Inhomogeneity Effects in Topological Superconductors

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We have constructed a quasiclassical framework on superconductors with strong spin-orbit couplings, applicable to Cu\(_x\)Bi\(_2\)Se\(_3\) [Y. Nagai, H. Nakamura, and M. Machida: arXiv:1305.3025]. The notable point is that in this framework the Bogoliubov-de Gennes Hamiltonians with suggested odd-parity pairing states turn to quasiclassical ones with usual spin-triplet Cooper pairs. Using this quasiclassical theory, we can investigate inhomogeneity effects such as the phenomena with vortices and surfaces in this superconductors and shed light on the pairing state of topological superconductors.

In this paper, we apply the quasiclassical framework to the surface bound states with the Dirac-cone energy dispersion originated from the topological invariant in the parent compound Bi\(_2\)Se\(_3\) in order to investigate the robustness of these bound states under the superconducting order parameter. The odd-parity gap functions can not open on the Dirac-cone-dispersion band in the Cu-doped Bi\(_2\)Se\(_3\) superconductor. We show that the massless Dirac quasiparticles originated from the normal-state topological invariant and the Majorana quasiparticles coexist with each other on the surface in the odd-parity topological superconductivity. Inhomogeneity effects can be easily investigated with the use of our quasiclassical framework in topological superconductors.

**KEYWORDS:** Topological superconductors, Dirac quasiparticles, Quasiclassical framework

1. Introduction

The discovery of topological superconductors has attracted much attention because of new topologically non-trivial states of condensed matters. Experimentalists have intensively explored evidence of the topological superconductivity by various tools, and theorists have debated theoretical framework to describe their various non-trivial superconducting properties [1–11]. Recently, we have constructed a convenient quasiclassical framework for the topological superconductivity characterized by strong spin-orbit coupling and clarified its theoretical correspondence to the spin-triplet superconductivity without the spin-orbit coupling [12].

The topological insulator Bi\(_2\)Se\(_3\) becomes a superconductor with the Cu-doping, and Cu\(_x\)Bi\(_2\)Se\(_3\) has been regarded as a key compound for the investigation of non-trivial topological superconductivity [13–18]. According to the result of the angular photoemission experiment [14], there are surface bound states originated from the normal-state topological invariant even in the doping material as shown in Fig. 1. In this paper, we apply the quasiclassical framework to the surface bound states with the Dirac-cone energy dispersion originated from the topological invariant in the parent compound Bi\(_2\)Se\(_3\) in order to investigate the robustness of these bound states under the superconducting order parameter. With the use of our surface quasiclassical theory, the \(8 \times 8\) matrix Dirac Bogoliubov-de Gennes (BdG) equations in the three-dimensional space become \(2 \times 2\) matrix ones in the two-dimensional space.
Fig. 1. Schematic diagram of the dispersion relations of the surface bound states in the topological insulator and the topological superconductor. \( \Delta_{\text{eff}} \) denotes the superconducting gap on the bulk band and \( \Delta_{\text{sur}} \) denotes that on the surface band.

2. Dirac-type Hamiltonian

Now, let us begin with the massive Dirac type BdG Hamiltonian on the topological superconductivity expressed as [17, 18]

\[
H = \int dr \left( \begin{array}{cc}
\bar{\psi}(r) & \bar{\psi}_c(r)
\end{array} \right) \left( \begin{array}{cc}
\hat{H}^-(r) & \Delta^-(r) \\
\Delta^+(r) & \hat{H}^+(r)
\end{array} \right) \left( \begin{array}{c}
\psi(r) \\
\psi_c(r)
\end{array} \right),
\]

(1)

where

\[
\hat{H}^\pm(r) = M_0 - i\partial_\gamma \gamma^1 - i\partial_\gamma \gamma^2 - i\partial_\gamma \gamma^3 \pm \mu \gamma^0.
\]

(2)

