Majorana Modes in Time-Reversal Invariant s-Wave Topological Superconductors

Shusa Deng, Lorenza Viola, and Gerardo Ortiz

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Majorana modes in time-reversal invariant s-wave topological superconductors

Shusa Deng,[1] Lorenza Viola,[1] and Gerardo Ortiz[2]

[1]Department of Physics and Astronomy, Dartmouth College, 6127 Wilder Laboratory, Hanover, NH 03755, USA
[2]Department of Physics, University of Indiana, Bloomington, Indiana 47405, USA

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We present a time-reversal invariant s-wave superconductor supporting Majorana edge modes. The multi-band character of the model together with spin-orbit coupling are key to realizing such a topological superconductor. We characterize the topological phase diagram by using a partial Chern number sum, and show that the latter is physically related to the parity of the fermion number of the time-reversal invariant modes. By taking the self-consistency constraint on the s-wave pairing gap into account, we also establish the possibility of a direct topological superconductor-to-topological insulator quantum phase transition.

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Since Majorana suggested the possibility for a fermion to coincide with its own antiparticle back in 1937 [1], the search for the Majorana particle has catalized intense effort across particle and condensed-matter physicists alike [2]. Particles either constitute the building blocks of a fundamental physical theory or may effectively emerge as the result of the interactions of a theory. A Majorana fermion is no exception to this principle, with neutrinos potentially epitomizing the first view [3], and localized quasiparticle excitations in matter illustrating the second [4]. Remarkably, Majorana fermions can give rise to the emergence of non-Abelian braiding [6]. Thus, in addition to their significance for fundamental quantum physics, interest in realizing and controlling Majorana fermions has been fueled in recent years by the prospect of implementing fault-tolerant topological quantum computation [7, 8]. As a result, a race is underway to conclusively detect and characterize these elusive particles.

A variety of condensed-matter systems hosting localized Majorana elementary excitations have been proposed, notably certain quantum Hall states [6] and so-called *topological superconductors* (TSs) [9, 10]. Unfortunately, these exotic states of matter require the explicit breaking of time-reversal (TR) symmetry and their physical realization seems to be at odds with existent materials. Such is the case, for instance, of superconductors with $p_x + ip_y$ spin-triplet pairing symmetry. This has not prevented researchers to pursue creative proposals that rely on a combination of carefully crafted materials and devices. Fu and Kane [11], in particular, suggested the use of a (topologically trivial) s-wave superconducting film on top of a three-dimensional topological insulator (TI), which by proximity effect transforms the non-trivial surface state of the TI into a localized Majorana excitation [4, 12] (see also [5] for related early contributions). While experimental realization of this idea awaits further progress in material science, alternative routes are being actively sought, including schemes based on metallic thin-film microstructures, quantum nanowires, and semiconductor quantum wells coupled to either a ferromagnetic insulator, or to a magnetic field in materials with strong spin-orbit (SO) coupling [13].

Our motivation in this work is to explore whether a path to TSs exists based on conventional *bulk* s-wave spin-singlet pairing superconductivity. We answer this question by explicitly constructing a model which, to the best of our knowledge, provides the first example of a 2D TS with s-wave pairing symmetry, and supports Majorana edge modes *without breaking TR symmetry* [14]. The key physical insight is the *multi-band* character of the model, in the same spirit of two-gap superconductors [15], but with the SO coupling playing a crucial role in turning a trivial two-gap superconductor into a topologically non-trivial one. Our results advance existing approaches in several ways. First, multi-band systems clearly expand the catalog of TI and TS materials. Following the discovery of s-wave two-band superconductivity in MgB_2 in 2001, a number of two-gap superconductors ranging from high-temperature cuprates to heavy-fermion and iron-based superconductors have already been characterized in the laboratory [16], giving hope for a near-future material implementation. Furthermore, from a theoretical standpoint, our TR-invariant model also supports a direct TI-to-TS (first-order) quantum phase transition (QPT), allowing one to probe these novel topological phases and their surface states by suitably tuning control parameters in the same physical system.

