A generic theory for Majorana zero modes in 2D superconductors

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It is well known that non-Abelian Majorana zero modes (MZMs) harbor at vortex cores in a p_x + i p_y topological superconductor, which can be realized in a 2D spin-orbit coupled system with a single Fermi surface and by proximity coupling to an s-wave superconductor. Here we show that existence of non-Abelian MZMs is unrelated to the bulk topology of a 2D superconductor, and propose that such exotic modes can be resulted in much broader range of superconductors, being topological or trivial. For a generic 2D system with multiple Fermi surfaces and gapped out by superconducting pairings, we show that at least a single MZM survives if there are only odd number of Fermi surfaces of which the corresponding superconducting orders have vortices, and such MZM is protected by an emergent Chern-Simons invariant, irrespective of the bulk topology of the superconductor. This result may enrich new experimental schemes for realizing non-Abelian MZMs. In particular, we propose a minimal scheme to realize the MZMs in a 2D superconducting Dirac semimetal with trivial bulk topology, which can be well achieved based on the recent cold atom experiments.

The quest for realization of non-Abelian Majorana zero modes (MZMs), driven by the pursuit of both fundamental physics and their potential application to fault-tolerant topological quantum computation [1, 2], has been spearheaded by the developments in p-wave superconductors. Early studies predicted that MZMs exist in ν = 5/2 fractional quantum Hall state [3], at the vortex cores in 2D spinless p_x + i p_y topological superconductors (SCs) [4], and at ends of a 1D p-wave SC [5]. More recently, it has been proposed that the hybrid systems of s-wave SC and spin-orbit (SO) coupled matters with odd number of Fermi surfaces (FSs) can favor effective p-wave pairing states, bringing the realization of MZMs to realistic solid state experiments [6–15]. Motivated by these proposals, numerous experimental studies have been performed to observe Majorana induced zero bias conductance anomalies with different heterostructures formed by s-wave SCs and semiconductor nanowires [16–19], magnetic chains [20], or topological insulators [21–23].

By far the experimental proposals for MZMs are built on the realization of topological SCs. Note that MZMs in SCs are topological defect modes [24–27], which correspond to nonlocal extrinsic deformations in the Hamiltonian of the topological system. For example, MZMs in the chiral p_x + i p_y SC harbor at vortices which exhibit nonlocal phase windings of the SC order (a global deformation in the original uniform Hamiltonian). This feature tells that the MZMs at vortices are not intrinsic topological excitations, but extrinsic modes of a SC. In this regard, one may conjecture that the existence of MZMs is not uniquely corresponding to the bulk topology of a SC, and there might be much broader range of experimental systems which can host such exotic modes, besides those based on topologically nontrivial SCs.

In this Letter, we show that the existence of MZMs localized in the vortex cores does not rely on the bulk topology of a 2D SC, with which we further propose a minimal experimental scheme to realize MZMs in a 2D system. For a generic 2D normal system with N FSs and gapped out by SC pairings. We show that the existence of the MZMs at the SC vortices is characterized by an emergent $\mathbb{Z}_2$ Chern-Simons invariant $\nu_3$:

$$\nu_3 = \sum_i n_i w_i \mod 2,$$

where $\Delta_{Q_i}(k)$ is the SC order projected onto the $i$-th FS and is generically momentum dependent, $w_i$ counts the phase winding of $\Delta_{Q_i}(k)$ in the $k$-space around the $i$-th FS loop, and $n_i$ denotes the integer vortex winding number (vorticity) attached to $\Delta_{Q_i}$, $\Delta_{Q_i} \rightarrow \Delta_{Q_i} e^{i n_i \theta}$, A single MZM is protected when the index $\nu_3 = 1$, while the bulk of the SC, characterized by Chern number if having no symmetry protection, can be topologically trivial. We then propose a minimal experimental scheme to realize MZMs based on a 2D superconducting Dirac semimetal whose bulk is topologically trivial. The doped 2D Dirac semimetals are topological metals with strong spin-orbit coupling and possess two FSs which can be fully gapped out by a two-component pairing density wave (PDW) SC order, rendering a trivial 2D superconducting phase with zero Chern number. However, we find that a protected MZM is obtained in the half-vortex regime, namely, only one of two SC order components in the PDW phase is attached with a single vortex, giving a nonzero $\nu_3$ index. The proposed 2D SO coupled Dirac semimetal can be well achieved with the recent cold atom experiments.

Generic theory. We start with the proof of the generic theorem given in Eq. (1) for the Chern-Simons invariant, which governs the existence of the MZM in a 2D (class D) superconductor. For a system with multiple normal bands and FSs, the superconducting pairings may occur within each FS (intra-FS pairings) and between different
FSs (inter-FS pairings). As we shall discuss later, the theorem (1) is not affected by inter-FS pairings. Thus for convenience, we consider below the generic SC Hamiltonian with only intra-FS pairings, given by

$$H = \sum_k C_k^\dagger \hat{H}_0 C_k + \sum_{i,k} \epsilon_{Q_i, +k} \hat{\Delta}_{Q_i} \epsilon_{Q_i, -k} + h.c., \quad (2)$$

where $C_k = (c_{\alpha k, \beta}, c_{\beta k, \gamma}, \cdots, c_{\gamma k, \alpha})^T$, with $\alpha$ incorporating the band and spin indices, the normal band Hamiltonian $\hat{H}_0(k)$ is considered to have $N$ FSs, and the pairing matrix element $\hat{\Delta}_{Q_i}(k) \propto (c_{Q_i/2+\mathbf{k}, \alpha} c_{Q_i/2-\mathbf{k}, \beta})$ regarding the $i$-th FS has a central-of-mass momentum $\mathbf{Q}_i$. Here for convenience we take that each FS is circular and centered at a momentum $\mathbf{Q}_i/2$. Note that we can always continuously deform the FSs to be circular without changing topology of the system, as long as the bulk gap keeps open during the deformation. In general the SC order exhibits spatial modulation in the real space, rendering the PDW or Fulde-Ferrell-Larkin-Ovchinnikov SC order exhibits spatial modulation in the real space, $\mathbf{Q}_i$, and the trace is performed on the filled bands.

