Current patterns and magnetic impurities in time-reversal breaking superconductors

Yukihiro Okuno

Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan

(Received )

We study the impurity effect in the time reversal symmetry (T) breaking superconductor based on the Bogoliubov-de Gennes (BdG) equations. In T-violating superconductors, spontaneous currents are induced around the impurity. The current patterns around the impurity reflect the structures of the Cooper pairs. We investigate impurity problem numerically for two kinds of T violating superconductors (px + ipy and d + is) and investigate the currents around the impurity. We also study the effects of the magnetic impurity in p-wave (px + ipy) superconductor, especially in view of the zero-energy crossing of energy levels related to the phase transition of the ground state.

KEYWORDS: time-reversal breaking state, px + ipy and d + is superconductor, B-dG equation, spontaneous current, bound state, magnetic impurity

§1. Introduction

One of the current important issues of the superconductivity is the occurrence of the time-reversal symmetry (T)-violating state. It has been investigated in connection with the local behavior of the order parameter at the interface of the Josephson junctions and the surface of the material. Another context of T violating state is the unconventional superconductor where time reversal symmetry is violated throughout the whole materials. Such examples are seen in the heavy fermion superconductors UPt3, U1−xThxBe13 (0.017 < x < 0.045) and the layered perovskite superconductor Sr2RuO4. In general the violation of time-reversal invariance is a property of the magnetism and indeed, it is found that the T-violating superconductor shows various magnetic properties. In such systems, inhomogeneities where the Meissner screening effects are insufficient allow the appeared spontaneous supercurrent. This happens, for example, at the surface of samples and also on the domain wall between the degenerate states of the superconductor. The defects of the crystal lattice, in particular impurities, can also lead to the appearance of the magnetic properties of the T-violating state, and it is known that the spontaneous suppercurent are induced in the vicinity

* E-mail: okuno@yukawa.kyoto-u.ac.jp
of an impurity in such a system. Such an induced current around the impurities can generate the local magnetic field in the superconducting state. The local magnetic field can be detected by a high resolution probe like spin polarized muons\cite{2,4} and indeed has lead to the observation of the intrinsic magnetism in the superconducting state of such $\mathcal{T}$-violating superconducting systems. There are some studies about the induced current around the impurity in $\mathcal{T}$-violating superconductor\cite{7,8,9,10}. We have already investigated a microscopic mechanism of such an induced current around the non-magnetic impurity with the Cooper pair of the type $p_x \pm ip_y$, which is a candidate of the Cooper pair symmetry of the Sr$_2$RuO$_4$\cite{11} and has angular momentum $L_z = \pm 1$. We see that the circular current generated around the impurities reflects the angular momentum of the Cooper pair. But still there are only few studies on how the induced currents around the impurity depend on the type of the Cooper pairs. So it is interesting to study the influence of the the structures of the Cooper pairs to the patterns of the induced currents around the impurity. Here in this paper we investigate the induced currents around a non-magnetic impurity with different types of Cooper pair, especially we pay attention to the angular momentum of the Cooper pair. Basically we can make a distinction between two kinds of $\mathcal{T}$-violating superconducting states whose Cooper pair have an intrinsic angular momentum like $p_x \pm ip_y$, $d_{zx} \pm id_{zy}$ ($L_z = \pm 1$), $d_{x^2-y^2} \pm id_{xy}$ ($L_z = \pm 2$) and those that have no angular momentum like $d + is$. Such a difference of the structure of the Cooper pairs will affect the pattern of the induced currents around the impurity. We also study the effects of the magnetic impurity in $p_x + ip_y$ superconductor and investigate the differences from the non-magnetic impurity. Especially we pay attention to the bound state and the ground state transition as well as the induced current.

The organization of this paper is as follow. In §2, we solve the Bogoliubov-de Gennes equation numerically and investigate the induced current around the impurity. In §3, we study the magnetic impurity effect on the $p_x + ip_y$ superconductor, §4 is the conclusion and discussion.

§2. Pattern of the induced current around a non-magnetic impurity

In order to investigate the induced current effect on the superconductor, we solve the Bogoliubov-de Gennes equation numerically\cite{12,13}. The formalism is given below. We start with the B.C.S Hamiltonian on the 2D square lattice

$$H = -t \sum_{<i,j>,\sigma} a_{i\sigma}^\dagger a_{j\sigma} + \sum_{<i,j>} (\Delta_{i,j} a_{i\uparrow}^\dagger a_{j\downarrow} + h.c.) + U \sum_\sigma a_{0\sigma}^\dagger a_{0\sigma} - \mu \sum_{i,\sigma} a_{i\sigma}^\dagger a_{i\sigma}$$  \hspace{1cm} (2.1)

where $t$ and $U$ is the hopping between the nearest-neighbor (n.n) sites and the impurity potential respectively and $\mu$ is the chemical potential of the system. We set the non-magnetic impurity at the site 0. The real space order parameter $\Delta_{i,j}$ is defined as

$$\Delta_{i,j} = V_{i,j} < a_{i\uparrow} a_{j\downarrow}>$$  \hspace{1cm} (2.2)
where \( V_{i,j} \) is the attractive pairing interaction between the site \( i \) and \( j \). The Hamiltonian (2.1) can be diagonalized by means of the unitary transformation \( U \)

\[
H = \sum_{m=1}^{N_L} \epsilon_m \gamma_m^\dagger \gamma_m + \sum_{m=1}^{N_L} \left( -\epsilon_m \right) \gamma_m^\dagger \gamma_m^\dagger \tag{2.3}
\]

where \( N_L \) is the number of the lattice sites and \( \epsilon_m (>0) \) is the excitation energy of the Bogoliubov quasiparticles. The fermion operators \( \gamma \) are related to the original electron operator \( a_{i,\sigma} \) by

\[
\begin{pmatrix}
  a_{1\uparrow} \\
  \vdots \\
  a_{N_L\uparrow} \\
  a_{1\downarrow}^\dagger \\
  \vdots \\
  a_{N_L\downarrow}^\dagger
\end{pmatrix}
= U
\begin{pmatrix}
  \gamma_{1\uparrow} \\
  \vdots \\
  \gamma_{N_L\uparrow} \\
  \gamma_{1\downarrow}^\dagger \\
  \vdots \\
  \gamma_{N_L\downarrow}^\dagger
\end{pmatrix}.
\tag{2.4}
\]

