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Topological invariants for the Fermi surface of a time-reversal-invariant superconductor

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A time-reversal-invariant (TRI) topological superconductor has a full pairing gap in the bulk and topologically protected gapless states on the surface or at the edge. In this paper, we show that in the weak pairing limit, the topological quantum number of a TRI superconductor can be completely determined by the Fermi-surface properties and is independent of the electronic structure away from the Fermi surface. In three dimensions, the integer topological quantum number in a TRI superconductor is determined by the sign of the pairing order parameter and the first Chern number of the Berry phase gauge field on the Fermi surfaces. In two dimensions and one dimension, the Z_2 topological quantum number of a TRI superconductor is determined simply by the sign of the pairing order parameter on the Fermi surfaces. Our results could directly aid the search for topological superconductors in real materials.

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I. INTRODUCTION

Since the discovery of quantum spin Hall effect,[1–4] topological insulators in both two dimensions (2D) and three dimensions (3D) have generated great interest both theoretically and experimentally.[5–9] Following this development, recent attention has focused on time-reversal-invariant (TRI) topological superconductors and superfluids.[10–13] There is a direct analogy between superconductors and insulators because the Bogoliubov-de Gennes (BdG) Hamiltonian for the quasiparticles of a superconductor is analogous to the Hamiltonian of a band insulator, with the superconducting gap corresponding to the band gap of the insulator. ^{3}He-B is an example of such a topological superfluid state. This TRI state has a full pairing gap in the bulk and gapless surface states consisting of a single Majorana cone.[10–12,14] In fact, the BdG Hamiltonian for ^{3}He-B is identical to the model Hamiltonian of a 3D topological insulator proposed by Zhang *et al.*[7] In 2D, the classification of topological superconductors is very similar to that of topological insulators. Time-reversal breaking superconductors are classified by an integer,[15,16] similar to quantum Hall insulators[17] while TRI superconductors are classified[10–13] by a Z_2 invariant in 1D and 2D but by an integer (Z) class in 3D. The integer-valued topological invariant in 3D can be written as a winding number over the entire momentum space.[12] Simplified criteria for inversion symmetric superconductors has been proposed in the literature.[18] An explicit expression of the Z_2 topological invariants in 1D and 2D has not been obtained in the literature.

Despite the similarity of topological insulators and topological superconductors, there is a key physical difference between them. Starting from a Fermi-liquid "normal state" with some attractive interaction, superconductivity is induced at low enough temperatures due to the Cooper instability of the Fermi surface. At least right below the transition temperature, Cooper pairing is only important around the Fermi surface, so the topological properties of such a superconductor are determined *completely* by the properties in the neighborhood of the Fermi surface, rather than that of the full Brillouin zone, as in the case of a topological insulator.

Motivated by such an observation, in this paper we obtain simple and explicit physical criteria for TRI topological superconductivity in one, two, and three dimensions in the *weak pairing limit*, where the pairing is only important in a small neighborhood of the Fermi surface. In 3D, the Fermi-surface topological invariant (FSTI) of a TRI superconductor is determined by the sign of the pairing order parameter and the first Chern number of each Fermi surface. Here the first Chern number of a Fermi surface is defined by the net flux of the Berry phase gauge field penetrating the Fermi surface. This is quantized as long as the Fermi surface is a smooth two-dimensional manifold. Based on this Fermi-surface criterion for the 3D topological superconductor, the Z_2 FSTI's in 1D and 2D can be obtained by dimensional reduction.[19] The criteria for a Z_2 nontrivial superconductor in the weak pairing limit is simple: a TRI superconductor is nontrivial (trivial) if there are an odd (even) number of Fermi surfaces with a negative pairing order parameter. For example, the superconductivity in a 2D Rashba system is nontrivial if the pairing on the two Fermi surfaces has opposite sign. Inspired by such Fermi-surface formulas, we also obtain an explicit expression of the Z_2 FSTI in 1D and 2D which applies to generic superconductors beyond the weak pairing limit. Our criteria is simple to compute and applies to generic TRI superconductors so that we expect it to be helpful in the search for topological superconductors.

II. TOPOLOGICAL INVARIANT IN 3D TRI SUPERCONDUCTORS

We start from a generic mean-field Hamiltonian of a 3D TRI superconductor, which can be written in momentum space as

$$H=\sum_{\mathbf{k}}\left[\psi_{\mathbf{k}}^{\dagger}h_{\mathbf{k}}\psi_{\mathbf{k}}+\frac{1}{2}(\psi_{\mathbf{k}}^{\dagger}\Delta_{\mathbf{k}}\psi_{-\mathbf{k}}^{\dagger T}+\text{H.c.})\right]\equiv\sum_{\mathbf{k}}\Psi_{\mathbf{k}}^{\dagger}H_{\mathbf{k}}\Psi_{\mathbf{k}},$$

with

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$$\Psi_{\mathbf{k}} = \frac{1}{\sqrt{2}}\begin{pmatrix} \psi_{\mathbf{k}} - i\mathcal{T}\psi_{-\mathbf{k}}^{\dagger} \\ \psi_{\mathbf{k}} + i\mathcal{T}\psi_{-\mathbf{k}}^{\dagger} \end{pmatrix}, \quad H_{\mathbf{k}} = \frac{1}{2}\begin{pmatrix} & h_{\mathbf{k}} + i\mathcal{T}\Delta_{\mathbf{k}}^{\dagger} \\ h_{\mathbf{k}} - i\mathcal{T}\Delta_{\mathbf{k}}^{\dagger} & \end{pmatrix}. \tag{1}$$

In general, $\psi_{\mathbf{k}}$ is a vector with N components and $h_{\mathbf{k}}$ and $\Delta_{\mathbf{k}}$ are $N\times N$ matrices. The matrix $\mathcal{T}$ is the time-reversal matrix satisfying $\mathcal{T}^{\dagger}h_{\mathbf{k}}\mathcal{T}=h_{-\mathbf{k}}^{T}$, $\mathcal{T}^2=-\mathbb{I}$, and $\mathcal{T}^{\dagger}\mathcal{T}=\mathbb{I}$. For further background and derivation see Appendix A. We have chosen a special basis in which the BdG Hamiltonian $H_{\mathbf{k}}$ has a special off-diagonal form. It should be noted that such a choice is only possible when the Hamiltonian has both time-reversal symmetry and particle-hole symmetry. These two symmetries also require $\mathcal{T}\Delta_{\mathbf{k}}^{\dagger}$ to be Hermitian, which makes the matrix $h_{\mathbf{k}}+i\mathcal{T}\Delta_{\mathbf{k}}^{\dagger}$ generically non-Hermitian. The matrix $h_{\mathbf{k}}+i\mathcal{T}\Delta_{\mathbf{k}}^{\dagger}$ can be decomposed by singular value decomposition (SVD) as $h_{\mathbf{k}}+i\mathcal{T}\Delta_{\mathbf{k}}^{\dagger}=U_{\mathbf{k}}^{\dagger}D_{\mathbf{k}}V_{\mathbf{k}}$ with $U_{\mathbf{k}}$, $V_{\mathbf{k}}$ unitary matrices and $D_{\mathbf{k}}$ a diagonal matrix with non-negative elements. One can see straightforwardly that the diagonal elements of $D_{\mathbf{k}}$ are actually the positive eigenvalues of $H_{\mathbf{k}}$. For a fully gapped superconductor, $D_{\mathbf{k}}$ is positive definite and we can adiabatically deform it to the identity matrix $\mathbb{I}$ without closing the superconducting gap. During this deformation the matrix $h_{\mathbf{k}}+i\mathcal{T}\Delta_{\mathbf{k}}^{\dagger}$ is deformed to a unitary matrix $Q_{\mathbf{k}}=U_{\mathbf{k}}^{\dagger}V_{\mathbf{k}}\in \mathrm{U(N)}$. As shown in Ref. 12, the integer-valued topological invariant characterizing topological superconductors is defined as the winding number of $Q_{\mathbf{k}}$,

$$N_W = \frac{1}{24\pi^2}\int d^3\mathbf{k}\,\epsilon^{ijk}\,\mathrm{Tr}[Q_{\mathbf{k}}^{\dagger}\partial_i Q_{\mathbf{k}} Q_{\mathbf{k}}^{\dagger}\partial_j Q_{\mathbf{k}} Q_{\mathbf{k}}^{\dagger}\partial_k Q_{\mathbf{k}}]. \tag{2}$$

