Topological phases and surface flat bands in superconductors without inversion symmetry

Andreas P. Schnyder$^1$ and Shinsei Ryu$^2$

$^1$Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany
$^2$Department of Physics, University of California, Berkeley, CA 94720, USA
(Dated: September 16, 2011)

We examine different topological phases in three-dimensional non-centrosymmetric superconductors with time-reversal symmetry by using three different types of topological invariants. Due to the bulk boundary correspondence, a non-zero value of any of these topological numbers indicates the appearance of zero-energy Andreev surface states. We find that some of these boundary modes in nodal superconducting phases are dispersionless, i.e., they form a topologically protected flat band. The region where the zero-energy flat band appears in the surface Brillouin zone is determined by the projection of the nodal lines in the bulk onto the surface. These dispersionless Andreev surface bound states have many observable consequences, in particular, a zero-bias conductance peak in tunneling measurements. We also find that in the gapless phase there appear Majorana surface modes at time-reversal invariant momenta which are protected by a $Z_2$ topological invariant.

PACS numbers: 73.43.-f, 73.20.-r, 03.65.Vf, 74.55.+v, 74.45.+c, 73.20.Fz

The hallmark of topological insulators and superconductors (SCs) is the existence of topologically protected conducting boundary modes. The recent experimental observation of these edge and surface states in spin-orbit induced $Z_2$ topological insulators in two and three dimensions [1], respectively, has lead to a surge of interest and excitement [2]. An exhaustive classification of topologically protected boundary modes occurring in gapped free fermion systems in terms of symmetry and spatial dimension was given in Refs. [3–5]. Interestingly, this classification scheme, which is known as the “periodic table” of topological insulators and SCs, predicts a three dimensional (3D) topological SC which satisfies time-reversal symmetry, but breaks spin-rotation symmetry. Indeed, the B phase of $^3$He is one example of this so-called “class DIII” topological superfluid, whose different topological sectors can be distinguished by an integer topological invariant. Recent transverse acoustic impedance measurements in $^3$He-B confirmed the existence of the predicted surface Majorana bound state [6].

However, finding an electronic analog of the superfluid B phase of $^3$He remains an outstanding challenge. In this paper we argue that some of the 3D non-centrosymmetric SCs might be examples of electronic topological SCs in symmetry class DIII [7]. We analyze the topological phase diagram of these systems and demonstrate quite generally that adjacent to fully gapped topological phases there exist non-trivial gapless superconducting phases with topologically protected nodal lines (rings). To characterize these gapless lines we introduce a set of topological invariants and show that, due to the bulk-boundary correspondence, the presence of topologically stable nodal rings implies the appearance of dispersionless zero-energy Andreev surface states. These topologically protected surface flat bands manifest themselves in scanning tunneling spectroscopy (STS) as a zero bias conductance peak, a feature which could be used as an experimental signature of the topological non-triviality.

In non-centrosymmetric SCs the absence of inversion in the crystal structure generates antisymmetric spin-orbit couplings (SOC) and leads to a mixing of spin-singlet and spin-triplet pairing states. These are the properties that give rise to topologically non-trivial quasi-particle band structures in these systems. Starting with CePt$_3$Si [8], a multitude of non-centrosymmetric SCs has recently been discovered, including, among others, Li$_3$Pd$_x$Pt$_{3-x}$B [9].

Model Hamiltonian As a generic phenomenological description applicable to any of the aforementioned materials we employ a single band model with antisymmetric SOC and treat superconductivity at the mean field level. Thus, let us consider $H = \sum_k \Psi_k^\dagger H(k) \Psi_k$ with $\Psi_k = (c_{k\uparrow}, c_{k\downarrow}, \alpha_{k\uparrow}, \alpha_{k\downarrow})^T$, where $\alpha_{k\sigma}$ is the electron creation operator with spin $\sigma$ and momentum $k$ and the Bogoliubov-de Gennes (BdG) Hamiltonian is given by

$$H(k) = \begin{pmatrix} h(k) & \Delta(k) \\ \Delta^\dagger(k) & -h^T(-k) \end{pmatrix}. \quad (1)$$

The normal state Hamiltonian $h(k)$ describes non-interacting electrons in a crystal without inversion center $h(k) = \varepsilon_k \sigma_0 + \gamma_k \cdot \sigma$, where $\varepsilon_k = \varepsilon_{k\uparrow}$ is the spin-independent part of the spectrum, $\sigma_1, 2, 3$ stand for the three Pauli matrices, and $\gamma_0$ denotes the $2 \times 2$ unit matrix. The second term in $h(k)$ represents an antisymmetric SOC with coupling constant $\gamma_k$.

Due to the presence of the parity breaking SOC $\gamma_k$, the order parameter in Eq. (1) is in general an admixture of spin-singlet $\psi_k$ and spin-triplet $d_k$ pairing states $\Delta(k) = (\psi_k \sigma_0 + d_k \cdot \sigma) (i\sigma_2)$, where $\psi_k$ and $d_k$ are even and odd functions of $k$, respectively. The direction of the spin-triplet component $d_k$ is assumed to be parallel to $\gamma_k$, as for this choice the antisymmetric SOC is not destructive for triplet pairing [10]. Hence, we parametrize the $\vec{d}$-vector and the SOC as $d_k = \Delta_l k_l$ and $\gamma_k = \alpha \Delta_{l,s}$, respectively. For the spin-singlet component we assume $s$-wave pairing $\psi_k = \Delta_s$ and choose the amplitudes $\Delta_{l,s}$ to be real and positive.

