Topological properties of spin-triplet superconductors and Fermi surface topology in the normal state

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We report intimate relations between topological properties of full-gapped spin-triplet superconductors with time-reversal invariance and the Fermi surface topology in the normal states. An efficient method to calculate the $\boldsymbol{Z}_2$ invariants and the winding number for the spin-triplet superconductors is developed and connections between these topological invariants and the Fermi surface structures in the normal states are pointed out. We also obtain a correspondence between the Fermi surface topology and gapless surface states in the superconducting states. The correspondence is inherent to spin-triplet superconductivity.

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Search for possible states of quantum matter is one of the central issues in condensed-matter physics. In addition to local order parameters, gapped states can be characterized by topological invariants which are constructed from the wave functions. The quantum-Hall state is a prominent example of such topological states in which the Hall conductance is identified with the topological number introduced by Thouless, Kohmoto, Nightingale, and den Nijs (TKNN).[1] While the TKNN number is nontrivial only when the time-reversal symmetry is absent, recently new topological invariants, namely, the $\boldsymbol{Z}_2$ invariants, were introduced in order to distinguish a topological state with time-reversal invariance from ordinary band insulators.[2–8] For such a "topological insulator," the bulk-edge correspondence between the topological invariants in the bulk and gapless edge (or surface) states on the boundary was discussed in a similar manner to the quantum-Hall state.[2,5,9] The topologically protected gapless state is an origin of dissipationless (spin) Hall effects which inspire an application to spintronics.[10,11]

In this paper, using the topological invariants, we study topological properties of another class of gapped systems, spin-triplet superconductors. Although conventional s-wave superconductors are topologically trivial, it is known that an unconventional superconductor can be topologically nontrivial.[12–14] In the following, we will develop a powerful method to evaluate the topological invariants for spin-triplet superconductors and find an intimate relation between the topological properties in the spin-triplet superconducting state and those in the normal state. In particular, from topological arguments based on the bulk-edge correspondence, we derive formulas between the gapless surface (edge) state on the boundary of the three-dimensional (3D) (two-dimensional (2D)) spin-triplet superconductor and the topological invariants of the Fermi surface in the normal state. Although the number N_0 of the gapless surface (or edge) states itself depends on the details of the gap function, it will be shown that the index $(-1)^{N_0}$ does not depend on them and is directly related to the Fermi surface topology in the normal state. We also introduce a tight-binding lattice model and confirm the results by numerical calculations.

In the following, we consider mainly full-gapped spin-triplet superconductors with time-reversal invariance. A generalization to those without time-reversal invariance will be mentioned in the last part of this paper briefly.

Let us start with the single-band description of a spin-triplet superconducting state with time-reversal invariance. (Generalization to the multiband description is presented later.) The Hamiltonian $\mathcal{H}$ of a spin-triplet superconductor in a single-band is given by

$$\mathcal{H} = \sum_{\boldsymbol{k},\sigma} \epsilon(\boldsymbol{k}) c_{\boldsymbol{k},\sigma}^{\dagger} c_{\boldsymbol{k},\sigma} + \frac{1}{2}\sum_{\boldsymbol{k},\sigma,\sigma'} [\Delta_{\sigma\sigma'}(\boldsymbol{k}) c_{\boldsymbol{k},\sigma}^{\dagger} c_{-\boldsymbol{k},\sigma'}^{\dagger} + \text{H.c.}], \tag{1}$$

where $c_{\boldsymbol{k},\sigma}^{\dagger}$ $(c_{\boldsymbol{k},\sigma})$ denotes a creation (annihilation) operator of the electron, $\epsilon(\boldsymbol{k})$ the dispersion of the electron in the normal state, and $\Delta(\boldsymbol{k})$ the gap function given by $\Delta(\boldsymbol{k}) = i\boldsymbol{d}(\boldsymbol{k}) \cdot \boldsymbol{\sigma}\sigma_2$. $\boldsymbol{d}(\boldsymbol{k})$ are odd functions and $\boldsymbol{\sigma}$ are the Pauli matrices. By rewriting $\mathcal{H}$ as

$$\mathcal{H} = \frac{1}{2}\sum_{\boldsymbol{k}} \boldsymbol{c}_{\boldsymbol{k}}^{\dagger} H(\boldsymbol{k}) \boldsymbol{c}_{\boldsymbol{k}}, \quad \boldsymbol{c}_{\boldsymbol{k}}^{\dagger} = (c_{\boldsymbol{k},\sigma}^{\dagger}, c_{-\boldsymbol{k},\sigma}), \tag{2}$$

it is found that the spin-triplet superconducting state is described by the 4×4 Bogoliubov-de Gennes (BdG) Hamiltonian

$$H(\boldsymbol{k}) = \begin{pmatrix} \epsilon(\boldsymbol{k}) \mathbf{1}_{2\times 2} & \Delta(\boldsymbol{k}) \\ \Delta(\boldsymbol{k})^{\dagger} & -\epsilon(\boldsymbol{k}) \mathbf{1}_{2\times 2} \end{pmatrix}. \tag{3}$$

