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 \[2\], thanks to their potential to realize non-Abelian braiding. As a result, a wealth of different approaches are being actively pursued theoretically and experimentally in the quest for topologically non-trivial quantum matter \[1, 3\], with recent highlights including broken time-reversal (TR) $p + ip$ superconductors, proximity-induced TR-invariant superconductivity in topological insulators, semiconductor-superconductor heterostructures, multiband superconductors and/or bilayer systems \[4, 6\], as well as potential signatures of Majorana fermions in hybrid nanowires \[7\] and doped topological insulators \[8\]. In this work a different paradigm is proposed, based on the possibility of 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 Gor’kov \[9\] 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 unconventional nodal superconductors may support zero-energy flat bands at the surface – notably, certain $d$-wave \[10\], $d_{xy} + p$ \[11\], $p \pm ip$ superconductors \[12\], and non-centrosymmetric superconductors with a mixture of $s$- and $d$-wave pairing \[13\]. Recently, a proposal for MFBs in nodeless s-wave (one-band) broken TR superconductors has also been put forward \[14\]. An outstanding feature that our work unveils is the anomalous, non-unique bulk-boundary correspondence (BBC) that gapless TSs exhibit: MFBs 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 \[15\], 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 closes non-linearly along certain directions, while it is linear (Dirac) along others.

Besides providing, to our knowledge, the first example of a TR-invariant $s$-wave gapless TS system, our findings suggest a general guiding principle for identifying and/or engineering materials supporting MFBs. 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 which may be advantageous for topological quantum computation \[16\]. The dispersionless character of a MFB implies a large peak in the low density of states (LDOS) at the surface. Thus, while detecting Majorana fermions through the appearance of 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 \[14, 17\].

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 $\psi_k^\dagger = (\psi_{k, \uparrow}^c, \psi_{k, \uparrow}^d, \psi_{k, \downarrow}^c, \psi_{k, \downarrow}^d)$, the relevant momentum-space Hamiltonian may be written as $H = \frac{1}{2} \sum_k (\psi_k^\dagger H_k \psi_k - 4\mu)$, where the $8 \times 8$ matrix

$$\hat{H}_k = s_z (m_k \tau_z - \mu) + \tau_x (\lambda_c \sigma_x + \lambda_d \sigma_z) - \Delta s_x \tau_y \sigma_x. \tag{1}$$

Here, $s_x, \tau_x, \sigma_x, \nu = x, y, z$, are the Pauli matrices in the
the heart of the mechanism leading to the MFB. 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 \( k_c \equiv (k_{x,c}, k_{y,c}) \) and \( k_{x,c} \in (0, \pi) \) [Fig. 1(a)].

In the limit \( \Delta = 0 \), our Hamiltonian reduces (up to unitary equivalence) to a topological insulator (TI) model [19]. A qualitative comparison of the spectrum with open boundary conditions (OBC) along \( \hat{z} \) with \( \Delta = 0 \) vs. \( \Delta \neq 0 \) 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 \( \lambda \neq 0 \) 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., \( (k_x - k_{x,c}) \)] and quadratically along \( k_y \) [i.e., \( (k_y - k_{y,c})^2 \)]. This peculiar behavior is at the heart of the mechanism leading to the MFB.

**Topological response.**— As a result of the gapless nature of the bulk excitation spectrum, topological invariants (such as the partial Chern number [2]) applicable to 2D TR-invariant gapped TS systems are no longer appropriate. This motivates the use of partial Berry-phase indicators [6]. In particular, we study the partial Berry phase of the two occupied negative bands of one Kramers’ sector only, \( \hat{H}_{1,k} \), for each \( k_z \) (or \( k_z \)), namely, \( B_{n,k_z}, n = 1, 2, \) since the Berry phase of all the negative bands of \( \hat{H}_{1,k} \) and \( \hat{H}_{2,k} \) is always trivial [6]. We can then compute the partial Berry phase parities for each \( k_z \) as

\[
P_{B,k_z} = (-1)^{m_{k_z} + 2|k_{y,c}|}/\pi, \quad B_{+k_z} \equiv B_{1,k_z} + B_{2,k_z},
\]

and define a \( Z_2 \) topological number as \( \prod_{k_z} P_{B,k_z} \). However, similar to the gapped case [6], the latter fails to identify quantum-critical lines between phases that share the same \( Z_2 \) 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 $k_z \neq k_{x,c}$ 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 \([1, 5, 20]\). To understand the BBC in our gapless model, we contrast the two following 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 $k_{s,c} < |k_z| \leq \pi (k_{s,c} \approx 1.8)$, 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 $k_z \neq k_{x,c}$ is always trivial (i.e., $P_{B,k_z} = 1$); and when $P_{B,k_z} = -1$, it corresponds to gapless bulk modes for that $k_{x,c}$.