In order to exemplify the topological properties of the BdG Hamiltonian (1), we consider a normal state tight-binding band structure on the cubic lattice $\varepsilon_k = t_1 (\cos k_x + \cos k_y + \cos k_z) - \mu$, with hopping amplitude $t_1$ and chemical potential $\mu$. We will set $(t_1, \mu, \alpha, \Delta_0) = (4, 0.48, 1.0, 1.0)$ henceforth. The specific form of the SOC $\gamma_k$ depends on the crystal structure [11], i.e., $\gamma_g g^{-1} k = \gamma_k$, where $g$ is any symmetry operation in the point group $G$ of

\[ g = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \]
the crystal. Having in mind Li$_2$Pd$_4$Pt$_{3-x}$B, we assume for the pseudovector $l_k$ the following form compatible with the symmetry requirements of the cubic point group $O$

$$l_k = \left( \begin{array}{c} \sin k_x \\ \sin k_y \\ \sin k_z \end{array} \right) - g_2 \left( \begin{array}{c} \sin k_x (\cos k_y + \cos k_z) \\ \sin k_y (\cos k_x + \cos k_z) \\ \sin k_z (\cos k_x + \cos k_y) \end{array} \right),$$

with the constant $g_2$, and where we neglect higher order terms. Furthermore, we also consider the point group $C_{4v}$, relevant for CePt$_3$Si, in which case $k_k$ reads

$$l_k = \left( \begin{array}{c} \sin k_y \hat{e}_x - \sin k_x \hat{e}_y \\ + g_2 \sin k_x \sin k_y \sin k_z (\cos k_x - \cos k_y) \hat{e}_z \end{array} \right).$$

It is important to note that the quasi-particle band topology of $H(k)$, as defined by Eq. (1), is mainly determined by the momentum dependence of $l_k$ along the Fermi surface sheets. Hence, the results we obtain are expected to remain qualitatively unchanged upon inclusion of further-neighbor hopping terms in the band structure $\hat{e}_k$.

**Topological Invariants**

To characterize the topological properties of $H(k)$ we introduce three different topological invariants. But before doing so, we observe that $H(k)$ satisfies both time-reversal symmetry (TRS), with $T^2 = -1$, and particle-hole symmetry (PHS), with $C^2 = +1$, which are the defining symmetry properties of symmetry class DIII in the terminology of Ref. [3]. Combining TRS and PHS yields a third discrete symmetry, the “chiral” symmetry $S = TC$, i.e., there is a unitary matrix $S$ which anticommutes with $H(k)$. It is important to note that while both TRS and PHS relate $H(k)$ to $H^T(-k)$, $S$ is a symmetry which is satisfied by $H(k)$ at any given point $k$ in the Brillouin zone (BZ).

As shown in Ref. [3] topological sectors in the fully gapped phases of $H(k)$ are distinguished by the winding number

$$\nu = \int_{BZ} \frac{d^3k}{24\pi^2} \epsilon^{\mu\nu\rho} \text{Tr} \left[ (q^{-1}\partial_\mu q)(q^{-1}\partial_\nu q)(q^{-1}\partial_\rho q) \right],$$

where the integral is over the 1st BZ and $q(k)$ is the off-diagonal block of the flat-band matrix of $H(k)$ [12].

In the nodal superconducting phases the winding number $\nu$ is no longer quantized. However, we can consider $H(k)$ restricted to 1D loops in reciprocal space and define a topological number in terms of a 1D momentum space loop integral to characterize the topology of the gapless phases. We observe that $H(k)$ confined to a generic momentum space loop no longer satisfies TRS nor PHS, but it still obeys chiral symmetry $S$. Hence, $H(k)$ restricted to a loop in the BZ belongs to symmetry class AIII [3] and its topological characteristics are described by the 1D winding number

$$N_L = \frac{1}{2\pi i} \oint_L dk \text{Tr} [q^{-1}(k)\nabla q(k)],$$

where the integral is evaluated along the loop $L$ in the BZ. Observe that for any closed loop $L$ that does not intersect with gapless regions in the BZ, $N_L$ is quantized to integer values. If $L$ is chosen such that it encircles a line node, then $N_L$ determines the topological stability (i.e., the topological charge) of the gapless line [13, 14].

Finally, we also consider $H(k)$ restricted to a time-reversal invariant (TRI) loop $L$, which is mapped onto itself under $k \rightarrow -k$. In that case we obtain a 1D Hamiltonian satisfying both TRS and PHS (i.e., belonging to symmetry class DIII). The topological properties of such a 1D system are characterized by the following $Z_2$ invariant [12]

$$W_L = \prod_K \text{Pf} [q^T(K)] / \sqrt{\det [q(K)]},$$

where $K$ denotes the two TRI momenta on the loop $L$ and Pf is the Pfaffian. Note that $W_L$ is either +1 or -1 for any TRI loop that does not cross gapless regions in the BZ.

