Anomalous Andreev bound state in non-centrosymmetric superconductors

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We study edge states of non-centrosymmetric superconductors where spin-singlet $d$-wave pairing mixes with spin-triplet $p$ (or $f$)-wave one by spin-orbit coupling. For $d_{xy}$-wave pairing, the obtained Andreev bound state has an anomalous dispersion as compared to conventional helical edge modes. A unique topologically protected time-reversal invariant Majorana bound state appears at the edge. The charge conductance in the non-centrosymmetric superconductor junctions reflects the anomalous structures of the dispersions, particularly the time-reversal invariant Majorana bound state is manifested as a zero bias conductance peak.

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Recently, physics of non-centrosymmetric (NCS) superconductors is one of the important issues in condensed matter physics [1, 2]. One of the remarkable features in NCS superconductors is that due to the broken inversion symmetry, superconducting pair potential becomes a mixture of spin-singlet even-parity and spin-triplet odd-parity [5]. Due to the mixture of spin-singlet and spin-triplet pairings, several novel properties such as the large upper critical field are expected [3, 6].

In these works, pairing symmetry of NCS superconductors is that due to the broken inversion symmetry, superconducting pair potential becomes a mixture of spin-singlet even-parity and spin-triplet odd-parity [5]. Due to the mixture of spin-singlet and spin-triplet pairings, several novel properties such as the large upper critical field are expected [3, 6].

Up to now, there have been several studies about superconducting profiles of NCS superconductors [3, 6, 12]. In these works, pairing symmetry of NCS superconductors has been mainly assumed to be $s + p$-wave. However, in a strongly correlated system, this assumption is not valid anymore. Microscopic calculations have shown that $d_{xy}$-wave spin-singlet pairing mixes with $f$-wave pairing based on the Hubbard model near half filling [13]. Also, a possible pairing symmetry of superconductivity generated at heterointerface LaAlO$_3$/SrTiO$_3$ [4] has been studied based on a similar model [16]. It has been found that the gap function consists of spin-singlet $d_{xy}$-wave component and spin-triplet $p$-wave one [15]. Therefore, now, it is a challenging issue to reveal novel properties specific to $d_{xy} + p$ or $d_{xy} + f$-wave pairing.

The generation of Andreev bound state (ABS) at the surface or interface is a significantly important feature in unconventional superconductors since tunneling spectroscopy via ABS [16] is a powerful method to identify pairing symmetry and mechanism of unconventional superconductors [17], it is quite important and interesting to clarify ABS and resulting tunneling conductance for $d_{xy} + p$-wave and $d_{xy} + f$-wave pairings.

In this Letter, we investigate ABS and tunneling conductance $\sigma_C$ in normal metal / NCS superconductor junctions. For both $d_{xy} + p$-wave and $d_{xy} + f$-wave cases, new types of ABS are obtained. In particular, for $d_{xy} + p$-wave case, due to the Fermi surface splitting by spin-orbit coupling, a single branch of topologically stable Majorana bound state appears. Recently, to search for Majorana fermions is one of the hottest issues in condensed matter physics [18, 19]. In stark contrast to the other Majorana fermions, the present one preserves time-reversal symmetry. From this difference, the “time-reversal invariant (TRI) Majorana bound state” has a peculiar flat dispersion. It shows a unique ZBCP in $\sigma_C$ depending on the spin-orbit coupling. Therefore, the experimental identification is feasible.

We start with the Hamiltonian of NCS superconductor

$$H_S = \begin{pmatrix} \hat{H}(k) & \hat{\Delta}(k) \\ -\hat{\Delta}^*(k) & -\hat{H}^*(-k) \end{pmatrix}$$

with $\hat{H}(k) = \xi_k + V(k) \cdot \hat{\sigma}$, $V(k) = \lambda(\hat{x}k_y - \hat{y}k_x)$, $\xi_k = \hbar^2 k^2/(2m) - \mu$. Here, $\mu$, $m$, $\hat{\sigma}$ and $\lambda$ denote chemical potential, effective mass, Pauli matrices and coupling constant of Rashba spin-orbit interaction, respectively [3]. The pair potential $\Delta(k)$ is given by

$$\Delta(k) = [d(k) \cdot \hat{\sigma}]\hat{\sigma}_y + i\psi(k)\hat{\sigma}_x.$$  

