Intrinsically s-wave like property of triplet superconductors with spin-orbit coupling

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We have studied a general property of unconventional superconductors with spin-orbit coupling by solving the Bogoliubov-de Gennes equation and found that the two of four eigenfunctions for triplet pairing coincide with those for s-wave pairing when a relation holds between pairing symmetry and spin-orbit coupling, indicative of an intrinsically s-wave like property of triplet superconductors. Applying the result, we have studied the tunneling conductance in normal metal / insulator / unconventional superconductor junctions with a candidate of pairing symmetry of CePt$_3$Si, $d(k) \propto \hat{x}k_y - \hat{y}k_x$. The effect of Rashba spin-orbit coupling (RSOC) is taken into account. We have found that the RSOC induces a peak at the energy gap like s-wave superconductors in the tunneling spectrum, which stems from the intrinsically s-wave like property of triplet component of CePt$_3$Si.

As a result, the tunneling spectrum has s- and p-wave like features. This may serve as a tool for determining the pairing symmetry of CePt$_3$Si.

The recent discovery of CePt$_3$Si has attracted much attention because it is the first heavy fermion superconductor without inversion symmetry. It is predicted that this effect causes the Rashba type spin-orbit coupling (RSOC). Theoretically superconductivity under broken mirror symmetry shows some novel phenomena due to the RSOC. However the effect of the other types of spin-orbit coupling (SOC), e.g., the Dresselhaus type SOC, in superconductors without inversion symmetry is not studied well. It is important to study the general case because the pairing symmetry and the type of SOC depend on the crystal structure. Frigeri et al. showed that the pairing symmetry of CePt$_3$Si is given by $d(k) \propto \hat{x}k_y - \hat{y}k_x$ where $\hat{x}$ and $\hat{y}$ are the unit vectors. This triplet pairing symmetry is, however, not conclusive. It is desirable to calculate the physical quantities of CePt$_3$Si with candidates of its pairing symmetry and compare them with experimental results.

All these motivate us to study the general property of unconventional superconductors (USs) with SOC. After we clarify it, we apply the result to the tunneling junctions with CePt$_3$Si and find a peak structure at the energy gap in tunneling spectrum even for the triplet pairing. This may serve as a tool for determining the pairing symmetry of CePt$_3$Si because the tunneling spectroscopy in superconducting junctions is a powerful method to study its pairing symmetry.

In normal metal / superconductor (N/S) junctions Andreev reflection (AR) is one of the most important process for low energy transport. Taking into account the AR, Blonder, Tinkham and Klapwijk (BTK) proposed the formula for the calculation of the tunneling conductance. This method makes it possible to clarify the energy gap profile of superconductors. It was extended to normal metal / unconventional superconductor (N/US) junctions in order to study the properties of unconventional superconductors. In fact, calculation or measurement of the tunneling conductance in N/US junctions are useful to study the symmetry of the pair potential of USs because the tunneling conductance is sensitive to the pairing symmetry due to the formation of Andreev resonant states. However, there is no theory considering the effect of the SOC in the tunneling junctions. In this paper we generalize the theory in Ref by incorporating the RSOC and apply it to junctions with a new superconductor CePt$_3$Si using the triplet pairing symmetry ($d(k) \propto \hat{x}k_y - \hat{y}k_x$).

We will first clarify a general property of USs with SOC by solving the Bogoliubov-de Gennes (BdG) equation. Applying the result, we calculate the tunneling conductance in normal metal / insulator / unconventional superconductor CePt$_3$Si junctions with a RSOC. We find that the RSOC induces a peak at the energy gap in the tunneling conductance even for the triplet pairing. The result can be explained by the general property of US with SOC. Further we estimate parameter values for the tunneling junctions with CePt$_3$Si. The present results may give useful information for the analysis in experiments to determine the pairing symmetry of CePt$_3$Si. Although we use a simple model for CePt$_3$Si which has a complicated bandstructure, we believe our results grasp the essence of the physics. Below we focus on the zero temperature regime.

