Analysis of impurity-induced circular currents for the chiral superconductor

\textbf{Sr}_2\textbf{RuO}_4

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(Received )

The microscopic mechanism of circular currents induced in the vicinity of a non-magnetic impurity is analyzed for the (time-reversal symmetry breaking) chiral superconducting state $d(k) = \hat{z}(k_x \pm ik_y)$ which is very likely realized in \textsc{Sr}_2\textsc{RuO}_4. From the analytic, not self-consistent solution of the Bogolyubov-de Gennes equations we find two types of quasiparticle states, a bound state and the continuum state. Through impurity scattering the condensate transfers angular momentum to the quasiparticle states which generate a circular current. At low temperature the continuum part of the quasiparticle spectrum gives the main contribution. The non-selfconsistent solution yields a state of finite angular momentum. The comparison with the corresponding Ginzburg-Landau theory reveals the existence of a compensating counterflow created by the superconducting condensate. The currents and magnetic fields appearing around the impurity have possibly been observed by muon spin relaxation measurements.

KEYWORDS: \textsc{Sr}_2\textsc{RuO}_4, $p$-wave superconductor, unitary state, time-reversal breaking state, B-dG equation, non-magnetic impurity, spontaneous current

§1. \textbf{Introduction}

\textsc{Sr}_2\textsc{RuO}_4 is the first example of copper-free layered perovskite superconductor\cite{1} This material is structurally identical with the layered perovskite \textsc{La}_2\textsc{CuO}_4, one of the parent compounds of high temperature superconductors. In spite of their structural similarity, there are clear differences in the electronic properties between the two systems. The cuprates are antiferromagnetic Mott insulators in their stoichiometric composition and turn into itinerant electron systems with superconductivity only upon doping carriers. On the other hand, the normal state of \textsc{Sr}_2\textsc{RuO}_4 displays Fermi liquid behavior with essentially two-dimensional character and renormalized due to strong correlation effects. Because superconductivity appears on the background of strong electron correlation, it is unlikely that the pairing channel is conventional $s$-wave type. It was early suggested that this

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system might choose spin-triplet p-wave pairing symmetry instead for various reasons. First it resembles the feature of a strongly correlated Fermi liquid like $^3$He which is a well-known p-wave superfluid. Second, Sr$_2$RuO$_4$ belongs to the Ruddelsen-Popper series Sr$_{n+1}$Ru$_n$O$_{3n+1}$ which consists almost exclusively of ferromagnetic compounds, so that the end member Sr$_2$RuO$_4$ may be subject to strong ferromagnetic spin fluctuations.

Indeed there is now overwhelming evidence for the realization of unconventional superconductivity in Sr$_2$RuO$_4$, and the pairing symmetry has most likely the form $d(k) = \hat{z}(k_x \pm ik_y)$ analog to the (spin-triplet) A-phase of $^3$He. The identification of the symmetry is basically possible due to two experiments. One is the measurement of the spin susceptibility in the superconducting state using $^{17}$O-NMR Knight shift. According to this experiment no change of the spin susceptibility appears with the onset of superconductivity indicating equal spin pairing (spin triplet) with the moments in the basal plane. Note that a strong reduction of the spin susceptibility is common to spin singlet superconductors. Furthermore, $\mu$SR zero field relaxation rate experiments show a pronounced increase of intrinsic magnetic field in the superconducting phase, suggesting that the pairing state breaks time reversal symmetry $T$. Both experiments are fully consistent with one single state, $d(k) = \hat{z}(k_x \pm ik_y)$, among the possible pairing states.

The observation of the enhancement of the internal magnetic field is directly related with $T$-violation. In the case of the state $d(k) = \hat{z}(k_x \pm ik_y)$ the Cooper pair has an orbital angular momentum parallel to the $z$-axis of the crystal. This pairing state belongs to the class of “ferromagnetic” $T$-violating superconducting states according to the symmetry classification by Volovik and Gorkov. It is natural to expect that the presence of this angular momentum appears in magnetic properties. In fact, however, the effect of the angular momentum is invisible in the homogeneous superconducting phase due to Meissner screening. It only occurs where the superconducting state is disturbed in some way that screening effects are insufficient. This happens for example at the surface of samples and also at domain wall between the phases $\hat{z}(k_x + ik_y)$ and $\hat{z}(k_x - ik_y)$. Furthermore defects of the crystal lattice, in particular impurities, can also lead to the appearance of the unusual magnetic properties of the $T$-violating state. It is the aim of this paper to analyze the effect of scattering by a single impurity on the quasiparticle states and the resulting magnetic properties. It is known that spontaneous supercurrents are generated in the vicinity of an impurity in such a state. This has probably been first investigated by Rainer and Vurio in the case of the A-phase of superfluid $^3$He.

