Abstract. We study the impurity effects on bound states in a single vortex core of a topological s-wave superconductor (SC), which is a two-dimensional electron gas with Rashba spin-orbit coupling, Zeeman coupling and s-wave superconductivity. We calculate the Gor'kov Green’s function in the presence of impurities in a way similar to Kopnin and Kravtsov (1976); We restrict the Hilbert space to that spanned by the eigenstates of the Bogoliubov-deGennes equation for a pure system, bounded near the vortex core. This topological s-wave SC has two types of vortices and each type is specified by the relative sign between the vorticity and Zeeman coupling. We find that the impurities affect bound states differently between the two types of vortices and bound states are more robust against impurities when vorticity and Zeeman coupling are opposite in signs.

1. Introduction

Topological superconductors (TSCs) have zero energy states called Majorana bound states at edges or topological defects [1, 2]. An idea has been proposed on implementation of topological quantum computation (TQC) [3], which utilizes non-Abelian statistics in the Majorana bound states in TSCs. TQC has advantage in low decoherence, compared to conventional quantum computations [4].

If we do not consider space groups, all possible TSCs are classified by Schnyder et al. [5, 6] into ten symmetry classes based on the random matrix classification by Altland and Zirnbauer [7]. Particularly, class D, where time reversal symmetry is broken, is one of Bogoliubov-deGennes (BdG) classes and TSCs in this class are proposed for various forms such as $\nu = 5/2$ fractional quantum Hall state [8], chiral p-wave SC [9] and cold-atoms with artificial gauge field [10]. However, realization of non-Abelian statistics in solids is challenging. Sr$_2$RuO$_4$ is expected to be a chiral p-wave SC [11], but the superconducting state in this material does not have continuous rotational symmetry, because of the point group symmetry $C_4$ in the crystal structure. Recent theories tell us that proximity effects can lead some engineered TSCs which are equivalent to $p+ip$ SCs [12, 13]. The example is an s-wave SC on a surface of three-dimensional (3D) topological insulator with a time-reversal breaking field [12], or a heterostructure of 2D electron gas with strong Rashba spin-orbit coupling (SOC), Zeeman coupling and s-wave superconductivity [13]. In this article, we focus on the latter engineered $p+ip$ SC and call it topological s-wave SC.

TQC using non-Abelian statistics is realized through an adiabatic exchange of Majorana states in their subspace. The adiabatic time scale is characterized by the inverse of the minigap ($\Delta_{\text{min}}$), which is the energy gap between the Majorana state and the first excited state. Thus
a large minigap as well as the Majorana bound state is necessary for realization of TQC. The topological s-wave SC is a promising system for TQC: the minigap for bound states in a vortex core is about $0.1 \sim 1K$, while a minigap of typical chiral p-wave SC is about $1 \sim 10mK$.

An important issue in a realistic situation is how robust this large minigap is against randomness such as impurities. In order to study the robustness of the minigap of the topological s-wave SC, the authors in the earlier work [14] introduced random potential into the BdG equation and calculate the energy spectrum. In their work, however, the effects of randomness have not been treated systematically enough in the sense that the random average has not been taken. Moreover, the difference in impurity effects on two types of vortices have not been considered seriously; In this SC, there are inequivalent vortices in the sense that one type of vortex is not transformed into the other by symmetry operations. The type of vortex is specified by the relative sign of the vorticity and the Zeeman coupling. We know that the robustness of bound states against impurities depends crucially on the type of vortex in chiral p-wave SC [15].

One of the standard approaches to treat the random impurity effects on inhomogeneous SC is to use the quasiclassical theory of superconductivity. The impurity effects on chiral p-wave SC mentioned above are studied within quasiclassical, continuous spectrum approximation. For the case of the topological s-wave SC, the large minigap implies that the spectra are discrete and the quasiclassical theory does not provide quantitative results. In addition, the quasiclassical theory itself has not been constructed for this system. Another approach is to use Green’s function through the Gor’kov equation. Kopnin and Kravtsov have developed a scheme of the Green’s function for an s-wave SC [16], but the form of the coherence factor is not clear in their scheme and thus it is inapplicable to other SCs, as it stands. With these backgrounds, we have derived a proper formula within the self-consistent Born Approximation, which updates the Kopnin-Kravtsov scheme. The details of this formulation are discussed in [17]. With use of this method, we can study the impurity effects on bound states systematically keeping the discreteness of the energy spectrum.