Let us start studying a general property of USs with SOC. Consider an effective Hamiltonian for BdG equation with SOC. The Hamiltonian reads

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

with $\hat{H}(k) = \xi_k + \mathbf{V}(k) \cdot \mathbf{\sigma}$, and $\hat{\Delta}(k) = i\Delta \mathbf{\sigma}_y$ for singlet pairing or $\hat{\Delta}(k) = (d(k) \cdot \mathbf{\sigma})i\mathbf{\sigma}_y$ for triplet pairing. Here $\xi_k$, $k$ and $\sigma$ denote electron band energy measured from the Fermi energy, electron momentum and Pauli matrices respectively. The second term of $\hat{H}(k)$, $\mathbf{V}(k) \cdot \mathbf{\sigma}$, represents the SOC. For example, $\mathbf{V}(k) \propto \hat{x}k_y - \hat{y}k_x$ corresponds to the RSOC and $\mathbf{V}(k) \propto \hat{x}k_y$ does the Dresselhaus type SOC. In this work we focus on the unitary states. We assume $d(k) \parallel \mathbf{V}(k)$ where both vectors have only real number components and $\mathbf{V}(-k) = -\mathbf{V}(k)$ which breaks inversion symmetry but conserves...
time reversal symmetry. The condition $\mathbf{d}(k) \parallel \mathbf{V}(k)$ gives the highest $T_C$ of the US. The BdG equation reads

$$\hat{H} \left( \hat{u}_\pm \right) = E_\pm \left( \hat{v}_\pm \right)$$  \hspace{1cm} (2)

for electron-like quasiparticles, and

$$\hat{H} \left( \sigma_y \hat{v}_\pm \sigma_y \right) = -E_\pm \left( \sigma_y \hat{v}_\pm \sigma_y \right)$$  \hspace{1cm} (3)

for hole-like quasiparticles, with $E_\pm = \sqrt{(\xi_k \pm |\mathbf{V}(k)|)^2 + |\Delta|^2}$, $\hat{u}_\pm = u_0^\pm \left( 1 \pm \hat{V}(k) \cdot \sigma \right)$ and $\hat{v}_\pm = v_0^\pm \frac{\Delta}{|\Delta|} \left( 1 \pm \hat{V}(k) \cdot \sigma \right)$. Here $u_0^\pm = \sqrt{\frac{1}{2} \left( 1 + \frac{E_\pm^2 - |\Delta|^2}{E_\pm} \right)}$, $v_0^\pm = \sqrt{\frac{1}{2} \left( 1 - \frac{E_\pm^2 - |\Delta|^2}{E_\pm} \right)}$, $\mathbf{V}(k) = \mathbf{V}(k) / |\mathbf{V}(k)|$ and $|\Delta|^2 = \frac{1}{2} T \nu |\Delta|^4$. This shows that there exist the independent four eigenfunctions: electron- and hole-like quasiparticles with the eigenvalues $E_\pm$.

Let us discuss the property of the four eigenstates. For singlet pairing, we can find

$$\hat{v}_\pm = v_0 \frac{\Delta}{|\Delta|} \left( 1 \pm \hat{V}(k) \cdot \sigma \right) = -i \sigma_y v_0 \left( 1 \pm \hat{V}(k) \cdot \sigma \right)$$  \hspace{1cm} (4)

with $\hat{\Delta} = i \Delta \sigma_y$ while for triplet pairing we get

$$\hat{v}_\pm = -i \sigma_y v_0 \left( \hat{V}(k) \cdot \sigma \right) \left( 1 \pm \hat{V}(k) \cdot \sigma \right)$$

$$= \mp i \sigma_y v_0 \left( 1 \pm \hat{V}(k) \cdot \sigma \right)$$  \hspace{1cm} (5)

with $\hat{\Delta} = \mathbf{d}(k) \cdot \sigma i \sigma_y$. Thus we can find that the eigenfunctions with ‘+’ have the same form for singlet and triplet pairings. This indicates that the two of the four eigenfunctions for triplet pairing coincide with those for singlet pairing when the magnitude of the gap, $|\Delta|$, has the same dependence on $k$, especially with those for $s$-wave pairing when $|\Delta|$ is independent of $k$. This feature gives an intrinsically s-wave like property of triplet superconductors with SOC. As an example of its manifestation, we will calculate the tunneling conductance in the normal metal / unconventional superconductor (CePt$_3$Si) junctions because CePt$_3$Si is considered to satisfy the above conditions to have an s-wave like property.