Then, the self-consistent equation for the gap \( \Delta_{i,j} \) (2.2) is given as

\[
\Delta_{i,j} = - \sum_{m=1}^{N_L} V_{i,j} \left[ U_{i,N_L+m,j,N_L+m}^* \right].
\tag{2.5}
\]

We solve the equation (2.1) - (2.5) iteratively until the self consistent conditions are satisfied. In the \( T \)-violating superconductor, the spatial variation of the gap function induces the supercurrent. The current in the \( a \) directions at the site \( i \) is expressed as follow,

\[
J_{ia} = \text{i} t \sum_{m=1}^{N_L} \left( U_{i+N_L+m,j,N_L+m} U_{i,m,N_L+m}^* - U_{i+m,N_L+m,j} U_{i+m,N_L+m}^* \right).
\tag{2.6}
\]

First, we solve the problem in the case of \( \eta_\pm = p_x \pm ip_y \), which has an angular momentum \( L_z = \pm 1 \) if the systems has cylindrical symmetry. We take the nearest neighbor interaction for \( V_{i,j} \) and shift the chemical potential from half filling in order to stabilize the p-wave pairing. We assume the state \( \eta_+ = p_x + ip_y \) is realized globally in the absence of impurity. In the calculation we take the lattice size \( 27 \times 27 \) with periodic boundary condition and we take the value \( V_{i,j} = 3t \), \( U = 100t \), the chemical potential \( \mu = -0.7t \).

The numerical result satisfies the relation,

\[
\begin{align*}
\Delta_{i,i+e_x} & = - \Delta_{i+e_x,i}, \\
\Delta_{i,i+e_y} & = - \Delta_{i+e_y,i},
\end{align*}
\tag{2.7}
\]

where \( e_x \) and \( e_y \) are unit vectors in the \( x \) and \( y \) direction respectively. This result shows that the odd parity state is realized and there are no even parity components within the numerical accuracy.
Each component of the $p_x$ and $p_y$ of the Cooper pairs at the site $i$ are defined as,

$$
\Delta p_x(i) \equiv \frac{1}{2}(\Delta_{i,i+e_x} - \Delta_{i,i-e_x}) \tag{2.8}
$$

$$
\Delta p_y(i) \equiv \frac{1}{2}(\Delta_{i,i+e_y} - \Delta_{i,i-e_y}) \tag{2.9}
$$

Due to the spatial variation of the order parameter, $\eta_- = p_x - ip_y$ component is induced near the impurity. We determine the weight of the $\eta_\pm$ for each site as,

$$
\eta_+(i) \begin{pmatrix} 1 \\ i \end{pmatrix} + \eta_-(i) \begin{pmatrix} 1 \\ -i \end{pmatrix} = \begin{pmatrix} \Delta p_x(i) \\ \Delta p_y(i) \end{pmatrix} \tag{2.10}
$$

We depict the spatial dependence of the order parameter in Fig.1(a-c). Fig.(1-a) shows the $\eta_+$ component which is dominant in the bulk and are suppressed around the impurity. In Fig.1b-c, we can see the admixture component $\eta_-$, which vanishes in the bulk and is induced around the impurity. The admixture component $\eta_-$ has phase winding 2, like $\eta_+(i) - e^{2i\theta} \eta_-(i)$, reflecting the difference of the angular momentum between dominant and admixture components of the Cooper pairs. The BdG equations have bound state which is localized around the impurity. The energy level of the bound state is not zero even in the unitary limit, if the system has not the electron-hole symmetry (see Appendix 1).

In Fig.2 we show the induced circular current. The spontaneous circular current are induced around the impurity and the current pattern are the reflection of the intrinsic angular momentum of the Cooper pairs. The intrinsic angular momentum turns into a circular current around an impurity due to scattering. Within this numerical calculation on the lattice systems, it is difficult to observe the ‘counter current’ which we discussed in Ref[10] because it is small and extends beyond the lattice treated model.

We also show another type of the $T$-violating superconductor. We take $d_{xy} + is$, which is easily realized by the next-nearest neighbor interaction. In this case, the Cooper pair has no angular momentum (equal admixture of the orbital momentum $L_z = \pm 2$) and is not a chiral state. We define the d-wave and (extended) s-wave components of the gap function as below,

$$
\Delta_d(i) = \frac{1}{4}(\Delta_{i,i+e_x+e_y} + \Delta_{i,i-e_x-e_y} - \Delta_{i,i-e_x+e_y} + \Delta_{i,i+e_x-e_y})
$$

$$
\Delta_s(i) = \frac{1}{4}(\Delta_{i,i+e_x+e_y} + \Delta_{i,i-e_x-e_y} + \Delta_{i,i-e_x+e_y} + \Delta_{i,i+e_x-e_y}) \tag{2.11}
$$

In the calculation we take the next-nearest neighbor interaction $V_{i,j} = V = 2t$ and the chemical potential $\mu = -0.7t$ as in the p-wave case. In Fig.3(a-c) we show the self-consistently determined order parameters. The magnitude of the bulk $d_{xy}$ and s-wave component is estimated as $\Delta_d = 0.6t$ and $\Delta_s = 0.22t$ within these parameters. Around the impurity the real parts of the s-wave order is generated. Not that also the s-wave component is influenced by the non-magnetic impurity, since it has a non-trivial phase dependence in the Brillouin zone. The real s-wave component is induced

4
along the diagonal direction and vanishes in the node directions of the d-wave gap, and change sign under 90-degree rotation as in previous studies, which are reflections of the sign change of the d-wave component. The induced current around the impurity is shown in Fig.4. In this case, the induced current is not circular but flows along the diagonal direction. The pattern of the current is understood from the Ginzburg-Landau theory.

