Higher-order topological odd-parity superconductors

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The topological property of a gapped odd-parity superconductor is jointly determined by its pairing nodes and Fermi surfaces in normal state. We reveal that the contractibility of Fermi surfaces without crossing any time-reversal invariant momentum and the presence of nontrivial Berry phase on Fermi surfaces are two key conditions for the realization of higher-order topological odd-parity superconductors (HOTOPSCs). When the normal state is a normal metal, we reveal the necessity of removable Dirac pairing nodes and provide a general and simple principle to realize HOTOPSCs. Our findings can not only be applied to analyze the topological property of odd-parity superconductors, but also be used as a guiding principle to design new platforms of higher-order topological superconductors, as well as higher-order topological insulators owing to their direct analogy in Hamiltonian description.

A defining characteristic of topological phases is their bulk-boundary correspondence, namely, a topologically nontrivial bulk will manifest itself through the boundary modes[1]. Recently, higher-order topological insulators (HOTIs) and superconductors (HOTSCs) have attracted considerable interest owing to the emergence of unconventional bulk-boundary correspondence[2–16]. As is known, the boundary modes of conventional topological insulators (TIs) and topological superconductor (TSCs) are located at their one-dimensional lower boundaries[17, 18], however, for an \( n \)-th order TI or TSC with \( n \geq 2 \), its boundary modes are located at its \( n \)-dimensional lower boundaries (accordingly, conventional TIs and TSCs are also dubbed first-order TIs and TSCs, respectively). In two dimensions (2D) and three dimensions (3D), such boundary modes are commonly dubbed corner modes or hinge modes, and have been predicated to exist in quite a few materials[19–24] and observed in a series of platforms, including photonic crystals[25–28], microwave resonators[29], circuit arrays[30], phononic crystals[31–33], bismuth[34], and iron-based superconductors[35]. More recently, these concepts have further been extended to cold atom systems[36, 37], Floquet systems[38–45], as well as non-Hermitian systems[46–51].

The boundary modes of HOTSCs are of particular interest for their potential application in topological quantum computation[52–54]. Thus far, a general approach to realize HOTSCs is "order transition"[55–70], that is, by breaking certain appropriate symmetries, the one-dimensional lower boundary modes will be gapped out in a nontrivial way, and accordingly, the first-order topological phase is transited to a higher-order topological phase. According to this approach, if the starting first-order topological phase is an odd-parity superconductor, to gap out its one-dimensional lower boundary modes, one has to introduce terms of even parity to break certain symmetries[36, 56–59]. This, while suggesting that superconductors with appropriate mixed-parity pairings are candidates of HOTSCs[36, 58], does not mean that odd-parity pairing only can not realize intrinsic HOTSCs. In fact, the authors in ref[58] have demonstrated that a Dirac semimetal with chiral \( p \)-wave pairing provides a realization of second-order TSC in 2D. Nevertheless, a general theory of intrinsic higher-order topological odd-parity superconductors (HOTOPSCs) is still lacking. In particular, we notice that when the normal state is a featureless normal metal, what kind of pairing and Fermi surface structure can realize intrinsic HOTOPSCs has not been explored.

As the topological property of an odd parity superconductor is jointly determined by its pairing nodes and Fermi surfaces in normal state[71, 72], in this work, we investigate the general conditions on pairing nodes and Fermi surfaces for the realization of HOTOPSCs. Our study reveals that there are two key conditions for the realization of HOTOPSCs. One is that the Fermi surfaces can continuously contract to a point without crossing any time-reversal invariant (TRI) momentum, and the other is the presence of nontrivial Berry phase on the Fermi surfaces. Importantly, when the normal state is a normal metal, we reveal the necessity of removable Dirac pairing nodes (RDPNs) and provide a general and simple principle to realize HOTOPSCs.

General theory.— Given \( H = \sum_k \Psi_k^\dagger H(k) \Psi_k \) with \( \Psi_k = (c_k, c_k^\dagger)^T \), the topological property of a superconductor is encoded in \( H(k) \) whose general form is given by

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

where \( \varepsilon(k) \) describes the normal state and \( \Delta(k) \) represents the pairing order parameter. In this work, we focus on inversion symmetric normal states and odd-parity pairings which satisfy \( \Delta(k) = -\Delta(-k) \). Apparently, \( \Delta(k) \) always vanishes at TRI momenta in the Brillouin zone, i.e., momenta satisfy \( k = -k + m \Gamma \) with \( \Gamma \) the reciprocal lattice vector and \( m = 0 \) or 1. This means that the pairing nodes at TRI momenta (TRIPNs) are unmovable and removable. When the normal state is a normal metal, the TRIPNs of a gapped odd-parity superconductor are of Dirac point nature, so when a Fermi surface encloses one TRIPN, it has a nontrivial Berry phase as the pairing order parameter shows a nonzero integer times of winding on it. The presence of nontrivial Berry phase on Fermi surfaces is the origin of nontrivial topology.