We consider a two dimensional ballistic N/US junctions. The band structure of CePt$_3$Si shows that the main contribution to the density of states stems from the $\beta$ band as shown in Ref. 12. The $\beta$ band has a three dimensional complicated structure. However, its volume is large for large $k_z$ and hence the most important part is the $\beta$ band for large $k_z$ where the dependence of the $\beta$ band on $k_z$ is weak. Therefore we focus on this part and assume the two dimensional N/US junctions as a first step. The N/US interface located at $x = 0$ (along the $y$-axis) has an infinitely narrow insulating barrier described by the delta function $U(x) = U\delta(x)$. We choose $\mathbf{d}(k) = \frac{\Delta}{|\Delta|} (\mathbf{k}_y - i \mathbf{k}_x)$ and $\mathbf{V}(k) = \lambda (\mathbf{k}_y - i \mathbf{k}_x)$ with Rashba coupling constant $\lambda$. The eigenfunctions of the Hamiltonian are $\mathcal{T} (u_0, -i\alpha_1 u_0, i\alpha_1 v_0, v_0)$, $\mathcal{T} (u_0, i\alpha_2 u_0, i\alpha_2 v_0, -v_0)$, $\mathcal{T} (i\alpha_2 v_0, v_0, -i\alpha_1 u_0)$, and $\mathcal{T} (i\alpha_2 v_0, -v_0, i\alpha_2 u_0)$ with $\alpha_1(2) = \frac{k_x(2)}{k_y(2)}$, $u_0 = u_0^+ = u_0^-$, $v_0 = v_0^+ = v_0^-$, $k_1 = -\frac{m_\parallel}{\hbar^2} + \frac{\hbar v_F}{\hbar} |\Delta|^2$, $k_2 = \frac{m_\parallel}{\hbar^2} + \frac{\hbar v_F}{\hbar} |\Delta|^2$ and $k_1(2) = k_1(2) e^{\pm i\theta_1(2)}$. Here we put $E_+ = E_-$, $\theta_1(2)$ is an angle of the wave with wave number $k_1(2)$ with respect to the interface normal, $k_F$ is Fermi wave number, and $m$ is effective mass in US. Velocity operator in the $x$-direction is defined as $v_x = \frac{\partial \mathcal{H}}{\partial k_x}$.

The wave function $\psi(x)$ for $x \leq 0$ (N region) is represented as

$$\psi(x \leq 0) = e^{ik_F x} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} + e^{-ik_F x} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

$$+ b e^{ik_F x} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} + c e^{-ik_F x} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$  \hspace{1cm} (6)

for an injection wave in up (down) spin states with $k_F = k_F \cos \theta$ where $\theta$ is an angle of the wave with wave number $k_F$ with respect to the interface normal in the N region. $a$ and $b$ are AR coefficients. $c$ and $d$ are normal reflection (NR) coefficients. Because we focus on the low energy transport compared to the Fermi energy, we neglect the difference of the wave number between electron and hole.

Similarly for $x \geq 0$ (US region) $\psi(x)$ is given by the linear combination of the eigenfunctions. Note that since the translational symmetry holds for the $y$-direction, the momenta parallel to the interface are conserved: $k_x = k_x$ sin $\theta = k_1$ sin $\theta_1 = k_2$ sin $\theta_2$.

The wave function follows the boundary conditions as

$$\psi(x)|_{x=+0} = \psi(x)|_{x=-0}$$  \hspace{1cm} (7)

$$v_x \psi(x)|_{x=+0} = -v_x \psi(x)|_{x=-0}$$

$$\frac{\hbar}{m} \frac{2 \nu m U}{\hbar^2} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \psi(0).$$  \hspace{1cm} (8)

Applying the BTK theory to our calculation, we obtain the dimensionless conductance represented in the form:

$$\sigma_S = \frac{4}{\pi} \int_{1/4}^{3/4} \left| a + b + c - d \right|^2 \cos \theta d\theta.$$  \hspace{1cm} (9)

We define the normalized conductance as $\sigma_T = \sigma_S / \sigma_N$ where $\sigma_N$ is given by the conductance for normal states,
i.e., $\sigma_S$ for $\Delta = 0$ and parameters as $\beta = \frac{2m\lambda}{\hbar^2 k_F}$ and $Z = \frac{2mU}{\hbar^2 k_F}$. $g$ is the effective mass in N divided by that in US.

In the following we study the normalized tunneling conductance $\sigma_T$ as a function of bias voltage $V$. For $Z = 10$ and $g = 0.1$, the magnitude of $\sigma_T$ at $eV = \Delta$ increases as increasing $\beta$ and finally a peak structure appears (Fig. 1 (a)). On the other hand we can’t find such a peak for $Z = 0$ and $g = 0.1$ (Fig. 1 (b)). Next we will study the case of a larger effective mass in US to check its effect on the conductance. Figure 2 shows the conductance for (a) $Z = 10$ and $g = 0.01$, and (b) $Z = 0$ and $g = 0.01$. In both cases a peak emerges at $eV = \Delta$ and becomes sharper for large $\beta$.