We assume that the normal state has the inversion symmetry and the time-reversal invariance, so $\epsilon(-\boldsymbol{k}) = \epsilon(\boldsymbol{k})$. From the time-reversal invariance of $H(\boldsymbol{k})$,

$$\Theta H(\boldsymbol{k}) \Theta^{-1} = H(-\boldsymbol{k})^{*}, \quad \Theta = \begin{pmatrix} i\sigma_2 & 0 \\ 0 & i\sigma_2 \end{pmatrix}, \tag{4}$$

$\boldsymbol{d}(\boldsymbol{k})$ should be real. Eigenstates of $H(\boldsymbol{k})$ with negative energies $E(\boldsymbol{k}) < 0$ are occupied in the ground state of the superconducting state.

The essential ingredient of our argument is the following "symmetry" for the spin-triplet superconductor. Since the parity of the gap function is odd, $\boldsymbol{d}(-\boldsymbol{k}) = -\boldsymbol{d}(\boldsymbol{k})$, the BdG Hamiltonian of the spin-triplet superconductor has the symmetry

$$\Pi H(\boldsymbol{k})\Pi^{\dagger} = H(-\boldsymbol{k}), \quad \Pi^2 = 1 \tag{5}$$

with

$$\Pi = \begin{pmatrix} \mathbf{1}_{2\times 2} & 0 \\ 0 & -\mathbf{1}_{2\times 2} \end{pmatrix} = \mathbf{1}_{2\times 2} \otimes \tau_3. \tag{6}$$

Using this, we will study topological properties for the spin-triplet superconductor.

Let us consider special points $\boldsymbol{k}=\Gamma_a$ in the Brillouin zone which are time-reversal invariant and satisfy $-\Gamma_a=\Gamma_a+\boldsymbol{G}$ for a reciprocal-lattice vector $\boldsymbol{G}$. In terms of the primitive reciprocal-lattice vectors $\boldsymbol{b}_j$, the time-reversal-invariant momenta Γ_a are expressed as

$$\Gamma_{a=(n_1,n_2)} = (n_1\boldsymbol{b}_1 + n_2\boldsymbol{b}_2)/2 \quad \text{for two dimensions}, \tag{7}$$

$$\Gamma_{a=(n_1,n_2,n_3)} = (n_1\boldsymbol{b}_1 + n_2\boldsymbol{b}_2 + n_3\boldsymbol{b}_3)/2 \quad \text{for three dimensions}, \tag{8}$$

with $n_j=0,1$. At these momenta, the time-reversal invariance [Eq. (4)] reduces to $\Theta H(\Gamma_a)\Theta^{-1}=H(\Gamma_a)^*$ since $H(\boldsymbol{k})$ satisfies $H(\boldsymbol{k}+\boldsymbol{G})=H(\boldsymbol{k})$. This implies that an occupied eigenstate $|u_n(\Gamma_a)\rangle$ $(n=1,2)$ has the same energy as its Kramers partner $\Theta|u_n(\Gamma_a)\rangle^*$. In addition, from the additional symmetry [Eq. (5)], we have $[H(\Gamma_a),\Pi]=0$. So the Kramers doublet of the occupied states has the same eigenvalue of Π. The eigenvalue of Π is given by

$$\pi_a = -\,\mathrm{sgn}\;\epsilon(\Gamma_a), \tag{9}$$

since $H(\Gamma_a)=\epsilon(\Gamma_a)\Pi$.

The eigenvalues $\{\pi_a\}$ have the following interesting properties: (a) they are defined only at the time-reversal momenta $\{\Gamma_a\}$; (b) they only take $\pi_a=\pm 1$; (c) their values can change only when the gap of the system closes. To see the last property (c), consider the quasiparticle spectrum $E(\boldsymbol{k}) = \pm\sqrt{\epsilon(\boldsymbol{k})^2+\boldsymbol{d}(\boldsymbol{k})^2}$ which is obtained by diagonalizing $H(\boldsymbol{k})$. The gap of the system $2|E(\boldsymbol{k})|$ closes when $\epsilon(\boldsymbol{k})=\boldsymbol{d}(\boldsymbol{k})=0$. At the time-reversal momenta, the $\boldsymbol{d}$ vector vanishes identically, $\boldsymbol{d}(\Gamma_a)=0$, so only $\epsilon(\Gamma_a)=0$ is required for gap closing. Therefore, the gap closes when π_a changes.