To compute the Chern-Simons invariant $\nu_3$ which is defined in 3D space, we parameterize the Bogoliubov de Gennes (BdG) Hamiltonian by taking the phase $\phi \in [0, 2\pi)$ of the SC order $\hat{\Delta}_{Q_i} e^{-i\phi}$ as a synthetic dimension of ring geometry $S^1$. Together with the 2D physical space, the bulk BdG Hamiltonian can then be written down in a synthetic 3D torus $T^3 = T^2 \times S^1$ spanned by $(\mathbf{k}, \phi)$. In the synthetic 3D space, the $Z_2$ Chern-Simons invariant [24, 30–32] can be calculated by

$$\nu_3 = -\frac{1}{4\pi^2} \int_{T^2 \times S^1} Q_3 \text{mod } 2 \quad (3)$$

$$Q_3 = \text{Tr} \left[ A_i^3 \right],$$

where the elements of one-form Berry connection are given by $A_i^\lambda(\mathbf{k}, \phi) = i\langle \psi_i | d\psi_i \rangle$, with $| \psi_i \rangle$ denoting the corresponding eigenvector of the BdG Hamiltonian, and the trace is performed on the filled bands.

A direct computation of the index $\nu_3$ for the generic case is not realistic. To simplify the study we shall take the advantage that the topology of the system is unchanged under any kind of continuous deformation without closing bulk gap. For this we further adiabatically deform the Hamiltonian $H$ to a new form $H' \equiv H[\hat{\Delta}_{Q_i} \rightarrow \hat{\Delta}_{Q_i} \cos \Theta_{S_i}(\mathbf{k})]$, where $\Theta_{S_i}(\mathbf{k})$ is a positive real smooth truncation function with $\hat{\Delta}_{Q_i}(\mathbf{S}_i) = 1$ inside the orientable vector area $\mathbf{S}_i$ enclosed by the $i$-th FS loop centered at $\mathbf{Q}_i$, and decays to zero at a short distance beyond this area. Since the system remains fully gapped for the continuous deformation, the invariant $\nu_3$ can be evaluated over $H'$. Denoting by $\hat{F}_i$ the vector area with $\Theta_{S_i}(\mathbf{k}) \neq 0$, It is straightforward to show that the invariant given in Eq. (3) can be reduced to the integral over the disjoint union $\bigcup_i \hat{F}_i \times S^1$ [32], which facilitates our further study.

While in general the Hamiltonian $\hat{H}_0$ incorporates multiple normal bands, we can consider the weak SC pairing regime, in which case only the states around each FS will be effectively paired up. Ignoring the pairing between a state around FS and that from other bands does not affect the topology of the system. In this way, the BdG $H'$ further reduces to an effective one-band form in the eigen-basis $u_k$ of $\hat{H}_0$. In particular, for the momentum $\mathbf{k} \in \hat{F}_i$ around a specific FS centered at momentum $\mathbf{Q}_i$, the effective BdG Hamiltonian takes the form

$$h_i(\mathbf{k}, \phi) = \left[ \begin{array}{cc} c_{Q_i+k} & \Delta_{Q_i}(\mathbf{k}) \Omega_i e^{-i\phi} \\ \Delta_{Q_i}(\mathbf{k}) \Omega_i e^{+i\phi} & -c_{Q_i-k} \end{array} \right]$$

where $\Delta_{Q_i}(\mathbf{k}) \equiv \langle u_k | \hat{\Delta}_{Q_i} | u^*_{-k} \rangle$ is the pairing term projected onto the $i$-th Fermi surface. Note that $\Delta_{Q_i}(\mathbf{k})$ has captured the original band topology. The eigenstates of $h_i$, take the form $| \psi_{i,k} \rangle = (\alpha_{k\pm} u_k, \beta_{k\pm} u^*_{-k})^T$. Then $\nu_3$ can be decomposed into $\nu_3 = \sum_i \nu_3^{(i)} (\text{"mod } 2^* \text{ temporarily omitted})$, and

$$\nu_3^{(i)} = -\frac{1}{4\pi^2} \int_{\hat{F}_i \times S^1} [\mathbf{A}_\phi \nabla_k \times \mathbf{A}_k + \mathbf{A}_k \times \nabla_k \mathbf{A}_\phi] d\phi d^2k$$

