Finite-size energy gap in weak and strong topological insulators

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The non-trivialness of a topological insulator (TI) is characterized either by a bulk topological invariant or by the existence of a protected metallic surface state. Yet, in realistic samples of finite size this non-trivialness does not necessarily guarantee the gaplessness of the surface state. Depending on the geometry and on the topological indices, a finite-size energy gap of different nature can appear, and correspondingly, exhibits various scaling behaviors of the gap. The spin-to-surface locking provides one of such gap-opening mechanisms, resulting in a power-law scaling of the energy gap. Weak and strong TIs show different degrees of sensitivity to the geometry of the sample. As a noteworthy example, a strong TI nanowire of a rectangular prism shape is shown to be more gapped than that of a weak TI of precisely the same geometry.

I. INTRODUCTION

The non-trivialness of a TI is often characterized by the presence of a gapless surface state.1,2 A one-to-one correspondence can be established between the (non-) trivialness of a bulk topological invariant and the presence vs. absence of the gapless surface state (bulk-surface correspondence). However, precisely speaking, for such a gapless state to be existent, both the trivial and non-trivial sides are semi-infinite, separated by an infinitely large interface. The above distinction can be made, therefore, only in such an idealized situation. TI samples, in reality, occupy only a finite domain of the space, and have also a variety of shapes surrounded generally by a curved or folded surface(s). In experiments it is also the case that some TI samples of nanometer scale size exhibit a clear gapless surface state, while other samples of the same chemical composition but of a different geometrical shape do not necessarily exhibit a clear signature of topological non-triviality. Such an issue will be addressed in this paper.

The main scope of the paper is concomitant with the observation that there are three different gap-opening mechanisms effective in the samples of finite size. The most primitive among them is the one due to mixing of the surface electronic wave functions on the opposing sides, e.g., of an infinitely large slab-shaped sample. Such an energy gap associated with the finite thickness of the gapped bulk, decays exponentially as a function of the thickness of the slab, and is in practice almost irrelevant except in extremely thin film samples.3 The low-energy (surface) electronic spectrum in the slab geometry suffers indeed only from this type of exponentially small finite-size energy gap.4–7 The second mechanism to open a gap in the surface electronic spectrum, which is also more relevant in magnitude, is the so-called “spin-to-surface locking.”8–11 The electronic spin in the a priori gapless surface state on a curved surface of TI has a tendency to be locked in-plane to the local tangent of the surface. In the cylindrically symmetric case, the spin-to-surface locking results in the half-integral quantization of the orbital angular momentum along the axis of the cylinder. The half-odd integer quantization gaps out the spectrum, and this gap decays only algebraically; qualitatively more relevant than the gap of the previous type. The spin-to-surface locking leads, indeed, irrespective of the presence of cylindrical symmetry, e.g., in a prism-shaped sample, to opening of the gap.

Another aspect of the topological insulator which we aim at exploring in this paper is the role of anisotropy, especially in the weak topological insulator (WTI) phase. This is much related to the third mechanism of gap-opening, which occurs due to the interplay of the anisotropy of WTI and the specific geometry we will focus on (case of the prism-shaped geometry). In three spatial dimensions (3D), $\mathbb{Z}_2$ topological insulator is known to be characterized by four $\mathbb{Z}_2$ indices,12–14 the principal (strong) index $\nu_0$ and other “weak” indices $\nu_1, \nu_2, \nu_3$, instead of a single $\mathbb{Z}_2$ index in the case of 2D. The principal index $\nu_0$ is used to distinguish a STI ($\nu_0 = 1$) from trivial and weak topological insulators ($\nu_0 = 0$). In a WTI at least one of its weak indices exhibits a nontrivial value (= 1). A WTI shows generally an even number of helical Dirac cones on its surfaces, but on the surface normal to its “weak vector” $\vec{\nu} = (\nu_1, \nu_2, \nu_3)$ it shows no Dirac cone. The WTI can be viewed as stacked layers of 2D $\mathbb{Z}_2$ topological insulators. In this regard the set of weak indices ($\nu_1\nu_2\nu_3$) can be regarded as the Miller index of such stacked layers. Since gapless surface states are expected to form only at the edge of the stacked layers, one can naturally understand that no Dirac cone is formed on a surface normal to $\vec{\nu}$ in this picture. To summarize, the WTI bears two Dirac cones on surfaces parallel to $\vec{\nu}$ and no Dirac cone on surfaces normal to $\vec{\nu}$. When this characteristic feature is combined with the specific (rectangular) prism geometry, the anisotropy of a WTI manifests as an alternating size-dependence of the energy gap; the magnitude of the gap is qualitatively different whether the number of “stacked layers” is even or odd. It will be demonstrated that weak and strong TIs show different degrees of sensitivity to the geometry of the sample.

The periodic table of topological insulators and superconductors classifies them by the nature of strong in-
dices characterizing the system. The weak indices are not shown, at least explicitly, on the table.\textsuperscript{15,16} Showing an even number of Dirac cones on its surfaces, WTI is a \textit{a priori} considered not to be robust. But recently, a few counter examples to this common belief have been proposed. One is the existence of protected gapless helical modes along a dislocation line in the WTI.\textsuperscript{17,18} More recently, a couple of papers have appeared, demonstrating that an even number of Dirac cones on the surface of WTI are actually not that fragile against disorder.\textsuperscript{19,20} Here, we point out that in a specific situation in the prism-shaped geometry the surface state of a WTI is in a sense “more strongly protected” from a finite-size energy gap than that of a STI.

The paper is organized as follows. In Sec. II we introduce our effective model Hamiltonian for 3D anisotropic topological insulators. The phase diagram of the model is determined by the calculation of topological numbers in the bulk. In Sec. III we discuss different origins of the finite-size energy gap, highlighting the role of spin-to-surface locking in the cylindrical geometry. In Sec. VI we demonstrate that in the more realistic rectangular-prism geometry, three types of gap-opening appear and disappear by a small change of model parameters, leading to an intricate size dependence of the gap. Sec. VI is devoted to Conclusions.

II. MODEL AND ITS PHASE DIAGRAM—ENGINEERING THE WEAK INDICES

As a concrete realization of strong and weak topological insulators with specific strong and weak indices, $\nu_0$ and $\vec{\nu} = (\nu_1,\nu_2,\nu_3)$, we consider as given in Eq. (1), a Wilson-Dirac type effective Hamiltonian for a 3D topological insulator implemented on a cubic lattice.\textsuperscript{21,22} Since we will be interested in the analysis of WTI phases with anisotropic weak indices, we choose the mass parameters $m_{2x}$, $m_{2y}$, $m_{2z}$ appearing in the Wilson term [see Eq. (2)] to be anisotropic.

A. The Wilson-Dirac type effective Hamiltonian

Let us consider the following Wilson-Dirac type effective Hamiltonian for a 3D topological insulator implemented on a cubic lattice:

$$H_{\text{bulk}} = \epsilon(k)1 + \tau_x m(k) + \tau_y \sigma_{\mu} A_{\mu} \sin k_{\mu},$$

where $\epsilon(k)$ is an even function of $k$, and

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

In Eqs. (1) and (2) a summation over the repeated index $\mu = (x,y,z)$ is not shown explicitly. The model specified by this couple of equations can be regarded as a tight-binding model with only the nearest neighbor hopping, determining the structure of the energy bands over the entire 3D Brillouin zone (BZ). Eq. (1) can be regarded as a $4 \times 4$ matrix, spanned by two types of Pauli matrices $\sigma$ and $\tau$ each representing physically real and orbital spins, respectively. Compared with a more generic representation of the Dirac Hamiltonian in terms of the “$\gamma$-matrices”, we have chosen in Eq. (1) ”$\gamma_0$” coupled to the mass term $m(k)$ associated only with an orbital spin $\tau_x$.

The mass term (2) represents (a half of) the band gap at time-reversal invariant momenta (TRIM), $k = k_0$, satisfying $-k_0 = k_0 + G$, with $G$ being a reciprocal lattice vector, corresponding either to a normal or an inverted gap, depending on the relative sign of $m_0$ and the coefficient of the quadratic (Wilson) term at a given TRIM. By investigating this feature of band inversion at the eight TRIM as varying the mass parameters, one can identify\textsuperscript{23} various weak and strong TI phases characterized by strong and weak indices, $\nu_0$ and $\vec{\nu} = (\nu_1,\nu_2,\nu_3)$.
Phase boundaries between such topologically distinguishable insulating phases correspond necessarily to closing of the bulk energy gap.