Now we study $Q_{\mathbf{k}}$ in the weak pairing limit. For simplicity, in the following, we will assume the Fermi surfaces are all nondegenerate and there are no lower dimensional zero-energy defects such as point or line nodes. All our conclusions can be easily generalized to more generic cases. When the Fermi surfaces are nondegenerate and the weak pairing term $\Delta_{\mathbf{k}}$ is only turned on around the Fermi surfaces, the matrix elements of $\mathcal{T}\Delta_{\mathbf{k}}^{\dagger}$ between different bands are negligible. Thus, to leading order we have

$$h_{\mathbf{k}} + i\mathcal{T}\Delta_{\mathbf{k}}^{\dagger} \simeq \sum_n (\epsilon_{n\mathbf{k}} + i\delta_{n\mathbf{k}})|n,\mathbf{k}\rangle\langle n,\mathbf{k}|$$

with

$$\delta_{nk} \equiv \langle n,\mathbf{k}|\mathcal{T}\Delta_{\mathbf{k}}^{\dagger}|n,\mathbf{k}\rangle \in \mathbb{R}, \tag{3}$$

where $|n,\mathbf{k}\rangle$ are the eigenvectors of $h_{\mathbf{k}}$. Physically, δ_{nk} is the matrix element of $\Delta_{\mathbf{k}}^{\dagger}$ between $|n,\mathbf{k}\rangle$ and its time-reversed partner $|\bar{n},-\mathbf{k}\rangle=\mathcal{T}^{\dagger}|n,\mathbf{k}\rangle$. In this approximation, the matrix $Q_{\mathbf{k}}$ is given by

$$Q_{\mathbf{k}} = \sum_n e^{i\theta_{n\mathbf{k}}}|n,\mathbf{k}\rangle\langle n,\mathbf{k}| \tag{4}$$

with $e^{i\theta_{n\mathbf{k}}}=(\epsilon_{n\mathbf{k}}+i\delta_{n\mathbf{k}})/|\epsilon_{n\mathbf{k}}+i\delta_{n\mathbf{k}}|$. In the weak pairing limit, we take $\delta_{n\mathbf{k}}$ to be nonzero only in a small neighborhood $-\epsilon \le E \le \epsilon$ of the Fermi level. As shown in Fig. 1, the phase $\theta_{n\mathbf{k}}$ changes from 0 to $\pm\pi$ across the Fermi level, with the sign determined by the sign of $\delta_{n\mathbf{k}}$. In the limit $\epsilon\to 0$, such a domain-wall configuration of $\theta_{n\mathbf{k}}$ can be expressed by the formula

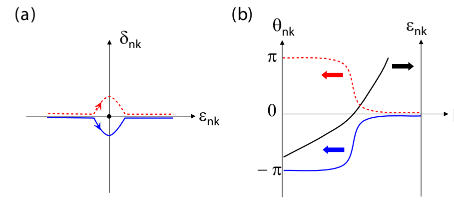

FIG. 1. (Color online) (a) The path of $\epsilon_{n\mathbf{k}}+i\delta_{n\mathbf{k}}$ in the complex plane for positive (red dashed) and negative (blue) $\delta_{n\mathbf{k}}$ around the Fermi surface. (b) $\theta_{n\mathbf{k}}$ and $\epsilon_{n\mathbf{k}}$ vs momentum $\mathbf{k}$. The change in $\theta_{n\mathbf{k}}$ across k_F is $-\pi$ $(+\pi)$ when $\delta_{n\mathbf{k}}$ is positive (negative), as shown by the red dashed (blue) curve.

$$\nabla\theta_{n\mathbf{k}} = -\pi\mathbf{v}_{n\mathbf{k}}\,\mathrm{sgn}(\delta_{n\mathbf{k}})\delta(\epsilon_{n\mathbf{k}}) \tag{5}$$

in which $\mathbf{v}_{n\mathbf{k}}=\nabla_{\mathbf{k}}\epsilon_{n\mathbf{k}}$ is the Fermi velocity. It should be noted that for a gapped superconductor $\delta_{n\mathbf{k}}$ remains nonzero for all $\mathbf{k}$ on the Fermi surfaces, so the sign of $\delta_{n\mathbf{k}}$ is fixed on each Fermi surface.

Once the behavior of $\theta_{n\mathbf{k}}$ in the Brillouin zone is simplified to Eq. (5) in the weak pairing limit, the winding number [Eq. (2)] can be simplified to the following simple FSTI:

$$N_W = \frac{1}{2}\sum_s \mathrm{sgn}(\delta_s)C_{1s}, \tag{6}$$

where s is summed over all disconnected Fermi surfaces and $\mathrm{sgn}(\delta_s)$ denotes the sign of $\delta_{n\mathbf{k}}$ on the sth Fermi surface. C_{1s} is the first Chern number of the sth Fermi surface (denoted by FS_s),

$$C_{1s} = \frac{1}{2\pi}\int_{\mathrm{FS}_s} d\Omega^{ij}[\partial_i a_{sj}(\mathbf{k}) - \partial_j a_{si}(\mathbf{k})] \tag{7}$$

with $a_{si}=-i\langle s\mathbf{k}|\partial/\partial k_i|s\mathbf{k}\rangle$ the adiabatic connection defined for the band $|s\mathbf{k}\rangle$ which crosses the Fermi surface and $d\Omega^{ij}$ the surface element two forms of the Fermi surface. More details of the derivation of Eq. (6) are included in Appendix B.

As an example, consider a two-band Hamiltonian $h_{\mathbf{k}}=\mathbf{k}^2/2m-\mu+\alpha\mathbf{k}\cdot\sigma$. For $\mu>0$, the system has two Fermi surfaces which are concentric spheres around $\mathbf{k}=0$. (The two-band model should be regularized on the lattice but the lattice regularization is unimportant as long as no other Fermi surfaces are introduced.) Denoting the electron states at the inner (outer) Fermi surface by $|\mathbf{k},+(-)\rangle$, we have $\sigma\cdot\mathbf{k}|\mathbf{k},\pm\rangle=\pm|\mathbf{k}||\mathbf{k},\pm\rangle$. It is easy to check that the two Fermi surfaces carry opposite Chern number $C_{\pm}=\pm 1$. Thus, according to Eq. (6), we can obtain a topological superconductor if the two Fermi surfaces have opposite signs of pairing. The time-reversal matrix is $\mathcal{T}=i\sigma_y$ in this system. If we have $\Delta_{\mathbf{k}}=i\Delta_0\sigma_y$, then $i\mathcal{T}\Delta_{\mathbf{k}}^{\dagger}=\Delta_0\mathbb{I}$ which has the same sign on the two Fermi surfaces and leads to $N_W=0$. On the other hand, if we have $\Delta_{\mathbf{k}}=i\Delta_0\sigma_y\sigma\cdot\mathbf{k}$, then $i\mathcal{T}\Delta_{\mathbf{k}}^{\dagger}=\Delta_0\sigma\cdot\mathbf{k}$ has opposite sign on the two Fermi surfaces so that $N_W=1$ if $\Delta_0>0$. If we take the limit $\alpha\to 0$, we obtain a topological superconductor with quadratic kinetic-energy term and pairing $\Delta_{\mathbf{k}}=i\Delta_0\sigma_y\sigma\cdot\mathbf{k}$, which is exactly the BdG Hamiltonian of the ^{3}He-B phase. This example also illustrates how the FSTI [Eq. (6)] can be generalized to systems with degeneracies on

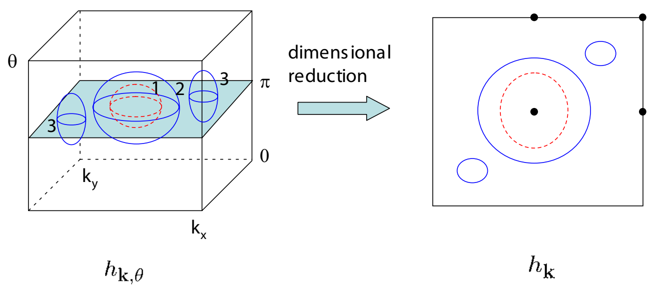

FIG. 2. (Color online) Dimensional reduction from a 3D TRI superconductor to a 2D TRI superconductor. The 2D TRI superconductor corresponds to the $\theta=\pi$ section of a 3D superconductor. The Fermi surfaces with blue (red dashed) color are those with positive (negative) pairing amplitude δ_s.

the Fermi surface: one can always add a small perturbation proportional to $\mathcal{T}\Delta_{\mathbf{k}}^{\dagger}$ to the Hamiltonian to lift the degeneracy while preserving the topological properties of the superconductor.

III. DIMENSIONAL REDUCTION TO 2D

The FSTI can be generalized to lower dimensions, i.e., 2D and 1D. The TRI topological superconductors in 2D and 1D are related to the one in 3D by *dimensional reduction*, similar to the procedure carried out in the context of TRI topological insulators in Ref. 19.

