$Z_2$ index theorem for Majorana zero modes in a class D topological superconductor

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We propose a $Z_2$ index theorem for a generic topological superconductor in class D. Introducing a particle-hole symmetry breaking term depending on a parameter and regarding it as a coordinate of an extra dimension, we define the index of the zero modes and corresponding topological invariant for such an extended Hamiltonian. It is shown that these are related with the number of the zero modes of the original Hamiltonian modulo two.

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Topological invariants are useful tools in various fields in physics. In particle physics, interesting phenomena such as chiral and gauge anomalies, instantons, vortices, Skyrmions and many other nonperturbative effects are related to the topological invariants \[1, 2\]. In condensed matter physics, they also play a crucial role in the classification of various kinds of phases of matter \[3–7\]. Some kinds of defects \[8\] or solitons \[2\] are also classified by the use of topological numbers.

Recently, index theorems \[9, 10\] for fermions coupled with a Higgs field in a monopole or vortex background \[11, 12\] have been attracting renewed interest in condensed matter physics. It is due to zero-energy Majorana bound states obeying non-Abelian statistics, pioneered by Read and Green \[13\] in a \[p\]-wave superconductor and by Kitaev \[14, 15\] in quantum computations. Extensive studies have recently predicted them in various kinds of superfluids and superconductors \[16–39\]. In a special case in which the systems have enhanced symmetry (chiral symmetry), it has been shown \[36\] that the index theorem ensures the existence of such zero modes. However, for generic topological superconductors, there are no index theorems which relate zero modes with a topological invariant.

In this paper, we propose a $Z_2$ index theorem for Majorana zero modes in a vortex of a generic topological superconductor in class D. We first introduce a particle-hole symmetry breaking term that depends continuously on a parameter and regarding it as a coordinate of an extra dimension and extend the $d$-dimensional Hamiltonian to $(d + 1)$-dimensional one with chiral symmetry. This enables us to define the index of the extended Hamiltonian and also the topological invariant corresponding to it. Since the index is equal to the number of zero modes of the original $d$-dimensional Hamiltonian modulo two, we thus have a $Z_2$ index theorem for the original system, implying that the Majorana zero mode in topological superconductors in class D is also protected topologically. We will give concrete calculations in two dimensional models, but the extension to an arbitrary higher dimensions is straightforward.

We investigate the Hamiltonian proposed by Fu and Kane \[21\] for the surface states of a topological insulator with a proximity effect of an $s$-wave superconductor,

$$\mathcal{H} = i\gamma^j \partial_j - \mu_1 \otimes \sigma^3 + \gamma^{a^2} \phi_a,$$

where $\gamma^j$ and $\gamma^{a^2}$ ($j, a = 1, 2$) form a set of $\gamma$ matrices $\gamma^\mu$ in four dimensions satisfying $\{\gamma^\mu, \gamma^\nu\} = 2\delta^{\mu\nu}$. We explicitly employ $\gamma^j = \sigma^1 \otimes \sigma^3$ and $\gamma^{a^2} = 1 \otimes \sigma^a$, where, in the tensor product of the Pauli matrices, the former (latter) describes the spin (Nambu) space. The pairing potential is included as $\phi = (\text{Re}\Delta(x), \text{Im}\Delta(x))$. Provided that $\phi_1 \phi_2 \neq 0$, the Hamiltonian \[1\] belongs to class D, since it has only particle-hole symmetry

$$C \mathcal{H} C^{-1} = -\mathcal{H},$$

where charge conjugation operator $C$ is defined by $C = i\gamma^2 \gamma^3 K$ with $K$ being complex conjugation $\bar{\phi}$. This symmetry ensures that all states with nonzero energies appear as paired states with $\pm$ energies. Let $\varepsilon_n$ be an eigenvalue of the Hamiltonian \[1\] labeled by an integer $n$. Then, it is natural to label the paired state with the opposite energy by $-n$, and hence, particle-hole symmetry can be characterized by the relation, $\varepsilon_{-n} = -\varepsilon_n$.