In 2D and 3D, it has been demonstrated that if the number of Fermi surfaces enclosing TRI momentum (for TRI systems, the number does not take into account the Kramers degeneracy) is odd, a gapped odd-parity superconductor is a first-
order TSC\cite{71,72}. This implies that to guarantee the first order topological property to be trivial, the Fermi surfaces must be contractible in the sense that it can continuously contract to a point without crossing any TRI momentum. Noteworthily, however, this does not mean that the Fermi surfaces can directly contract to a point without closing the bulk gap as there may exist other Dirac pairing nodes at generic momentum. In fact, as HOTOPSCs are essentially distinct to trivial superconductors in topology, one can conjecture that to realize HOTOPSCs, the presence of nontrivial Berry phase on Fermi surfaces should be necessary. There are two ways to achieve this, one is that the Fermi surfaces enclose Dirac pairing nodes away from TRI momentum, and the other is that the underlying normal state is a topological semimetal for which the band touchings themselves will contribute nontrivial Berry phase, like in ref.\cite{58}. Thus, if the normal state is a normal metal, the existence of Dirac pairing nodes away from TRI momentum should be necessary for realizing HOTOPSCs.

Second-order topological odd-parity superconductors (SOTOPSCs) in 2D.--- In 2D, a novel class of models with odd-parity pairing and trivial Chern number (so trivial first-order topological property) can be constructed by a novel approach called Hopf map\cite{73}. According to this approach, we let

$$H(k) = d_1(k)\tau_1 + d_2(k)\tau_2 + d_3(k)\tau_3 \quad (2)$$

with $d_i(k) = z(k)^\dagger\tau_i z(k)$, where $z_1(k) = f_1(k) + if_2(k)$, $z_2(k) = g_1(k) + ig_2(k)$ and $\tau_{1,2,3}$ are Pauli matrices in particle-hole space. To describe an odd-parity superconductor, we let $f_{1,2}(k)$ be real and even functions of momentum, i.e., $f_1(k) = f_1(-k)$, and let $g_{1,2}(k)$ be real and odd functions of momentum, i.e., $g_1(k) = -g_1(-k)$. It is noteworthy that this choice of $f_i$ and $g_i$ is distinct to the conventional Hopf map\cite{72,77}. A comparison of Eq.(1) and Eq.(2) reveals

$$\Delta(k) = d_1(k) - id_2(k) = 2[f_1(k) + if_2(k)][g_1(k) - ig_2(k)],$$

$$\varepsilon(k) = d_3(k) = f_1^2(k) + f_2^2(k) - g_1^2(k) - g_2^2(k). \quad (3)$$

Before giving concrete expressions to $f_i(k)$ and $g_i(k)$, we make a general discussion about the Hamiltonian above. Clearly, the different parity of $f_i(k)$ and $g_i(k)$ guarantees $\Delta(k) = -\Delta(-k)$, confirming that it describes an odd-parity superconductor. Moreover, according to the expression of $\Delta(k)$ in Eq.(3), one can find that Dirac pairing nodes will show up at generic momentum when $f_1(k) = 0$ and $f_2(k) = 0$ can simultaneously be satisfied. In contrast to TRIMPNs, such Dirac pairing nodes are removable. Focusing on the Fermi surface determined by $\varepsilon(k) = 0$, one can further find that the number of disconnected Fermi surfaces must be even and the removable Dirac pairing nodes (RDPNs), if they exist, are located within the disconnected Fermi surfaces or between two near neighbour disconnected Fermi surfaces (see Fig.1 for a graphic illustration), which guarantees that the Fermi surfaces can not continuously contract to a point without closing the bulk gap. When each disconnected Fermi surface encloses an odd number of Dirac pairing nodes, the presence of nontrivial Berry phase on Fermi surfaces will also be satisfied.

