Topological odd-parity superconductors

Masatoshi Sato

The Institute for Solid State Physics, The University of Tokyo, Kashiwanaoh 5-1-5, Kashiwa, Chiba, 277-8581, Japan,
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In this letter, we investigate topological phases of full-gapped odd-parity superconductors, which are distinguished by the bulk topological invariants and the topologically protected gapless boundary states. Using the particle-hole symmetry, we introduce \( Z_2 \) invariants characterizing topological odd-parity superconductors without or with time-reversal invariance. For odd-parity superconductors, a combination of the inversion and the \( U(1) \) gauge symmetry is manifestly preserved, and the combined symmetry enables us to evaluate the \( Z_2 \) invariants from the knowledge of the Fermi surface structure. Relating the \( Z_2 \) invariants to other topological invariants, we establish characterization of topological odd-parity superconductors in terms of the Fermi surface topology. Simple criteria for topological odd-parity superconductors in various dimensions are provided. Implications of our formulas for nodal odd-parity superconductors are also discussed.

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Recently, there has been considerable interest in topological phases which are characterized by the bulk topological invariants and the topologically protected gapless boundary states. The prototype of the topological phase is the integer quantum Hall states, where the band TKNN integers or Chern numbers give the integer quantum Hall states, where the band edge states at the same time \([2]\). While the time-reversal Hall effects \([1]\), and they ensure the stability of the integer quantum Hall states, where the band edge states at the same time \([2]\). While the time-reversal symmetry breaking (TRSB) is necessary to have non-trivial Chern numbers, there exist another topological invariants called the \( Z_2 \) invariants which classify the topological phases of the time-reversal invariant (TRI) insulators \([3,4,5,6]\). When the \( Z_2 \) invariants are non-trivial, there exist an odd number of the Kramers pairs of gapless edge modes in two dimensions, and an odd number of the Kramers degenerate band crossings (Dirac cones) on the surface in three dimensions, respectively.

The concept of topological phases is also applicable to superconducting states \([7,8,11,12]\) because there is a direct analogy between superconductors and insulators: The Bogoliubov de-Gennes (BdG) Hamiltonian for a quasiparticle of a superconductor is analogous to the Hamiltonian of a band insulator, and the superconducting gap corresponds to the gap of the band insulator. Indeed, the TRSB chiral \( p \)-wave superconductors have non-trivial Chern numbers, and they support topologically protected chiral gapless edge states in analogy with the integer quantum Hall states \([7]\). Topological phases of noncentrosymmetric superconductors and \( s \)-wave superfluids, which support non-abelian anyons, were also investigated in \([8,11,12]\).

In addition to the analogous properties, there are topological features inherent to superconductors. Superconductors possess the particle-hole symmetry (PHS) exchanging the quasiparticle with the anti-quasiparticle, which provides additional topological characteristics to superconductors. In particular, for general superconductors without spin rotation symmetry, there arise extra \( Z_2 \) invariants in one dimensional TRSB and TRI systems, and an integer winding number in three dimensional TRI one \([10]\). As a result, the topological superconductors are characterized by the one dimensional \( Z_2 \) invariants and the two dimensional Chern number for the TRSB case, and the one and two dimensional \( Z_2 \) invariants and the three dimensional winding number for the TRI one, respectively.

In this letter, assuming the inversion symmetry in the normal state, we present a theory of topological odd-parity superconductors. For TRI single-band odd-parity superconductors, it has been revealed that the topological properties are characterized by the Fermi surface topology in the normal state \([13]\). Here we extend these results to general odd-parity superconductors without or with time-reversal invariance, by using the one-dimensional \( Z_2 \) invariants obtained from the PHS. We develop a method to link the \( Z_2 \) invariants to the topology of the Fermi surface, where a combination of the inversion and the \( U(1) \) gauge symmetry plays an essential role. Moreover, making connections between the \( Z_2 \) invariants and the other topological invariants mentioned above, we provide characterization of topological odd-parity superconductors in terms of the topology of the Fermi surface.