**Topological Phase diagram**

Numerical evaluation of the topological numbers (4) and (5) yields the topological phase diagram of $H(k)$, which is shown in Fig. 1 as a function of second order SOC $g_2$ and relative strength of singlet and triplet pairing components. Fully gapped phases with different topological properties (i.e., the phases labeled by $\nu = \pm1$, 0, −5, +7) are separated in the phase diagram by regions of nodal superconducting phases (grey shaded and dotted areas). The fully gapped phases with $\nu = \pm1$ are electronic analogs of $^3$He-B. The nodal superconducting phases exhibit topologically stable nodal rings, which are centered around high symmetry axes of the BZ (see Figs. 2a and 3a). In order to determine the topological character of these nodal lines (and hence of the corresponding gapless phases) it is sufficient to consider the topological invariant $N_L$ only for loops $L$ that run along high symmetry axes. Thus, for the cubic point group $O$ we choose the loops $C_1 : \Gamma \rightarrow M \rightarrow X \rightarrow \Gamma$ and $C_2 : \Gamma \rightarrow M \rightarrow R \rightarrow \Gamma$, whereas for the tetragonal point group $C_{4v}$ we consider $C_3 : \Gamma \rightarrow Z \rightarrow R \rightarrow X \rightarrow \Gamma$ and $C_4 : \Gamma \rightarrow Z \rightarrow A \rightarrow M \rightarrow \Gamma$. For the cubic point group we find that whenever $(N_{C_1}, N_{C_2}) = (\pm1, 0)$ there are topologically stable nodal rings centered around the (100) axis (and symmetry related directions). When $(N_{C_1}, N_{C_2}) = (0, \pm1)$ the gapless lines are oriented along the (111) axis, whereas when $(N_{C_1}, N_{C_2}) = (\pm1, \pm1)$ the rings are located around the...
Andreev surface states: A non-zero quantized value of any of the three topological numbers \(\mathbf{4}, \mathbf{5}\), and \(\mathbf{6}\) implies the existence of zero-energy Andreev surface states. First of all, in fully gapped phases with topologically non-trivial character there appear linearly dispersing Majorana surface modes \(\mathbf{3}, \mathbf{15}, \mathbf{17}\). In order to understand the appearance of zero-energy Andreev surface states in the gapless phases, we now make use of the topological invariant \(N_C\) with a cleverly chosen loop \(\mathcal{L}\). Let us consider Eq. \(\mathbf{1}\) in a slab configuration with \((lmn)\) face. In this geometry the Hamiltonian \(H_{(lmn)}\) retains translational invariance along the two independent directions parallel to the \((lmn)\) surface. Hence, \(H_{(lmn)}(k)\) can be viewed as a family of 1D systems parameterized by the two surface momenta \(k_{\parallel 1} = (k_{\parallel 1}, k_{\parallel 2})\). Since \(H_{(lmn)}(k)\) obeys chiral symmetry (but breaks in general TRS and PHS), its topological properties are given by the 1D winding number of class AII

\[
N_{(lmn)}(k) = \frac{1}{2\pi i} \int dk_{\perp} \text{Tr} \left[ g^{-1}(k) \partial \perp q(k) \right],
\]

where \(k_{\perp}\) is the bulk momentum perpendicular to the surface, and \(\partial \perp = \partial / \partial k_{\perp}\). Note that \(N_{(lmn)}\) is the same as \(N_C\), \(\mathbf{7}\), Eq. \(\mathbf{5}\), with \(\mathcal{L}\) chosen along \(k_{\perp}\), following a non-contractible cycle of the BZ torus \(T^3\).

Now, the key observation is that the above line integral is closely related to the loop integral \(N_C\), with \(\mathcal{L} = C_1\), that determines the topological charge of the superconducting nodal lines. That is, for those surface momenta \(k_{\parallel 1}\) for which the loop along \(k_{\perp}\) in Eq. \(\mathbf{5}\) passes through just one non-trivial nodal ring, \(N_{(lmn)}(k)\) is equal to the topological charge of this given nodal ring. Hence, if we plot \(N_{(lmn)}(k)\) as a function of surface momenta (see Figs. \(\mathbf{2}, \mathbf{3}\)), we find that the boundaries separating regions with different winding number are identical to the projection of the nodal lines onto the \((lmn)\) plane. Furthermore, since a non-zero quantized value of \(N_{(lmn)}\) implies the existence of zero energy states at the end points of the 1D Hamiltonian \(H_{(lmn)}(k)\) \(\mathbf{3}, \mathbf{18}\), we find that there are zero-energy Andreev bound states on the \((lmn)\) surface located within the projected nodal rings. This conclusion is corroborated by numerical computations of the zero-energy surface states both for the point group \(O\) and \(C_{4v}\) (see Figs. \(\mathbf{2}, \mathbf{3}\)). When two nodal rings overlap in the \((lmn)\) projection of the BZ, then the quantized value of \(N_{(lmn)}\) in the overlapping region is determined by the additive contribution of the topological charges of the two rings. In particular, one can have a situation where the two contributions cancel, in which case there is no zero-energy surface state within the overlapping region.

Finally, using an analogous argument as in the previous paragraph, we can also employ the \(Z_2\) number \(\mathbf{6}\) to deduce the presence of zero energy modes at TRI momenta of the surface BZ \(\mathbf{12}\). One example of this is the Kramers pair of surface zero modes located at the center of the surface BZ in Fig. \(\mathbf{2}\) (cf. Refs. \(\mathbf{16}, \mathbf{17}\)). Remarkably, this is a surface Ma-

FIG. 2. (color online) Nodal rings (a) and (111) surface states (c,d) for the point group \(O\) with \((g_3, \Delta_3) = (0.3, 0.5)\). This parameter choice corresponds to the red dotted region in Fig. \(\mathbf{1}\). (b) Topological invariant \(N_{(111)}\), Eq. \(\mathbf{7}\), as a function of surface momentum \(k_{\parallel 1}\). Grey and dark blue indicate \(N_{(111)} = \pm 1\), while light blue is \(N_{(111)} = 0\). (c) Band structure for a slab with (111) face as a function of surface momentum \(k_{\parallel 2}\) with \(k_{\parallel 1} = 0.75\pi\). (d) Energy dispersion of the lowest lying state with positive energy. The color scale is such that black corresponds to zero energy. The states at zero energy make use of the topological invariant \(N_{(111)}\) such that black corresponds to zero energy. The states at zero energy in (c) and (d) are localized at the surface. The flat bands in (c) and (d) are singly degenerate (i.e., one branch per surface), whereas the linearly dispersing zero mode at the center of the BZ in (d) is doubly degenerate.

