Manipulating quantum channels in weak topological insulator nano-architectures

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Weak topological insulator (WTI) nanostructures are shown to be platforms for realizing one-dimensional (1D) helical channels that could be strongly protected. Two-dimensional surface states originating from an even number of Dirac cones are a priori considered to be fragile, while such 1D states that appear in the presence of an appropriate nanostructure could be robust against disorder. Whether this is indeed the case depends on the number of stacked atomic layers in the nanostructure; in WTI nanofilms the 1D channel is robust against localization due to disorder and becomes perfectly conducting when the number of stacked layers is odd. By studying response of the system against flux insertion numerically, we design and characterize quantum junctions at which multiple 1D channels meet and couple to one another under a certain traffic rule.

I. INTRODUCTION

Three-dimensional (3D) topological insulators are classified into weak and strong[14] The strong topological insulator (STI) exhibits a single Dirac cone in the surface Brillouin zone (BZ), which is immune to backscattering by non-magnetic impurities[14] The immunity to backscattering also implies that an electronic state in the single Dirac cone cannot be confined in a finite area. Instead, it is extended to the entire surface of STI[6] making all its facets metallic. On contrary, the weak topological insulator (WTI) exhibits an even number of (typically two) Dirac cones in the surface BZ, which can be confined; among surfaces of a WTI sample oriented in different directions there are also gapped surfaces, i.e., surfaces that exhibit no surface state of topological origin. Topological non-triviality is always manifest in STI, while in WTI it is either manifest or hidden[7,8] one can actually switch it on and off. This controllability of the topological non-trivialness sometimes makes WTI more useful than STI. In a previous work[7] we have demonstrated that one can possibly construct a nano-circuit of protected 1D helical modes on the surface of the WTI by simply patterning it with the use of lithography and etching.

Here, in this paper we quantify the nature of such 1D helical modes that appear in nano-architectures built on the surface of a WTI. We first consider as a toy example of such a nano-architecture, the case of a WTI nanofilm, as represented in FIG. 1 (a). In the figure, the film thickness is somewhat exaggerated for clarity, and here we consider a typical and realistic situation[19] in which the top and bottom surfaces of the film are gapped. As shown in the figure, this has been encoded in the choice of weak indices: \( \nu = (\nu_1, \nu_2, \nu_3) = (0, 0, 1) \). For this case, the WTI nanofilm consists of unit atomic layers stacked in the z-direction, where each layer can be regarded as a 2D quantum spin-Hall (QSH) insulator having a counter-propagating pair of 1D (gapless) helical edge channels. Let \( N_z \) be the number of unit atomic layers. In the limit of decoupled such 2D QSH states there are \( N_z \) pairs of 1D helical edge channels, each circulating around the corresponding 2D QSH layer. When such \( N_z \) 2D QSH layers are coupled to form a WTI in the bulk, 1D helical edge modes are also coupled, to form surface states of the bulk WTI which appears only on side surfaces of the film. In the film geometry, here represented as a flattened rectangular prism of height \( N_z \), i.e., the film thickness is \( N_z \), conducting properties of such WTI surface states is a drastic function of \( N_z \), since such surface states are confined in a finite width \( N_z \) of side surfaces[10,11]. If \( N_z \) is odd, there remains, after recombination, one helical channel that is gapless, extended and perfectly conduct-
ing. If $N_z$ is even, all the channels are gapped and tend to get localized.

Once the electronic properties of such WTI films are properly addressed, we proceed to analyzing the case of WTI terraces. In FIG. 1 (b) a simplest example of such terraces is modeled by two prisms of different heights $N_1$ and $N_2$ joined together through a side surface. A scenario similar to the nanofilm case applies, here, to this case of single step geometry; when the height of the step is an odd-integer multiple of atomic layers, there appears a robust 1D channel along the step. If one thinks of a more generic WTI nanostructure, multiple sets of such 1D channels are expected to appear, and couple to each other. If isolated, each set of 1D channels acts according to the even/odd rule we find in the case of the prism, while when they get together, interact, and eventually recombine, it is less trivial to tell what would happen.

In panel (c) of FIG. 1 we give an example of multiple 1D channels: steps that run in parallel; one stemming from the top, the other from the bottom surface. Let us assume that $\Delta N_1$ and $\Delta N_2$ are both odd, giving rise to 1D channels that are robust against disorder. If $N_1$ and $N_2$ are also odd, the robust 1D channels are extended to side surfaces either on the $N_1$ or to the $N_2$ side. An interesting question is how the two channels incident at the step recombine to either of the side surfaces at the junction of quantum channels formed at both ends of the step. If two channels at the step are spatially well separated ($N_2 \gg 1$) they do not interact and will act as two independent, perfectly conducting channel. In the opposite limit: $N_2 \sim 1$, we address in this paper, two odd-number channels run parallel close to each other. In this situation it is a priori not clear whether or not this pair of an odd-number of channels merge together to become a single set of gapped even-number channels. To probe the nature of helical modes along the step and around the side surfaces, we study response of the system to a magnetic flux. We try different ways of inserting a flux: e.g., $\Phi_1$ and $\Phi_2$ in FIG. 1 (c) to obtain further insight on how different 1D channels couple and recombine to each another.

Recently, an experimental realization of WTI in a bismuth-based layered compound Bi$_{14}$Rh$_3$I$_9$ has been reported. In spite of the number of realizations of 3D topological insulators, there have not been many proposals for realizing a WTI in stoichiometric compounds. WTI may be realized in superlattice systems. Features specific to WTI can be also seen in the so-called topological crystalline insulators (TCI). Unlike the standard topological insulators protected by time-reversal symmetry, TCI is protected by crystalline symmetry.

