Impurity effects in a two-dimensional topological superconductor: A link of $T_c$-robustness with a topological number

Yuki Nagai, Yukihiro Ota, and Masahiko Machida

CCSE, Japan Atomic Energy Agency, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8587, Japan

Impurity effects are probes for revealing an unconventional property in superconductivity. We study effects of non-magnetic impurities, in a 2D topological superconductor with $s$-wave pairing, the Rashba spin-orbit coupling, and the Zeeman term. Using a self-consistent $T$-matrix approach, we calculate a phenomenological formula for the Thouless-Kohmoto-Nightingale-Nijs (TKNN) invariant in interacting systems, as well as density of states, with different magnetic fields. This quantity weakly depends on the magnetic field, when a spectral gap opens, whereas this changes drastically, when in-gap states occurs. Furthermore, in the latter case, we find that the Anderson’s theorem (robustness of $s$-wave superconductivity against non-magnetic impurities) breaks down. We discuss the origin, from the viewpoints of both unconventional superconductivity and the TKNN invariant.

1. Introduction

Topological materials, such as semiconductors with the quantum Hall effect$^1$ and topological insulators$^2$ attract a great deal of attention in condensed matter physics. Their essential character is classified by topological invariants.$^3$ Among them, topological superconductors$^4-8$ are notable materials, and their feature is studied by different theoretical ways.$^9-11,13$ Their topologically-protected features allow us to implement applications, such as quantum engineering.$^{14}$

The impurity effect in superconductivity is a probe for classifying types of superconducting states, as well as tunneling spectroscopy.$^{15}$ Impurities lead to phenomena never occurring in clean superconductors.$^{16}$ A gapless behavior in the density of states (DOS) via non-magnetic impurity scattering,$^{17,18}$ for example, is witness of unconventional superconductivity.

One of the celebrated statements about superconducting alloys is the Anderson’s theorem:$^{16}$ the robustness of $T_c$ in $s$-wave superconductivity against non-magnetic impurities. This prediction is related to the absence of low-energy excitations in conventional superconductivity. Here, we pose a simple question: Is a topological superconductor conventional? Intuitively, such a superconductor should be robust against impurities, from its topological nature. Moreover, if the superconductivity occurs under $s$-wave pairing, the Anderson’s theorem implies that this material is free from non-magnetic impurities. A topological $s$-wave superconductor is predicted by Sato, Takahashi, and Fujimoto.$^{11,12}$ We notice that, however, this prediction indicates the system is regarded as a chiral $p$-wave model; the topological $s$-wave superconductivity can have unconventional features. To construct theory of dirty topological superconductors is desirable for answering this intriguing issue. This approach is also useful for development of quantum engineering based on topological superconductors, since typical materials in experiments would be dirty.

![s-wave superconductivity](image)

**Fig. 1.** Schematic diagram of our main result; robustness of $T_c$ against non-magnetic impurities, in an $s$-wave superconductor with the Rashba spin-orbit coupling and the Zeeman magnetic field.$^{15}$ The brighter region (zero-TKNN) is more robust than the darker region. Inside the zero-TKNN region, a topological invariant, Thouless-Kohmoto-Nightingale-Nijs (TKNN) invariant is zero, without impurities. Otherwise, the robustness reduces continuously.

In this paper, we study effects of non-magnetic impurities, in a topological superconductor with $s$-wave pairing, the Rashba spin-orbit coupling, and the Zeeman term.$^3$ Our idea for revealing the impurity effects is to use a formula relevant to Thouless-Kohmoto-Nightingale-Nijs (TKNN) invariant.$^{19,20}$ In addition to standard arguments in superconducting alloys. We obtain this formula phenomenologically, using an expression for the TKNN invariant derived by Niu, Thouless, and Wu.$^{21}$ We call it NTW-TKNN formula. The value of this formula is a leading term of a generic TKNN invariant in interacting systems,$^{25-24}$ under momentum-independent self-energy. We find that its numerical calculations are more stable than the generic formula, when the superconducting pair breaking occurs via non-magnetic impurities. The NTW-TKNN formula and low-energy behaviors in DOS (the presence of in-gap states) are calculated by the self-consistent $T$-
matrix approximation, changing the magnetic field. The critical temperature $T_c$ is evaluated by self-consistent calculations of the gap equation.