Exact solution with periodic boundary conditions.— We consider a TR-invariant two-band Hamiltonian of the form $H = H_{\mathsf{cd}} + H_{\mathsf{so}} + H_{\mathsf{sw}} + H.c.$, where

$$
\begin{aligned}
H_{\mathsf{cd}} &= \frac{1}{2}\sum_j (u_{cd}\psi_j^\dagger \tau_x \psi_j - \mu \psi_j^\dagger \psi_j) - t\sum_{\langle i,j\rangle} \psi_i^\dagger \tau_x \psi_j, \\
H_{\mathsf{so}} &= i\lambda \sum_{j,\nu=\hat{x},\hat{y}} \psi_j^\dagger \tau_z \sigma_\nu \psi_{j+\nu}, \\
H_{\mathsf{sw}} &= \sum_j (\Delta_c c_{j,\uparrow}^\dagger c_{j,\downarrow}^\dagger + \Delta_d d_{j,\uparrow}^\dagger d_{j,\downarrow}^\dagger), \qquad (1)
\end{aligned}
$$

represent the two-band (c and d) dynamics, the SO interaction, and s-wave superconducting fluctuations, respectively. In the above equations, μ is the chemical potential, u_{cd} represents an onsite spin-independent "hybridization term" between the two bands, fermionic creation operators at lattice site j (unit vectors $\hat{x}, \hat{y}$) and spin $\sigma =\uparrow,\downarrow$ are specified as $c^\dagger_{j,\sigma}$ or $d^\dagger_{j,\sigma}$, depending on the band, and (Δ_c, Δ_d) denote the mean-field s-wave pairing gaps. By letting $\psi_j \equiv (c_{j,\uparrow}, c_{j,\downarrow}, d_{j,\uparrow}, d_{j,\downarrow})^T$, the Pauli matrices τ_ν and σ_ν act on the orbital and spin part, respectively. Notice that we have implicitly assumed that the intraband SO coupling strengths obey $\lambda_c = -\lambda_d \equiv \lambda$. In this way, in the limit where $\mu = 0 = \Delta_c = \Delta_d$, H reduces to a known model for a TI [17].

For general parameter values and periodic boundary conditions (PBC), H can be block-diagonalized by Fourier transformation in both x and y. That is, we can rewrite $H = \frac{1}{2}\sum_{\mathbf{k}}(\hat{A}^\dagger_{\mathbf{k}} \hat{H}_{\mathbf{k}} \hat{A}_{\mathbf{k}} - 4\mu)$, with $\hat{A}^\dagger_{\mathbf{k}} = (c^\dagger_{\mathbf{k},\uparrow}, c^\dagger_{\mathbf{k},\downarrow}, d^\dagger_{\mathbf{k},\uparrow}, d^\dagger_{\mathbf{k},\downarrow}, c_{-\mathbf{k},\uparrow}, c_{-\mathbf{k},\downarrow}, d_{-\mathbf{k},\uparrow}, d_{-\mathbf{k},\downarrow})$, and $\hat{H}_{\mathbf{k}}$ an 8×8 matrix. An analytical solution exists in the limit where the pairing gaps are π-shifted, $\Delta_c = -\Delta_d \equiv \Delta$, since $\hat{H}_{\mathbf{k}}$ decouples into two 4×4 matrices. By introducing new canonical fermion operators, $a_{\mathbf{k},\sigma} = \frac{1}{\sqrt{2}}(c_{\mathbf{k},\sigma} + d_{\mathbf{k},\sigma})$, $b_{\mathbf{k},\sigma} = \frac{1}{\sqrt{2}}(c_{\mathbf{k},\sigma} - d_{\mathbf{k},\sigma})$, we may rewrite $H = \frac{1}{2}\sum_{\mathbf{k}}(\hat{B}^\dagger_{\mathbf{k}} \hat{H}'_{\mathbf{k}} \hat{B}_{\mathbf{k}} - 4\mu)$, with $\hat{B}^\dagger_{\mathbf{k}} = (a^\dagger_{\mathbf{k},\uparrow}, b^\dagger_{\mathbf{k},\downarrow}, a_{-\mathbf{k},\uparrow}, b_{-\mathbf{k},\downarrow}, a^\dagger_{-\mathbf{k},\downarrow}, b^\dagger_{-\mathbf{k},\uparrow}, a_{\mathbf{k},\downarrow}, b_{\mathbf{k},\uparrow})$, and $\hat{H}'_{\mathbf{k}} = \hat{H}'_{1,\mathbf{k}} \oplus \hat{H}'_{2,\mathbf{k}}$, with $\hat{H}'_{1,\mathbf{k}}$, $\hat{H}'_{2,\mathbf{k}}$ being TR of one another,

$$\hat{H}'_{1,\mathbf{k}} = \begin{pmatrix} m_{\mathbf{k}}\sigma_z - \mu + \lambda_{\mathbf{k}}\cdot\vec{\sigma} & i\Delta\sigma_y \\ -i\Delta\sigma_y & -m_{\mathbf{k}}\sigma_z + \mu + \lambda_{\mathbf{k}}\cdot\vec{\sigma}^* \end{pmatrix}.$$