![FIG. 1. Two representative configurations of Fermi surfaces and RDPNs that realize SOTOPSCs in 2D. The circles in black represent the Fermi surfaces, and the dots with different color represent RDPNs with opposite winding number.](image)

While we have infinite choices on $f_i(k)$ and $g_i(k)$, in this work we let

$$f_i(k) = f_i(k_1) = (\cos k_1 + \lambda_i),$$

$$g_i(k) = g_i(k_1) = \sin k_1. \quad (4)$$

Accordingly, we have $d_1(k) = 2\sum_{i=1,2}(\cos k_1 + \lambda_i)\sin k_1$, $d_2(k) = 2(\cos k_1 + \lambda_1)\sin k_2 - 2(\cos k_2 + \lambda_2)\sin k_1$, and $d_3(k) = \sum_{i=1,2}(\cos k_1 + \lambda_i)^2 - \sin^2 k_1$. Meanwhile, the energy spectra are

$$E(k) = \pm \sum_{i=1,2}[(\cos k_1 + \lambda_i)^2 + \sin^2 k_1], \quad (5)$$

one can find that the bulk gap vanishes only when $|\lambda_1| = |\lambda_2| = 1$. As an even-parity term can be taken as a Dirac mass, the presence of two Dirac masses in Eq.(5) guarantees the first-order topological property to be trivial.

According to Eq.(2), when $|\lambda_{1,2}| < 1$, the RDPNs are located at $k = (\pm Q_1, \pm Q_2)$ with $Q_{1,2} = \pi - \arccos \lambda_{1,2}$, and one can find that the configuration of Fermi surfaces and RDPNs belongs to the type shown in Fig.1(a). When $|\lambda_1| = 1$ or $|\lambda_2| = 1$, the RDPNs coincide in pairs and annihilate. Once $|\lambda_1| > 1$ or $|\lambda_2| > 1$, they are removed. For each pairing node, we can assign a winding number to characterize its topological property.

$$w_n = \frac{1}{2\pi} \int dk \frac{d_1 \partial_2 d_2 - d_2 \partial_1 d_1}{d_1^2 + d_2^2} = \frac{1}{2\pi} \int dk \frac{g_1 \partial_2 g_2 - g_2 \partial_1 g_1}{g_1^2 + g_2^2} - \frac{f_1 \partial_2 f_2 - f_2 \partial_1 f_1}{f_1^2 + f_2^2}, \quad (6)$$

where $C$ denotes a closed contour enclosing only one pairing node. As $f_i$ and $g_i$ decouple from each other, this indicates that the creation or annihilation of RDPNs does not affect the topological property of TRIMPNs. Such a property is in fact also crucial for the realization of SOTOPSCs. As a counter example, if we keep the form of $\varepsilon(k)$ and let $\Delta(k) = f_2g_1 + if_1g_2$, while the locations of pairing nodes are same, now all RDPNs have same winding number, consequently the creation or annihilation of RDPNs will directly change the topological property of TRIMPNs since the net
winding number of all Dirac pairing nodes should be zero. For this case, when $|\lambda_{1,2}| < 1$, the Hamiltonian in fact realizes a first-order TSC with large Chern number, instead of a SOTOPSC we want.

To see that the Hamiltonian indeed realizes a SOTOPSC when RDPNs exist, i.e., $|\lambda_{1,2}| < 1$, let us focus on the special case with $\lambda_1 = \lambda_2$ for an intuitive understanding. When $\lambda_1 = \lambda_2 = \lambda$, there are two special lines in the Brillouin zone, $k_1 = k_2$ and $k_1 = -k_2$, on which chiral symmetry is preserved and thus a winding number can be defined. On the $k_1 = k_2$ line (the case with $k_1 = -k_2$ can similarly be analyzed), the Hamiltonian reduces to

$$H_R(q) = d_1(q)\tau_1 + d_3(q)\tau_3,$$  

(7)

where $q$ represents the momentum along the line $k_1 = k_2$, $d_1(q) = 4(\cos q + \lambda_1)\sin q$, and $d_3(q) = 2(\cos q + \lambda_1)^2 - 2\sin^2 q$. The winding number characterizing the topological property of $H_R(q)$ is given by

$$w_R = \frac{1}{2\pi} \int_{-\pi}^{\pi} dq \frac{d_3\partial_4 d_4 - d_1\partial_q d_2}{d_1^2 + d_3^2} = \left\{ \begin{array}{cl} 2, & |\lambda| < 1, \\ 0, & |\lambda| < 1. \end{array} \right.$$  

(8)

The result indicates when $\lambda_1 = \lambda_2$ and $|\lambda_{1,2}| < 1$, the Hamiltonian describes a weak TSC. Accordingly, if the system is of a ribbon geometry and open boundary condition is taken in the $\hat{x}_1 + \hat{x}_2$ (or $\hat{x}_1 - \hat{x}_2$) direction, then gapless modes will show up on the edges. On each edge, the number of left-moving modes and right-moving modes must be equal as the bulk Chern number is zero. As shown in Fig. 2(a), when $|\lambda| < 1$, each edge indeed harbors four left-moving modes and four right-moving modes, confirming the expectation. It is noteworthy that the number of gapless modes is four times the winding number given in Eq. (8), which is because the $d_2$ term has four zeroes along the line $k_1 = -k_2$. As a comparison, if open boundary condition is not along the $\hat{x}_1 + \hat{x}_2$ (or $\hat{x}_1 - \hat{x}_2$) direction, one can expect the absence of gapless edge states. In Fig. 2(b), the result for open boundary condition in the $\hat{x}_1$ direction is presented, which clearly demonstrates the absence of gapless edge states within the energy gap.

