Topological indices, defects and Majorana fermion in chiral superconductors

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(Dated: May 22, 2014)

We study theoretically the role of topological invariants to protect the Majorana fermions in a model of two-dimensional chiral superconductors which belong to class D of topological periodic table. A rich phase diagram is revealed. Each phase is characterized by the topological invariants for 2d (Z) and 1d (Z\textsubscript{2}), which lead to the Majorana fermion at the edge of the dislocation and the core of the vortex. Interference of the Majorana fermions originated from the different topological invariants is studied. The stability of the Majorana fermion with respect to the interlayer coupling, i.e., in 3d, is also examined.

PACS numbers: 74.20.-z, 74.62.Dh, 71.10.Pm

Keywords: topological superconductor, Majorana fermion, vortex, dislocation

Topological classification of the electronic states in solids has shed a new light on the band structure of solids and also the superconductivity \cite{1}. Initiated by the proposal of Z\textsubscript{2} topological invariant and the quantum spin Hall effect in two-dimensional spin-orbit coupled system \cite{2} and its extension to three dimensions \cite{3}, the more generic topological classification scheme, i.e., topological periodic table, is now available based on the three symmetries, i.e., time-reversal (\Theta), particle-hole (\Xi), and chiral (\Pi) symmetries \cite{4,5}. Here \Xi symmetry is due to the periodic table, is now available based on the three symmetries, i.e., time-reversal (\Theta), particle-hole (\Xi), and chiral (\Pi) symmetries \cite{4,5}. Here \Xi symmetry is due to the periodicity called Bott periodicity which relates the different topological invariants for \textit{d} and \textit{D} systems, i.e., in 3d, is also examined.

This topological periodic table provides the powerful guiding principle also for the topological superconductors (TSs). Especially, the Majorana fermions expected to appear at the edge or the core of the vortex in TSs attract intensive interests from the viewpoint of the quantum information technology \cite{9,14}. Therefore, it is an important theoretical issue to design the Majorana fermions in realistic systems. Proximity-induced superconductivity in 3d TI \cite{13}, the superconductivity in a doped TI Cu\textsubscript{2}Bi\textsubscript{2}Se\textsubscript{3} \cite{16,17}, the possible TS in noncentrosymmetric systems with the Rashba spin splitting \cite{18,22}, and \textit{p} wave superconductivity in Sr\textsubscript{2}RuO\textsubscript{4} \cite{24} are the promising candidates as the host of the Majorana fermions. As pointed out in ref. \cite{25}, most of the theoretical proposals for the Majorana fermions are based on the two models, i.e., \textit{p}-wave pairing in the one-dimensional spinless fermions (Kitaev model \cite{25}) and the \textit{p}+\textit{i}\textit{p} pairing superconductor.

In this paper, we study theoretically the topological invariants and their relation to the protected Majorana bound states in a model of class D chiral superconductors containing both the Kitaev model and \textit{p}+\textit{i}\textit{p} superconductor in the limiting cases. The topological invariant for class D is 0 for \delta = 3, Z for \delta = 2, and Z\textsubscript{2} for \delta = 1. Therefore, there is no "strong TS" in 3d, while the 2d system is characterized by \textit{Z} topological invariant and the 1d system by Z\textsubscript{2} topological invariant. The purpose of the present Letter is to reveal the topological phase diagram characterized by these invariants, and the associated Majorana fermions at the textures such as dislocations and vortices.

We consider a generalized model of \textit{p}+\textit{i}\textit{p} wave superconductor on a square lattice in 2d. The Hamiltonian can be written as \textit{H} = \sum\textit{k} \textit{C}^\dagger\textit{k} \textit{H}(\textit{k}) \textit{C}_{\textit{k}} with

\begin{equation}
H(\textit{k}) = 
\begin{pmatrix}
2\ell_x \cos k_x + 2\ell_y \cos k_y - \mu & d_x \sin k_x - i d_y \sin k_y \\
\mu - 2\ell_x \cos k_x - 2\ell_y \cos k_y & d_x \sin k_x + i d_y \sin k_y
\end{pmatrix},
\end{equation}

and \textit{C}^\dagger = (c_{\textit{k}}^\dagger, c_{-\textit{k}}). This 2 \times 2 Hamiltonian matrix can
be expressed as $H(k) = H(k_x, k_y) = h(k) \cdot \sigma$ where $\sigma = (\sigma^x, \sigma^y, \sigma^z)$ is the vector of Pauli matrices. Since $(C^\dagger_{-k})^T = \sigma^2 C_k$, $H(k)$ should satisfy

$$H(k) = -\sigma^x H(-k)^T \sigma^x$$

(2)

where $T$ means the transpose. This condition leads to the relation [24]

$$h_{x,y}(k) = -h_{x,y}(-k), \quad h_z(k) = h_z(-k).$$

(3)

Therefore, for the time-reversal invariant momenta (TRIM), which satisfy $k \equiv -k$, only $h_z(k)$ cannot be nonzero, i.e., $h(k)$ points either in $+z$ or $-z$ directions as long as the gap opens, i.e., $|h(k)| > 0$. There are 4 TRIMs in this 2d model, i.e., $k_x = (0,0), (\pi,0), (0,\pi)$ and $(\pi,\pi)$, and the sign $s_0 = \pm 1$ of the corresponding $h_z$. As will be discussed, $s_0$ determines the $Z_2$ topological invariants and the parity of the $Z$ invariant.