Due to the same symmetry reason as the 3D case, the BdG Hamiltonian $H_{\mathbf{k}}$ of a 2D TRI superconductor can also be written in the form of Eq. (1) so that one can also define a matrix $Q_{\mathbf{k}} \in \mathrm{U(N)}$ for the 2D case. Since $\Pi_2[\mathrm{U(N)}]=0$, we can always find a smooth deformation $Q_{\mathbf{k},\theta}$, $\theta\in[0,\pi]$ which interpolates between $Q_{\mathbf{k}}$ and the identity $\mathbb{I}$,

$$Q_{\mathbf{k},\theta}=\begin{cases}\mathbb{I}, & \theta=0\\ Q_{\mathbf{k}}, & \theta=\pi.\end{cases} \tag{8}$$

It should be noted that $Q_{\mathbf{k}}$ satisfies $\mathcal{T}^{\dagger}Q_{\mathbf{k}}\mathcal{T}=Q_{-\mathbf{k}}^{T}$ due to time-reversal symmetry. Thus, if we define $Q_{\mathbf{k},-\theta}=\mathcal{T}^{\dagger}Q_{-\mathbf{k},\theta}^{T}\mathcal{T}$ for $\theta\in[0,\pi]$, we obtain $Q_{\mathbf{k},\theta}$ for $\theta\in[-\pi,\pi]$ which is continuous and periodic in $\theta\to\theta+2\pi$. Considering θ as a momentum in an additional dimension, $Q_{\mathbf{k},\theta}$ describes a 3D TRI superconductor, which is characterized by the winding number [Eq. (2)]. If there are two different interpolations $Q_{\mathbf{k},\theta}$ and $Q'_{\mathbf{k},\theta}$ which both interpolate between $Q_{\mathbf{k}}$ and $\mathbb{I}$, it can be shown that time-reversal symmetry requires their winding numbers to be different by an even number: $N_W(Q)-N_W(Q')=0 \bmod 2$. Thus the parity $(-1)^{N_W(Q)}$ is independent of the choice of interpolation path and is a Z_2 topological invariant uniquely determined by $Q_{\mathbf{k}}$.

Now we study the expression of such a Z_2 invariant in the weak pairing limit. In this limit, the interpolation of $Q_{\mathbf{k}}$ to $Q_{\mathbf{k},\theta}$ is equivalent to interpolating the 1D Fermi circles of the 2D normal-state Hamiltonian $h_{\mathbf{k}}$ to Fermi surfaces in a 3D Brillouin zone parameterized by (k_x,k_y,θ). We can simply extrapolate the pairing on the Fermi circles to the Fermi surfaces, as illustrated in Fig. 2. If the Fermi surfaces remain nondegenerate during the interpolation, we obtain the Z_2 FSTI as the parity of the winding number given by Eq. (6),

$$N_{2D}=(-1)^{N_W}=(-1)^{1/2\Sigma_s \mathrm{sgn}(\delta_s)C_{1s}}=\prod_s[i\ \mathrm{sgn}(\delta_s)]^{C_{1s}}.$$

Such a formula can be further simplified by noticing the following two properties of the Chern number C_{1s} carried by the Fermi surfaces: (i) the Chern number of each Fermi surface satisfies $(-1)^{C_{1s}}=(-1)^{m_s}$, where m_s is the number of TRI points enclosed by the sth Fermi surface. (ii) The net Chern number of all Fermi surfaces vanishes, $\Sigma_s C_{1s}=0$. We leave a more detailed demonstration of these two conclusions to Appendix C and only sketch the physical reasons for them here. The conclusion (i) comes from the fact that a Fermi surface which only encloses one TRI point, such as Fermi surface 1 in Fig. 2, always encloses a singularity at the TRI point due to Kramers' degeneracy. One can prove that the Chern number is always odd by making use of time-reversal symmetry. The Fermi surfaces enclosing multiple TRI points can be adiabatically deformed into several Fermi surfaces, each enclosing a single TRI point. The conclusion (ii) is a consequence of the Nielsen-Ninomiya theorem[20] which states that the total chirality of a 3D lattice system must be zero.

Using these properties of C_{1s}, we finally obtain the following expression for the Z_2 FSTI which is independent of the interpolation to 3D:

$$N_{2D}=\prod_s[\mathrm{sgn}(\delta_s)]^{m_s}. \tag{9}$$

The criterion shown in Eq. (9) is quite simple: a 2D TRI superconductor is nontrivial (trivial) if there are an odd (even) number of Fermi surfaces each of which encloses one TRI point in the Brillouin zone and has negative pairing.

IV. DIMENSIONAL REDUCTION TO 1D AND GENERIC EXPRESSION OF Z_2 INVARIANT

Following the same logic, the dimensional reduction can be carried out again to obtain the Z_2 FSTI in 1D. This results in an identical formula to Eq. (9). Since in 1D each Fermi "surface" (which consists of two points at k_F and $-k_F$) always encloses one TRI invariant point, the FSTI is simply

$$N_{1D}=\prod_s[\mathrm{sgn}(\delta_s)], \tag{10}$$

where s is summed over all the Fermi points between 0 and π. In other words, a 1D TRI superconductor is nontrivial (trivial) if there are an odd number of Fermi points between 0 and π with negative pairing. Two examples with trivial and nontrivial pairing are shown in Fig. 3.

Interestingly, from Fig. 3 we can get an alternative understanding of the 1D topological superconductor, which can apply to a generic 1D TRI superconductor beyond the weak pairing limit. As discussed earlier in Fig. 1, the sign of the pairing δ_s determines the winding of the phase $\theta_{n\mathbf{k}}$ across the Fermi point. On the other hand, we have shown that time-reversal symmetry requires $\mathcal{T}^{\dagger}Q_{\mathbf{k}}\mathcal{T}=Q_{-\mathbf{k}}^{T}$, from which we can find that $\theta_{n\mathbf{k}}=\theta_{\bar{n}-\mathbf{k}}$ if $|n,\mathbf{k}\rangle$ and $|\bar{n},-\mathbf{k}\rangle$ label a Kramers' pair. Thus, along the path from $k=0$ to $k=\pi$, the change in $\theta_{n\mathbf{k}}$

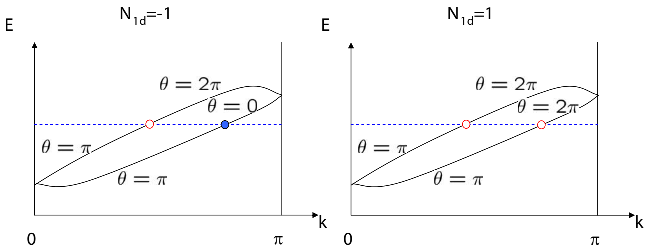

FIG. 3. (Color online) Simple examples of (a) nontrivial and (b) trivial pairing in a 1D system. The red (open) and blue (closed) dots are Fermi points with negative and positive pairing, respectively. The phase $\theta=\theta_{n\mathbf{k}}$ is taken to be the same at $k=0$ for the two bands. At $k=\pi$, θ of the two bands are differ by (a) 2π for nontrivial pairing and (b) by 0 for trivial pairing.

and $\theta_{\bar{n}\mathbf{k}}$ must be the same modulo 2π: $\int_0^\pi dk(\partial_k\theta_{nk}-\partial_k\theta_{\bar{n}k})=2\pi n,\ n\in\mathbb{Z}$. In the examples shown in Fig. 3 we have $n=1$ for the nontrivial pairing and $n=0$ for the trivial pairing. Such a parity difference of the winding number of $\theta_{n\mathbf{k}}$ turns out to be generic and can be captured by the following Z_2 FSTI:

$$N_{1\mathrm{D}}=\frac{\mathrm{Pf}(\mathcal{T}^\dagger Q_{k=\pi})}{\mathrm{Pf}(\mathcal{T}^\dagger Q_{k=0})}\exp\left(-\frac{1}{2}\int_0^\pi dk\ \mathrm{Tr}[Q_k^\dagger\partial_k Q_k]\right), \quad (11)$$

where we have used $\mathcal{T}^\dagger Q_k\mathcal{T}=Q_{-k}^T\Rightarrow\mathcal{T}^\dagger Q_k=-(\mathcal{T}^\dagger Q_{-k})^T$ so that $\mathcal{T}^\dagger Q_k$ is antisymmetric for $k=0,\ \pi$ and the Pfaffian is well defined. It is straightforward to show that $N_{1\mathrm{D}}=\pm 1$ is a Z_2 quantity and also a topological invariant. More details on the properties of the Z_2 FSTI [Eq. (11)] and its relation to the FSTI [Eq. (10)] are given in Appendix D. Equation (11) is the topological superconductor analog of Kane and Mele's Z_2 invariant in quantum spin Hall insulators.[21] Following the same approach as Refs. 22 and 23, one can obtain three Z_2 invariants in 2D, one of which is the "strong topological invariant" $N_{2\mathrm{D}}=N_{1\mathrm{D}}(k_y=0)N_{1\mathrm{D}}(k_y=\pi)$, with $N_{1\mathrm{D}}[k_y=0(\pi)]$ the 1D topological invariant defined for the $k_y=0(\pi)$ system, respectively. This topological invariant is robust to disorder and is equivalent to the one described by Eq. (9).

