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Majorana Flat Bands in s-Wave Gapless Topological Superconductors

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We demonstrate how the non-trivial interplay between spin-orbit coupling and nodeless s-wave superconductivity can drive a fully gapped two-band topological insulator into a time-reversal invariant gapless topological superconductor supporting symmetry-protected Majorana flat bands. We characterize topological phase diagrams by a $2 \times 2$ partial Berry-phase invariant, and show that, despite the trivial crystal geometry, no unique bulk-boundary correspondence exists. We trace this behavior to the anisotropic quasiparticle bulk gap closing, linear vs. quadratic, and argue that this provides a unifying principle for gapless topological superconductivity. Experimental implications for tunneling conductance measurements are addressed, relevant for lead chalcogenide materials.

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The emergence of “topologically protected” Majorana edge modes is a hallmark of topological superconductors (TSs) [1]. Aside from their fundamental physical significance, Majorana modes are key building blocks in topological quantum computation [2], due to their potential to realize non-Abelian braiding. As a result, a wealth of different approaches are being pursued theoretically and experimentally in the quest for topological quantum matter [1], with recent highlights including broken time-reversal (TR) $p + ip$ superconductors, proximity-induced TR-invariant superconductivity in topological insulators (TIs), semiconductor-superconductor heterostructures, multiband superconductors and/or bilayer systems [3, 4], as well as experimental signatures of Majorana fermions in hybrid nanowires [5] and doped TIs [6]. Here, we propose a different paradigm, based on topological gapless superconductivity in nodeless (s-wave) superconductors.

Gapless superconductivity is a physical phenomenon where the quasiparticle energy gap is suppressed (that is, it vanishes at particular momenta), while the superconducting order parameter remains finite, strictly non-zero. This concept was anticipated on phenomenological grounds by Abrikosov and Gorkov [7] in the context of TR pair-breaking effects in s-wave superconductors. Although certain unconventional superconductors may display similar behavior, their gapless nature results from the nodal character of the superconducting order parameter. In this work, the physical mechanism leading to a vanishing excitation gap is the spin-orbit coupling (SOC) in an otherwise nodeless, TR-invariant (centrosymmetric) multiband superconductor with bulk s-wave pairing.

A consequence of such a state of matter is the emergence of surface Majorana flat bands (MFBs) if the spatial dimension $D \geq 2$. It has been appreciated that protected zero-energy flat bands may exist in unconventional nodal superconductors – notably, at the surface of certain $d_{xy} + d_{x^2-y^2}$-wave [8], $d_{xy}$-wave [9], and $d_{xy} + p$-wave superconductors [10]; superconductors with a mixture of d- and s-wave pairing [11]; $p \pm ip$ superconductors [12] and superconducting helical magnets with effective $p$-wave pairing [13] – as well as in the vortex core of topological defects [14]. Recently, a proposal for MFBs in nodeless s-wave (one-band) broken TR superconductors has also been put forward [15]. To the best of our knowledge, our model provides the first example of a TR-invariant s-wave gapless TS. We show that the number of Majorana edge modes in the non-trivial MFB phase (as opposed to just the parity of the number of Majorana pairs) is protected by a local chiral symmetry, a feature that is both crucial to understand robustness against perturbations and may be advantageous for topological quantum computation [16]. The dispersionless character of a MFB implies a large peak in the local density of states (LDOS) at the surface. Thus, while detecting Majorana fermions through a zero-bias conductance peak in scanning tunneling microscopy (STM) experiments is not viable in gapped $D \geq 2$ TSs, an unambiguous experimental signature is predicted in the gapless case [15, 17].

In addition to the above practical significance, an outstanding feature that our work unveils is the anomalous, non-unique bulk-boundary correspondence (BBC) that gapless TSs may exhibit: MFBs may emerge only along particular crystal directions, with no surface modes existing along others. While such an anomalous BBC is reminiscent of the directional behavior typical of topological crystalline phases [18], it does not stem simply from special crystal symmetries. Rather, the physical mechanism is rooted in the anisotropic momentum dependence of the band degeneracy: the quasiparticle gap may close non-linearly along certain directions, while it is linear (Dirac) along others. Only in the former case may a MFB exist at the corresponding edge. Accordingly, our findings suggest a general guiding principle for identifying and/or engineering materials supporting MFBs.

