Triplet Cooper Pair Formation by Anomalous Spin Fluctuations in Non-centrosymmetric Superconductors

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A microscopic theory for the spin triplet Cooper pairing in non-centrosymmetric superconductors like CePt\textsubscript{3}Si and CeTSi\textsubscript{3} (T=Rh, Ir) is presented. The lack of inversion symmetry leads to new anomalous spin fluctuations which stabilize the triplet part in addition to the singlet part originating from the centrosymmetric spin fluctuations. It is shown that both parts have similar nontrivial momentum dependence of $A_1$ type. Therefore the mixed singlet-triplet gap function has accidental line nodes on both Fermi surface sheets which are stable as function of temperature. This gap function explains the salient features of CePt\textsubscript{3}Si and CeTSi\textsubscript{3} superconductors.

KEYWORDS: non-centrosymmetric system, antisymmetric spin-orbit coupling, superconductivity

Since its discovery in the heavy fermion compound CeCu\textsubscript{2}Si\textsubscript{2},\textsuperscript{1} unconventional superconductivity has attracted much attention in the field of correlated electron systems. For systems with inversion symmetry, the pairing states of superconductivity are classified as spin-singlet of even-parity or spin-triplet of odd-parity. Recalling that a phonon-mediated mechanism is established for s-wave spin-singlet superconductivity, the possibility of spin-triplet superconductivity, as realized, e.g. in UPt\textsubscript{3} and Sr\textsubscript{2}RuO\textsubscript{4}, is considered as a characteristic feature of the correlated electron system.

It has been suggested that the spin-triplet superconductivity is destroyed by breaking the inversion symmetry.\textsuperscript{2} However, recently, the unconventional superconductivity has been observed in several non-centrosymmetric heavy fermion compounds like CePt\textsubscript{3}Si,\textsuperscript{3} CeRhSi\textsubscript{3},\textsuperscript{4} CeIrSi\textsubscript{3},\textsuperscript{5} and CeCoGe\textsubscript{3}.\textsuperscript{6} These compounds have tetragonal crystal structures without the inversion symmetry, and the superconductivity is found around each antiferromagnetic phase.\textsuperscript{4–7} The evidence of unconventional superconductivity is at least shown by the existence of a line node of the superconducting gap in CePt\textsubscript{3}Si, which is observed by NMR,\textsuperscript{8} thermal transport,\textsuperscript{9} and penetration depth.\textsuperscript{10} Furthermore, the common remarkable property of the unconventional superconductivity is the large upper critical magnetic field exceeding the Pauli limiting field.\textsuperscript{3–5,11} The observed upper critical field has opened up the possibility of the spin-triplet superconductivity in non-centrosymmetric systems in contrast to the theoretical expectation.\textsuperscript{2}

The lack of inversion symmetry of non-centrosymmetric systems leads to an antisymmetric spin-orbit interaction.\textsuperscript{12} A general superconducting order parameter is described by the even spin-singlet gap function $\psi(\mathbf{k})$ and odd spin-triplet gap function $\mathbf{d}(\mathbf{k})$.\textsuperscript{13} The coexistence of $\psi(\mathbf{k})$ with $\mathbf{d}(\mathbf{k})$ is unavoidable in principle in the non-centrosymmetric superconductor because of the lack of inversion symmetry. For the non-centrosymmetric superconductor with a large upper critical field, Sigrist \textit{et al.} have reconsidered the possibility of spin-triplet pairing and concluded that a Cooper pair satisfying $\mathbf{d}(\mathbf{k}) \| g_{\mathbf{k}} (g_{\mathbf{k}}$: Rashba field) does not suffer the suppression of pairing coming from the lack of inversion symmetry.\textsuperscript{14} Based on this spin-triplet state, many theoretical proposals have been made for the superconducting properties. However, the pairing mechanism remains an unsettled problem except for a few attempts.\textsuperscript{15–17}

On the other hand, a spin fluctuation property characteristic of the non-centrosymmetric system has been developed recently.\textsuperscript{18} Unlike the centrosymmetric system, the anomalous spin fluctuations do not vanish in the non-centrosymmetric system under the condition, that the symmetry of the momentum dependence is equivalent to the symmetry of spin-product included in the spin fluctuation. Furthermore, not only usual (centrosymmetric) spin fluctuations but also anomalous (non-centrosymmetric) spin fluctuations enhance on approaching the magnetic instability. Therefore, it is expected that the latter play an essential role in the pairing mechanism of superconductivity.