Known examples of 3D topological insulators are layered materials, exhibiting, in the leading order approximation, uniaxial anisotropy in the crystal c-axis.\textsuperscript{24–28} To reflect this feature in the effective tight-binding model, i.e., in Eqs. (1), (2) we assume that our model parameters have the same uniaxial anisotropy.\textsuperscript{21} Especially, the three mass parameters $m_{2x}$, $m_{2y}$, $m_{2z}$ are classified to two types: $m_{2\perp}$ and $m_{2\parallel}$, depending on whether the corresponding hopping direction is either parallel or perpendicular to the stacked layers of the crystal. Clearly, the correspondence depends on the relative orientation of the crystal growth axis and our cartesian coordinates; e.g., when the crystal c-axis is oriented to the direction of z-axis,

$$m_{2\perp} = m_{2z}, \quad m_{2\parallel} = m_{2x} = m_{2y}, \quad A_\perp = A_z, \quad A_\parallel = A_x = A_y. \quad (3)$$

Independently of this choice of the relative orientation, our control parameters for specifying topologically different phases are relative magnitudes of $m_0$, $m_{2\perp}$ and $m_{2\parallel}$. Then, by studying the feature of band inversion at eight TRIM as a function of these control parameters,\textsuperscript{23} one can deduce the phase diagram of the model. FIG. 1 shows such a phase diagram depicted in the $(m_0/m_{2\parallel}, m_{2\perp}/m_{2\parallel})$-plane.

### B. Phase diagram

FIG. 1 shows the phase diagram of the Wilson-Dirac type effective tight-binding Hamiltonian given in Eqs. (1), (2). The uniaxial anisotropy of the hopping parameters, as given by Eqs. (3), is taken into account. Each of the STI and WTI phases are characterized by four $\mathbb{Z}_2$ indices. The calculated winding number $N_3$ (see Appendix A) is also shown. Solid lines, separating neighboring topologically distinct phases, indicate closing of the bulk energy gap. Duplicate lines appearing at the phase boundary correspond to simultaneous formation of two bulk 3D Dirac cones. The duplication is due to the uniaxial choice of the hopping parameters. To see such specific features, let us focus below on a few particular examples of the STI and WTI phases.

Let us first concentrate on the isotropic line $m_{2\perp}/m_{2\parallel} = 1$ in the phase diagram (indicated as a thick green line in FIG. 1). The change of the winding number $N_3$ on this line is shown in the first panel of FIG. 11. Notice that on this line different STI and WTI phases show only symmetric weak indices. At the phase boundaries between STI and WTI phases, a double and single solid lines cross, indicating simultaneous closing of three Dirac cones in the bulk. This occurs at X, Y, Z: $k_X = (\pi, 0, 0)$, $k_Y = (0, \pi, 0)$, $k_Z = (0, 0, \pi)$, three symmetric points (TRIM) in the 3D BZ.

Stopping at $m_0/m_{2\parallel} = -1$, let us now vary $m_{2\perp}/m_{2\parallel}$, i.e., introduce anisotropy in the mass parameters. On the line $m_0/m_{2\parallel} = -1$ (a thick red line in FIG. 1), the system is in a STI phase with $\nu_0 = 1$ and $\nu = (0,0,0)$, when $m_{2\perp}/m_{2\parallel} > 1/4$. The anisotropy appears in the weak indices below this critical value, $m_{2\perp} = -m_0/4$, corresponding to band crossing occurs at the Z-point, and the system enters a WTI-A phase with $\nu_0 = 0$ and $\nu = (0,0,1)$ when $m_{2\perp}/m_{2\parallel} < 1/4$. In later sections we will quantify various manifestations of this quantum phase transition in the finite size effects. The situation is similar on the line $m_0/m_{2\parallel} = -5$ (a thick blue line in FIG. 1), above and below the critical point $m_{2\perp}/m_{2\parallel} = 1/4$, although in this second example the transition occurs from an isotropic to an anisotropic WTI phase, each named, respectively, WTI-B and WTI-C phases.

| geometry        | x-PBC | y-PBC | z-PBC |
|-----------------|-------|-------|-------|
| surfaceless     | 1     | 1     | 1     |
| slab            | 1     | 1     | 0     |
| (rectangular) prism | 0     | 1     | 0     |
| cubic           | 0     | 0     | 0     |

TABLE I. Definition of the surfaceless, slab, (rectangular) prism and cubic geometries. Here, to avoid confusion in the terminology, we define these different types of geometries in terms of the switching on and off of the periodic boundary conditions (PBC) in the $x$, $y$, and $z$-directions. In the Table, “1” and “0” signifies that the PBC in the corresponding direction is, respectively, on and off. In the latter case, PBC is replaced by the fixed boundary condition (FBC).

### III. Different origins of the finite-size energy gap

A single Dirac cone on the surface of a STI is topologically protected,\textsuperscript{2} and also robust against disorder.\textsuperscript{29,30} In reality, TI samples always have a finite thickness between the two surfaces of opposing sides. Imagine a slab-shaped sample (cf. Table I), which we assume infinitely large, neglecting the existence of side surfaces. In such a slab geometry, STI bears a pair of surface Dirac cones, each localized in the vicinity of the two opposing surfaces. These two “Dirac cones” do not communicate, and consequently remain gapless, as far as the thickness of the slab is much larger than the penetration of the surface state into the bulk [see Appendix B for an extensive discussion on the penetration of the surface wave function in the slab geometry; see also Refs.\textsuperscript{4–7}].

In a sense this gaplessness is also protected by the very slab geometry. In the case of a sample of more realistic shape with typically side surfaces (cf., cases of a prism and a cube; see Table I), the same protection is no longer valid. The side surfaces open a priori gapless channels allowing for communication between the two initial Dirac
cones on two surfaces of the slab. Since this communication through gapless side surfaces is much stronger than the one through the gapped bulk (cf. case of the slab geometry), it leads to opening of a size gap qualitatively more relevant than the latter case.

Of course, the effects of such side surfaces appear in the transport characteristics only when an electron can really “see” the ends of the sample. In a macroscopic sample in which the (single-particle) relaxation length, determined, e.g., by the inelastic scattering length, does not exceed the size of the system, finite-sizes effects, corresponding to a length scale smaller than the former, are naturally smeared out. In the following sections we consider nanowire samples that have a nano-meter scale cross section, with its circumference sufficiently smaller than the relaxation length. Here, we concentrate on the cylindrical geometry, imposing additionally a rotational (cylindrical) symmetry. We also assume that the system extends to infinity, or (by taking only two of four end (cylindrical) symmetry. We also assume that the system is often cited with another adjective “helical”. The word, really “see” the ends of the sample. In a macroscopic geometry, it leads to opening of a size gap qualitatively more relevant than the latter case.

A. Spin-to-surface locking on the cylindrical surface

The protected surface state of a topological insulator is often cited with another adjective “helical”. The word, helical, stems from a specific feature, often referred to as spin-to-momentum locking,\textsuperscript{32} that the helical state exhibits in momentum space. Here, we highlight another characteristic of the helical surface state, the “spin-to-surface locking”, which manifests in real space, and when the surface is curved. The electronic spin in a helical state is often cited with another adjective “helical”. The word, really “see” the ends of the sample. In a macroscopic geometry, it leads to opening of a size gap qualitatively more relevant than the latter case.

The spin-to-surface locking can be also regarded as a consequence of (spin) Berry phase of $\pi$. In the case of rotationally symmetric (cylindrical) wire, the orbital angular momentum along the axis of the wire is quantized to be half-odd integers. This half-odd integral quantization gaps out the spectrum of electronic motion along the wire. The spin-to-surface locking leads, indeed, irrespective of the presence of rotational symmetry, to opening of the Dirac spectrum.