Our analysis is based on the solution of the Bogolyubov-de Gennes equations for the single impurity problem. In this formulation we can show how quasiparticle states of different angular momentum around the impurity are coupled together and give rise to a circular current and magnetic field. This feature can already been observed by solving the problem on a phenomenological level with Ginzburg-Landau (GL) theory. Thus before giving a detailed microscopic analysis we
will introduce the problem by GL theory.

§2. Impurity problem in the Ginzburg-Landau theory

We begin our discussion of the superconducting state around an impurity by the discussion within the framework of GL theory. This allows us to recognize some of the basic features of the problem. The order parameter of the superconducting state has two complex components so that we can write in general the gap function $d$ as

$$d(k) = \eta^+ d_+(k) + \eta^- d_-(k)$$ (2.1)

with $d_{\pm}(k) = \hat{z}(k_x \pm i k_y)$. The free energy expansion in these two components has the form

$$f = -(|\eta^+|^2 + |\eta^-|^2) + \frac{1}{2}(|\eta^+|^4 + |\eta^-|^4) + 2|\eta^+|^2|\eta^-|^2 + |D\eta^+|^2 + |D\eta^-|^2 + \frac{1}{2}((D^-\eta^+)(D^+\eta^-) + (D^-\eta^-)(D^+\eta^+))^2 + B^2$$ (2.2)

where $D_\mu = -i \nabla_\mu / \kappa - A_\mu$, $D_{\pm} = D_x \pm i D_y$ and $B = \nabla \times A$. The free energy density $f$ is given in units of $B_c^2 / 4\pi$ ($B_c$: thermodynamical critical field), and lengths are measured in units of the penetration depth $\lambda$ and $B$ in the unit $\sqrt{2}B_c = \phi_0 / (2\pi \lambda \xi)$, and $\kappa = \lambda / \xi$. This form of the free energy density corresponds to the weak-coupling approach with a single cylindrical symmetric Fermi surface.

The uniform state is immediately obtained by minimizing the free energy with respect to the order parameter,

$$(\eta^+, \eta^-) = \eta_0(1, 0) \quad \text{or} \quad \eta_0(0, 1)$$ (2.3)

with $|\eta_0|^2 = 1$. Either the state $d_+(k)$ or $d_-(k)$ are stabilized in the homogeneous phase. The gradient terms, however, show us that this needs not to be true in general if the superconducting phase is inhomogeneous as we will see immediately. We will in the following assume that the homogeneous bulk phase is $(\eta^+, \eta^-) = \eta_0(1, 0)$.

Let us now add a term to the free energy introducing the effect of the single impurity located at $r = 0$,

$$f_{\text{imp}} = \frac{S}{2} (|\eta^+|^2 + |\eta^-|^2) \delta(r)$$ (2.4)

where we use coefficient $S$ to describe the strength of the scattering potential, noting that conventional impurity scattering is pair breaking for unconventional superconductors, in general, leading to a local suppression of the order parameter. We will analyze the behavior of the order parameter in the vicinity of the impurity by assuming weak distortion of the order parameter for distances sufficiently far from the impurity. Thus we introduce two complex functions $u_+(r)$ and $u_-(r)$ with
\( \eta_+ = \eta_0 + u_+(r) \) and \( \eta_- = u_-(r) \). Neglecting in addition the effect of a finite vector potential on the order parameter we obtain the following coupled GL equation in first order in the impurity coupling strength.

