Robustness against non-magnetic impurities in topological superconductors

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Abstract. We study the robustness against non-magnetic impurities in a three-dimensional topological superconductor, focusing on an effective model (massive Dirac Bogoliubov-de Gennes (BdG) Hamiltonian with $s$-wave on-site pairing) of Cu$_x$Bi$_2$Se$_3$ with the parameter set determined by the first-principles calculation. With the use of the self-consistent $T$-matrix approximation for impurity scattering, we discuss the impurity-concentration dependence of the zero-energy density of states. We show that a single material variable, measuring relativistic effects in the Dirac-BdG Hamiltonian, well characterizes the numerical results. In the nonrelativistic limit, the odd-parity fully-gapped topological superconductivity is fragile against non-magnetic impurities, since this superconductivity can be mapped onto the $p$-wave superconductivity. On the other hand, in the ultrarelativistic limit, the superconductivity is robust against the non-magnetic impurities, since the effective model has the $s$-wave superconductivity. We derive the effective Hamiltonian in the both limit.

1. Introduction
The discovery of topological insulators triggers off a number of the studies on topological aspects of matter [1]. Specifically, the interplay of topology and superconductivity leads to intriguing issues in low-temperature physics. One of the key topics is to seek a bulk topological superconductor. A strong candidate for this superconductor is Cu$_x$Bi$_2$Se$_3$ [2]; the copper intercalation into a topological insulator Bi$_2$Se$_3$ induces superconductivity. Thus, identifying the characters of Cu$_x$Bi$_2$Se$_3$ is highly desirable now.

An advantageous way of clarifying superconducting properties is to ask whether a superconductor is conventional or not. A distinct feature of a topological superconductor shows up on the boundaries with different topological states (e.g., vacuum); the closing of the gap at interface indicates the presence of gapless edge modes [1]. An intrinsic feature of unconventional superconductivity (e.g., $p$-wave) is the presence of gapless states around non-magnetic impurities, owing to the violation of Anderson’s theorem. In specific models for topological superconductivity [3, 4], non-magnetic impurities induce the gapless states in the quasiparticle spectrum; one may claim that the topological superconductor is unconventional.

In this paper, we study the robustness of a topological superconductor against non-magnetic impurities, focusing on a set of the material variables for Cu$_x$Bi$_2$Se$_3$. Our approach is divided into two parts. First, we build up an effective theory to intuitively understand our system. Second, we examine the presence of gapless excitations, by numerical calculations with a self-consistent $T$-matrix approach. We show that the system has two aspects, i.e., both conventional and unconventional properties, depending on the amount of a relativistic effect in
the normal Hamiltonian. In other words, an analogy between Cu$_2$Bi$_2$Se$_4$ and an unconventional superconductor is dominated by the mass-to-momentum ratio in the Dirac-type Hamiltonian.

2. Model and formulation

2.1. Dirac Bogoliubov-de Gennes Hamiltonian

The Dirac Bogoliubov-de Gennes (BdG) Hamiltonian matrix $[2, 3, 5]$ is

$$
\mathcal{H}(\mathbf{k}) = \begin{pmatrix}
    h_0(\mathbf{k}) & \Delta_{\text{pair}}(\mathbf{k}) \\
    \Delta_{\text{pair}}^\dagger(\mathbf{k}) & -h_0^*(\mathbf{-k})
\end{pmatrix},
$$