The $T_c$ reduction behavior in this topological superconductor is characterized well in terms of the NTW-TKNN formula. When a spectral gap opens in the DOS under impurities, the NTW-TKNN formula quite weakly depends on the magnetic field. We find that a robust topological superconducting state emerges in this magnetic-field region. In contrast, when in-gap states occur in the DOS, this quantity depends on it strongly. In this case, we have a topological superconducting state fragile against non-magnetic impurities. We also find a trivial state, whose NTW-TKNN formula in clean limit (i.e., the TKNN invariant) has a non-zero value, in the latter magnetic-field region. This indicates that an $s$-wave state is suffered from non-magnetic impurities. Therefore, we find that robustness of $s$-wave superconductivity against non-magnetic impurities (Anderson’s theorem) breaks down, when the TKNN invariant has a non-zero value (See, Fig. 1). In other words, a class of $s$-wave superconductivity is sensitive to non-magnetic impurities, unlike unconventional superconductivity.

The origin of this violation is clarified from two viewpoints. First, we find a similar mechanism to chiral $p$-wave. Second, the low-energy excitations related to gapless edge modes, whose number is characterized by the TKNN invariant, is relevant to the reduction of the $T_c$ and conductivity against non-magnetic impurities (Anderson’s theorem) breaks down, when the TKNN invariant has a non-zero value. Therefore, we find that robustness of $s$-wave superconductivity against non-magnetic impurities (Anderson’s theorem) breaks down, when the TKNN invariant has a non-zero value. Therefore, we find that robustness of $s$-wave superconductivity against non-magnetic impurities (Anderson’s theorem) breaks down, when the TKNN invariant has a non-zero value.
with $V = \text{diag}(V_0, V_0, -V_0, -V_0)$ and the $k$-mesh size $N$. The self-energy is

$$\Sigma(\Omega) = n_{\text{imp}}T(\Omega) - n_{\text{imp}}V,$$

(4)

with impurity concentration $n_{\text{imp}}$. The anomalous ($f_k$) and the normal ($g_k$) Green’s functions are $2 \times 2$ block matrices of $G_k(\Omega)$,

$$G_k(\Omega) = \begin{pmatrix} f_k(\Omega) & f_k(\Omega) \\ g_k(\Omega) & \bar{g}_k(\Omega) \end{pmatrix}.$$  

(5)

The pair potential $\Delta$ is evaluated by the gap equation

$$i\Delta r_2 = V_{\text{int}} \frac{T}{N} \sum_{n=-n_c}^{n_c} \sum_k f_k(i\omega_n),$$

(6)

with pairing interaction strength $V_{\text{int}}$ and the fermionic Matsubara frequency $i\omega_n = \pi T(2n + 1)$. We use the cutoff parameter $n_c$ such that $\omega_n = 10\pi$. The DOS is

$$N(E) = \frac{1}{2\pi N} \sum_k \text{tr}[\text{Im} g_k(E)].$$

(7)

The evaluation of $T_c$ depending on $n_{\text{imp}}$ is performed, with fully self-consistent calculations, i.e., solving Eqs. (3)–(6) self-consistently. In the calculations of $\mathcal{W}$ and $N(E)$, we self-consistently solve Eqs. (3)–(5) for given $\Delta$ and $\mu$, to compare our results with the arguments by Sato et al.\[11\]

4. Results

4.1 NTW-TKNN formula and density of states

Now, we show the results for the NTW-TKNN formula. Figure 2 shows the magnetic-field dependence, with different impurity concentrations. The impurity strength is $V_0 = 3t$ and the pair potential is $\Delta = 0.35t$. We examine two kinds of the chemical potential, $\mu = 3.5t$ and $\mu = t$. In Eq. (2), the number of the meshes for the $k$-summation is 480 $\times$ 480, and the energy-integration range is $-2.5t \leq \omega \leq 2.5t$. Without impurities ($n_{\text{imp}} = 0$), the NTW-TKNN formula takes an integer for each magnetic field. This result is consistent with the exact analysis.\[11\] The TKNN invariant is an even number for a non-topological magnetic-field region.\[11\] Otherwise, a topological superconducting state occurs. In the zero TKNN-invariant region, $\mathcal{W}$ is not significantly changed, compared to the case when $\mathcal{W}|_{n_{\text{imp}} = 0}$ takes a non-zero value. We can find that the DOS is robust against the non-magnetic impurities in this region, as well. These behaviors correspond to the Anderson’s theorem.

