Topological $D+p$-wave superconductivity in Rashba systems

Tomohiro Yoshida$^1$ and Youichi Yanase$^2$

$^1$Department of Physics, Gakushuin University, Tokyo 171-8588, Japan
$^2$Department of Physics, Kyoto University, Kyoto 606-8502, Japan

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We show two-dimensional “strong” topological superconductivity in $d$-wave superconductors (SCs). Although the topological invariant of the bulk wave function cannot be defined in $d_{x^2-y^2}$-wave and $d_{xy}$-wave SCs because of nodal excitations, the bulk energy spectrum of $d$-wave SCs on a substrate is fully gapped in a magnetic field. Then the superconducting state is specified by a nontrivial Chern number, and hence topologically nontrivial properties are robust against disorders and interactions. We discuss high-temperature topological superconductivity in cuprate SCs recently fabricated on a substrate. Furthermore, we show that the three-dimensional noncentrosymmetric $d$-wave SC is a Weyl SC hosting topologically protected Weyl nodes. Noncentrosymmetric heavy-fermion SCs, such as CeRhSi$_3$ and CeIrSi$_3$, are candidates for Weyl SCs.

I. INTRODUCTION

Topological insulators and superconductors (SCs) have evolved into a new research field in modern condensed matter physics$^{1,2}$. In particular, distinct properties of topological SCs accompanied by Majorana fermions obeying non-Abelian statistics$^{3,4}$ have attracted broad interest$^{5-22}$. Although conventional $s$-wave SCs are topologically trivial in most cases, effectively spinless band structures may produce topological superconductivity. For example, a surface state of a topological insulator$^{23,24}$, low-carrier-density Rashba systems$^{14,15}$, and magnetic atom chains$^{26,27}$ may host topological superconductivity, and experimental indications have been obtained$^{22,23}$.

Although a particular band structure is needed for the above $s$-wave topological superconductivity, topological superconductivity may be realized in non-$s$-wave SCs in a wider range of conditions. However, the topological superconducting state induced by such unconventional Cooper pairing has not been established so far. This is mainly because the condition for odd-parity superconductivity is hardly satisfied in real materials although many theoretical proposals for topological superconductivity assume odd-parity SCs$^{3-6,16-18}$. Indeed, few materials host odd-parity superconductivity$^{24,25}$. Unfortunately, experimental evidence of the topological edge state has not yet been reported in the rare candidate for a chiral $p$-wave SC, Sr$_2$RuO$_4$ $^{26}$. Although UPt$_3$ is considered to be an odd-parity spin-triplet SC$^{25}$, the nodal gap structure obscures the definition of the bulk topological invariant. Odd-parity superconductivity has been proposed in the doped-topological insulator Cu$_2$Bi$_2$Se$_3$ $^{17,18}$, but the experimental evidence is still under debate$^{26,27}$.

In contrast to odd-parity $p$-wave or $f$-wave superconductivity, even-parity $d$-wave superconductivity occurs in a variety of strongly correlated electron systems$^{28-32}$. Therefore, a design for topological superconductivity based on the $d$-wave SC may lead to a major breakthrough. However, canonical $d$-wave SCs are not topological SCs in the strong sense$^{33}$ owing to the nodal superconducting gap. In this paper, we propose a method for making a two-dimensional (2D) gapless $d$-wave SC be a gapped “strong” topological SC. We also show a Weyl SC based on a three-dimensional (3D) $d$-wave SC.

![FIG. 1. (Color online) (a) Schematic of a $d$-wave SC on a substrate. (b) Magnetic-field dependence of the bulk superconducting gap defined by $E_{\text{min}} = \text{Min}_{\kappa} |E_n(k)|$, where $E_n(k)$ are eigenvalues of the BdG Hamiltonian. Squares were obtained for $t = 1$, $t' = 0.25$, $\mu = -0.56$, $\alpha = 0.3$, $\Delta_1 = 0.01$, and $\Delta_2 = 0.002$ ($D+p$-wave SC); circles, for $\Delta_1 = 0$ (purely $d$-wave SC).](image-url)