In this Letter, we study the superconducting transition in a correlated electron system without inversion symmetry. The roles of usual and anomalous spin fluctuations in the superconductivity and the nodal structure of gap functions are examined within the weak-coupling theory. We also compare the superconductivity of centrosymmetric systems with that of non-centrosymmetric ones around the magnetic instability.

The latter is described by the following Hamiltonian $H = H_0 + H_1$ for correlated electrons:

\begin{equation}
H_0 = \sum_{\mathbf{k}\sigma\sigma'} \left[ (\varepsilon_{\mathbf{k}} - \mu) \sigma 0 + g_{\mathbf{k}} \cdot \sigma \right] c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma'},\quad (1)
\end{equation}

\begin{equation}
H_1 = U \sum_i n_{i\uparrow} n_{i\downarrow},\quad (2)
\end{equation}

where $c_{\mathbf{k}\sigma}$ and $c_{\mathbf{k}\sigma}^\dagger$ are annihilation and creation operators of an electron with a momentum $\mathbf{k}$ and a spin $\sigma$. 
Here, $\varepsilon_k$ and $\mu$ are the energy dispersion of electrons and the chemical potential, respectively, while $\mathbf{g}_k = -\mathbf{g}_{-k}$ describes the Rashba field coming from the antisymmetric spin-orbit interaction, which breaks the inversion symmetry. Then, eigenenergies of $H_0$ are given by $\varepsilon_{k\pm} = \varepsilon_k \pm |\mathbf{g}_k| - \mu$. In $H_1$, $U$ is the screened on-site interaction.

In the following, we consider a two-dimensional tetragonal system with a dispersion energy $\varepsilon_k = 2t_y(\cos k_x + \cos k_y) + 4t_2 \cos k_x \cos k_y$ and a Rashba-field $\mathbf{g}_k = g(\sin k_y, -\sin k_x, 0)$, which is a periodic form of the simplest one $(k_y, -k_x, 0)$. Closings parameters as $t_2/t_1=0.35$ and $g/t_1=0.2$, we can reproduce quasi-two-dimensional Fermi surfaces of CePt$_3$Si obtained by band calculations. Furthermore, the reason why the two-dimensional system is used instead of the realistic three dimensional system is based on the following knowledge. It is known that the unconventional superconducting phase shrinks with increasing the dimensionality in the centrosymmetric system. Recalling that the superconducting transition temperature 1.6 K in a non-centrosymmetric system CeIrS$_3$ is in the same order as the highest superconducting transition temperature 2.7 K of CeCoIn$_5$ among Ce-based compounds, it is suggestive that unconventional superconductivity is more favorable in two dimensional system than in three dimensional one, independent of the inversion symmetry.

From the specific heat data and $2\Delta/T_c$ value used to fitting to the NMR relaxation rate in CeIrS$_3$, the strong-coupling theory is suggested. However, the weak-coupling theory will be sufficient to examine the mechanism of superconductivity. In general, the matrix gap function $\Delta(k)$ is decomposed into a spin-singlet $\psi(k)$ and a spin-triplet $d(k)$-vector as $\Delta(k) = \{\psi(k)\sigma_0 + d(k) \cdot \hat{\sigma}\}|\hat{\sigma}_y|$. In non-centrosymmetric superconductors, only spin-triplet component satisfying $|d(k) \cdot \mathbf{g}_k| = |d(k)||\mathbf{g}_k|$ is not affected by the suppression of pairing coming from the lack of inversion symmetry. Then, the spin-triplet component will be given by $d(k) = \phi(k)\mathbf{g}_k$, where the symmetry of momentum dependence of $\phi(k)$ is the same as that of the spin-singlet $\psi(k)$. Under this condition for $d(k)$, the normal and anomalous matrix Green’s functions, $G(k, \omega_n)$ and $F(k, \omega_n)$, respectively, are defined with $\mathbf{g}_k = \mathbf{g}_k / |\mathbf{g}_k|$ as

$$G(k, \omega_n) = G_+(k, \omega_n)\sigma_0 + G_-(k, \omega_n)\mathbf{g}_k \cdot \hat{\sigma} \quad (0.3)$$

$$F(k, \omega_n) = \left[ F_+(k, \omega_n)\sigma_0 + F_-(k, \omega_n)\mathbf{g}_k \cdot \hat{\sigma}\right] |\Theta_\mathbf{q}\quad (0.4)$$