In the following, we consider a general Hamiltonian \( H \) \([18]\) for full gapped odd-parity superconducting states,

\[
H = \frac{1}{2} \sum_{k \alpha \alpha'} (c_{k \alpha} \dagger, c_{-k \alpha}) H(k) \left( c_{-k \alpha'} \right),
\]

\[
H(k) = \begin{pmatrix}
\varepsilon(k)_{\alpha \alpha'} - \Delta(k)_{\alpha \alpha'} & -\varepsilon'(-k)_{\alpha' \alpha'} \\
\Delta(k)_{\alpha' \alpha} & \varepsilon'(-k)_{\alpha' \alpha'}
\end{pmatrix},
\]

where \( c_{k \alpha} \) \((c_{k \alpha} \dagger)\) denotes the creation (annihilation) operator of electron with momentum \( k \). The suffix \( \alpha \) labels other degrees of freedom for electron such as spin, orbital

*Electronic address: msato@issp.u-tokyo.ac.jp
degrees of freedom, sub-lattice indeces, and so on. $\mathcal{E}(k)$ is an hermitian matrix describing the normal dispersion of the electron. Here we assume that the system in the normal state is symmetric under the inversion $c_{k_{\alpha}} \rightarrow \sum_{n_{\alpha}} P_{n_{\alpha},k_{\alpha} - c_{k_{\alpha}}}$ with $P^2 = 1$, so $P \mathcal{E}(k) P = \mathcal{E}(-k)$. For an odd-parity superconductor, the gap function $\Delta(k)$ satisfies $P \Delta(k) P^* = -\Delta(-k)$. In addition, the Fermi statistics of electron implies $\Delta^T(k) = -\Delta(-k)$.

An important ingredient of our theory is the PHS of the BdG Hamiltonian $\mathcal{H}$,

$$CH(k)C^\dagger = -H^*(k), \quad C = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{2}$$

From (2), we can say that if $|u_n(k)|$ is a quasiparticle state with positive energy $E_n(k) > 0$ satisfying $H(k)|u_n(k)| = E_n(k)|u_n(k)|$, then $C|u_n^*(k)|$ is a quasiparticle state with negative energy $-E_n(-k) < 0$. In the following, we use a positive (negative) $n$ for $|u_n(k)|$ to represent a positive (negative) energy quasiparticle state, and set

$$|u_{-n}(k)| = C|u_n^*(k)|. \tag{3}$$

To define the topological invariants, we introduce the gauge fields $A_i^{(+)}(k) = i \sum_{n \geq 0} \langle u_n(k) | \partial_k | u_n(k) \rangle$. We also denote their sum as $A_i(k) = A_i^{(+)}(k) + A_i^{(-)}(k)$. From (2), we have

$$A_i^{(+)}(k) = A_i^{(-)}(-k). \tag{4}$$

Using this and the fact that $A_i(k)$ is the total derivative of a function, we can prove that the Wilson loop of $A_i^{(-)}(k)$ along the TRI closed path $C$ in the Brillouin zone (BZ)

$$W[C] = \frac{1}{2 \pi} \oint_C \partial_k A_i^{(-)}(k) \tag{5}$$

is quantized as $e^{2\pi i W[C]} = \pm 1$. Therefore, we can introduce a $Z_2$ invariant $(-1)^{\nu[C]}$ by $(-1)^{\nu[C]} = e^{2\pi i W[C]}$. As we will discuss later, $(-1)^{\nu[C]} = (-1)^{n}$ corresponds to a topological non-trivial (trivial) phase of the superconducting state.

Now consider the TRI closed path $C_{ij}$ passing through the TRI momenta $\Gamma_i$ and $\Gamma_j$ in Fig.1. The TRI momentum satisfies $\Gamma_i = -\Gamma_i + G$ with a reciprocal lattice vector $G$, and because of the periodicity of the BZ, $C_{ij}$ forms a closed path. In the following, we evaluate the $Z_2$ invariant $(-1)^{\nu[C_{ij}]}$ along $C_{ij}$ by developing the method in 13.