for each $\hat{F}_i$, where $\mathbf{A}_\phi = i\langle \psi_i | \nabla_\phi | \psi_i \rangle$, and $\mathbf{A}_k \equiv (A_{k\pm}, A_{k\pm}^\dagger) = i\langle \psi_i | \nabla_k | \psi_i \rangle$, with $\nabla_k \equiv (\partial_{k\pm}, \partial_{k\pm})$. The above result can be further simplified by taking the limit $\Delta_{Q_i} \rightarrow 0^+$, in which case the gap becomes infinitesimal at the Fermi surface, and the contribution to $\nu_3$ will completely come from the FS states. It can be derived directly on $\hat{F}_i$ that $\mathbf{A}_{\phi} = -n_i \Theta_{S_i}$ and $\mathbf{A}_k = (1 - 2\Theta_{S_i}) \mathbf{A}_{0,k} + \Theta_{S_i} (\nabla_k \arg \Delta_{Q_i} + \mathbf{A}_{0,k}^\dagger)$, where $\Theta_{S}$ is a step function equal to 1 within $S_i$ and 0 otherwise, $\mathbf{A}_{0,k} = i u_k \nabla_k u_k$ represents the Berry connection for the normal band, and $\mathbf{A}_{0,k}^\dagger$ is the defect gauge field as a consequence of the multivalueness of $\arg \Delta_{Q_i}$ [32, 33]. Substituting these results into the formula of $\nu_3$ yields

$$\nu_3 = \sum_i \frac{n_i}{2\pi} \int_{\hat{F}_i} \Theta_{S_i} \nabla_k \times (\nabla_k \arg \Delta_{Q_i} + \mathbf{A}_{0,k}^\dagger) \cdot d^2k. \quad (5)$$

The above result is exactly the one given in Eq. (1) by observing that the curl of gradient of SC phase vanishes, while the contribution from the defect gauge field $\mathbf{A}_{0,k}^\dagger$ renders the phase winding of SC order in the momentum space around FS loop [32]. This completes the proof. The theorem is still valid if the system has dominant pairing between two different FSs, while then the phase winding of the inter-FS pairing has to be computed in both FSs simultaneously, contributing a trivial number to $\nu_3$. 
The above result shows that the existence of MZMs at vortex cores is essentially protected not by the bulk topology of the 2D SC, but by an emerging Chern-Simons invariants \( \nu_3 \), implying that a non-Abelian MZM can exist in a trivial SC. A famous example can be obtained from a Rashba spin-orbit coupled semiconductor with Zeeman splitting and in proximity to a conventional \( s \)-wave SC \([8, 9]\). To obtain a chiral topological SC the chemical potential has to lie within the Zeeman gap and cross the bulk band for once. According to the theorem shown here, even the chemical potential is above the Zeeman gap and crosses two FSs, MZMs can in principle be generated if the SC orders in the two FSs are independent and only one of them is attached with vortex.

2D Dirac metal.—The theorem in (1) suggests that MZMs can exist in broader range of physical systems. In the following we propose a minimal scheme, which can be readily achieved based on a recent cold atom experiment \([34, 35]\), for the realization of MZMs. The Hamiltonian takes the form

\[
H_0 = \sum_k \left( c_{k\uparrow}^\dagger c_{k\downarrow} \right) H_0 \left( c_{k\uparrow} c_{k\downarrow}^\dagger \right) \tag{6}
\]

\[
H_0 = \left( m_z - 2t_x \cos k_x - 2t_y \cos k_y \right) \sigma_z + 2t_{so} \sin k_x \sigma_x - \mu,
\]

where \( c_{k\sigma} (c_{k\sigma}^\dagger) \) is annihilation (creation) operator with spin \( \sigma = \uparrow, \downarrow \), \( t_{x,y} \) is the spin-conserved hopping along \( x/y \) direction, \( t_{so} \) is the spin-flip hopping amplitude, \( m_z \) denotes the effective Zeeman coupling, and \( \mu \) is the chemical potential. The Hamiltonian in Eq. (6) describes a topological Dirac metal for \(|m_z| < 2(t_x + t_y)\), with two Dirac points at \( Q_k = (0, 0) \pm \left( \pm \frac{\pi}{3} \right) \) and possesses non-trivial spin texture on the Fermi surfaces (Fig. 1). Note that here the 2D Dirac metal is driven by spin-orbit interaction, and is distinct from graphene, of which the Dirac points are protected by symmetry only if spin-orbit coupling is absent \([36]\).

Superconducting phase diagram \& MZM.—With the above model, the superfluid (superconductor) states can be studied by considering an attractive Hubbard interaction. The total Hamiltonian is \( H = H_0 - U \sum_n n_{\uparrow}^n n_{\downarrow}^n \) for \( U > 0 \). For the multiple Fermi surfaces corresponding to various Dirac cones, generically one shall consider both the inter-cone (BCS) and the intra-cone (PDW) pairing orders, described by \( \Delta_{2Q} = U/N \sum_k \left( c_{k\uparrow} c_{k\downarrow} \right) \), with \( Q = \pm \frac{\pi}{3} \) or \( 0 \) \([35, 37–39]\) and \( N \) is total number of lattice sites. Generally, the order parameter in real space takes the form

\[
\Delta(r) = \Delta_0 + \Delta_{2Q_+} e^{2iQ_+ r} + \Delta_{2Q_-} e^{2iQ_- r}
\]

and the BCS and PDW orders may compete with each other. Owing to the different spin-momentum lock at the Fermi surfaces of the two Dirac cones [Fig. 1 (b)], the inter-cone BCS pairing cannot fully gap out the bulk spectrum, and leaves four nodal points. On the other hand, the intra-cone PDW order can fully gap the bulk in the expense of reducing the translation symmetry. The two types of orders may compete to dominate in different parameter regimes.