FIG. 3. (color online) Same as Fig. \(\mathbf{2}\) but for the point group \(C_{4v}\), for a slab with (012) face, and with \((g_2, \Delta_2) = (0.0, 0.5)\). This parameter choice corresponds to the white dotted area in Fig. \(\mathbf{1}\).
The zero-energy surface flat bands in time-reversal symmetric non-centrosymmetric SCs are topologically protected against the opening of a gap and are therefore stable against weak symmetry preserving deformations. Conversely, any perturbation that leads to a gap opening of the surface states is expected to be accompanied by the breaking of the symmetries of the time-reversal symmetric SC, i.e., TRS or certain types of translational invariance. One possible scenario, for example, is that interactions might lead to spontaneous TRS breaking at the boundary of the SC, such as to the coexistence of TRS breaking and TRS preserving order parameters near the surface. This would be observable in experiments, for instance, as a splitting of the zero-bias conductance peak.

In conclusion, using three different topological invariants, we examined the topological properties of general 3D non-centrosymmetric superconductors with TRS. We showed that in nodal superconducting phases there always appear dispersionless Andreev surface bands. We established a correspondence between these zero-energy surface flat bands and the topologically protected nodal lines in the bulk, thereby revealing the topological origin of the surface flat band. In particular, we demonstrated that the projection of the nodal lines on the surface coincides with the boundary of the surface flat band. We emphasize that the presented formalism (or a generalization thereof) can be applied to any 3D unconventional SC that preserves TRS. One particularly interesting family of compounds is Li$_2$Pd$_x$Pt$_{3-x}$B. In these SCs the substitution of Pd by Pt seems to be related to the relative strength of singlet and triplet pairing states. Hence, it might be possible to observe in Li$_2$Pd$_x$Pt$_{3-x}$B the transition between two topologically distinct quantum phases as a function of Pt concentration.

Acknowledgments The authors thank B. Béni, A. Furusaki, L. Klam, A. Ludvig, R. Nakai, P. Horsch, and M. Sigrist for discussions. A.P.S. is grateful to the Aspen Center for Physics for hospitality during the preparation of this work. S.R. is supported by Center for Condensed Matter Theory at UCB.

1. M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L. W. Molenkamp, X.-L. Qi, S.-C. Zhang, Science 318, 766 (2007); D. Hsieh, D. Qian, L. Wray, Y. Xia, Y. Hor, R. Cava, and M. Hasan, Nature 452, 970 (2008).
2. M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010); X.-L. Qi and S.-C. Zhang, arXiv:1008.2026 (unpublished).
3. A. P. Schnyder, S. Ryu, A. Furusaki, A. W. W. Ludwig, Phys. Rev. B 78 195125 (2008); AIP Conf. Proc. 1134 10 (2009).
4. A. Y. Kitaev, AIP Conf. Proc. 1134 22 (2009).
5. S. Ryu, A. P. Schnyder, A. Furusaki, A. W. W. Ludwig, New Journal of Physics 12 065010 (2010).
6. S. Murakawa, Y. Tamura, Y. Wada, M. Wasai, M. Saitoh, Y. Aoki, R. Nomura, Y. Okuda, Y. Nagato, M. Yamamoto, S. Higashitani, and K. Nagai, Phys. Rev. Lett. 103, 155301 (2009).
7. Topological SCs in class DIII may also be found among non-centrosymmetric SCs with triplet pairing, see, e.g., G. E. Volovik and L. P. Gorkov, Sov. Phys. JETP 61, 843 (1985).
8. E. Bauer, G. Hilscher, H. Michor, Ch. Paul, E. W. Scheidt, A. Gribanov, Yu. Seropogin, H. Noël, M. Sigrist, and P. Rogl, Phys. Rev. Lett. 92, 027003 (2004).
9. K. Togano, F. Badica, Y. Nakamori, S. Orimo, H. Takeya, and K. Hirata, Phys. Rev. Lett. 93, 247004 (2004); F. Badica, T. Kondo, and K. Togano, J. Phys. Soc. Jpn. 74, 1014 (2005).
10. P. A. Frigeri, D. E. Agterberg, A. Koga, and M. Sigrist, Phys. Rev. Lett. 92, 097001 (2004).
11. K. V. Samokhin, Annals of Physics 324 2385 (2009).
12. See supplementary material for details of the calculation.
13. B. Béni, Phys. Rev. B 81, 134515 (2010).
14. M. Sato, Phys. Rev. B 73 214502 (2006).
15. X.-L. Qi, T. L. Hughes, S. Raghu, and S.-C. Zhang, Phys. Rev. Lett. 102 187001 (2009).
16. A. B. Vorontsov, I. Vekhter, and M. Eschrig, Phys. Rev. Lett. 101, 127003 (2008).
17. M. Eschrig, C. Iniotakis, and Y. Tanaka, arXiv:1001.4286.
[18] S. Ryu and Y. Hatsugai, Phys. Rev. Lett. 89, 077002 (2002).

[19] For a similar Majorana Andreev state at edges of 2D nodal superconductors, see M. Sato and S. Fujimoto, Phys. Rev. Lett. 105, 217001 (2010).

[20] Y. Tanaka and S. Kashiwaya, Phys. Rev. Lett. 74, 3451 (1995).

[21] S. Kashiwaya and Y. Tanaka, Rep. Prog. Phys. 63, 164 (2000).