Here, \( \gamma^i \) is a 4 \times 4 Dirac gamma matrix, which can be described as \( \gamma^0 = \hat{\sigma}_z \otimes 1 \), \( \gamma^{1,2,3} = i\hat{\sigma}_y \otimes \hat{s}_i \), and \( \gamma^5 = \hat{\sigma}_x \otimes 1 \) with 2 \times 2 Pauli matrices \( \hat{\sigma}_i \) in the orbital space and \( \hat{s}_i \) in the spin space, \( \psi(r) \) is the Dirac spinor, \( \bar{\psi}(r) \equiv \psi^\dagger(r)\gamma^0 \), \( \bar{\psi}_c(r) \equiv \bar{\psi}_c^\dagger(r) \), and \( \psi_c \equiv C\bar{\psi}^T \), where \( C \equiv i\gamma^2 \gamma^0 \) is the representative matrix of charge conjugation. \( \Delta^- \) is the gap function and \( \Delta^+ \equiv \gamma^0(\Delta^-)^\dagger \gamma^0 \). Considering only the on-site pairing interaction, the possible gap form is reduced into six types of functions as seen in Table I of Ref. [17]. These gap functions are classified into scalar, pseudo-scalar, and polar vector (four-vector) associated with the Lorentz transformation,

\[
\Delta^- = \Delta_0, \Delta_0 \gamma^5, \Delta_0 \mu \gamma^5,
\]

(3)

where, \( \Delta_0 \) is a scalar magnitude of the gap functions, the Feynman slash \( \mu \) is defined by \( \sum_\mu \gamma^\mu a_\mu \), and the gap function including \( \mu \) is characterized as a unit four-vector \( a_\mu \). From the Hamiltonian Eq. (1), the correspondent 8 \times 8 BdG equations are given as

\[
\begin{pmatrix}
\hat{h}_0(r) - \mu & \hat{\Delta}(r) \\
\hat{\Delta}^+(r) & \hat{h}_0(r) + \mu
\end{pmatrix}
\begin{pmatrix}
u(r) \\
u_c(r)
\end{pmatrix} = E
\begin{pmatrix}
u(r) \\
u_c(r)
\end{pmatrix},
\]

(4)

where \( \gamma^0 \hat{h}_0 = \tilde{h}_0 \pm \mu \), and \( \hat{\Delta} = \gamma_0 \Delta^- \). Note that \( \nu \) in the conventional Nambu eigen-state form, \( (u, v)^T \) is related to \( u_c \) as \( v \equiv i\gamma^2 u_c \).

3. Surface bound states in normal states

3.1 Surface bound states at the \( \Gamma \)-point

Topological insulators have gapless quasiparticle states at a surface. We consider the surface perpendicular to \( z \)-axis and the material fills the region of \( z > 0 \). The boundary condition is given by
\[ u(z = 0) = u_c(z = 0) = 0. \] Assuming the translational symmetry along \( x \) and \( y \), the Dirac Hamiltonian (4) is expressed as

\[ \left[ H_0(k_x, k_y, -i\partial_z) + H_1(k_x, k_y) \right] u(k_x, k_y, z) = [E + \mu] u(k_x, k_y, z), \tag{5} \]

where \( H_0(k_x, k_y, -i\partial_z) \equiv M(k_x, k_y, -i\partial_z)\gamma^0 - i\partial_z\gamma^0\gamma^3 \) and \( H_1(k_x, k_y) \equiv \gamma^0(k_x\gamma^1 + k_y\gamma^2) \). The equation for \( u_c \) is solved by substituting \( \mu \rightarrow -\mu \) into the above equation. In the case of \( E = -\mu \), the eigenvalue equation with respect to \( H_0 \) becomes

\[ \left[ M(k_x, k_y, \lambda_i) + \sigma \lambda_i \right] \psi_i = 0, \tag{6} \]

where \( \psi_i \) is the \( i \)th eigenvectors of \( \gamma^3 \) with the eigenvalue \( \epsilon_i = i\sigma \) with \( \sigma = \pm 1 \) expressed as