![FIG. 1: (color online) Normalized tunneling conductance with $g = 0.1$ for (a) $Z = 10$ and (b) $Z = 0$.](image1)

Let us explain the origin of the peak at $eV = \Delta$ in Figs. 1 and 2. A coherent peak at $eV = \Delta$ in the tunneling conductance also appears in N/S junctions, even in the presence of RSOC\cite{11}. The two of four eigenfunctions of the BdG equation with RSOC for the pair potential we consider coincide with those for s-wave pair potential. We can choose the electron-like and hole-like quasiparticle states with wave number $k_2$ as the two eigenfunctions. Actuantly, using the expressions of $\hat{u}_\pm$ and $\hat{v}_\pm$, we get the eigenfunctions of the Hamiltonian for s-wave pairing: $T (u_0, -i\alpha_1^{-1}u_0, i\alpha_1^{-1}v_0, v_0)$, $T (u_0, i\alpha_2^{-1}u_0, -i\alpha_2^{-1}v_0, v_0)$, $T (i\alpha_1 v_0, v_0, -u_0, i\alpha_1 u_0)$, $T (i\alpha_2 v_0, -v_0, u_0, i\alpha_2 u_0)$.

This implies that US with RSOC has an intrinsically s-wave like property. As $\beta$ increases, the contribution of the eigenstates with wave number $k_2$ is much more dominant than that with wave number $k_1$ because $k_2$ ($k_1$) is an increasing (decreasing) function of $\beta$. Therefore the behavior of the conductance becomes similar to the one for the s-wave pairing with increasing RSOC in US. Note that near zero voltage the Mig gap Andreev resonant states greatly change the spectrum compared to the one for the s-wave junctions\cite{10,11}. Thus there is a qualitative difference in the conductance between two pairing states near zero voltage. For understanding the underlying physics, it is useful to check the case of very large RSOC, though it may be unphysical. Figure 3 displays the tunneling conductance with the same parameters in Fig. 1 (a) with very large RSOC. Apparently an s-wave-like tunneling spectrum emerges as increasing $\beta$, which confirms the above explanation.

![FIG. 3: (color online) Normalized tunneling conductance for $Z = 10$ and $g = 0.1$.](image2)

Note that this feature is unique to the pair potential considered. As a reference, we will consider the case of other pairing symmetries with the same parameters as in
Fig. 1 (a). We choose

\[ \hat{\Delta}(k) = \begin{pmatrix} \Delta_{r} & 0 \\ 0 & \Delta_{i} \end{pmatrix} \] (10)

in Fig. 1 (a) and

\[ \hat{\Delta}(k) = \begin{pmatrix} \Delta_{r} & 0 \\ 0 & \Delta_{i} \end{pmatrix} \] (11)

in Fig. 1 (b). In both cases there is no qualitative change by the RSOC in the tunneling conductance.

Now let us examine the parameter values suitable to CePt3Si. In the case of CePt3Si, we estimate \( g \sim 0.01 \) from the specific-heat measurement\(^1\) and \( \beta \sim 0.3 \) from the band calculation\(^12\). The corresponding results are shown by solid curves in Fig. 2 (a) and (b), where the conductance clearly reflects the features of s- and p-wave superconductors: a broad peak around zero voltage and a peak at the energy gap. Recent NMR study of CePt3Si showed that \( 1/T_1 \) of CePt3Si exhibits a small peak just below \( T_\text{c} \) like the Hebel-Slichter peak in s-wave superconductors\(^17\). This similarity between CePt3Si and s-wave superconductors is consistent with our results.

In summary we solved the BdG equation for US with SOC and found that the two of four eigenfunctions for triplet pairing have the same form as those for singlet pairing under the following conditions: (i) \( \mathbf{d}(\mathbf{k}) \) and \( \mathbf{V}(\mathbf{k}) \) have only real components. (ii) \( \mathbf{d}(\mathbf{k}) \parallel \mathbf{V}(\mathbf{k}) \). (iii) \( \mathbf{V}(-\mathbf{k}) = -\mathbf{V}(\mathbf{k}) \). Moreover, if (iv) the magnitude of the gap, \( |\Delta| \), is independent of \( \mathbf{k} \), the two of four eigenfunctions for triplet pairing coincide with those for s-wave pairing. This feature gives an intrinsically s-wave like property of triplet superconductors with SOC. Note that this is essentially different from the recent work where the mixture of singlet and triplet pairing is discussed\(^18\). We found that triplet superconductor itself has a singlet-like property. As an example of its manifestation, we studied the tunneling conductance in N/US junctions with RSOC and a candidate of pairing symmetry of CePt3Si. This compound is considered to satisfy the above four conditions\(^3\). We found that the RSOC induces a peak at the energy gap in the tunneling conductance as found in s-wave superconductor junctions, which results in the s- and p-wave like features in the tunneling spectrum. This may serve as a tool for determing the pairing symmetry of CePt3Si.

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