The above properties suggest a connection between the $\boldsymbol{Z}_2$ invariants introduced in Ref. 2 and $\{\pi_a\}$. The $\boldsymbol{Z}_2$ numbers are calculated from the quantities $\{\delta_a\}$ (Ref. 6)

$$\delta_a = \frac{\sqrt{\det[w(\Gamma_a)]}}{\mathrm{Pf}[w(\Gamma_a)]}, \tag{10}$$

where $w(\Gamma_a)_{nm}$ is the antisymmetric U(2) matrix connecting the occupied states $|u_n(\Gamma_a)\rangle$ $(n=1,2)$ with their Kramers partners $\Theta|u_n(\Gamma_a)\rangle^*$, $w(\Gamma_a)_{nm}\equiv\langle u_n(\Gamma_a)|\Theta|u_m(\Gamma_a)\rangle^*$, and Pf denotes its Pfaffian. While the quantities $\{\delta_a\}$ depend on the gauge (or phase choice) of the occupied states, their gauge-independent combinations define the $\boldsymbol{Z}_2$ invariants, ν for two dimensions and ν_μ $(\mu=1,2,3,0)$ for three dimensions:[6] $(-1)^{\nu}=\prod_{n_j=0,1}\delta_{a=(n_1,n_2)}$ for two dimensions, and $(-1)^{\nu_0}=\prod_{n_j=0,1}\delta_{a=(n_1,n_2,n_3)}$ and $(-1)^{\nu_k}=\prod_{n_{j\neq k}=0,1;n_k=1}\delta_{a=(n_1,n_2,n_3)}$ $(k=1,2,3)$ for three dimensions. We notice here that the quantities $\{\delta_a\}$ have properties similar to those of $\{\pi_a\}$: (A) they are defined only at the time-reversal-invariant momenta; (B) they only take $\delta_a=\pm 1$ since $\mathrm{Pf}[w(\Gamma_a)]^2=\det[w(\Gamma_a)]$; (C) with fixing the gauge (or phase choice) of the occupied states, their values can change only when the gap of the system closes. The last property (C) is obvious because their gauge-independent combinations ν and ν_μ can change only when the gap of the system closes.

These similarities suggest that the relation $\delta_a=\pi_a$ holds with a suitable phase choice of the occupied states. Indeed, we can prove it by using a similar technique developed in Ref. 6 with the replacement of the inversion symmetry P by the symmetry Π in the argument. As a result, we obtain useful formulas of the $\boldsymbol{Z}_2$ invariants for the time-reversal-invariant spin-triplet superconductor,

$$(-1)^{\nu} = \prod_{n_j=0,1} \mathrm{sgn}\;\epsilon(\Gamma_{a=(n_1,n_2)}) \quad \text{for two dimensions}, \tag{11}$$

$$(-1)^{\nu_0} = \prod_{n_j=0,1} \mathrm{sgn}\;\epsilon(\Gamma_{a=(n_1,n_2,n_3)}),$$

$$(-1)^{\nu_k} = \prod_{n_{j\neq k}=0,1;n_k=1} \mathrm{sgn}\;\epsilon(\Gamma_{a=(n_1,n_2,n_3)}) \quad \text{for three dimensions}. \tag{12}$$

Note that the $\boldsymbol{Z}_2$ numbers ν and ν_μ are mod 2 integers, which are identified with $\nu+2$ and $\nu_\mu+2$, respectively. Thus the $\boldsymbol{Z}_2$ numbers are nontrivial (trivial) when they are odd (even).

Here we find that the right-hand sides of Eqs. (11) and (12) have their own topological meanings related to the Fermi surface structure in the normal state: For Eq. (11), by using the relation $\epsilon(-\boldsymbol{k})=\epsilon(\boldsymbol{k})$, it is found that

$$\prod_{n_j=0,1} \mathrm{sgn}\;\epsilon(\Gamma_{a=(n_1,n_2)}) = (-1)^{p_0(S_F)}, \tag{13}$$

where $p_0(S_F)$ is the number of different connected components of the Fermi surface in the normal state. Also for Eq. (12), we obtain

$$\prod_{n_j=0,1} \mathrm{sgn}\;\epsilon(\Gamma_{a=(n_1,n_2,n_3)}) = (-1)^{\chi(S_F)/2},$$

$$\prod_{n_{j\neq k}=0,1;n_k=1} \mathrm{sgn}\;\epsilon(\Gamma_{a=(n_1,n_2,n_3)}) = (-1)^{p_0(C_k)}, \tag{14}$$

where $\chi(S_F)$ is the Euler characteristic of the Fermi surface and $p_0(C_k)$ is the number of different connected components of the intersection C_k between the Fermi surface and the time-reversal-invariant plane with $\boldsymbol{k}=\boldsymbol{b}_k/2$. (For a single connected Fermi surface, the Euler characteristic is given by $\chi(S_F)=2(1-g)$ with g the genus of the Fermi surface. When there are multiple connected components of the Fermi surface, $\chi(S_F)$ is the sum of the Euler characteristics of each component.) We illustrate $p_0(S_F)$, $\chi(S_F)$, and $p_0(C_k)$ in Figs. 1 and 2. Equations (13) and (14) are confirmed by these examples. These quantities, $p_0(S_F)$, $\chi(S_F)$, and $p_0(C_k)$, are topological invariants of the Fermi surface and they do not change the values under deformations of the Fermi surface unless the Fermi surface crosses one of the time-reversal-invariant momenta. Therefore, Eqs. (11)–(14) make connec-