Due to the spin-orbit coupling, the spin-triplet component $d(k)$ is aligned with the polarization vector of the Rashba spin orbit coupling, $d(k) = |V(k)| \hat{V}(k)$ [3]. Then, the triplet component is $d(k) = \Delta(f(k))(\hat{x}k_y - \hat{y}k_x)/k$ with $k = \sqrt{k^2}$ while singlet component reads $\psi(k) = \Delta_s f(k)$ with $\Delta_s \geq 0$ and $\Delta_s \geq 0$.

$f(k)$ is given by $f(k) = 2k_x k_y/k^2$ for $d_{xy} + p$-wave and $f(k) = (k_x^2 - k_y^2)/k^2$ for $d_{xy} + f$-wave. The superconducting gaps are $\Delta_1 = |\Delta_1(k)|$ and $\Delta_2 = |\Delta_2(k)|$ for
the two spin-split band with \( \bar{\Delta}_1(k) = (\Delta_s + \Delta_t)f(k) \) and \( \bar{\Delta}_2(k) = (\Delta_t - \Delta_s)f(k) \), respectively, in homogeneous state \[3\].

Let us consider a wave function including ABS localized at the surface. Consider a two-dimensional semi-infinite superconductor on \( x > 0 \) where the surface is located at \( x = 0 \). The corresponding wave function is given by \[1\]

\[
\Psi_S(x) = \left[ c_1^+ \psi_1^+ \exp(iq_{1x}^+x) + c_1^- \psi_1^- \exp(-iq_{1x}^-x) + c_2^+ \psi_2^+ \exp(iq_{2x}^+x) + c_2^- \psi_2^- \exp(-iq_{2x}^-x) \right] \exp(ik_yy),
\]

\[
q_{1(2)x} = k_{1(2)x} \pm \frac{k_{1(2)x}}{k_{1(2)x}} \left( \frac{E^2 - |\bar{\Delta}_1(\bar{k}_{1(2)x})|^2}{\lambda^2 + 2h^2\mu/m} \right),
\]

with \( k_{1(2)x} = k_{1(2)x} = \sqrt{k_{1(2)}^2 - k_y^2} \) for \( |k_y| \leq k_{1(2)} \) and \( k_{1(2)x} = -k_{1(2)x} = i\sqrt{k_y^2 - k_{1(2)}^2} \) for \( |k_y| > k_{1(2)} \), and \( k_{1(2)x} = (\pm k_{1(2)x}, k_y) \). Here, \( k_1 \) and \( k_2 \) are the Fermi wavenumbers for the smaller and larger Fermi surface given by \(-m\lambda/h^2 + \sqrt{(m\lambda/h^2)^2 + 2m\mu/h^2} \) and \( m\lambda/h^2 + \sqrt{(m\lambda/h^2)^2 + 2m\mu/h^2} \), respectively. The wave functions are given by \( T_1 \psi_1^\pm = (1, -\alpha_{-1,1}, \alpha_{-1,1}^\dagger, \Gamma_{1\pm}) \) and \( T_2 \psi_2^\pm = (1, \alpha_{+1,1}, \alpha_{-1,1}^\dagger, \Gamma_{2\pm}) \) with

\[
\Gamma_{1(2)\pm} = \frac{\bar{\Delta}_{1(2)}(k_{1(2)x})}{E \pm \sqrt{E^2 - |\bar{\Delta}_{1(2)}(k_{1(2)x})|^2}}\]

and \( \alpha_{1(2)\pm} = (\pm k_{1(2)x} - ik_y) / k_{1(2)} \). \( E \) is the quasiparticle energy measured from the Fermi energy.