V. SUMMARY AND MORE DISCUSSION

In summary, we have presented the criteria for TRI topological superconductivity in the physical dimensions one, two, and three. When the Fermi surfaces are nondegenerate, the criteria are very simple. In three dimensions, the winding number is an integer which is determined by the sign of pairing order parameter and the Chern number of the Fermi surfaces. In one and two dimensions, a pairing around the Fermi surface is nontrivial if there are an odd number of Fermi surfaces with a negative pairing order parameter. We also obtained an explicit formula for the Z_2 invariants applicable to generic 1D and 2D TRI superconductors. Our results provide simple and physical criteria that can be used in the search for topological superconductors. Our FSTI's suggest to search for topological superconductors in the nonconventional superconductors with strong inversion symmetry breaking and strong correlation. The strong inversion symmetry breaking is necessary to generate spin-split Fermi surfaces and strong electron-electron Coulomb interactions prefer the pairing to have a nonuniform sign in the Brillouin zone.[24]

ACKNOWLEDGMENTS

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APPENDIX A: BACKGROUND AND DERIVATION OF THE BdG HAMILTONIAN

We first list some basic properties of time-reversal-invariant superconductors in generic dimensions and then go on to derive the form of Eq. (1) from the main text. Consider a general TRI superconductor with the Hamiltonian

$$H=\sum_{\mathbf{k}}\left[\psi_{\mathbf{k}}^\dagger h_{\mathbf{k}}\psi_{\mathbf{k}}+\frac{1}{2}(\psi_{\mathbf{k}}^\dagger\Delta_{\mathbf{k}}\psi_{-\mathbf{k}}^{\dagger T}+\mathrm{H.c.})\right]$$
$$\equiv\sum_{\mathbf{k}}(\psi_{\mathbf{k}}^\dagger,\psi_{-\mathbf{k}}^T)H(\mathbf{k})\begin{pmatrix}\psi_{\mathbf{k}}\\ \psi_{-\mathbf{k}}^{\dagger T}\end{pmatrix} \quad (A1)$$

with

$$H(\mathbf{k})=\begin{pmatrix}h(\mathbf{k}) & \Delta(\mathbf{k})\\ \Delta^\dagger(\mathbf{k}) & -h^T(-\mathbf{k})\end{pmatrix}. \quad (A2)$$

The normal-state Hamiltonian $h(\mathbf{k})$ is time-reversal invariant, which means there is a matrix $\mathcal{T}$ satisfying

$$\mathbb{T}^{-1}\psi_{\mathbf{k}}\mathbb{T}=\mathcal{T}^\dagger\psi_{-\mathbf{k}},\quad \mathcal{T}^\dagger h_{\mathbf{k}}\mathcal{T}=h_{-\mathbf{k}}^T,\quad \mathcal{T}=-\mathcal{T}^T,\quad \mathcal{T}^\dagger\mathcal{T}=\mathbb{I}. \quad (A3)$$

From the transformation property of $\psi_{\mathbf{k}}$ we can obtain

$$\mathbb{T}^{-1}\psi_{\mathbf{k}}^\dagger\mathbb{T}=\psi_{-\mathbf{k}}^\dagger\mathcal{T} \quad (A4)$$

so that

$$\mathbb{T}^{-1}\begin{pmatrix}\psi_{\mathbf{k}}\\ \psi_{-\mathbf{k}}^{\dagger T}\end{pmatrix}\mathbb{T}\equiv\begin{pmatrix}\mathcal{T}^\dagger & \\ & \mathcal{T}^T\end{pmatrix}\begin{pmatrix}\psi_{\mathbf{k}}\\ \psi_{-\mathbf{k}}^{\dagger T}\end{pmatrix}=\begin{pmatrix}\mathcal{T}^\dagger & \\ & -\mathcal{T}\end{pmatrix}\begin{pmatrix}\psi_{\mathbf{k}}\\ \psi_{-\mathbf{k}}^{\dagger T}\end{pmatrix} \quad (A5)$$

and the time-reversal symmetry of the Hamiltonian requires

$$T^\dagger H(\mathbf{k})T=H(-\mathbf{k})^T$$

with

$$T=\begin{pmatrix}\mathcal{T} & \\ & -\mathcal{T}^\dagger\end{pmatrix}. \quad (A6)$$

On the other hand, the following identity:

$$\begin{pmatrix}\psi_{\mathbf{k}}\\ \psi_{-\mathbf{k}}^{\dagger T}\end{pmatrix}^\dagger=\begin{pmatrix} & \mathbb{I}\\ \mathbb{I} & \end{pmatrix}\begin{pmatrix}\psi_{-\mathbf{k}}\\ \psi_{\mathbf{k}}^{\dagger T}\end{pmatrix} \quad (A7)$$

requires the particle-hole symmetry of the BdG Hamiltonian,

$$C^{\dagger}H(\mathbf{k})C = -H(-\mathbf{k})^T$$

with

$$C = \begin{pmatrix} & \mathbb{I} \\ \mathbb{I} & \end{pmatrix}. \tag{A8}$$

The two symmetries [Eqs. (A6) and (A8)] require the pairing matrix $\Delta(\mathbf{k})$ to satisfy

$$\Delta(\mathbf{k}) = -\Delta^T(-\mathbf{k}), \quad (\mathcal{T}\Delta^{\dagger}(\mathbf{k}))^{\dagger} = \mathcal{T}\Delta^{\dagger}(\mathbf{k}). \tag{A9}$$

If we define

$$\chi = iTC^{\dagger} = \begin{pmatrix} & i\mathcal{T} \\ -i\mathcal{T}^{\dagger} & \end{pmatrix}, \tag{A10}$$

then we have

$$\chi^{\dagger}H(\mathbf{k})\chi = CT^{\dagger}H(\mathbf{k})TC^{\dagger} = CH(-\mathbf{k})^TC^{\dagger} = -H(\mathbf{k}). \tag{A11}$$

The "chirality operator" χ can be diagonalized by

$$\chi = V^{\dagger}\begin{pmatrix} \mathbb{I} & \\ & -\mathbb{I} \end{pmatrix}V$$

with

$$V = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathbb{I} & -\mathbb{I} \\ \mathbb{I} & \mathbb{I} \end{pmatrix}\begin{pmatrix} \mathbb{I} & \\ & -i\mathcal{T} \end{pmatrix}. \tag{A12}$$

To derive Eq. (1) from the main text we transform the basis to the eigenbasis of χ to get the Hamiltonian form

$$\widetilde{H}(\mathbf{k}) = VH(\mathbf{k})V^{\dagger} = \begin{pmatrix} & h_{\mathbf{k}} + i\mathcal{T}\Delta_{\mathbf{k}}^{\dagger} \\ h_{\mathbf{k}} - i\mathcal{T}\Delta_{\mathbf{k}}^{\dagger} & \end{pmatrix}. \tag{A13}$$

As is mentioned in main text, the matrix $A_{\mathbf{k}} = h_{\mathbf{k}} + i\mathcal{T}\Delta_{\mathbf{k}}^{\dagger}$ can be decomposed by SVD

$$A_{\mathbf{k}} \equiv h_{\mathbf{k}} + i\mathcal{T}\Delta_{\mathbf{k}}^{\dagger} = U_{\mathbf{k}}^{\dagger}D_{\mathbf{k}}V_{\mathbf{k}} \tag{A14}$$

in which $D_{\mathbf{k}}$ is a diagonal matrix with nonnegative real diagonal components and $U_{\mathbf{k}}$ and $V_{\mathbf{k}}$ are unitary. The Hamiltonian $\widetilde{H}(\mathbf{k})$ can be diagonalized as

$$\widetilde{H}(\mathbf{k}) = \begin{pmatrix} & U_{\mathbf{k}}^{\dagger}D_{\mathbf{k}}V_{\mathbf{k}} \\ V_{\mathbf{k}}^{\dagger}D_{\mathbf{k}}U_{\mathbf{k}} & \end{pmatrix}$$

$$= \begin{pmatrix} U_{\mathbf{k}}^{\dagger} & \\ & V_{\mathbf{k}}^{\dagger} \end{pmatrix}\begin{pmatrix} & D_{\mathbf{k}} \\ D_{\mathbf{k}} & \end{pmatrix}\begin{pmatrix} U_{\mathbf{k}} & \\ & V_{\mathbf{k}} \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}}\begin{pmatrix} U_{\mathbf{k}} & U_{\mathbf{k}} \\ -V_{\mathbf{k}}^{\dagger} & V_{\mathbf{k}}^{\dagger} \end{pmatrix}\begin{pmatrix} D_{\mathbf{k}} & \\ & -D_{\mathbf{k}} \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} U_{\mathbf{k}}^{\dagger} & -V_{\mathbf{k}} \\ U_{\mathbf{k}}^{\dagger} & V_{\mathbf{k}} \end{pmatrix}. \tag{A15}$$