[22] Y. Tanaka, Y. Mizuno, T. Yokoyama, K. Yada, and M. Sato Phys. Rev. Lett. 105, 097002 (2010).

[23] K. Yada, M. Sato, Y. Tanaka, and T. Yokoyama Phys. Rev. B 83, 064505 (2011).

[24] M. Sato, Y. Tanaka, K. Yada, and T. Yokoyama, Phys. Rev. B 83, 224511 (2011).

[25] H. Q. Yuan, D. F. Agterberg, N. Hayashi, P. Badica, D. Vanderselde, K. Togano, M. Sigrist, and M. B. Salamon, Phys. Rev. Lett. 97, 017006 (2006).

Supplementary Materials

We first discuss basic symmetry properties of superconductors with time-reversal invariance and then go on to derive the topological numbers (3), (5), and (6) from the main text. We shall keep the analysis as general as possible, such that it may be applied to arbitrary superconducting systems. In Section [23] we will then specialize to the Bogoliubov-de Gennes Hamiltonian (1) describing a single-band non-centrosymmetric superconductor.

Appendix A: Symmetries of the Bogoliubov-de Gennes Hamiltonian

Let us consider a general time-reversal invariant superconductor belonging to symmetry class DIII in the terminology of Refs. [3, 26, 27]

\[ H(k) = \begin{pmatrix} h(k) & \Delta(k) \\ \Delta^T(k) & -h^T(-k) \end{pmatrix}, \]  

(A1)

with the \( N \)-band normal state Hamiltonian \( h(k) \) and the superconducting gap matrix \( \Delta(k) \), which obeys \( \Delta(k) = -\Delta^T(-k) \) because of Fermi statistics. With \( N \) bands (orbitals) and two spin degrees of freedom, the total dimension of the Bogoliubov-de Gennes Hamiltonian at momentum \( k \) is \( 4N \times 4N \). A class DIII superconductor satisfies two independent anti-unitary symmetries: time-reversal symmetry \( T = KU_T \), with \( T^2 = -1 \), and particle-hole symmetry \( C = KC_U \), with \( C^2 = +1 \). Here, \( K \) stands for the complex conjugation operator. Time-reversal symmetry constrains \( H(k) \) as

\[ U_T H^*(-k) U_T^* = +H(k), \]  

(A2)

with \( U_T = \text{diag}(u_T, u_T \sigma \) and \( u_T \) is a \( 2N \times 2N \) unitary matrix that implements time-reversal invariance of the normal state Hamiltonian, i.e., \( u_T^* h(-k) u_T = h(k) \) and \( u_T^* \Delta^T(k) u_T = -\Delta(k) \). Observe, Eq. (A2) implies \( u_T^* \Delta^T(k) = \Delta(k) u_T^* \). Particle-hole symmetry acts on the Bogoliubov-de Gennes Hamiltonian \( H(k) \) as

\[ U_C H^*(-k) U_C^* = -H(k), \]  

(A3)

where \( U_C = \sigma_1 \otimes \mathbb{I}_{2N}, \sigma_{1,2,3} \) stand for the three Pauli matrices, and \( \mathbb{I}_{2N} \) is the \( 2N \times 2N \) unit matrix. Combining time-reversal and particle-hole symmetry we obtain a third discrete symmetry, which is given by

\[ U_S^* H(k) U_S = -H(k), \]  

(A4)

with \( U_S = iU_T U_C \). In other words, there is a unitary matrix \( U_S \) that anticommutes with \( H(k) \) and thereby endows the Hamiltonian with a “chiral” structure. Namely, in the basis in which \( U_S \) is diagonal, \( H(k) \) takes block off-diagonal form

\[ \tilde{H}(k) = V H(k) V^T = \begin{pmatrix} 0 & D(k) \\ D^T(k) & 0 \end{pmatrix}, \]  

(A5)

where the unitary transformation \( V \) is given by

\[ V = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{I}_{2N} + i u_T \\ \mathbb{I}_{2N} - i u_T \end{pmatrix}, \]  

(A6)

and the block off-diagonal component reads \( D(k) = h(k) + i \Delta(k) u_T \). In the off-diagonal basis the unitary matrix \( U_T \) is given as

\[ U_T = V U_T V^T = \sigma_1 \otimes u_T. \]  

Thus, time-reversal symmetry acts on \( D(k) \) as follows

\[ u_T D^T(-k) u_T^* = D(k). \]  

(A7)

To compute the \( \mathbb{Z}_2 \) invariant, Eq. (6), it is advantageous to perform a second basis transformation which brings \( U_T \) into the simple form \( \bar{U}_T = W U_T W^T = \sigma_1 \otimes \mathbb{I}_{2N} \). This can be achieved with the help of the unitary matrix \( W = \text{diag}(\mathbb{I}_{2N}, u_T) \). In this new basis the Bogoliubov-de Gennes Hamiltonian reads

\[ \bar{H}(k) = W \tilde{H}(k) W^T = \begin{pmatrix} 0 & \bar{D}(k) \\ \bar{D}^T(k) & 0 \end{pmatrix}, \]  

(A8)

with the block off-diagonal component

\[ \bar{D}(k) = D(k) u_T^* = h(k) u_T^* - i \Delta(k). \]  

(A9)

We note that time-reversal symmetry operates on \( \bar{D}(k) \) as \( \bar{D}^T(-k) = -\bar{D}(k) \).