For an odd-parity superconductor, the combination of the inversion symmetry and the $U(1)$ gauge symmetry, $c_{k_{\alpha}} \rightarrow i U_{n_{\alpha}} c_{k_{\alpha}}$, is manifestly preserved, although each symmetry is spontaneously broken by the condensation $\Delta(k)$. Therefore, the BdG Hamiltonian $H(k)$ has the following symmetry

$$P^* H(k) P = H(-k), \quad P = \begin{pmatrix} P & 0 \\ 0 & -P^* \end{pmatrix}. \tag{6}$$

From this symmetry, we have $[H(\Gamma_i), \Pi] = 0$ for the TRI momentum $\Gamma_i$. Thus, the quasiparticle state $|u_{\pi}(\Gamma_i)|$ at $\Gamma_i$ is simultaneously an eigenstate of $\Pi$. From $|u_{\pi}(\Gamma_i)| = \pi_i(\Gamma_i) |u_{\pi}(\Gamma_i)|$. Evaluation of $(-1)^{\nu[C_{ij}]}$ is done by using the unitary matrices, $V_{mn}(k) = \langle u_m(k) | \Pi C | u_n^*(k) \rangle$, and $W_{mn}(k) = \langle u_m(-k) | C | u_n^*(k) \rangle$. Since we have $\text{tr}(V^\dagger \partial_k V) = 2i A_i(k)$ from (3), $\nu[C_{ij}]$ is rewritten as

$$\nu[C_{ij}] = \frac{1}{\pi i} \int_{\Gamma_i} d\Gamma_j \partial_k A_i(k) = \frac{1}{\pi} \ln \left( \frac{\sqrt{\text{det} V(\Gamma_i)}}{\sqrt{\text{det} V(\Gamma_j)}} \right). \tag{7}$$

Here we have used (4) and $\text{tr}(V^\dagger \partial_k V) = \partial_k \ln \text{det} V$. Furthermore, because $V_{mn}(\Gamma_i)$ is recast into $V_{mn}(\Gamma_i) = \langle u_m(\Gamma_i) | \Pi C | u_n^*(\Gamma_i) \rangle = \pi_m(\Gamma_i) \langle u_m(\Gamma_i) | C | u_n^*(\Gamma_i) \rangle = \pi_m(\Gamma_i) W_{mn}(\Gamma_i)$, we obtain

$$\text{det} V(\Gamma_i) = \prod_n \pi_n(\Gamma_i) \text{det} W, \tag{8}$$

where $\text{det} W$ is independent of $\Gamma_i$ because $\partial_k \ln \text{det} W = \text{tr}(V^\dagger \partial_k V) = i [A_i(k) - A_i(-k)] = 0$. Due to the PHS, $|u_{\pi}(\Gamma_i)|$ and $|u_{-\pi}(\Gamma_i)|$ share the same eigenvalue of $\Pi$ and each eigenvalue appears twice in the product in (8). Therefore, taking the square root, we find $\sqrt{\text{det} V(\Gamma_i)} = \prod_{n < 0} \pi_n(\Gamma_i) \sqrt{\text{det} W}$. As a result, (7) reduces to

$$(-1)^{\nu[C_{ij}]} = \prod_{n < 0} \pi_n(\Gamma_i) \pi_n(\Gamma_j), \tag{9}$$

where we have used $\pi_0^2(\Gamma_j) = 1$.

In order to attribute the Fermi surface properties to the $Z_2$ invariants, we make the weak-paring assumption 13. For ordinary superconductors, the superconducting gap is much smaller than the Fermi energy. Therefore, we reasonably assume that the typical energy scale of the gap function $\Delta(\Gamma_i)$ at the TRI momentum is much smaller than that of $\mathcal{E}(\Gamma_i)$. Under this assumption, we can take $\Delta(\Gamma_i) \rightarrow 0$ without the gap closing. Because of

FIG. 1: The TRI momenta $\Gamma_i$, and the TRI closed path $C_{ij}$ connecting $\Gamma_i$ and $\Gamma_j$ in the BZ. a) 1 dim BZ. The solid line denotes $C_{12}$. b) 2 dim BZ $T^2$. The solid line denotes $C_{12}$, and the dotted one $C_{14}$. c) 3 dim BZ. The solid line is $C_{12}$.\]
The topological nature of $(-1)^{p(C_{ij})}$, this adiabatic process does not change the value of $(-1)^{p(C_{ij})}$.