The Ginzburg-Landau free energy is given as,

$$f = \int d^2r \left[ \sum_{j=d,s} (\alpha_j |\Delta_j|^2 + \beta_j |\Delta_j|^4 + K_j |\Pi_j||\Delta_j|^2) + \gamma_1 |\Delta_d|^2 |\Delta_s|^2 + \frac{1}{2} \gamma_2 (\Delta^2_d \Delta^2_s + \Delta^2_d \Delta^2_s) + \hat{K} (\Pi_X^* \Delta_s \Pi_X \Delta^*_d - \Pi_Y^* \Delta_s \Pi_Y \Delta^*_d + c.c) + g_s \delta(r) |\Delta_s|^2 + g_d \delta(r) |\Delta_d|^2 \right],$$  

(2.12)
where $g_s$ and $g_d$ are the impurity potential for s and d-wave respectively and X and Y are directed to the diagonal (1,1) and (-1,1) respectively and $\Pi = -i(\nabla_X, \nabla_Y)$. The current are expressed as,

$$j(r) = (-2e)[(K_s\Delta^* s \Pi^* \Delta^* s + K_d\Delta^* d \Pi^* \Delta^* d)$$

$$+ \tilde{K}\{(\Delta^* s \Pi^* X \Delta_d + \Delta^* d \Pi^* X \Delta_s)\hat{e}_X + c.c\}$$

$$- \tilde{K}\{(\Delta^* s \Pi^* Y \Delta_d + \Delta^* d \Pi^* Y \Delta_s)\hat{e}_Y + c.c\}]$$

(2.13)

where $\hat{e}_X$ and $\hat{e}_Y$ are the unit vectors in the $X -$ and $Y -$ direction respectively. The parts which come from the mixing gradient term ($\tilde{K}$ term ) is important for the induced current. The d-wave gap are most affected by the non-magnetic impurity, and the suppression of the gap occurs in the diagonal direction. So the current in the diagonal direction is most remarkable. Due to the sign change of the d-wave gap, the direction of the current is reversed between $X -$ and $Y -$ direction.

If we consider the conservation of the current, the overall feature of the induced current should be given like Fig.5, which we cannot see unfortunately them easily in the numerical data due to the their small value. But it is a natural feature because the superconducting state is admixture of the orbital angular momentum of Cooper pair, $L_z = 2$ and $L_z = -2$ (and s-wave component $L_z = 0$). The direction of the current circle is the appearance of the mixture of $L_z = 2$ and $L_z = -2$ of the Cooper pair.

The induced current is clearly distinguished from that of the chiral $p_x + ip_y$ one. In chiral $p_x + ip_y$ case, the induced current forms the magnetic moment around the impurity, but in the $d_{xy} + is$ case, the induced current is arranged like a quadrupole, which is just the reflection of the angular momentum of $d_{xy}$ component. We discuss the magnetic field generated by this type of Cooper pair $(d + is)$ in Appendix 2. The $d_{x^2-y^2} + is$, state which are often discussed in the context of the high temperature superconductor, will give the same type of the induced current with 90 degree rotation.
Fig. 3. The self-consistent gap function for the $d_{xy} + is$ superconductor. Fig.(3-a) and (3-b) shows the spatial variation of the $d_{xy}$ and $s$-wave components, respectively. Fig.(3-c) is the induced real component of the $s$-wave gap which is absence in the bulk.

about the $z$ axis.

In this section we consider the superconductor which violates the $\mathcal{T}$ symmetry in the bulk. It is possible that the $\mathcal{T}$-violating superconducting state in realized locally around the impurity. The induced current pattern will be the same as that of the corresponding $\mathcal{T}$-violating bulk one. So if we can detect the magnetic field pattern around the impurity, we can distinguish the symmetry of the Cooper pair. But it is difficult to produce the locally $\mathcal{T}$-violating superconducting state only by the non-magnetic or magnetic impurity without spin-orbit interaction. We can understand the reason in the GL treatment. Based on GL free energy (2.12) and we assume the bulk state is the real $d$-wave components only. The spatial variation of the order parameter induces the $s$-wave component near the impurity. If the impurity effect is not so strong, we expand the GL equation by the impurity potential. We can easily see the first order of the impurity potential, only the real part of the $s$-wave and $d$-wave component coupled to the impurity potential. So the phase of the
induced s-wave is real with in the first order of the impurity potential and does not violate the $T$ symmetry.

§3. Magnetic impurity in $p_x+ip_y$ superconductor

In this section we discuss the magnetic impurity effects in chiral state, $p_x+ip_y$ superconductor. Here we limit our considerations to a classical spin, $S \gg 1$. In the singlet case we can take the direction of the impurity spin parallel to the $z$-axis by suitable unitary transformation. In the case of the triplet superconductor, we cannot perform the same operation due to the lack of the spin rotation symmetry. But we take the direction of the magnetic impurity in the $z$ direction due to
the physical condition as we explains below. The spontaneous circular current will flow around the
magnetic impurity and the magnetic field generated by the induced current will fix the direction of
impurity spin to the z-axis. So we take the magnetic impurity as a classical Ising type and neglect
the transversal components of the impurity spin.