Model Hamiltonian. — We consider a two-band (say, orbitals $c$ and $d$) TR-invariant s-wave superconductor on a 2D square lattice. By letting $k \equiv (k_x, k_z)$ denote the wave-vector in the first Brillouin zone and
\[ \psi_k = (c_{k,\uparrow}, d_{k,\uparrow}, c_{-k,\uparrow}, c_{-k,\downarrow}, d_{-k,\downarrow}, d_{-k,\downarrow}) \]

the relevant momentum-space Hamiltonian may be written as

\[ H = \frac{1}{2} \sum_k (\psi_k^\dagger \hat{H}_k \psi_k - 4\mu), \]

where the 8 \times 8 matrix

\[ \hat{H}_k = s_z (m_k \sigma_z - \mu) + \tau_z (\lambda_{k_x} \sigma_x + \lambda_{k_z} \sigma_z) - \Delta s_x \tau_y \sigma_x. \] (1)

Here, \( s_x, s_y, s_z, \nu = x, y, z \), are the Pauli matrices in the Nambu, orbital, and spin space, respectively, and tensor-product notation is understood. Physically, \( m_k \equiv u_{cd} - 2t (\cos k_x + \cos k_z) \), with \( u_{cd} \) and \( t \) representing the orbital-dependent on-site potential and the intraband hopping strength; \( \mu \) is the chemical potential; \( \lambda_{k_x} \equiv (\lambda_{k_x^\uparrow}, \lambda_{k_x^\downarrow}) = -2\lambda (\sin k_x, \sin k_z) \) describes the interband SOC, and \( \Delta \) is the mean-field gap, with the superconducting pairing term being an interband s-wave spin-triplet of the form

\[ H_{sw} = i \Delta \sum_j (c_{j,\uparrow}^\dagger c_{j,\downarrow} + c_{j,\downarrow}^\dagger c_{j,\uparrow}) + H.c., \Delta \in \mathbb{C}. \]

In addition to TR, particle-hole, and inversion symmetries \[\text{[4]}, \text{the Hamiltonian in Eq. (1) obeys a special (unitary) chiral symmetry, } \hat{H}_k, U_k \hat{H}_k^\dagger = 0, \text{ where } U_k \equiv s_z \otimes \tau_x \otimes I \text{ and } I \text{ denotes the 2 \times 2 identity matrix } \text{[19]}. \]

This symmetry will play an essential role in describing MFBs. We may decouple \( \hat{H}_k \) into two 4 \times 4 blocks by applying a suitable unitary transformation \( U \), followed by a reordering of \( P \) of the fermionic operator basis. Specifically, let \( U = \frac{1}{\sqrt{2}} \left[ \begin{array}{cc} [I \otimes (I + i\sigma_y)] & [I \otimes (I - i\sigma_y)] \end{array} \right] \), with \( P \psi_k \equiv (c_{k,\uparrow}^\dagger, d_{k,\uparrow}, c_{-k,\uparrow}, d_{-k,\uparrow}, c_{k,\downarrow}^\dagger, d_{k,\downarrow}, c_{-k,\downarrow}, d_{-k,\downarrow}) \). Then \( H \) is transformed into \( H' = \frac{1}{2} \sum_k (\psi_k^\dagger \hat{H}_k \psi_k - 4\mu) \), with \( \hat{H}'_{1,k} = (PU) H_k (PU)^\dagger \equiv \hat{H}'_{1,k} \oplus \hat{H}'_{2,k} \). As in \[\text{[4]}, \hat{H}'_{1,k} \text{ and } \hat{H}'_{2,k} \text{ may be regarded as TR partners, and}

\[ \hat{H}'_{1,k} = \left( m_k \sigma_z - \mu + \lambda_k \cdot \sigma \right) \frac{-i \Delta \sigma_y}{i \Delta \sigma_y} \left( s_z \sigma_x + \mu + \lambda_k \cdot \sigma \right), \]

with \( \sigma \equiv (\sigma_x, \sigma_y) \). The exact quasiparticle excitation spectrum obtained by diagonalizing \( \hat{H}'_{1,k} \) is given by:

\[ \epsilon_{n,k} = \pm \sqrt{m_k^2 + \Omega^2 + |\lambda_k|^2 \pm 2 \sqrt{\mu^2 + \Omega^2 (\lambda_{k_x}^2 + \lambda_{k_z}^2)}}, \] (2)

where we assume the order \( \epsilon_{1,k} \leq \epsilon_{2,k} \leq \ldots \leq \epsilon_{4,k} \leq \epsilon_{4,k} \), and \( \Omega^2 \equiv \mu^2 + \Delta^2 \). If no SOC is present, \( \lambda = 0 \), then \( \epsilon_{n,k} = \pm |m_k| \pm |\Omega| \), hence the gap closes (\( \epsilon_{2,k} = 0 \)) for \( |m_k| = |\Omega| \). By comparing \( \epsilon_{2,k} \) and \( \epsilon_{3,k} \), one can see that as long as \( |u_{cd}| \sim |\Omega| \), there is a continuous region of gapless bulk modes, which corresponds to a gapless two-band superconductor with overlapping excitation spectrum \[\text{[20]}. \]

If \( \lambda = 0 \), the situation is simplest at \( \mu = 0 \), in which case \( \epsilon_{n,k} = \pm \sqrt{\lambda_{k_x}^2 + \left( \frac{m_k^2 + \lambda_{k_z}^2}{4|\Omega|} \pm \Delta^2 \right)} \), and \( \epsilon_{2,k} = 0 \) when \( \lambda_{k_z} = 0 \), and \( \lambda_{k_x}^2 + m_k^2 = \Delta^2 \). For instance, if \( \lambda = t \neq 0 \), this leads to \( k_x \equiv k_{x,c} \in [0, \pi] \), and \( k_z \equiv k_m = \pm \text{arccos} \left( \frac{|u_{cd}| - 2 t \cos k_{x,c}}{4|u_{cd}| - 2 t \cos k_{x,c}} \right) \). Let \( (k_x, k_z) \equiv (k_{x,c}, k_m) \) denote the modes for which the bulk excitation spectrum closes. We then expect only a finite set of values \( k_m \) when \( \lambda \neq 0 \) for arbitrary \( \mu \). The quantum critical lines are determined by \( \Delta = \pm m_{k_c} \), with \( k_c \equiv (k_{x,c}, k_{z,c}) \) and \( k_{x,c} \in [0, \pi] \) \[\text{[4]}, \text{Fig. (1)(a)}\].

In the limit \( \Delta = 0 \), our Hamiltonian reduces (up to unitary equivalence) to a TI model \[\text{[21].} \text{A qualitative comparison of the spectrum with open boundary conditions (OBC) along } z \text{ with } \Delta = 0 \text{ vs. } \Delta 
eq 0 \text{ is shown in Fig. (1)(b)-(c). Remarkably, we may consider our gapless TS to arise from doping a TI with fully-gapped, nodeless (spin-triplet) s-wave superconductivity. More intuitively, an alternative route to realize our gapless TS is by turning on a suitable SOC in a two-band gapless superconductor, as the effect of \( \lambda = 0 \) is to separate the overlapping excitation spectrum and only leave a vanishing gap at a finite number of points. Thus, our nontrivial quasiparticle spectrum is a combined effect of SOC and superconducting order parameter. The most striking aspect of such a spectrum is the fact that the quasiparticle gap closing is anisotropic: the gap vanishes linearly along \( k_x \) [i.e., \( k_z \equiv k_{x,c} \)] and quadratically along \( k_z \) [i.e., \( k_x \equiv k_{z,c} \)] \[\text{[20]}, \text{as we shall soon see, this peculiar behavior will manifest directly into an anomalous BBC}. \]

Topological response.— As a result of the gapless nature of the bulk excitation spectrum, topological invariants (such as the partial Chern number \[\text{[4]}\]) applicable to 2D TR-invariant gapped TS systems are no longer appropriate. This motivates the use of partial Berry-phase indicators \[\text{[4]}\]. In particular, we study the partial Berry phase of the two occupied negative bands of one Kramers’ sector only, \( H_{1,k} \), for each \( k_z \) (or \( k_x \)), namely, \( B_{n,k_z}, n = 1, 2 \), since the Berry phase of all the negative bands of \( H_{1,k} \) and \( H_{2,k} \) is always trivial \[\text{[4]}\]. We can then compute the partial Berry phase parity for each \( k_z \) as