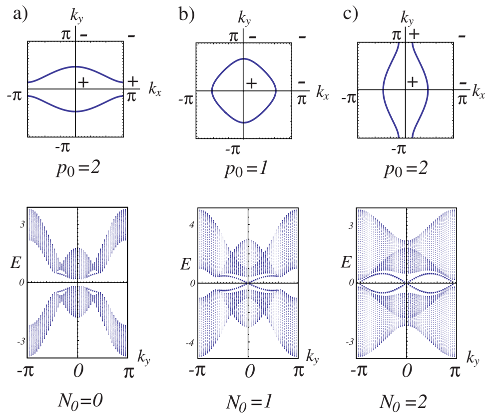

FIG. 1. (Color online) The Fermi surfaces in the normal state and the edge states in 2D time-reversal-invariant spin-triplet superconducting state. (Top row) The Fermi surfaces and $\pi_a=\pm$ at the time-reversal-invariant momenta. $p_0[=p_0(S_F)]$ is the number of the connected components of the Fermi surface. (Bottom row) The energy spectra of the corresponding superconducting states described by Eq. (25) with edges at $i_x=0$ and $i_x=50$. Here k_y denotes the momentum in the y direction and N_0 the number of gapless helical edge states. We set the parameters of the lattice model [Eq. (25)] as (a) $t_x=0.4$, $t_y=1$, $\mu=-1$, and $d=0.5$, (b) $t_x=t_y=1$, $\mu=-1$, and $d=0.5$, and (c) $t_x=1$, $t_y=0.4$, $\mu=-1$, and $d=0.5$, respectively.

tions between the topological invariants in two different phases, i.e., the $\boldsymbol{Z}_2$ invariants in the superconducting phase and $p_0(S_F)$, $\chi(S_F)$, and $p_0(C_k)$ in the normal phase:

$$(-1)^{\nu}=(-1)^{p_0(S_F)} \quad \text{for two dimensions}, \tag{15}$$

$$(-1)^{\nu_0}=(-1)^{\chi(S_F)/2},$$

$$(-1)^{\nu_k}=(-1)^{p_0(C_k)} \quad \text{for three dimensions}, \tag{16}$$

An important physical consequence of our formulas (15) and (16) is that one can obtain useful information about gapless surface (or edge) states in the spin-triplet superconductor from the knowledge of the Fermi surface topology. From the bulk-edge correspondence, a nontrivial $\boldsymbol{Z}_2$ number of a bulk gapped system implies the existence of a gapless state localized on the boundary.[5] For time-reversal-invariant systems in two dimensions, the gapless state is nonchiral and its Kramers doublet forms a helical pair.[11,15] The helical-edge pair also satisfies the Majorana condition in the present case because of the particle-hole symmetry of the superconducting system. From a topological argument similar to that in Ref. 5, it is shown that an odd (even) number of gapless helical Majorana pairs exist on each edge when $(-1)^{\nu}=-1$ ($(-1)^{\nu}=1$). Thus from Eq. (15), we find the following connection between the number N_0 of the gapless helical Majorana pairs on each edge and the topological invariant $p_0(S_F)$ of the Fermi surface,

$$(-1)^{N_0}=(-1)^{p_0(S_F)}. \tag{17}$$

This formula implies that when $p_0(S_F)$ is odd N_0 cannot be zero and at least one gapless helical Majorana state should exist on each edge.

For 3D time-reversal-invariant spin-triplet superconductors, the gapless boundary state is a 2D massless Majorana fermion. By generalizing the argument in Ref. 5 to this case, we have the following two properties of the surface state. (1) The number N_0 of 2D gapless Majorana fermions on a boundary surface is related to the topological number ν_0 by the equation $(-1)^{N_0}=(-1)^{\nu_0}$. (2) When $(-1)^{\nu_0}=1$, a nontrivial ν_i implies the existence of 2D gapless Majorana fermions on