The Bogoliubov-de Gennes equation with the simple Ising-like magnetic impurity is given like
below,
\[ \begin{align*}
    h_0(r) u_{\sigma}(r) + \sigma J S z \delta(r) u_{\sigma}(r) + \sum_{\sigma'} \int dr' \Delta_{\sigma,\sigma'}(r, r') v_{\sigma - \sigma'}(r') &= E_i u_{\sigma}(r), \\
    -h_0(r) v_{\sigma}(r) + \sigma J S z \delta(r) v_{\sigma}(r) - \sum_{\sigma'} \int dr' \Delta_{\sigma,\sigma'}^*(r, r') u_{\sigma'}(r') &= E_i v_{\sigma}(r),
\end{align*} \]
(3.1)
where \( J \) is the exchange energy and \( S_z \) is the impurity spin. The BdG equation is decoupled by
\((u_\uparrow(r), v_\uparrow(r))\) and \((u_\downarrow(r), v_\downarrow(r))\) due to the absence of the transversal component of the impurity
spin. By the solution of \((u_\uparrow(r), v_\uparrow(r))\) with the eigenvalue \( E_i \), we can construct the solution of the
pair \((u_\downarrow(r), v_\downarrow(r))\) with the eigenvalue \(-E_i\) like \((u_\downarrow^*(r), u_\uparrow^*(r))\) and this is an one to one correspondence. First, we neglect the spatial dependence of the gap function, and fix \( \Delta(k) = \Delta_0\) for the hole-like states it is just the opposite way around. This property is responsible for the
fact that these states carry a circular current. The solution of the bound state with an eigenvalue

\[ \left( \begin{array}{c}
    u_{B\uparrow}(r) \\
    v_{B\downarrow}(r)
\end{array} \right) = \left( \begin{array}{c}
    \frac{2J_0 N_0 e^{-\Delta_0^2 - \epsilon_-^2}}{\Delta_0^2 - \epsilon_-^2} f_1(k_F r) \\
    -\frac{2J_0 N_0 i}{\Delta_0^2 - \epsilon_-^2} f_2(k_F r) e^{-i\theta}
\end{array} \right) \quad \text{or} \quad \left( \begin{array}{c}
    -\frac{2J_0 N_0 \Delta_0}{\Delta_0^2 - \epsilon_-^2} i f_2(k_F r) e^{i\theta} \\
    \frac{2J_0 N_0}{\Delta_0^2 - \epsilon_-^2} f_1(k_F r)
\end{array} \right) \]
(3.2)
where \( N_0 \) is the density of state at the Fermi level and \( c = \pi N_0 J S_z \) and \( I_0^2 = \frac{2 \Delta_0}{\pi N_0 (1 + c^2)^{\frac{3}{2}}} \), and the functions \( f_1(k_F r) \) and \( f_2(k_F r) \), where \( k_F \) is the Fermi wave number, are approximately given for the distance \( r \gg 1/k_F \), as
\[ f_1(k_F r) \approx \frac{\pi}{2} \sqrt{\frac{2}{\pi k_F}} \cos(k_F r - \frac{\pi}{4}) e^{-\frac{\sqrt{\Delta_0^2 - \epsilon_-^2}}{v_F} r}, \]
(3.3)
\[ f_2(k_F r) \approx \frac{\pi}{2} \sqrt{\frac{2}{\pi k_F}} \cos(k_F r - \frac{3\pi}{4}) e^{-\frac{\sqrt{\Delta_0^2 - \epsilon_-^2}}{v_F} r}. \]
\( \epsilon_- \) is an eigenvalue of the bound state and is given as
\[ \epsilon_- = -\frac{\Delta_0}{\sqrt{1 + c^2}}. \]
(3.4)
We can see the mixing of the angular momentum of the wave functions in (3.2). Here the above
eigenvalue and the bound states are derived by the assumption of the electron-hole symmetry and
the infinite band width of the conduction electron. We can easily see that for the electron-like state
the particle wave function couples to the hole wave function of an angular momentum reduced by
1. For the hole-like states it is just the opposite way around. This property is responsible for the
fact that these states carry a circular current. The solution of the bound state with an eigenvalue
$\epsilon_+ = \frac{\Delta_0}{\sqrt{1+c^2}}$ is given as, $(u_{\text{B} \downarrow}(r), v_{\text{B} \uparrow}(r)) = (v^*_{\text{B} \downarrow}(r), u^*_{\text{B} \uparrow}(r))$, as we said. The spectral density, $A_\sigma(r=0, \omega) = Z^{(+)}_\sigma(0)\delta(\omega-\epsilon) + Z^{(-)}_\sigma(0)\delta(\omega+\epsilon)$, at the impurity site due to the bound state is given like, $Z^{(+)}_\downarrow = Z^{(-)}_\uparrow = \frac{2\pi N_0 \Delta_0 c}{(1+c^2)^{3/2}}$, and $Z^{(-)}_\downarrow = Z^{(+)}_\uparrow = 0$.

The current composed by the bound state is given below,

$$j_\theta^B = \frac{4e\Delta_0 N_0|c|}{\pi m(1+c^2)^{3/2}} \frac{f_2(k_F r)^2}{r}$$

(3.5)

In contrast to the non-magnetic impurity there is finite electron-like contribution of the current at the absolute zero temperature. This is due to the fact that the attractive nature of the exchange impurity potential ($J > 0$) for the down spin electrons.

We can also calculate the contribution of the continuum state to the induced current as in the non-magnetic impurity case. In the unitary limit ($c \to \infty$), the current from the continuum is given by,

$$j_\theta^c \sim -\frac{e\Delta_0}{2m\pi^2 v_F}(2\pi - 1)\frac{\cos^2(k_F r - \frac{3}{4})}{r^2} \left(1 + e^{-\frac{2\Delta_0}{v_F r}}\right),$$

(3.6)

where $v_F$ is the Fermi velocity. The power-law decay $1/r^2$ is because of the fact that the current is carried by the quasiparticle belonging to the continuum spectrum.

Basically, the feature and the mechanism of the induced current is not different from the non-magnetic case and the contribution of the continuum spectrum is important. The direction of the current composed by the bound state is opposite to that of the continuum one.

We can see the induced circular current also flows around the magnetic impurity and it does not contradict the assumption we first set up.

Due to the spin degree of freedoms magnetic impurities cause another effect to the superconducting state. In the s-wave superconductor, there is a zero temperature first-order phase transition depending on the magnitude of the impurity exchange potential $J$. The total spin of the electron change from spin unpolarized state, $< s_z > = 0$, to the polarized one $< s_z > = -\frac{1}{2}$, which was noticed by Sakurai.