Let us focus on the 1-TKNN-invariant region in Fig. 2(a) ($0.5t < h < 3.5t$). We find that the NTW-TKNN formula weakly depends on $h$ but is almost constant up to $h \sim 1t$, whereas $\mathcal{W}$ strongly depends on $h$ (a decreasing behavior) for $h > 2t$. For understanding these behaviors more clearly, we turn into the results for the DOS (Fig. 3), with $\mu = 3.5t$. In the calculations of the DOS, the $k$-mesh size is 960 $\times$ 960. Figures 3(a) and 4(a) show that the spectral gap opens for every impurity concentration, when the change of the NTW-TKNN formula is moderate against $h$ (i.e., $h = 1t$). However, when $\mathcal{W}$ is decreasing ($h > 2t$), the spectral gap closes and in-gap states occurs for high impurity concentration ($n_{\text{imp}} = 0.02$), as shown in Figs. 3(b) and 4(b).

4.2 Robustness of $T_c$

Now, we examine the robustness of $T_c$ against non-magnetic impurities, in terms of the NTW-TKNN formula. We can find that $T_c$ is robust for the zero-TKNN-invariant regions ($0 < h < 0.5t$ in Fig. 2(a) and $0 < h < 1r$ in Fig. 2(b)). We confirm the Anderson’s theorem, again. When the topological $s$-wave superconducting state (i.e., a state with an odd TKNN invariant) occurs, the behaviors of $T_c$ against $n_{\text{imp}}$ are strongly correlated with the NTW-TKNN formula. Figure 5(a) shows that $T_c$ is not so reduced, with increasing the impurity concentrations, when $\mathcal{W}$ is almost constant [$h = 1t$ in Fig. 2(a)]. However, when $h = 2t$ (i.e., the value of the
4.3 Generic TKNN invariant for non-zero spectral gap

The previous results indicate that the superconducting order survives well, when $h < 2 \Gamma$. Let us consider this claim, in terms of the generic TKNN invariant in interacting systems. Under the condition that the self-energy $\Sigma$ is independent of $k$, the relationship of the generic formula $W_{\text{gen}}$ to $W$ is $W_{\text{gen}} = W + \delta W$, with

$$
\delta W = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \int_{-\pi}^{\pi} \frac{d\omega'}{2\pi} \text{Tr} \left[ (-1)^{\sum_{ij} \partial H_i / \partial k_j} \left( \frac{\partial H_i}{\partial k_j} G_k(i\omega) \frac{\partial H_j}{\partial k_l} G_k(i\omega) \right) \right].
$$

(8)

Figure 6 shows the magnetic-field dependence of $W_{\text{gen}}$ for $\mu = 3.5 \Gamma$, $\Delta = 0.35 \Gamma$, and $h < 2 \Gamma$, with different impurity concentrations. The physical parameter set is the same as in Fig. 2(a). We find that the topological feature without non-magnetic impurities does not change, even in the presence of impurity scattering. We can find that the calculations of $W_{\text{gen}}$ are unstable when the spectral gap is closed (e.g., $h > 2 \Gamma$). This difficulty may come from a singular behavior of $d\Sigma(i\omega)/d\omega$ on the imaginary axis. In addition, we speculate that the in-gap state excitations shown in Fig. 4(b) can be an obstacle to assess a topological property via $W_{\text{gen}}$. Berry’s connection 1-form built up by the occupied bands (negative eigenstates) of the BdG Hamiltonian would be ill-defined, since the in-gap states can induce transition from the negative eigenstates to the positive ones, and vice versa.