\[
\begin{align*}
\epsilon_1 &= i, \psi_1^T = (1/\sqrt{2}) \begin{pmatrix} 0 & i & 0 & 1 \end{pmatrix}, \\
\epsilon_2 &= i, \psi_2^T = (1/\sqrt{2}) \begin{pmatrix} -i & 0 & 1 & 0 \end{pmatrix}, \\
\epsilon_3 &= -i, \psi_3^T = (1/\sqrt{2}) \begin{pmatrix} 0 & -i & 0 & 1 \end{pmatrix}, \\
\epsilon_4 &= -i, \psi_4^T = (1/\sqrt{2}) \begin{pmatrix} i & 0 & 1 & 0 \end{pmatrix}.
\end{align*}
\tag{7-10}
\]

Here, we assume \( u(z) = \sum_{i=1}^{4} c_i \exp[\lambda_i z] \psi_i \). \( \lambda_i \) dependence of \( M(k_x, k_y, \lambda_i) \) determines the existence condition of the bound states, since the surface bound states exist only if \( \text{Re}\lambda > 0 \) under the condition \( \lim_{z \to \infty} u(z) = 0 \). If \( M(k) = M_0(k_x, k_y) + M_1 k_x^2 \), we have \( \lambda_i = (\sigma \pm \sqrt{1 + 4M_0M_1})/(2M_1) \) and the surface bound state exists when \( M_0M_1 < 0 \). Then, the general solution with respect to \( H_0 \) with \( M_1 < 0 \) and \( E = -\mu \) becomes

\[ u(k_x, k_y, z, E = -\mu) = \frac{1}{\sqrt{A}} \sum_{i=1}^{2} c_i e^{\sqrt{A} \sinh(Kz)} \psi_i, \tag{11} \]

where \( K = (\sqrt{1 + 4M_0M_1})(2M_1) \) with \( A = \int_{0}^{\infty} dz \exp(z/M_1)|\sinh(Kz)|^2 \).

3.2 Surface bound states with the rotational symmetry

We can obtain the eigenvector with respect to \( H_0 + H_1 \) at \( E \neq -\mu \) with the use of the above general solution with respect to \( H_0 \). By substituting the above solution into Eq. (5), the eigenvalue equations become

\[ \begin{pmatrix} 0 & -ik_+ \\ ik_- & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E' \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}, \tag{12} \]

with \( k_\pm \equiv k_x \pm ik_y \) and \( E' \equiv E + \mu \). Therefore, we obtain the surface-bound states expressed as

\[ u_N(k_x, k_y, r, E') = \frac{1}{\sqrt{2A}} e^{ik_+r_\perp} e^{i\phi} \sinh(Kz) \left[ \psi_1 + ie^{-i\phi} \text{sgn}(E') \psi_2 \right], \tag{13} \]

with \( k_\perp = (k_x, k_y) = \sqrt{k_x^2 + k_y^2}(\cos \phi, \sin \phi) \) and \( r_\perp = (x, y) \).

3.3 Surface bound states with the six-fold rotational symmetry

Considering the Hamiltonian for Bi$_2$Se$_3$ on the triangular lattice [13, 18], the eigenvalue equations become

\[ \begin{pmatrix} 0 & -iP_+(k_x, k_y) \\ iP_-(k_x, k_y) & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E' \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}, \tag{14} \]
with
\[ P_{\pm}(k_x, k_y) \equiv P_1(k_x, k_y) \pm iP_2(k_x, k_y), \] (15)
\[ P_1(k_x, k_y) \equiv \frac{2}{3} \sqrt{3} \sin \left( \frac{\sqrt{3}}{2} k_x \right) \cos \left( \frac{k_y}{2} \right), \] (16)
\[ P_2(k_x, k_y) \equiv \frac{2}{3} \left[ \cos \left( \frac{\sqrt{3}}{2} k_x \right) \sin \left( \frac{k_y}{2} \right) + \sin (k_y) \right]. \] (17)