The physical picture of the phase transition is that the electron is captured by the magnetic impurity due to the large enough exchange energy, $J$. So there is a competition between the pairing-condensation energy and the magnetic impurity interaction. The feature of the transition can be understood from the level crossing of the bound state. We express the solution of the BdG equation of the pair $(u_n(r), v_n(r))$ as $\gamma_n$ and as $\gamma'_m$ for the solution of the pair $(u_m(r), v_m(r))$. We set the $n > 0$ for the eigenvalue $E_n > 0$ and $n < 0$ for $E_n < 0$. The difference of the number of up spin electrons and that of down spin electrons, $M_z$ is expressed as,

$$M_z = \sum_{n<0} 1 - \sum_{k} 1 + \sum_{n>0} \gamma_n^\dagger \gamma_n - \sum_{m>0} \gamma_m^\dagger \gamma_m$$

(3.7)

where the summation $\sum_k$ runs over the wave number space. The spin of the ground state is given by, $\sum_{n<0} 1 - \sum_k 1$, and changes its value when the number of the negative energy states are decreased.
or increased, namely it is the level crossing across the Fermi level. We can see the energy level of the bound state for the $p_x + ip_y$ superconductor is $\epsilon_B = -\Delta_0 / \sqrt{1 + c^2}$. It does not cross the Fermi level however large the exchange energy of the impurity is. So it can be concluded that a phase transition, as found in an s-wave superconductor, is absent in this case. This conclusion is also applicable for the d-wave superconductor and was already pointed out by Salkola. However, we used various assumptions like electron-hole symmetry and impurity s-wave scattering. These are rather ideal conditions for the actual magnetic impurity systems. If we give up these restrictions, the situation is changed. For example, if we allow the electron-hole asymmetry like $N(\xi) = N_0 + N'\xi$, where $N(\xi)$ is the density of state and $N'$ is the introduced phenomenological parameter for the electron-hole asymmetry. Then the level of the bound state is given as,

$$\epsilon_\pm = \pm \frac{(1 - N' DJS_z)}{\sqrt{(\pi N_0 JS_z)^2 + (1 - 2N' DJS_z)^2}} \Delta_0$$

(3.8)

where $D$ is the half of the band width. We can see that the level crossing can occur at the critical strength, $J_{cS_z} = 1 / N' D$.

We can also see that p-wave scattering at the impurity can also cause the phase transition to the spin polarized state. For example, we take the magnetic impurity potential as,

$$\hat{J}(k, k') = J_s \sigma_z + J_p (e^{i(\phi - \phi')} + e^{-i(\phi - \phi')}) \sigma_z$$

(3.9)

where $J_s$ and $J_p$ is the s-wave and p-wave scattering term, respectively, and $\phi$ and $\phi'$ is the angle of $k$ and $k'$ respectively. In this case the energy levels of the bound states solution for the pair $(u_{n\uparrow}(r), v_{n\downarrow}(r))$ are given like below (see Appendix3),

$$\epsilon_1 = -\frac{(1 - cd)\Delta_0}{\sqrt{(c + d)^2 + (1 - cd)^2}}$$

(3.10a)

$$\epsilon_2 = -\frac{\Delta_0}{\sqrt{1 + d^2}}$$

(3.10b)

where $c = \pi N_0 J_s S$ and $d = \pi N_0 J_p S$. We can see from (3.10a) that the impurity spin can be compensated when $c > 1/d$. Another bound state is also accompanied by introducing the p-wave scattering (3.10b). We take another impurity potential like below,

$$\hat{J}(k, k') = U_s + J_p (e^{i(\phi - \phi')} + e^{-i(\phi - \phi')}) \sigma_z$$

(3.11)

where $U$ is the s-wave scalar potential. In this case, the levels of the bound state is given like,

$$\epsilon_1 = -\frac{1 - cd}{\sqrt{(c + d)^2 + (1 - cd)^2}} \Delta_0$$

(3.12a)

$$\epsilon_2 = -\frac{\Delta_0}{\sqrt{1 + d^2}}$$

(3.12b)

$$\epsilon_3 = \pm \frac{1 + cd}{\sqrt{(c - d)^2 + (1 + cd)^2}} \Delta_0$$

(3.12c)
where \( c = \pi N_0 U_s \) and in (3.12c) we take plus sign for \( (c > d) \) and minus sign for \( (c < d) \). The form of (3.12a) can also be possible for the level crossing. In the unitary limit for the scalar potential \( c \rightarrow \infty \), the level crossing occurs at infinitesimal p-wave magnetic potential. The bound state energy level with the unitary limit in s-wave scattering, \( c \rightarrow \infty \), is \( \pm d\Delta_0/\sqrt{1 + d^2} \) and does not coincide with the zero energy level. The above scenario is applicable to the d-wave superconductor with d-wave scattering from the impurity. The p-wave and d-wave scattering is given naturally from the nearest neighbor exchange interaction of the impurity like \( J_0 \sum_\tau S_0 \sigma_{0+\tau} \). Where summation \( \tau \) is taken at the nearest neighbors of the impurity site 0 and \( S_0 \) is the impurity spin and \( \sigma \) the electron spin. Basically, the impurity resonance peak at the zero energy level in unitary limit splits by many factors like electron-hole asymmetry and p-wave scattering. The resonance peak splitting of the DOS in Tsuchiura\(^{21}\) may be related to the anisotropic scattering from the impurity. The anisotropic scattering from the impurity is not negligible in actual transition metal systems like the cuprate superconductors. So actually there is also a first order phase transition of the ground state in this p-wave case as in the conventional s-wave superconductor. But the critical strength of the impurity exchange potential \( J_c \) is not determined only by the competition of the condensation energy and the exchange energy as in the s-wave case but various factors should be considered.