The phase diagram are obtained by self-consistent calculation with proper parameters so that the Dirac points are located at \( Q_{\pm} = \left( 0, \pm \frac{2\pi}{3} \right) \) (see more details in the Supplementary Material \([32]\), as shown in Fig. 2. It can be found that the BCS pairing is generically suppressed and only the PDW phase with equal magnitude of \( |\Delta_{2Q_{\pm}}| \) exists. With increasing chemical potential, the Dirac cone becomes less isotropic (Fig. 1) and the Fermi surfaces are less well-nested. As a consequence, a narrow gapless region with nonzero PDW orders \( |\Delta_{2Q_{\pm}}| \neq 0 \) is obtained for \( \mu > 0.05 \) [Fig. 2(a)], while the spectrum becomes fully gapped when \( |\Delta_{2Q_{\pm}}| \) increases exceeding

Figure 1. (a) The band structure of 2D topological Dirac metal with two Dirac points located at \( Q_{\pm} \), the gray thick loops around two Dirac points represent the Fermi surfaces, and the color represents the average value of the spin component \( \langle s_z \rangle \). (b) Schematic of the spin orientations, shown by blue arrows, at the Fermi surfaces around the Dirac points. Parameters: \( t_{x,y} = t_{so} = m_z = 1 \) and the corresponding Dirac node momenta \( Q_{\pm} = -Q_{\pm} = (0, 2\pi/3) \).

Figure 2. (a) Mean field phase diagram of the Dirac-Hubbard Hamiltonian versus attractive Hubbard interaction \( U \) and chemical potential \( \mu \). The BCS order is always suppressed and \( \Delta_{2Q} = 0 \). In the "Dirac metal" phase, all \( \Delta_{2Q} = 0 \); in the narrow "Gapless" region, \( \Delta_{2Q_{\pm}} \) are finite but not strong enough to fully gap the system. In the "PDW" phase, the system is fully gapped; (b) Magnitude of PDW order \( \Delta_{2Q_{\pm}} \). The parameters for numerics are the same as those in Fig. 1.
with two unit vorticities of opposite vorticities.

In Fig. 3 (a,c) we consider the half vortex regime.

The physical origin of the existence of MZMs can be viewed as a direct consequence of bulk-boundary correspondence, as illustrated in Fig. 3(b). Consider the region far away enough form the vortex core so that at each azimuthal angle $\phi$ we can find a microscopic large region with approximately constant SC phase $\theta$. This region can be thought of as a 2D system in $(r, k_{||}; \phi)$ with fixed $\phi = \theta$, periodic boundary along $k_{||}$ direction and open boundary along $r$ direction. Combining all such 2D systems with $\phi \in [0, 2\pi)$ yields an effective 3D space with periodic boundary with respect to $k_{||}$ and $\phi$, while open boundary along $r$ axis due to the existence of vortex. With this picture when the parameterized 3D system has a nontrivial Chern-Simons invariant $\nu_3$, which is the case for half-vortex regime based on a direct numerical check, MZM is obtained as a boundary zero mode at the vortex core.

In conclusion, we have developed a generic theory for MZM modes at the vortex cores in 2D superconductors. Our results show that the MZMs are generically protected by an emerging Chern-Simons invariant which can be nontrivial even the bulk of the superconductor is topologically trivial. The result that existence of MZMs is unrelated to the superconducting bulk topology enriches broader range of experimental systems to host non-Abelian MZMs, in particular for the Dirac materials which have even number of Fermi surfaces. As a minimal experimental scheme based on a trivial superconductor/superfluid, we have proposed to realize non-Abelian MZMs with a SO coupled 2D Dirac semimetal which can be fullled gapped out by PDW pairing orders. The protected MZMs have been shown to exist in the half-vortex regime.

Such a Dirac semimetal system can be readily realized with the recent cold atom experiment [34, 35]. While in the present study we have focused on the MZMs without symmetry protection, it is of great interests to generalize the present theory to the superconductors with protection by symmetry, like time reversal, mirror, or other symmetries.

**Note added**: In completing the present manuscript, we are informed of another interesting work by Z. Yan et al., which presents a different model for the realization of MZMs in a trivial 2D superconductor [41].

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In this Supplementary Material we provide the details on the selfconsistent mean field study and the proof of the Chern-Simons invariant. With the PDW orders, the original Brillouin zone (BZ) will be folded up into sub-BZ. In the present study, we choose $Q_\pm$ for PDW orders. With the PDW orders, the original Brillouin zone (BZ) will be folded up into sub-BZ. In the present study, we choose $Q_+ = -Q_- = (0, 2\pi/3)$, so the folded BZ is 1/3 of the original BZ, and the mean field Hamiltonian can be written as

$$H_{MF} = \frac{1}{2} \sum_k \Psi^\dagger_k H_{MF}(k) \Psi_k,$$

Supplementary Material:
A generic theory for Majorana zero modes in 2D superconductors

In this Supplementary Material we provide the details on the selfconsistent mean field study and the proof of the Chern-Simons invariant.
\[ H_{\text{MF}}(k) = \begin{bmatrix} \hat{H}_0(k) & \hat{\Delta}(k) \\ \hat{\Delta}^\dagger(k) & -\hat{H}_0^T(-k) \end{bmatrix}, \]  