Now let us start with the $Z_2$ invariant. For this purpose, let us consider the 1d Hamiltonian with fixed $k_x = \pi$ in eq. (1), i.e.,

$$H(k_x = \pi, k_y) = 
\begin{pmatrix}
-2t_x + 2t_y \cos(k_y) & -\mu \\
\mu & 2t_x - 2t_y \cos(k_y)
\end{pmatrix},$$

(4)

which is nothing but the Kitaev model for a one dimensional topological superconductor [9]. The $Z_2$ topological invariant $\nu_x$ is related to the “polarization” $2\nu_x$.

$$\frac{\nu_x}{2} = P(k_x) = \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} a_y(k_x, k_y) \mod 1.$$ 

(5)

given by the Berry phase vector potential $a_j(k_x, k_y) = -i \frac{1}{\hbar} \sum_{n:occ} \langle\mu|\partial_j\psi_n|\mu\rangle$, and is given by $(-1)^{y_x} = s_{x(\pi,0)}^y s_{y(\pi,\pi)}$. Therefore, we can easily obtain the $Z_2$ topological invariant $\nu_x$ as

$$\nu_x = \begin{cases} 1 & \text{for } |t_x + \frac{\mu}{2}| < |t_y| \\ 0 & \text{for } |t_x + \frac{\mu}{2}| > |t_y| \end{cases}$$

(6)

The topological invariant $\nu_x'$ for $k_x = 0$ can be also calculated in a similar way. From these equations, it is clear that strengths of $d_x$ and $d_y$ are not related to the topological numbers if they have finite values. The $Z_2$ invariants $\nu_y, \nu_y'$ are obtained in the similar way.

On the other hand, the $Z$ topological invariant $\nu$ is nothing but the Chern number, i.e., the wrapping number of the mapping from the 1st Brillouine zone of $k$ to the unit sphere $h(k)/|h(k)|$ and is given by

$$\nu = \int_{BZ} \frac{dk_x dk_y}{2\pi} \left\{ \partial_{k_x} a_y(k_x, k_y) - \partial_{k_y} a_x(k_x, k_y) \right\}.$$ 

(7)

Equations (5) and (7) lead to the relation [3, 21, 25, 26]

$$\nu_x + \nu_x' = \nu_y + \nu_y' = \nu \mod 2.$$ 

(8)

In summary, our model is characterized by $Z$ topological invariant $\nu$ and two $Z_2$ topological invariants $\nu_x$ and $\nu_y$. This is the general result, and superconductors in class $D$ in 2d are characterized by $\nu : \nu_x \nu_y$. From the above consideration, these topological invariants depend on the hopping integrals $t_x, t_y$ and the chemical potential $\mu$, while do not depend on the pairing amplitudes $d_x, d_y$ as long as they are finite. Therefore, we show in Fig. 1 the phase diagram of the present model in the plane of $(t_x, t_y)$ for fixed $\mu$. The lines where the energy gap closes divide the $(t_x, t_y)$-plane into nine domains. Electronic states are characterized by topological invariants in each domain. When $|\mu|$ is larger than $|t_x| + |t_y|$, i.e., domain $V$, the pairing state is topologically trivial since it corresponds to the strong coupling limit. In the domain $I, IV, V, VI, VIII$, and $IX$, the anisotropy between $t_x$ and $t_y$ is large and hence the system behaves basically as the weakly coupled chains of 1d Kitaev models, and the system has only 1d $Z_2$ topological invariants but $Z$ topological invariant $\nu = 0$, so they are weak topological states.

Now we turn to the consequences of the topological invariants. The $Z_2$ invariant $\nu_x (\nu_y)$ ensures that the propagating Majorana fermion channels appear at the edge along $x$ direction ($y$ direction). They have zero-energy

FIG. 1: The topological phase diagram of a model in eq. (1) for chiral superconductors in 2d characterized by $\nu : \nu_x \nu_y$. The lines where the energy gap closes divide the $(t_x, t_y)$-plane into nine domains. The system is the strong topological superconductors ($\nu = 1$) in the domains $\text{I, II, III, VII and VIII}$, while it is weak topological superconductor in the domains $\text{I, IV, V, VI and IX}$ with $\nu = 0$ but some of $Z_2$ invariants being nonzero. In the domain $V$, the system is the trivial strong coupling superconductor.

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In this equation, we define $G$ vector $B$ energy states are localized at each edge dislocation. Probability distribution of the zero-energy states. Zero-energy states exist, which are 2-fold degenerate because the 2 edge dislocations are present in the system. The right figure of Fig. 3 indicates the probability distribution for the zero-energy states. The zero energy Majorana bound state appear at each of the edge dislocations.

It is clear that zero-energy states exist, which are 2-fold degenerate because the 2 edge dislocations are present in the presence of edge dislocations.