Here, $\lambda_{\mathbf{k}} = -2\lambda(\sin k_x, \sin k_y)$, $m_{\mathbf{k}} = u_{cd} - 2t(\cos k_x + \cos k_y)$, and $\vec{\sigma} \equiv (\sigma_x, \sigma_y)$. The excitation spectrum obtained from diagonalizing either $\hat{H}'_{1,\mathbf{k}}$ or $\hat{H}'_{2,\mathbf{k}}$ is

$$\epsilon_{n,\mathbf{k}} = \pm\sqrt{m^2_{\mathbf{k}} + \Omega^2 + |\lambda_{\mathbf{k}}|^2 \pm 2\sqrt{m^2_{\mathbf{k}}\Omega^2 + \mu^2|\lambda_{\mathbf{k}}|^2}}, \quad (2)$$

where the order $\epsilon_{1,\mathbf{k}} \le \epsilon_{2,\mathbf{k}} \le 0 \le \epsilon_{3,\mathbf{k}} \le \epsilon_{4,\mathbf{k}}$ is assumed and $\Omega^2 \equiv \mu^2 + \Delta^2$. QPTs occur when the gap closes ($\epsilon_{2,\mathbf{k}} = 0$, for general $\Delta \neq 0$), leading to the critical lines determined by $m_{\mathbf{k}_c} = \pm\Omega$, where the critical modes $\mathbf{k}_c \in \{(0,0), (0,\pi), (\pi,0), (\pi,\pi)\}$. It is worth noticing that through a suitable unitary transformation (see Eq. (4) of Ref. [18]), the SO interaction in Eq. (1) is formally mapped into $p_x + ip_y$ and $p_x - ip_y$ intraband interaction, hinting at the existence of non-trivial topological phases, as we demonstrate next.

Topological response.— Since H preserves TR invariance, bands which form TR-pairs have opposite bulk Chern numbers (CNs) C_n, leading to $\sum_{n\in\text{occupied}} C_n = 0$ (including both $\hat{H}'_{1,\mathbf{k}}$ and $\hat{H}'_{2,\mathbf{k}}$). Thus, introducing a new $\mathbb{Z}_2$ topological invariant is necessary in order to distinguish between trivial and TS phases. In Ref. [19], the parity of the sum of the *positive* CNs was considered, whereas in Ref. [20] an integral of the Berry curvature over *half* the Brillouin zone for all the occupied bands was used. Here, we propose a different $\mathbb{Z}_2$ invariant which is *guaranteed* to work in the presence of TR: taking advantage of the decoupled structure between TR-pairs, we use the CNs of the *two occupied negative bands of* $\hat{H}'_{1,\mathbf{k}}$ *only* (say, C_1 and C_2) and define the following parity invariant:

$$P_C \equiv (-1)^{\text{mod}_2(C_+)}, \quad C_+ \equiv C_1 + C_2. \quad (3)$$

Let $|\psi_{n,\mathbf{k}}\rangle$ denote the band-n eigenvector of $\hat{H}'_{1,\mathbf{k}}$. Then the required CNs C_n, $n = 1, 2$, can be computed as [21]

$$C_n = \frac{1}{\pi}\int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \,\text{Im}\,\langle \partial_{k_x}\psi_{n,\mathbf{k}} | \partial_{k_y}\psi_{n,\mathbf{k}}\rangle. \quad (4)$$