Therefore, we obtain the surface-bound states on the triangular lattice expressed as
\[ u_{in}^N(k_x, k_y, r, E') = \frac{1}{\sqrt{2A}} e^{ik_zr+ie^{ik_zr}} \sinh (Kz) \left[ \psi_1 + ie^{-i\Phi(k_x, k_y)} \text{sgn}(E')\psi_2 \right]. \] (18)

with
\[ e^{-i\Phi(k_x, k_y)} \equiv \frac{P_1(k_x, k_y) - iP_2(k_x, k_y)}{\sqrt{P_1(k_x, k_y)^2 + P_2(k_x, k_y)^2}} \] (19)

4. Surface quasiclassical theory

The quasiclassical theory is founded on an assumption that the coherence length \( \xi \) is much longer than the Fermi wave length \( 1/k_F (\xi k_F \gg 1) \) [19]. The assumption is valid, when the order parameter amplitude \( |\Delta_0| \) is much smaller than the Fermi energy \( E_F (|\Delta_0|/E_F \ll 1) \), and the condition is fully fulfilled in BCS weak-coupling superconductivity. In this theory, the wave function is expressed by a product of the fast oscillating one characterized by the Fermi momentum \( p_F \) and the slowly varying one by the coherence length \( \xi \), and the quasiclassical solution of the BdG equations is given as
\[ \begin{pmatrix} u(r) \\ u_c(r) \end{pmatrix} \sim \begin{pmatrix} u^N(r, k_{F\perp}) f(r_\perp, k_{F\perp}) \\ u_c^N(r, k_{F\perp}) g(r_\perp, k_{F\perp}) \end{pmatrix}, \] (20)
where \( u^N, u_c^N \) are normal-state eigenvectors at the Fermi level expressed as,
\[ \hat{h}_0(r) u^N(r, k_{F\perp}) = \mu u^N(r, k_{F\perp}), \] (21)
\[ \hat{h}_0(r) u_c^N(r, k_{F\perp}) = -\mu u_c^N(r, k_{F\perp}). \] (22)

Here, the chemical potential is supposed to be larger than the mass \( (\mu > M_0) \). As shown in Ref. 12, there are two solutions in a bulk. On the other hand, there is an only one solution at a surface as shown in Eq. (13). The eigenvectors are given as
\[ u^N(r, k_{F\perp}) = u^N(k_{Fx}, k_{Fy}, r, \mu), \] (23)
\[ u_c^N(r, k_{F\perp}) = u^N(k_{Fx}, k_{Fy}, r, -\mu). \] (24)

With the use of the above wave function, we reach \( 2 \times 2 \) matrix eigenvalue problem with respect to two functions \( (f_1, g_1) \) from \( 8 \times 8 \) BdG equations. The diagonal term is converted as
\[ \int_0^\infty dz u^N(r, k_{F\perp}) (\hat{h}_0 - \mu) u^N(r, k_{F\perp}) f = -iv_{F\perp} \cdot \nabla_{\perp} f, \] (25)
with \( v_F \equiv (\cos \phi, \sin \phi) \) and \( \nabla_{\perp} \equiv (\partial_x, \partial_y) \). Thus, we have effective two-dimensional \( 2 \times 2 \) quasiclassical BdG equations represented as
\[ \begin{pmatrix} -iv_{F\perp} \cdot \nabla_{\perp} & \Delta_{\text{sur}}(r_\perp, k_{F\perp}) \\ \Delta_{\text{sur}}(r_\perp, k_{F\perp})^* & iv_{F\perp} \cdot \nabla_{\perp} \end{pmatrix} \begin{pmatrix} f(r_\perp, k_{F\perp}) \\ g(r_\perp, k_{F\perp}) \end{pmatrix} = E \begin{pmatrix} f(r_\perp, k_{F\perp}) \\ g(r_\perp, k_{F\perp}) \end{pmatrix}. \] (26)
The correspondence between the original BdG gap functions $\tilde{\Delta}$, the effective ones $\Delta_{\text{eff}}(p_F)$ and the surface effective ones $\Delta_{\text{surf}}(k_{F\perp})$ in quasiclassical theory. “P-scalar” denotes a pseudo scalar whose parity is odd and “$i$-polar” denotes a polar vector pointing the $i$ direction in four dimensional space.