The above results demonstrate the asymmetry between the $\hat{z}$ and $\hat{x}$ directions notwithstanding their geometrical equivalence — in direct correspondence with the anisotropic momentum dependence of the bulk excitation gap, as remarked earlier [21]. We stress that although the choice of Hamiltonian in Eq. (11) is directly motivated by our earlier work [4], different physical realizations may be envisioned as long as a similar mechanism is in place: notably, a gapless TR-invariant TS may be obtained by changing $H_{sw}$ to interband s-wave spin-singlet, $H'_{sw} = \sum_j \Delta \left( \epsilon^{j,\downarrow}_c d^{j,\downarrow} c^{j,\uparrow}_c + \text{H.c.} \right)$, while also ensuring that the strength of the SOC is sufficiently anisotropic, e.g., $(\lambda_{k_z},\lambda_{k_z}) = (2 \lambda_z, \sin k_{x}, \lambda_z \sin k_{z})$, with $\lambda_z \ll \lambda_x$. Based on these observations, we conjecture that the momentum asymmetry of the excitation gap closing is a necessary condition for a MFB.

**Observable signatures of Majorana flat band.** — The tunneling current between a STM and the sample material is proportional to the surface LDOS of electrons \([22]\). 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 additionally compare to a typical gapped TS, e.g., the TR-invariant model discussed in Ref. [4]. 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 higher), 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 possible 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 $H_p = \sum_{j,k_z,k'_z,\sigma} u_p e^{i jx, k_z, \sigma} d^{j, \sigma}_{j,k'_z,\sigma} + \text{H.c.}$, where $k'_z \in \{ -k_z, \pi - k_z \}$, $u > 0$. 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 $H_{1, k_z}$, say $\gamma_{k_z, \ell}$ ($\ell = L, R$), may be taken to be eigenstates of $\mathcal{K}$ which, written in second-quantized language on the cylinder defined in BC1, reads $\mathcal{K} = \sum_j i d^{j, \ell}_{k_z} d^{j, -k_z, \uparrow} + e^{i jx, k_z, \uparrow} e^{jx, -k_z, \downarrow} + \text{H.c.}$. Specifically, $\mathcal{K} \gamma_{k_z, \ell} = \pm \gamma_{k_z, \ell}$, 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

**Fig. 2:** (Color online) Excitation spectrum of $H$ [Eq. (1)] for $\mu = 0, t = \lambda = u_{cd} = 1$. Top (bottom) panels correspond to BC1 (BC2), whereas right vs. left columns correspond to $(P_{B,0}, P_{B,\pi}) = (1, 1)$ vs. $(1, -1)$. System size: $N_x = N_z = 40$. 

**Table:**

| Phase | Majorana Modes | Bulk Excitation | Surface LDOS |
|-------|-----------------|-----------------|--------------|
| BC1   | Yes             | Yes             | Yes          |
| BC2   | No              | No              | No           |
ary may belong to different sectors of $H$ only does the
boundary, the propagating along opposite directions. Panels (c)
and (d): LDOS and DOS for a gapped TS in 2D and 1D.
System size: $(N_x, N_z) = (80, 400)$ (a), $(N_x, N_z) = (400, 80)
(b), (N_x, N_z) = (80, 400)$ (c), $N_x = 80$ (d).

Next, consider TR-breaking perturbations due to
a random direction on the $\hat{z}$ plane is similar to the one
under $h_z$. Similar again to our previous analysis \cite{6}, we
can infer that a MFB responds to a uniform Zeeman
field along a certain direction in a similar way as to a
magnetic impurity fields along the same direction. Thus,
in a realistic setting where in-plane magnetic impurities
may be unavoidable, the MFB will still be robust.

Conclusion.— Majorana modes in gapless TSs can
manifest themselves through new signatures, such as the emergence of a MFB which depends crucially on the
nature of the boundary. Such an anomalous, non-unique,
BBC in 2D (3D) gapless TSs allows for a more unam-
biguous signature in tunneling experiments than gapped
TSs may afford. The anisotropic, linear vs. non-linear,
vanishing of the quasiparticle bulk excitation gap at par-
ticular momenta is the organizing principle behind such
MFBs. Our model provides an explicit realization of a
TR-invariant two-band gapless TS, where the required
nontrivial excitation spectrum arises from the interplay of
conventional $s$-wave superconductivity with a SOC
whose form is directly motivated by band-structure stud-
ies in Pb$_2$Sn$_{1-x}$Te \cite{22}. We thus expect that materials in
this class may be natural candidates for the experimental
search of TR-invariant gapped \cite{6} or gapless TSs.

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