\[ P_{B,k_z} = (-1)^{\text{mod}_{2} (B_{+1,k_z})} \]

define a \( Z_2 \) topological number as \( \Pi_{k_z} P_{B,k_z} \). How-
ever, similar to the gapped case \( \Pi \), the latter fails to identify quantum-critical lines in phases that share the same \( \mathbb{Z}_2 \) number. For the purpose of identifying all the phase transitions and characterizing the whole phase diagram in Fig. 1(a), a \( \mathbb{Z}_2 \times \mathbb{Z}_2 \) indicator is necessary. Specifically, we define our topological invariant as \( \{P_{B, k_z = 0}, P_{B, k_z = \pi}\} \) [marked in each phase on Fig. 1(a)], which correctly signals a phase transition whenever a jump of either \( P_{B, k_z = 0} \) or \( P_{B, k_z = \pi} \) occurs. Since, as expected for a consistent bulk behavior, it turns out that \( \{P_{B, k_z = 0}, P_{B, k_z = \pi}\} = \{P_{B, k_z = 0}, P_{B, k_z = \pi}\} \), we shall just write the \( \mathbb{Z}_2 \times \mathbb{Z}_2 \) invariant as \( \{P_{B, 0}, P_{B, \pi}\} \) henceforth. Note that while ultimately such a \( \mathbb{Z}_2 \times \mathbb{Z}_2 \) invariant involves only the partial Berry phase at \( k = k_c \), the reason for the more general definition of the topological numbers at \( k_z \neq k_z, c \) is related to the BBC, as we discuss next.

**Bulk-boundary correspondence.** — In a gapped TR-invariant TS, the BBC defines the relation between bulk topological invariants and the (parity of the) number of TR pairs of edge states \( \Pi, \Pi \). To understand the BBC in our gapless model, we contrast two situations: BC1—periodic boundary conditions (PBC) along \( \hat{z} \), and OBC along \( \hat{x} \); BC2—PBC along \( \hat{x} \), and OBC along \( \hat{z} \). Fig. 2 shows how the excitation spectrum changes as a function of \( \Delta \) for BC1 (top panels) and BC2 (bottom panels) for representative parameter choices in phases labelled by \( \{P_{B, 0}, P_{B, \pi}\} = (1, 1) \) [panels (a) and (c)], and \( \{P_{B, 0}, P_{B, \pi}\} = (1, -1) \) [panels (b) and (d)]. In (a) there are two pairs of Majorana modes on each boundary for \( k_z = 0 \), but no Majorana edge modes in (c); likewise, in (b) there is a MFB for \( k_m < |k_z| \leq \pi \) (\( k_m \approx 1.8 \)), but again no Majorana edge modes in (d). As further investigation under BC1 reveals, when \( P_{B, k_z} = -1 \) a single TR-pair of Majorana edge modes exists for that \( k_z \)-value on each boundary. Thus, a MFB is generated when there is a dense set of \( k_z \) for which \( P_{B, k_z} = -1 \). On the contrary, the partial Berry phase for \( k_x \neq k_x, c \) is always trivial (i.e., \( P_{B, k_x} = 1 \)); and when \( P_{B, k_x, c} = -1 \), it corresponds to gapless bulk modes for that \( k_x, c \).

The above results demonstrate the asymmetry between the \( \hat{x} \) and \( \hat{z} \) directions notwithstanding their geometrical equivalence – in direct correspondence with the anisotropic momentum dependence of the bulk excitation gap, as anticipated. We stress that although the choice of Hamiltonian in Eq. 1 is motivated by our earlier work \( \Pi \), different physical realizations of s-wave gapless TR-invariant TSs may be envisioned as long as a similar mechanism is in place: notably, we may change \( H_{\text{sw}} \) to interband s-wave spin-singlet, \( H_{\text{sw}}' = \frac{1}{2} \sum_{j \neq j'} \Delta \left[c_{j, \sigma}^\dagger c_{j', \sigma} - c_{j', \sigma}^\dagger c_{j, \sigma}\right] + \text{H.c.} \], while also ensuring that the strength of the SOC is sufficiently anisotropic, e.g., \((\lambda_{k_z}, \lambda_{k_x}) = \frac{-2(\lambda_x \sin k_x, \lambda_z \sin k_z)}{\lambda_x} \). Based on these observations, we conjecture that the momentum asymmetry of the (bulk) excitation gap closing is a necessary condition for anomalous BBC, and that MFBs are necessarily associated with higher-than-linear closing. Direct calculation confirms that this conjecture holds across a variety of models supporting surface flat bands: in particular, anomalous BBC is observed in spin-triplet \( p_x + i p_y \) TSs \( \Pi \), in both s-wave and \( d_{x^2-y^2} \)-wave spin-singlet TSs \( \Pi \), as well as a TR-broken TI model \( \Pi \). Interestingly, MFBs emerge along both spatial directions in \( d_{xy} \) TSs \( \Pi \), consistent with the symmetric (quadratic) closing of the bulk gap.