In the process $\Delta(\Gamma_i) \to 0$, the BdG Hamiltonian at $\Gamma_i$ reduces to $H(\Gamma_i) \to \text{diag}(\mathcal{E}(\Gamma_i), -\mathcal{E}^T(\Gamma_i))$. By using an eigenstate $|\varphi(\Gamma_i)\rangle$ of $\mathcal{E}(\Gamma_i)$ satisfying $\mathcal{E}(\Gamma_i)|\varphi(\Gamma_i)\rangle = \varepsilon(\Gamma_i)|\varphi(\Gamma_i)\rangle$, an occupied state of $H(\Gamma_i)$ is given by $(|\varphi(\Gamma_i)\rangle, 0)^T$ for $\varepsilon(\Gamma_i) < 0$, and $(0, |\varphi(\Gamma_i))\rangle^T$ for $\varepsilon(\Gamma_i) > 0$. Therefore, denoting the parity of $|\varphi(\Gamma_i)\rangle$ as $P|\varphi(\Gamma_i)\rangle = \varepsilon(\Gamma_i)|\varphi(\Gamma_i)\rangle$, we find

$$\prod_{n<0} \sigma_n(\Gamma_i) = \prod_{\alpha} \xi(\Gamma_i) \prod_{\alpha} \text{sgn} \varepsilon(\Gamma_i),$$

where the sum of $\alpha$ is taken for all eigenstates of $\mathcal{E}(\Gamma_i)$. We notice here that the product of the parity, $\prod \xi(\Gamma_i)$, is independent of $\Gamma_i$ since it is determined solely from $\text{det} P$ and the dimensionality of the matrix $\mathcal{E}(\Gamma_i)$. Thus if we substitute (10) into (9), the contributions from the parity at $\Gamma_i$ and $\Gamma_j$ cancel each other, then we obtain the final expression,

$$(-1)^{p(C_{ij})} = \prod_{\alpha} \text{sgn} \varepsilon(\Gamma_i) \text{sgn} \varepsilon(\Gamma_j).$$

This formula is very powerful: It enables us to calculate the $Z_2$ invariants only from the knowledge of the band energy $\varepsilon(\Gamma_i)$ of electron in the normal state. We also notice that the right hand side of (11) has its own topological meaning. By denoting the number of intersection points between the Fermi surface and $C_{ij}$ as $i_0(S_F \cap C_{ij})$, the right hand side is found to be $(-1)^{i_0(S_F \cap C_{ij})/2}$ [19]. Therefore, when $i_0(S_F \cap C_{ij})$ is odd (even), the $Z_2$ invariant in (11) is non-trivial (trivial).

To see the physical meaning of the $Z_2$ invariants, consider a full gapped one-dimensional odd-parity superconductor. In one dimension, we have a single $Z_2$ invariant $(-1)^{p(C_{12})}$ where $C_{12}$ is the TRI closed path in [11]. When $(-1)^{p(C_{12})} = -1$ (+1), the system is topologically non-trivial (trivial), and there exist an odd (even) number of the zero energy states on the boundary [10]. Without loss of generality, we can consider the simplest non-trivial topological phase with a single boundary zero mode. See Fig[2]. The PHS ensures the topological stability of the zero mode against small perturbation: From the PHS, a non-zero mode with energy $E$ must be paired with a non-zero mode having the opposite energy $-E$. Therefore, a zero mode can be a non-zero mode only in pairs. This implies that the single zero mode in Fig[2] can not acquire non-zero energy and it is stable against small perturbation. The $Z_2$ nature of the topological phase is evident if we add another zero mode as depicted in Fig[10]. In this case, we have a pair of zero modes, so they can be non-zero modes by small perturbation as demonstrated in Fig[10]. This argument consistently indicates that the topological phase ensured by the PHS is distinguished by the $Z_2$ invariant.