To be explicit let us consider the continuum limit of Eqs. (1) and (2), or an effective $k \cdot p$ Hamiltonian at the $\Gamma$-point ($k = 0$),

$$H_{\text{bulk}} = \epsilon(p)1 + \tau_z m(p) + A r y \sigma_{\mu} p_{\mu},$$

where $m(p) = m_0 + m_2 p^2$. Here, we focus on the isotropic case: $m_2 = m_2$ and $A_{\mu} = A$ for $\mu = x, y, z$. We also assume $\epsilon(p) = 0$, for simplicity. We then consider the eigenvalue problem for Eq. (4), i.e.,

$$H_{\text{bulk}}|\psi\rangle = E|\psi\rangle,$$

in the cylindrical coordinates:

$$r = \sqrt{x^2 + y^2}, \quad \phi = \arctan \frac{y}{x}. \quad (6)$$

Note that our TI sample occupies the interior of a cylinder of radius $R$. As shown in the Appendix C, any surface solutions $|\alpha\rangle$ of Eq. (5) can be expressed as a linear combination of the two basis solutions,

$$|r+\rangle_{\text{dv}} = \rho(r)|\tau_z+\rangle|r+\rangle_{\text{dv}},$$

$$|r-\rangle_{\text{dv}} = \rho(r)|\tau_z-\rangle|r-\rangle_{\text{dv}}, \quad (7)$$

where $|\tau_z\pm\rangle$ is an eigenstate of $\tau_z$ with the corresponding eigenvalue $\pm 1$ and

$$|r\pm\rangle_{\text{dv}} = \frac{1}{\sqrt{2}} \left[ e^{-i\phi/2} \pm e^{i\phi/2} \right]$$

are two real spin eigenstates pointing either to the centripetal (+$r$) or to the centripetal (−$r$) direction. In Eqs. (7), $\rho(r)$ is the radial part of the surface wave function localized in the vicinity of the surface of the cylinder, given explicitly in Eq. (C12). In Eqs. (7), (8) the subscript “dv” is added to make explicit that these spinors are double-valued. In terms of $|r\pm\rangle_{\text{dv}}$, the surface solution $|\alpha\rangle$ reads

$$|\alpha\rangle = \alpha_+(\phi)|r+\rangle_{\text{dv}} + \alpha_-(\phi)|r-\rangle_{\text{dv}}. \quad (9)$$

Here, the explicit form of the coefficients $\alpha_\pm(\phi)$ is determined by solving the eigenvalue problem for the following surface effective Hamiltonian,

$$H_{\text{surf}} = A \left[ -\frac{1}{R} \left[ -i \frac{\partial}{\partial \phi} \right] \sigma_3 + p_z \sigma_y \right],$$

i.e.,

$$H_{\text{surf}} \alpha(\phi) = E \alpha(\phi), \quad (10)$$

where

$$\alpha(\phi) = \begin{bmatrix} \alpha_+(\phi) \\ \alpha_-(\phi) \end{bmatrix}. \quad (12)$$

Notice here that thanks to the rotational symmetry with respect to the axis of the cylinder the orbital angular momentum $L_z$ is a good quantum number, which can be simultaneously diagonalized with $H_{\text{surf}}$ and $p_z$. In the following, we focus on such surface eigenstates of $L_z$, which can be represented in terms of $\alpha(\phi)$ introduced in Eqs. (11), (12) as

$$\alpha(\phi) = \alpha_{L_z,p_z}(\phi)$$

$$= \begin{bmatrix} \alpha_+(\phi) \\ \alpha_-(\phi) \end{bmatrix} = e^{iL_z\phi} \begin{bmatrix} \alpha_+(0) \\ \alpha_-(0) \end{bmatrix}. \quad (13)$$

$\alpha_+(0)$ is specified by the orientation of the surface crystal momentum specified by $p_z$ and $p_\phi = L_z/R$. The corresponding eigenenergy $E$ of $H_{\text{surf}}$ is then specified by $p_\phi$ and $p_z$ as

$$E = E(p_\phi, p_z) = \pm A \sqrt{p_\phi^2 + p_z^2}. \quad (14)$$
The state $|\alpha\rangle$ thus given, and specified by the $\alpha(\phi)$ given in Eq. (9), signifies a simultaneous eigenstate of $H_{\text{bulk}}, L_z$ and $p_z$, which may be also represented $|L_z, p_z\rangle$. Eq. (9) implies that such a state is an equal-weight superposition of the centrifugal and the centripetal spin components given in Eqs. (8), since $|\alpha_{+}(0)| = |\alpha_{-}(0)|$. This signifies that when an electron is on the surface of the cylinder at an angle $\phi$ in the configuration space, its spin state is constrained onto the local tangent of the cylinder at this position (spin-to-surface locking). While an electron travels around the cylinder in the configuration space, the corresponding spin frame also completes a $2\pi$ rotation in the spin space.

B. Half-integral quantization of the orbital angular momentum and the resulting finite-size energy gap

Let us reconsider the statue of the angle $\phi$ in different steps of the formulation. In the original bulk effective Hamiltonian (4) the angle $\phi$ purely specifies the position of an electron in the configuration space. This is also the case in its eigenstate $|\alpha\rangle$. Therefore, $|\alpha\rangle$ must be single-valued with respect to the $2\pi$-rotation of $\phi$,

$$|\alpha\rangle|_{\phi\to\phi+2\pi} = |\alpha\rangle. \quad (15)$$

On contrary, $\phi$ in $|r\pm\rangle_{dv}$ specifies the direction of real SU(2) spin. Therefore, $|r\pm\rangle_{dv}$ is double-valued with respect to the $2\pi$-rotation of $\phi$,

$$|r\pm\rangle_{dv}|_{\phi\to\phi+2\pi} = -|r\pm\rangle_{dv}. \quad (16)$$

In Eq. (9) these two boundary conditions are compatible, only if

$$\alpha(\phi + 2\pi) = -\alpha(\phi), \quad (17)$$

i.e., the coefficients $\alpha_{\pm}(\phi)$ are also anti-periodic. In the light of Eq. (13), this requires,

$$L_z = \pm \frac{1}{2}, \pm \frac{3}{2}, \ldots, \quad (18)$$

i.e., the orbital angular momentum $L_z$ is quantized to be half-odd integers.

Notice also that the double-valuedness of $|r\pm\rangle_{dv}$ is not essential for the half-integral quantization of $L_z$. One can equally employ the single-valued version of Eq. (8),

$$|r\pm\rangle_{sv} = \frac{1}{\sqrt{2}} \left[ \begin{array}{c} 1 \\
\pm e^{i\phi} \end{array} \right], \quad (19)$$

which is related to $|r\pm\rangle_{dv}$ by a simple phase factor,

$$|r\pm\rangle_{sv} = e^{i\phi/2} |r\pm\rangle_{dv}. \quad (20)$$

In this single-valued basis the surface effective Hamiltonian acquires an additional phase factor $\pi$, the spin Berry phase, as

$$\tilde{H}_{\text{surf}} = A \left[ -\frac{1}{R} \left( -i \frac{\partial}{\partial \phi} \pm \frac{1}{2} \right) \sigma_x + p_z \sigma_y \right]. \quad (21)$$

Then, if one employs the same representation (13) for the coefficients $\alpha, L_z$ takes formally integral values, $L_z = 0, \pm 1, \pm 2, \ldots$. The corresponding eigenenergy $E = E(p_{\phi}, p_z)$ can be also written formally in the same way as in Eq. (14). But in that case, $p_{\phi}$ in the same formula must be reinterpreted as

$$p_{\phi} = \frac{L_z + 1/2}{R}. \quad (22)$$

This energy gap due to spin-to-surface locking, or eventually to the doubling of the original two Dirac cones through “side surfaces” of the cylinder, decays only algebraically as a function of (inversely proportionally to) the circumference of the cylinder. This enhanced finite-size energy gap is in marked contrast with that of the slab due to mixing of the two surface wave functions sitting mainly on the opposing sides of the slab and separated by the bulk energy gap.

IV. CASE OF THE RECTANGULAR PRISM GEOMETRY

In the previous section, we have considered an idealized case of the cylindrical geometry, to demonstrate how spin-to-surface locking leads to opening of the finite-size energy gap. With the rotational (cylindrical) symmetry hypothesized, the cylindrical geometry was best suited for analytic considerations of the surface state. Here, we attempt to realize an equivalent situation in numerical experiments in terms of the tight-binding simulation. For that purpose, we consider rather prism-shaped samples whose cross section on the plane normal to the axis of the (right) prism is a rectangle rather than a circle. From the viewpoint of topology, such a rectangular prism shape is a natural implementation of the cylinder-like geometry on the cubic lattice.

In addition to that aspect as a substitute of a cylinder, there is also a more positive reason we focus here on this rectangular prism geometry. In the last few sections, throughout the comparison of slab and cylinder, we have seen that preventing the communication of two Dirac cones sitting on the opposing sides of the sample helps protecting the gaplessness of Dirac cones. We have so far discussed such switching on and off of this communication channel by changing the system’s (global) geometry. Here, in this section, a new element comes into...
cases type of the phase parity of $N_z$ size gap; $N_z$ dependence gap opening mechanism
(a) WTI even $N_z^{-1}$ (iii) doubling of Dirac cones due to confinement
(b) WTI odd “0” (exponentially small) (i) mixing of the opposing sides through gapped bulk
(c) STI irrelevant $(N_z + N_x)^{-1}$ (ii) spin-to-surface locking

TABLE II. Three typical behaviors of the finite-size energy gap in the rectangular-prism shaped samples.