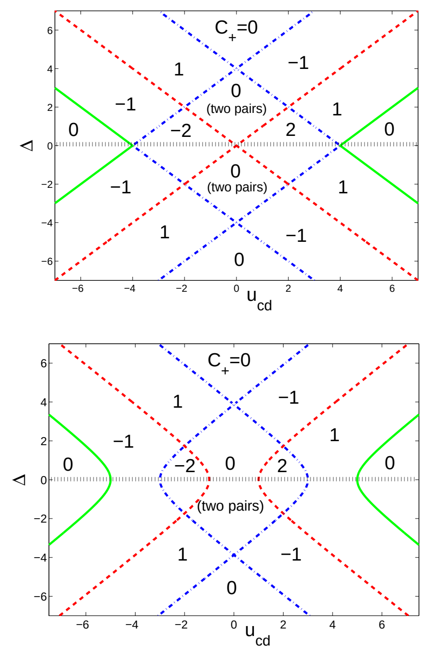

FIG. 1: (Color online) Topological characterization of the phase structure of Hamiltonian H via the partial CN sum C_+ as a function of u_{cd} and Δ, with $t = 1$ and arbitrary $\lambda \neq 0$, for representative chemical potentials $\mu = 0$ (top) and $\mu = -1$ (bottom). The black (dashed) line represents an insulator or metal phase, depending on the filling, with $\Delta = 0$. CNs are calculated for $(N_x, N_y) = (100, 100)$ lattice sites. Note that we may have two pairs of edge modes with $C_+ = 0$.

The resulting topological phase structure is shown in Fig. 1 by treating the pairing gap Δ as a *free* control parameter. In an actual physical system, Δ cannot be changed at will, but only be found self-consistently by minimizing the free energy (or ground-state energy at zero temperature). While we shall return on this issue later, we first focus on understanding the physical meaning of the above invariant and on establishing a bulk-boundary correspondence for our model.

Interestingly, there is a direct connection between the invariant P_C and the fermion number parity of the TR-invariant modes. Without loss of generality, let $\mu = 0$, and focus on the ground-state fermion number parity of the four TR-invariant points in the first

Brillouin zone, $\mathbf{k}_c$. Since $\hat{H}'_{1,\mathbf{k}}$ and $\hat{H}'_{2,\mathbf{k}}$ are decoupled, we need only concentrate on the ground-state parity property of $\hat{H}'_{1,\mathbf{k}}$. Let us introduce the new basis: $u_{\mathbf{k}_c} \equiv \{a^\dagger_{\mathbf{k}_c,\uparrow}|\text{vac}\rangle, b^\dagger_{\mathbf{k}_c,\downarrow}|\text{vac}\rangle, |\text{vac}\rangle, a^\dagger_{\mathbf{k}_c,\uparrow}b^\dagger_{\mathbf{k}_c,\downarrow}|\text{vac}\rangle\}$. In this basis, $\hat{H}'_{1,\mathbf{k}}$ becomes $\widehat{H}_{1,\mathbf{k}_c} = m_{\mathbf{k}_c}\sigma_z \oplus \Delta\sigma_x$, with eigenvalues $\pm m_{\mathbf{k}_c}, \pm\Delta$, and an identical matrix for $\hat{H}'_{2,\mathbf{k}_c}$ in the TR-basis. When $|m_{\mathbf{k}_c}| > |\Delta|$, the ground state of each mode $\mathbf{k}_c$ is in the sector with odd fermion parity, $P_{\mathbf{k}_c} = e^{i\pi(a^\dagger_{\mathbf{k}_c,\uparrow}a_{\mathbf{k}_c,\uparrow}+b^\dagger_{\mathbf{k}_c,\downarrow}b_{\mathbf{k}_c,\downarrow})} = -1$, otherwise it is in the sector with even fermion parity $P_{\mathbf{k}_c} = 1$. By analyzing the relation between $|m_{\mathbf{k}_c}|$ and $|\Delta|$ for each $\mathbf{k}_c$, we can see that the TS (trivial) phases with $P_C = -1(1)$ correspond to the ground state with $\prod_{\mathbf{k}=\mathbf{k_c}} P_{\mathbf{k_c}} \equiv P_F = -1(1)$. Thus, our $\mathbb{Z}_2$ invariant coincides with the fermion number parity of the four TR-invariant modes *from one representative of each Kramer's pairs*, consistent with the fact that only a partial CN sum can detect TS phases in the presence of TR symmetry. While the relation between non-trivial topological signatures (such as the fractional Josephson effect) and the local fermion parity of Majorana edge states has been discussed in the literature [7, 22, 23], invoking the fermion number parity of the TR-invariant modes in *bulk periodic systems* to characterize TS phases has not, to the best of our knowledge.