\[
\begin{align*}
  u_+(r) + \eta_0 u_+(r) - \frac{\nabla^2}{\kappa^2} u_+(r) - \frac{\nabla^2}{2\kappa^2} u_-(r) + \eta_0 S \delta(r) &= 0 \\
  u_-(r) - \frac{\nabla^2}{\kappa^2} u_-(r) - \frac{\nabla^2}{2\kappa^2} u_+(r) &= 0.
\end{align*}
\]  \hspace{1cm} (2.5)

where we use \( \nabla = \nabla_x \pm i \nabla_y \). This linear equation system is easily solved by using Fourier transformation. If we set \( \eta_0 = e^{i\chi} \), we obtain the following solution,

\[
\begin{align*}
  e^{-i\chi} u_+(r) &= \int_0^\infty dq \frac{-S(1 + \frac{q^2}{\kappa^2})}{2 + \frac{3}{\kappa^2} q^2 + \frac{3}{4\kappa^4} q^4} 2\pi J_0(qr) = g_1(r) \\
  e^{-i\chi} u_-(r) &= -e^{-2i\theta} \int_0^\infty dq \frac{S}{2 + \frac{3}{\kappa^2} q^2 + \frac{3}{4\kappa^4} q^4} 2\pi J_2(qr) = g_2(r) e^{-2i\theta}.
\end{align*}
\]  \hspace{1cm} (2.6)

The important point of this solution is the fact that \( \eta_- \)-component is induced around the impurity and has a phase winding of \(-2 \times 2\pi\). Any spatial variation of \( \eta_+ \) drives \( \eta_- \) which carries a phase winding.

This feature leads now to a spontaneous circular current which we easily find by variation of the free energy with respect to the vector potential and the Maxwell equation \( \nabla \times B = j \). Since no current is flowing in the homogeneous case we express the current \( j \) in first order in \( S \),

\[
j = i \eta_0^* [\hat{\sigma}_0 \nabla u_+ + \frac{1}{2} (\hat{\sigma}_z + i \hat{\sigma}_x) \nabla u_- ] + c.c.
\]  \hspace{1cm} (2.7)

where \( \sigma_0 \) is the \( 2 \times 2 \) unit matrix and \( \sigma_\mu \) the Pauli matrices. Also here we neglect the vector potential. With the above solution we find the circular current as

\[
\begin{align*}
  j_\theta(r) &= \frac{1}{\kappa} \left( \frac{\partial g_2(r)}{\partial r} + \frac{2}{r} g_2(r) \right) \\
  &= \frac{-1}{\kappa} \int_0^\infty dq \frac{2\pi S q^4}{2 + \frac{3}{\kappa^2} q^2 + \frac{3}{4\kappa^4} q^4} J_1(qr) \\
  &= \frac{4\pi S \kappa^2}{\beta - \alpha} (\beta^2 K_1(\sqrt{\beta} \kappa r) - \alpha^2 K_1(\sqrt{\alpha} \kappa r))
\end{align*}
\]  \hspace{1cm} (2.8)

where \( \alpha = 2 - \frac{2}{\sqrt{3}} \), \( \beta = 2 + \frac{2}{\sqrt{3}} \) and \( K_1(x) \) is the modified Bessel function of first order. This expression shows that the flow direction of the current changes as we move away from the impurity.
The current generated near the impurity is compensated again farther out. This kind of counter flow has been reported also by Rainer and Vurio in the A-phase of $^3$He.\textsuperscript{12}

At distances far from the impurity the current decays exponentially, $j_\theta(r) = -S\kappa^{5/4}/\sqrt{3\pi^3}\kappa/z\exp(-\sqrt{\alpha\kappa r})$ with a length scale comparable to the coherence length. At short distances the expression in eq.(2.8) suggests a $1/r$-divergence. This behavior is certainly not appropriate for short distances. Thus, we need to introduce a cutoff into the integral in eq.(2.8) which leads to $j_\theta(r) \propto r$ for $r \to 0$.

The current and counter current flow in a narrow range around the impurity. The resulting total angular momentum of this flow pattern or, equivalently, the magnetic moment vanish due to the exact canceling of the two circular currents,

$$M = \frac{1}{2} \int d^2r \times j(r) = 0 \quad (2.9)$$

Since the canceling of the current occurs on a length scale shorter than London penetration depth (in type II superconductors) the Meissner screening effect does not play an important role for the counter flow. Among the two length scales $1/\kappa\sqrt{\beta}$ and $1/\kappa\sqrt{\alpha}$, the shorter one describes the building up of the magnetic moment due to the order parameter distortion around the impurity and the longer one the decay of the $\eta_-$-component which due to the phase winding introduces the compensating counter flow. Note that this winding does not introduce a topological charge like a finite flux of a vortex, since the winding order parameter component does not exist in the bulk. As a consequence there can not be a finite magnetic flux associated with the impurity state although there is a local magnetic field.