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FIG. 2. Surface wave function in the rectangular prism geometry [Eq. (24)]; WTI phase ($m_{2z}/m_{2||} = 0.2$) with $N_z$ even. Upper: the square of the wave function $|\psi(z,x)|^2$ with $N_z = 20$, $N_x = 20$ and $k_y = 0$ is plotted in the $(z,x)$-plane. Spin and orbital indices are summed over. $A_\perp = A_\parallel = 1$. Lower: $|\psi(x,y,z)|^2$ is plotted in the 3D $(x,y,z)$-space. The front, upper and right surfaces correspond, respectively, to the ones normal to $(-1,0,0)$, $(0,1,0)$ and $(0,0,1)$. Fixed boundary condition (FBC) in the $z$- and $x$-directions. PBC in the $y$-direction.

FIG. 3. Plots of the surface wave function in the rectangular prism geometry analogous to FIG. 2. Case of $N_z$ odd ($N_z = 19$). WTI phase. $N_z = 20$, $k_y = 0$, $A_\perp = A_\parallel = 1$. FBC in the $z$- and $x$-directions. PBC in the $y$-direction.

The system we consider here has a shape of rectangular prism extended in the $\hat{y}$-direction. We assume that the prism is infinitely long, or periodic, without end surfaces. Each cross section of the system at fixed $y$ is restricted to a rectangular area of size $N_z \times N_x$ in the $(z,x)$-plane:

$$1 \leq z \leq N_z, \quad 1 \leq x \leq N_x.$$ (24)

play, the weak indices. As mentioned in the Introduction, the weak indices have the potentiality of excluding a gapless Dirac cone from a surface oriented in a particular direction, i.e., that of the weak vector, $\vec{\nu} = (\nu_1, \nu_2, \nu_3)$.

Folded surfaces of the rectangular prism geometry are more adapted for implementing a weak vector as a means for eradicating the “dangerous” gapless channels from the targeted side surfaces. Another characteristic of the WTI surface state is that it exhibits even number of Dirac cones. These two features combine to make gaplessness of the surface state of a prism-shaped WTI a rather subtle issue, which depends intricately on the geometry and on the nature of weak indices. Depending on the relative orientation between the weak vector and the surfaces of the rectangular prism and on the size of the prism, non-compatibility of the surface wave function with a specific boundary condition imposed by the geometry leads to, or not to opening of a finite-size energy gap.

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FIG. 4. Plots of the surface wave function in the STI case ($m_{2z}/m_{2\parallel} = 0.3$); plots similar to FIG. 2 and FIG. 3. Here, the surface wave function is extended over all the four facets of the prism.

The system has two surfaces ($\hat{x}$-surfaces) at $x = 1$ and $x = N_x$ normal to $\hat{x} = (1,0,0)$ and two others ($\hat{z}$-surfaces) at $z = 1$ and $z = N_z$ normal to $\hat{z} = (0,0,1)$. We assume translational symmetry in the $\hat{y}$-direction; $k_y$ is a good quantum number. As for the anisotropy of bulk topological insulators, we consider the case of mass parameters with uniaxial-type anisotropy as given in Eq. (3). In the WTI phase, this corresponds to the case of stacked 2D TI layers piled up in the $z$-direction.

In the following, we will mainly focus on the WTI phase with a specific weak vector $\vec{\nu} = (0,0,1)$ normal to the $\hat{z}$-surfaces. Then, gapless Dirac cones are completely eliminated from these surfaces, at least in the limit of infinitely large surfaces. In the prism geometry (24), the wave function of the corresponding surface state has a finite amplitude only on $\hat{x}$-surfaces, barely penetrates into the $\hat{z}$-side. The Dirac cones forced to be localized in each of the $\hat{x}$-surfaces are subject to a particular boundary condition imposed by this combination of the prism geometry and the weak vector. Compatibility or non-compatibility of the surface wave function with this specific boundary condition leads to an even/odd feature with respect to $N_z$ (width of the $\hat{x}$-surfaces) of the finite-size energy gap in the WTI phase. After reviewing three typical situations we encounter in the analysis of the size gap in the WTI and STI phases, we describe the nature of even/odd feature in the spirit of $k \cdot p$ approximation.

A. Even/odd feature in the WTI phase

The three typical situations we investigate are the cases of

- WTI with $N_z$ even [case (a)],
- WTI with $N_z$ odd [case (b)], and
- STI [case (c)].

The three cases are also listed in Table II. In our model, Eqs. (1), (2), and in the geometry employed, the three situations can be realized by a small change of parameters. As for the concrete choice of parameters, we use here the following double standard. We first use the “theoretical values” that varies on the lines indicated in
FIG. 1 for the demonstration of crossover from type (c) to type (a), and from type (c) to type (b) behaviors. We believe that use of these theoretical values help understanding the nature of the phenomenon in the light of the phase diagram. Then, in the actual computation of the size gap, we also use “experimental values” of the parameters that are deduced from experimental data for Bi$_2$Se$_3$. 21,34

The three situations can be easily contrasted by the shape of the surface wave function. In the WTI phase (FIG. 2 and FIG. 3) the amplitude of the surface wave function concentrates on the two $\vec{x}$ surfaces. The weak vector $\vec{v}$ is here pointed in the direction $\hat{z}$, expels the surface state from the sides normal to $\hat{z}$. In the STI phase (FIG. 4), on contrary, the surface state is extended over all the four surfaces. In these figures the square of the total amplitude of the surface wave function,

$$|\psi(z,x)|^2 = \sum_{j=1}^{4} |\psi_j(z,x)|^2,$$

is plotted at each point on a cross section (the system is translationally invariant in the $y$-direction).

Let us focus on more detailed structures of the shape of the surface wave function in the WTI phase, and compare the cases of $N_z$ even (FIG. 2) and $N_z$ odd (FIG. 3). On the two $\vec{x}$ surfaces, the wave function shows a regular pattern, vanishing practically at every other layer, when $N_z$ is odd, whereas in FIG. 2 it is concave shaped (case of $N_z$ even).

This even-odd feature appears more clearly in the behavior of the finite-size energy gap (see FIG. 5). On the (red) line $m_0/m_{2||} = -1$ of the phase diagram (FIG. 1), slightly below [WTI-A: (0,100)] and above [STI: (1,000)] the phase boundary at $m_{2||}/m_0 = -1/4$ the gap is plotted as a function $N_z$ (the number of stacking layers). In the WTI case: $m_{2z}/m_{2||} = 0.2$, $E_0 = E_0(N_z)$ shows an even/odd feature, and for $N_z$ even the gap scales as $\sim (N_z + 1)^{-1}$. In the STI case: $m_{2z}/m_{2||} = 0.3$, a weak even/odd feature for small $N_z$ is washed out as $N_z$ increases, and the gap scales as $\sim (N_z + N_y)^{-1}$. In a sense, depending on the parity of the number of stacked layers, the system becomes either trivial (gapped, when $N_z$ even) or gapless (when $N_z$ odd). Physically, this even/odd feature stems from the fact that WTI can be treated as a function of $N_z$ pattern, vanishing practically at every other layer, when $N_z$ is odd, whereas in FIG. 2 it is concave shaped (case of $N_z$ even), even the gap scales $\sim (N_z + 1)^{-1}$. Physically, this even/odd feature stems from the fact that WTI can be treated as a function of $N_z$ pattern, vanishing practically at every other layer, when $N_z$ is odd, whereas in FIG. 2 it is concave shaped (case of $N_z$ even), even the gap scales $\sim (N_z + 1)^{-1}$.

A single Dirac cone cannot be confined (cf. Klein tunneling). This applies to the STI phase we have considered in Sec. III, in which any surface state, instead of being terminated at the end of a plane, continues to the adjacent ones, covering the entire surface. In the WTI phase, typically two Dirac cones appear on its surfaces, i.e., there are “valleys.” In that case, one can confine them in a finite area of the surface. Let us sketch explicitly how this is possible.

A typical situation we focus on below is the case in which two side faces of the prism is normal to the weak vector $\vec{v}$, implying that there is no Dirac cone on these surfaces. In such a situation, the wave function of the WTI surface state has a finite amplitude only on the remaining two surfaces parallel to $\vec{v}$, barely penetrates into the side normal to $\vec{v}$. The key observation here is that the latter can be regarded as a “boundary condition” for the wave function that lives mainly on the primary parallel surfaces.