$G_\pm(k, \omega_n)$ and $F_\pm(k, \omega_n)$ are given by

$$G_\pm(k, \omega_n) = \frac{1}{2} \begin{bmatrix} -\omega_n - \varepsilon_k & \pm \omega_n - \varepsilon_k \\ \omega_n^2 + E_k^2 & \omega_n^2 + E_k^2 \end{bmatrix} \quad (0.5)$$

$$F_\pm(k, \omega_n) = \frac{1}{2} \begin{bmatrix} \Delta_k^\pm + (\omega_n^2 + E_k^2)^{1/2} & \pm (\omega_n^2 + E_k^2)^{1/2} \\ \Delta_k^\pm - (\omega_n^2 + E_k^2)^{1/2} & \pm (\omega_n^2 + E_k^2)^{1/2} \end{bmatrix} \quad (0.6)$$

with $\Delta_k^\pm = \psi(k) \pm \phi(k)|\mathbf{g}_k|$ and $E_k^\pm = \sqrt{\omega_n^2 \pm \Delta_k^\pm}$.

Within the weak-coupling theory for superconductivity, only the static spin susceptibility is required. For simplicity, we neglect the feedback effect of superconductivity on the spin fluctuation below $T_c$. Therefore, in this case the spin fluctuation is just the static spin susceptibility in the normal state. Including the electron repulsion $U$ within RPA, the matrix of static spin susceptibility is calculated with the above Green’s function as $\chi(q) = \left[ 1 - 2U \chi^{(0)}(q) \right]^{-1} \chi^{(0)}(q)$, where the matrix element $\chi^{(0)}_{\alpha\beta}(q)$ for $\alpha, \beta = x, y, z$ is given by

$$\chi^{(0)}_{\alpha\beta}(q) = \frac{1}{8N_0} \sum_k \sum_\xi \sum_\zeta \Gamma^{\alpha\beta}_{\xi\zeta}(k; q) \frac{f(E_{k+q\xi}) - f(E_{k+q\zeta})}{E_{k+q\xi} - E_{k+q\zeta}} \quad (0.7)$$

with the Fermi distribution function $f(\xi)$ and a vertex

$$\Gamma^{\alpha\beta}_{\xi\zeta}(k; q) = \frac{\varepsilon_{\xi\zeta}^2 E_{k+q\xi}}{\varepsilon_{\xi\zeta}^2 E_{k+q\zeta}} \quad (0.8)$$

$$+ \xi \left( \tilde{g}_{k\alpha} \tilde{g}_{k+q\beta} + \tilde{g}_{k\beta} \tilde{g}_{k+q\alpha} - \varepsilon_{\alpha\beta} \frac{1}{2} (\xi \tilde{g}_{k+q\beta} - \xi \tilde{g}_{k\alpha}) \right).$$

Similarly, the charge fluctuation is described by $\chi^{(0)}(q) = \chi^{(0)}_{\alpha\beta}(q)/[1 + 2U \chi^{(0)}_{\alpha\beta}(q)]$, which is obtained by the replacement of $\Gamma^{\alpha\beta}_{\xi\zeta}(k; q)$ by $\Gamma^{\alpha\beta}_{\xi\zeta}(q; k) = 1 + \xi \varepsilon_{\xi\zeta} \tilde{g}_{k+q\xi} / \chi^{(0)}_{\alpha\beta}(q)$.

We comment on the spin fluctuations in the tetragonal system. In the centrosymmetric system, the matrix $\chi(q)$ is diagonal. We denote $\chi_{\alpha\alpha}(q)$ and $(\chi_{xx}(q) + \chi_{yy}(q))/2$ as usual (centrosymmetric) spin fluctuations. On the other hand, in the non-centrosymmetric case, $(\chi_{xx}(q) - \chi_{yy}(q))/2$, $(\chi_{xy}(q) + \chi_{yx}(q))/2$, and $(\chi_{xx}(q) - \chi_{xy}(q))/2$ also remain zero with characteristic $q$-dependences of $q_x^2 - q_y^2$, $q_x q_y$, $q_x$, and $q_y$, respectively. We call these four contributions as anomalous spin fluctuations. The characteristic $q$-dependences of anomalous (non-centrosymmetric) spin fluctuations are caused by the Rashba field $\mathbf{g}_k$ under the symmetry constraint. Considering the matrix $\chi(q)$, not only usual spin fluctuations but also anomalous spin fluctuations develop around a magnetic instability.