Postulating \( \Psi_S(x) = 0 \) at \( x = 0 \), we can determine the ABS. We consider the case for \( |k_y| < k_2 \). We first focus on the ABS for \( d_{xy} + p \)-wave case. For \( \Delta_t > \Delta_s \), the dispersion \( \varepsilon_b \) of ABS is given by

\[
\varepsilon_b = \begin{cases} 
\pm |k_{1(2)}(\pm k_y^2 + k_{1(2)}^2), \sqrt{2m\mu/h^2} & \text{if } k_c < |k_y| \leq k_{1(2)} \\
0 & \text{if } k_1 < |k_y| \end{cases}
\]

with \( \gamma = (k_1/k_2 + k_2/k_1 + (\Delta_s/\Delta_t)(k_2/k_1 - k_1/k_2)), \eta = |\Delta_s(1 - k_1/k_2) + \Delta_t(1 + k_1/k_2)|/|\Delta_1[1 + (k_1/k_2)]^2 + \Delta_2[1 - (k_1/k_2)]^2|, \) \( k_c = k_1 \sqrt{\Delta_1(1 - k_1/k_2) + \Delta_2\sqrt{\Delta_1 + \Delta_2} - (k_1/k_2)^2} \). On the other hand, for \( \Delta_s > \Delta_t \), the resulting \( \varepsilon_b \) is given by \( \varepsilon_b = 0 \). The dispersion \( \varepsilon_b \) of ABS changes drastically at \( \Delta_s = \Delta_t \), where one of the energy gaps, i.e. \( \Delta_2 \), becomes zero. It should be remarked that the present ABSs do not break the time reversal symmetry.

The resulting \( \varepsilon_b \) is plotted for various cases in Fig. 1 with \( \Delta_0 = \Delta_s + \Delta_t \). For convenience, we introduce dimensionless constant \( \beta = 2m\lambda/(h^2k_f) \) with \( k_f = \sqrt{2m\mu/h^2} \). We also plot \( \Delta_1 \) and \( \Delta_2 \). Both \( \Delta_1 \) and \( \Delta_2 \) become zero at \( k_y = 0 \). At \( |k_y| = k_2, \Delta_2 \) is always zero. However, \( \Delta_1 \) then becomes zero only for \( \beta = 0 \). First, we look at the \( \Delta_t > \Delta_s \) case. For \( \Delta_s = 0 \) with \( \beta = 0, \varepsilon_b = \pm c_k \) with some constant \( c \) for small \( k_y \) (curve a in Fig. 1) as shown in the case of \( s + p \)-wave pairing\[8–13\] since \( \eta = 0 \) is satisfied. This type of ABS is called helical edge mode \[11\] \( \Delta_2 \). However, this condition is satisfied only for \( \Delta_s = 0 \) and \( \beta = 0 \). In fact, \( \varepsilon_b \) near \( k_y = 0 \) becomes absent in general as shown in curves a in Figs. 1(B), (D) and (E). At \( k = \pm k_c, \varepsilon_b \) coincides with \( \pm 2 \). For nonzero \( \beta, \varepsilon_b \) becomes exactly zero for \( |k_y| > k_1 \) as shown in curves a in Figs. 1(D) and (E). The present line shapes of \( \varepsilon_b \) are completely different from those of \( s + p \)-wave superconductors. On the other hand, for \( \Delta_s > \Delta_t, \varepsilon_b = 0 \) for any \( k_y \) similar to the case of spin-singlet \( d_{xy} \) or spin-triplet \( p_x \)-wave pairing\[14, 17\].

We notice here that the zero energy bound state for \( |k_y| > k_1 \) is a Majorana bound state. The wave function for the zero energy edge state \( \Psi_m(k_y) \) can be written as

\[
\Psi_m(k_y) = (u_1(k_y), u_2(k_y), v_1(k_y), v_2(k_y))
\]

where

\[
u_1(k_y) = -i\sigma v_2(k_y) = \frac{(\alpha f_1 - \beta f_2) \exp(ik_yy - i\frac{\pi}{2})}{\sqrt{\sigma \alpha}}
\]

\[
u_2(k_y) = i\sigma v_1(k_y) = \frac{(f_1 + \beta f_2) \exp(ik_yy - i\frac{\pi}{2})}{\sqrt{\sigma \alpha}}
\]