FIG. 1: The spectrum of the Hamiltonian in the case of $q = 3$ vorticity. (a) Three Majorana zero modes, marked by an oval, appear when $\mu = 0$. (b) Two of these get finite $\pm$ energies if a nonzero chemical potential is switched on, but an unpaired state is protected from it, sitting exactly at the zero energy due to particle-hole symmetry.

Let us assume that there is a vortex at the origin which is described by $\phi = \Delta(r)(\cos \Theta(\theta), \sin \Theta(\theta))$, where $(r, \theta)$
is the polar coordinates in two dimensions and the phase satisfies $\Theta(2\pi) = \Theta(0) + 2\pi q$ with $q$ being an integer. We assume that $\Delta(0) = 0$ and $\Delta(\infty) = \Delta_0 > 0$. Then, it has been argued [19, 20] that a Majorana zero mode appears for odd $q$, whereas for even $q$ no zero modes are allowed. This can be understood from the perturbation theory based on a simpler model with $\mu = 0$ which belongs to class BDI due to additional chiral symmetry [22, 23]. In this case of $\mu = 0$, the exact $q$ zero modes wave functions can be obtained similarly to [12]. We can also apply the index theorem to this special model [10, 56], and show that the index computed by the exact zero modes mentioned above and the topological invariant, i.e., the winding number of the pairing potential, indeed coincide, both of which are given by $-q$. This result matches the classification scheme due to Teo and Kane [11]. On the other hand, in the case of $\mu \neq 0$, index theorems cannot apply any longer due to the absence of chiral symmetry. Instead, perturbative arguments strongly suggest that even number of zero modes disappear in pairs with nonzero $+\epsilon$ energy, whereas an unpaired state is protected to stay at the zero energy due to the particle-hole symmetry. These imply that the number of Majorana zero modes in class D is classified by $\mathbb{Z}_2$, even or odd $q$ [11, 20, 23, 11]. These features are illustrated in Fig. 1.

Beyond perturbative arguments, we propose an index theorem valid for class D superconductors without chiral symmetry. To this end, we define, in the former part of the paper, an analytical index for a generic model [11] with a nonzero chemical potential. Firstly, we introduce symmetry breaking term [22, 11] to the Hamiltonian [11] such that

$$
\mathcal{H}(\tau) = i\gamma^j \partial_j - \mu 1 \otimes \sigma^3 + \gamma^{a+2} \phi_a - \lambda(\tau) \gamma_b, \quad (2)
$$

where $\gamma_b$ could be any hermitian matrix with $C\gamma_b C^{-1} = \gamma_b$, which may be several products of the $\gamma$ matrices. One of simpler choices is $\gamma_b = \gamma_5 \equiv (-i)^2 \gamma^1 \gamma^2 \gamma^3 A$. For simplicity and for convenience, we will restrict our discussions only to this case, $\gamma_b = \gamma_5$. As for $\lambda(\tau)$, we assume that it is an odd function of $\tau$, $\lambda(-\tau) = -\lambda(\tau)$, and hence $\lambda(0) = 0$. We also assume that $\lambda(\infty) = \lambda_0$ is finite. Then, particle-hole symmetry can be generalized to

$$
CH(\tau)C^{-1} = -\mathcal{H}(-\tau).
$$

Provided that the spectrum of $\mathcal{H}(\tau)$ is a smooth function of $\tau$, it can be labeled by the same quantum number $n$ for the $\tau = 0$ Hamiltonian such that $\mathcal{H}(\tau) \varphi_n(\tau, x) = \varepsilon_n(\tau) \varphi_n(\tau, x)$, where $\varepsilon_n(0) = \varepsilon_n$. From the point of view of the spectrum, the generalized particle-hole symmetry leads to the new relationship,

$$
\varepsilon_{-n}(\tau) = -\varepsilon_n(\tau). \quad (3)
$$

In this sense, the states labeled by $\pm n$ can be still regarded as the paired states. The spectral flow as a function of $\tau$ is shown in Fig. 2.