In two and three dimensions, we have multiple one-dimensional $Z_2$ invariants corresponding to possible $C_{ij}$ in Fig[10]-c). When the $Z_2$ invariant $(-1)^{p(C_{ij})}$ is non-trivial, we have a gapless state on the surface perpendicular to $C_{ij}$: By fixing the momenta along the surface perpendicular to $C_{ij}$, the part of the system can be considered as a one-dimensional gapful system [10]. Therefore, from the topological argument above, it is concluded that there exist a gapless mode on the surface.

Following the classification in [10], the two-dimensional Chern numbers $\nu_{\text{Ch}}$ also characterize the topological phase of the TRSB superconductors. Now make a connection between the Chern number $\nu_{\text{Ch}}$ and the $Z_2$ invariants in two dimensions. $\nu_{\text{Ch}}$ is defined by

$$\nu_{\text{Ch}} = \frac{1}{2\pi} \int_{T^2} \mathcal{F}(-\mathbf{k}),$$

where $\mathcal{F}(-\mathbf{k})$ is the field strength of $A_i(-\mathbf{k})$, and $T^2$ the two-dimensional BZ in Fig[10]. Noting that the field strength $\mathcal{F}(\mathbf{k})$ of $A_i(\mathbf{k})$ is identically zero, we find $\mathcal{F}(\mathbf{k}) = \mathcal{F}(\mathbf{k})$ from [4]. Thus the Chern number is linked to the $Z_2$ invariants as

$$\nu_{\text{Ch}} = \frac{1}{2\pi} \int_{T^2} \mathcal{F}(-\mathbf{k}) = \frac{1}{\pi} \int_{T^2} \mathcal{F}(\mathbf{k}) = \frac{1}{\pi} \oint_{\mathcal{T}^2} dk_i A_i(-\mathbf{k}) = [\nu(C_{12}) - \nu(C_{34})],$$

where $\mathcal{T}^2$ is the upper half of $T^2$. Consequently, from (11), we have the following relation between $\nu_{\text{Ch}}$ and the topology of the Fermi surface,

$$(-1)^{\nu_{\text{Ch}}} = \prod_{\alpha, i=1,2,3,4} \text{sgn} \varepsilon(\Gamma_i) = (-1)^{p_0(S_F)},$$

where $p_0(S_F)$ is the number of the connected components of the Fermi surface on $T^2$, and in the second equality, we have used the result in [13]. This formula provide a criterion for non-zero $\nu_{\text{Ch}}$: If $p_0(S_F)$ is odd, then $\nu_{\text{Ch}}$ is non-zero. This simple criterion immediately reproduces the non-zero $\nu_{\text{Ch}}$ for the chiral $p$-wave superconductor [7] since it has a single Fermi surface. In a similar manner, it is found that the Chern numbers in three dimensions are also characterized by the topology of the Fermi surface.

Now consider TRI odd-parity superconductors. Because of the time-reversal invariance $\Theta$ with $\Theta^2 = -1$, the occupied states of the BdG Hamiltonian $H(\mathbf{k})$ are divided into two Kramers pairs, $\{|u_n(\mathbf{k})\rangle, |u_n^{\dagger}(\mathbf{k})\rangle\}$ ($s = I, II$),

$$|u_n(\mathbf{k})\rangle = \Theta |u_n^{\dagger}(\mathbf{k})\rangle.$$

FIG. 2: $Z_2$ classification of edge state. a) Topologically protected zero mode. b) and c) Topologically trivial edge modes.
Since the Kramers pair, \(|u_1^1(\Gamma_i)\rangle \equiv |u_{2n}(\Gamma_i)\rangle\) and \(|u_1^{2n+1}(\Gamma_i)\rangle \equiv |u_{2n+1}(\Gamma_i)\rangle\) at \(\Gamma_i\) share the same eigenvalue of \(\Pi\), \([9]\) leads to \((-1)^{\nu[C_{ij}]^{(II)}} = 1\). In other words, \((-1)^{\nu[C_{ij}]^{(II)}}\) is always trivial for TRI odd-parity superconductors. However, use of the time-reversal invariance as well makes it possible to define non-trivial \(Z_2\) invariants.