2. Formulation

Hamiltonian for a 2D electron system with s-wave pairing, Rashba SOC and Zeeman coupling is given by [13]

$$H = \int dr \hat{\psi}^\dagger(r) \hat{H}_0(r) \hat{\psi}(r) + \int dr \left[ \Delta(r) \psi_1^\dagger(r) \psi_1^0(r) + \text{h.c.} \right],$$  

$$\hat{H}_0(r) = \left(\frac{\hbar^2}{2m} - \mu + \alpha(p \times \hat{\sigma})_z + V_z \hat{\sigma}_z \right), \quad \hat{\psi}^\dagger(r) = (\psi_1^\dagger(r), \psi_0^\dagger(r)),$$

where $\mu$ is the chemical potential, $\alpha$ strength of Rashba type SOC, $V_z$ Zeeman coupling. $\Delta(r)$ is s-wave pairing. We assume that there is a single vortex and the pairing function takes the form: $\Delta(r) = \Delta_0 \rho^{i\kappa\theta}(\kappa = \pm 1)$, $\kappa$ denotes vorticity. This system is in a topological phase when $V_z > \sqrt{\mu^2 + \Delta_0^2}$. $\Delta_0$ denotes the magnitude of s-wave pair potential in the bulk. The BdG equation in this system can be derived as follows:

$$\hat{H}_{\text{BdG}}(r) \hat{u}_K(r) = E_K \hat{u}_K(r),$$

$$\hat{H}_{\text{BdG}}(r) = \begin{bmatrix} \hat{H}_0(r) & \hat{\Delta}(r) \\ \hat{\Delta}^\dagger(r) & -\hat{H}_0^*(r) \end{bmatrix}, \quad \hat{\Delta}(r) = \Delta(r) \hat{\sigma}_y.$$

The symbol $\hat{\cdot}$ denotes a 4 by 4 matrix, $\cdot$ a 2 by 2 matrix and the basis is taken as $\hat{u}_K^\dagger(r) = (u_{K1}^\dagger(r), u_{K2}^\dagger(r), v_{K1}^\dagger(r), v_{K2}^\dagger(r))$. We take the cylindrical coordinate and each eigenstate $K$ is labeled by $(l, \nu)$, which denotes a set of angular momentum $l$ and quantum number $\nu$ of radial direction. In order to solve the BdG equation, we adopt Fourier-Bessel expansion [14].
We take the system size $R = 100\xi_0$ and two cut-offs: $l_c = 50, N_c = 400$ for $l, \nu$ respectively. We put $\Delta(r) = \Delta_0 \tanh(r/\xi_0)$ and $\xi_0 = v_F/\Delta_0$. This system has two kinds of bound states with energies below $\Delta_0$: one is bounded in the vortex core known as the Caroli-deGennes-Matricon (CdGM) mode, and the other is near the edge of the system. It is known that the sign of $V_z$ and vorticity correspond to the signs of the angular velocities of the edge mode and CdGM mode, respectively [18] and we note that the sign of $V_z$ plays a similar role in this TSC as the sign of chirality in chiral p-wave SC. We investigate the impurity effects on the CdGM mode for both signs of $V_z$ and the negative vorticity ($\kappa = -1$). In the following part, we call parallel (anti-parallel) vortex when the signs of $V_z$ and vorticity are same (opposite). To study random impurity effects, we use the Gor’kov equation [17]. We take into account a mode $\nu = 0$ bounded in the vortex core only and omit this label $\nu$ hereafter.

Within the self-consistent Born approximation, Green’s function and self energies are

$$\tilde{G}(r, r'; \omega_n) = \sum_l \frac{\hat{\tau}_z \tilde{u}_l(r) \tilde{u}_l^*(r)}{E_l - \sigma_l(i\omega_n) - i\omega_n},$$  \hspace{1cm} (5)

$$\sigma_l(\omega_n) = \frac{\gamma}{2\pi} \sum_\nu M_{l,\nu} \frac{M_{l,\nu}}{E_\nu - \sigma_\nu - i\omega_n},$$  \hspace{1cm} (6)

$$M_{l,\nu} = \int rdr |\tilde{u}_l(r) \tilde{u}_l^*(r)|^2,$$  \hspace{1cm} (7)

where $\gamma = \Gamma_n/(\pi N_n) = 2v_F \Gamma_n/k_F$. $\Gamma_n$ denotes the impurity scattering rate in the normal state and $N_n$ the density of states per spin at the Fermi level in the normal state. $k_F$ and $v_F$ denote, respectively, the Fermi wavenumber and the Fermi velocity. $\tilde{u}_l(r)$ is the radial part of $\tilde{u}_l(r)$. The present scheme is similar to that derived by Kopnin and Kravtsov [16] for the s-wave SC. In contrast to their scheme, our scheme has the coherence factor (Eq. (7)) and is applicable to various kinds of SCs such as chiral p-wave SCs. We calculate the density of states from this Green’s function:

$$N(\omega) = \sum_l N_l(\omega) = \int dr \Im \frac{1}{\pi} \Tr \tilde{\tau}_z \tilde{G}(r, r; \omega_n)|_{i\omega_n \to \omega + i\delta}.$$  \hspace{1cm} (8)

We evaluate the width of spectrum, denoted as $\Gamma$ and defined as half the width at half maximum (HWHM) (Fig. 1). $\Gamma$ corresponds to the impurity scattering rate of CdGM mode.