Appendix B: Flat Band Hamiltonian and Winding Number

For the derivation of the topological invariants it is convenient to adiabatically deform \( H(k) \), Eq. (A1), into a flat band Hamiltonian \( Q(k) \). The only assumptions that we need for computing \( Q(k) \) are: (i) the Hamiltonian has a full spectral gap and (ii) there is a unitary matrix \( U_S \) anticommuting with \( H(k) \). Thus, the following derivation of \( Q(k) \) is applicable to any chiral symmetric Hamiltonian with a full bulk gap, in particular also to the three-dimensional topological superconductors in symmetry class AIII, DIII, and CI [3, 28, 29, 32].

In what follows, we work in a basis in which \( H(k) \) takes block off-diagonal form. The flat band Hamiltonian is defined in terms of the projection operator \( P(k) \) which projects onto filled Bloch eigenstates of \( H(k) \) at a given momentum \( k \). The
projector $P(k)$, in turn, is defined in terms of the eigenfunctions of $\tilde{H}(k)$

$$
\begin{pmatrix}
0 & D(k) \\
D^\dagger(k) & 0
\end{pmatrix}
\begin{pmatrix}
\chi^\pm_a(k) \\
\eta^\pm_a(k)
\end{pmatrix}
= \pm \lambda_a(k)
\begin{pmatrix}
\chi^\pm_a(k) \\
\eta^\pm_a(k)
\end{pmatrix},
$$

(B1)

where $a = 1, \ldots, 2N$ is the combined band and spin index. We assume there is a spectral gap around zero energy with $|\lambda_a(k)| > 0$, and for definitiveness we choose $\lambda_a(k) > 0$ for all $a$. Multiplying equation (B1) from the left by $\tilde{H}(k)$ yields

$$
DD^\dagger \chi^\pm_a(k) = \lambda_a^2 \chi^\pm_a, \quad D^\dagger D \eta^\pm_a = \lambda_a^2 \eta^\pm_a.
$$

(B2)

Hence, the eigenfunctions $(\chi^\pm_a, \eta^\pm_a)$ can be obtained from the eigenvectors of $DD^\dagger$ or $D^\dagger D$

$$
DD^\dagger u_a = \lambda_a^2 u_a, \quad D^\dagger D v_a = \lambda_a^2 v_a.
$$

(B3)

The eigenvectors $u_a, v_a$ are taken to be normalized to one, i.e., $u_a^\dagger u_a = v_a^\dagger v_a = 1$, for all $a$ (here, the index $a$ is not summed over). The eigenstates of $D^\dagger D$ follow from the eigenstates of $DD^\dagger$ via

$$
v_a = N_a D^\dagger u_a,
$$

with the normalization factor $N_a$. Using Eq. (B3) one can check that $v_a$ is indeed an eigenvector of $D^\dagger D$,

$$
D^\dagger D v_a = D^\dagger D (N_a D^\dagger u_a) = N_a \lambda_a^2 D^\dagger u_a = \lambda_a^2 v_a,
$$

(B5)

for all $a$. The normalization factor $N_a$ is given by

$$
u_a D D^\dagger u_a = \lambda_a^2 \nu_a^\dagger u_a = \lambda_a^2 \Rightarrow N_a = \frac{1}{\lambda_a},
$$

(B6)

for all $a$. It follows that the eigenfunctions of $\tilde{H}(k)$ are

$$
\begin{pmatrix}
\chi^\pm_a(k) \\
\eta^\pm_a(k)
\end{pmatrix} = \frac{1}{\sqrt{2}}
\begin{pmatrix}
u_a \\
\pm \nu_a
\end{pmatrix} = \frac{1}{\sqrt{2}} \left( \pm D^\dagger u_a / \lambda_a \right).
$$

(B7)

With this, the projector $P(k)$ onto the filled Bloch states becomes

$$
P = \frac{1}{2} \sum_a \begin{pmatrix}
u_a & -\nu_a^\dagger \\
-\nu_a^\dagger & \nu_a
\end{pmatrix} = \frac{1}{2} \begin{pmatrix} I_{2N} & 0 \\
0 & I_{2N}\end{pmatrix} - \frac{1}{2} \sum_a \begin{pmatrix} 0 & \nu_a^\dagger u_a \\
\nu_a u_a^\dagger & 0 \end{pmatrix}.
$$

(B8)

Finally, we obtain for the flat band Hamiltonian $Q$, which is defined as $Q = 4N - 2P$ ([5]),

$$
Q = \sum_a \begin{pmatrix} 0 & \nu_a^\dagger u_a \\
\nu_a u_a^\dagger & 0 \end{pmatrix} = \sum_a \begin{pmatrix} 0 & u_a^\dagger D \\
D^\dagger u_a & 0 \end{pmatrix}.
$$

(B9)

In other words, the off-diagonal block of $Q(k)$ reads

$$
q(k) = \sum_a \frac{1}{\lambda_a} u_a(k) u_a^\dagger(k) D(k),
$$

(B10)

where $u_a(k)$ denotes the eigenvectors of $DD^\dagger$. For a system with completely degenerate bands, $\lambda_a = \lambda$, for all $a$, the above formula simplifies to

$$
q(k) = \frac{1}{\lambda(k)} \sum_a u_a(k) u_a^\dagger(k) D(k) = \frac{1}{\lambda(k)} D(k).
$$

(B11)

Examples of topological insulators and superconductors with completely degenerate bands are the Dirac representatives of Ref. [5].