The paper is organized as follows. In Sec. II we introduce the effective Hamiltonian we employ in the subsequent studies. In Sec. III we discuss even/odd features in the case of WTI nanofilm. In Sec. IV, we extend this observation to characterize different variations of the 1D helical modes emergent in WTI nanostructures, typically at a step or at steps. It is shown to be possible to realize various types of non-trivial junctions that involve 1D perfectly conducting channels in WTI nanostructures. Sec. V is devoted to conclusions.

II. MODEL

To represent a bulk TI we consider the following Wilson-Dirac type effective Hamiltonian:

$$h(k) = \tau_z m(k) + \tau_x \sigma_\mu A_\mu \sin k_\mu,$$

where

$$m(k) = m_0 + 2m_2(1 - \cos k_\mu).$$

In Eqs. (1), (2) a summation over the repeated index $\mu = x, y, z$ is not shown explicitly. Eq. (1) can be regarded as a 4 x 4 matrix, spanned by two types of Pauli matrices $\sigma$ and $\tau$ each representing physically real and orbital spins. Eqs. (1), (2) can be regarded as a lattice version of the continuum Dirac Hamiltonian

$$h_\Gamma(k) = \tau_z m(k) + \tau_x \sigma_\mu A_\mu k_\mu,$$

at the $\Gamma$-point, where $m(k) = m_0 + 2m_2k_\mu^2$. Here, in Eqs. (1), (2) the lattice is chosen to be simple cubic for simplicity. Indeed, Eqs. (1), (2) represent a tight-binding Hamiltonian with only onsite and nearest neighbor hopping terms defined on the cubic lattice. On top of Eqs. (1), (2) we also consider on-site potential disorder of strength $W$. On each site $(x, y, z)$ of the cubic lattice a random potential of magnitude $V(x, y, z)$ is introduced, and distributed uniformly in the range of $[-W/2, W/2]$.

In Eqs. (1), (2) terms breaking the symmetry between the valence and the conduction band are not introduced explicitly, while such an accidental symmetry is automatically eliminated on introduction of the potential disorder. In terms of the symmetry class, the model specified by Eqs. (1), (2) belongs to the so-called DIII symmetry class with an accidental particle-hole and chiral symmetries, while the symmetry class changes to AII in the presence of the disorder potential.

By varying the mass parameters in Eq. (2) one can realize various weak and strong TI phases characterized by strong and weak indices, $\nu_0$ and $\nu = (\nu_1, \nu_2, \nu_3)$. Here, to achieve a situation in which the weak vector $\nu$ is given by $\nu = (0, 0, 1)$, we choose the mass parameters such that

$$m_{2x} = m_{2y} = m_{2||}, \quad m_{2z}/m_{2||} = 0.1, \quad m_0/m_{2||} = -2.$$

III. WTI NANOFILM: CASE OF EVEN VS. ODD NUMBER OF ATOMIC LAYERS

The specificity of the WTI surface states is that it exhibits even/odd features in regard to the number of
FIG. 2: Spectral flow in WTI nanofilms. Evolution of the spectrum $E(\phi)$ as a function of the flux $\phi = 2\pi(\Phi/\Phi_0)$ is shown in the clean limit ($W = 0$) [panels (a), (b)], and at moderate disorder ($W = 2$) [panels (c), (d)]. Panels (a), (c) are for the case of $N_z$ odd ($N_z = 3$), while (b), (d) are for the case of $N_z$ even ($N_z = 2$).

The nature of surface states can be revealed by observing their response to an inserted flux. Here, we assume that the flux is inserted through surfaces normal to the $z$-direction (the gapped surfaces) so that the flux would not touch the surface state (see FIG. 1). The role of the flux is then to twist the boundary condition around the gapped surfaces. The flow of the spectrum as a function of the flux encodes information on the response of the surface states against disorder; i.e., whether the surface states are localized or extended.

In the WTI prism geometry considered here surface electrons are confined onto side surfaces. On this closed “quasi-1D ring” the electrons form 1D helical modes. The nature of such 1D helical modes are governed by the width $N_z$ of the quasi-1D ring. The spectrum of the 1D modes in the clean limit is already much different in the cases of $N_z$ odd and $N_z$ even. When $N_z$ is odd, there always remains a gapless helical pair, while when $N_z$ is even, the entire spectrum including the contribution from such surface 1D modes is gapped (the surface 1D modes are gapped out by the finite-size effect). This even/odd feature in the clean limit is discussed in the next subsection. In the presence of disorder, such a difference in the behavior of surface 1D modes is further accentuated. When $N_z$ is odd, the 1D modes remain to be perfectly conducting, which is indeed a very remarkable behavior. While, when $N_z$ is even, all the 1D channels tend to get localized. These two contrasting behaviors can indeed be triggered by our diagnosis based on the observation of the flow of the spectrum as a function of the flux inserted.

Each eigenstate on the closed quasi-1D ring is characterized by a fictitious momentum along the circumferen-

atomic layers stacked in the direction of $\nu$. Here, we focus on the prism geometry as depicted in FIG. 1(a), and quantify such an even/odd feature in spectrum and in the behavior of the wave function in the presence of disorder.
FIG. 3: Spatial profile of typical wave functions in WTI nano-films in the presence of moderate disorder ($W = 2$). Panels (a), (b): Contrasting behaviors in the cases of $N_z$ odd and even. (a) When $N_z$ is odd ($N_z = 3$), the wave function is extended over the entire side surfaces. (b) When $N_z$ even ($N_z = 2$) the wave function is localized around one corner of the prism. Panels (c), (d): the magnetic flux introduced to examine the spectral flow shown in FIG. 2 induces also a bound state surrounding the flux tube piercing the bulk WTI. (c) $N_z = 3, \phi = 0.7\pi$; (d) $N_z = 2, \phi = 0.9\pi$.

A. Surface effective theory

To have further insight on the contrasting behaviors in spectral flow revealed in FIG. 2 in cases of $N_z$ odd and even, we start by analyzing this issue based on the effective theory for WTI surface states. Such an effective theory has been employed in the analyses of Ref. 27,34–36, while more recently it has been explicitly derived from the bulk effective Hamiltonian 37. The central ingredients of the theory are two Dirac cones that appear in the surface BZ for side surfaces, i.e., for surfaces that is parallel to $\nu$.