Although the extended Hamiltonian [22] does not have chiral symmetry, we can employ the spectral flow for the index theorem. To see this, we introduce a kinetic term for the parameter $\tau$ and define

$$
\mathcal{H}^{(3)} = i\sigma^2 \otimes 10_\tau + \sigma^1 \otimes \mathcal{H}(\tau) = i\Gamma^j \partial_j + \Gamma^{a+3} \phi_a + i\Gamma^1 \Gamma^2 \Gamma^6 \mu, \quad (4)
$$

where $j, a = 1, 2, 3$. Newly defined $\Gamma$-matrices obey $\{\Gamma^\mu, \Gamma^\nu\} = 2\delta^{\mu\nu}$. $\mathcal{H}^{(3)}$ can be regarded as a Hamiltonian defined in three dimensions spanned by the coordinates $x_1, x_2$ and $x_3 \equiv \tau$. We have also introduced $\phi_3 = \lambda$ and regarded it as a component of a generalized order parameter $\phi = (\text{Re} \Delta, \text{Im} \Delta, \lambda)$. Note that the extended Hamiltonian [24] has chiral symmetry $\Gamma_7 \mathcal{H}^{(3)} = -\mathcal{H}^{(3)} \Gamma_7$, where $\Gamma_7 = (-i)^3 \Gamma^1 \cdots \Gamma^6$. Therefore, if the Hamiltonian [24] has zero modes, they have definite chirality.

The eigenvalue equation for the zero modes is $\mathcal{H}^{(3)} \Phi = 0$, which is given by $\mathcal{H}(\tau)$ as follows:

$$
\partial_\tau \Phi = \sigma^3 \otimes \mathcal{H}(\tau) \Phi. \quad (5)
$$

To solve this equation, let us set $\Phi_n(\tau, x) = f_n(\tau) \varphi_n(\tau, x)$. Then, $\partial_\tau \Phi_n = (\partial_\tau f_n) \varphi_n + f_n (\partial_\tau \lambda) \lambda_n \varphi_n$, since the Hamiltonian $\mathcal{H}(\tau)$ depends on $\tau$ only through $\lambda(\tau)$. Provided that $\partial_\tau \lambda$ can be neglected in the adiabatic approximation and that $\varphi_n(\tau, x)$ is normalizable, it turns out that $f_n$ is given by

$$
f_n^\pm(\tau) = e^{\pm \int \tau' \varepsilon_n(\tau')} f_\epsilon^\pm, \quad (a)
$$

where $f_\epsilon$ is a constant spinor with $\Gamma_7 f_\epsilon^\pm = \pm f_\epsilon^\pm$. If a given state for $n \neq 0$ satisfies $\varepsilon_n(+\infty) > 0$ and $\varepsilon_n(-\infty) < 0$, which is the case of $n = 1$ and $n = -1$ modes in Fig. 2 (a), the states labeled by $n$ and $-n$ are normalizable zero modes with chirality $-1$. Likewise, if $\varepsilon_n(+\infty) < 0$ and $\varepsilon_n(-\infty) > 0$, $\pm n$ states are normalizable zero modes with

![FIG. 2: The spectral flow of the Hamiltonian for a generic case of $\mu \neq 0$. The $n = 0$ state crosses the $E = 0$ line at least $\tau = 0$. (a) If any other eigenvalue crosses it at a finite $\tau$, say, $\varepsilon_n(\tau_0) = 0$, the spectral symmetry [3] ensures that $\varepsilon_n(-\tau_0) = 0$. (b) If the model parameters are changed, the above $\pm n$ modes may come not to cross the zero energy. Even in this case, the index changes by even integers because of the symmetry [3].](image-url)
chirality $+1$. Now, define the index of the Hamiltonian $H^{(3)}$ by

$$ \text{ind } H^{(3)} = N_+ - N_- $$

(6)