5. Discussion

We argue the origin of the fragile behaviors of $T_c$ and the violation of the Anderson’s theorem. First, we consider this point to be typical arguments of the impurity effects in unconventional superconductors. The Anderson’s theorem breaks down when the $k$-averaged anomalous self-energy vanishes. Let us use the non-self-consistent Born approximation, for simplicity. The anomalous self-energy is

$$
\Sigma_{\text{Born}}(\Omega) = -(n_{\text{imp}} V_0^2 / N) \Sigma_k f_k(\Omega).
$$

This quantity vanishes in...
chiral $p$-wave superconductors. Now, we obtain
\[ \Sigma^A_{\text{Born}}(\Omega) = i\Delta \sigma_2 n_{\text{imp}} V^2 \frac{1}{N} \sum_k D^{-1}(k)[C(k) - (h - \Omega)^2], \] (9)
with $C = a^2|L_{12}|^2 + |\Delta|^2 + s^2$ and $D = \det(\Omega - \mathcal{H})$. We find that $C$ is strictly positive for non-zero $\Delta$. We also find that $D^{-1}$ is strictly negative when $\Omega$ is the Matsubara frequency ($\Omega = i\omega_n$). The latter statement can be shown that the spectrum of the BdG Hamiltonian is constructed by pairs of the positive and the negative eigenvalues ($E_k, -E_k$), owing to its particle-hole symmetry. Therefore, when $h \rightarrow 0$, the anomalous self-energy never vanishes. This corresponds to the Anderson’s theorem. In contrast, when $h$ increases, $\Sigma^A_{\text{Born}}$ can be so small that the robustness of $T_c$ dies out. Hence, the Anderson’s theorem is violated, when the magnetic field is large.

Next, we focus on the TKNN invariant. The quantity is related to the number of gapless edge modes.\(^{11}\) The zero TKNN invariant means no gapless mode, for example. When the TKNN invariant is $\pm 2$, we have two modes. Under the open boundary condition along the $x$-direction, one mode has a gapless behavior at $k_x = 0$, while the other is zero at $k_y = \pi$.\(^{11}\) Thus, the non-zero TKNN invariant means the presence of low-energy edge modes, even if $s$-wave pairing potential induces the superconductivity.

Although the $T_c$ reduction by impurity scattering is a phenomena in the bulk system, we find an intriguing coincidence in Fig. 2; the NTW-TKNN formula differs from a constant value, for the magnetic field generating the gapless edge modes on the surfaces in the clean limit. The non-constant behaviors of NTW-TKNN formula (2) with respect to $h$ imply the disappearance of the robustness against non-magnetic impurities (See Sec.4.2). Therefore, we suggest that the occurrence of the gapless edge modes on the surfaces be relevant to the low-energy excitations around impurities, leading to pair-breaking effects. We will test this conjecture elsewhere.\(^{28}\)

Before closing this section, we refer to two topics related to the present study. First, we focus on an analogy with vortex physics of a chiral $p$-wave superconductor. The chiral $p$-wave superconductivity has two kinds of the vortices, one of which has the vorticity parallel to the internal angular momentum of the Cooper pair, while the other of which has the anti-parallel vorticity. We note that the effect of non-magnetic impurities is suppressed inside a vortex core, only in the anti-parallel case.\(^{29}\) This behavior originates from the fact that the total topological number, i.e., the summation of the vorticity and the chirality is zero. A similar effect is expected in the present topological superconductor, when the TKNN invariant is 1; the impurity effects inside a vortex core may depend on the direction of a vortex (i.e., the total topological number composed of the TKNN invariant and the vorticity). Second, a two-dimensional topological superconductor can be realized in superlattice structures made of CeCoIn\(_5\) and YbCoIn\(_5\).\(^{30}\) Mizukami et al.\(^{10}\) show that a number of the superconducting layers can be controlled and the Rashba spin-orbit coupling
can be induced in a multi-layer structure. A theoretical prediction\textsuperscript{31} suggests the emergence of a topological spin-singlet state. The application of our approach to this system is an intriguing future work.

6. Summary

In summary, we studied the non-magnetic impurity effects in a topological \textit{s}-wave superconductor, in terms of NTW-TKNN formula (2). Our numerical calculations show that the NTW-TKNN formula is almost constant in the presence of impurities, whenever a spectral gap opens in the DOS. We examined \( T_c \) versus impurity concentrations. The self-consistent calculations indicate that \( T_c \) is robust when the NTW-TKNN formula is almost constant in the presence of impurities, whereas \( T_c \) significantly reduces when this quantity depends on the magnetic field. For a non-zero even TKNN invariant, a fragile behavior is shown. Hence, we conclude that the Anderson’s theorem breaks down even for a \textit{s}-wave superconductor and its violation is characterized well by the value of the NTW-TKNN formula. The present approach suggests that intriguing effects occur via incorporation between a topological order and spatial inhomogeneity.

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