3. Result

We numerically calculate the density of states using Eqs. (5)-(8). In this calculation, $|V_z| = 2.0\Delta_0$, $\mu = 0.2\Delta_0$ are fixed parameters, while $m a^2/\Delta_0$, $\Gamma_n/(\pi \Delta_0)$ are taken as 0.1, 0.4, 0.9, 1.6 and $10^{-5}, 10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}$ respectively.

3.1. vortex type study

Figure 2 (a) (2 (b)) shows the width calculated from the spectra of bound states scattered by impurities when the Zeeman coupling $V_z$ and vorticity have the opposite (same) sign. The details of parameters are written in the caption. As an overall feature, we find that the impurity scattering rates in Fig. 2 (b) ($V_z < 0$) are larger than those in Fig. 2 (a) ($V_z > 0$). This reminds us of impurity effects on two types of vortices in chiral p-wave SC; the type is specified by the relative signs of the vorticity and the chirality and bound states are more robust against impurities when the vorticity and chirality have opposite sign. In this topological s-wave SC,
we thus understand the difference between these figures by recalling that the sign of $V_z$ in this SC corresponds to that of the chirality in chiral p-wave SC.

We note that the robustness of bound states is crucial to realization of adiabatic manipulation of vortices in TQC. To quantify the robustness against impurities (or equivalently, realizability of adiabatic dynamics), we define “the minigaps” in the presence of impurities by subtracting the widths of the first excited state and the zero mode from the minigap without impurities.

Figure 3 (a) (3 (b)) shows the dependence of minigaps on the normal scattering rates for the anti-parallel (parallel) vortex for various values of $ma^2/\Delta_0$. Figure 2 (a) and 2 (b) shows that scattering rates at low energies are suppressed for small $ma^2/\Delta_0$. When the signs of Zeeman coupling and vorticity are opposite (Fig. 3 (a)), on the other hand, the minigaps decrease steeply as $\Gamma_n$ increases. When the signs of Zeeman coupling and vorticity are opposite (Fig. 3 (a)), on the other hand, the minigaps maintain their magnitudes even for the strong $\Gamma_n$.

3.2. Rashba SOC dependence of anti-parallel vortex

Now we return to Fig. 2 and discuss the energy dependence of the scattering rate, particularly in the anti-parallel vortex. We can see that $\Gamma$ for the states with finite excitation energy decreases with the energy increasing regardless of the values of $ma^2/\Delta_0$ in the parallel vortex (Fig. 2 (b)). Figure 2 (a) shows that scattering rates at low energies are suppressed for small $ma^2/\Delta_0$. As $ma^2/\Delta_0$ increases, energy dependences become similar to those in Fig. 2 (b). Figure 2 (a) implies that the type of CdGM mode changes as $ma^2/\Delta_0$ changes.

Although the relative signs of the vorticity and the Zeeman coupling are common for all data in Fig. 2 (a), different strengths of Rashba SOC cause this difference, which has not
been observed in the cases of an s-wave SC and chiral p-wave SCs. We also find the $m\alpha^2/\Delta_0$ dependence of low energy scattering in Fig. 3 (a). As $\Gamma_n$ increases, the minigaps for large $m\alpha^2/\Delta_0$ decrease, while the minigaps for small $m\alpha^2/\Delta_0$ are robust against impurities. For some values of $\Gamma_n$, the relative magnitude of the minigaps is reversed.

4. Discussion
We find that the scattering rates at low energies are suppressed for some values of Rashba SOC in an anti-parallel vortex. This suppression is due to small $M_{l,l}$, i.e. coherence factor. Such a suppression as this for the anti-parallel vortex is theoretically expected in chiral p-wave superconducting vortices, where the rotational symmetry is found to be crucial for the coherence factors to be small [15]. The 2D electron system in a semiconductor has the rotational symmetry, but the symmetry of chiral p-wave SCs such as Sr$_2$RuO$_4$ is affected by point groups of crystals. Therefore this suppression of the impurity scattering will be observed more clearly in the topological s-wave SC than the chiral p-wave SC.

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