We now examine the effect of both usual and anomalous spin fluctuations on the pairing mechanism in the non-centrosymmetric tetragonal system. Using the standard procedure, the following gap equation is obtained,

$$[ \psi(k) \quad d_x(k) \quad d_y(k) ]^T = \frac{1}{N_0} \sum_q \begin{bmatrix} V_{xx}(q) & V_{xz}(q) & V_{xy}(q) \\ V_{yx}(q) & V_{yy}(q) & V_{yx}(q) \\ V_{yx}(q) & V_{yy}(q) & V_{yy}(q) \end{bmatrix} \begin{bmatrix} F_s(k - q) \\ F_s'(k - q) \\ F_y(k - q) \end{bmatrix}$$

where $V_{\xi\zeta}(q)$ is the pairing interaction due to corresponding fluctuation exchange given by

$V_{xx}(q) = -U^2[\chi_{xx}(q) + \chi_{yy}(q) - \chi_{cc}(q)] - U$,

$V_{xx}(q) = U[\chi_{cc}(q) + \chi_{zz}(q) - \{\chi_{xx}(q) - \chi_{yy}(q)\}]$,

$V_{yy}(q) = U[\chi_{cc}(q) + \chi_{zz}(q) - \{\chi_{xx}(q) - \chi_{yy}(q)\}]$,

$V_{yy}(q) = -U^2[\chi_{yy}(q) + \chi_{yz}(q)]$,

$V_{yy}(q) = -V_{xx}(q) = iU^2[\chi_{yy}(q) - \chi_{yz}(q)]$,

$V_{yy}(q) = -V_{yy}(q) = iU^2[\chi_{xx}(q) - \chi_{yz}(q)]$.

Similar relations between the pairing interactions and spin fluctuations in non-centrosymmetric systems are obtained from a different approach. In order to get a favorable form of the gap equation, $F_s(k)$ and $F_y(k)$ are introduced by $T \sum_q F(k, \omega_n) = [F_s(k)\sigma_0 + F(k)\hat{\sigma}]|\Theta_\mathbf{q}|$, where $F_s(k) = \left[ \psi(k)\varphi_s(k) + d(k) \cdot \mathbf{g}_k \varphi_s(k) \right] / 2$ and $F_s(k) = \left[ \psi(k)\varphi_s(k) + d(k) \cdot \mathbf{g}_k \varphi_s(k) \right] / 2$.
$\tilde{g}_{kk}(\omega(q)\varphi_-(k) + d(k) \cdot \tilde{g}_k \varphi_+(k))/2$ are obtained with
$\varphi_\pm (k) = \tanh \frac{\tilde{g}_k}{2E_{k+}} \pm \tanh \frac{\tilde{g}_k}{2E_{k-}}$.

In the centrosymmetric case, only $V_{ss}(q)$ and $V_{xx}(q) = V_{yy}(q)$ remain, and the usual spin fluctuations in $V_{ss}(q)$ and $V_{xx}(q)$ contribute to the spin-singlet and spin-triplet pairing mechanisms, respectively. For non-zero Rashba field, the anomalous spin fluctuations contribute only to the spin-triplet pairing interactions $V_{\alpha\beta}(q)$ and the mixing interactions $V_{\alpha\alpha}(q) = -V_{\alpha\beta}(q)$ for $\alpha, \beta=x, y$. We also note that the mixing interactions between spin-singlet and spin-triplet pairs are described by antisymmetric spin fluctuations, $\chi_{yz}(q) = -\chi_{zy}(q)$, which relate with the Dzyaloshinski-Moriya interaction. Therefore, the anomalous spin fluctuations are essential to form the spin-triplet pairs in the non-centrosymmetric system, if they are constructive for superconductivity.

In the following, we show the results of numerical calculation. When the system is in the normal state, the gap equation reduces to an eigenvalue problem. When the maximum eigenvalue of a representation reaches unity, superconductivity belonging to this representation appears. For actual calculation, we introduce a cutoff energy $\omega_c = 0.2t_1$ for electrons forming the Cooper pair. Furthermore, we fix the superconducting transition temperature at $T_c = 0.02t_1$. In Fig. 1, it is shown that by increasing the on-site repulsion $U$ toward an incommensurate magnetic instability at $U_c = 2.551t_1$, every maximum eigenvalue $\lambda_T$ of $\Gamma$-representation for the eigenvalue problem increases, and $\lambda_{A_1}$ reaches unity first among all tetragonal group representations. This means that the superconductivity of $A_1$ representation in $C_{4v}$ appears around the incommensurate magnetic instability.