**Observable signatures of Majorana flat band.** — The tunneling current between a STM and the material is proportional to the surface LDOS of electrons \( \Pi \). Results of LDOS calculations are shown in Fig. 3 together with the corresponding bulk density of states (DOS): a huge (small) peak for the LDOS (DOS) is seen at zero energy under BC1 in (a), whereas no zero-energy peak occurs under BC2 in (b). While the quantitative difference between the LDOS vs. DOS peaks in panel (a) does indicates that the zero-energy modes are located on the boundary, the qualitative difference between panels (a) and (b) reinforces the asymmetric behavior under the two boundary conditions shown in Fig. 2. It is instructive to compare to a typical gapped TS, e.g., the TR-invariant model discussed in Ref. \( \Pi \). Although in this case Majorana edge modes exist in a nontrivial phase regardless of the direction along which OBC are assigned, no peak in LDOS (DOS) is seen at zero energy for \( D > 1 \) [panels (c)-(d)]; in 2D (and 3D), the contribution to the LDOS from the finite number of Majorana edge modes is washed out by the extensive one from the bulk modes as the system size grows. Thus, a mechanism other than the existence of a finite number of Majoranas is needed to explain a zero-bias peak in 2D (3D) fully-gapped superconductors.

**Robustness of Majorana flat band.** — Let us first consider a TR-preserving perturbation of the form \( H_p = \sum_{j, k_x, k_z, k_z'} u_p (c_{j, k_x, k_z, \sigma}^\dagger c_{j, k_x, k_z, \sigma} + d_{j, k_x, k_z, \sigma}^\dagger d_{j, k_x, k_z, \sigma}) + \text{H.c.} \),
where \( k'_z \in \{ -k_z, \pi - k_z \} \), \( u_p \in \mathbb{R} \). Since \( H_p \) allows Majorana modes at \( k_z \) and \( k'_z \) to couple with each other, it could significantly change the number of edge modes in principle. However, the zero-energy modes on the left (right) boundary of \( H_{k_z} \), say \( \gamma_{k_z, \ell} \) (\( \ell = L, R \)), may be taken to be eigenstates of \( \mathcal{K} \), i.e., \( \gamma_{k_z, \ell} = \pm \gamma_{k_z, \ell} \), when there is only one edge mode on each boundary for \( k_z \).

Thus, when there is only one pair of zero-energy modes in the bulk, at \( k_z = \pm k_m \), all the zero-energy edge modes on the same boundary can be continuously deformed one into another, which guarantees that they belong to the same sector of \( \mathcal{K} \). Therefore, any local perturbation that preserves both chirality and TR cannot lift the degeneracy of the zero-energy modes belonging to the same sector of \( \mathcal{K} \), leaving the MFB stable. However, the protection from \( \mathcal{K} \) may fail when there is an even number of pairs of zero-energy bulk modes: e.g., in the phase \(( P_{B,0}, P_{B,\pi} ) = (-1, -1) \), the MFB is not robust against \( H_p \), since now Majoranas on the same boundary may belong to different sectors of \( \mathcal{K} \). Thus, not only does the parity of the number of Kramers’ pairs of Majoranas play an important role, but also the number of edge modes in the MFB is conserved as long as both symmetries are respected and there is only one pair of bulk gapless modes.