Then, these paired zero modes contribute to the index for $H^{(3)}$ always by two. On the other hand, if $\epsilon_n(\pm \infty)$ has the same sign, such $\pm n$ states cannot be zero modes, since the wave functions are not normalizable. Therefore, these states give no contribution to the index. It Thus turns out that $n \neq 0$ modes can change the index by even integers. Contrary to these modes, the number of zero modes of $H^{(3)}$ unless $\epsilon_0(\infty) = 0$, determines whether the index is even or odd. Thus, it turns out that the number of zero modes of $H$ in Eq. (1), which we denote as $N_0(H)$, is given by the index of $H^{(3)}$ in Eq. (6) as

$$ N_0(H) = \text{ind } H^{(3)} \mod 2 $$

(7)

So far we have discussed the index of the extended Hamiltonian $H^{(3)}$ and its modulo-two relationship with the number of zero modes of the original Hamiltonian $H$. The rest of the present paper is devoted to calculations of the corresponding topological invariant. For the Hamiltonian with chiral symmetry such as $H^{(3)}$, it is possible to define the topological invariant equal to the index and to claim the index theorem \cite{9, 11, 36} such that

$$ \text{ind } H^{(3)} = -\frac{1}{2} \int dS_j J^i(x, 0, \infty), $$

(8)

where $dS_j$ is an infinitesimal surface elements at the boundary $(x \to \infty)$ of the Euclidean space $R^3$, and $J^i$ is the axial vector current defined by

$$ J^i(x, m, M) = \lim_{y \to x} \Gamma_0 \left( \frac{1}{m - iH^{(3)}} - \frac{1}{M - iH^{(3)}} \right) \delta(x - y). $$

The first term in the above parentheses becomes the index in the limit $m \to 0$ when integrated over the two-dimensional surface at infinity. The second term has been introduced as a Pauli-Villars regulator in order for the current to be regularized \cite{11, 36}. It should be set $M \to \infty$ after the calculations. When we calculate the r.h.s. of Eq. (8), it may be easy to use the plane wave basis. Possible terms contributing to the index are

$$ J^i(x, 0, \infty) = - \int \frac{d^3k}{(2\pi)^3} G^3 \text{tr } \Gamma_7 \Gamma^i \left( -i\Gamma^j k_j - i\Gamma^a + 3 \phi_a + \Gamma^1 \Gamma^2 \Gamma^6 \mu (K - \mu \Gamma) \Lambda (K - \mu \Gamma) \Lambda (K - \mu \Gamma), \right) $$

where

$$ G^{-1} = \left[ \left( \frac{k_0^2 + k_j^2 + \lambda^2 - \mu}{2} \right)^2 + k_j^2 + \Delta^2 \right] \left[ \left( \frac{k_0^2 + k_j^2 + \lambda^2 + \mu}{2} \right)^2 + k_j^2 + \Delta^2 \right], $$

$$ K = k_j^2 + \phi_a^2 + \mu^2, \quad \Gamma = 2i (\Gamma^2 \Gamma^6 k_1 + \Gamma^6 \Gamma^1 k_2 + \Gamma^1 \Gamma^2 \lambda), \quad \Lambda = i \Gamma^3 \Gamma^a + 3 \partial_k \phi_a. $$

The first step of the calculations is to take the trace of the $\Gamma$-matrices by the use of $\text{tr } \Gamma_7 \Gamma^a \Gamma^b \Gamma^c \Gamma^d \Gamma^{ab} \Gamma^{cd} = (2i)^3 \epsilon^{ijklmnp} \cdot \Gamma^{mnp}$ \cite{42}. Lengthy but straightforward calculations lead to

$$ J^i = 2\delta^{ijk} \epsilon^{abc} \phi_a \partial_j \phi_b \partial_k \phi_c \int \frac{d^3k}{(2\pi)^3} G^2 \Delta $$

$$ - \delta^{ijk} \mu^2 \delta^{abc} \lambda \partial_k \phi_a \partial_l \phi_b \int \frac{d^3k}{(2\pi)^3} G^2. $$