Thus we see that the eigenvalues of the Hamiltonian are given by the eigenvalues of $D_{\mathbf{k}}$ and $-D_{\mathbf{k}}$. For a gapped Hamiltonian, all the eigenvalues of D_k are positive so that we can adiabatically deform $D_{\mathbf{k}}$ to $\mathbb{I}$, which deforms the Hamiltonian to the form

$$\widetilde{H}(\mathbf{k}) \simeq \begin{pmatrix} & Q_{\mathbf{k}} \\ Q_{\mathbf{k}}^{\dagger} & \end{pmatrix}, \quad Q_{\mathbf{k}} \equiv U_{\mathbf{k}}^{\dagger}V_{\mathbf{k}} \in \mathrm{U(N)}. \tag{A16}$$

It can be seen from the derivation above that $Q_{\mathbf{k}}$ is uniquely determined by the BdG Hamiltonian $H_{\mathbf{k}}$, up to a $\mathbf{k}$-independent $\mathrm{U(N)}\times\mathrm{U(N)}$ rotation

$$Q_{\mathbf{k}} \to gQ_{\mathbf{k}}h, \quad g,h \in \mathrm{U(N)}. \tag{A17}$$

All physical information carried by $Q_{\mathbf{k}}$, such as the topological invariants, is insensitive to this global $\mathrm{U(N)}\times\mathrm{U(N)}$ rotation.

APPENDIX B: DETAILED DERIVATION OF THE 3D FERMI-SURFACE FORMULA

In this section we will show the detailed calculation of the 3D Fermi-surface formula. Beginning with the generic form of the winding number in 3D we will show how to derive Eq. (6) from the main text. The general formula for the integer-valued topological number is

$$N_W = \frac{1}{24\pi^2}\int d^3\mathbf{k}\,\epsilon^{ijk}\,\mathrm{Tr}[Q_{\mathbf{k}}^{\dagger}\partial_iQ_{\mathbf{k}}Q_{\mathbf{k}}^{\dagger}\partial_jQ_{\mathbf{k}}Q_{\mathbf{k}}^{\dagger}\partial_kQ_{\mathbf{k}}]. \tag{B1}$$

First of all, if $\Delta_{\mathbf{k}}=0$ for some region of $\mathbf{k}$, the winding number density vanishes in that region. To see that, notice that for $\Delta_{\mathbf{k}}=0$, $Q_{\mathbf{k}}$ is an adiabatic deformation of $A_{\mathbf{k}}=h_{\mathbf{k}}$ so that $Q_{\mathbf{k}}$ is Hermitian and $Q_{\mathbf{k}}^2=Q_{\mathbf{k}}^{\dagger}Q_{\mathbf{k}}=\mathbb{I}$. Consequently the winding number density is given by

$$\rho_W = \frac{1}{24\pi^2}\epsilon^{ijk}\,\mathrm{Tr}[Q_{\mathbf{k}}\partial_iQ_{\mathbf{k}}Q_{\mathbf{k}}\partial_jQ_{\mathbf{k}}Q_{\mathbf{k}}\partial_kQ_{\mathbf{k}}]. \tag{B2}$$

By making use of $\partial_i(Q_{\mathbf{k}}^2)=Q_{\mathbf{k}}\partial_iQ_{\mathbf{k}}+\partial_iQ_{\mathbf{k}}Q_{\mathbf{k}}=0$, i.e., $\{Q_{\mathbf{k}},\partial_iQ_{\mathbf{k}}\}=0$, one can prove that $\rho_W=0$. This confirms our statement that in the weak pairing limit, when only the pairing around Fermi surfaces is considered, the topological invariant N_W is completely determined by the physics in the neighborhood of the Fermi surfaces.

As discussed in Eq. (4) of the main text, in the weak pairing limit $Q_{\mathbf{k}}$ can be written as

$$Q_{\mathbf{k}} = \sum_n e^{i\theta_{n\mathbf{k}}}|n,\mathbf{k}\rangle\langle n,\mathbf{k}| \tag{B3}$$

with $e^{i\theta_{n\mathbf{k}}}=(\epsilon_{n\mathbf{k}}+i\delta_{n\mathbf{k}})/|\epsilon_{n\mathbf{k}}+i\delta_{n\mathbf{k}}|$ and $\delta_{n\mathbf{k}}=\langle n,\mathbf{k}|\mathcal{T}\Delta_{\mathbf{k}}^{\dagger}|n,\mathbf{k}\rangle$. To the leading order, near the Fermi surface we have

$$e^{i\theta_{n\mathbf{k}}} \simeq \frac{v_F(k_{\perp}-k_F)+i\delta_{nk_F}}{\sqrt{v_F^2(k-k_F)^2+\delta_{nk_F}^2}}. \tag{B4}$$

In the limit $\delta_{nk_F}\to 0$, we have

$$\lim_{\delta_{nk_F}\to 0}\theta_{n\mathbf{k}} \to \pi\,\mathrm{sgn}(\delta_{nk_F})\eta(k_F-k_{\perp}) \tag{B5}$$

with $\eta(x)$ the step function satisfying $\eta(x)=1$, $x\geq 0$ and $\eta(x)=0$, $x<0$. Thus we obtain

$$\partial_{k_{\perp}}\theta_{n\mathbf{k}} = -\pi\,\mathrm{sgn}(\delta_{n\mathbf{k}})\delta(k_{\perp}-k_F). \tag{B6}$$

In the vector form, this equation can be written as Eq. (5) of the main text,

$$\nabla\theta_{n\mathbf{k}} = -\pi\mathbf{v}_{n\mathbf{k}}\,\mathrm{sgn}(\delta_{n\mathbf{k}})\delta(\epsilon_{n\mathbf{k}}). \tag{B7}$$

Now we simplify the winding number formula by using Eq. (B3). After some algebra we obtain

$$N_W = \frac{i}{2\pi^2}\int d^3k\sum_{n,s}\epsilon^{ijk}\Bigg[\partial_i\theta_n\left(a_j^{ns}\sin\frac{\theta_{ns}}{2}\right)\left(a_k^{sn}\sin\frac{\theta_{sn}}{2}\right) - \frac{2i}{3}\sum_p\left(a_i^{pn}\sin\frac{\theta_{pn}}{2}\right)\left(a_j^{ns}\sin\frac{\theta_{ns}}{2}\right)\left(a_k^{sp}\sin\frac{\theta_{sp}}{2}\right)\Bigg], \tag{B8}$$

where $\theta_{ns}=\theta_n-\theta_s$ and $a_i^{ns}=-i\langle n,\mathbf{k}|\partial_i|s,\mathbf{k}\rangle$ is the non-Abelian adiabatic connection. When we restrict the pairing to an energy shell $-\epsilon<\epsilon_{n\mathbf{k}}<\epsilon$ and take the $\epsilon\to 0$ limit, the only nonvanishing term is the one with $\partial_i\theta_n$ which has a δ function on the Fermi surface. This leads to

$$\begin{aligned}N_W &= -\frac{i}{2\pi^2}\int_{FS} d^2\mathbf{k}_\parallel\int_{k_F-\epsilon/v_F}^{k_F+\epsilon/v_F} dk_\perp\sum_{n,s}\partial_\perp\theta_n\sin^2\frac{\theta_{ns}}{2}(a_1^{ns}a_2^{sn}-a_2^{ns}a_1^{sn})\\ &= -\frac{i}{2\pi^2}\int_{FS} d^2\mathbf{k}_\parallel\sum_{n,s}\left[\int d\theta_\beta\sin^2\frac{\theta_n-\theta_s}{2}\right](a_1^{ns}a_2^{sn}-a_2^{ns}a_1^{sn})\\ &= -\frac{i}{2\pi^2}\int_{FS} d^2\mathbf{k}_\parallel\sum_{n,s}\frac{\theta_n-\sin(\theta_n-\theta_s)}{2}\Bigg|_{\theta_n^-}^{\theta_n^+}(a_1^{ns}a_2^{sn}-a_2^{ns}a_1^{sn}),\end{aligned} \tag{B9}$$

where $\theta_n^{\pm}$ are the values of θ_n right outside and inside the Fermi surface, respectively. When there is only one band that crosses the Fermi surface, $\theta_n^+=\theta_n^-$ for all other bands. Labeling the single band crossing the Fermi surface with $n=0$, we have

$$N_W = -\frac{i}{2\pi^2}\int_{FS} d^2\mathbf{k}_\parallel\sum_{s\neq 0}\frac{\theta_0-\sin(\theta_0-\theta_s)}{2}\Bigg|_{\theta_0^-}^{\theta_0^+}(a_1^{0s}a_2^{s0}-a_2^{0s}a_1^{s0}). \tag{B10}$$

