and the second term is the proximity induced exchange coupling to the magnetization profile \( \mathbf{m}(r) \) with constant magnitude \( M \). Such a magnetization texture will occur naturally in films of magnetic materials, which we assume to be placed on top the topological insulator. The structure can in some limits be manipulated by an external magnetic field. We stress that the induced magnetization affects only the surface states and leaves the bulk conductivity of the 3D-STI unaffected - thus opening a possible path for disentangling the surface and bulk contributions to the conductivity.

The in-Plane Configuration The lower domain wall sketched in Fig. 1 has the explicit form \( \mathbf{m}(r) = (\cos \vartheta(x), \sin \vartheta(x), 0) \). We assume the angle \( \vartheta(x) \) has the analytical form \( \cos \vartheta(x) = \tanh(x/w) \). This shape can be obtained within a mean-field model with ferromagnetic exchange constant \( J \) and anisotropy constant \( K \), so that the length of the domain wall becomes \( w = \sqrt{J/K} \) [18]. Our problem is effectively one-dimensional and \( k_y \) is a good quantum number. We make the ansatz for the wave-function \( |\Psi(x, y)\rangle = e^{i\vartheta(x)} e^{ik_y y} |\psi(x)\rangle \), by which
The $m_y$-component is eliminated by the gauge factor, and end up with

$$H_{IP} = i\hbar v_\sigma \mathbf{\partial}_z + (i\hbar k_y - M \tanh(x/w))\sigma_x .$$

(2)

From now on, we choose units such that $\hbar = 1$ and restore them only in the final results.

In the homogeneous parts, we observe that the magnetization shifts the Dirac cone along the $k_y$-direction, which is also evident in the spectrum of this system shown in Figure 2a. The red and green cones correspond to the dispersions far away from the DW, so that the wave vectors in transport direction for the left (L) and the right (R) side obey $k^2_{L/R} = E^2 - (k_y \pm M)^2$ when we consider an eigenstate with energy $E$. The current operator is $j = (j_x, j_y) = v(-\sigma_y, \sigma_x)$. We find for incoming plane-wave states that the current points along $(k_{L/R}, k_y \pm M)$ corresponding to an angle $\gamma_{L/R} = \arctan((k_y \pm M)/k_{L/R})$ (see inset Fig. 2a).

We can solve the full eigenproblem $H_{IP}|\psi\rangle = E|\psi\rangle$ analytically by the substitution $z \equiv \frac{1}{\tau} (1 - \tanh \frac{x}{w})$, which gives two decoupled differential equations for $|\psi\rangle = (\varphi^+, \varphi^-)$. In order to bring these equations into hypergeometric form, we make the ansatz $\varphi^+(z) = (1 - z)^{-\frac{1}{2}k_Lw}z^{-\frac{1}{2}k_Rw} \phi(z)$ and find that

$$\{z(1-z)\partial^2_z + (\gamma - (\alpha + \beta) + 1)\partial_z - \alpha\beta\} \phi = 0$$

(3)

with the coefficients $\alpha = 1 + (M - ik_0)w$, $\beta = -(M + ik_0)w$ and $\gamma = 1 - ik_0w$, using $k_0 = \frac{1}{2}(k_L + k_R)$. This equation is known [19] and we directly write the solution

$$\varphi^+(z) = e^{-\frac{1}{2}(\gamma_M - \frac{z}{\sqrt{k_Rw}})}(1 - z)^{-\frac{1}{2}k_Lw}z^{-\frac{1}{2}k_Rw} 2F_1(\alpha, \beta, \gamma, z),$$

(4)

where $2F_1$ is the hypergeometric function. The solution for $\varphi^+$ can be obtained directly by using the symmetry $T_M T_{k_y} \sigma_y, H_{IP} \rangle = 0$, so that $\varphi^+_n(z) = -i T_M T_{k_y} \varphi^+_n(z)$ (we define symmetry operations as $T_M: M \rightarrow -M$ and similar for $k_y$ and $x$). The prefactor of this solution is chosen such that it directly reflects the symmetry properties of the system, i.e. $T_M T_{k_y} \sigma_y, |\phi^+_{k_y}\rangle = |\phi^+_{k_y}\rangle$.