The integer-valued topological invariant characterizing topological superconductors is now simply given by the winding number of $q(k)$. It can be defined in any odd spatial dimension. In three dimensions we have

$$
u_3 = \int_{BZ} \frac{d^3k}{24\pi^2} \text{Tr} \left[ (q^{-1} \partial_\nu q)(q^{-1} \partial_\nu q)(q^{-1} \partial_\nu q) \right],
$$

(B12)

and in one spatial dimension it reads

$$\nu_1 = \frac{1}{2\pi i} \int_{BZ} dk \text{Tr} \left[ q^{-1} \partial_k q \right].$$

(B13)

Alternatively, it is also possible to define the winding number in terms of the unflattened off-diagonal block $D(k)$ of the Hamiltonian. For example, for the winding number in one spatial dimension this reads

$$
u_1 = \frac{1}{4\pi i} \int_{BZ} dk \text{Tr} \left[ D^{-1} \partial_k D - \{D^\dagger\}^{-1} \partial_k D^\dagger \right] = \frac{1}{2\pi} \text{Im} \int_{BZ} dk \text{Tr} \left[ \partial_k \ln D \right].
$$

(B14)

**Appendix C: $\mathbb{Z}_2$ Invariant for Symmetry Class DIII**

In this section we compute the $\mathbb{Z}_2$ topological invariant for symmetry class DIII in $d = 1$ and $d = 2$ spatial dimensions. It is most convenient to perform this derivation in the basis (A8), in which the $4N \times 4N$ Bogoliubov-de Gennes Hamiltonian takes the form

$$
H(k) = \begin{pmatrix} 0 & D(k) \\
-D^\dagger(k) & 0 \end{pmatrix}, \quad D(k) = -D^T(-k).
$$

(C1)

In this representation, the time-reversal symmetry operator is given by $T = K U_T = K i \sigma_2 \otimes 1_{2N}$ and the flat band Hamiltonian reads

$$
Q(k) = \begin{pmatrix} 0 & q(k) \\
q^\dagger(k) & 0 \end{pmatrix}, \quad q(k) = -q^T(-k).
$$

(C2)

The presence of time-reversal symmetry allows us to define the Kane-Mele $\mathbb{Z}_2$ invariant ([5, 32, 37]),

$$
W = \prod_K \frac{\text{Pf} \left[ w(K) \right]}{\sqrt{\text{det} \left[ w(K) \right]}},
$$

(C3)

with $K$ a time-reversal invariant momentum and Pf the Pfaffian of an anti-symmetric matrix. Here, $w(K)$ denotes the "sewing matrix"

$$
w_{ab}(k) = \langle u_a^\dagger(-k) T u_b^\dagger(k) \rangle,
$$

(C4)

where $a, b = 1, \ldots, 2N$ and $u_{a}^\dagger(k)$ is the $a$-th eigenvector of $Q(k)$ with eigenvalue $\pm 1$. The Pfaffian is an analog of
the determinant that can be defined only for $2n \times 2n$ anti-
symmetric matrices $A$. It is given in terms of a sum over all
elements of the permutation group $S_{2n}$

$$\text{Pf}(A) = \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} \text{sgn}(\sigma) \prod_{i=1}^{n} A_{\sigma(2i-1), \sigma(2i)}.$$ 

Due to the block off-diagonal structure of Eq. (C2), a set of
eigen Bloch functions of $Q(k)$ can be constructed as [5]

$$|u^{\pm}_a(k)\rangle_N = \frac{1}{\sqrt{2}} \left( \pm q^\dagger(k) n_a \right),$$  \hspace{1cm} (C5)

or, alternatively, as

$$|u^{\pm}_a(k)\rangle_S = \frac{1}{\sqrt{2}} \left( \pm q(k) n_a \right),$$  \hspace{1cm} (C6)

where $n_a$ are $2N$ momentum independent orthonormal vec-
tors. For simplicity we choose $(n_a)_b = \delta_{ab}$. In passing, we
note that both $|u^{\pm}_a(k)\rangle_N$ and $|u^{\pm}_a(k)\rangle_S$ are well-defined globally over the entire Brillouin zone. To compute the $\mathbb{Z}_2$ topo-
logical number we choose the basis $|u^{\pm}_a(k)\rangle_N$. Combining Eqs. (C4) and (C5) yields

$$w_{ab}(k) = \frac{1}{2} \left( n^a_1 q^\dagger(-k) \right) i \sigma_2 \otimes \mathbb{I}_{2N} \mathcal{C} \left( \pm q^\dagger(k) n_b \right) = \frac{1}{2} \left( n^a_1 q^\dagger(-k) \right) \left( \frac{q^T(k) n_b}{-n_b} \right) = \frac{1}{2} \left( n^a_1 q^T(k) n_b - n^a_1 q(-k) n_b \right) = q^T_{ab}(k).$$  \hspace{1cm} (C7)

In the second last line we used Eq. (C2), i.e., $q(-k) = -q^T(k)$. In conclusion, the $\mathbb{Z}_2$ topological number in spatial di-
ensions $d = 2$ and $d = 1$ is given by

$$W = \prod_{K} \text{Pf} \left[ q^\dagger(K) \right].$$  \hspace{1cm} (C8)

where $K$ denotes the four (two) time-reversal invariant mo-
menta of the two-dimensional (one-dimensional) Brillouin

\section*{Appendix D: Flat Band Hamiltonian for the Non-centrosymmetric Superconductor, Eq. (1)}

Let us now apply the formalism developed in the pre-
ceeding sections to the Bogoliubov-de Gennes Hamiltonian [11] from the main text, describing a single band non-
centrosymmetric superconductor [38, 39]. First, we note that
time-reversal symmetry for $H(k)$, Eq. (1), is implemented by $U_T H^*(\mathbf{-k}) U_T^\dagger = +H(k)$ with $U_T = \sigma_0 \otimes i \sigma_2$. Hence, we need to set $U_T = i \sigma_2$ in Eq. (A2). It then follows from
Eq. (A6) that $H(k)$ can be brought into block off-diagonal
form by the unitary transformation

$$V = \frac{1}{\sqrt{2}} \left( \mathbb{I}_2 - \sigma_2 \right).$$  \hspace{1cm} (D1)