(\text{S1})

where the basis for the folded BZ is denoted as

\[ \Psi_k = (c_{Q_\uparrow} + k^\uparrow, c_{Q_\uparrow} - k^\uparrow, (\uparrow \to \downarrow); c_{Q_\downarrow}^\dagger - k^\uparrow, c_{Q_\downarrow}^\dagger + k^\uparrow, c_{Q_\uparrow}^\dagger - k^\uparrow)^T, \]

with \( k_x \in [-\pi, \pi) \) and \( k_y \in [-\pi/3, \pi/3) \). The explicit form of \( \hat{H}_0(k) \) is obtained by restricting the momentum of the 2D topological Dirac metal Hamiltonian \( \hat{H}_0(k) = (m_c - 2t_x \cos k_x - 2t_y \cos k_y)\sigma_z + 2t_{so} \sin k_x \sigma_x - \mu \) within a sub-BZ. The order parameter \( \hat{\Delta} \) in the matrix form reads

\[ \hat{\Delta} = \begin{bmatrix} \Delta_{Q_\uparrow} & \Delta_{Q_\downarrow} \\ -\Delta_{Q_\downarrow} & \Delta_{Q_\uparrow} \end{bmatrix}, \]

(\text{S2})

with

\[ \Delta_{Q} = \begin{bmatrix} \Delta_{2Q_\uparrow} & \Delta_{2Q_\downarrow} & \Delta_0 \\ \Delta_{2Q_\downarrow} & \Delta_0 & \Delta_{2Q_\uparrow} \\ \Delta_0 & \Delta_{2Q_\uparrow} & \Delta_{2Q_\downarrow} \end{bmatrix}. \]

Utilizing Eq. (S1) and Eq. (S2), one can iteratively solve the Hamiltonian and compute \( \Delta_{2\nu} \)'s until convergence. The mean field phase diagram versus attractive interaction strength \( U \) and chemical potential \( \mu \) are shown in Fig. 2 in the main text.

**S-2. Derivations for the Generic Reduced Formula of the Chern-Simons Invariant**

Now we are going to prove that, for a 2D superconductor with vortices, the Chern-Simons invariant \( \nu_3 \) [24, 30, 31] defined in the base space \( (k_x, k_y, \phi) \in T^2 \times S^1 \), with \( \phi \) denoting the emergent dimension for vorticity,

\[ \nu_3 = -\frac{1}{4\pi^2} \int_{T^2 \times S^1} Q_3 \mod 2, \]

\[ Q_3 = \text{Tr} \left[ AdA - \frac{2i}{3} A^3 \right], \]

where \( A_{\lambda\lambda'}(k, \phi) = i\langle \psi_{\lambda'} | d\psi_{\lambda} \rangle \) is the one-form Berry connection (\( | \psi_{\lambda} \rangle \) is the corresponding eigenvector of the Hamiltonian, and the trace is performed on the filled bands), takes the following simple form

\[ \nu_3 = \frac{1}{2\pi} \sum_i n_i \oint_{\partial S_i} \nabla_k \text{arg} \Delta_{Q_i}(k) \cdot dk \mod 2, \]

where the orientable area \( S_i \) denotes the region enclosed by the \( i \)-th Fermi surface \( (\partial S_i = FS_i \text{ in the main text}) \), \( \Delta_{Q_i} \) is the superconductor order parameter projected onto the \( i \)-th Fermi surface, and \( n_i \) denotes the integer vortex winding number attached to \( \Delta_{Q_i} \).

For a general BdG Hamiltonian

\[ H = \sum_{k \in T^2} C_k^\dagger \hat{H}_0(k) C_k + \sum_{i, k} c_{Q_\uparrow}^\dagger + k^\uparrow, \hat{\Delta}_{\alpha}^{\alpha \beta} c_{Q_\downarrow}^\dagger - k^\uparrow, c_{Q_\uparrow}^\dagger - k^\uparrow + h.c., \]

where \( C_k = (c_{\alpha, k}, c_{\beta, k}, \cdots, c_{\gamma, k}, \cdots)^T \), with \( \alpha \) incorporating the band and spin indices. Suppose that the normal band Hamiltonian \( \hat{H}_0(k) \) has multiple bands \( \epsilon_n(k) \), and only one of such bands, with (normalized) eigenvector \( u_k \), cuts the chemical potential, and we call this band middle band. The middle band gives rise to \( N \) Fermi surfaces with possible Berry phases, and \( \Delta_{Q_i} \) are pairing terms that can fully gap the whole system. The following results can be easily generalized to the system with multiple middle bands.

We assume that each Fermi surface is circular and centered at some momentum \( Q_i/2 \), otherwise one can always continuously deform the original Hamiltonian to the current form without gap closing. One can imagine that each Fermi surface is equipped with a PDW order parameter \( \Delta_{Q_i} \), and we further assume that the system is fully gapped
only if all the $\hat{\Delta}_Q$'s are non-vanishing. Here we consider some of $\hat{\Delta}_Q$'s acquire a winding $\hat{\Delta}_Q \rightarrow \hat{\Delta}_Q e^{-i n_i \phi}$ with $\phi \in [0,2\pi)$ and $n_i \in \mathbb{Z}$. Together with the 2D physical space, the bulk BdG Hamiltonian can then be written down in a synthetic 3D torus $T^3 = T^2 \times S^1$ spanned by $(k, \phi)$.