We carry out the numerical calculation of the BdG equation as in the non-magnetic impurity. In Fig.6 we show the spatial dependence of the gap function. Basic feature is not different from that of the non-magnetic impurity case. The magnetic impurity induces the spatial dependence of the spin density. In Fig.7 we show the spin density around the magnetic impurity. The peak \( < s(r = 0) > \) is cut off in order to illustrate the fine details. In Fig.(7-a) the impurity potential \( J_S = 5t \) and is not the electron spin-unpolarized state \( (< s_z > = 0) \). On the other hand, (7-b) is the spin-polarized state \( (< s_z > = -\frac{1}{2}) \) with \( J_S = 10t \). There is a compensating spin-density cloud of opposite sign in the neighborhood of the magnetic moment in order to screen the spin polarization as in the d-wave case\(^{21}\). On the other hand, for the spin-polarized state, the compensating spin-density cloud is much smaller than that of unpolarized one due to the imbalance of the spin up and down electron. Just at the impurity site, \( r = 0 \), the bound state contribution to the spin density \( < s(r = 0) > \) changes at the transition point from the up spin to the down spin. So there exists the discontinuity of \( < s(r = 0) > \) at the transition. But the main contribution of the \( < s(r = 0) > \) comes from the continuum part of the spectrum.

\section*{§4. Conclusion and Discussion}

In this paper we have investigated the non-magnetic impurity effect by solving the BdG equation numerically for chiral \( p_x + ip_y \) and the non-chiral but \( T \)-violating \( d_{xy} + is \) superconductor in §2. We see induced currents of the \( p_x + ip_y \) and \( d_{xy} + is \) superconductors. Both of the \( T \)-violating superconductor can generate the induced spontaneous currents around the impurities. The induced current can generate localized magnetic field in the superconductor. But the patterns of the induced
currents are quite different reflecting the property of the Cooper pairs. In the chiral superconductor $p_x + ip_y$, circular currents around the impurity are induced spontaneously. On the other hand, in the $d_{xy} + is$ superconductor, the current pattern has quadrapolar shape reflecting the mixture of the angular momentum $L_z = 2$ and $L_z = -2$.

In §3 we investigate the magnetic impurity in $p_x + ip_y$ superconductor. In this case, the circular current is induced as in the non-magnetic impurity case. But the bound states also carry the current in contrast to the non-magnetic case. The level of the bound state is not different as in the non-magnetic case and the phase transition of the ground state is absent when the ‘ideal’ conditions, such as electron-hole symmetry and s-wave scattering from the impurity, are satisfied in the p-wave case. But if some conditions are violated, then there is a transition to the electron spin-polarized state. Especially, we pay attention to the anisotropic scattering from the impurity.
which cause the phase transition to the spin polarized state.

In this paper, we take a classical impurity spin and neglect the transversal components of the magnetic impurity spin. So we do not consider the Kondo effect in the usual sense. It is expected that in the $\mathcal{T}$ violating superconductor the induced current pins the impurity spin to the parallel direction of the generated magnetic field. This effect would weaken the Kondo effects in addition to the presence of the superconducting gap. But if the Zeeman energy is small, then the Kondo effect should be taken into account. It is interesting to investigate the competition of the Kondo effect and this Zeeman energy in $\mathcal{T}$-violating superconductor. Other than this effect, in the triplet superconductor, there are many interesting effects in connection to the Kondo effect. Especially due to the lack of the spin symmetry of the superconducting state and the mixture of the finite angular momentum channels other than s-state (angular momentum $m = 0$ channel), the Kondo effect in the triplet superconductor may have different features from the s-wave case. This problem is left for future studies. Also the spin-orbit interaction shows interesting effects. The spin-orbit interaction directly couples to the orbital part of the Cooper pair and give different effects for the $p_x + ip_y$ and $p_x - ip_y$ state. So the induced components, $p_x - ip_y$, around the impurity in $p_x + ip_y$ superconductor will be affected by the spin-orbit interaction. Also this problem will be discussed elsewhere.
Acknowledgment

The author is grateful to M. Sigrist for many helpful discussion and suggestions. He also thanks to M. Matsumoto and Y. Onishi for discussion and K. K. Ng for reading this manuscript Numerical computation in this work was carried out at the Yukawa Institute Computer Facility. The author has been supported by COE fellowship from the Ministry of Education, Science, Sports and Culture of Japan.

Appendix 1

Electron-hole asymmetry shifts the the energy levels of the bound states. Here we concentrate the $p_x + ip_y$ type of Cooper pairs. As for impurity potential, we take the contact type s-wave scattering like $U \delta(r)$. The Fourier transformed BdG equation is written as,

$$\xi_k u_{k\sigma} + \Delta_k v_{k-\sigma} + \frac{U}{V} \sum_k u_{k\sigma} = \epsilon u_{k\sigma}$$

$$-\xi_k v_{k-\sigma} + \Delta_k^* u_{k\sigma} - \frac{U}{V} \sum_k v_{k-\sigma} = \epsilon v_{k-\sigma}$$

where $u_k$ and $v_k$ are electron and hole part of the wave function, respectively, $\xi_k$ is quasi-particle dispersion and $\Delta_k$ is gap function. We introduce the variable $I_0 = (U/V) \sum_k u_{k\sigma}$ and $I_0' = (U/V) \sum_k v_{k-\sigma}$, and the self-consistent equation for $I_0$ and $I_0'$ are given as

$$I_0 = \frac{U}{V} \sum_k u_{k\sigma} = \frac{U}{V} \sum_k \frac{(\epsilon + \xi_k)I_0 - \Delta_k I_0'}{\epsilon^2 - \xi_k^2 - |\Delta_k|^2} = I_0 \frac{U}{V} \sum_k \frac{\epsilon + \xi_k}{\epsilon^2 - \xi_k^2 - |\Delta_k|^2}$$

$$I_0' = \frac{U}{V} \sum_k v_{k-\sigma} = \frac{U}{V} \sum_k \frac{\Delta_k^* I_0 - (\epsilon - \xi_k)I_0'}{\epsilon^2 - \xi_k^2 - |\Delta_k|^2} = I_0' \frac{U}{V} \sum_k \frac{-\epsilon + \xi_k}{\epsilon^2 - \xi_k^2 - |\Delta_k|^2}$$