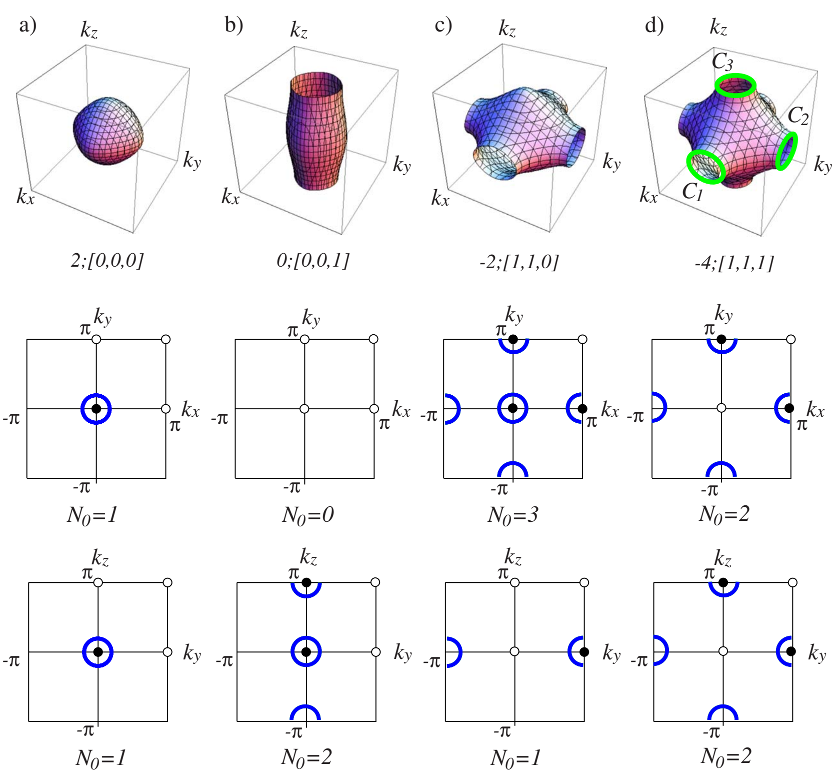

FIG. 2. (Color online) Various Fermi surface topologies in three dimensions and the corresponding gapless surface states for the 3D time-reversal-invariant spin-triplet superconductor with $\boldsymbol{d}(\boldsymbol{k})=\sin k_x\hat{\boldsymbol{x}}+\sin k_y\hat{\boldsymbol{y}}+\sin k_z\hat{\boldsymbol{z}}$. (Top row) Fermi surfaces in the first Brillouin zone and their topological invariants, $\chi(S_F);[p_0(C_1),p_0(C_2),p_0(C_3)]$. The green circles are C_j ($j=1,2,3$) for (d). (Middle and bottom rows) The corresponding surface states on the Brillouin zone for 001 surface (middle) and 100 surface (bottom) in the superconducting state. The blue solid circles symbolize the Dirac cones of the 2D gapless Majorana fermions and the energies of the surface states become zero at the time-reversal-invariant momenta enclosed by the blue circles. N_0 denotes the number of 2D gapless Majorana states on each surface.

TABLE I. Topological invariants of the Fermi surface and the possible number N_0 of gapless boundary states for full-gapped time-reversal-invariant spin-triplet superconductors. (a) 2D case. Here $p_0(S_F)$ denotes the number of connected components of the Fermi surface and N_0 the possible number of gapless helical Majorana pairs on an edge. (b) 3D case. Here $\chi(S_F)$ is the Euler characteristic of the Fermi surface, $p_0(C_k)$ the number of different connected components of the intersection C_k between the Fermi surface and the time-reversal-invariant plane with $\boldsymbol{k}=\boldsymbol{b}_k/2$, and m_i integers. The surface $\boldsymbol{G}$ is perpendicular to the reciprocal-lattice vector $\boldsymbol{G}$ and N_0 is the possible number of 2D Majorana fermion on the surface $\boldsymbol{G}$.

	(a)	
$(-1)^{p_0(S_F)}=-1$	$N_0=1,3,5,\cdots$	
$(-1)^{p_0(S_F)}=1$	$N_0=0,2,4,\cdots$	
	(b)	
$(-1)^{\chi(S_F)/2}=-1$	$N_0=1,3,5,\cdots$	
$(-1)^{\chi(S_F)/2}=1$	On a surface $\boldsymbol{G}=\Sigma_i(p_0(C_i)+2m_i)\boldsymbol{b}_i$	$N_0=0,2,4,\cdots$
	On a surface $\boldsymbol{G}\neq\Sigma_i(p_0(C_i)+2m_i)\boldsymbol{b}_i$	$N_0=2,4,6,\cdots$

surfaces determined by ν_i. To specify the surfaces, consider a surface $\boldsymbol{G}$ which is perpendicular to a reciprocal-lattice vector $\boldsymbol{G}$. If the surface $\boldsymbol{G}$ satisfies $\boldsymbol{G}\neq\Sigma_i(\nu_i+2m_i)\boldsymbol{b}_i$ for any integers m_i, then there exist 2D gapless Majorana fermions on the surface. Combining the former property with Eq. (16), we have a relation between the gapless surface state of a 3D time-reversal-invariant spin-triplet superconductor and its Fermi surface topology as

$$(-1)^{N_0}=(-1)^{\chi(S_F)/2}, \tag{18}$$

where N_0 the number of the 2D gapless Majorana fermions on the boundary surface. Moreover, taking into account the latter property as well, we obtain the following predictions. (i) When the Fermi surface satisfies $(-1)^{\chi(S_F)/2}=-1$, an odd number of 2D gapless Majorana fermions exist on each boundary surface. In particular, at least one gapless Majorana fermion exists on each boundary surface. (ii) When the Fermi surface satisfies $(-1)^{\chi(S_F)/2}=1$, the number of the 2D gapless Majorana fermions on a boundary surface is even. Then if the surface $\boldsymbol{G}$ satisfies $\boldsymbol{G}\neq\Sigma_i[p_0(C_i)+2m_i]\boldsymbol{b}_i$ with arbitrary integers m_i, at least two 2D massless Majorana fermions exist on the boundary surface $\boldsymbol{G}$. On the other hand, if $\boldsymbol{G}=\Sigma_i[p_0(C_i)+2m_i]\boldsymbol{b}_i$ with integers m_i, no gapless Majorana fermion is possible on the surface $\boldsymbol{G}$.