Consider a continuous deformation $H \rightarrow H'$, with $H' = H[\hat{\Delta}_Q, \hat{\Delta}_Q(x, \Omega^Q_i(x))]$, where $\Omega^Q_i(x)$ is a positive real smooth truncation function with $\Omega^Q_i(x) \equiv 1$, and decays to zero at a short distance from the Fermi surface, as shown in Fig. S1(a). We denote the region with $\Omega^Q_i(x) \neq 0$ as $\mathcal{F} = \bigsqcup_i \mathcal{F}_i$ (disjoint union of $N$ orientable areas $\mathcal{F}_i$) and $\mathcal{F} = T^2 - \mathcal{F}$, note that $\mathcal{S}_i \subset \mathcal{F}_i$, as shown in Fig. S1(b). Since the whole system remains fully gapped for a continuous deformation $H \rightarrow H'$, we have ("mod 2" temporarily omitted)

$$\nu_3 = -\frac{1}{4\pi^2} \int_{T^2 \times S^1} Q_3[H] = -\frac{1}{4\pi^2} \int_{T^2 \times S^1} Q_3[H'].$$

One can easily see that

$$\int_{\mathcal{F} \times S^1} Q_3[H'] = 0,$$

since in the region $\mathcal{F}$, $A_\phi = 0$ and $\partial_\phi A_{k_x,k_y} = 0$, then $\text{Ad}A = \text{Tr}[A_k (\partial_{k_x} A_\phi - \partial_{k_y} A_\phi) + A_k (\partial_\phi A_{k_x} - \partial_{k_y} A_\phi)] dk_x \wedge dk_y \wedge d\phi = 0$, also $A^3 \sim \text{Tr}[A_k A_{k_x} A_\phi - A_{k_x} A_k A_\phi] dk_x \wedge dk_y \wedge d\phi = 0$, hence,

$$\nu_3 = -\frac{1}{4\pi^2} \sum_i \int_{\mathcal{F}_i \times S^1} Q_3[H'].$$

While in general the Hamiltonian $\tilde{H}_0$ incorporates multiple normal bands, we can consider the weak SC pairing regime, in which case only the states around each Fermi surface will be effectively paired up. Ignoring the pairing between a state around the Fermi surface and that from other bands does not affect the topology of the system. In this way, the BdG $H'$ further reduces to an effective one band Hamiltonian projected to the middle band. For $\mathcal{F}_i$, the effective BdG Hamiltonian takes the form

$$h_{Q_i}(k, \phi) = \begin{bmatrix} \epsilon_{Q_i+k} & \Delta_{Q_i}(k) \Omega_{Q_i}(k) e^{i \phi} \\ \Delta_{Q_i}^*(k) \Omega_{Q_i}(k) e^{-i \phi} & -\epsilon_{Q_i-k} \end{bmatrix},$$

where $\Delta_{Q_i} \equiv \langle u_{k} | \hat{\Delta}_Q | u^*_{-k} \rangle$ is the superconductor order parameter projected onto the $i$-th Fermi surface. Furthermore, in each $\mathcal{F}_i$, only one $\Delta_{Q_i}$ is non-vanishing and captures the Berry curvature in the corresponding $\mathcal{F}_i$ only, so the Chern-Simons invariant $\nu_3$ can be written as a sum of the corresponding "Chern-Simons invariant" in different $\mathcal{F}_i$. Since
$A_{k_x,k_y,\phi}$ are local functions of $(k_x, k_y, \phi)$, and for effective only one band, $A_{k_x,k_y,\phi}$ are just numbers, hence $A^3 = 0$, thus we can decompose $\nu_3$ as

$$\nu_3 = \frac{-1}{4\pi^2} \sum_i \int_{\tilde{F}_i \times S^1} Q_3[h_Q(k, \phi)] = \frac{-1}{4\pi^2} \sum_i \int_{\tilde{F}_i \times S^1} A dA[h_Q_i].$$

In this case, the Chern-Simons invariant reduces to the Hopf invariant that captures the linking number of the inverse images of two points in the target space $S^2$ of $h_Q(k, \phi)$.

For brevity, we consider below a particular $\tilde{F} = \tilde{F}_i$ for some $i$ and ignore the subscript $i$. To proceed, one needs the eigenvectors of $h_Q(k, \phi)$. In the original basis, the eigenvectors for the middle band are of the form $|\psi_k\rangle = (\alpha_{k} \pm u_k, \beta_{k} \pm u^*_{-k})^T$, where $\alpha_{k} \pm u_{k}, \beta_{k} \pm u^*_{-k}$ are the eigenvectors of $h_Q(k, \phi)$ written in the eigen-basis. For $h_Q(k, \phi)$, there are nonetheless two choices of eigenvectors (without normalization),

$$\left(\frac{\alpha_{+k,\pm}}{\beta_{+k,\pm}}\right) \propto \left(\frac{\xi_k + \sqrt{\xi_k^2 + |\Delta_Q(k)\Omega_Q(k)|^2}}{\Delta^*_Q(k)\Omega_Q(k)e^{i\phi}}\right)$$

(S3)

or

$$\left(\frac{\alpha_{-k,\pm}}{\beta_{-k,\pm}}\right) \propto \left(\frac{-\xi_k + \sqrt{\xi_k^2 + |\Delta_Q(k)\Omega_Q(k)|^2}}{\Delta^*_Q(k)\Omega_Q(k)e^{i\phi}}\right),$$

(S4)

where $\xi_k \equiv \frac{\epsilon_Q + k + \Omega_k}{2}$. One can check that both of them are the eigenvectors of $h_Q(k, \phi)$. Actually, for Fermi surfaces, there are two cases with $\xi_k > 0$ or $\xi_k < 0$ inside the region $\tilde{S}$. For these two different cases, we choose different eigenvector, i.e., Eq. (S3) for $\xi_k > 0$ and Eq. (S4) for $\xi_k < 0$.