with the normal-state Hamiltonian $h_0(\mathbf{k}) = \varepsilon(\mathbf{k}) + d_0(\mathbf{k})\gamma^0 + \sum_{i=1}^3 d_i(\mathbf{k})\gamma^i\gamma^0$ and the $4 \times 4$ pairing potential matrix $\Delta_{\text{pair}}$. The $4 \times 4$ complex matrices $\gamma^\mu$ ($\mu = 0, 1, 2, 3$) are the Gamma matrices in the Dirac basis. Using the orbital $2 \times 2$ Pauli matrices $\sigma^i$ and the spin $2 \times 2$ Pauli matrices $s^i$, we have $\gamma^0 = \sigma^3 \otimes 1_2$ and $\gamma^i = i\sigma^i \otimes s^i$. In the diagonal block of $h_0$, we have $\varepsilon = -\mu + \bar{D}_1\epsilon_c(\mathbf{k}) + (4/3)\bar{D}_2\epsilon_{\perp}(\mathbf{k})$ and $d_0 = M_0 - \bar{B}_1\epsilon_c(\mathbf{k}) - (4/3)\bar{B}_2\epsilon_{\perp}(\mathbf{k})$, with $\epsilon_c = 2 - 2\cos(k_z)$, $\epsilon_{\perp} = 3 - 2\cos(\sqrt{3}k_x/2)\cos(k_y/2) - \cos(k_y)$. The diagonal block has contributions from the spin-orbit couplings, $d_1 = (2/3)\bar{A}_2\sqrt{3}\sin(\sqrt{3}k_x/2)\cos(k_y/2)$, $d_2 = (2/3)\bar{A}_2[\cos(\sqrt{3}k_x/2)\sin(k_y/2) + \sin(k_y)]$, and $d_3 = \bar{A}_1\sin(k_z)$. The material variables $\bar{D}_1$, $\bar{D}_2$, $\bar{B}_1$, $\bar{B}_2$, $\bar{A}_2$, $\bar{A}_1$ are determined by the data from the first-principle calculations in [9]. The other material variable $M_0$ and the chemical potential $\mu$ are changed, since they are related to a doping level. In this paper, we focus on a pseudo-scalar-type order parameter in the superconducting part,

$$
\Delta_{\text{pair}} \gamma^2 = i\gamma^0 f^{\text{us}}.
$$

This pairing potential indicates the topological fully-gapped $s$-wave superconductivity [3]. We mention that a scalar-type gap function (a non-topological fully-gapped $s$-wave state) is robust against non-magnetic impurities [3]. This behavior is consistent with Anderson’s theorem for $s$-wave superconductivity.

2.2. Indicator of relativistic effects

We show the indicator of relativistic effects [3]. The linearized normal-state Hamiltonian is

$$
h_0(\mathbf{k}) \sim \gamma^0 \left[ M_0 + A_2(k_x\gamma^1 + k_y\gamma^2) + A_1k_z\gamma^3 \right].
$$

We define the indicator of the relativistic effects as

$$
\beta = \frac{\bar{A}_2k_F}{|M_0|} = \sqrt{\left( \frac{\mu}{M_0} \right)^2 - 1}.
$$

The Dirac-BdG Hamiltonian has two distinct behaviors, depending on $\beta$. In the limit of $\beta \to 0$, we have a nonrelativistic limit (i.e. large-mass limit). In the limit of $\beta \to \infty$, we have an ultrarelativistic limit (i.e. massless limit).

2.3. Self-consistent T-matrix approximation

We consider the non-magnetic impurity effects with the use of the self-consistent $T$-matrix approximation. We assume that the impurities are randomly distributed, leading to the impurity potential

$$
V(r) = \sum_i \delta(r - r_i)V^{\text{NM}}, \quad V^{\text{NM}} = V_0 \begin{pmatrix}
    1_{2 \times 2} & 0 \\
    0 & \begin{pmatrix} 1_{2 \times 2} \end{pmatrix}
\end{pmatrix}.
$$
The $T$-matrix is written as

$$T(\Omega) = \left[ 1 - V^{NM} \frac{1}{N} \sum_k G_k(\Omega) \right]^{-1} V^{NM}, \quad (6)$$

where $N$ is the number of meshes in momentum space and $G_k(\Omega)$ is the Green’s function with self-energy $\Sigma(\Omega)$. We have

$$G_k(\Omega) = \frac{1}{\Omega - H(k) - \Sigma(\Omega)} = \begin{pmatrix} g_k(\Omega) & f_k(\Omega) \\ f_k^*(\Omega) & g_k^*(\Omega) \end{pmatrix}, \quad \Sigma(\Omega) = n_{imp}T(\Omega) - n_{imp}V^{NM}, \quad (7)$$

with the impurity concentration $n_{imp}$. Solving 6 and 7 self-consistently, we obtain the density of states (DOS) as

$$N(E) = \frac{1}{2\pi} \frac{1}{N} \sum_k \text{tr}[\text{Im} \lim_{\eta \to 0} g_k(E + i\eta)]. \quad (8)$$

Similarly, we obtain the DOS of the normal state $N_{\text{normal}}(E)$, setting $f^{\text{imp}} = 0$. Note that the second term in the self energy in 7 corresponds to the renormalization of the chemical potential $\mu$, since in our calculations $\mu$ is fixed.