II. TWO-DIMENSIONAL TOPOLOGICAL SUPERCONDUCTIVITY

A setup for the 2D topological SC is schematically shown in Fig. 1(a). We consider a $d$-wave SC on a substrate, which has been realized in high-$T_c$ cuprate SCs, La$_{2-x}$Sr$_x$CuO$_{4-y}$, YBa$_2$Cu$_3$O$_{6+y}$, La$_2$CuO$_{4+\delta}$, and Pr$_{2-x}$Ce$_x$CuO$_{4+\delta}$. Interestingly, electrostatic control of the superconducting state by use of the gate voltage has been achieved in these SCs. Because of the asymmetric potential due to the substrate and/or the gate voltage, $p$-wave Cooper pairs are admixed with $d$-wave ones through spin-orbit coupling$^{34,35}$. This noncentrosymmetric $D+p$-wave SC is still gapless, since the gap node is topologically protected in the presence of time-reversal symmetry$^{36,37}$. On the other hand, Fig. 1(b) indicates a fully gapped bulk energy spectrum when time-reversal symmetry is broken by a magnetic field along the $c$ axis. Thus, we can define the strong topological index of gapped...
quantum phases classified by the so-called topological periodic table\textsuperscript{26–29}. In the following part, we demonstrate that the 2D $D+p$-wave SC is a topological SC specified by the nontrivial topological number in symmetry class $D$.

We study 2D $D+p$-wave SCs by adopting the Bogoliubov-de Gennes (BdG) Hamiltonian, $\mathcal{H} = \frac{1}{2} \sum_{k} \Psi_{k}^{\dagger} \mathcal{H}(k) \Psi_{k}$, where

\begin{equation}
\mathcal{H}(k) = \begin{pmatrix}
\mathcal{H}_{0}(k) & \Delta(k) \\
\Delta^\dagger(k) & -\mathcal{H}_{0}^*(k)
\end{pmatrix},
\end{equation}

and $\Psi_{k} = (c_{k}^d, \ldots, c_{-k}^s)$, with $c_{k}$ being the annihilation operator of electrons with momentum $k$ and spin $s$. The normal-part Hamiltonian is given by $\mathcal{H}_{0}(k) = \xi(k)\sigma_{0} - \mu_{B} H_{z} \sigma_{z} + \alpha g(k) \cdot \sigma$. We assume a dispersion relation $\xi(k) = -2t(cos k_{x} + cos k_{y}) + 4t' cos k_{x} cos k_{y} - \mu$, which reproduces the Fermi surface of high-$T_{c}$ cuprate SCs. Effects of the magnetic field $H_{z}$ are taken into account through the Zeeman coupling term. The asymmetric potential due to the substrate and/or the gate voltage gives rise to Rashba spin-orbit coupling with $g$-vector, $g(k) = (-\sin k_{y}, \sin k_{x}, 0)$\textsuperscript{24}. As a result of the Rashba spin-orbit coupling, the order parameter is described as $\Delta(k) = i\psi(k) + d(k) \cdot \sigma \sigma_{y}$, where a spin-singlet component $\psi(k)$ and a spin-triplet component $d(k)$ are admixed. In this paper we study the $D+p$-wave superconducting state by adopting a simple form, $\psi(k) = \Delta_{s}(cos k_{x} - cos k_{y})$ and $d(k) = \Delta_{t}(sin k_{y}, sin k_{x}, 0)$. Both the $d$-wave component and the $p$-wave component belong to the $B_{1}$ representation of the noncentrosymmetric $C_{4v}$ point group, and thus these two components admix with each other as explicitly shown in a microscopic calculation\textsuperscript{24}. Since we focus on dominantly $d$-wave SCs, we assume that $|\Delta_{s}| > |\Delta_{t}|$. As shown in Fig. 1(b), the superconducting gap $E_{\text{min}}$ linearly increases with $H_{z}$ when $\Delta_{t} \neq 0$, while $E_{\text{min}} = 0$ for $\Delta_{t} = 0$. Thus, the fully gapped superconducting state is realized by cooperation of the magnetic field, Rashba spin-orbit coupling, and parity mixing in Cooper pairs.