Open boundary conditions and edge states.— A hallmark of a TS is the presence of an *odd* number of pairs of gapless helical edge states, satisfying Majorana fermion statistics. Thus, in order to understand the relation between P_C (or P_F) and the parity of the number of edge states, *i.e.*, a bulk-boundary correspondence, we study the Hamiltonian H on a cylinder. That is, we retain PBC only along x, and correspondingly obtain the excitation spectrum, ϵ_{n,k_x}, by applying a Fourier transformation in the x-direction only. For simplicity, let us again focus on the case $\mu = 0$. The resulting excitation spectrum is depicted in Fig. 2 for representative parameter choices. Specifically, for *odd* P_C ($C_+ = 1$ in panel (a) and $C_+ = -1$ in panel (b), respectively), H supports one TR-pair of helical edge states on each boundary, corresponding to the Dirac points $k_x = 0$ (a) and $k_x = \pi$ (b). Different possibilities arise for *even* P_C. While $C_+ = 0$ can clearly also indicate the absence of edge states, in panel (c) one TR-pair of helical edge states exists on each boundary for both Dirac points $k_x = 0, \pi$ (for a total of two pairs, as also explicitly indicated in Fig. 1). In panel (d) ($C_+ = 2$), both TR-pairs of helical edge states correspond to the Dirac point $k_x = 0$ instead. Since, as remarked, our Hamiltonian exhibits particle-hole symmetry, the equation $\gamma_{\epsilon_{n,k_x}} = \gamma^\dagger_{-\epsilon_{n,k_x}}$ holds for each eigenvalue ϵ_{n,k_x}, where $\gamma_{\epsilon_{n,k_x}}$ is the associated quasi-particle annihilation operator. Thus, for zero-energy edge states, $\gamma_0 = \gamma_0^\dagger$, indicating that the edge states in our system satisfy Majorana fermion statistics.

Phase diagram with self-consistent pairing gap.— Within BCS mean-field theory, let $V \equiv V_{\mathbf{k},\mathbf{k}'} > 0$ denote the effective attraction strength in each band. Then the pairing gap $\Delta = \Delta_c = -V\langle c_{\mathbf{k},\uparrow}c_{-\mathbf{k},\downarrow}\rangle = -\Delta_d$, and the ground-state energy can be written as $E_g = 2N_xN_y(\Delta^2 V) + \sum_{\mathbf{k}}(\epsilon_{1,\mathbf{k}} + \epsilon_{2,\mathbf{k}} - 2\mu)$. The first (constant) term is the condensation energy, which was neglected in H. By using Eq. (2) and minimizing E_g, we obtain the stable self-consistent pairing gap Δ as a function of the remaining control parameters [24]. The resulting zero-temperature phase diagram is shown in Fig. 3. For $\mu = 0$ (top panel), the average fermion number is consistent with half-filling, and thus with an insulating phase when $\Delta = 0$. In particular, when $0 < |u_{cd}| < 4$, the ground state is known to correspond to a TI phase [17]. Interestingly, without self-consistency, the TI *cannot* be turned into a TS directly, as shown in the top panel of Fig. 1. However, after self-consistency is taken into account, the topologically trivial phase with $C_+ = \pm 2$ disappears, and a first-order QPT can connect the two phases. For $\mu = -1$ (bottom panel), the average fermion number is found to be less than half-filling, realizing a metallic phase when $\Delta = 0$. Derivatives of the ground-state energy indicate that *all* QPTs, except the TI-to-TS phase transition, are continuous.