We introduce two edge dislocations with the Burgers vector $B = \pm e_x$. We represent two edge dislocations by adding lattice sites between them. Edge dislocations are separated by a half system size. Calculations were done on a 40 unit cell system with a periodic boundary condition along $x$- and $y$-directions. The parameters are $t_x = 0.5$, $t_y = 0.5$, $d_x = 0.6$, $d_y = 0.6$, $\mu = 0.2$. In these parameters, the topological invariants are 1 : 11. In this case: $G = \frac{1}{2\pi}(e_x | b_x + b_y)$ and $B = \pm e_x$. $B \cdot G = 1$ is satisfied, so zero-energy states appear at edge dislocations.

The results of our numerical calculations are shown in Fig. 4. The left figure of Fig. 4 indicates the energy levels of our model in the presence of edge dislocations. It is clear that zero-energy states exist, which are 2-fold degenerate because the 2 edge dislocations are present in the system. The right figure of Fig. 4 indicates the probability distribution of the zero-energy states. Zero-energy states are localized at each edge dislocation.

In the presence of edge dislocations with the Burgers vector $B = \pm e_x$, zero-energy states appear in the domain $I, II, VI, VII$ and $IX$ in Fig. 4 in the case of $\mu > 0$ and zero-energy states appear in the domain $I, III, VIII$ and $IX$ in Fig. 4 in the case of $\mu < 0$. In particular, zero-energy states in the domain $I$ and $IX$ can be intuitively interpreted as follows. The weak topological superconductors in these domains are adiabatically connected to a stack of the Kitaev models $[9]$ for a 1d topological superconductor along $y$-direction. In the presence of edge dislocations, the edges of 1d topological superconductor appear at edge dislocations as shown in Fig. 2. So zero-energy states appear there. In general, the existence of zero-energy states is proved by the same method as in ref. [3].

Next we consider the interference of the $Z$ and $Z_2$ topological invariants, which is realized in the present model. When $Z$ is nonzero, the zero energy Majorana bound state is realized at the core of the vortex. It is expected that, if the dislocations are in the crystal, they act as the pinning centers of the vortex, and hence there are two reasons for the existence of the Majorana bound states when $Z_2$ invariant is 1. This situation occurs in the domains $II, III, VII$, and $VIII$ in Fig. 1, and the interference of these two mechanisms is an issue. Figure 3 summarizes the calculated results, in which there are dislocations and vortex cores at same positions. The probability distributions are plotted for the zero energy states if any. To introduce a periodic boundary condition, we introduce two vortices with the winding number 1 and two vortices with the winding number -1. We consider the two cases of topological invariants $1: 00$ (upper panels) and $1: 11$ (lower panels). The parameters are $t_x = 0.5$, $t_y = 0.5$, $d_x = 0.6$, $d_y = 0.6$, $\mu = 0.2$ for the former, while they are $t_x = 0.5$, $t_y = 0.5$, $d_x = 0.6$, $d_y = 0.6$, $\mu = 0.2$ for the latter. Calculations were done on a 40×40 unit cell system with a periodic boundary condition along $x$ and $y$-directions. There are dislocations and vortex cores at same positions in the right panels while only dislocations are there in the left panels. They are separated from each other by a half system size. In the case of the topological invariants $1: 00$, zero-energy states do not appear at edge dislocations. Zero-energy states appear when the dislocations and vortices exist at the same time because of the $Z$ invariant $\nu = 1$ and vortices. We have also confirmed that the zero-energy states appear with only the vortices. In the case of the topo-
to the state in the domain in the case, the electronic state is adiabatically connected
parameters because the state in the domain \( t \) in Fig. 1. If \( t \) case of
zeros |\( x \), \( y \), and \( z \)-directions. We found that these zero-energy
The authors acknowledge the fruitful discussion with Yukio Tanaka, and Sho Nakosai. This work is supported
by Grant-in-Aid for Scientific Research (Grants No. 17071007, No. 17071005, No. 19048008, No. 19048015,
No. 22103005, No. 22340096, and No. 21244053) from the Ministry of Education, Culture, Sports, Science and
logical invariants 1 : 11, zero-energy states appear when
exist but vortices do not exist. The interaction between zero-energy states at edge dislocations and at vortex cores eliminates zero energy
states when dislocations and vortex cores exist at the same positions.

We generalize this model into the model in 3d. The 3d model is constructed as a stack of 2d models with
a hopping integral \( t_z \) along the z-direction as shown in Fig.2. \( t_z \) causes the finite region where the energy gap
The authors acknowledge the fruitful discussion with Yukio Tanaka, and Sho Nakosai. This work is supported
by Grant-in-Aid for Scientific Research (Grants No. 17071007, No. 17071005, No. 19048008, No. 19048015,
No. 22103005, No. 22340096, and No. 21244053) from the Ministry of Education, Culture, Sports, Science and
Technology of Japan, Strategic International Cooperative Program (Joint Research Type) from Japan Science and Technology Agency, and Funding Program for World-Leading Innovative RD on Science and Technology (FIRST Program).

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