Analytical Result on Electronic States around a Vortex Core in a Noncentrosymmetric Superconductor

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We analytically study electronic bound states around a single vortex core in a noncentrosymmetric superconductor such as CePt\textsubscript{3}Si without mirror symmetry about the ab plane. Considering a mixed spin-singlet-triplet Cooper pairing model, we obtain a formula about the local density of states (LDOS) around a vortex core in any direction of the magnetic field. The LDOS under a magnetic field perpendicular to the c axis is quite different from that of typical s-wave or d-wave superconductors. From the ellipticity of the spatial pattern of the LDOS around a vortex core, one can experimentally estimate the pairing symmetry of CePt\textsubscript{3}Si, such as the position of the gap nodes and the ratio of the singlet component to the triplet component in the order parameter.

KEYWORDS: CePt\textsubscript{3}Si, Unconventional superconductivity, Vortex core, Local density of states, Broken inversion symmetry, Quasiclassical theory

In a time reversal invariant system, the lack of inversion symmetry is connected with the presence of an antisymmetric spin-orbit coupling.\textsuperscript{1} Unconventional superconductivity in strongly correlated systems exists in heavy Fermion superconductors. The discovery of the noncentrosymmetric heavy Fermion superconductor CePt\textsubscript{3}Si\textsuperscript{2} has attracted considerable attention. Many theoretical and experimental studies on unconventional superconductivity without inversion symmetry have been reported for a few years.\textsuperscript{2–10} The vortex structure of the mixed state in this system was recently studied on the basis of the Ginzburg-Landau theory and the London theory.\textsuperscript{6,7} The vortex core structure was also studied by means of the quasiclassical theory of superconductivity, which enables us to calculate the physical quantities more microscopically.\textsuperscript{8} However, no studies have been attempted to investigate the possible anisotropic spatial structure of the quasiparticle distribution around a vortex core in such a system. In this paper, we analytically investigate the local density of states (LDOS) around a single vortex core in a noncentrosymmetric superconductor and devise a formula for LDOS that is applicable in any arbitrary direction of the magnetic field, thus revealing an anisotropic quasiparticle structure. An anisotropic pairing symmetry is reflected by the real-space LDOS pattern because of the presence of quasiparticles around a vortex core.\textsuperscript{11,12} Therefore, for understanding the Cooper pairing without inversion symmetry, it is important to investigate the LDOS pattern. The LDOS can be probed experimentally by STM.\textsuperscript{13,14} If the LDOS pattern presented in this paper is consistent with that observed by STM, we can obtain information on the position of the gap nodes and the ratio of the singlet component to the triplet component in this material. In other words, this can serve as one of the methods to experimentally investigate the pair potential directly in CePt\textsubscript{3}Si. Thus, we can also show that our theoretical formulation is capable of wide application.

We consider a mixed spin-singlet-triplet model to study the noncentrosymmetric superconductor. Considering the results of numerical calculations by Hayashi et al.,\textsuperscript{8} we assume that the spatial variations of the s-wave pairing component of the pair potential are the same as those of the p-wave pairing component. $\Delta = [\Psi \hat{\sigma}_0 + d_k \cdot \hat{\sigma}] i \hat{\sigma}_y = \Delta(r) \begin{bmatrix} \Psi \hat{\sigma}_0 - k_y \hat{\sigma}_x + k_x \hat{\sigma}_y \end{bmatrix} i \hat{\sigma}_y$, where the s-wave pairing component $\Psi$, the d vector $d_k = \Delta(-k_y, k_x, 0)$, the Pauli matrices in the spin space $\hat{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$, the unit matrix $\hat{\sigma}_0$, and the unit vector $\hat{k}$ in the momentum space will be discussed later. Here, the ratio of the singlet to the triplet component is defined in the bulk region as $\hat{\Psi} = \Psi / \Delta$. This mixed s+p-wave model is proposed for CePt\textsubscript{3}Si.$^5$