where for final form we used the fact that the angular integral over the gap function $\Delta_k$ vanishes. The $\xi_k$ term in the numerator does not vanish due to the electron-hole asymmetry. The solutions of (4.3) are divided into two types ($I_0 \neq 0$ and $I_0' = 0$ ) and ($I_0 = 0$ and $I_0' \neq 0$ ). Here we introduce the electron-hole asymmetry phenomenologically like $N(\xi) = N_0 + N' \xi$, where $N(\xi)$ is the density of state. Then with neglecting the $k$-dependence of the $|\Delta_k|^2$ in denominator of (4.3), which are approximately valid in the $p_x + ip_y$ case, in the unitary limit $U \to \infty$, the energy level of the bound state ($\epsilon < |\Delta_k|$ ) is given like,

$$\epsilon \sim \pm \frac{|2 \Delta' D|}{\sqrt{(N_0 \pi)^2 + (2N' D)^2}}$$

where $D$ is the half of the band-width. The energy level does not coincide to zero energy level but splits due to the electron-hole asymmetry. The above argument is also applicable to the d-wave superconductor.
Appendix 2

In this Appendix we discuss the magnetic field generated around the impurity in the d + is type Cooper pair. Our discussion is based on the GL theory. In the case of the coexistence of the d and s wave with $\mathcal{T}$-violating superconductor, the GL free energy in the weak coupling approximation is written as

$$
\begin{align*}
    f &= -2\alpha_s |\Delta_s|^2 - \alpha_d |\Delta_d|^2 + \beta (|\Delta_s|^4 + \frac{3}{8} |\Delta_d|^4 + 2 |\Delta_s|^2 |\Delta_d|^2 + \frac{1}{2} (\Delta_s^* \Delta_d^2 + \Delta_s^2 \Delta_d^*))^2] \\
    &+ K [2|\Pi\Delta_s^*| + |\Pi\Delta_d^*| + (\Pi_x^* \Delta_x \Delta_d^* - \Pi_y^* \Delta_y \Delta_d^* + c.c)] + g ((|\Delta_s|^2 + |\Delta_d|^2)) \delta(r)
\end{align*}
$$

(4.5)

where $\alpha_s = \ln \frac{T_d}{T}$ and $\alpha_d = \ln \frac{T_d}{T}$ and we set the same strength of the impurity potential for d and s wave order parameter.

The derived GL equations are,

$$
\begin{align*}
    -2\alpha S + \frac{8}{3} (|S|^2 + |D|^2) S + \frac{3}{4} D^2 S^* + 2\Pi^2 S + (\Pi^2_x - \Pi^2_y) D + g S \delta(r) &= 0 \\
    -D + \frac{4}{3} (|S|^2 + 2|S|^2) D + \frac{4}{3} S^2 D^* + \Pi^2 x D^* + (\Pi^2_x - \Pi^2_y) S + g D \delta(r) &= 0 \\
    j &= [2S^* \Pi S + D^* \Pi D + (\Pi_x D^* + \Pi_x S^*) \hat{x} - (\Pi_y D^* + \Pi_y S^*) \hat{y} + c.c]
\end{align*}
$$

(4.6) (4.7) (4.8)

here $\alpha = \frac{\alpha_d}{\alpha_s}$ and $\Pi = -i \nabla$. $D$ and $S$ is the order parameters for d- ans s-wave, respectively, which are normalized by $\Delta_0 = \sqrt{\frac{2}{\alpha_d}}$ and the length scale is also normalized by $\sqrt{\frac{K}{\alpha_d}}$. For the realization of the bulk $\mathcal{T}$-violating state we impose the condition $1 > \alpha > \frac{2}{3}$. We expand $S$ and $D$ in first order of impurity potential, $g$, like $S = i(S_0 + S_1)$ and $D = (D_0 + D_1)$, where $S_0$ and $D_0$ are the values of the homogeneous case and are given as $S_0^2 = \frac{3}{8}(3\alpha - 2)$ and $D_0^2 = 3(1 - \alpha)$. The Fourier transformed form of $S_1$ and $D_1$ are rather complex and are given like

$$
\begin{align*}
    S'(q, \phi) &= 2\sqrt{-6 + 9 \alpha g} (16 \alpha^2 + 3 q^2 (-4 + q^2) - 2 \alpha (8 - 9 q^2) - q^2 (4 - 2 \alpha + q^2) \cos(4\phi)) \frac{C(q, \phi)}{C(q, \phi)} \\
    S''(q, \phi) &= 4\sqrt{3 - 3 \alpha g} \cos(2\phi) (16 + 48 \alpha^2 - 16 q^2 + 3 q^2 + 8 \alpha (-7 + 3 q^2) - q^4 \cos(4\phi)) \frac{C(q, \phi)}{C(q, \phi)} \\
    D'(q, \phi) &= 8\sqrt{3 - 3 \alpha g} (-16 \alpha + 24 \alpha^2 - 10 q^2 + 21 \alpha q^2 + 3 q^4 - q^2 (2 - \alpha + q^2) \cos(4\phi)) \frac{C(q, \phi)}{C(q, \phi)} \\
    D''(q, \phi) &= 4\sqrt{-6 + 9 \alpha g} \cos(2\phi) \left( -2 (8 + 16 \alpha^2 - 6 q^2 + q^4 + 6 \alpha (-4 + q^2)) + q^4 \cos(2\phi)^2 \right) \frac{C(q, \phi)}{C(q, \phi)}
\end{align*}
$$

(4.9)

where we set $(q_x, q_y) = (q \cos(\phi), q \sin(\phi))$ and decompose like $S_1 = S' + iS''$ and $D_1 = D' + iD''$. The denominator factor, $C(q, \phi)$, is given as,

$$
C(q, \phi) = 512\alpha - 1280\alpha^2 + 768\alpha^3 + 320q^2 - 896\alpha q^2 + 480\alpha^2 q^2 - 48q^4 - 48\alpha q^4 - 19q^6 + 4q^2 \left( 16 + 24\alpha^2 + 4q^2 + 3q^4 + 4\alpha (-8 + q^2) \right) \cos(4\phi) - q^6 \cos(8\phi)
$$