In the following simulations we choose the parameters as in Eq. 4 to realize a WTI with indices $\nu = (0, 0, 1)$. We then put this system into a geometry as shown in FIG. 1 (a), i.e., a prism of height $N_z$ and with a constant cross sectional area of size $N_x \times N_y$. As a result, surface electronic states associated with the two Dirac cones that appear on side surfaces of the prism are regrouped into those of sub-bands. The entire spectrum takes the following form; see Appendix for its justification:

$$E = \pm \sqrt{(A_z \sin q)^2 + (A_{||} k_{||})^2} \equiv E^{\pm}(q, k_{||}),$$

where both (i) $q$ and (ii) $k_{||}$ take discrete values due to quantization associated, respectively, with (i) confinement of the surface wave function into a width of $N_z$, ...
and (ii) the circular motion around the prism of circumference \( \xi \simeq 2(N_x + N_y) \). Naturally, the effect of (i) \( N_z \)-quantization is more important, since here we have in mind a situation in which \( N_z \ll \xi \).

Let us first focus on the quantization of \( q \). This \( N_z \)-quantization regroups the spectrum represented by Eq. 5) into sub-bands specified by a band index \( m \) such that

\[
E^{\pm}(q_m, k ||) \equiv E^\pm_m(k ||),
\]

i.e., \( q \) has been quantized as

\[
q = \frac{m\pi}{N_z + 1} \equiv q_m,
\]

where \( 2m \) is an integer, or \( m = 0, \pm 1, \pm 2, \ldots \). Yet, an essential observation is here to be added. Depending on the parity of \( N_z \), not all the values of \( q \) in Eq. (7) are allowed:

1. If \( N_z \) is odd, the allowed values of \( m \) in Eq. 7) are restricted to integers: \( m = 0, \pm 1, \pm 2, \ldots \). Since \( q \) appears squared in Eq. (5), or more explicitly,

\[
E^{\pm}_m(k ||) = \pm \sqrt{(A_z \sin \left( \frac{m\pi}{N_z + 1} \right))^2 + (A||k ||)^2},
\]

the \( m = 0 \) sub-band is non-degenerate, while all the remaining sub-bands are doubly degenerate: \( E^+_m(k ||) = E^-_m(k ||) \). Note that the non-degenerate \( m = 0 \) sector represents a linearly dispersing, gapless sub-band:

\[
E^+_0 = \pm A||k ||,
\]

while the remaining degenerate sub-bands are all gapped.

2. If \( N_z \) is even, \( m \) in Eq. (7) is an half odd integer: \( m = \pm \frac{1}{2}, \pm \frac{3}{2}, \ldots \), \( (N_x - 1) \). This signifies in contrast to the \( N_z \) odd case all the sub-bands are without exception doubly degenerate: \( E^+_m(k ||) \equiv E^-_m(k ||) \). Since these degenerate sub-bands are also all gapped, the entire spectrum is also gapped. The bottom of the lowest-energy sub-band is located at

\[
E^+_0(k || = 0) = A_z \sin \left( \frac{\pi}{2(N_z + 1)} \right).
\]

The second source of the quantization is (ii) the circular motion around the prism, which is applied to discretization of \( k || \). Here, let us take account of also the effect of the flux inserted. Then, the periodic boundary condition associated with the circular motion is twisted by two types of AB effect: extrinsic and intrinsic. The intrinsic effect is due to the flux \( \phi = 2\pi(\Phi_1/\Phi_0) \), while the intrinsic effect refers to the Berry phase \( \pi \) associated with the so-called spin connection. In any case, the boundary condition associated with the circular motion is given by

\[
e^{i(k || \xi - \phi)} = -1,
\]

where \( \xi \) is the circumference of this orbital motion. Eq. (11) determines the quantization rule for \( k || \), which reads

\[
k || = \frac{2\pi}{\xi} \left( n - \frac{1}{2} + \frac{\phi}{2\pi} \right) \equiv k_n(\phi).
\]

Generally, introduction of a flux breaks time reversal symmetry of the system. Only at \( \phi = 0 \) and at \( \phi = \pi \) the symmetry remains to hold, implying that all the states at these values of \( \phi \) are two-fold degenerate (Kramers degeneracy). Since

\[
k_n(0) = \frac{2\pi}{\xi} \left( n - \frac{1}{2} \right) = -k_{-n+1}(0)
\]

and \( k || \) appears squared in Eq. (5), a pair of circular modes with \( k || = k_n \) and \( k || = k_{-n+1} \) are Kramers partners at \( \phi = 0 \):

\[
E^+_m(n, \phi = 0) = E^\pm_m(-n+1, \phi = 0),
\]

where

\[
E^\pm_m(n, \phi) \equiv E^\pm_m(q_m, k_n(\phi))
\]

\[
= \pm \sqrt{(A_z \sin q_m)^2 + (A\| \frac{2\pi}{\xi} \left( n - \frac{1}{2} + \frac{\phi}{2\pi} \right))^2}
\]

The two partners evolve, however, differently on introduction of \( \phi \). At \( \phi = \pi, \) both \( n \)th and \( (-n + 1) \)th modes find a new partner:

\[
k_n(\pi) = \frac{2\pi}{\xi} n = -k_{-n}(\pi),
\]

\[
k_{-n+1}(\pi) = \frac{2\pi}{\xi} (-n + 1) = -k_{n-1}(\pi),
\]

i.e.,

\[
E^\pm_m(\pi) = E^\pm_{m,n}(\pi), \quad E^\pm_{m,n+1}(\pi) = E^\pm_{m,n-1}(\pi).
\]