In a system without inversion symmetry, there is a Rashba-type spin-orbit coupling with the form$^4,5,10$

\begin{equation}
\mathcal{H}_1 = \sum_{\mathbf{k}, \eta, \eta'} \alpha \mathbf{g}_k \cdot \hat{\sigma}_{\eta \gamma} \hat{c}_{\eta}^{\dagger} \hat{c}_{\eta'}^{\dagger},
\end{equation}

where $\mathbf{g}_k = \sqrt{2 \eta / \eta'}(-k_y, k_x, 0)$. Here, $\hat{c}_{\mathbf{k}}^{\dagger}$ ($\hat{c}_{\mathbf{k}}$) is the creation (annihilation) operator for the quasiparticle state with momentum $\mathbf{k}$ and spin $\sigma$ and $\alpha (>0)$ denotes the strength of the spin-orbit coupling. We use units in which $\hbar = k_B = 1$. The $\mathbf{g}_k$ vector, which is an antisymmetric vector ($\mathbf{g}_{-k} = -\mathbf{g}_k$), is parallel to the d vector.$^3$

We calculate the LDOS around a vortex core on the basis of the quasiclassical theory of superconductivity.$^{15–17}$ We consider the quasiclassical Green function $\tilde{\Psi}$ that has matrix elements in the Nambu (particle-hole) space as

\begin{equation}
\tilde{\Psi}(\mathbf{r}, \tilde{\mathbf{k}}, i \omega_n) = \begin{pmatrix} \hat{g} & \hat{f} \\ -\hat{f} & \hat{g} \end{pmatrix},
\end{equation}

where $\omega_n$ is the Matsubara frequency. Throughout the
paper, “hat” $\hat{a}$ denotes a $2 \times 2$ matrix in the spin space, and “check” $\check{a}$ denotes a $4 \times 4$ matrix composed of the $2 \times 2$ Nambu space and the $2 \times 2$ spin space.$^{10}$

The Eilenberger equation, which includes the spin-orbit coupling term, is given as$^{3,10,18,20}$

$$i\nu_F(k) \cdot \nabla \check{g} + [i\omega_n, \tau_3 - \alpha g_k \cdot \check{S} - \Delta, \check{g}] = 0,$$  \hspace{1cm} (3)

where

$$\check{g} = \begin{pmatrix} g_0 \sigma_0 & 0 \\ g_{-\sigma_0} & 0 \end{pmatrix} = \begin{pmatrix} g_{-\sigma_0} & 0 \\ 0 & -g_{\sigma_0} \end{pmatrix},$$  \hspace{1cm} (4)

$$g_k = \sqrt{\frac{3}{2}} (-\hat{k}_y, \hat{k}_x, 0), \ \check{\tau}_3 = \begin{pmatrix} 0 & 0 \\ 0 & -\sigma_0 \end{pmatrix},$$  \hspace{1cm} (5)

$$\check{S} = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma^{tr} \end{pmatrix}, \ \Delta = \begin{pmatrix} 0 & \Delta \\ -\Delta & 0 \end{pmatrix}.$$  \hspace{1cm} (6)

Here, $\nu_F(k)$ is the Fermi velocity, $\sigma^{tr} = -\sigma_y \sigma_y$, and the commutator $[a, b] = ab - ba$. $\check{g}$ should be subject to the normalization condition$^{15,18}$ $g_0^2 = 1$, where 1 is a $4 \times 4$ unit matrix. We neglect the impurity effect and the vector potential because CePt$_3$Si is a clean extreme-type-II superconductor.$^2$

The Eilenberger equation can be simplified by introducing a parametrization for the propagators that satisfy the normalization condition. Propagators are defined as $\check{F}_\pm = \frac{1}{2}(1 \pm \check{g})$, which were originally introduced in the studies of vortex dynamics.$^{21}$ Using these propagators, we obtain the matrix Riccati equations as follows:

$$\nu_F \cdot \tilde{\nabla} \tilde{a}_+ + 2\omega_n \tilde{a}_- + \tilde{a}_+ \Delta_\downarrow \tilde{a}_- - \hat{\Delta} + i(\tilde{a}_+ \sigma_0 + \alpha g_k \cdot \sigma \tilde{a}_+) = 0,$$  \hspace{1cm} (7)

$$\nu_F \cdot \tilde{\nabla} \tilde{b}_- - 2\omega_n \tilde{b}_- - \tilde{b}_- \Delta_\downarrow \tilde{b}_+ + \Delta_\uparrow - i(\tilde{b}_- \sigma_0 + \alpha g_k \cdot \sigma \tilde{b}_-) = 0,$$  \hspace{1cm} (8)