Eq. 4 exhibits the different types of solutions illustrated in Fig. 2a, depending on whether $k_{L/R}$ are real or imaginary. In particular, the bound state spectrum follows for $k_L$ and $k_R$ being imaginary and we straightforwardly find $|2|\Delta| + 1$ bound states at energy $E_{n,0} = \pm \frac{2w}{\hbar^2} \sqrt{2\Delta - n}$, where we defined $\Delta \equiv \frac{w}{\hbar^2} = \frac{Mw}{2\hbar^2}$ with the magnetic length $l_M$. The dispersion along $k_y$ is $E_{n,k_y} = E_{n,0}\sqrt{1 - \frac{2w^2k_y^2}{(\Delta - n)^2}}$ and the states merge with the continuum at $k_y^{(n)}_{\text{max}} = (\Delta - n)^2/(w\Delta)$. Here, $n = 0$ describes a zero energy flat band for $|k_y| \leq M$ as also seen in Fig. 2a. Note that the square-root dependence of the energy on the quantum number $n$ is typical for Dirac Fermions, as for example in the case of Landau levels for Dirac Fermions [20].

The scattering solutions are described by real $k_{L/R}$ and are pairwise degenerate. We can use parity symmetry in the $x$-$y$-plane, i.e. $[H_{IP}, T_{k_y} \sigma_y] = 0$, in order to obtain the second orthogonal solution, $|\psi^{(IP)}_{-k_y, k_y}\rangle = -iT_{k_y} T_{k_y} \sigma_y |\psi^{(IP)}_{k_y, k_y}\rangle$. Here, $|\psi^{(IP)}_{k_y, k_y}\rangle$ describes an incoming wave from the left that is partially reflected and transmitted to the right side, and likewise, $|\psi^{(IP)}_{-k_y, k_y}\rangle$ describes an incoming wave from the right side. From the asymptotic behavior of Eq. 4, we can extract the transmission and reflection amplitudes and find the transmission probability

$$T_{IP}(E, k_y) = \frac{\sinh(\pi k_Lw) \sinh(\pi k_Rw)}{\sinh^2(\pi\Delta) + \sinh^2\left(\frac{\pi}{2} (k_L + k_Rw)\right)},$$

(5)

and the reflection probability $R_{IP} = 1 - T_{IP}$. In the regime of small externally applied voltage $V$, we calculate the linear conductance $G$ using the Landauer formula $G = G_Q \sum_{k_y} T(E_F, k_y)$, where $G_Q = e^2/h$ is the fundamental conductance quantum [21]. In the absence of the domain wall, the conductance for transport along the $x$-direction is $G_0 = G_Q \frac{W E_F}{\pi e^2}$ and $W$ is the transverse dimension of the ballistic contact.

To quantify the change of the conductance due to the presence of the domain wall, we define the domain wall resistance as

$$\delta G = -\frac{G_{DW} - G_0}{G_0} = \delta G_M + \delta G_{DW}.$$

(6)

We split this into two contributions: $\delta G_{DW}$ depends on the specific domain wall profile while $\delta G_M = \frac{M}{E_F} > 0$ is the fraction of totally reflecting channels (red shaded area in Fig. 2b) to the total number of transport channels (yellow + red areas). Essentially, $\delta G_M$ encodes the
For sharp walls, i.e. \( w \ll l_M \), we observe that \( \delta G_M \) strongly dominates, except for short walls where \( w \lesssim l_M \). As the Fermi level moves deeper into the metallic regime, we also see an overall decrease of the change in conductance. The limiting behaviors can be obtained analytically. For sharp walls, i.e. \( w \ll l_M \), we can approximately solve the integral and find \( \delta G_{\text{DW}} \rightarrow \frac{1}{2} \delta G_M \). Since \( \delta G_{\text{DW}} \) decreases when the wall width increases, we can conclude \( \delta G_{\text{DW}} \leq \frac{1}{2} \delta G_M \). In the limit of wide walls, i.e. \( w \gg l_M \), using the saddle point method, we find
\[
\delta G_{\text{DW}} \approx \frac{1}{2} \delta G_M \left( \frac{k_F^2}{2E_F} \right)^2 \frac{1}{w^2}.
\]