Indeed, all the Kramers pairs at \( \phi = 0 \) change their partners as \( \phi \) evolves from 0 to \( \pi \), and as argued in Ref[14] this change of the partner is the origin of a characteristic spectral flow \( \left\{ E_j(\phi) \right\} \). Here, \( \left\{ E_1(\phi), E_2(\phi), E_3(\phi), \ldots \right\} \) is an energy spectrum at a given value of \( \phi \), with energy eigenvalues \( E_1(\phi), E_2(\phi), E_3(\phi), \ldots \) sorted in the increasing (or decreasing) order. A spectral flow \( \left\{ E_j(\phi) \right\} \) is the entire image of the trajectories of such a set of eigenvalues when \( \phi \) is varied over one cycle of AB oscillation, \( \phi \in [-\pi, \pi] \). In FIG. 2 and in the subsequent figures only half of the flow is shown, since here \( E(-\phi) = E(\phi) \) is guaranteed by time reversal symmetry of the original model. In Eqs. 10 and 17 the case of \( m = n = 0 \).
needs a separate consideration\textsuperscript{12} The following relation holds:

\[ E_{0,0}^+(\pi) = E_{0,0}^-(\pi) \]  

(18)

instead of Eq. \textsuperscript{17}.

Let us focus on spectral flow shown in FIG. 2. First recall that the spectrum is doubly degenerate at \( \phi = 0 \) and at \( \phi = \pi \), and this degeneracy is ensured by the Kramers theorem. This holds true both in the clean limit [panels (a) and (b)] and in the presence of disorder [panels (c) and (d)]. In the case of \( N_z \) even, additional degeneracies occur at an intermediate \( \phi \) [see panel (b)], and these crossings are not protected. In the presence of disorder such accidental degeneracies are indeed lifted [panel (d)]. When \( N_z \) is odd, typically a single \( m = 0 \) non-degenerate subband appears in the relevant low-energy regime; such a situation is indeed predominant in panels (a), (c). Then, the spectral flow is free from accidental crossings as mentioned above. Generally, degenerate subbands with \( m \neq 0 \) may also appear in a relatively high-energy region and be superposed on top of \( m = 0 \) non-degenerate subband. However, mixing with such pseudo two-fold degenerate subbands does not destroy the non-trivial spectral flow. Here, non-trivialness refers to the fact that the spectral flow is a connected line traversing the entire gap region as shown in the case of panel (c). The reason why this is so is essentially due to the same logic leading to the \( Z_2 \) classification of 2D QSH states.\textsuperscript{13} In the case of \( N_z \) even, anti-crossings at an intermediate \( \phi \) make the spectral flow trivial, i.e., the spectrum consists of disconnected lines.

B. Even/odd features in the spectral flow

Based on the observations so far established in the light of the surface effective theory, let us re-examine the spectral flow shown in the four panels of FIG. 2 in more detail. Panels (a), (c) show a calculated spectral flow in the case of \( N_z \) odd \( (N_z = 3) \), while panels (b), (d) correspond to the case of \( N_z \) even: \( N_z = 2 \). Panels (a), (b) represent a spectral flow in the clean limit, while (c), (d) are those of the disordered case: \( W = 2 \). Other model parameters are chosen such that \( N_x = N_y = 12 \) and \( A_\parallel = A_z = 2 \) (measured in units of \( m_\parallel \)).

1. Case of \( N_z \) odd: extended, perfectly conducting

Let us first focus on FIG. 2 panel (a): case of \( N_z = 3 \) in the clean limit. In the range of energies shown in the figure, the low-lying part of three sub-bands with \( m = 0 \) and \( m = \pm 1 \) of Eq. \textsuperscript{8}, are relevant, contributing to the spectral flow. The \( m = 0 \) sub-band is non-degenerate and gapless, which is responsible for the non-trivialness of the flow. In the \( E > 0 \) sector, the bottom of the degenerate \( m = \pm 1 \) sub-bands are located at

\[ E_1^+(k_\parallel = 0) = A_z \sin \left( \frac{\pi}{N_z+1} \right) = 2 \sin \frac{\pi}{4} = \sqrt{2}. \]  

(19)

The simple zigzag pattern below this threshold energy is purely due to the \( m = 0 \) sub-band, while above this energy the two contributions are superposed.

In the pure \( m = 0 \) regime the pitch of the zigzag pattern is given as

\[ \Delta E_{\text{pitch}} = A_\parallel \frac{2\pi}{\xi} = \frac{\pi}{12} \approx 0.2618 \]  

(20)

[see Eq. \textsuperscript{15}]. In the presence of disorder [FIG. 2 panel (c)] this pitch is modified by the mixing of \( m = 0 \) and \( m = \pm 1 \) sub-bands, while the connectedness of the zigzag pattern is maintained; the spectral flow remains non-trivial, traversing the valence and conduction bands. Crossing of the spectra at \( \phi = 0 \) and \( \phi = \pi \) is a consequence of the time reversal symmetry (Kramers degeneracy), which is unaffected by introduction of non-magnetic impurities considered here. Robustness of the continuous zigzag pattern is a clear signature that a pair of surface helical channels are robust against disorder, and the corresponding wave function is extended despite the presence of disorder [FIG. 3 panel (a)].

2. Case of \( N_z \) even: all the states get localized

If \( N_z \) is even, the situation is much different. First, the spectrum is gapped by a finite-size quantization [see Eq. \textsuperscript{10}]. The half width of this gap is in the present choice of parameters \( E_1^+(k_\parallel = 0) = 1 \) [c.f. FIG. 2, panel (b)]. Above this threshold energy, two pseudo degenerate sub-bands with \( m = \pm \frac{1}{2} \) become available for edge/surface conduction. In the clean limit [panel (b)] these two sub-bands form a zigzag pattern somewhat resembling the case of \( N_z \) odd. Note that the two sub-bands are not completely degenerate; they interfere due to the existence of corners, and as a result their spectrum repel each other. Also importantly, there is a crossing once per each period \( \phi \in [0, \pi] \) between these pseudo degenerate sub-bands at a (non-protected) intermediate value of \( \phi \) (recall the arguments in the previous subsection). Crossings occur with a counter-propagating partner, and between neighboring \( k_n \) modes [see Eq. \textsuperscript{12}].