### 3. Effective Hamiltonian

Let us examine an effective Hamiltonian, depending on $\beta$. First, we focus on the nonrelativistic limit ($\beta \to 0$). Using the Dirac basis with respect to the Gamma matrices, the eigenvalue equations of the Dirac-BdG Hamiltonian are

$$\begin{pmatrix} \mu' & k' \cdot s & 0 & \Delta^{12} \\ k' \cdot s & -2M_0 - \mu' & 0 & 0 \\ 0 & \Delta^{21} & \mu' & k' \cdot s^* \\ \Delta^{21} & 0 & k' \cdot s^* & 2M_0 + \mu' \end{pmatrix} \begin{pmatrix} F \\ G \\ F' \end{pmatrix} = E \begin{pmatrix} F \\ G \\ F' \end{pmatrix}, \quad (9)$$

with $k' = (\bar{A}_2 k_x, \bar{A}_3 k_y, \bar{A}_1 k_z)$ and the effective chemical potential $\mu' \equiv \mu - M_0$. The indicator $\beta$ is zero when $\mu'$ is zero. The “large-component” ($F$ and $F'$) equations are

$$\begin{align*}
\mu' F + k' \cdot s G + \Delta^{12} G' &= EF, \\
\mu' F' + k' \cdot s^* G' + \Delta^{21} G &= EF',
\end{align*} \quad (10, 11)$$

whereas the “small-component” ($G$ and $G'$) equations are

$$\begin{align*}
G &= \frac{k' \cdot s}{E + 2M_0 + \mu'} F + \frac{\Delta^{21}}{E + 2M_0 + \mu'} F', \\
G' &= \frac{k' \cdot s^*}{E - 2M_0 - \mu'} F' + \frac{\Delta^{21}}{E - 2M_0 - \mu'} F.
\end{align*} \quad (12, 13)$$

Substituting the small components ($G$ and $G'$) into 10 and 11, we obtain the equations composed only of the large components. Imposing the conditions that $E/|M_0| \ll 1$, $\mu'/|M_0| \ll 1$, and $f^{\text{imp}}/|M_0| \ll 1$, we find that

$$\begin{pmatrix} \frac{k'^2}{2M_0} - \mu' - \frac{|f^{\text{imp}}|^2}{2M_0} & \frac{|f^{\text{imp}}|^2}{2M_0} k' \cdot s (i s^2) \\ -\frac{f^{\text{imp}}}{2M_0} k' \cdot s (i s^2) & \frac{k'^2}{2M_0} + \mu' + \frac{|f^{\text{imp}}|^2}{2M_0} \end{pmatrix} \begin{pmatrix} F \\ F' \end{pmatrix} = E \begin{pmatrix} F \\ F' \end{pmatrix}. \quad (14)$$
These effective equations indicate that the spin-orbit coupling term makes the effective gap function anisotropic. This $p$-wave gap function is equal to that of the B-phase in superfluid $^3$He [6, 7, 8]. Since Anderson’s theorem is not valid in the $p$-wave superconductivity, the topological fully-gapped $s$-wave superconductor in the nonrelativistic limit is not robust against non-magnetic impurities. The equivalence to the B-phase also indicates that the topological nature in this limit originates from the property of the Cooper-pair wavefunction.

Next, we focus on the ultrarelativistic limit ($\beta \rightarrow \infty$). The Weyl basis with respect to the Gamma matrices is convenient. We use the over-line symbol to specify the quantities in the Weyl basis. The linearized Dirac BdG equations is

$$
\begin{pmatrix}
-\mathbf{k}' \cdot \mathbf{s} - \mu' & M_0 & \tilde{\Delta}^{11} & 0 \\
0 & k' \cdot \mathbf{s} - \mu & 0 & \tilde{\Delta}^{22} \\
\tilde{\Delta}^{11*} & M_0 & 0 & 0 \\
0 & \tilde{\Delta}^{22*} & 0 & -M_0
\end{pmatrix}
\begin{pmatrix}
\mathbf{\tilde{F}} \\
\mathbf{\tilde{G}} \\
\mathbf{\tilde{F}}' \\
\mathbf{\tilde{G}}'
\end{pmatrix}
= E
\begin{pmatrix}
\mathbf{\tilde{F}} \\
\mathbf{\tilde{G}} \\
\mathbf{\tilde{F}}' \\
\mathbf{\tilde{G}}'
\end{pmatrix},
$$