Since the BdG Hamiltonian belongs to symmetry class $D^{28–30}$, the 2D gapped state is specified by the Chern number $\nu$\textsuperscript{45,46}.

\begin{equation}
\nu = \frac{i}{2\pi} \int \text{d}k \epsilon^{ij} \sum_{E_{n}(k) < 0} \partial_{k_{i}} \langle u_{n}(k) | \partial_{k_{j}} u_{n}(k) \rangle,
\end{equation}

where $|u_{n}(k)\rangle$ is the wave function of Bogoliubov quasi-particles with energy $E_{n}(k)$. Figure 2 shows the topological phase diagram as a function of the chemical potential and magnetic field. Interestingly, the Chern number is nontrivial, $\nu = 4$, in a large parameter regime near half-filling, where $d$-wave superconductivity is likely induced by the antiferromagnetic spin fluctuation\textsuperscript{28–30}. Thus, in the magnetic field the $d$-wave SC on the substrate is a strong topological SC specified by the nontrivial bulk topological invariant. As expected from the bulk-edge correspondence, four chiral Majorana modes appear near the edge as shown in Fig. 3. The high transition temperatures of cuprate SCs may enable experimental observations of Majorana states by use of the available technology.

The topological superconducting state demonstrated above is outside the classification scheme of gapless $d$-wave superconducting states\textsuperscript{26}. The $Z_{2}$ index obtained by Sato and Fujimoto\textsuperscript{26} is equivalent to the parity of the Chern number in the gapped phase, that is, $\nu_{2} = (\nu)^{\nu}$. Thus, the $Z_{2}$ index $\nu_{2}$ is trivial in the phase with $\nu = 4$ or 6. According to Fig. 2 a nontrivial $Z_{2}$ index is obtained when the chemical potential is close to the band edge ($\nu = 1$). However, an unfeasible fine-tuning of the chemical potential may be needed, and the $d$-wave superconductivity mediated by the antiferromagnetic spin fluctuation is not likely to occur in such a low-carrier-density
region\textsuperscript{30}. On the other hand, the topological superconducting state with $\nu = 4$ is stabilized near half-filling without any fine-tuning of parameters.

A gapped $d$-wave superconducting state in one-dimensional nanowires has been studied, and its topologically nontrivial properties are specified by the winding numbers\textsuperscript{48}. We think that the 2D topological SC proposed in this paper may be more feasible than the one-dimensional nanoscale SC.

III. THREE-DIMENSIONAL WEYL SUPERCONDUCTIVITY

Next, we investigate 3D $d$-wave SCs. The $d$-wave superconductivity occurs in many Ce-based heavy-fermion SCs having 3D Fermi surfaces\textsuperscript{34,49}. The crystal structure of CePt$_3$Si\textsuperscript{49}, CeRhSi$_3$\textsuperscript{50}, CeSi$_2$\textsuperscript{51}, and CeCoGe\textsuperscript{52} lacks inversion symmetry, and hence the 3D $D+p$-wave state may be stabilized in these SCs. We show here that this superconducting state realizes a Weyl SC\textsuperscript{53–57}, that is, an analog of the Weyl semimetal attracting great attention recently\textsuperscript{55–64}.

We again adopt the BdG Hamiltonian in Eq. (1), and assume here an isotropic dispersion relation in the cubic lattice, $\xi(k) = -2t(\cos k_x + \cos k_y + \cos k_z) - \mu$. In contrast to the 2D model adopted above, next-nearest-neighbor hopping is ignored for simplicity. Slicing the 3D Brillouin zone at a fixed $k_z$, we consider an effective 2D model parametrized by $k_z$. Then the $k_z$-dependent Chern number $\nu(k_z)$ is defined as a topological invariant of the 2D model by Eq. (2). Note that the 2D model depends on $k_z$ through the $k_z$-dependent chemical potential, $\mu'(k_z) = \mu + 2t \cos k_z$. Although we set $t'=0$, the topological phase diagram of the 2D model is qualitatively the same as Fig. 2. Indeed, the Chern number changes $\nu(k_z) = 0 \rightarrow 1 \rightarrow 0 \rightarrow 4 \rightarrow 0 \rightarrow 1 \rightarrow 0$ with increasing $\mu'(k_z)$.