Since $\theta_0^{\pm}$ and θ_s all have the values 0 or π, the second term $\sin(\theta_0-\theta_s)$ vanishes, and we have

$$\begin{aligned}N_W &= -\frac{i}{4\pi^2}\int_{FS} d^2\mathbf{k}_\parallel\sum_{s\neq 0}\Delta\theta_0(a_1^{0s}a_2^{s0}-a_2^{0s}a_1^{s0})\\ &= \frac{1}{4\pi}\sum_{FS}\mathrm{sgn}(\delta_{s\mathbf{k}})\int_{FS} d^2\mathbf{k}_\parallel(\partial_1a_2^{00}-\partial_2a_1^{00})\\ &= \frac{1}{2}\sum_s\mathrm{sgn}(\delta_s)C_{1s}.\end{aligned} \tag{B11}$$

It should be noted that (i) the superconducting gap on the Fermi surface is given by $|\delta_{n\mathbf{k}}|$ so that $\mathrm{sgn}(\delta_{n\mathbf{k}})$ is the same for all the $\mathbf{k}$ on the same Fermi surface, otherwise the superconducting gap would vanish for some $\mathbf{k}$. (ii) The Chern number of the sth Fermi surface C_{1s} is defined with the normal vector along the direction of $\mathbf{v}_F$, which is opposite for an electron pocket and a hole pocket.

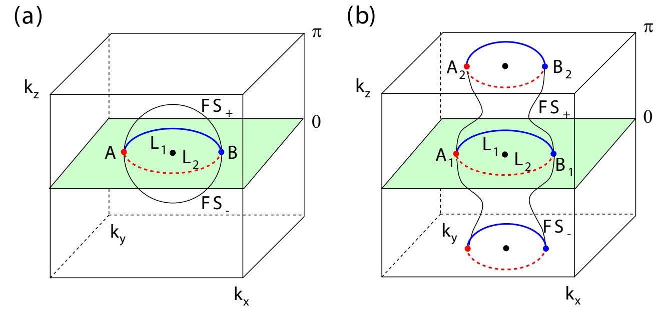

FIG. 4. (Color online) (a) Schematic picture of a Fermi surface enclosing one TRI point (0,0,0). The Fermi surface is separated to two parts FS_+ and FS_- by $k_z=0$ plane. The interface between the two parts is further split into curves L_1 (red dashed curve) and L_2 (blue curve) which are time-reversal partners of each other. The interface of L_1 and L_2 are given by points A and B. (b) Schematic picture of a Fermi surface enclosing two TRI points (0,0,0) and $(0,0,\pi)$. Similar to (a), the Fermi surface is separated to FS_+ and FS_-, and the interface between FS_+ and FS_- is split into L_1 (red dashed curve) and L_2 (blue curve), which intersect at two pairs of points A_1, B_1 and A_2, B_2.

APPENDIX C: PROOF OF CHERN-NUMBER PROPERTIES USED IN THE DIMENSIONAL REDUCTION TO 2D

In the main text, we have used the following two properties of the Fermi-surface Chern number to obtain the 2d Z_2 formula: (1) the Chern number of each Fermi surface satisfies $(-1)^{C_{1s}}=(-1)^{m_s}$, where m_s is the number of TRI points enclosed by the sth Fermi surface. (2) The net Chern number of all Fermi surfaces vanishes, $\Sigma_s C_{1s}=0$. In this section, we will prove both properties.

1. Proof of property 1

We first study a simple Fermi surface enclosing one TRI point, e.g., the Γ point, as shown in Fig. 4(a). Denote the states at the Fermi level as $|s,\mathbf{k}\rangle$. The Berry phase gauge potential is defined by $a_i^{ss}=-i\langle s,\mathbf{k}|\partial_i|s,\mathbf{k}\rangle$. In the following, we will denote $a_i=a_i^{ss}$ for simplicity. The time-reversal invariance of the normal-state Hamiltonian $h_\mathbf{k}$ requires the time-reversed state $T(|s,\mathbf{k}\rangle)$ to also be on the Fermi surface. When the bands are nondegenerate on the Fermi surface, in general, we have

$$T(|s,\mathbf{k}\rangle) = e^{i\varphi_\mathbf{k}}|s,-\mathbf{k}\rangle \tag{C1}$$

$$\begin{aligned}\Rightarrow a_i(-\mathbf{k}) &= -i\langle s,-\mathbf{k}|\frac{\partial}{\partial(-k_i)}|s,-\mathbf{k}\rangle\\ &= iT(\langle s,\mathbf{k}|)e^{i\varphi_\mathbf{k}}\partial_i[e^{-i\varphi_\mathbf{k}}T(|s,\mathbf{k}\rangle)]\\ &= \partial_i\varphi_\mathbf{k} + i(\langle s,\mathbf{k}|\partial_i(|s,\mathbf{k}\rangle))^*\\ &= \partial_i\varphi_\mathbf{k} + a_i(\mathbf{k}).\end{aligned} \tag{C2}$$

Thus the gauge curvature is

$$f_{ij}(\mathbf{k}) = \partial_i a_j(\mathbf{k}) - \partial_j a_i(\mathbf{k}) = -f_{ij}(-\mathbf{k}). \quad \text{(C3)}$$

We denote the upper half of the Fermi surface with $k_z \geq 0$ as FS_+ and the lower half as FS_-. Thus

$$C_{1s} = \frac{1}{2\pi}\int_{FS} d\Omega^{ij} f_{ij}(\mathbf{k}) = \frac{1}{2\pi}\int_{FS_+} d\Omega^{ij} f_{ij}(\mathbf{k}) + \frac{1}{2\pi}\int_{FS_-} d\Omega^{ij} f_{ij}(\mathbf{k}).$$

Since the two form $d\Omega^{ij}$ denoting the normal direction of the Fermi surface is also odd in $\mathbf{k}$, the contributions of FS_+ and FS_- to the Chern number are equal so that

$$C_{1s} = \frac{1}{\pi}\int_{FS_+} d\Omega^{ij} f_{ij}(\mathbf{k}). \quad \text{(C4)}$$

Since FS_+ is a manifold with boundary, the Chern form is equivalent to a boundary integral,

$$C_{1s} = \frac{1}{\pi}\oint_{\partial FS_+} dl^i a_i(\mathbf{k}) \quad \text{(C5)}$$

in which ∂FS_+ is the boundary of FS_+, i.e., the $k_z=0$ section of the Fermi surface and dl^i is the tangent vector to ∂FS_+. However, it should be noted that Eq. (C5) holds only if $a_i(\mathbf{k})$ is continuous in the whole FS_+. In a generic gauge transformation $a_i(\mathbf{k}) \to a_i(\mathbf{k}) + \partial_i \phi_{\mathbf{k}}$ on the boundary ∂FS_+, the right-hand side of Eq. (C5) can change by an even number,

$$\frac{1}{\pi}\oint_{\partial FS_+} dl^i a_i(\mathbf{k}) \to \frac{1}{\pi}\oint_{\partial FS_+} dl^i a_i(\mathbf{k}) + \frac{1}{\pi}\oint_{\partial FS_+} dl^i \partial_i \phi_{\mathbf{k}} = \frac{1}{\pi}\oint_{\partial FS_+} dl^i a_i(\mathbf{k}) + 2n, \quad n \in \mathbb{N}. \quad \text{(C6)}$$

Thus we have

$$C_{1s} = \frac{1}{\pi}\oint_{\partial FS_+} dl^i a_i(\mathbf{k}) \bmod 2 \quad \text{(C7)}$$

in a generic gauge choice.