§3. Bogolyubov-de Gennes Formulation

We turn now to the description of the impurity problem in the Bogolyubov-de Gennes (BdG) formulation in order to understand the origin of the spontaneous currents on the level of quasiparticle states. It is possible to perform most of the calculations analytically, if we do not require self-consistency of the pair potential, but leave it constant also in the vicinity of the impurity. We will discuss the shortcomings in the approximation later.

The uniform pair potential $\hat{\Delta}(k) = i(\hat{\sigma} \cdot d(k))\sigma_y$ is given by

$$d(k) = \Delta_0(k_x + ik_y)\hat{z} \quad (3.1)$$

The BdG equation can be written in the following non-local form

$$\begin{align*}
h_0(r)u_{iso}(r) + \sum_{\sigma'} \int d\mathbf{r}' \hat{\Delta}_{\sigma',\sigma}(\mathbf{r},\mathbf{r}')v_{i\sigma}(\mathbf{r}') &= E_iu_{i\sigma}(\mathbf{r}) \\
-h_0(r)v_{i\sigma}(r) - \sum_{\sigma'} \int d\mathbf{r}' \hat{\Delta}^*_{\sigma',\sigma}(\mathbf{r},\mathbf{r}')u_{i\sigma}(\mathbf{r}') &= E_iu_{i\sigma}(\mathbf{r})
\end{align*} \quad (3.2)$$
with \( u_\sigma(r) \) and \( v_\sigma(r) \) is the particle- and hole-like part of the wavefunction. The part \( h_0 \) includes besides the kinetic energy also the potential of the non-magnetic impurity located at the origin,

\[
h_0(r) = h_{\text{kin}} + U\delta(r)
\]

with \( h_{\text{kin}} = -\frac{\nabla^2}{2m} - \epsilon_F \) where \( \epsilon_F \) is the Fermi energy. Moreover, \( U \) denotes the potential strength of the impurity for which we assume the contact type s-wave scattering.

Because we neglect the spatial dependence of the gap function, in particular the suppression of the pair potential around the impurity, we can simplify the equation by Fourier transformation to momentum space.

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

(3.4)

\[
-\xi_k v_{k-\sigma} + \Delta^*_k u_{k\sigma} - \frac{U}{V} \sum_k v_{k-\sigma} = \epsilon v_{k-\sigma}
\]

(3.5)

where \( \Delta_k = \Delta_0 \exp(i\phi) \) (we neglect the gap’s dependence on the magnitude of the wave vector \( |k| \) and take the value of the gap at the Fermi level for simplicity.), \( \xi_k = k^2/2m - \epsilon_F \). By introducing the variables \( I_0 = (U/V) \sum_k u_{k\sigma} \neq 0 \) and \( I_0' = (U/V) \sum_k v_{k-\sigma} \neq 0 \), we can express the wave functions as

\[
\begin{align*}
    u_{k\sigma} &= \frac{(\epsilon + \xi_k)I_0 - \Delta_k I_0'}{\epsilon^2 - \xi_k^2 - \Delta_0^2} \\
    v_{k-\sigma} &= \frac{\Delta^*_k I_0 - (\epsilon - \xi_k)I_0'}{\epsilon^2 - \xi_k^2 - \Delta_0^2}.
\end{align*}
\]

(3.6)

Both \( I_0 \) and \( I_0' \) should be determined self-consistently leading to the equations for the energy,

\[
\begin{align*}
    I_0 &= \frac{U}{V} \sum_k u_{k\sigma} = \frac{U}{V} \sum_k \frac{(\epsilon + \xi_k)I_0 - \Delta_k I_0'}{\epsilon^2 - \xi_k^2 - \Delta_0^2} = I_0 \frac{U}{V} \sum_k \frac{\epsilon}{\epsilon^2 - \xi_k^2 - \Delta_0^2} \\
    I_0' &= \frac{U}{V} \sum_k v_{k-\sigma} = \frac{U}{V} \sum_k \frac{\Delta^*_k I_0 - (\epsilon - \xi_k)I_0'}{\epsilon^2 - \xi_k^2 - \Delta_0^2} = I_0' \frac{U}{V} \sum_k \frac{-\epsilon}{\epsilon^2 - \xi_k^2 - \Delta_0^2}
\end{align*}
\]

(3.8)

where for final form we used the fact that the angular integral over the gap function \( \Delta_k \) vanishes and that close to the Fermi surface the assumption of electron-hole symmetry is satisfied, i.e. the normal state density of state is constant. Actually, there is no qualitative change if we include particle-hole asymmetry.