In Table I, we summarize the relations between the Fermi surface topology and the boundary gapless state.[16] Later, we will check these results by using concrete models.

For 3D time-reversal-invariant spin-triplet superconductors, it is also known that there exists another topological invariant $\nu_{\rm w}$ called the winding number.[17,18] Now we will derive a useful formula for $\nu_{\rm w}$ and show that $\nu_{\rm w}$ also has an intimate relation to the Fermi surface topology. In the single-band description, the winding number $\nu_{\rm w}$ is given by

$$\nu_{\rm w}=\frac{1}{12\pi^2}\int_{T^3}dk^3\epsilon^{ijk}\epsilon^{abcd}\hat{\eta}_a\partial_i\hat{\eta}_b\partial_j\hat{\eta}_c\partial_k\hat{\eta}_d, \tag{19}$$

where T^3 denotes the first Brillouin zone and $\hat{\eta}_a(\boldsymbol{k})=\eta_a(\boldsymbol{k})/\sqrt{\eta_a(\boldsymbol{k})^2}$ with $\eta_a(\boldsymbol{k})=[\boldsymbol{d}(\boldsymbol{k}),\epsilon(\boldsymbol{k})]$. $\nu_{\rm w}$ counts the number of times the unit vector $\hat{\eta}_a$ wraps the 3D sphere S^3 ($\hat{\eta}_a^2=1$) when we sweep T^3. In order for $\hat{\eta}_a$ to wind S^3, it is necessary to pass the poles of S^3 defined by $\boldsymbol{\eta}\equiv(\eta_1,\eta_2,\eta_3)\equiv\boldsymbol{d}=0$. So consider the set of zeros $\boldsymbol{k}^*$ satisfying $\boldsymbol{\eta}(\boldsymbol{k}^*)=0$. From the topological nature of $\nu_{\rm w}$, we can rescale $\epsilon(\boldsymbol{k})$ as $\epsilon(\boldsymbol{k})\to a\epsilon(\boldsymbol{k})$ ($a\ll1$) without changing the value of $\nu_{\rm w}$. Then it is found that only neighborhoods of the zeros contribute to $\nu_{\rm w}$ if a is small enough. By expanding η_a as $\eta_i=\partial_j d_i(\boldsymbol{k}^*)(\boldsymbol{k}-\boldsymbol{k}^*)_j+\cdots,(i=1,2,3)$, $\eta_4=\epsilon(\boldsymbol{k}^*)(\ll1)$, the contribution from the zero $\boldsymbol{k}^*$ is evaluated as

$$\nu_{\rm w}(\boldsymbol{k}^*)=-\frac{1}{2}{\rm sgn}[\epsilon(\boldsymbol{k}^*)]{\rm sgn}\{\det[\partial_j d_i(\boldsymbol{k}^*)]\}. \tag{20}$$

[When $\det[\partial_j d_i(\boldsymbol{k}^*)]=0$, Eq. (20) is generalized to

$$\nu_{\rm w}(\boldsymbol{k}^*)=-\frac{1}{2}{\rm sgn}[\epsilon(\boldsymbol{k})]i(\boldsymbol{k}^*), \tag{21}$$

where $i(\boldsymbol{k}^*)$ denotes the Poincaré-Hopf index[19] of the zero $\boldsymbol{k}^*$.] Summing up the contributions of all zeros, we have

$$\nu_{\rm w}=\sum_{\boldsymbol{\eta}(\boldsymbol{k}^*)=0}\nu_{\rm w}(\boldsymbol{k}^*). \tag{22}$$

From Eq. (22), we can show that $\nu_{\rm w}$ is also related to $\chi(S_F)$. For simplicity, suppose that the set of zeros $\boldsymbol{k}^*$ contains only the time-reversal-invariant points $\{\Gamma_a\}$. [Γ_a is always zero since it satisfies $\boldsymbol{d}(\Gamma_a)=0$.] Dividing the set of zeros into two subsets, $\Gamma_\pm\equiv\{\Gamma_a;{\rm sgn}\,\epsilon(\Gamma_a)=\pm1\}$, we obtain $\nu_{\rm w}=-\Sigma_{\Gamma_a\in\Gamma_+}i(\Gamma_a)/2+\Sigma_{\Gamma_a\in\Gamma_-}i(\Gamma_a)/2$. Then by using the Poincaré-Hopf theorem $\Sigma_{\boldsymbol{k}^*}i(\boldsymbol{k}^*)=0$,[20] it is recast into $\nu_{\rm w}=\Sigma_{\Gamma_a\in\Gamma_-}i(\Gamma_a)$. Here $i(\Gamma_a)$ is an odd integer because of $\boldsymbol{d}(-\boldsymbol{k})=-\boldsymbol{d}(\boldsymbol{k})$. Therefore, $\nu_{\rm w}$ is an odd (even) integer if Γ_- has an odd (even) number of elements. From this, we obtain the relation