(4.10)
The current in the first order of $g$ is given as

$$j(r) = (-4S_0\partial_x S''(r) - 2D_0\partial_x D''(r) + 2S_0\partial_x D'(r) - 2D_0\partial_x S'(r))\hat{x}$$  \hspace{1cm} (4.11)

$$+ (-4S_0\partial_y S''(r) - 2D_0\partial_y D''(r) + 2S_0\partial_y D'(r) - 2D_0\partial_y S'(r))\hat{y}$$  \hspace{1cm} (4.12)

The magnetic field can be calculated by the Biot-Savart formula like,

$$B(q) = \frac{q \times j(q)}{q^2}$$

$$=-\frac{q_x q_y (S_0 D'(q) - D_0 S'(q))}{q^2}$$  \hspace{1cm} (4.13)

We can easily see the sign of the magnetic field changes by 90 degree rotation in $(q_x, q_y)$ space from (4.9) and (4.13), so the feature of the generated magnetic field is the quadrapole like. The feature is consistent to our numerical calculations in §2.

**Appendix 3**

The energy levels of the bound states with p-wave scattering from the impurity are determined as below. We take the same form of the magnetic impurity potential as (3.9). Then as in the Appendix 1 from the Fourier transformed form of the BdG equation we get

$$u_{\uparrow,N}(k) = \frac{(\epsilon_N + \xi_k)(I_0 + I_1 e^{i\phi} + I_1 e^{-i\phi}) + \Delta_k (J_0 + J_1 e^{i\phi} + J_1 e^{-i\phi})}{\epsilon^2_N - \xi^2_k - \Delta_0^2}$$  \hspace{1cm} (4.14a)

$$v_{\downarrow,N}(k) = \frac{\Delta^*(k) (I_0 + I_1 e^{i\phi} + I_1 e^{-i\phi}) + (\epsilon_N - \xi_k)(J_0 + J_1 e^{i\phi} + J_1 e^{-i\phi})}{\epsilon^2_N - \xi^2_k - \Delta_0^2}$$  \hspace{1cm} (4.14b)

here we define $I_0 = J_S \sum_{k'} u_{\uparrow,N}(k')$, $I_1 = J_p S \sum_{k'} u_{\uparrow,N}(k') e^{-i\phi}$, $I_1' = J_p S \sum_{k'} u_{\uparrow,N}(k') e^{i\phi}$, $J_0 = J_S \sum_{k'} v_{\downarrow,N}(k')$, $J_1 = J_p S \sum_{k'} v_{\downarrow,N}(k') e^{-i\phi}$ and $J_1' = J_p S \sum_{k'} v_{\downarrow,N}(k') e^{i\phi}$, where $\phi'$ is the angle of $k'$. Assuming $|\epsilon_N| < \Delta_0$, we get the bound energies from the linear equations from $I_0, I_1, I_1', J_0, J_1$ and $J_1'$. The energy levels of the bound states with the impurity potential (3.11) are given by replacing $J_0$ to $-J_0$ in the above expression (4.14).

---

[1] M. Sigrist: Prog. Theor. Phys. 99 (1998) 899.
[2] R.H. Heffner, J.O. Willis, J.L. Smith, P. Birrer, C. Baines, F.N. Gygax, B. Hitti, E. Lippelt, H.R. Ott, A. Schenk and D. E. MacLaughlin: Phys. Rev. B. 40 (1989) 806.
[3] Y. Maeno: Physica C 282-287 (1997) 206.
[4] G.M. Luke, Y. Fudamoto, K.M. Kojima, M.I. Larkin, J. Merrin, B. Nachumi, Y.J. Uemura, Y. Maeno, Z.Q. Mao, Y. Mori, H. Nakamura, and M. Sigrist: Nature 394 (1998) 558.
[5] G. E. Volovik and L. P. Gorkov: Sov. Phys. JETP 61 (1985) 843.
[6] M. Sigrist and K. Ueda: Rev. Mod. Phys. 63 (1991) 239.
[7] C.H. Choi and P. Muzikar: Phys. Rev. B. 39 (1989) 9664.
[8] V.P. Mineev: JETP Lett. 49 (1989) 719.
[9] D. Rainer and M. Vuorio: J. Phys. C: Solid State Phys. 10 (1977) 3093.
[10] Y. Okuno, M. Matsumoto, M. Sigrist: J. Phys. Soc. Jpn 68 (1999) 3054.
[11] Y. Onishi, Y. Ohashi, Y. Shingaki and K. Miyake: J. Phys. Soc. Jpn 65 675.
[12] Y. Kusama and Y. Ohashi: J. Phys. Soc. Jpn 68 (1999) 987.
[13] M. Franz, C. Kallin and A. J. Berlinsky: Phys. Rev. B 54 (1996) R6897.
[14] H. Tanaka, K. Kuboki and M. Sigrist: Int. J. Mod. Phys. B 12 (1998) 2447.
[15] A. V. Balatsky: Phys. Rev. Lett 80 (1998) 1972.
[16] A. Sakurai: Prog. Theor. Phys. 44, (1970) 1472.
[17] M. I. Salkola, A. V. Balatsky and J. R. Schrieffer: Phys. Rev. B 55 (1997) 12648.
[18] S. Nakajima: Introduction to the Superconductivity (in Japanese) Baifukan (1971).
[19] H. Shiba: Prog. Theor. Phys. 40 (1968) 435.
[20] D. Poilblanc, D. J. Scalapino and W. Hanke: Phys. Rev. Lett. 72 (1994) 884.
[21] H. Tsuchiura, Y. Tanaka, M. Ogata and S. Kashiwaya: condmat-9911117.