Now, as we switch on disorder [see panel (d)], a crucial difference arises from the case of \( N_z \) odd [panels (c)]. The zigzag is broken apart into many pieces; the spectral flow is indeed trivial in this case. In FIG. 3 (b) the spatial profile of the corresponding wave function is shown. In consistency with the trivial spectral flow the wave function is localized in the vicinity of one corner of the prism.
C. Bound states

In the spectral flow shown in the four panels of FIG. 2, one can recognize a separate branch that are superposed on top of the spectral flow we have so far focused on. This separate branch stems from a bound state induced by the flux insertion. This can be verified explicitly by inspecting the spatial profile of the corresponding wave function as shown in FIG. 3 (c), (d). The figure indicates that such bound states are localized around a plaquette through which the flux is inserted. That is, they can be regarded as localized states on the surface.
of a prism-shaped hole (i.e. flux tube) corresponding to the
plaquette, where the circumference of $\xi_b$ of the hole is $\xi_b \simeq 4a$ with a being the lattice constant. The reason
why such bound states appear in the spectrum can be read from Eq. (15), while here the typical length scale is $\xi_b$ associated with the quantization of $k_\parallel = k_n$ [see Eq. (12)]. As $a$ is chosen to be unity in the simulation, $\xi_b \simeq 4$. The fact that $\xi_b$ is on the order of $N_x$ implies that $q$-quantization and $k_\parallel$-quantization are equally important. This is contrasting to the case of surface states on side surfaces, in which $N_x \ll \xi$ holds, indicating that the $q$-quantization is much more important. In the low-energy regime shown in FIG. 2 only the $n = 0$ (or $n = 1$ on the $0 < \phi < 0$ side) sector is relevant.

When $N_x$ is odd, $q$-quantization allows for a zero mode: $m = 0$ in Eq. (7). The separate branch that appears in the spectral flow shown in FIG. 2(a), (c), and the spatial profile of the wave function shown in FIG. 3(c) are due to such a bound state with $m = 0$, $n = 0$. Since

$$q_0 = 0, \quad k_0(\phi) = \frac{2\pi}{\xi_b} \left( -\frac{1}{2} + \frac{\phi}{2\pi} \right), \quad (21)$$

this bound state becomes “gapless” at $\phi = \pi$. Taking $\xi_b \simeq 4$ into account, one can also estimate the rough energy “dispersion” $E(\phi)$ of this bound state from Eq. (15) as

$$E_{\text{bound}}^{(0)\pm} = E_{0,0}^\pm(\phi) = \pm A_\parallel \frac{\pi - \phi}{4}. \quad (22)$$

In the spectral flow shown in FIG. 2(a), (c), the separate branch due to bound state shows indeed such a linear dispersion in the vicinity of the gap closing at $\phi = \pi$. In the high energy part of the spectral flow in the clean limit [FIG. 2(a)], one can also recognize the second sets of bound states, which are due to $m = \pm 1$, $n = 0$.

When $N_x$ is even, $q$-quantization has no zero mode. The separate branch that can be seen in FIG. 2(b), (d) are due to bound states with $m = \pm \frac{1}{2}$, $n = 0$. The spatial profile of the wave function in this case is shown in FIG. 3(d). From Eq. (15), one can make a rough estimate of $E(\phi)$ for such “massive” bound states:

$$E_{\text{bound}}^{(m)\pm}(\phi) = \pm \sqrt{A_z \sin \left( \frac{m\pi}{N_x + 1} \right)^2 + A_\parallel^2 \left( \frac{\pi - \phi}{4} \right)^2}. \quad (23)$$

where $m = \pm \frac{1}{2}$ in the present case with $N_x = 2$, i.e.,

$$E_{\text{bound}}^{(1/2)\pm}(\pi) = \pm A_z \sin \left( \frac{\pi}{2(N_x + 1)} \right) = \pm 1. \quad (24)$$

Setting $m = \pm 1$, one can apply the same formula, Eq. (23), to the second excited bound states in the case of $N_x$ odd; e.g., for $N_x = 3$,

$$E_{\text{bound}}^{(1)\pm}(\pi) = \pm A_z \sin \left( \frac{\pi}{N_x + 1} \right) = \pm \sqrt{2}. \quad (25)$$

Though such estimates as given in Eqs. (22), (23), (24), (25) are very rough ones, they still show a qualitatively good agreement with the calculated spectral flow presented as four panels in FIG. 2.

IV. PERFECTLY CONDUCTING CHANNELS EMERGENT IN WTI NANO-ARCHITECTURES

Let us consider the “step geometries” as depicted in FIG. 1(b), (c). A pair of 1D helical modes appear along a step (or steps) etched on the surface of a WTI. One can regard this also as a set of two WTI prisms we have studied in the last section of different height coupled together. To probe the nature of helical modes along the step and around the side surfaces, we study response of the system to flux $\Phi_1$ and $\Phi_2$ introduced on either side of the step, independently. In the following, we compare the cases of a single step [case of FIG. 1(b)], and of two steps running in parallel [panel (c)].

A. Case of the single step: a robust perfectly conducting channel running along the step

Let us consider two WTI prisms with different height $N_z = N_1$ and $N_z = N_2$ joined together via side surfaces. The gapped surfaces are on the top and bottom surfaces. Here, we put them together aligning the bottom surfaces [see FIG. 1(b)]. Then, if $N_1 \neq N_2$, a step of height $\Delta N = N_1 - N_2$ appears on the top surface. If $\Delta N$ is odd, there appears a pair of 1D protected helical modes along the step, while if $\Delta N$ is even, this is no longer the case; pseudo 1D modes are gapped out by the finite size effect, and do not appear in the low energy spectrum. Indeed, this odd/even feature with respect to $\Delta N$ stems from the difference of spectrum in the two cases [see Eq. (8)].