Since the section $k_z=0$ of the Fermi surface is also symmetric under time reversal, we can split it to two parts L_1 and L_2, which are the time reverse of each other, as shown in Fig. 4(a). Noticing that the tangential vector dl^i is opposite for $\mathbf{k}$ and $-\mathbf{k}$, and by making use of Eq. (C2) we have

$$\oint_{L_1} dl^i a_i(\mathbf{k}) = -\oint_{L_2} dl^i a_i(\mathbf{k}) - \oint_{L_2} dl^i \partial_i \varphi_{\mathbf{k}}$$

$$\Rightarrow C_{1s} = \frac{1}{\pi}\oint_{\partial FS_+} dl^i a_i(\mathbf{k}) = \frac{1}{\pi}\left(\oint_{L_1} + \oint_{L_2}\right) dl^i a_i(\mathbf{k}) = -\frac{1}{\pi}\oint_{L_2} dl^i \partial_i \varphi_{\mathbf{k}}. \quad \text{(C8)}$$

One can always split the boundary so that there are only two points A and B on the interface between L_1 and L_2. Due to time-reversal symmetry, the two points must be the time-reversed partners of each other and the formula above becomes

$$C_{1s} = -\frac{1}{\pi}(\varphi_A - \varphi_B) \bmod 2 \quad \text{(C9)}$$

Denote the momentum of A and B as $\mathbf{k}_A$ and $\mathbf{k}_B = -\mathbf{k}_A$, according to the definition Eq. (C1) we have

$$T(|s,\mathbf{k}_A\rangle) = e^{i\varphi_A}|s,\mathbf{k}_B\rangle,$$

$$T(|s,\mathbf{k}_B\rangle) = e^{i\varphi_B}|s,\mathbf{k}_A\rangle$$

$$\Rightarrow T[T(|s,\mathbf{k}_A\rangle)] = T(e^{i\varphi_A}|s,\mathbf{k}_B\rangle) = e^{-i\varphi_A}e^{i\varphi_B}|s,\mathbf{k}_A\rangle. \quad \text{(C10)}$$

On the other hand, we have $T^2=-1$ for each state so that

$$e^{i(\varphi_A - \varphi_B)} = -1 \Rightarrow C_{1s} = 1 \bmod 2 \quad \text{(C11)}$$

Thus we have proved that $(-1)^{C_{1s}} = (-1)^{m_s} = -1$ for $m_s = 1$.

For the Fermi surfaces enclosing more TRI points, as shown in Fig. 4(b), the proof is similar. Due to the time-reversal symmetry, we can always reduce the Chern number to an integral over the upper half of the Fermi surface FS_+ as in Eqs. (C4) and (C5). Generically, FS_+ has two boundaries at $k_z=0$ and $k_z=\pi$ so that

$$C_{1s} = \frac{1}{\pi}\int_{FS_+} d\Omega^{ij} f_{ij}(\mathbf{k}) = \frac{1}{\pi}\left(\oint_{\partial_\pi FS_+} - \oint_{\partial_0 FS_+}\right) dl^i a_i(\mathbf{k}), \quad \text{(C12)}$$

where $\partial_{0,\pi} FS_+$ stands for the boundary of FS_+ at $k_z=0$ and $k_z=\pi$, respectively. In the same way as above, the boundary at $k_z=0$ can each be separated into two parts L_1 and L_2, with several pairs of interface points A_i, B_i, $i=1,2,\ldots,p_0$. By the same derivation as above one can prove $\varphi_{A_i} - \varphi_{B_i} = \pi \bmod 2\pi$ and

$$\frac{1}{\pi}\oint_{\partial_0 FS_+} dl^i a_i(\mathbf{k}) = -\frac{1}{\pi}\sum_{i=1}^{p} (\varphi_{A_i} - \varphi_{B_i}) = p_0 \bmod 2. \quad \text{(C13)}$$

The same argument works for the $k_z=\pi$ boundary. Denoting the number of interface points at the $k_z=\pi$ boundary by p_π, we have

$$C_{1s} = p_\pi - p_0 \bmod 2. \quad \text{(C14)}$$

If the boundary $\partial_{0,\pi} FS_+$ encloses $m_{0,\pi}$ number of TRI points, respectively, we have $p_0 = m_0 \bmod 2$, $p_\pi = m_\pi \bmod 2$. Thus

$$(-1)^{C_{1s}} = (-1)^{p_\pi - p_0} = (-1)^{m_\pi + m_0} = (-1)^{m_s} \quad \text{(C15)}$$

with $m_s = m_\pi + m_0$ the total number of TRI points enclosed by the Fermi surface. Thus we have proved the property 1.

2. Proof of property 2

To prove property 2, we take a simple s-wave pairing

$$\Delta_{\mathbf{k}} = \Delta_0 \mathcal{T} \tag{C16}$$

with Δ_0 a real number. For such a pairing the matrix $A_{\mathbf{k}} = h_{\mathbf{k}} + i\mathcal{T}\Delta_{\mathbf{k}}^\dagger = h_{\mathbf{k}} + i\Delta_0 \mathbb{I}$ so that the pairing on all the Fermi surfaces has the same sign,

$$\delta_s = \langle s,\mathbf{k}|\mathcal{T}\Delta_{\mathbf{k}}^\dagger|s,\mathbf{k}\rangle = \Delta_0, \quad \forall\, s. \tag{C17}$$

Consequently, the topological invariant in the weak pairing limit is given by

$$N_W(\Delta_0) = \frac{1}{2}\sum_s \text{sgn}(\delta_s) C_{1s} = \frac{\text{sgn}(\Delta_0)}{2}\sum_s C_{1s}. \tag{C18}$$

On the other hand, the BdG Hamiltonian [Eq. (A13)] for this simple pairing can be diagonalized easily to obtain the eigenvalues

$$E_{n\mathbf{k}}^{\pm} = \pm\sqrt{\epsilon_{n\mathbf{k}}^2 + \Delta_0^2}. \tag{C19}$$

Thus for finite Δ_0, the spectrum of the BdG Hamiltonian is always gapped so that the winding number $N_W(\Delta_0)$ remains invariant for all $\Delta_0 > 0$. Thus we can compute N_W in the limit $\Delta_0 \to +\infty$. The unitary matrix $Q_{\mathbf{k}}$ is given by

$$Q_{\mathbf{k}} = \sum_n |n,\mathbf{k}\rangle \frac{\epsilon_{n\mathbf{k}} + i\Delta_0}{\sqrt{\epsilon_{n\mathbf{k}}^2 + \Delta_0^2}}\langle n,\mathbf{k}|,$$

$$\Rightarrow \lim_{\Delta_0 \to +\infty} Q_{\mathbf{k}} = i\sum_n |n,\mathbf{k}\rangle\langle n,\mathbf{k}| = i\mathbb{I}. \tag{C20}$$

Obviously, the winding number $N_W(\Delta_0 \to +\infty) = 0$ so that $N_W(\Delta_0) = 0$ for any Δ_0. According to Eq. (C18) we have proven property 2,

$$\sum_s C_{1s} = 0. \tag{C21}$$

APPENDIX D: PROPERTIES OF THE 1D Z_2 TOPOLOGICAL INVARIANT [Eq. (11)]

In this section, we will study some basic properties of the Z_2 topological invariant defined in Eq. (11) of the main text and show how it is reduced to the Fermi-surface formula (10) in the weak pairing limit. We start from Eq. (10) of the main text,

$$N_{1d} = \frac{\text{Pf}(\mathcal{T}^\dagger Q_{k=\pi})}{\text{Pf}(\mathcal{T}^\dagger Q_{k=0})}\exp\left(-\frac{1}{2}\int_0^\pi dk\, \text{Tr}[Q_k^\dagger \partial_k Q_k]\right). \tag{D1}$$

First of all, $\mathcal{T}^\dagger Q_k$ is antisymmetric since

$$\mathcal{T}^\dagger h_{\mathbf{k}} \mathcal{T} = h_{-\mathbf{k}}^T,$$

$$\mathcal{T}^\dagger(\mathcal{T}\Delta_{\mathbf{k}}^\dagger)\mathcal{T} = \Delta_{\mathbf{k}}^\dagger \mathcal{T} = -\Delta_{-\mathbf{k}}^{\dagger T}\mathcal{T} = (\mathcal{T}\Delta_{-\mathbf{k}}^\dagger)^T \Rightarrow \mathcal{T}^\dagger Q_k \mathcal{T}$$
$$= Q_{-k}^T \Rightarrow \mathcal{T}^\dagger Q_k = Q_{-k}^T \mathcal{T}^\dagger = -(\mathcal{T}^\dagger Q_{-k})^T. \tag{D2}$$

Thus the Pfaffian is well defined at $k=0$ and $k=\pi$.