with \( \alpha = (k_y - \sqrt{k_y^2 - k_{1y}^2}) / k_1, \beta_1 = (\alpha k_y/k_2 + 1), \beta_2 = (\alpha + k_y/k_2) \) and \( \sigma = \text{sgn}(k_y) \). The functions \( f_1 \) and \( f_2 \) decays exponentially as a function of \( x \) and are even function of \( k_y \). The Bogoliubov quasiparticle creation operator for this state is constructed in the usual way as \( \gamma^\dagger(k_y) = u_1(k_y)c_1^\dagger(k_y) + u_2(k_y)c_1(k_y) + v_1(k_y)c_1(-k_y) + v_2(k_y)c_1(-k_y) \). Since \( u_1(k_y) = v_1^\dagger(-k_y) \) and \( u_2(k_y) = v_2^\dagger(-k_y) \) are satisfied, it is possible to verify that \( \gamma^\dagger(k_y) = \gamma(-k_y) \). This means the generation of Majorana bound state at the edge for \( |k_y| > k_1 \). For \( \Delta_s > \Delta_t, \) a similar Majorana bound state also appears for \( |k_y| > k_1 \). On the other hand, for \( |k_y| \leq k_1 \), Majorana bound state has double branches and it is reduced to be conventional zero energy ABS.

Unlike Majorana fermions studied before\[18, 19\], the present single Majorana bound state is realized with time reversal symmetry. The TRI Majorana bound state has the following three characteristics. a) It has a unique flat dispersion: To be consistent with the time-reversal invariance, the single branch of zero mode should be symmetric under \( k_y \rightarrow -k_y \). Therefore, by taking into account the particle-hole symmetry as well, the flat dispersion is required. On the other hand, the conventional time-reversal breaking Majorana bound state has a linear dispersion. b) The spin-orbit coupling is necessary to obtain the TRI Majorana bound state. Without spin-orbit coupling, the TRI Majorana bound state vanishes. c) The TRI Majorana bound state is topologically stable under small deformations of the Hamiltonian\[20\].

We also calculate ABS for \( d_{x^2-y^2} + f \)-wave case. In this case, ABS exists only for \( \Delta_s < \Delta_t \). In Fig. 2, \( \varepsilon_b \) is plotted similarly to Fig. 1. As a reference, corresponding
The Hamiltonian $\hat{H}_N$ in a normal metal is given by putting $\Delta(k) = 0$ and $\lambda = 0$ in $\hat{H}_S$. We assume an insulating barrier at $x = 0$ expressed by a delta-function potential $U\delta(x)$. The wave function for spin $\gamma = (\uparrow, \downarrow)$ in the normal metal $\Psi_N(x)$ is given by

$$
\Psi_N(x) = \exp(ik_F y)[(\psi_{\gamma\uparrow} + \sum_{\rho=\uparrow,\downarrow} a_{\gamma\rho} \psi_{\rho\uparrow}) \exp(ik_F x) + \sum_{\rho=\uparrow,\downarrow} b_{\gamma\rho} \psi_{\rho\downarrow} \exp(-ik_F x)]
$$

with $T\psi_{\gamma\uparrow} = T\psi_{\gamma\downarrow} = (1, 0, 0, 0)$, $T\psi_{\rho\uparrow} = T\psi_{\rho\downarrow} = (0, 1, 0, 0)$, $T\psi_{\rho\uparrow} = (0, 0, 1, 0)$, and $T\psi_{\rho\downarrow} = (0, 0, 0, 1)$. The corresponding $\Psi_S(x)$ is given by Eq. (2). The coefficients $a_{\gamma\rho}$ and $b_{\gamma\rho}$ are determined by the boundary condition $\Psi_S(0) = \Psi_S(0)$, and $h\bar{v}_{Sx}\Psi_S(0) - h\bar{v}_{Nx}\Psi_N(0) = -2iU\bar{\tau}_3\Psi_S(0)$ with $h\bar{v}_{S(N)x} = \partial H_{S(N)}/\partial k_x$, and diagonal matrix $\bar{\tau}_3$ given by $\bar{\tau}_3 = \text{diag}(1, 1, -1, -1)$.