Let us consider a situation in which $N_1$ is odd and $N_2$ is even, say, $N_1 = 3$ and $N_2 = 2$. Since $\Delta N$ is odd, there appears a pair of 1D protected modes along the step. Here, one can apply the same arguments leading to Eq. (8) for surface states emergent at the step. Naturally, these 1D helical modes cannot be confined in a finite segment of the step. They must be extended over to side surfaces of the prism. Surface states on such side surfaces become pseudo-gapless [i.e., excepting the $k_\parallel$-discretization due to Eq. (12)] when $N_z$ is odd [case of Eqs. (8) with $m = 0$]. In the situation we consider, this happens on the $N_1$-side [FIG. 1(b)]. Thus, in the region of $E > 0$ but below the bottom of the surface sub-band on the $N_2$-side located at the energy given by Eq. (10), the 1D modes along the step form a closed loop solely with the pseudo 2D surface modes on the $N_1$-side [see FIG. 1(c)]. Above this threshold energy (i.e., the bottom of the sub-band on the $N_2$-side) an electron propagating via a 1D channel along the step and incident at a quantum junction that appear at the end of the step can turn either to the $N_1$- or to the $N_2$-side [see FIG.
At energies $E$ above the bottom of second sub-band on the $N_1$-side, given by Eq. (19), there seem to be a priori three, two and one pair of channels, incident, respectively, from the $N_1$-, $N_2$- and the step sides to the quantum junction.

In the presence of disorder, however, not all of these channels survive. To see the robustness of different channels against disorder, here, we have studied the spectral flow in the system under insertion of a magnetic flux in two different configurations. In Figs. 4 and 5 such a spectral flow is presented in panel (a) under a flux configuration of $(\phi_1, \phi_2) = (\phi, 0)$, where $\phi_1 = 2\pi(\Phi_1/\Phi_0)$ and $\phi_2 = 2\pi(\Phi_2/\Phi_0)$ represent, respectively, a flux inserted on the $N_1$- ($N_2 = 3$) side, and on the $N_2$- ($N_2 = 1$) side. In panel (b) of Figs. 4 and 5 a different configuration is studied, where $(\phi_1, \phi_2) = (0, \phi)$. Two panels of FIG. 6 represent a spectral flow in the clean limit ($W = 0$), while a moderate strength of disorder ($W = 2$) is introduced in the examples shown in FIG. 6. As one can clearly see in FIG. 6 a nontrivial spectral flow is still persistent in panel (a), i.e., the spectral flow is non-trivial in this case, while the flux dependence is almost extinct in panel (b); the spectral flow is trivial in this case. This indicates that in the single step geometry as depicted in FIG. 1 (b) with $N_1$ odd (= 3), $N_2$ even (= 2), and $\Delta N_1 = 1, \Delta N_2 = 0$, an electron in the 1D protected channel at the step is selectively transmitted to the $N_1$-side in the presence of disorder: $W \neq 0$.

### B. Two step geometry: an even number of channels running in parallel

In the previous examples, only surfaces consisting of an odd number of channels are robust against disorder, and such surfaces occur when the layer number $N$ is odd. A natural question that arises here is what happens in a geometry as depicted in FIG. 1 (c) if $N_1, N_2, \Delta N_1, \Delta N_2$ are all odd? If surfaces of both the $N_1$- and $N_2$-sides are robust against disorder, and are capable of providing with channels available for an electron incident at the step? We consider typically the case of $N_1 = 3, N_2 = 1, \Delta N_1 = 1, \Delta N_2 = 1$.

FIG. 6 shows response of such a system against flux insertion both on the $N_1$- and $N_2$-sides [see configuration of the two types of flux insertion $\Phi_1$ and $\Phi_2$ in FIG. 4 (b)]. The two panels of FIG. 6 show evolution of the spectrum at $W = 2$ as a function of the flux $\phi$ when the flux is inserted either on the $N_1$- or on the $N_2$-side; $(\phi_1, \phi_2) = (\phi, 0)$ in panel (a), and $(\phi_1, \phi_2) = (0, \phi)$ in panel (b).

We begin by pointing out two specific features that can be seen in the two panels of FIG. 6. First, both panels show a non-trivial spectral flow, in which each member of a Kramers pair at $\phi = 0$ changes its partner at $\phi = \pi$. This means that there exists a robust perfectly conducting channel both around the prism 1 and around the prism 2. Provided that $\Delta N_1$ and $\Delta N_2$ are both odd ($\Delta N_1 = \Delta N_2 = 1$), one expects a priori an even number (= 2) of channels running in parallel at the connection of two prisms. Yet, the obtained spectral flow implies that the two channels behave as if there were an odd number of channels. We will clarify this point later.
Secondly, the two spectra are complementary in the sense that those partners that are sensitive to $\Phi_1$ are insensitive to $\Phi_2$, and vice versa. Note that at $\phi = 0$ the two plots coincide, since the two simulation is done for the same configuration of impurities.

Let us now overview what is supposed to happen in the system, leaving its justification to arguments given later. Those states that are sensitive to the flux in FIG. 6 (a) stem from states that goes around the prism 1 [1c and 1a modes in FIG. 7 panel (b)], while those which are insensitive (at least around $\phi = 0$) to the flux are states that goes around the prism 2 (2c and 2a, *ibid.*). To check these assumptions, here, we have designed the system such that the circumference $L_2$ of 2c and 2a modes is twice as long as that of 1c and 1a ($= L_1$); *i.e.*, $L_2 \simeq 2L_1$. Note that separation of the levels associated with a 1D channel due to finite size is inversely proportional to its circumference. In panel (a) those pairs that are sensitive to the flux are spaced by a distance twice as large as those which are insensitive to the flux. Since the former is assumed to stem from 1c and 1a, while the latter from 2c and 2a, this makes perfectly sense.