Since $Q_k \in \text{U(N)}$, we have $\det Q_k = e^{i\phi_k}$ which is a U(1) phase. Since $\text{Tr}[Q_k^\dagger \partial_k Q_k] = \text{Tr}[\log Q_k] = \log\det Q_k = i\varphi_k$, we have $\int_0^\pi dk\, \text{Tr}[Q_k^\dagger \partial_k Q_k] = i[\varphi(\pi) - \varphi(0)] \bmod 2\pi$ so that

$$\exp\left[-\int_0^\pi dk\, \text{Tr}(Q_k^\dagger \partial_k Q_k)\right] = e^{-i[\varphi(\pi)-\varphi(0)]} = \frac{\det(\mathcal{T}^\dagger Q_{k=0})}{\det(\mathcal{T}^\dagger Q_{k=\pi})}. \tag{D3}$$

Thus

$$N_{1d}^2 = \frac{\det(\mathcal{T}^\dagger Q_{k=\pi})}{\det(\mathcal{T}^\dagger Q_{k=0})}\exp\left(-\int_0^\pi dk\, \text{Tr}[Q_k^\dagger \partial_k Q_k]\right) \equiv 1 \tag{D4}$$

so that N_{1d} always takes the value of ± 1.

Now we show that N_{1d} is a topological invariant. For an infinitesimal deformation $Q_k > Q_k' = Q_k + \delta Q_k$, the phase factor $\exp(-\frac{1}{2}\int_0^\pi dk\, \text{Tr}[Q_k^\dagger \partial_k Q_k])$ only depends on the deformation of Q_k at $k=0$ and π,

$$\exp\left[-\frac{1}{2}\int_0^\pi dk\, \text{Tr}(Q_k'^\dagger \partial_k Q_k')\right]$$
$$= \exp\left[-\frac{1}{2}\int_0^\pi dk\, \text{Tr}(Q_k^\dagger \partial_k Q_k)\right] e^{-i/2[\delta\varphi(\pi)-\delta\varphi(0)]}. \tag{D5}$$

On the other hand, the change in Pfaffian is given by

$$\text{Pf}(\mathcal{T}^\dagger Q_{k=0,\pi}') = e^{i/2\,\delta\varphi_{k=0,\pi}}\,\text{Pf}(\mathcal{T}^\dagger Q_{k=0,\pi}'). \tag{D6}$$

Consequently, we see that $\delta N_{1d} = 0$ in any smooth deformation of the unitary matrix $Q_{\mathbf{k}}$ as long as time-reversal symmetry is preserved.

In the weak pairing limit, the general formula (D1) can be reduced to the Fermi-surface formula given by Eq. (10) of the main text. In the weak pairing limit, assume there are M Fermi points k_s, $s = 1, 2, \ldots, M$ between 0 and π. As discussed in the main text, we require that the Fermi level does not cross any band at $k=0$ or π. As discussed in Fig. 1 of the main text, each Fermi point leads to a domain wall of θ_{sk} for the corresponding band s crossing the Fermi level. According to Eq. (B3) in the weak pairing limit we have

$$\det Q_k = \exp\left(i\sum_n \theta_{nk}\right). \tag{D7}$$

Across each Fermi point k_{Fs}, the phase θ_{sk} will jump by $-\pi\,\text{sgn}(v_{Fs}\delta_{sk_s})$ and the θ_{nk} for other bands remain invariant. It should be noted that the sign of v_F enters the expression since the winding of θ_{sk} is given by $-\pi\,\text{sgn}(\delta_{sk_s})$ *along the direction of the Fermi velocity* v_{Fs}. Consequently, the phase $\log\det Q_k = i\Sigma_n \theta_{nk}$ is changed by $-i\pi\,\text{sgn}(v_{Fs}\delta_{sk_s})$ across the sth Fermi point and the net change in $\log\det Q_k$ from 0 to π is given by

$$\int_0^\pi dk\partial_k \log \det Q_k = -i\pi\sum_{s=1}^{M} \text{sgn}(v_F\delta_{sk_s})$$

$$\Rightarrow \exp\left[-\frac{1}{2}\int_0^\pi dk\, \text{Tr}(Q_k^\dagger \partial_k Q_k)\right] = \prod_s e^{-i\pi/2\,\text{sgn}(v_{Fs}\delta_{sk_s})} \equiv \prod_s [-i\,\text{sgn}(v_{Fs}\delta_{sk_s})] = \prod_s [\text{sgn}(\delta_{sk_s})]\prod_s [-i\,\text{sgn}(v_{Fs})]. \quad \text{(D8)}$$

When there are m Fermi points with positive v_{Fs} and n Fermi points with negative v_{Fs}, $n-m$ gives the number of bands which are above the Fermi level at $k=0$ but below the Fermi level at $k=\pi$. If we denote $N_2(0)$ and $N_2(\pi)$ as the number of bands occupied at $k=0$ and $k=\pi$, respectively, then $n-m = N_2(\pi)-N_2(0)$. Since all bands are paired in Kramers pairs at $k=0, \pi$, $N_2(0)$, and $N_2(\pi)$ must be even. Thus we have

$$\prod_s [-i\,\text{sgn}(v_{Fs})] = (-i)^m i^n = e^{i/2\pi(n-m)} = (-1)^{N_2(\pi)-N_2(0)/2}. \quad \text{(D9)}$$

Now we study the Pfaffian $\text{Pf}(\mathcal{T}^\dagger Q_{k=0,\pi})$. Since we have assumed the Fermi level does not cross the bands at $k=0, \pi$, in the weak pairing limit we have $\Delta_{k=0,\pi}=0$. If the normal-state Hamiltonian h_k is diagonalized to

$$h_k = U_k^\dagger \begin{pmatrix} \epsilon_1(k) & & \\ & \cdots & \\ & & \epsilon_N(k) \end{pmatrix} U_k. \quad \text{(D10)}$$

Q_k can be obtained by

$$Q_k = U_k^\dagger \begin{pmatrix} \mathbb{I}_{N_1\times N_1} & \\ & -\mathbb{I}_{N_2\times N_2} \end{pmatrix} U_k \quad \text{(D11)}$$

in which N_1 and N_2 are the number of unoccupied and occupied bands, respectively. The Pfaffian $\text{Pf}(\mathcal{T}^\dagger Q_k)$ can be obtained as

$$\text{Pf}(\mathcal{T}^\dagger Q_k) = \text{Pf}\left[\mathcal{T}^\dagger U_k^\dagger \begin{pmatrix} \mathbb{I}_{N_1\times N_1} & \\ & -\mathbb{I}_{N_2\times N_2} \end{pmatrix} U_k\right] = \text{Pf}\left[U_k^{\dagger T}\mathcal{T}^\dagger U_k^\dagger \begin{pmatrix} \mathbb{I}_{N_1\times N_1} & \\ & -\mathbb{I}_{N_2\times N_2} \end{pmatrix}\right] \cdot \det U_k. \quad \text{(D12)}$$

By making use of the time-reversal-invariance condition $\mathcal{T}^\dagger Q_k \mathcal{T} = Q_{-k}^T$, one can prove that

$$\left[U_k^{\dagger T}\mathcal{T}^\dagger U_k^\dagger \begin{pmatrix} \mathbb{I}_{N_1\times N_1} & \\ & -\mathbb{I}_{N_2\times N_2} \end{pmatrix}\right] = 0 \quad \text{(D13)}$$

for $k=0, \pi$ so that the matrix $U_k^{\dagger T}\mathcal{T}^\dagger U_k^\dagger$ is block diagonal. Consequently, we have

$$\text{Pf}\left[U_k^{\dagger T}\mathcal{T}^\dagger U_k^\dagger \begin{pmatrix} \mathbb{I}_{N_1\times N_1} & \\ & -\mathbb{I}_{N_2\times N_2} \end{pmatrix}\right] = (-1)^{N_2/2}\text{Pf}(U_k^{\dagger T}\mathcal{T}^\dagger U_k^\dagger) = (-1)^{N_2/2}\text{Pf}(\mathcal{T}^\dagger)\cdot \det U_k^\dagger. \quad \text{(D14)}$$

Thus

$$\text{Pf}(\mathcal{T}^\dagger Q_k) = (-1)^{N_2/2}\text{Pf}(\mathcal{T}^\dagger) \quad \text{(D15)}$$

for $k=0, \pi$. It should be noted that the number of occupied bands N_2 is always even for $k=0, \pi$ due to Kramers degeneracy.

Combining Eqs. (D8), (D9), and (D15) we obtain

$$N_{1d} = \prod_s [\text{sgn}(\delta_{sk_s})]. \quad \text{(D16)}$$

Thus we have proved that the general Z_2 invariant [Eq. (11)] in the main text is equivalent to Eq. (10) in the main text in the weak pairing limit.

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