| Parity   | $\Delta_{\text{eff}}(p_F)$ | $\Delta_{\text{surf}}(k_{F\perp})$ |
|----------|----------------------------|----------------------------------|
| Scalar   | $\gamma^5$                 | singlet                         |
| $t$-polar| $\gamma^0\gamma^5$        | singlet                         |
| P-scalar | 1                          | triplet: $d = (v_x, v_y, v_z)$  |
| $x$-polar| $\gamma^1\gamma^5$        | triplet: $d = (0, -v_z, v_y)$   |
| $y$-polar| $\gamma^2\gamma^5$        | triplet: $d = (v_z, 0, -v_x)$   |
| $z$-polar| $\gamma^3\gamma^5$        | triplet: $d = (-v_y, v_x, 0)$   |

All the converted gap functions are listed in Table I. As an example exhibited in Table I, the pseudo scalar gap function is equivalent to the spin-triplet gap function $\Delta_{\text{eff}}$ whose $d$-vector rotates in momentum space in the bulk superconductor ($d = (v_x, v_y, v_z)$). Here, $v$ denotes the velocity. On the other hand, we should note that the effective surface gap function originated from the pseudo scalar gap function $\Delta_{\text{surf}}$ is zero as shown in Table I, since the off-diagonal term with the pseudo-scalar gap function is converted as

$$\int_0^{\infty} dz u_{c}^N(r, k_{F\perp})\gamma^0 \Delta^\dagger u_{c}^N(r, k_{F\perp})f = 0.$$ (27)

This shows that the normal-state surface bound states written as Eq. (13) are robust against the pseudo-scalar gap functions because the gap can not open as shown in Fig. (1). We should note that even the surface bound states with the six-fold symmetry expressed as Eq. (18) are robust, since the off-diagonal term with the wave function $u_{\text{int}}^N(k_x, k_y, r, E')$ becomes zero.

### 5. Discussion

We discuss the reason why the surface bound states do not open the superconducting gap due to the odd-parity gap functions. We note that the spin rotates on the Fermi surface originated from the surface bound states in the normal states expressed as Eq. (13), which is well known as “spin-momentum locking” [5]. The spin of the quasiparticle with the momentum $k_F$ is anti-parallel to that with the momentun $-k_F$ as shown in Fig. 2. Therefore, the Cooper pairs with parallel spins such as the spin-triplet superconductivity cannot form on this spin-momentum locking Fermi surface. The odd-parity gap functions can not open on the Dirac-cone-dispersion band in the Cu-doped Bi$_2$Se$_3$ superconductor as shown in Fig. (1). This indicates that there are the robust Dirac-type surface states expressed as Eq. (13) and the robust Majorana surface states due to the odd-parity superconductivity. Inhomogeneity effects due to the interaction between the Dirac quasiparticles and the Majorana quasiparticles on the surface of the topological superconductor can be treated by our quasiclassical treatment.

### 6. Conclusion

We constructed a surface two-dimensional quasiclassical theory which consists of the normal-state surface bound states. These surface bound states do not open the superconducting gap due to the odd-parity gap functions, since the Cooper pairs with parallel spins such as the spin-triplet superconductivity can not form on this spin-momentum locking Fermi surface. We showed that the massless Dirac quasiparticles originated from the normal-state topological invariant and the Majorana quasiparticles coexist on the surface in the odd-parity topological superconductivity. Inhomogeneity
effects due to the interaction between the Dirac quasiparticles and the Majorana quasiparticles on the surface of the topological superconductor can be treated by out quasiclassical treatment.

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