These being said, let us come back to the question: why are the even number of channels incident at the steps robust against disorder? Why do they behave like an odd number of channels, showing a nontrivial spectral flow? Our short answer is the following: if we focus on some energy $E$, say, in the spectrum shown in FIG. 6 (a), there exists indeed an odd number of (here, only one) channel(s) at the step. To elaborate what this actually implies, let us divide the spectrum in energy into two regions. The two regions do not coexist, but are connected smoothly. At a given energy $E$, there exists, and always exist, only a single state (at some value of $\phi$), *either* on the $N_1$- or on the $N_2$-side (or sometimes in between).

Let us try to formulate how this *segregation* occurs by zooming up a part of the spectral flow shown in the red frame of FIG. 6 panel (a). FIG. 7 panel (a) shows an enlarged image of this part of the flow. Those parts of the spectrum which are sensitive to the flux $\phi_1$ are due to states that goes around the prism 1, moving either in the clockwise, or in the anti-clockwise direction [1c and 1a modes in FIG. 7 panel (b)]. On contrary, those parts of the spectrum that are insensitive to the flux $\phi_1$ are due to states that goes around the prism 2 (2c and 2a modes).

However, in the presence of the step region at which two prisms are coupled, the eigenstates of the system become a combination of 1c/1a and 2c/2a states; they are mixed and recombined in the step region. In FIG. 7 (a) two Kramers pairs: 1c/1a and 2c/2a, are incident at $\phi = 0$ apart in energy. Here, we consider the spectral flow of the system under a flux inserted in the configuration of $(\phi_1, \phi_2) = (\phi, 0)$. As $\phi_1 (= \phi)$ is increased, 1c/1a pair breaks; 1c is the upward branch, which intersects with the 2c/2a pair located initially above. As schematically illustrated in panel (b), the spectral feature in the vicinity of this intersection can be understood as the result of anti-crossing between 1c and, intrinsically, a linear combination of 2c and 2a. Since the spin quantization axis of the two helical pairs: 1c/1a and 2c/2a, are not not necessarily aligned, one expects *a priori* recombination of such
modes at the step region. In principle, $1c$ is coupled to either $2c$ or $2a$, or to both. Let us introduce the linear combination:

$$|2b⟩ = c_{2c}|2c⟩ + c_{2a}|2a⟩,$$

$$|2b⟩ = c_{2a}^*|2c⟩ - c_{2a}|2a⟩,$$

(26)

where $c_{2c}$ and $c_{2a}$ are some constants normalized such that $|c_{2c}|^2 + |c_{2a}|^2 = 1$, and assume that $1c$ is coupled to $2b$ at the step region. Then, this signifies that $2b$ is orthogonal to $1c$, and $2b$ represents a branch that is unaffected by the proximity to $1c$. Indeed, $2b$ state remains flat, insensitive to the flux, and there is no anti-crossing between $1c$ and $2b$. Only at $φ = π$ it reunites with $2b$. In contrast to the flat $2b$-subband, $1c$ and $2b$ show a clear anti-crossing feature. The two branches of the anti-crossing may be presented as

$$|1c2b⟩ = c_{1c}|1c⟩ + c_{2b}|2b⟩,$$

$$|1c2b⟩ = c_{2b}^*|1c⟩ - c_{1c}^*|2b⟩,$$

(27)

where $c_{1c}$ and $c_{2b}$ are some constants that vary as a function of $φ$. So actually, $c_{1c} = c_{1c}(φ)$ and $c_{2b} = c_{2b}(φ)$. The constants $c_{1c}$ and $c_{2b}$ are also normalized such that $|c_{1c}|^2 + |c_{2b}|^2 = 1$. Let us assume that $1c2b$ represents the bonding branch focused in FIG. 7 panels (a) and (b), while $1c2b$ corresponds to the anti-bonding branch. To illustrate the evolution of $|1c2b⟩$ as a function of branch, we have plotted in FIG. 8 the spatial profile of the corresponding wave function at different values of $φ/π$ ($= 0.3, 0.45, 0.6$). One can see that a dominant weight of the wave function is on the $N_2$-side at $φ/π = 0.3$, which is shifted to the $N_1$-side as $φ/π$ is increased.

FIG. 8: Evolution of the $|1c2b⟩$ state: snap shots of the wave function at (a) $φ/π = 0.3$, (b) $φ/π = 0.45$, (c) $φ/π = 0.6$.

FIG. 9: Spectral flow in the two step geometry in case of the configuration of $φ_1$ and $φ_2$ such that (a) $(φ_1,φ_2) = (φ,φ)$. (b) $(φ_1,φ_2) = (φ,−φ)$.

In the arguments developed so far two sets of helical modes $1c/1a$ and $2c/2a$ that are incident on the two sides of the step region come into play; see inset of FIG. 7 (b). They circulate, propagating in opposite directions, around prism 1, or prism 2. When they meet at the step region, how are they coupled to each other? Is $1c$ coupled to $2a$ or to $2c$? In Eq. 26 we simply assumed that
1c is coupled to the 2\(c\)-combination, while in this combination what a percentage actually comes from 2\(c\), and what a percentage from 2\(a\)? In this last part, we clarify this point by studying yet another type of spectral flow. Two panels of FIG. [9] show such a spectral flow in the cases of flux configurations such that \((\phi_1, \phi_2) = (\phi, \phi)\) in panel (a), i.e., case of the flux introduced in the same direction on the \(N_1\) and \(N_2\) sides, while \((\phi_1, \phi_2) = (\phi, -\phi)\) in panel (b), i.e., case of the flux inserted in the opposite directions. Whether the spectrum responds either in the upward or downward direction is a combined effect of the direction of the propagating 1D channel and that of the flux introduced. Therefore, by changing the relative sign of \(\phi_2\) with respect to \(\phi_1\), one can bring together different combinations of channels in the flow of the spectrum (see FIG. [10]).