Let us consider a simple and concrete example. In the WTI-A phase, shown in FIG. 1, only two $\vec{x}$-surfaces are compatible with the presence of gapless Dirac cones; the remaining $\hat{z}$-surfaces are normal to $\vec{v}$, implying that there is no Dirac cone on these surfaces. In such a situation, the wave function of the WTI surface state has a finite amplitude only on the remaining two surfaces parallel to $\vec{v}$, barely penetrates into the side normal to $\vec{v}$. The key observation here is that the latter can be regarded as a “boundary condition” for the wave function that lives mainly on the primary parallel surfaces.

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B. Effective surface $k \cdot p$ theory

A single Dirac cone cannot be confined (cf. Klein tunneling). This applies to the STI phase we have considered in Sec. III, in which any surface state, instead of being terminated at the end of a plane, continues to the adjacent ones, covering the entire surface. In the WTI phase, typically two Dirac cones appear on its surfaces, i.e., there are “valleys.” In that case, one can confine them in a finite area of the surface. Let us sketch explicitly how this is possible.

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be constructed by superposing contributions from one valley surrounding a Dirac point at \(k_1\) and from another located at \(k_2\). As our system is translationally invariant in the \(y\)-direction, \(\psi(y, z)\) is expressed in the form of

\[
\psi(y, z) = e^{i k_y y} \chi(z),
\]

where \(\chi(z)\) should be chosen to satisfy the boundary conditions (26). This is allowed only when the \(y\)-components of \(k_1\) and of \(k_2\) are identical as \(k_1 = (k_0, k_1)\) and \(k_2 = (k_0, k_2)\). This is indeed the case in the WTI-A phase, where \(k_0 = 0, k_1 = 0\) and \(k_2 = \pi\). The superposition yields

\[
\chi(z) = e^{i(k_1+p_1)z} - e^{i(k_2+p_2)z},
\]

where \(p_1\) and \(p_2\) are small displacements from the corresponding Dirac points. Note that this automatically satisfies the boundary condition at \(z = 0\). If \(\chi(z)\) with \(p_1 = p_2 = 0\) (i.e., the superposition of the wave functions just at the two Dirac points) is compatible with the other boundary condition at \(z = N_z + 1\), the resulting wave function has the zero energy eigenvalue at \(k_y = k_0\), resulting in the gapless surface states. This occurs typically at \(N_z\) odd, and in the WTI-A phase with \(k_1 = 0\) and \(k_2 = \pi\). Contrastingly, if finite displacements (i.e., \(p_1, p_2 \neq 0\)) are necessary to satisfy the boundary condition, a finite size gap inevitably appears. Naturally, the latter applies to the case of \(N_z\) even. These two contrasting behaviors explain the nature of the even/odd feature demonstrated in FIG. 5.

Let us further quantify the case of \(N_z\) even. To fulfill the requirement of Eq. (26) we set \(p_1 = -p_2 = q\). The boundary condition at \(z = N_z + 1\) is satisfied, if

\[
q = \pm \frac{n}{2(N_z + 1)} \pi,
\]

and \(n\) being an odd integer. The lowest energy solution with \(n = 1\) determines the energy gap to be,

\[
E_0 = \frac{A}{2(N_z + 1)} \pi,
\]

i.e., \(E_0\) scales as \((N_z + 1)^{-1}\) for \(N_z\) even within the range of validity of the \(k \cdot p\)-approximation. Eq. (30) allows for comparing the above simple effective theory with the calculated spectrum. This is done in FIG. 5 by plotting the energy gap obtained by numerical diagonalization of the corresponding tight-binding model against the postulated scaling of Eq. (30).

A similar comparison can be made for the shape of the surface wave function. Plugging Eq. (29) with \(n = 1\) back into Eq. (28) one finds,

\[
|\chi(z)|^2 = 4 \sin^2 \left[ \frac{N_z \pi}{2(N_z + 1)} z \right].
\]

The shape of this envelop function is to be compared with the calculated value of the amplitude of the surface state eigenspinor at \(x = 1\), which is shown in FIG. 6.

It is suggestive to apply the above \(k \cdot p\) effective theory to the case of WTI-B and WTI-C phases. (see FIG. 1). These two topologically different WTI phases appear on the blue line \(m_0/m_2|| = -5\) in the phase diagram with the phase boundary at \(m_{z1}/m_{z2||} = -1/4\). The crossover of the finite-size energy gap at the transition between these two WTI phases is precisely in parallel with the one between STI and WTI-A phases (on the red line: \(m_0/m_{z2||} = -1\) in FIG. 1) we have considered so far. In the case of WTI-B and WTI-C phases, The constituent surface Dirac cones on the \(k = (k_y, k_z)\)-plane appear at \(k_1 = (\pi, 0)\) and at \(k_2 = (0, \pi)\) in the WTI-B phase, and at \(k_1 = (\pi, 0)\) and at \(k_2 = (\pi, \pi)\) in the WTI-C phase. Here, the relative position of the two Dirac cone is essential. In the case of WTI-C phase, one can construct the surface wave function (28) compatible with the specific boundary condition (26) precisely in parallel with the previous case of the WTI-A phase, simply by replacing \(k_0 = 0\) with \(k_0 = \pi\), leading to the same even/odd feature. Notice that the surface Dirac cone in the WTI-C phase appears in the spectrum of prism geometry \(E = E_{\text{prism}}(k_y)\) at \(k_y = \pi\).

In the case of WTI-B phase, the two Dirac cones at \(k_1 = (\pi, 0)\) and at \(k_2 = (0, \pi)\) are projected onto a different point on the \(k_y\) axis, making the previous construction [Eqs. (27), (28)] impossible. This is, of course, consistent with the fact that in the WTI-B phase the surface states are not confined to the \(x\)-surfaces. This observation, in turn, reveals that the relative orientation of the two (even number of) Dirac cones in the WTI is indeed imposed by the weak indices. On surfaces parallel to the weak vector \(\vec{v}\), they must appear in line in the direction of \(\vec{v}\).

### C. Effects of disorder

Let us comment here on the robustness of the surface states discussed in the previous subsections against disorder. A motivation for this is that since disorder leads generally to repulsion of the energy levels, one naturally questions whether the finite-size effects discussed so far are still meaningful when the size gap is perturbed by the effects of level repulsion by disorder. The effects of disorder is taken into account by introducing a random potential \(V(\mathbf{r})\), which obeys a uniform distribution in the period \([-W/2, W/2]\) at each site \(\mathbf{r}\) of the cubic lattice, i.e., a scalar random potential, \(\propto 1\) in the real and orbital spin space, which is also cite-diagonal:

\[
V = \sum_{\mathbf{r}} V(\mathbf{r}) \mathbf{1} \otimes |\mathbf{r}\rangle \langle \mathbf{r}|, \quad V(\mathbf{r}) \in [-W/2, W/2]
\]

is added to the tight-binding Hamiltonian (1) represented in the real space. In Eq. (32) the summation over \(\mathbf{r}\) should be taken over all the lattice sites on the cubic lattice, \(\mathbf{r} = (x, y, z)\) with \(x = 1, 2, \cdots, N_x, y = 1, 2, \cdots, N_y\) and \(z = 1, 2, \cdots, N_z\). In the actual computation we set
FIG. 7. Surface wave function in the presence of disorder. Comparison of the WTI and STI cases: $m_2/m_2\parallel = 0.2$ (upper) vs. $m_2/m_2\parallel = 0.3$ (lower). Here, the simulation is done for a system of size, $N_x \times N_y \times N_z = 10 \times 10 \times 10$; i.e., $N_z$ is even.

$W = 1$, $m_0 = -1$, $A_\perp = A_\parallel = 1$ in units of $m_2\parallel$ (which is set to be unity).

In FIG. 7 plots similar to FIG. 2, FIG. 3 and FIG. 4 performed in the presence of disorder are shown. In the upper panel (WTI case) the surface wave function is localized mainly on one facet of the prism. This is contrasting to the clean cases (FIG. 2, FIG. 3) and to the STI case (lower), in which the surface state is extended over all the four facets of the prism. The stripe-shaped structure is also still visible, indicating that the surface wave functions of a specific shape discussed in the previous subsection possess some robustness against disorder.