To define non-trivial \(Z_2\) invariants, let us introduce the gauge field \(A_i^{(\pm)}(k)\) as defined in \([11]\). Here \(\tilde{e}_{2n}(\Gamma_i)\) is an eigenvalue of \(\mathcal{E}(\Gamma_i)\), and we have set \(\varepsilon_{2n}(\Gamma_i) = \varepsilon_{2n+1}(\Gamma_i)\) by using the Kramers degeneracy. In terms of the topology of the Fermi surface, the right hand side of \([17]\) is expressed by \((-1)^{\nu(S_F)/4}\).

For the TRI odd-parity superconductors, we also have two-dimensional \(Z_2\) invariants \((-1)^{\nu[\mathcal{I}]}\) which were originally used to characterize topological insulators \([13]\), and three dimensional winding number \(\nu_w\) defined in \([19]\). Using the formula \([17]\), we can connect these topological invariants to the Fermi surface topology: First, since the \(Z_2\) invariant \((-1)^{\nu[\mathcal{I}]}\) for topological insulators is defined as a product of \(e^{2\pi iw}\mathcal{I}\), it is also a product of our \(Z_2\) invariants \((-1)^{\nu[C_{ij}]^{(II)}}\).

Therefore, in two dimensions, the formula \([17]\) leads to

\[
(-1)^{\nu[\mathcal{I}]} = \prod_{\alpha, i=1,2,3,4} \text{sgn} \varepsilon_{2\alpha}(\Gamma_i) = (-1)^{\nu_w(S_F)/2}.
\]

In a similar manner, the \(Z_2\) invariant \((-1)^{\nu[\mathcal{I}]}\) for three dimensional topological insulators \([4, 5, 6]\) is represented by a product of our one-dimensional \(Z_2\) invariants \((-1)^{\nu[C_{ij}]^{(II)}}\). Moreover, the winding number \(\nu_w\) satisfies

\[
(-1)^{\nu_w} = (-1)^{\nu[\mathcal{I}]}\]

where \(\nu(S_F)\) is the Euler characteristics of the Fermi surface \([13]\). While the formulas \([18]\) and \([19]\) have already been reported for TRI single-band spin-triplet superconductors and multi-band odd-parity superconductors with \(P = 1\), here they are extended to general TRI odd-parity superconductors \([20]\). Furthermore, owing to the PHS, we have an additional formula \([17]\), which was not known before.

So far, we have considered full-gapped odd-parity superconductors, but our formulas \([11]\) and \([17]\) are applicable to a nodal odd parity superconductor as well if the TRI path \(C_{ij}\) does not intersect a node of the superconducting gap. As was discussed above, fixing the momenta along the surface perpendicular to \(C_{ij}\), we can consider the part of the system as a one-dimensional gapful odd-parity superconductor. When the \(Z_2\) invariant \((-1)^{\nu[C_{ij}]^{(II)}}\) or \((-1)^{\nu[C_{ij}]^{(II)}}\) is non-trivial, a gapless surface state is predicted on the surface perpendicular to \(C_{ij}\).

To conclude, in this letter, we present a description of topological odd-parity superconductors in terms of the Fermi surface topology in the normal state. All the topological invariants for odd-parity superconductors are directly related to the topology of the Fermi surface by \([11]\) and \([17]\) for the TRSB case, and \([17, 18]\) and \([19]\) for the TRI one, respectively, which provide simple criteria for topological odd-parity superconductors.

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[18] In the classification of \([14]\), the Hamiltonian is in class D for the TRSB case, and in class DII for TRI one.
respectively.

[19] In this letter, the degeneracy of the Fermi surface is taken into account to count $i_0(S_F \cap C_i) \cdot p_0(S_F)$ and $\chi(S_F)$. So, they are different from those in [13] by factor 2.

[20] The recent preprint [17] also discussed the generalization of (19) for the TRI case in a different manner.