The Berry connections are $A_{\eta} = i\langle \psi_k | \partial_{\eta} | \psi_k \rangle$, with $\eta = x, y, \phi$, or explicitly

$$A_{\pm,\phi} = i(\alpha_{\pm, k} \pm u^T_k, \beta_{\pm, k} \pm u^*_{-k}) \partial_{\phi} \left(\begin{array}{c} \alpha_{\pm, k} - u_k \\ \beta_{\pm, k} - u^*_{-k} \end{array}\right) = \begin{cases} i\beta_{+k} \partial_{\phi} \beta_{+k} &= -n|\beta_{+k}|^2 \Delta_Q^{\to 0} - n\Theta_S, \quad \text{for} \quad \xi_k > 0 \text{ in } \tilde{S}, \\ i\alpha^*_{-k} \partial_{\phi} \alpha_{-k} &= +n|\alpha_{-k}|^2 \Delta_Q^{\to 0} + n\Theta_S, \quad \text{for} \quad \xi_k < 0 \text{ in } \tilde{S}. \end{cases}$$

$$A_{\pm, k} = (A_{\pm, k_x}, A_{\pm, k_y}) = i(\alpha_{\pm, k} \pm u^T_k, \beta_{\pm, k} \pm u^*_{-k}) \nabla_k \left(\begin{array}{c} \alpha_{\pm, k} - u_k \\ \beta_{\pm, k} - u^*_{-k} \end{array}\right) = i|\alpha_{\pm, k}^2 - |\beta_{\pm, k}^2|| u_k \nabla_k u_k + i(\alpha_{\pm, k}^2 \nabla_k u_{\pm, k} + \beta_{\pm, k}^2 \nabla_k u_{\pm, k}) = \pm(1 - 2\Theta_S)A_{0,k} + A_{\pm,1,k},$$

here we have used the trick $\Delta_Q \rightarrow 0$ without closing the bulk gap, the upper (lower) sign means $\xi_k > 0$ ($\xi_k < 0$) inside the region $\tilde{S}$, $\Theta_S \equiv \Theta(\xi_k > 0)$ ($\Theta(\xi_k < 0)$) for the case $\xi_k > 0$ ($\xi_k < 0$), and denotes the step function is 1 inside the region $\tilde{S}$ and 0 else, and $\nabla_k \equiv (\partial_{k_x}, \partial_{k_y})$. In the last line, we denote $A_{0,k} \equiv iu_k \nabla_k u_k$, and

$$A_{\pm,1,k} \equiv i(\alpha_{\pm, k} \nabla_k \alpha_{\pm, k} + \beta_{\pm, k} \nabla_k \beta_{\pm, k}) = \pm \frac{\Delta_Q \Omega_Q \nabla_k (\Delta_Q \Omega_Q) - \Delta^*_Q \Omega_Q \nabla_k (\Delta^*_Q \Omega_Q)}{4\sqrt{\xi_k^2 + \Omega_Q^2 |\Delta_Q|^2}} \frac{\Delta_Q^{\to 0} \pm i\Theta_S}{2|\Delta_Q \Omega_Q|^2}.$$

Let’s denote $\vec{v} = \frac{\Delta_Q \Omega_Q \nabla_k (\Delta^*_Q \Omega_Q) - \Delta^*_Q \Omega_Q \nabla_k (\Delta_Q \Omega_Q)}{2|\Delta_Q \Omega_Q|^2}$, direct substitution of $\Delta_Q = \Delta_k e^{i\theta_k}$ seems to give $\vec{v} = \nabla_k \theta_k$. But note that $\theta_k$ is a multivalued field, for a general SC order parameter with phase winding $m$, there will be a branch cut from $2\pi m \rightarrow 0$. Consider the region close to the branch cut, $\theta_k$ behaves like $2\pi m \Theta$, where $\Theta$ is a step function, so the correct result should be [33]

$$\vec{v} = \nabla_k \theta_k + A_d,$$
where the vector field $A_d$ is the defect gauge field compensating for the discontinuity in $\theta_k$ and the properties are

$$
\nabla_k \times \nabla_k \theta_k = 0,
$$

(S5)

$$
\oint_{\partial S} \nabla_k \theta_k \cdot dk = 2\pi m,
$$

(S6)

$$
\nabla_k \times A_d = 2\pi m \delta(k) \cdot \hat{z} = \nabla_k \theta_k \cdot dk,
$$

(S7)

$$
\oint_{\partial S} A_d \cdot dk = \begin{cases} 0 & \text{if $\partial$ avoids the branch cut} \\ 2\pi m & \text{otherwise} \end{cases},
$$

(S8)

where $\partial S$ is the boundary of the region containing the origin. Eq. (S7) is corresponded to the boundary of the branch cut. In order to make these results consistent, the chain rule of differentiation must be modified to

$$
\nabla_k e^{i\theta_k} = i(\nabla_k \theta_k + A_d) e^{i\theta_k}.
$$

Note that $\bar{v}$ is invariant under the gauge transformations

$$
\theta_k \rightarrow \theta_k + \lambda_k, \\
A_d \rightarrow A_d - \nabla_k \lambda_k.
$$

An example is that, for a $p + ip$ SC, the SC order parameter can be expressed as $\Delta = \Delta_k e^{i\phi_k}$, with the azimuthal angle $\phi_k \in [0, 2\pi)$. In this case, the field $\theta_k = \phi_k$ is discontinuous over the positive $k_x$-axis, thus $\nabla_k \theta_k = \hat{\phi}/k - 2\pi \Theta(k_x) \delta(k_y) \hat{k}_y$. Note that we expect $\bar{v} = \hat{\phi}/k$, hence $\bar{v} = \nabla_k \theta_k + A_d$, and $A_d = 2\pi \Theta(k_x) \delta(k_y) \hat{k}_y$.