D. STI more gapped than WTI !?

We finally discuss the $N_z$-dependence of the size gap. As shown in Table II, there are three different types of behaviors in the $N_z$-dependence of the size gap, each corresponding to the three different gap-opening mechanisms we have highlighted in this paper. Here, let us focus again (cf. FIG. 5) on the (red) line $m_0/m_2\parallel = -1$ in the phase diagram (FIG. 1) slightly above and below the phase boundary at $m_2\perp/m_0 = -1/4$, and compare the STI: (1,000) and WTI-A: (0,001) phases. In the following demonstrations (FIG. 8, FIG. 9, FIG. 10), however, we use slightly different set of parameters inspired by the corresponding material parameters of Bi$_2$Se$_3$, but focus on the same phase boundary between STI and WTI-A. Here, the tight-binding parameters are specially adjusted to reproduce the band structure in the vicinity of $Z$-point obtained by the first-principle calculation.
The employed parameters are given explicitly as

\[ m_0 = -0.1, \quad m_\perp = m_\perp = 0.1, \quad m_\parallel = 1, \]

\[ A_\perp = A_\perp = 0.1, \quad A_\parallel = 0.3. \]  \tag{33}

Here, the parameters are normalized in units of \( m_\parallel \approx 2.60 \text{ eV} \). This set of parameters corresponds to the case of the STI phase. To achieve a weak phase we modify the value of \( m_\parallel \) in Eq. \( \text{(33)} \) as \( m_\parallel \to 0.01 \). This indeed falls on the WTI-A phase in Fig. 1. The spectrum of the \textit{strong} phase is “gapped”, showing a finite-size energy gap due to spin-to-surface locking, which decays only algebraically, \( E_0 \sim (N_x + N_z)^{-1} \neq 0 \). In the \textit{weak} phase, and in the case of \( N_z \) odd considered here, the spectrum is “gapless”, decaying exponentially as a function of the distance \( N_x \) between the two \textit{ideally} gapless patches (log \( E_0 \propto -N_x \), \( E_0 \simeq 0 \)). This is indeed a comparison of the cases (b) and (c) in Table II. In Fig. 8, the logarithm of the energy gap \( E_0 \) is plotted vs. \( N_x \) taking into account such an expected exponential decay in the WTI-A phase. But here, a systematic deviation from a simple exponential decay can be clearly seen, implying that this is rather a damped oscillation.

As mentioned in Appendix B, the magnitude of the finite-size energy gap in the slab is directly related to the (complex) penetration depth of the surface wave function, or \( \rho_{1,2} \) given in Eq. \( \text{(B10)} \). One can indeed verify,

\[ E_0(N_x) \propto |\rho_1^{N_x+1} - \rho_2^{N_x+1}|. \]  \tag{34}

Recall that in the WTI-A phase considered here two Dirac cones, one at \( k_1 = (0,0) \) and the other at \( k_2 = (0,\pi) \), are well grounded on the \( \hat{z} \)-surfaces. The corresponding surface wave functions exhibit different penetration depths at each Dirac point, which are specified by Eq. \( \text{(B10)} \). The solutions of Eq. \( \text{(B10)} \) at \( k_1 = (0,0) \) are

\[ \rho = \rho_{1,2}(k_1) \simeq 0.826 \pm 0.238 i, \]  \tag{35}

while they are given by

\[ \rho = \rho_{1,2}(k_2) \simeq 0.843 \pm 0.166 i, \]  \tag{36}

at \( k_2 = (0,\pi) \), \textit{i.e.}, in the two cases, they become a pair of complex numbers. In the slab, the finite-size energy gap is \( \kappa = (k_x, k_z) \)-resolved; \( E_0 = E_0(\kappa) \), simply the minimal value of which determines the actual magnitude of the finite-size energy gap. In the case of rectangular prism, contributions from \( k = k_1 \) and from \( k = k_2 \) are superposed to cope with the boundary condition. Notice also that here the surface wave function at \( k = k_1 \) and at \( k = k_2 \) are both oscillatory [Eqs. \( \text{(35)} \) and \( \text{(36)} \)]. These two features combine to give the oscillatory pattern of log \( E_0 \) in the WTI case in Fig. 8. In the figure, two theoretical curves for log \( E_0 \) are shown in solid curves for comparison, not showing a quantitative agreement with the actual data. The two curves correspond to the finite-size energy gap given as in Eq. \( \text{(34)} \) at \( k = k_1 \) (green) and at \( k = k_2 \) (cyan) estimated under the hypothesis that the system is slab-shaped. The actual \( N_x \)-dependence of log \( E_0 \) is somewhat in between.

Fig. 9 is a plot similar to Fig. 8, making the same comparison of the STI and WTI-A phases for the same \( N_z \) odd case except that the model parameters are slightly modified from Eq. \( \text{(33)} \). We replace one of the velocity parameters \( A_\parallel \) with \( A_\perp = 0.7 \), leaving \( A_\parallel = 0.3 \) (the same value as before). This replacement makes the corresponding solutions of Eq. \( \text{(B10)} \) two real solutions, indicating that the surface wave function exhibits a simple exponential decay. In the WTI-A phase, we have chosen as before \( m_\parallel = 0.01 \). The behavior of log \( E_0 \) in the WTI case is qualitatively different from the previous case. At the two Dirac points, \( k = k_1 \) and \( k = k_2 \), in the WTI phase, the solutions of Eq. \( \text{(B10)} \) are

\[ \rho_1(k_1) \simeq 0.821, \quad \rho_2(k_1) \simeq 0.587 \]  \tag{37}

at \( k_1 = (0,0) \), while they are given by

\[ \rho_1(k_2) \simeq 0.905, \quad \rho_2(k_2) \simeq 0.532 \]  \tag{38}

at \( k_2 = (0,\pi) \). The actual magnitude of the size gap is determined by the largest value of \( \rho_{1,2} \), which is the value of \( \rho_1 \) at \( k = k_2 \). Indeed, the actual \( N_x \)-dependence of log \( E_0 \) approaches to this scaling behavior \( E_0 \propto \rho_1(k_2)^{N_x} \), shown in a solid straight line in Fig. 9) for large enough \( N_x \).

Through these two examples we can convince ourselves that in this configuration imposed by the combination of the prism geometry and a specific choice of the weak vector, which can be achieved by adjusting the direction of crystal growth direction with respect to the prism, the strong topological insulator is qualitatively more gapped than a weak topological insulator.

In the last figure, Fig. 10, we make a comparison between the cases (a) and (c) in Table II, in contrast to
In the STI case the size gap shows a power law decay, 
$E_0 \sim \left( N_z + N_x \right)^{-1} \neq 0$, due to spin-to-surface locking. In the WTI-A phase, the size gap implied by Eq. (30) does not scale as a function of $N_z$, but given simply by

$$E_0 = \frac{A_z}{2(N_z + 1)} \pi = 0.1 \times \frac{\pi}{22} \tag{39}$$

In FIG. 10 this value is indicated as a horizontal grid line (in blue). For sufficiently large value of $N_z$, the data looks almost constant at a value not much far from the one of Eq. (39).

We have seen so far that from the viewpoint of the scaling behavior of finite-size energy gap, the statue of the strong and weak phases could be reversed. Here, to illustrate this feature we have considered only a very representative range of parameters, but the same feature is generic to the vicinity of transitions between STI and WTI phases with a suitable choice of the surface directions and the number of quintuple layers.

V. CONCLUSIONS

We have studied the finite-size energy gap in 3D weak and strong topological insulators. Employing the standard Wilson-Dirac type effective model, we have developed both numerical and analytical considerations. It has been demonstrated that anisotropy of the model and the geometry of the system are among other model parameters crucial elements for determining the qualitative nature of the finite-size energy gap. The two elements manifest in a correlated manner. The weak topological insulator (WTI) has a specific property of (i) expelling the gapless surface state from surfaces normal to its weak vector $\vec{\nu}$ ($\approx$ weak indices, i.e., no Dirac cone on the surface normal to $\vec{\nu}$, (ii) but on surfaces parallel to the weak vector, it bears two Dirac cones [more Dirac cones than a strong topological insulator (STI)]. We have seen in this paper through the study of finite-size effects that these two, seemingly competing characteristics of the WTI operate, in fact, in a cooperative way (c.f., $\vec{k} \cdot \vec{p}$-description of the surface state in the WTI phase; Sec. IV-B). The condition of no Dirac cone on the side normal to $\vec{\nu}$ imposes the relative orientation of the two Dirac cones on the side parallel to $\vec{\nu}$. The weak indices are also much related to the anisotropy of the model parameters. To encompass different scaling behaviors of the finite-size energy gap, we have manipulated the weak indices by varying the model parameters, guided by the phase diagram shown in FIG. 1.