with $\tilde{\Delta}^{11} = -i s^2 f^{ps}$ and $\tilde{\Delta}^{22} = i s^2 f^{ps}$. Taking $M_0 \rightarrow 0$, we find that the BdG equations are divided into a left-handed sector ($\tilde{G}$ and $\tilde{G}'$) and a right-handed sector ($\tilde{F}$ and $\tilde{F}'$),

$$
\begin{pmatrix}
k' \cdot \mathbf{s} - \mu & i s^2 f^{ps} \\
- i s^2 f^{ps*} & -k' \cdot \mathbf{s}^* + \mu
\end{pmatrix}
\begin{pmatrix}
\mathbf{\tilde{G}} \\
\mathbf{\tilde{G}}'
\end{pmatrix}
= E
\begin{pmatrix}
\mathbf{\tilde{G}} \\
\mathbf{\tilde{G}}'
\end{pmatrix},
$$

$$
\begin{pmatrix}
-k' \cdot \mathbf{s} - \mu & i s^2 f^{ps} \\
- i s^2 f^{ps*} & -k' \cdot \mathbf{s}^* + \mu
\end{pmatrix}
\begin{pmatrix}
\mathbf{\tilde{F}} \\
\mathbf{\tilde{F}}'
\end{pmatrix}
= E
\begin{pmatrix}
\mathbf{\tilde{F}} \\
\mathbf{\tilde{F}}'
\end{pmatrix}.
$$

When the chemical potential is large and positive, one can only consider the left-handed sector ($\tilde{G}$ and $\tilde{G}'$) to discuss the superconducting properties, since the Fermi wave-length $k_F = \mu$ in normal states characterizes the quasiparticle excitations. In both of the sectors, the formulae are obtained at $\Gamma$ point ($\mathbf{k} = 0$). The effective Hamiltonian is equivalent to in an $s$-wave superconductor, except $\mathbf{k} = 0$. This result indicates that the topological fully-gapped $s$-wave superconductor in the ultra-relativistic limit is robust against non-magnetic impurities, owing to Anderson’s theorem. We note that the difference between the topological and non-topological fully-gapped $s$-wave superconductors occurs at zero-momentum, where the quasiparticles with zero-momentum feel the sign change of the gap functions between the left- and right-handed sectors and induce surface bound states in the topological superconductors.

4. Numerical calculations of gapless excitations

Now, we show the numerical results. The $\mathbf{k}$-mesh size is $256 \times 256 \times 256$. The unitary-like scattering model with $V_0 = 10$eV is adopted. The gap amplitude is $f^{ps} = 0.1$eV. The smearing factor for the DOS is $\eta = 0.5$meV. The material parameters are set by $(D_1, D_2, B_1, B_2, A_1, A_2) = (0.0024, 19.6/a^2, 0.216, 56.6/a^2, 0.32, 4.1/a)$, in unit of eV, with $a = 4.076$. These parameters are determined by the data from the first-principles calculations in [9]. We remark that they are different from in [2, 3]. We calculate the zero-energy DOS $N(E = 0)$, changing the impurity concentration $n_{\text{imp}}$. The zero-energy DOS of the normal state, $N_{\text{normal}}(E = 0)$ is also calculated, by setting $f^{ps} = 0$.

Figure 1 shows that $\beta$ characterizes well the robustness against the non-magnetic impurities. In the nonrelativistic region ($\beta = 0.88$ in figure 1), the non-magnetic impurities easily induce the zero-energy DOS. The zero-energy DOS drastically increases above the specific impurity concentration, which depends on $\beta$. We note that the $T_c$ robustness against impurities depends on the point where the zero-energy DOS becomes finite. As shown in Fig. 1, the robustness monotonically increases with increasing $\beta$. These results indicate that the system has two aspects, $p$- and $s$- wave features, depending on the amount of relativistic effects.
5. Summary

In conclusion, we studied the robustness against the non-magnetic impurities, in a bulk topological $s$-wave superconductor. The calculations were performed for the data from the first-principles calculations of Cu$_2$Bi$_2$Se$_3$ [9]. We found that the results are summarized well by a single variable $\beta$, characterizing relativistic effects in the normal Hamiltonian. In the nonrelativistic region, the full-gapped topological $s$-wave superconductor is not robust against the non-magnetic impurities. In contrast, in the ultrarelativistic region, this superconducting state is robust against non-magnetic impurities. Consequently, the present system has two aspects, $p$- and $s$- wave features, with a typical set of the material variables of Cu$_2$Bi$_2$Se$_3$.

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