The defining characteristic of a SOTOPSC in 2D is the presence of Majorana corner modes (MCMs) [54–59]. By choosing open boundary condition in both the $\hat{x}_1$ and $\hat{x}_2$ directions, we indeed find when $|\lambda| < 1$, each corner of the finite-size system harbors one Majorana zero mode (MZM), as shown in Fig. 2(c). Here the presence of MCMs can intuitively be understood by noting that the $d_2$ term is odd under the mirror reflection about the line $k_1 = k_2$. From a low-energy perspective, this implies that the Dirac mass gapping out the gapless edge modes will have opposite sign if the respective edges are located at different sides of the $\hat{x}_1 + \hat{x}_2$ (or $\hat{x}_1 - \hat{x}_2$) direction. As a result, if the $\hat{x}_1 + \hat{x}_2$ (or $\hat{x}_1 - \hat{x}_2$) direction places in between a corner, the corner is a domain wall of Dirac mass and consequently harbors a MZM. While such an intuitive picture relies on $\lambda_1 = \lambda_2$, the existence of MCMs does not rely on it. Through detailed numerical calculation, we confirm that the MCMs persist as long as $|\lambda_{1,2}| < 1$, so the phase diagram in Fig. 2(d) [78].

Before ending this part, we point out that the SOTOPSC follows a $Z_2$ classification because when two MZMs appear at the same corner, there is no symmetry to protect them from coupling, and so splitting. This implies when there exist many RDPNs and disconnected Fermi surfaces in the Brillouin zone, if the structure of Fermi surfaces and pairing nodes can continuously evolve to the two types of representative configurations given in Fig. 2b without closing the bulk gap, the system realizes a robust SOTOPSC. Furthermore, it is worthy to point out that to the best of our knowledge, Eq. (2) is the first “d · r” model that realizes a second-order TSC (SOTSC) in 2D. If putting two copies of the model together, i.e.,

$$H(k) = d_1(k)\tau_1 s_3 + d_2(k)\tau_2 + d_3(k)\tau_3$$  

(9)

with $s_{1,2,3}$ the Pauli matrices in spin space, one also obtains a minimal-model realization of TRI SOTSCs in 2D.

*SOTOPSCs in 3D.—* The scenario in two dimensions can naturally be generalized to higher dimensions. To see this, we construct the following Hamiltonian,

$$H(k) = \tilde{d}_1(k)\tau_1 s_1 + \tilde{d}_2(k)\tau_1 s_3 + \tilde{d}_3(k)\tau_2 + \tilde{d}_4(k)\tau_3$$  

(10)

where $\tilde{d}_{1,2}(k) = d_{1,2}(k), \tilde{d}_3(k) = \sin k_3$, and $\tilde{d}_4(k) = d_3(k) - t(\cos k_3 - 1)$. The Hamiltonian describes a three-dimensional TRI odd-parity superconductor, with $\tilde{d}_{1,2,3}(k)$ corresponding to the pairings, and $\tilde{d}_4(k)$ characterizing the energy dispersion of the normal state.
For this Hamiltonian, RDPNs also exist only when $|\lambda_{1,2}| < 1$. With the increase of dimension to 3D, the topological invariant characterizing Dirac pairing nodes needs to be generalized as

$$\nu_n = \frac{1}{4\pi} \oint_S d^2k \frac{\epsilon_{ijk} \partial_i \phi_k \partial_j \phi_k \partial_k}{(\partial^2_{i} + \partial^2_{j} + \partial^2_{k})^{3/2}}$$

(11)

where $S$ denotes a closed surface enclosing one pairing node, $k_i$ and $k_j$ are local coordinates characterizing $S$, and $\epsilon_{ijk}$ with $\{i, j, k\} = \{1, 2, 3\}$ is the Levi-Civita symbol. One can check that for this Hamiltonian, the creation or annihilation of RDPNs also does not change the topological property of TRIMPNs, fulfilling the requirement on RDNPs.