In order to clarify the topological properties of the 3D $D+p$-wave SC, it is useful to consider the winding number, introduced as follows. The magnetic mirror symmetry preserved in the system ensures the symmetry of the BdG Hamiltonian, $TM_{xz}\hat{\mathcal{H}}(k)M_{xz}^{-1}T^{-1} = \hat{\mathcal{H}}(-k_x, k_y, -k_z)$, where $TM_{xz}$ is the product of the time-reversal symmetry $T$ and the mirror symmetry with respect to the $xz$-plane $M_{xz}$. Thus, the BdG Hamiltonian preserves the combined anti-symmetry $\Gamma \hat{\mathcal{H}}(k) \Gamma^{-1} = -\hat{\mathcal{H}}(k_x, -k_y, k_z)$, with $\Gamma = PTM_{xz}$ and $P$ being the particle-hole symmetry. This symmetry reduces to chiral symmetry on the magnetic-mirror-invariant planes, namely, at $k_y = 0$ and $\pi$. The mirror symmetry ensures that the BdG Hamiltonian is off-diagonal in the basis where $\Gamma$ is diagonal:

$$U\hat{\mathcal{H}}(k)U^{-1} = \begin{pmatrix} 0 & q(k) \\ q^\dagger(k) & 0 \end{pmatrix}. \quad (3)$$

Then we can define the integer winding number,

$$W(k_y, k_z) = \frac{1}{4\pi i} \int_{-\pi}^{\pi} dk_z \text{Tr}[q^{-1}(k)\partial_{k_z} q(k) - q^{-1}(k)\partial_{k_z} q^\dagger(k)], \quad (4)$$

at $k_y = 0$ and $\nu = 0, 1, 2, 3$. Hereafter, we denote $W(k_z) = W(0, k_z)$ and $W'(k_z) = W(\pi, k_z)$. The winding numbers of 2D $D+p$-wave SCs, $W$ and $W'$, are defined in the same way as Eq. (4), and they are shown in Fig. 2.

When the Fermi surface encloses the $\Gamma$ point in the first Brillouin zone ($k = 0$), we obtain the $k_z$-dependent topological numbers in Fig. 4. The Chern number changes $\nu(k_z) = 4 \rightarrow 0 \rightarrow 1 \rightarrow 0$ with increasing $|k_z|$, while the winding number changes as $W(k_z) = 0 \rightarrow 2 \rightarrow 1 \rightarrow 0$. Note that $\nu(k_z) = \nu(-k_z)$ and $W(k_z) = W(-k_z)$. Figure 4 does not show the trivial winding number, $W'(k_z) = 0$.

A discrete jump of topological numbers indicates a nodal gap structure, since the topological number does not change without closing the bulk excitation gap. Indeed, we find point nodes in the superconducting gap at $k_z$ where the Chern number changes. For parameters in Fig. 4, four point nodes appear at $k_z/\pi = \pm 0.555$, where the Chern number changes as $4 \rightarrow 0$. The positions of the nodal points are $k = (k', 0, \pm 0.555\pi)$ and symmetric momentum, and we obtain

$$\cos k' = \frac{1}{\alpha^2(\Delta_s^2 + \Delta_t^2)} \left[ \alpha^2 \Delta_s^2 - \alpha \Delta_1 \sqrt{\alpha^2 \Delta_t^2 + (\mu_B H_s)^2}(\Delta_s^2 + \Delta_t^2) \right]. \quad (5)$$