For example, in the \((\phi, \phi)\)-configuration, combinations such as \((1c, 2a)\) and \((2c, 1a)\), e.g., pairs of co-propagating modes, get close to one another in the spectral flow. However, as one can see in FIG. [9] (a), the two branches show clear anti-crossing, making the flow of the spectrum disconnected. These co-propagating pairs are indeed coupled, and recombine at the step region. On contrary, in the \((\phi, -\phi)\)-configuration [FIG. [9] (b)], combinations such as \((1c, 2c)\) and \((1a, 2a)\), i.e., a pair of counter-propagating modes meet in the spectral flow, and show practically no conspicuous anti-crossing. These imply that at the step region the co-propagating combinations such as \((1c, 2a)\) and \((2c, 1a)\) are coupled, while counter-propagating combinations such as \((1c, 2c)\) and \((1a, 2a)\) are not coupled, i.e., in terms of Eq. (26) \(c_{2c} \simeq 0, c_{2a} \simeq 1\), implying actually, \(|2b\rangle = |2a\rangle\). The co-propagating combinations compose the \(\phi\)-dependent part, while the counter-propagating combinations are responsible for the \(\phi\)-independent, i.e., the flat part of the spectral flow shown in Figs. [6] and [7], ensuring together the connectedness of the nontrivial spectral flow.

V. CONCLUDING REMARKS

We have studied protected helical conducting channels that appear in WTI nanofilms, WTI terraces, and WTI nano-architectures, and their robustness against disorder. After a close inspection of the nanofilm case in Sec. III, we have highlighted the cases of WTI terraces and steps in Sec. IV. In contrast to the case of a single step, an electron incident at the step region in the two-step geometry is transmitted either to the \(N_1\)- or to the \(N_2\)-side, depending on its energy \(E\). For an electron incident at a quantum junction at the end of the step region a non-trivial (energy dependent) traffic rule emerges. As a result, an even number of channels incident at the step region are robust against disorder, behaving as perfectly conducting channels, as if they were an odd number of channels. In nano-circuits fabricated on surfaces of a WTI, a number of 1D channels appear, meet and couple in a non-trivial manner. Nontrivial quantum junctions appear, at which more than two channels meet in a nontrivial manner. Here, we have shown an example in which incident 1D channels stay extended in spite of such coupling. The obtained results indicate robustness of the 1D helical channels established in simple nano-structures such as WTI nanofilms and steps is a more generic feature that can be applied to more involved and realistic nano-architectures.

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Appendix A: Derivation of Eqs. (5), (7), (8)

The low-energy electron states that appear on the side surface of \(1 \leq z \leq N_x\) are described by the following effective Hamiltonian

\[
H_{eff} = \sum_{z=1}^{N_x} |z\rangle \left[ A_{||}k_{||} 0 0 -A_{||}k_{||} \right] |z\rangle \\
+ \sum_{z=1}^{N_x-1} \left( |z+1\rangle \left[ \begin{array}{ccc} 0 & 0 & -\frac{1}{2}A_{z} \\ \frac{1}{2}A_{z} & 0 & 0 \end{array} \right] |z\rangle + H.c. \right) . \tag{A1}
\]

where \(|z\rangle \equiv \{|z\rangle_\uparrow, |z\rangle_\downarrow\}\) represents two-component state vector for the \(z\)th 1D helical channel, and \(k_{||}\) represents a component of the momentum in the direction the side surface is extended, say, \(x\) or \(y\).
where $\zeta = x$ or $y$. In the expression Eq. (A2)
\begin{equation}
\begin{bmatrix}
\alpha_z \\
\beta_z
\end{bmatrix} = \psi(z) \begin{bmatrix} a \\ b \end{bmatrix}, \tag{A3}
\end{equation}
where the transverse function $\psi(z)$ must satisfy the boundary condition of
\begin{equation}
\psi(0) = 0, \quad \psi(N_z + 1) = 0. \tag{A4}
\end{equation}
By superposing plane wave solutions stemming from two Dirac cones: $(k_z, k_\parallel) = (q, k_\parallel), (\pi - q, k_\parallel)$, one can construct a wave function compatible with Eqs. (A3) and (A4) such that
\begin{equation}
\begin{bmatrix}
\alpha_z \\
\beta_z
\end{bmatrix} \propto (e^{iqz} - e^{i(\pi-q)z}) \begin{bmatrix} a \\ b \end{bmatrix}
\propto (e^{iqz} - (-1)^z e^{-iqz}) \begin{bmatrix} a \\ b \end{bmatrix}, \tag{A5}
\end{equation}
where $\psi(z)$ satisfies
\begin{equation}
\begin{bmatrix} A_{\parallel}k_\parallel & iq \\
-iq & -A_{\parallel}k_\parallel
\end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = E \begin{bmatrix} a \\ b \end{bmatrix}. \tag{A6}
\end{equation}
From Eq. (A6), one finds
\begin{equation}
E = \pm \sqrt{(A_{\parallel}q)^2 + (A_{\parallel}k_\parallel)^2}. \tag{A7}
\end{equation}
Allowed discrete values of $q$ given in Eq. (7) are specified by the second equality of Eq. (A4) by the vanishing of $\psi(z)$ at $z = N_z + 1$, i.e.
\begin{equation}
q = \frac{m\pi}{N_z + 1} = q_m, \tag{A8}
\end{equation}
where $m$ is either an integer or a half-odd integer. For an odd $N_z$, $m$ takes an integral value; $m = 0, \pm 1, \pm 2, \cdots, \pm \frac{N_z-1}{2}$. While for $N_z$ even, $m$ becomes a half-odd integer; $m = \pm \frac{1}{2}, \pm 1, \cdots, \pm \frac{N_z}{2}$. Substituting Eq. (A8) into Eq. (A7), one completes the derivation of Eq. (5) and (8).