The Fermi surface is determined by $\hat{d}_4(k) = 0$. One can find when $t > t_c = 1 - (\lambda_1^2 + \lambda_2^2)/4$, the Fermi surface only encloses the RDPNs located at the $k_3 = 0$ plane (see Fig.3(a)). While the Fermi surface can continuously contract to a point without crossing any TRI momentum, it can not continuously contract to a point without closing the bulk gap before the annihilation of RDPNs, indicating that the Hamiltonian realizes a HOTOPSC when $t > t_c$ and $|\lambda_{1,2}| < 1$. It is noteworthy that while in the following we only consider $t > t_c$, the phases in the regime $t < t_c$ and $|\lambda_{1,2}| < 1$ are also of great interest, e.g., a weak HOTOPSC will emerge when the Fermi surfaces enclose all RDPNs at both the $k_3 = 0$ and $k_3 = \pi$ planes.[78]

To confirm the realization of HOTOPSC when $t > t_c$ and $|\lambda_{1,2}| < 1$, we consider that the system takes open boundary condition in both the $\hat{x}_1$ and $\hat{x}_2$ directions, and periodic boundary condition in the $\hat{x}_3$ direction. As shown in Fig.3(b)(c), the numerical results reveal that each hinge of the sample harbors a pair of Majorana helical modes, confirming the realization of a TRI SOTOPSC in 3D.

While it is apparent that this scenario can further be generalized to even higher dimensions, we notice that the results in 2D and 3D strongly suggest that when the normal state is a normal metal, only SOTOPSCs can be realized. This limitation can be understood by noting the fact that for normal state being a normal metal, the Fermi surface can have nontrivial Berry phase only when it encloses Dirac pairing nodes, but this goes back to the scenario above. Therefore, to realize third-order topological odd-parity superconductors (TOTO-SCs), the underlying normal state needs to be a topological semimetal which itself has some topological structure.

**TOTO-SCs in 3D.**— A TOTO-SC in 3D can be realized by stacking two dimensional SOTOPSCs layer by layer in a dimerized way, as illustrated in Fig.3(d). As an example, we construct the below Hamiltonian,

$$H(k) = d_1(k) \tau_1 s_4 + d_2(k) \tau_2 + d_3(k) \tau_3 s_3 + (\cos k_3 + \lambda_3) \tau_3 s_1 + \sin k_3 \tau_1 s_1,$$

(12)

where $\sigma_{1,2,3}$ are Pauli matrices, e.g., in orbital space. One can see that the first three terms realize the two dimensional SOTOPSC, while the last two terms realize a Kitaev chain in the layer-stacking direction. The experience from Kitaev model tells us that the situation presented in Fig.3(d) corresponds to the limiting case $\lambda_3 = 0$.[72] For this special case, the outer two layers decouple from the inner layers, so MCMs will show up if each layer realizes a SOTOPSC. The experience from Kitaev model also tells us that the model is within the same phase for $|\lambda_3| < 1$.[79] Thus the Hamiltonian in Eq.(12) realizes a TOTO-SC when $|\lambda_{1,2,3}| < 1$.[78]

The normal state of the Hamiltonian in Eq.(12) is described by $H_N(k) = d_3 \sigma_z + (\cos k_3 + \lambda_3) \sigma_z$, which turns out to be a nodal-line semimetal in the regime $|\lambda_{1,2,3}| < 1$. If weakly doping the normal state, each piece of Fermi surfaces is a thin torus enclosing a nodal line. Along the poloidal direction, there is a global $\pi$-Berry phase.[80] When $|\lambda_{1,2}| < 1$, one can further find that the annihilation of nodal lines just corresponds to the transition from a TOTO-SC to a trivial superconductor, indicating that here the topological structure of the normal state plays a crucial role.

**Conclusion.**— We have revealed that there are two basic requirements for the realization of HOTOPSCs. One is the contractibility of Fermi surfaces without crossing any TRI momentum, and the other is the presence of nontrivial Berry phase on the Fermi surfaces. We have also revealed a general and simple principle to realize SOTOPSCs when the normal state is a normal metal. Furthermore, we have shown that the realization of SOTOPSCs requires the underlying normal state to be a topological semimetal. Our findings can not only be applied to analyze the topological property of intrin-
sic (or effective) odd-parity superconductors, but also guide us to find new promising routes to realize HOTSCs and their concomitant Majorana modes. In fact, we note that in a recent preprint[8], there the proposal based on a combination of Rashba spin-orbit coupling and $s + id$ pairings just provides an effective realization of our model in Eq. (2).

Finally, it is worthy to point out that all models proposed in this work can also be taken to describe HOTIs owing to the direct analogy between superconductors and insulators in Hamiltonian description, in other words, Eqs. (2), (9) and (10) are also minimal models of HOTIs.

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