The quantity of interest is the angle averaged charge conductance $\sigma_C$ given by

$$
\sigma_C = \frac{\int_{-\pi/2}^{\pi/2} f_C(\phi) d\phi}{\int_{-\pi/2}^{\pi/2} f_{NC}(\phi) d\phi},
$$

$$
f_C(\phi) = [2 + \sum_{\gamma,\rho} (|a_{\gamma\rho}|^2 - |b_{\gamma\rho}|^2) \cos^2 \frac{\phi}{2}],
$$

where $f_{NC}(\phi)$ denotes the angle resolved charge conductance in the normal state with $\Delta(k) = 0$. Here, $\phi$ denotes the injection angle measured from the normal to the interface with $\sin \phi = k_y/k_f$. To characterize transparency of the junction interface, we introduce dimensionless constant $Z = 2mU/h^2 k_f$.

We plot bias voltage $eV = E$ dependence of $\sigma_C$ for $d_{xy} + p$-wave case in Fig. 3 for various $Z$. First we concentrate on low transparent junction with $Z = 5$ by changing the value of $\Delta_x$ and $\Delta_t$. At $\Delta_t = \Delta_s$, one of the energy gap of the Fermi surface closes corresponding to the quantum phase transition. Then, the resulting $\sigma_C$ has a gradual change from the quantum critical point. For the case without spin-orbit coupling ($\beta = 0$) with $\Delta_t > \Delta_s$, $\sigma_C$ has a gap like structure around zero bias due to the absence of Majorana bound state as shown in Figs. 1(A) and 1(B). For $\Delta_t > \Delta_s$, ZBCP appears reflecting the zero energy ABS [17]. In the presence of spin-orbit coupling, $\sigma_C$ always has a ZBCP independent of the ratio of $\Delta_s$ and $\Delta_t$ as shown in Fig. 3(B). For $\Delta_t > \Delta_s$, the ZBCP originates from purely TRI Majorana bound state. The width of the ZBCP for $\Delta_t > \Delta_s$ is enhanced with the increase of $\beta$, since the region of $k_y$ where the TRI Majorana bound state exists is expanded with $\beta$. For $\Delta_s > \Delta_t$, both the conventional ABS and TRI Majorana bound state contribute to the formation of ZBCP. We also plot corresponding $\sigma_C$ for high ($Z = 1$) and intermediate ($Z = 2$) transparent junctions. For $\Delta_t > \Delta_s$, $\sigma_C$ has a broad dip-like structure around $eV = 0$ for $Z = 1$, while it is slightly enhanced around $eV = 0$ for $Z = 2$ (curves a and b in Figs. 3(C) and (D)). On the other hand, for $\Delta_s > \Delta_t$, $\sigma_C$ always has a ZBCP (curves d and e in Figs.3(C) and (D)). The presence of
TRI Majorana bound state gives a clear ZBCP with the increase of $Z$. As a reference, the tunneling conductance $\sigma_C$ for $d_{x^2-y^2} + f$-wave and $s+p$-wave cases are plotted in Fig. 4 for $Z = 5$. ABS exists only for $\Delta_s < \Delta_t$. The $\sigma_C$ for $d_{x^2-y^2} + f$-wave has a ZBCP splitting reflecting the complex dispersion $\epsilon_b$ shown in Fig. 4(A). On the other hand, for $s + p$-wave case, $\sigma_C$ has a broad ZBCP shown in Fig. 4(B). Summarizing Figs. 3 and 4, $\sigma_C$ for each paring state are qualitatively different from each other, which can be used to identify these pairings.

In conclusion, we have studied the ABS and resulting charge transport for $d_{xy} + p$-wave and $d_{x^2-y^2} + f$-wave superconductors. We find that the obtained dispersion of ABS in both cases have an anomalous structure. For $d_{xy} + p$-wave case, a novel TRI Majorana bound state is generated due to the spin-orbit coupling. The resulting charge conductance can serve as a guide to identify the TRI Majorana bound state and paring symmetry of NCS superconductors by tunneling spectroscopy.

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