The transformed Hamiltonian is given by

$$V H(k)V^\dagger = \left( \begin{array}{cc} 0 & D(k) \\ D^\dagger(k) & 0 \end{array} \right),$$  \hspace{1cm} (D2)

with the off-diagonal block

$$D(k) = \left( \begin{array}{cc} B_k + A l_k^z & A(l_k^x + i l_k^y) \\ A(l_k^x + i l_k^y) & B_k - A l_k^z \end{array} \right) = B_k \sigma_0 + A l_k \cdot \sigma,$$  \hspace{1cm} (D3)

and where we have introduced the short-hand notation

$$A = \alpha + i \Delta, \quad B_k = \varepsilon_k + i \Delta_s.$$  \hspace{1cm} (D4)

Alternatively, we can also choose to work in the basis (A8), in
which case the off-diagonal component reads

$$\tilde{D}(k) = \left( \begin{array}{cc} A(l_k^z - i l_k^y) & -B_k - A l_k^z \\ -B_k + A l_k^z & A(l_k^y + i l_k^x) \end{array} \right).$$  \hspace{1cm} (D5)

For the computation of the flat band Hamiltonian $Q(k)$ it is,
however, more convenient to use Eq. (D2).

Repeating the steps of section [3] we calculate the eigenvectors $u_a(k)$ of

$$D_k D_k^\dagger = |A|^2 l_k^2 + |B_k|^2 + (AB_k + B_k^* A^* l_k \cdot \sigma),$$  \hspace{1cm} (D6)

where $l_k = |l_k|$. The eigenfunctions $u_a(k)$ of $D_k D_k^\dagger$ can be obtained by diagonalizing $l_k \cdot \sigma$. Hence, when $(l_k^x, l_k^y) \neq (0, 0)$, we find that the eigenvectors $u_a(k)$ are given by

$$u_{1/2}(k) = \frac{1}{\sqrt{2 l_k(l_k^x + i l_k^y)}} \left( \pm l_k^y - i l_k^x \right).$$  \hspace{1cm} (D7)

According to Eq. (B11), the off-diagonal block of the flat
band Hamiltonian $Q(k)$ is defined in terms of the eigenvectors $u_a(k)$. Thus, we need to compute

$$\sum_{a=1,2} \frac{1}{\lambda_{a k}} u_a(k) u_a^\dagger(k) = \frac{1}{2 \lambda_{1 k} \lambda_{2 k}} \left[ (\lambda_{1 k} + \lambda_{2 k}) \sigma_0 + (\lambda_{2 k} - \lambda_{1 k}) l_k \cdot \sigma \right].$$  \hspace{1cm} (D8)
with the two positive eigenvalues $\lambda_{1k} = |B_k - A_lk|$ and $\lambda_{2k} = |B_k + A_lk|$. Note that the last term in the second line of Eq. (D8) contains removable singularities at the points $k_0$ where $L_{k_0} = 0$. For those points in the Brillouin zone one needs to carefully take the limit $k \to k_0$ to obtain the correct value of Eq. (D8). Finally, by use of Eq. (B11) together with Eqs. (D3) and (D8) we find for the off-diagonal block of the flat band Hamiltonian

$$q(k) = \frac{1}{2\lambda_{1k}\lambda_{2k}} \left\{ A_lk(\lambda_{2k} - \lambda_{1k}) + B_k(\lambda_{1k} + \lambda_{2k}) \right\} \sigma_0 + \left\{ A_lk(\lambda_{1k} + \lambda_{2k}) + B_k(\lambda_{2k} - \lambda_{1k}) \right\} l_k \cdot \sigma. \quad \text{(D9)}$$

Now, for the $\mathbb{Z}_2$ invariant we need to bring $q(k)$ into the basis in which $U_T = i\sigma_2 \otimes 1_2$. This is achieved by letting

$$q(k) \to -iq(k)\sigma_2. \quad \text{(D10)}$$

Using Eq. (C8) we get

$$W = \prod_K \text{Pf} \left[ i\sigma_2 q^T(K) \right] = \prod_K \frac{B_K}{\sqrt{B_K^2}}, \quad \text{(D11)}$$

where we have made use of the fact that $l_k$ is an antisymmetric function, i.e., $l_{-k} = -l_k$.

### 1. $\mathbb{Z}_2$ surface state

As discussed in the main text, the $\mathbb{Z}_2$ number (D11) can be used to deduce the presence of Andreev surface states at time-reversal invariant momenta of the surface BZ. To exemplify this, let us consider Hamiltonian (1) in a slab geometry with $(lmn)$ face. At the four time-reversal invariant momenta $K_\parallel$ of the $(lmn)$ surface BZ the $\mathbb{Z}_2$ invariant is defined by

$$W_{(lmn)}(K_\parallel) = \prod_{K_\perp} \frac{\text{Pf} \left[ i\sigma_2 q^T(K_\perp, K_\parallel) \right]}{\sqrt{\det \left[ i\sigma_2 q^T(K_\perp, K_\parallel) \right]}}, \quad \text{(D12)}$$

Eq. (D12) is quantized to $+1$ or $-1$, with $W_{(lmn)}(K_\parallel) = -1$ indicating the presence of Kramers degenerate surface modes at the surface momentum $K_\parallel$ (see Fig. 5).