The ballistic domain wall resistance \( \delta G_{\text{DW}} \) decays with the inverse square of the domain wall width, but the contribution \( \delta G_M = \frac{M}{E_F} \) is also present in this limit and is the dominating one. Experimentally, one could subtract \( \delta G_M \) (for example determined in the absence of the DW) in order to obtain the contribution from the domain wall profile.

As the Fermi level comes close to the band edge \( E_F \approx M \), we have \( \delta G \rightarrow 1 \), i.e. the domain wall blocks all transport channels. However, when the Fermi level \( E_F \) approaches \( M \) and eventually reaches the crossing point of the left and right Dirac cones (crossing of red and green line in Fig. 2), the number of states available for transport drastically reduces and one reaches the point of minimal conductivity. At this point, transport is due to few evanescent modes, which is beyond the present study.

The out-of-Plane Configuration. The OOP wall has the magnetization profile \( m(\mathbf{r}) = (0, \sin \phi(x), \cos \phi(x)) \) which, in the language of the 2D-Dirac equation, describes a mass domain wall connecting two quantum anomalous Hall states of opposite chirality. We perform a spin rotation around the \( y \)-axis by \( \frac{\pi}{2} \) utilizing the unitary spin rotation matrix \( U = e^{-i\frac{\pi}{2} \sigma_y} \) to obtain the representation \( U H_{\text{OOP}} U^\dagger = H_{\text{IP}}(k_y = 0) - \hbar v_F \mu_2 \), which allows us to reuse the previous results. As inferred from the symmetry \( \{ H_{\text{IP}}, \sigma_z \} = 0 \), we see that \( k_y \sigma_z \) only couples pairs of positive and negative energy. Thus, we only have to diagonalize \( 2 \times 2 \) sub-blocks and straightforwardly obtain the full energy dispersion \( E_k = \pm \sqrt{M^2 + \hbar^2 v_F^2 (k_x^2 + k_y^2)} \) with corresponding eigenstates not presented here. The same applies to the bound states except for the zero energy state for \( k_y = 0 \), which is invariant under the operation of \( \sigma_z \), and thus directly yields the linearly dispersing chiral state plotted as black straight line in Fig. 2.

In the asymptotic expansion of \( |\psi_{k_y, k_x}| \) far away from the domain wall, we find that finite \( k_y \) only modifies the spinor structure and therefore the transmission coefficients remain independent of \( k_y \). Thus, the transmission probability can be directly obtained from \( \bar{\langle \psi \rangle} \) by setting \( k_L = k_R = k_x \), viz.,
\[
T_{\text{OOP}}(k_x) = \frac{\sin^2(\pi k_x w)}{\sin^2(\pi \Delta) + \sin^2(\pi k_x w)}.
\]

We observe that \( T_{\text{OOP}} \) features oscillations in \( w \) with period \( l_M \), and in particular, for DWs with \( \Delta \in \mathbb{N} \), i.e. the reflection is completely suppressed for any \( k_y \) and \( k_x \).