As a next step, we carry out the integration over the momentum $k_j$ in the above and over the space coordinates $x_j$ in Eq. (8). In particular in the latter integration, since the generalized order parameter $\phi$ depends cylindrically on the coordinates $(r, \theta, \tau)$, it may be natural to regard the boundary of $R^3$ as a cylinder illustrated in Fig. 3. For convenience, let us divide it into two pieces I $(r \to \infty)$ and II $(r \to \pm \infty)$. The calculations on these two regions are quite similar to those in \cite{42} when $\mu = 0$. However, in the case of $\mu \neq 0$, we have to choose appropriate $\lambda_0 \equiv \lambda(\infty)$ to make the calculations valid. To see this, let us set $\Delta \to \Delta_0$ and $\lambda \to 0$, respectively, in the regions I and II. Then, we see that in the region I, $G$ in Eq. (8) is always finite because of finite $\Delta_0$. On the other hand, it becomes singular in the region II if $|\lambda_0| < |\mu|$. Indeed, in this case, $G^{-1}$ in Eq. (8) vanishes at some momentum at the core of the vortex $r = 0$, where $\Delta(0) = 0$. Therefore, we restrict our discussions to the case of $|\lambda_0| \geq |\mu|$. After some straightforward calculations, we arrive at

$$ \text{ind } H^{(3)} = \frac{1}{2\mu} (|\lambda_0| - |\mu|) \frac{1}{2\pi} \int d\theta \epsilon^{abc} \hat{\phi}_a \partial_b \hat{\phi}_c = -\text{sgn}(\lambda_0) q, $$

(10)
where $\hat{\phi}^a \equiv \phi^a / \Delta_0$, the subscript $a, b$ are restricted to 1, 2, and the $\theta$-integration is over $S^1$ at $r \to \infty$ in the region II, which becomes $q$. It turns out that the index is basically determined only by the vorticity $q$, and is the same as the the index of $\mathcal{H}$ when $\mu = 0$, which has been calculated in ref. \cite{36} as $\text{ind} \mathcal{H} = -q$: The artificially introduced parameter $\lambda$ just change the sign of the index. It follows that the index is topological: It is indeed protected from infinitesimal changes of the three parameters $\mu$, $q$, and $\lambda_0$. Eqs. \cite{10} and \cite{7} are $\mathbb{Z}_2$ index theorem for a generic model in class D.

As we have mentioned, the topological invariant \cite{10} is invalid if $|\lambda_0| < |\mu|$. In this case, the zero mode equation \cite{5} may not have normalizable solutions. This can be checked by the use of perturbations to this equation. Let us consider two possibilities of small parameters $\mu$, $q$, and $\lambda_0$. If one regards $\mu$ as a small parameter and applies the first order perturbation to $\mu = 0$ solutions, one has indeed one normalizable solution. On the other hand, in the case of small $\lambda$, one can obtain the first order wave function cannot be normalized. This implies that in the case $|\lambda| \ll |\mu|$, the relationship between the spectral flow of $\mathcal{H}(\tau)$ and the zero mode of $\mathcal{H}^{(3)}$ does not hold. Therefore, we conclude, from these observations, together with the calculations of the topological invariant, that the present formulation of the $\mathbb{Z}_2$ index theorem requires $|\lambda_0| \geq |\mu|$.

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\begin{itemize}
\item\[\lambda \tau x \equiv x_{\tau=0}\]
\end{itemize}

FIG. 3: The cylindrical surface of the integration in Eq. \cite{3}. "I" denotes the side of the cylinder $r \to \infty$, whereas "II" denote two discs at $\tau \to \pm \infty$.
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