where

$$\tilde{g} = -\tilde{N} \begin{pmatrix} (1 - \tilde{a}_+ \tilde{b}_-) & 2 \tilde{a}_+ \\ -2 \tilde{b}_- & -(1 - \tilde{b}_- \tilde{a}_+) \end{pmatrix},$$  \hspace{1cm} (9)

$$\tilde{N} = \begin{pmatrix} (1 + \tilde{a}_+ \tilde{b}_-) & 0 \\ 0 & (1 + \tilde{b}_- \tilde{a}_+) \end{pmatrix}.$$  \hspace{1cm} (10)

We consider a single vortex along the $Z$ axis that tilts from the crystal $c$ axis by an angle $\phi$. Now, we consider the $X$ axis on the $a-b$ plane. We assume the spherical Fermi surface and consider the moment vector $k = k(\cos \theta \sin \chi, \sin \theta \sin \chi, \cos \chi)$ in this coordinate system fixed to the magnetic field. To obtain the quasiclassical Green functions, we consider the trajectories of the quasiparticle on the $X-Y$ plane.$^{23}$ Because of a translational symmetry along the vortex, the trajectory of a quasiparticle with a moment $|k_F|$ and $k_Z \neq 0$ contributes to the quasiclassical Green functions in the same manner as that of a quasiparticle with a moment $|k_F|$ projected on the $k_X-k_Y$ plane. In other words, the quasiclassical Green functions in a three-dimensional system can be converted into a set of quasiclassical Green functions in a two-dimensional system having a momentum with different amplitude. Therefore, we determine the coordinates

$$\begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$  \hspace{1cm} (11)

to solve eqs. (7) and (8) along the direction of momentum in a two-dimensional system; the momentum is in the $x$ direction. Here, $y$ is the axis referred to as an impact parameter, $x$ is the axis perpendicular to $y$, and $r = \sqrt{x^2 + y^2} = \sqrt{X^2 + Y^2}$; the origin of these axes is at the vortex center.

Using the perturbative method developed by Kramer et al.$^{22,24}$ we can obtain the quasiclassical Green function around the vortex core in a low energy region ($|\omega_n| \ll |\Delta_\infty|$). Here, $\Delta_\infty$ is a pair potential in the bulk region. By expanding the matrix Riccati equations in the first order of $\alpha$, $y$, $|\Delta(r)|$, and $|\omega_n|$, we obtain the approximate solution as$^{25}$

$$\tilde{g} = \tilde{O}_C e^{-2(\sqrt{k_{\perp} \cdot \check{k}_F} + \hat{\Psi})F(x)} + \tilde{O}_D e^{-2(\sqrt{k_{\perp} \cdot \check{k}_F} + \hat{\Psi})F(x)} \frac{2 \tilde{F}_D}{2 \tilde{F}_C} + \hat{\tilde{g}},$$  \hspace{1cm} (12)

where

$$\tilde{F}_C, D = \frac{1}{v_F} \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} \left[ \frac{|\Delta(r')|}{|x'|} \sqrt{\tilde{k}_{\perp} \tilde{k}_D} \mp \hat{\tilde{\Psi}} \right] e^{-2(\sqrt{k_{\perp} \cdot \check{k}_F} + \hat{\tilde{\Psi}})F(x')}.$$  \hspace{1cm} (13)

Here, $k_\pm = \tilde{k}_x \pm \hat{k}_y$ and $F(x) = \int_0^{\infty} dx' \Delta(x')/v_F$. The first and second terms in eq. (12) are the Green functions referred to as $\tilde{g}_{I, II}$ on Fermi surfaces I and II; this is because the spin orbit coupling splits the Fermi surface into two surfaces by lifting the spin degeneracy.$^{4,5}$ Fermi I has a nodeless pair potential, and Fermi II has a pair potential with the line node (e.g., see Fig. 1 in ref. 10).