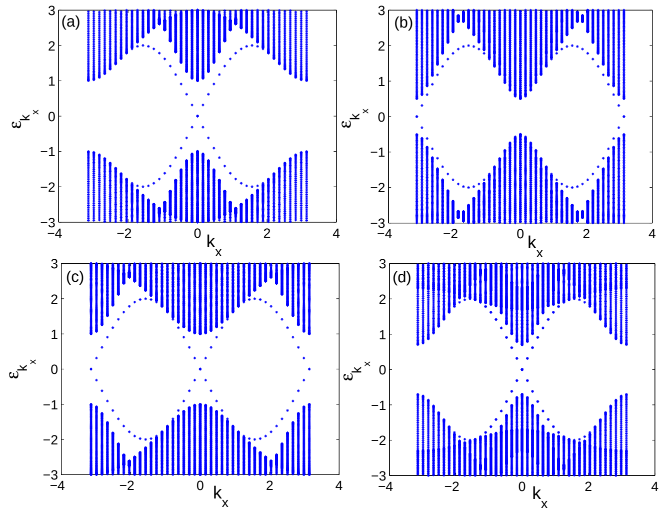

FIG. 2: (Color online) Excitation spectrum of Hamiltonian H on a cylinder for $\mu = 0, t = 1, \lambda = 1$. Panel (a), $C_+ = 1$: $\Delta = 2$, $u_{cd} = 3$; Panel (b), $C_+ = -1$: $\Delta = 2.5$, $u_{cd} = 2$; Panel (c), $C_+ = 0$: $\Delta = 2$, $u_{cd} = 1$; Panel (d), $C_+ = 2$: $\Delta = 0.8$, $u_{cd} = 1.5$. Note that the bulk gap scales as $\min(\lambda, \Delta)$. The number of lattice sites $(N_x, N_y) = (40, 100)$.

Discussion.— A number of remarks are in order. First, while the choice of SO coupling strengths and s-wave pairing gaps obeying $\lambda_c = -\lambda_d$ and $\Delta_c = -\Delta_d$ affords a fully analytical treatment, relaxing these conditions may be necessary to make contact with real materials. Numerical results on a cylinder show that the level crossing of the Majorana edge states in the TS phase is *robust* against perturbations around $\lambda_c = -\lambda_d$, including the

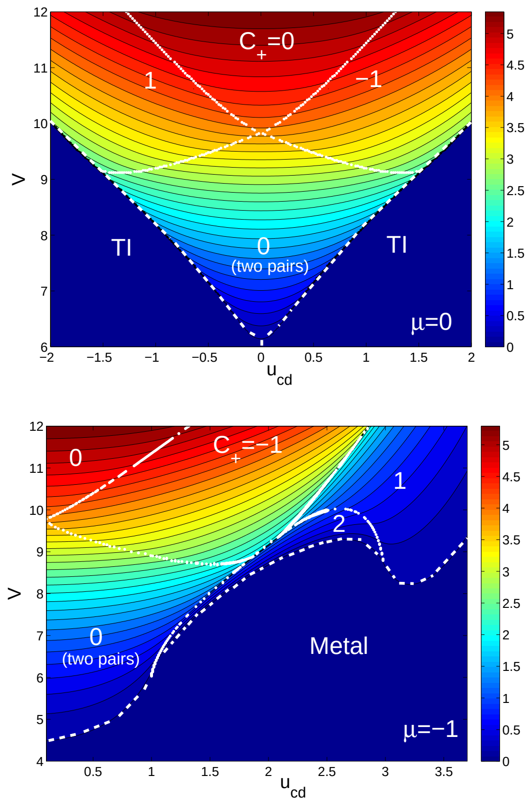

FIG. 3: (Color online) Phase diagram as a function of u_{cd} and V with the pairing gap Δ calculated self-consistently. The magnitude of Δ is represented by a color, whose scale is indicated on the side. The number of lattice sites $(N_x, N_y) = (80, 80)$.

possibility that the SO coupling vanishes in one of the bands. TS behavior also persists if $|\Delta_c| - |\Delta_d| \neq 0$, as long as the phase difference between pairing gaps is π. In the presence of a phase mismatch ε, edge modes are found to become gapped, with a minimal gap that scales linearly with ε. Interestingly, however, preliminary results indicate that adding a suitable Zeeman field can allow (at the expense of breaking TR invariance) gapless Majorana excitations to be restored, with a precise tuning of the phase difference being no longer required. It is also worth noting that one can reinterpret the band index in H as a layer index, and so H may be thought of as describing a *bilayer* of superconductors with phase-shifted pairing gaps, and an interlayer coupling H_{cd}. Beside establishing a *formal* similarity with the scenario discussed by Fu and Kane [11], such an interpretation may offer additional implementation flexibility, as the possibility to control the superconducting and SO couplings by an applied gate voltage has been demonstrated recently [25].

Second, we have thus far restricted to 2D systems in order to simplify calculations. Preliminary results indicate that a qualitatively similar behavior (that is, the possibility of even/odd numbers of pairs of gapless Majorana surface states) also exists for 3D systems obtained from a natural extension of our 2D Hamiltonian. It is especially suggestive to note that a π phase shift in the order parameter across two bands is also believed to play a key role in iron pnictide superconductors [26], hinting at possible relationships between TS behavior and so-called $s_{\pm}$ *pairing symmetry.* While a more detailed investigation is underway, it is our hope that multi-band superconductivity may point to new experimentally viable venues for exploring topological phases and their exotic excitations.

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