The ballistic domain wall resistance reads \( \delta G_{\text{OOP}} = \frac{1}{2E_F} \int_{k_y} \text{d} k_y R_{\text{OOP}}(\sqrt{k_y^2 - k_0^2}) \) with the Fermi wavevector \( \hbar v_{\text{F}} \). Since the spectrum is identical on both sides of the wall, \( \delta G_M = 0 \) here. This result is plotted in Fig. 3 and we recognize the oscillations in \( \Delta \) originating from \( T_{\text{OOP}} \). For the special points where the domain wall width is an integer multiple of the magnetic length, we find the domain wall to be completely transparent for the Dirac Fermions and \( \delta G \) drops to zero.

The change in conductance is plotted in Fig. 3 and we recognize the oscillations in energy. Thus, we only have to diagonalize \( 2 \times 2 \) sub-blocks and straightforwardly obtain the full energy dispersion \( E_k = \pm \sqrt{M^2 + \hbar^2 v_F^2 (k_x^2 + k_y^2)} \) with corresponding eigenstates not presented here. The same applies to the bound states except for the zero energy state for \( k_y = 0 \), which is invariant under the operation of \( \sigma_z \), and thus directly yields the linearly dispersing chiral state plotted as black straight line in Fig. 2.

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the Fermi level comes close to the band edge $E_F \approx M$, we have $\delta G_{\text{OOP}} \rightarrow 1$, as for the IP-configuration.

In the limit of wide walls $\Delta, k_F w \gg 1$, we obtain the approximate result

$$\delta G_{\text{OOP}} \xrightarrow{\Delta \gg 1} \frac{\log 2}{(\pi k_F w)^2} \mathcal{F}(\Delta), \quad (10)$$

with the modulation function $\mathcal{F}(\Delta) = \frac{2 \sin^2(\pi \Delta)}{1 + \sin^2(\pi \Delta)}$ which inherits the periodicity from $T_{\text{OOP}}$, in particular, $\mathcal{F}(\Delta)$ vanishes for integer $\Delta$. We see that the envelope decreases with $1/w^2$, similar to the result for the IP DW, Eq. (7). We find that the approximate formula fits well already for $\Delta \gtrsim 0.5$ and show in Fig. 3 the comparison between the full integration and the approximation (10).

In a realistic system, there is always impurity scattering which mixes channels with different $k$ and therefore reduces $\delta G_{\text{OOP}}$. However, as long as the wall width is much smaller than the mean free path, i.e. $w \ll \lambda_{\text{mfp}}$, our ballistic treatment is approximately correct. Impurities induce a finite scattering between the channels, however, due to the chiral nature of the electron dispersion, back-scattering is reduced. Thus, in the OOP case and when the DW conductance $\delta G$ is vanishing for reflectionless DW potentials, we expect $\delta G$ to remain significantly reduced in comparison to reflecting DWs for $\Delta \notin \mathbb{N}$.

**Supersymmetry.** The special characteristics of the domain wall resistance in the OOP geometry - the periodicity in $\Delta$ and the perfect transmission - can be understood as a supersymmetry encoded in the Hamiltonian $H_{\text{OOP}}$. Using the language of supersymmetry [24][25], we introduce the generalized creation $a^{\dagger}_{\Delta} = -\partial_{\xi} + \Delta \tanh(\xi)$ and annihilation operators $a_{\Delta} = \partial_{\xi} + \Delta \tanh(\xi)$ with dimensionless $\xi = x/w$. Introducing spin raising and lowering matrices $\sigma_{\pm} = (\sigma_x \pm i\sigma_y)/2$, the supercharges [24] are $Q_\Delta = a_{\Delta} \sigma_+ + a^\dagger_{\Delta} \sigma_-$. Using the supersymmetric hierarchy and the operators defined by $H_{\text{OOP}}$, the Hamiltonian reads

$$\mathcal{H} = \mathcal{U} H_{\text{OOP}} \mathcal{U}^\dagger = -Q_\Delta - Q^\dagger_\Delta + k_\nu \sigma_z.$$  