Near the vortex core ($|r| \ll \xi$), we use the following approximations,

$$\tilde{F}_C, D \sim \frac{-\tilde{g}|\sqrt{k_{\perp} \cdot \check{k}_F} + \hat{\tilde{\Psi}}|}{\sin \chi} + \frac{\check{i} \tilde{\omega}_n}{\sqrt{k_{\perp} \cdot \check{k}_D + \hat{\tilde{\Psi}}}},$$  \hspace{1cm} (15)

where

$$F(x) = \frac{1}{v_F} \int_0^{\infty} dx' \Delta(x') \sim 0,$$  \hspace{1cm} (16)

$$\frac{1}{v_F} \int_{-\infty}^{\infty} dx' e^{-2aF(x')} \sim \frac{1}{a \Delta_\infty},$$  \hspace{1cm} (17)

$$\int_0^{\infty} dx' \Delta(x') e^{-2aF(x')} \sim \Delta_\infty.$$  \hspace{1cm} (18)

Here, we use the dimensionless variables as $\tilde{\omega}_n = \omega_n/\Delta_\infty$ and $\tilde{y} = y/\xi_0$ with $\xi_0 = v_F/\Delta_\infty$. Therefore, the LDOS around the vortex core is

$$\tilde{\nu}(\tilde{r}, \tilde{\varphi}) = -\left\langle \Re \{ \tilde{t}_{\varphi} \tilde{F}(i\tilde{w}_n \rightarrow \tilde{\varphi} + 0^+) \} \right\rangle \tilde{k},$$  \hspace{1cm} (19)

$$= \tilde{t}_0(0) \int_0^\pi \sin \chi d\chi \int_0^{2\pi} \frac{d\theta}{4(\sqrt{k_{\perp} \cdot \check{k}_F} + \hat{\tilde{\Psi}})}.$$
Here, we consider the rotation about the \( x \) axis; this rotation \( \tilde{\Psi} \) diverges around the vortex perpendicular to the \( c \) axis. The pattern about Fermi I in Fig. 1(a) can be regarded as a result of the shape of the order parameter, such as two circles with a shift of the centers (shown in Fig. 1(a) in ref. 10). If the relation \( \tilde{\Psi} < |\cos\theta| \) between \( \tilde{\Psi} \) and \( \theta \) does not exist in the case of \( h_\perp \), the pattern about Fermi II is similar to that in a d-wave superconductor\(^{11,12}\) because of the presence of four nodes in the pair potential on the circular line \( \chi = \pi \) on the Fermi surface. However, the actual pattern about Fermi II (Fig. 1(b)) is similar to \( a \) part of that in a d-wave superconductor because of the presence of this relation between \( \tilde{\Psi} \) and \( \theta \) originating from the three-dimensional anisotropic pair potential. These results show that the quasiparticles on Fermi I are bound around a vortex, while those on Fermi II move in the direction associated with one node to the direction associated with the other node. We also \cal-

Therefore, we obtain the parametric equations:

\[
\tilde{X}_\pm = -\frac{\tilde{\epsilon} \sin \theta}{(1 \pm \tilde{\Psi})^2} \quad \text{and} \quad \tilde{Y}_\pm = \frac{\tilde{\epsilon} \cos \theta}{(1 \pm \tilde{\Psi})^2}
\]  

from eqs. (22), (24), and (25). This result is consistent with the numerical calculation by Hayashi et al.\(^8\) because this spatial LDOS pattern is in the form of two concentric circles. This result shows that the quasiparticles rotate around a vortex core, and the LDOS exhibits the two-gap property. The ratio of the singlet component to the triplet component, \( \tilde{\Psi} \), determines the ratio of the radius between the two concentric circles.

Second, we consider the system in a magnetic field perpendicular to the \( c \) axis (\( \phi = \pi/2 \)). In this case, \( \chi = \pi \) follows from eq. (26). Therefore, we obtain the following parametric equations:

\[
\tilde{X}_\pm = \frac{-\tilde{\epsilon} \sin \theta}{(|\cos \theta| \mp \tilde{\Psi})^3} \left\{ 3 |\cos \theta| \pm \tilde{\Psi} \right\} \quad \text{and} \quad \tilde{Y}_\pm = \frac{-2 \tilde{\epsilon} \sin^2 \theta \text{sign} |\cos \theta|}{(|\cos \theta| \pm \tilde{\Psi})^3} + \frac{\tilde{\epsilon} \cos \theta}{(|\cos \theta| \pm \tilde{\Psi})^2}
\]