Similarly, the MFB is robust against another natural TR-preserving perturbation, namely, intraband s-wave pairing, \( H_s = \Delta_c \sum_j (c_j^\dagger \gamma \sigma_y c_j + \Delta_d \sum_j d_j^\dagger d_{j+1}^\dagger + \text{H.c.} ) \), \( \Delta_c, \Delta_d \in \mathbb{R} \), which anti-commutes with \( U_K \).

Next, consider TR-breaking perturbations due to a static magnetic field \([ 4, 20 ] \), \( H_v = h_v \sum_j \psi_j^\dagger \mathbf{\sigma}_\nu \psi_j \), where \( \nu = \hat{x}, \hat{y}, \hat{z} \) (\( \hat{y} \)) correspond to in-plane (out-of-plane) directions. The response to an in-plane field is similar in both directions, with the MFB remaining flat. Fig. 4(a). Under a magnetic field \( h_y \), instead, the MFB becomes unstable. Fig. 4(b). The effect of the magnetic field along different directions may be understood through its relation with chirality. Specifically, the \( \hat{x} \) and \( \hat{z} \)-components of \( H_y \) anti-commute with \( \mathcal{K} \), whereas \( H_y \) commutes with \( \mathcal{K} \). Accordingly, chirality-protection is lost in this case. The LDOS in the presence of Zeeman fields along in-plane (\( \hat{z} \)) and out-of-plane (\( \hat{y} \)) directions is shown in Fig. 4(c)-(d): the peak at zero energy stays almost unchanged as \( h_z \) increases, whereas it is strongly suppressed when \( h_y \neq 0 \). This is consistent with the results from the excitation spectrum shown above. Moreover, the behavior of the LDOS under a magnetic field along an arbitrary direction on the \( \hat{x}-\hat{z} \) plane is similar to the one under \( h_z \). We may then infer that a MFB responds to a uniform Zeeman field along a certain direction in a similar way as to a magnetic imparity field along the same direction. Thus, the MFB will be robust in the presence of in-plane magnetic impurities, which may be unavoidable in real materials. Lastly, we investigated the effect of on-site disorder along the boundary, \( H_d = \sum_j v_j (c_j^\dagger \gamma \sigma_y c_j + d_j^\dagger d_{j+1}^\dagger + d_{j-1}^\dagger d_{j+1}^\dagger ) + \text{H.c.} \), where \( v_j \in \mathbb{R} \) is a Gaussian random potential. The MFBs are robust against weak disorder so long as chirality is preserved, with the zero-energy peak in the LDOS remaining qualitatively intact.

**Conclusion.**— Majorana modes in gapless TSs can manifest themselves through new signatures, such as the emergence of a chirality-protected MFB which may depend crucially on the nature of the boundary. Such an anomalous, non-unique, BBC in 2D (3D) gapless TSs allows for a more unambiguous signature in tunneling experiments than gapped TSs may afford. The anisotropic, linear vs. non-linear, vanishing of the quasiparticle bulk...
excitation gap at particular momenta is the unifying principle behind such anomaly. Our model provides an explicit realization of a TR-invariant two-band gapless TS, where an anisotropic excitation spectrum arises from the interplay of conventional s-wave superconductivity with a SOC whose form is motivated by band-structure studies in Pb$_2$Sn$_{1-x}$Te. Thus, we expect that materials in this class may be natural candidates for the experimental search of TR-invariant gapped or gapless TSs.

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[19] Using $U_K$ to define a chiral symmetry operator $K$ by its action on the Nambu basis vector, i.e. $K (\psi_k) K^{-1} = \sum I (U_K I) (\psi_k) I$, we obtain the following fermionic transformation properties: $K c(d)_{k,\uparrow} K^{-1} = c^\dagger (-d^\dagger)_{-k,\uparrow}$, $K c^\dagger (d^\dagger)_{k,\uparrow} K^{-1} = c(-d)_{-k,\uparrow}$, and $K c(d)_{k,\downarrow} K^{-1} = c^\dagger (-d^\dagger)_{-k,\downarrow}$, $K c^\dagger (d^\dagger)_{k,\downarrow} K^{-1} = c(-d)_{-k,\downarrow}$.


[23] Interestingly, $\prod_k P_{B,k,\vec{k}_z} = \prod_k P_{B,\vec{k}_z,k}$, which indicates consistent bulk properties as a whole, although the topological numbers for each $k_x$, $k_z$ may differ individually.