Now, return to our proof for the Chern-Simons invariant. Consider the defect gauge field, we have

$$
A_{\pm, 1, k} = \pm \Theta_{\bar{S}}(\nabla_k \arg\Delta_Q + A_d).
$$

In our effective one band case, since $A_d A = [A_{k_x}(\partial_{k_x} A_{k_y} - \partial_{k_y} A_{k_x}) + A_{k_y}(\partial_{k_y} A_{k_x} - \partial_{k_x} A_{k_y}) + A_k(\partial_{k_y} A_{k_x} - \partial_{k_x} A_{k_y})] dk_x \wedge dk_y \wedge d\phi$, and $\partial_\phi A_{k_x, k_y} = 0$, one can readily show that

$$
\nu_3 = \sum_i \nu_3^{(i)} \mod 2,
$$

and

$$
\nu_3^{(i)} = -\frac{1}{2\pi} \left( \frac{1}{2\pi} \int_0^{2\pi} d\phi \right) \int_{\mathcal{F}_i} [A_{i, \pm, \phi} \nabla_k \times A_{i, \pm, k} + A_{i, \pm, k} \times \nabla_k A_{i, \pm, \phi}] \cdot d^2 k

= \pm n_i \frac{1}{2\pi} \int_{\mathcal{F}_i} \left[ \Theta_{\bar{S}_i} \nabla_k \times A_{i, \pm, k} + A_{i, \pm, k} \times \nabla_k \Theta_{\bar{S}_i} \right] \cdot d^2 k.
$$

For the part involving $A_{i, 0, k}$, we have

$$
\nu_3^{(i)}[A_{i, 0, k}] = \frac{n_i}{2\pi} \int_{\mathcal{F}_i} \left[ \Theta_{\bar{S}_i} \nabla_k \times [(1 - 2\Theta_{\bar{S}_i}) A_{i, 0, k}] + (1 - 2\Theta_{\bar{S}_i}) A_{i, 0, k} \times \nabla_k \Theta_{\bar{S}_i} \right] \cdot d^2 k

= -\frac{n_i}{2\pi} \int_{\mathcal{F}_i} \left[ \Theta_{\bar{S}_i} \nabla_k \times A_{i, 0, k} - A_{i, 0, k} \times \nabla_k \Theta_{\bar{S}_i} + 2\Theta_{\bar{S}_i} \nabla_k \Theta_{\bar{S}_i} \times A_{i, 0, k} + 2\Theta_{\bar{S}_i} A_{i, 0, k} \times \nabla_k \Theta_{\bar{S}_i} \right] \cdot d^2 k

= -\frac{n_i}{2\pi} \left( \int_{\bar{S}_i} \nabla_k \times A_{i, 0, k} \cdot dk - \int_{\partial \bar{S}_i} A_{i, 0, k} \cdot dk \right).
$$

Since the Chern-Simons invariant is gauge-independent, we can consider a smooth gauge, using the Stokes’ theorem, $\nu_3^{(i)}[A_{i, 0, k}]$ just vanishes.
Next we need to consider for $\pm \Theta S_i (\nabla_k \arg \Delta Q_i + A_{i,d})$, which can be divided into two parts $\pm \Theta S_i A'_i$, with $A'_i = \nabla_k \arg \Delta Q_i$ or $A_{i,d}$.

\[
\nu_3^{(i)}[A'_i] = \frac{n_i}{2\pi} \int_{\mathcal{F}_i} \left[ \Theta S_i \nabla_k \times [\Theta S_i A'_i] + \Theta S_i A'_i \times \nabla_k \Theta S_i \right] \cdot d^2 k
\]

\[
= \frac{n_i}{2\pi} \int_{\mathcal{F}_i} \left[ \Theta S_i \nabla_k \times A'_i + \Theta S_i \nabla_k \Theta S_i \times A'_i + \Theta S_i A'_i \times \nabla_k \Theta S_i \right] \cdot d^2 k
\]

\[
= \frac{n_i}{2\pi} \int_{\mathcal{F}_i} \Theta S_i \nabla_k \times A'_i \cdot d^2 k = \frac{n_i}{2\pi} \int_{\mathcal{S}_i} \nabla_k \times A'_i \cdot d^2 k.
\]

Since $\nabla_k \times \nabla_k \arg \Delta Q_i = 0$, $\nu_3^{(i)[\nabla_k \arg \Delta Q_i]}$ vanishes. Next, by the property (S7) of $A_{i,d}$,

\[
\nu_3^{(i)[A_{i,d}]} = \frac{n_i}{2\pi} \int_{\mathcal{S}_i} \nabla_k \times A_{i,d} \cdot d^2 k = \frac{n_i}{2\pi} \int_{\partial S_i} \nabla_k \arg \Delta Q_i \cdot \delta(k) \cdot d^2 k = \frac{n_i}{2\pi} \int_{\partial S_i} \nabla_k \arg \Delta Q_i \cdot dk.
\]

Note that this is not Stokes’ theorem. Gathering all the results together, we have

\[
\nu_3 = \frac{1}{2\pi} \sum_i n_i \int_{\partial S_i} \nabla_k \arg \Delta Q_i(k) \cdot dk \mod 2.
\]

Note that the pairing $\Delta Q_i(k)$ has captured the band topology. For the case with SC pairings between two different Fermi surfaces, using the similar arguments as in [35], the formula is still applicable. This completes the proof.