We observe that the operator defined by $\mathcal{H} = \{Q_\Delta, Q^\dagger_\Delta\} = \frac{1}{2} \{a_{\Delta}, a^\dagger_{\Delta}\} + \frac{1}{2} \{a^\dagger_{\Delta}, a_{\Delta}\} \sigma_z = H^2 - k_\nu^2$ is diagonal and essentially the square of our original Hamiltonian. Solving the eigenvalue equation for $\mathcal{H}$ is equivalent to the one for $H$. Note that in this representation, $\frac{1}{2} \{a_{\Delta}, a^\dagger_{\Delta}\} \sigma_z$ removes the zero-point energy, thus allowing for the zero energy state, see Fig. 2. Obviously, $[\mathcal{H}, Q_\Delta] = 0$, which expresses the supersymmetry between the two components $\varphi_{\uparrow, \downarrow}$ of the spinor. Explicitly, $H_{\uparrow} = a_{\Delta} a^\dagger_{\Delta}$ and $H_{\downarrow} = a^\dagger_{\Delta} a_{\Delta}$ are supersymmetric partner Hamiltonians, which are iso-spectral, except that $H_{\uparrow}$ has one additional bound state. Furthermore, the reflection and transmission coefficients defined by $H_{\uparrow, \downarrow}$ differ only by a phase [24].

For the tanh-DW profile, a second symmetry exists, $[H - \Delta^2, a_{\Delta} e^{\mp i\Delta \sigma_z}] = 0$. This means that $H_{\uparrow, \downarrow}$ are part of a hierarchy of form-invariant supersymmetric partner Hamiltonians, each differing from its neighbor by $\Delta \rightarrow \Delta + 1$. All Hamiltonians in this hierarchy have the same transmission-/reflection probabilities which readily explains the oscillations in $\delta G_{\text{OOP}}$ as $w/l_M$ varies. Due to the scaling in $\xi = x/w$, there is an additional smooth dependence on $w$ which yields the factor $1/w^2$ in $\delta G_{\text{OOP}}$, Eq. (10). Furthermore, if $\Delta \in \mathbb{N}$, the constant potential is part of the hierarchy and thus all Hamiltonians in the hierarchy are reflectionless as well. Note, however, that the constant potential is not realized in our system, since the scaling becomes singular for $w \rightarrow 0$. Finally, the number of bound states differs by 1 between two neighbors in the hierarchy, which explains that the number of bound states is given by $[\Delta]$. We point out that similar reasoning can be used for the IP wall configuration, there however, the supersymmetric hierarchy is constructed in $(\Delta, k_\nu)$-space and thus, the $k_\nu$-integration performed in $\delta G$ averages out the characteristic signature of the hierarchy.

We remark that $\mathcal{H}_{\uparrow, \downarrow}$ describes essentially a free particle in the Pöschl-Teller potential, which is known to be reflectionless for certain parameters. In the reflectionless case however, a transmitted wave still acquires a phase which has consequences on a wave packet passing such a potential: it narrows and is ahead in time as compared to a freely moving wave-packet [26]. For optical systems, these potentials have been realized recently using arrays of evanescently coupled waveguides [27].

**Conclusions.** We have analytically calculated the ballistic DW conductance for in-plane and out-of-plane magnetic domain walls induced into the surface states of a topological insulator. For the in-plane DW, the DW conductance is dominated by the spectrum mismatch imposed by the opposite magnetization directions within the domains. For the out-of-plane DW, we unexpectedly find oscillations in the wall-width dependence with period $l_M$ (magnetic length). In particular, integer $w/l_M$ constitute a family of reflectionless potentials. We can understand these features using the idea of supersymmetry and find them to be a result of the dispersion of the topological surface states together with the specific tanh DW-profile. Detecting the oscillatory DW resistance could be a unique signature of the chiral Dirac surface states. This could be realized by placing an additional top-gate on the ferromagnetic insulator which can be used to tune the exchange field $M$. The oscillations would still be visible if the ratio $E_F/M$ changes slowly enough.

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