$$(-1)^{\nu_{\rm w}}=\prod_{n_j=0,1}{\rm sgn}\,\epsilon(\Gamma_{a=(n_1,n_2,n_3)}). \tag{23}$$

Combining this with Eqs. (14) and (18), we find that $\nu_{\rm w}$ is also related to the Euler characteristic $\chi(S_F)$ and the number N_0 of 2D gapless surface states as

$$(-1)^{\nu_{\rm w}}=(-1)^{\chi(S_F)/2}=(-1)^{N_0}. \tag{24}$$

Let us now illustrate our results with simple and important examples. In Fig. 1, we illustrate possible Fermi surfaces in the normal state and the corresponding $p_0(S_F)$ in two dimensions. We also present the energy spectra for the corresponding superconducting states with edges. To obtain the energy spectra, we use the lattice model of the superconducting state with $\boldsymbol{d}=d(\sin k_x\hat{\boldsymbol{x}}+\sin k_y\hat{\boldsymbol{y}})$,

$$\mathcal{H}=\frac{1}{2}\sum_{ij}\boldsymbol{c}_i^{\dagger}H_{ij}\boldsymbol{c}_j,\quad H_{ij}=\begin{pmatrix} t_{ij} & i\boldsymbol{d}_{ij}\cdot\boldsymbol{\sigma}\sigma_2 \\ -i\boldsymbol{\sigma}\sigma_2\boldsymbol{d}_{ji} & -t_{ij}\end{pmatrix},\quad (25)$$

where $\boldsymbol{c}_i^{\dagger}=(c_{i\sigma}^{\dagger},c_{i\sigma})$ and t_{ij} and $\boldsymbol{d}_{ij}$ are given by $t_{ij}=-t_x(\delta_{i,j+\hat{x}}+\delta_{j,i+\hat{x}})-t_y(\delta_{i,j+\hat{y}}+\delta_{j,i+\hat{y}})-\mu\delta_{ij}$, $(d_x)_{ij}=-i(d/2)(\delta_{j,i+\hat{x}}-\delta_{i,j+\hat{x}})$, $(d_y)_{ij}=-i(d/2)(\delta_{j,i+\hat{y}}-\delta_{i,j+\hat{y}})$, and $(d_z)_{ij}=0$. The spectra are calculated for the system with two edges at $i_x=0,50$ under the periodic boundary condition in the y direction. In Fig. 1, k_y denotes the momentum in the y direction. While no gapless edge state exists in Fig. 1(a), it is found that there exist gapless edge states in the bulk gap in Figs. 1(b) and 1(c). The relation Eq. (17) holds in Fig. 1.

In Fig. 2, we show various Fermi surfaces in the first Brillouin zone and their topological numbers $\chi(S_F)$ and $p_0(C_i)$ $(i=1,2,3)$ in three dimensions. In addition, we present gapless 2D Majorana surface states for the superconducting states with $\boldsymbol{d}(\boldsymbol{k})=\sin k_x\hat{\boldsymbol{x}}+\sin k_y\hat{\boldsymbol{y}}+\sin k_z\hat{\boldsymbol{z}}$. This figure also confirms the connection between the gapless surface states and the Fermi surface topology. The relation $(-1)^{\chi(S_F)/2}=(-1)^{N_0}$ holds for all the cases. Furthermore, in the cases with $(-1)^{\chi(S_F)/2}=1$ [i.e., Figs. 2(b) and 2(d)], there exist a nonzero even number of 2D gapless Majorana fermions on a surface $\boldsymbol{G}\neq\Sigma_i(p_0(C_i)+2m_i\boldsymbol{b}_i)$ with integers m_i. Note that in Fig. 2, only the 001 surface in Fig. 2(b) does not satisfy this condition. In this case, we have $\boldsymbol{G}=\boldsymbol{b}_3$ and it coincides with $\Sigma_i p_0(C_i)\boldsymbol{b}_i=\boldsymbol{b}_3$. From Eq. (22), we find that ν_{w}'s for this gap function are (a) $\nu_{\mathrm{w}}=1$, (b) $\nu_{\mathrm{w}}=0$, (c) $\nu_{\mathrm{w}}=-1$, and (d) $\nu_{\mathrm{w}}=-2$, respectively. These values are also consistent with Eq. (24).