We also see point nodes at $k = (0, 0, \pm 0.705\pi)$ and $k = (0, 0, \pm 0.856\pi)$, as expected from Fig. 4. Thus, the number of point nodes coincides with the jump of the Chern number. This means that all of the point nodes are specified by the topological Weyl charge $\omega = \pm 1$, which is the monopole charge of the Berry flux\textsuperscript{53–60}. Therefore, the $D+p$-wave SC with a 3D Fermi surface is classified as a Weyl SC.
FIG. 5. (Color online) Surface energy spectra of a 3D $D+p$-wave SC at (a) $k_z/\pi=0$ \([\nu(k_z),W(k_z)]=(4,0)\], (b) $k_z/\pi=0.6$ \([0,2]\], (c) $k_z/\pi=0.71$ \([1,1]\], and (d) $k_z/\pi=0.8$ \([1,1]\]. Parameters are the same as in Fig. 4. (e) Schematic of zero-energy surface states. Solid (blue) lines show Majorana loop and Majorana arcs. Double Majorana arcs are illustrated by thick lines. Circles represent projections of Weyl nodes.

The bulk-surface correspondence ensures topologically stable Majorana surface states in Weyl SCs. We show surface energy spectra of the 3D $D+p$-wave SC in Fig. 5. At momentum $k_z$ where the Chern number is $\nu(k_z)=4$ \([Fig. 5(a)]\), four chiral Majorana modes appear, similarly to the 2D $D+p$-wave state (see Fig. 3). At $k_z$ where $\nu(k_z)=0$ \([Fig. 5(b)]\), two chiral Majorana modes in Fig. 5(a) disappear. Instead, double Majorana surface modes emerge at $k_y=0$, and they are indicated by the nontrivial winding number $W(k_z)=2$ in accordance with the index theorem.\(^{41}\) The total chirality of topological surface states is 0, as ensured by the trivial Chern number $\nu(k_z)=0$. When $|k_z|$ is increased so that \([\nu(k_z),W(k_z)]=(1,1)\), a single chiral Majorana mode is observed at $k_y=0$ as indicated by the winding number \([Figs. 5(c) \text{ and } 5(d)]\). Figure 5(c) shows additional zero-energy states, while Fig. 5(d) does not. Indeed, a pair annihilation of zero-energy states occurs, accompanying the sign change in the velocity of the Majorana mode at $k_y=0$. This pair annihilation gives rise to a high surface density of states as shown in the superconducting Weyl semimetal.\(^{65}\) When $|k_z|$ is increased further, the surface state disappears.

Summarizing these results we obtain a schematic of the topological surface states in Fig. 5(e). One Majorana loop and several Majorana arcs appear on the surface of the 3D $D+p$-wave SC in the presence of the magnetic field along the $c$ axis. Majorana arcs terminate at the projection of Weyl nodes as expected. The surface states obtained here are quite different from those in chiral SCs,\(^ {54–57} \) which are other candidates for Weyl SCs.

IV. SUMMARY

In this paper, we show that the 2D $D+p$-wave SC is a strong topological SC in the presence of Rashba spin-orbit coupling and a Zeeman field. We demonstrate Majorana edge modes protected by a nontrivial Chern number. The topological invariant and topological edge states elucidated in this paper are different from those in nodal $d$-wave SCs.\(^ {42–44} \) The latter are specified by a weak topological index and accompanied by a flat edge band. Although the flat edge band is fragile against disorders, the chiral Majorana modes obtained in this paper are robust against disorders and interactions.\(^ {6,9,66} \) We also show that the 3D $D+p$-wave SC is a Weyl SC in the Zeeman field. The bulk energy spectrum hosts at least six pairs of Weyl nodes, which are specified by the topological Weyl charge, $\omega=\pm1$. Topological surface states are characterized by the Majorana loop and Majorana arcs.

The $d$-wave superconducting state is stabilized in a variety of strongly correlated electron systems, such as the high-$T_c$ cuprate SC,\(^ {28,29} \) heavy-fermion SC\(^ {31} \), and organic SCs.\(^ {32} \) Furthermore, Rashba spin-orbit coupling is introduced into the 2D high-$T_c$ cuprate SC\(^ {48–50} \) and 3D heavy-fermion SC\(^ {49–52} \) by intrinsically or externally breaking the space inversion symmetry. Artificial control of dimensionality has also been achieved in heavy-fermion superlattices.\(^ {67–69} \) We suggest that the topological SC and Weyl SC may be realized in these systems by applying a magnetic field.

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