For the eigenvector of $\lambda_{A_1} = 1$ at the critical interaction constant $U_{A_1}$, $k$-dependences of the corresponding normalized gap functions along Fermi-surfaces of $\varepsilon_k$ are shown in Figs. 2(a) and 2(b), respectively. Ignoring all anomalous spin fluctuations with $U = U_{A_1}$ in the gap equation, the $k$-dependences of the gap functions change to Figs. 2(c) and 2(d), respectively, where $\lambda_{A_1}$ decreases to 0.573 although the same interaction constant as Figs. 2(a) and 2(b) are used. Comparing these figures, the singlet gap function $\psi(k)$ is not affected by the anomalous spin fluctuations, as expected from eq. (0.10). Therefore, it is stabilized by the usual spin fluctuations with a momentum corresponding to the ordering wave vector at $U_c$, which spans from one peak position of $\psi(k)$ along a Fermi-line $\varepsilon_k = 0$ in Fig. 2(a) to other peak position of $|\psi(k)|$ along a Fermi-line $\varepsilon_k = 0$ in Fig. 2(b). On the other hand, the magnitude of spin-triplet gap functions are enhanced by switching on the anomalous spin fluctuations, and becomes almost the same size as that of spin-singlet gap. Thus, the anomalous spin fluctuations are constructive for the superconductivity, and they are responsible for the stabilization of spin-triplet gap function. We note that the effect of anomalous spin fluctuations on superconductivity does not depend on $\omega_c$.
\( \psi(k) \) and \( d(k) \), nodal structures for \( \Delta_{k\pm} \) are also expected. Considering that \( \Delta_{k\pm} \) are the gap functions in the band picture, they reflect directly to thermal and dynamical quantities in the superconducting state. For various temperatures below \( T_c = 0.02 t_1 \), the \( k \)-dependences of \( \Delta_{k\pm} \) along Fermi surfaces of \( \varepsilon_{k\pm} \) are shown in Fig. 3, where pairing interactions are fixed to those at \( T = T_c \). We stress that the \( k \)-dependences of gap functions reflect fully the characteristic momentum dependences of spin fluctuations without assuming the common simple form of \( \Delta_{k\pm} = \Delta_1 \pm \Delta_3 g_{k\pm} \). Recalling that the representation of the superconductivity is \( A_1 \) in \( C_{4v} \), both gap functions \( \Delta_{k\pm} \) exhibit accidental line nodes. The positions of nodes almost do not move with decreasing temperature, and the temperature dependence of \( \psi(k_1) \) and \( d(k_2) \cdot g_{k_2} \) is of common BCS type as shown in the inset. Therefore, the existence of the accidental node in gap function explains \( T \)-dependences of NMR relaxation rate, thermal conductivity, and penetration depth in the superconducting state of CePt\(_3\)Si and CeIrSi\(_3\),\(^8\)\(^-\)\(^10\),\(^24\) In order to check our scenario, it is desirable to observe the gap function in detail by the thermal conductivity experiment, in addition to the observation of anomalous spin fluctuations.

Finally, we comment on the superconductivity in non-centrosymmetric correlated electron systems. As already mentioned, the spin-singlet and spin-triplet gap functions coexist in the non-centrosymmetric superconductor. If only the usual antiferromagnetic spin fluctuations are enhanced, the spin-triplet gap function will be induced by the primary order parameter corresponding to the spin-singlet gap function, as shown in Figs. 2(c) and 2(d).\(^16\) However, in the case that the anomalous spin fluctuations are also enhanced,\(^18\) the superconducting state is quite different from the former case, although it will not be so different from that of the usual unconventional line-node superconductivity. With respect to its relation to magnetism, we note that unconventional superconductivity appears due to the spin fluctuations enhanced around the magnetic instability in a similar manner as in a centrosymmetric superconductor. On the other hand, the spin-triplet gap function develops due to the anomalous spin fluctuations characteristic of the non-centrosymmetric structure.

In summary, we have studied the mechanism of superconductivity in the non-centrosymmetric system. It has been shown that the spin-triplet gap function surviving the suppression of pairing due to the absence of centrosymmetry is developed by the anomalous spin fluctuations, which are enhanced around a magnetic instability. Reflecting the anisotropic momentum dependences of anomalous spin fluctuations, the gap functions have non-trivial \( A_1 \) \( k \)-dependence with accidental line node. This pairing mechanism gives a reasonable explanation for the superconductivity in a non-centrosymmetric superconducting systems CePt\(_3\)Si and CeTSi\(_3\), showing a huge upper critical field, a line-node gap structure, and an incommensurate magnetic structure.