Spin-to-surface locking is a characteristic feature of the topological insulator surface state, operational both in the WTI and STI phases, leading also to a finite-size energy gap that exhibits a specific power-law decay as a function of the system’s linear dimension. Clearly, this is more relevant than a usual exponential decay associated with the overlap of two surface wave functions, e.g., sitting on the opposing sides of the slab geometry. By its nature the finite-size energy gap due to spin-to-surface locking is not effective in the slab, but effective in the prism-shaped geometry. In the prism-shaped WTI samples, the interplay of these three ingredients; the weak vector, the spin-to-surface locking and the rectangular-prism geometry leads to intricate finite-size effects, depending on the model parameters. Three different gap opening mechanisms pointed out in this paper: (i) mixing of the surface wave functions, (ii) spin-to-surface locking, and (iii) commensurability with the boundary condition, are all effective in determining the intricate size dependence of the energy gap in the rectangular-prism geometry.

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Appendix A: Topological numbers

Notice that our model specified by Eqs. (1), (2) has inversion symmetry. This allows us to find the strong and weak $\mathbb{Z}_2$-indices with the use of Fu-Kane’s formula. Here, we mention that in the specific case of $\epsilon(\vec{k}) = 0$ (in most of the analyses in this paper we employ this condition for mathematical simplicity) one can introduce a $Z$-type winding number $N_3$. The strong index $\nu_0$ is related to $N_3$ as $\nu_0 = N_3 \mod 2$.

In terms of the periodic table\cite{15,35–39} our starting bulk effective Hamiltonian (1) falls on the class AII. This class of models has the symmetry, $\Theta^2 = -1$, $C^2 = 0$ and $\Gamma_5 = 0$, where $\Theta$, $C$ and $\Gamma_5$ represent, respectively, the time-reversal, particle-hole and chiral symmetries, and in this terminology “0” indicates that the system does not possess that type of symmetry. The periodic table says that class AII models are characterized by $\mathbb{Z}_2$-type bulk topological invariants in 3D. For the specific case of $\epsilon(\vec{k}) = 0$ in our model, the symmetry of the model is upgraded to the class DIII, i.e., $\Theta^2 = -1$, $C^2 = 1$ and $\Gamma_5 = 1$, where for the specific Hamiltonian, Eq. (1), $C$ and $\Gamma_5$ are given by $C = \sigma_y \tau_y K$ and $\Gamma_5 = \tau_y$. This symmetry class allows for $Z$-type bulk topological classification in 3D, characterized by a $Z$-type winding number $N_3$ to be defined below.

To construct the winding number $N_3$ explicitly, let us first represent the bulk Hamiltonian (1), using an explicit matrix representations for the orbital Pauli matrices $\tau_x$.
where \( E(k) = \pm \sqrt{m(k)^2 + P_\mu(k)^2} \), and
\[
Q(k) = \frac{m(k) - iP_\mu(k)\sigma_\mu}{|E(k)|}.
\] (A3)

Note that the matrix \( Q \) defined above is a \( 2 \times 2 \) \( SU(2) \) matrix, satisfying \( Q^\dagger Q = 1 \) and \( \det Q = 1 \). Then, one can introduce an integral winding number \( N_3 \) characterizing the mapping of the 3D Brillouin zone onto this \( SU(2) \) matrix as
\[
N_3 = \frac{1}{24\pi^2} \int_{\text{BZ}} d^3k \epsilon_{\mu\nu\lambda} \text{Tr} [\Gamma_\mu \Gamma_\nu \Gamma_\lambda], \tag{A4}
\]
where \( \Gamma_\mu = Q^\dagger \partial_{k_\mu} Q \). The integration should be done over the entire 3D Brillouin zone. We have evaluated this winding number numerically over the entire range of parameters shown in FIG. 1 to verify that
\[
\nu_0 = N_3 \mod 2 \tag{A5}
\]
indeed holds. The explicit values of \( N_3 \) in the different STI and WTI phases are also shown in FIG. 1. The same calculated value is also shown continuously in FIG. 11 as a function of a control parameter, either \( m_0/m_{2\parallel} \) or \( m_{2\perp}/m_{2\parallel} \) on a few specific lines in FIG. 1.

\section*{Appendix B: Penetration of the surface wave function in the slab geometry}

To quantify the surface electronic state in the slab geometry, let us concentrate on one surface of the slab. Also, we choose this flat surface normal to the \( \hat{x} \)-direction. To find the wave function which is localized in the vicinity of the surface we divide the bulk Hamiltonian (1) into two parts:
\[
H_{\text{bulk}}(k) = H_{\parallel}(k_{\parallel}) + H_{\perp}(k_x), \tag{B1}
\]
where \( k_{\parallel} = (k_y, k_z) \) and
\[
H_{\parallel}(k_{\parallel}) = \tau_x m_{\parallel}(k_{\parallel}) + \tau_y (\sigma_y A_y \sin k_y + \sigma_z A_z \sin k_z), \tag{B2}
\]
with \( m_{\parallel}(k_{\parallel}) \) defined as
\[
m_{\parallel}(k) = m_0 + 2m_{2\parallel} + 2m_{2\parallel}(1 - \cos k_y) + 2m_{2\parallel}(1 - \cos k_z), \tag{B3}
\]
and
\[
H_{\perp}(k_x) = -2\tau_x m_{2\parallel} \cos k_x + \tau_y \sigma_z A_z \sin k_x. \tag{B4}
\]

This and the following procedure is in parallel with the case in which we deal with the continuum model, a more standard situation in the context of \( k \cdot p \) approximation, discussed in Appendix C, but here we solve the lattice model directly without taking the continuum limit.\textsuperscript{43,44} Physically the decomposition (B1) is based on the picture that each \((y, z)\)-plane described by \( H_{\parallel}(k_{\parallel}) \) is coupled by \( H_{\perp}(k_x) \) to the neighboring layers. In the present geometry, \( k_{\parallel} = (k_y, k_z) \) is a good quantum number. Here,
we assume that the system is extended in the half space: \( x \geq 1 \), and impose a boundary condition: \( \psi(x = 0) = 0 \). A surface solution in such a geometry can be constructed by composing a linear combination of base solutions of the form, \( \psi(x) = \rho^2 \psi_0 (|\rho| < 1) \). For such damped (instead of plane-wave) solutions, Eq. (B4) modifies to

\[
H_\perp(p) = -2\tau_x m_2 \rho + \frac{\rho^{-1}}{2} + \tau_y \sigma_x A_x \rho - \frac{\rho^{-1}}{2}.
\]

In the surface energy spectrum \( E = E(k) \), protected gapless Dirac points can appear at either of the four TRIM: \( k_{\text{TRIM}} = (0,0), (\pi,0), (0,\pi), (\pi,\pi) \). At such TRIM of the surface BZ, the hopping terms in \( H(k) \) become inert;

\[
H(k) = \tau_x m(k) k_{\text{TRIM}} = \tau_x m(k) k_{\text{TRIM}}.
\]  

This significantly simplifies the derivation of \( \psi(k) \) at \( k = k_{\text{TRIM}} \). Notice also that Eq. (B2) with (B3) can be regarded as a lattice Hamiltonian for a 2D \( \mathbb{Z}_2 \) TI with an effective mass parameter \( m_2 > 0 \) (\( m_2 < 0 \)) corresponds, respectively, to the non-trivial (\( \nu = 0 \)) phases, where \( \nu \) is the 2D \( \mathbb{Z}_2 \) index. A situation described by this couple of equations realizes in the limit \( N_2 \to 1 \).

Let us construct the surface wave function,

\[
\psi(k, x) = \rho^2 \psi_0(k),
\]

explicitly at \( k = k_{\text{TRIM}} \). At TRIM, \( \psi_0(k) \) satisfies,

\[
H_{\text{bulk}} \psi_0 = \left[ \tau_x m(k_{\text{TRIM}}) + H_\perp(p) \right] \psi_0 = 0,
\]

i.e., \( \psi_0 \) is a zero-energy eigenstate of

\[
\tau_x H_{\text{bulk}} = m_\parallel(k_{\text{TRIM}}) - m_2 \rho (\rho + \rho^{-1}) + \tau_x \sigma_x A_x \frac{\rho - \rho^{-1}}{2}.
\]

Similarly to the case of the continuum model (see Appendix C), this zero-energy condition is proven to be necessary for constructing a surface solution compatible with the boundary condition at \( x = 0 \) in the form of Eq. (B12). Clearly, any of the four simultaneous eigenstates of \( \tau_x \) and \( \sigma_x \), \( \psi_{\pm\pm} = |\tau_x|^2 |\sigma_x|^2 \), is an eigenstate of the reduced operator (B9). Then the zero-energy condition can be used, in turn, to determine \( \rho \) as

\[
\rho = \frac{m_\parallel \pm \sqrt{m_\parallel^2 + 4m_2^2 A_x^2 / 4}}{2(m_2 \pm A_x / 2)} \equiv \rho_{1,2}
\]

where

\[
m_\parallel = m_\parallel(k_{\text{TRIM}}) \equiv m_0(k_{\text{TRIM}}) + 2m_2.
\]