where \( \tilde{\Psi} < |\cos \theta| \) (in the case of \( h_\perp \)) using eqs. (22), (24), and (25) with regard to Fermi I \((h_+ \)\) and II \((h_- \)\). In Fig. 1, we show these LDOS patterns around the vortex core for a fixed energy \( \tilde{\epsilon} \). The pattern about Fermi I in Fig. 1(a) can be regarded as a result of the shape of the order parameter, such as two circles with a shift of the centers (shown in Fig. 1(a) in ref. 10). If the relation \( \tilde{\Psi} < |\cos \theta| \) between \( \tilde{\Psi} \) and \( \theta \) does not exist in the case of \( h_\perp \), the pattern about Fermi II is similar to that in a d-wave superconductor\(^{11,12}\) because of the presence of four nodes in the pair potential on the circular line \( \chi = \pi \) on the Fermi surface. However, the actual pattern about Fermi II (Fig. 1(b)) is similar to \( a \) part of that in a d-wave superconductor because of the presence of this relation between \( \tilde{\Psi} \) and \( \theta \) originating from the three-dimensional anisotropic pair potential. These results show that the quasiparticles on Fermi I are bound around a vortex, while those on Fermi II move in the direction associated with one node to the direction associated with the other node. We also cal-

\[
\tilde{\Psi} = 0.5, \quad \epsilon/\Delta_\infty = 0.01.
\]
calculate the distribution of the LDOS from eq. (20) by numerical integration (Fig. 2). The LDOS in Fig. 1 is consistent with that in Fig. 2. In the limit $\Psi \to 0$, the

LDOS patterns in a magnetic field perpendicular to the $c$ axis become rather isotropic because the line nodes in a gap disappear. Therefore, the strongly anisotropic LDOS patterns, as shown in Fig. 2(b), suggest that the triplet channel and the singlet channel are mixed.

We can estimate the ratio of the singlet component to the triplet component, $\Psi$, from the spatial LDOS pattern shown in Fig. 2(b). From eqs. (32) and (33), we calculate the ratio of the intercept $X_0$ on the $X$ axis to the intercept $Y_0$ on the $Y$ axis in the LDOS pattern for Fermi II. The ratio between these intercepts $r$ is written as

$$r = \frac{(-5\Psi + \sqrt{24 + \Psi^2})^3}{108(1 - \Psi)^2(-\Psi + \sqrt{\Psi^2 + 24}) \left(1 - \left(\frac{\Psi + \sqrt{\Psi^2 + 24}}{6}\right)^2\right)^2}$$

where $r = Y_0/\sqrt{X_0}$ (Fig. 3); this ratio does not depend on the energy $\epsilon$. In other words, we can obtain the ratio $\Psi$ from the ellipticity $r$ of the shape around a vortex. We can also obtain the position of the gap-node $\theta_{\text{node}}$ with the relation $|\cos \theta_{\text{node}}| = \Psi$. Now, CePt$_3$Si has a tetragonal crystal structure. We have also investigated how the present result is influenced by an anisotropic mass tensor; thus, we found that the LDOS pattern is not significantly affected by the ellipsoidal Fermi surface.

In conclusion, we investigated the local density of states around a vortex core in a noncentrosymmetric superconductor. We derived an analytical formula of the LDOS in any direction of the magnetic field. In a magnetic field parallel to the $c$ axis, we found that the LDOS pattern is in the form of two concentric circles; this is consistent with the numerical calculation by Hayashi et al.\(^8\) In a magnetic field perpendicular to the $c$ axis, we found that the LDOS pattern about Fermi I is as shown in Fig. 1(a) and that about Fermi II extends far from the vortex center as shown in Figs. 1(b) and 2(b); this pattern is similar to that of a d-wave superconductor, but it is different from a four-fold d-wave superconductor. The anisotropic LDOS patterns indicate the mixed singlet-triplet channels. We can obtain the ratio of the singlet component to the triplet component in CePt$_3$Si from the ellipticity of the shape around a vortex as shown in Fig. 1(b). While we found that the effect of the deformation from the spherical to the ellipsoidal Fermi surface is not quite significant, it may be important in the future to investigate a more realistic band structure. Our analytical formulation presented in this paper is advantageous because it can be easily generalized to a system with anisotropic Fermi surfaces.

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