So far we have considered the single-band superconductor. However, the formulas (11) and (12) can be generalized to multiband systems. To see this, consider a multiband system which has the inversion symmetry and the time-reversal invariance in the normal state. If we assume that the parity operator transforms only the momentum as $\boldsymbol{k}\to-\boldsymbol{k}$,[21] then the Hamiltonian in the normal state is given by a $2N\times 2N$ matrix $\mathcal{E}(\boldsymbol{k})$ satisfying $\mathcal{E}(-\boldsymbol{k})=\mathcal{E}(\boldsymbol{k})$. ($N$ is the number of the bands.) Odd-parity superconducting states for this system are described by the generalized BdG Hamiltonian

$$H(\boldsymbol{k})=\begin{pmatrix}\mathcal{E}(\boldsymbol{k}) & \Delta(\boldsymbol{k})\\ \Delta(\boldsymbol{k})^{\dagger} & -\mathcal{E}(\boldsymbol{k})\end{pmatrix},\quad (26)$$

where the gap function $\Delta(\boldsymbol{k})$ is a $2N\times 2N$ matrix with odd parity, $\Delta(-\boldsymbol{k})=-\Delta(\boldsymbol{k})$. $H(\boldsymbol{k})$ has the property

$$\Pi H(\boldsymbol{k})\Pi^{\dagger}=H(-\boldsymbol{k}),\quad \Pi^2=1\quad (27)$$

with $\Pi=\mathbf{1}_{2N\times 2N}\otimes\tau_3$ and for $\boldsymbol{k}=\Gamma_a$, $H(\boldsymbol{k})$ becomes $H(\Gamma_a)=\mathcal{E}(\Gamma_a)\otimes\tau_3$. Thus in a similar manner as the single-band case, it is shown that

$$(-1)^{\nu}=\prod_{n_j=0,1}\prod_{m=1}^{N}\mathrm{sgn}\{E_{2m}[\Gamma_{a=(n_1,n_2)}]\}\quad \text{for two dimensions},\quad (28)$$

$$(-1)^{\nu_0}=\prod_{n_j=0,1}\prod_{m=1}^{N}\mathrm{sgn}\{E_{2m}[\Gamma_{a=(n_1,n_2,n_3)}]\},$$

$$(-1)^{\nu_k}=\prod_{n_{j\neq k}=0,1;n_k=1}\prod_{m=1}^{N}\mathrm{sgn}\{E_{2m}[\Gamma_{a=(n_1,n_2,n_3)}]\}$$

$$\text{for three dimensions},\quad (29)$$

where $E_n(\Gamma_a)$ $(n=1,\cdots 2N)$ are the eigenvalues of $\mathcal{E}(\boldsymbol{k})$ at $\boldsymbol{k}=\Gamma_a$ and we have set $E_{2m}(\Gamma_a)=E_{2m-1}(\Gamma_a)$ using the Kramers degeneracy. For a filled or empty band in the normal state, the signatures of $E_n(\Gamma_a)$ are the same for all the time-reversal points, so their contributions to Eqs. (28) and (29) are canceled. Therefore, in order to evaluate the $\boldsymbol{Z}_2$ numbers, it is enough to consider bands with the Fermi surfaces. Again it is evident that topological properties of the spin-triplet superconducting state are closely related to the topology of the Fermi surface.

Finally we make several comments in order. (a) Although we have assumed that the normal state has the inversion symmetry, our formulas (11) and (12) [or (28) and (29)] could be useful even for the systems which do not have the inversion symmetry in the normal state. Adiabatic continuity allows us to calculate the topological invariants if the system is adiabatically connected to materials which have the inversion symmetry in the normal state. The topological invariants for a class of noncentrosymmetric superconductors can be calculated in this manner.[22,23] (b) For spin-singlet superconductors, due to the inversion symmetry, their $\boldsymbol{Z}_2$ numbers are calculated by the technique developed in Ref. 6. However, it is found that all the $\boldsymbol{Z}_2$ numbers are trivial.[24] Therefore, the correspondence between the Fermi surface topology and the gapless surface state discussed in this paper are inherent to spin-triplet superconductors. (c) In this paper we have focused on the time-reversal-invariant spin-triplet superconductors. Here we mention a generalization to the time-reversal-breaking case in brief. For 2D chiral spin-triplet superconductors such as a $p+ip$ state, the topological properties are determined by the TKNN number ν_{TKNN}. In a similar manner to ν_{w}, in the single-band description it can be shown that the TKNN number is related to the Fermi surface topology by the equation

$$(-1)^{\nu_{\mathrm{TKNN}}}=(-1)^{p_0(S_F)},\quad (30)$$

where $p_0(S_F)$ is the number of the connected components of the Fermi surface.[24] This relation gives a simple explanation of the quantum phase transition from the weak paring phase to the strong one discussed in Ref. 25. This phase transition is accompanied with disappearance of the Fermi surface, thus $p_0(S_F)=1\to p_0(S_F)=0$. From the above relation, this causes a change of ν_{TKNN} which brings about different topological properties between the weak and strong phases.

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