Here, \( m_0(k_{\text{TRIM}}) \) represents the magnitude of bulk energy gap at \( k = k_{\text{TRIM}} \). In Eq. (B10) the meaning of two double signs may need some explanation; the one in the numerator is arbitrary, each choice corresponding to \( \rho_{1,2} \). The one in the denominator represents + for \( \psi_0 = \psi_{++} \) and \( \psi_{--} \), whereas, the same sign represents – for \( \psi_0 = \psi_{+-} \) and \( \psi_{-+} \). The structure of Eq. (B9) with the understanding that \( \tau_x \sigma_x = \pm 1 \) indicates that \( \rho \) satisfies the zero-energy condition, so does \( \rho^{-1} \). With a suitable choice of \( \psi_0 \), satisfying both \( |\rho_1| < 1 \) and \( |\rho_2| < 1 \), the surface solution can be constructed as

\[
\psi(x) = (\rho_1^2 - \rho_2^2) \psi_0.
\]

In a separate paper we study in detail various aspects of the finite-size effects in a slab-shaped sample. The magnitude of the finite-size energy gap in the slab is determined by the overlap of the two surface wave functions sitting on the opposing sides of the slab. It is, therefore, naturally expected that the magnitude of the gap (in a slab of width \( N_x \)) is essentially determined by the penetration depth, or the amplitude of the wave function (B12) at the depth of \( x = N_x \). Here, in this model one can verify that the correlation of theses two quantities is a bit stronger than this. The magnitude of the size energy gap \( E_0(N_x) \) is indeed directly proportional to \( |\psi(N_x)| \) as given in Eq. (34).  

Appendix C: Derivation of the effective surface Hamiltonian in the cylinder geometry

To find the surface effective Hamiltonian on the cylinder in the spirit of the \( k \cdot p \) approximation, one first divides the bulk 3D effective Hamiltonian (4) into two parts; one perpendicular, the other parallel to the cylindrical surface:

\[
H = H_\perp(p_r) + H_\parallel(p_\phi, p_z), \tag{C1}
\]

where \( H_\perp = H|_{p_r=0} \), and \( p_r = -i \partial / \partial r \). \( H_\perp \) and \( H_\parallel \) read explicitly,

\[
H_\perp = \left( m_\perp \tau_x + Ap_r \sigma_y \cos \phi + Ap_y \sin \phi \right)
\]

\[= \tau_x \left[ m_\perp + iAp_r \sigma_z \varphi \cdot \sigma \right], \tag{C2}
\]

\[
H_\parallel = \left( m_\parallel \tau_x + Ar_y \left( p_\phi \sin \phi \sigma_x + \cos \phi \sigma_y \right) + p_z \sigma_z \right)
\]

\[= m_\parallel \tau_x + Ar_y \left[ p_\phi \dot{\varphi} \sigma_z + p_z \sigma_z \right], \tag{C3}
\]

where

\[
m_\perp = m_0 - m_2 \left[ \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} \right], \tag{C4}
\]

and \( m_\parallel = m_2 (p_\phi^2 + p_z^2) \), with

\[
p_\phi = -i \frac{1}{r} \frac{\partial}{\partial \varphi}, \quad p_z = -i \frac{\partial}{\partial z}. \tag{C5}
\]

We have also introduced \( \dot{\varphi} = (\cos \phi, \sin \phi) \), and \( \dot{\varphi} = (\cos \phi, \sin \phi) \).

We then consider a solution of the eigenvalue equation,

\[
H_\perp (\psi_\perp) = E_\perp (\psi_\perp) \tag{C6}
\]
of the form, $\psi_\perp \sim e^{\kappa(r-R)}$, i.e., we set $p_r = -i\kappa$ ($\kappa > 0$) in Eq. (C2). $E_\perp$ is the value of energy eigenvalue at the Dirac point. In order to cope with the boundary condition $|\psi_\perp\rangle_{r=R} = 0$ on the surface of the cylinder, one can verify that this must be zero ($E_\perp = 0$). This implies,

$$\tau_x H_\perp |\psi_\perp\rangle = 0.$$  \hspace{1cm} (C7)

Notice that in the second line of Eq. (C2) $\hat{\sigma} \cdot \sigma$ can be diagonalized by pointing the real-spin spinor in the direction of $\hat{r}$ as Eqs. (8). Then, one can satisfy Eq. (C7) by four simultaneous eigenstates of $\tau_y$ and $\hat{r} \cdot \sigma$, i.e.,

$$|\psi_\perp\rangle = \rho(r)|\tau_z\pm\rangle|\vec{r}\pm\rangle_{dv},$$  \hspace{1cm} (C8)

if $\kappa$ is a solution of

$$E_\perp = m_\perp \pm A\kappa = m_0 - m_2 \kappa^2 \pm A\kappa = 0.$$  \hspace{1cm} (C9)

$|\vec{r}\pm\rangle_{dv}$ has been given in Eqs. (8). The double sign in Eq. (C9) signifies $+$ ($-$) when the combination of two signs in $|\tau_y\pm\rangle|\vec{r}\pm\rangle$ in Eq. (C8) are the same (opposite). One has to consider a linear combination of the eigenstates of the form,

$$\rho(r) \sim e^{\kappa_1(r-R)} - e^{\kappa_2(r-R)}$$  \hspace{1cm} (C10)

where $\kappa_1$ and $\kappa_2$ are solutions of Eq. (C9) with $E_\perp = 0$, i.e.,

$$\kappa = \pm A \pm \sqrt{A^2 + 4m_0 m_2} \equiv \kappa_{1,2},$$  \hspace{1cm} (C11)

where the double sign in front of $A$ corresponds to the one in Eq. (C9). The second one is arbitrary, each choice determining the subscript of $\kappa_{1,2}$. Here, the surface state should be localized in the inner vicinity of the surface of the cylinder. For that one needs a solution of the form of Eq. (C10) with $\kappa_{1,2}$ whose real part both being positive. This is in one-to-one correspondence with

- the choice of $+$ sign in front of $A$ in Eq. (C11), assuming that $A/m_2$ is positive, and
- the condition $m_0 m_2 < 0$.

Thus, the two basis solutions that span the subspace of the surface solutions of Eq. (5) that are also compatible with the boundary condition are identified as $|\vec{r}\pm\rangle_{dv}$, introduced in Eqs. (7). For preciseness, we normalize Eq. (C10) as

$$\rho(r) = \sqrt{\kappa_1 \kappa_2 (\kappa_1 + \kappa_2)} \frac{e^{\kappa_1(r-R)} - e^{\kappa_2(r-R)}}{|\kappa_1 - \kappa_2|}.$$  \hspace{1cm} (C12)

Any surface solution $|\alpha\rangle$ of Eq. (5), satisfying

$$H_{\parallel}|\alpha\rangle = E|\alpha\rangle,$$  \hspace{1cm} (C13)

can be expressed as a linear combination of these two basis solutions as

$$|\alpha\rangle = \alpha_+|\vec{r}+\rangle_{dv} + \alpha_-|\vec{r}-\rangle_{dv},$$  \hspace{1cm} (C14)

or as in Eq. (9).

Finally, following the prescription of the standard degenerate perturbation theory, we consider the secular equation for Eq. (C13), i.e.,

$$\begin{bmatrix} \langle \vec{r} + |H_\parallel|\vec{r}+\rangle \rangle & \langle \vec{r} + |H_\parallel|\vec{r}-\rangle \rangle \end{bmatrix} \begin{bmatrix} \alpha_+ \\ \alpha_- \end{bmatrix} = E \begin{bmatrix} \alpha_+ \\ \alpha_- \end{bmatrix},$$  \hspace{1cm} (C15)

where we have omitted the subscript “dv”, for simplicity. We define the coefficient matrix $\langle \vec{r} \pm |H_\parallel|\vec{r}\pm\rangle$ in the secular equation Eq. (C15) as the surface effective Hamiltonian $H_{surf}$. Noticing the relations such as

$$\langle \vec{r} \pm |\vec{r}\pm\rangle \rangle = \sigma_y,$$  \hspace{1cm} (C16)

$$\langle \vec{r} \pm |\vec{r}\pm\rangle \rangle = \sigma_z,$$  \hspace{1cm} (C17)

the explicit form of $H_{surf}$ is found as given in Eq. (10).

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