We immediately see that the equations for \( I_0 \) and \( I_0' \) are decoupled and give rise to different solutions. The states associated with \( I_0 \neq 0 \) can be considered as particle-like while the ones for \( I_0' \neq 0 \) are hole-like. Within both sectors there are two types of solutions, discrete energy states and states belonging to a continuous spectrum (Fig.2). The former consist of one midgap bound
state in both sectors and an electron-(hole)-like state above (below) the band top (bottom) which
 correspond to antibound states (for repulsive impurity scattering). In the following we will neglect
 these anti-bound states, since they are very far from the Fermi level and will not have much influence
 on the properties we are interested in. It is useful to separate the discussion of the midgap bound
 states and the states of the continuum.

3.1 Midgap bound states

From Fig.2 we recognize that there is one discrete midgap state for both case \( I_0 \neq 0 \) and \( I_0' \neq 0 \)
with the energies

\[
\epsilon_\pm = \mp \frac{\Delta_0}{\sqrt{1 + c^2}}
\]

respectively where \( c = \pi N_0 U \) and \( N_0 \) is the density of states at the Fermi level. Note, that for
strong scattering \( (U \to \infty) \) the bound state energy are both zero and for weak scattering \( (U \to 0) \)
the bound states are located close to the gap edge \( \pm \Delta_0 \). For the case particle-like bound state
\( (I_0 \neq 0) \) we obtain the wave function

\[
u_\sigma^-(r) = \frac{I_0}{2\pi} \int_0^\infty dk k \frac{\epsilon_- + \xi_k}{\xi_k^2 - \Delta_0^2} J_0(kr) \approx -\frac{2I_0N_0\epsilon_-}{\sqrt{\Delta_0^2 - \epsilon_-^2}} f_1(k_Fr)
\]

\[
u_\sigma^+(r) = -\frac{I_0'}{2\pi} \int_0^\infty dk k \frac{\Delta_0}{\epsilon_+^2 - \xi_k^2 - \Delta_0^2} iJ_1(kr)e^{-i\theta} \approx -\frac{2I_0'N_0\Delta_0}{\sqrt{\Delta_0^2 - \epsilon_+^2}} i f_2(k_Fr)e^{-i\theta}
\]

\[
u_\sigma^+(r) = -\frac{I_0'}{2\pi} \int_0^\infty dk k \frac{\epsilon_+ - \xi_k}{\epsilon_+^2 - \xi_k^2 - \Delta_0^2} J_0(kr) \approx \frac{2I_0'N_0\epsilon_+}{\sqrt{\Delta_0^2 - \epsilon_+^2}} f_1(k_Fr)
\]

and for the hole-like bound state \( (I_0' \neq 0) \)

where \( k_F \) is the Fermi wave number, \( \theta \) is the angle of position vector \( r \) and \( J_0(kr), J_1(kr) \) is the
Bessel function of 0th and 1st order, respectively. The form of the function \( f_1(k_Fr) \) and \( f_2(k_Fr) \)
for large distances \( (r >> 1/k_F) \) is approximatively given by

\[
f_1(k_Fr) \approx \frac{\pi}{2} \sqrt{\frac{2}{\pi k_F}} \cos(\pi k_F r) - \frac{\pi}{4} e^{-\sqrt{\Delta_0^2 - \epsilon_+^2}} \frac{\sqrt{\Delta_0^2 - \epsilon_+^2}}{k_F} r
\]

\[
f_2(k_Fr) \approx \frac{\pi}{2} \sqrt{\frac{2}{\pi k_F}} \cos(\pi k_F r) - \frac{3\pi}{4} e^{-\sqrt{\Delta_0^2 - \epsilon_+^2}} \frac{\sqrt{\Delta_0^2 - \epsilon_+^2}}{k_F} r
\]
where $\epsilon = \Delta_0/\sqrt{1+c^2}$ and $v_F$ is Fermi velocity.

The variables $I_0$ and $I'_0$ are determined by the normalization condition,

$$\sum_k (u_k^2 + v_k^2) = 1 \quad (3.13)$$

leading to $I_0^2 = I'_0^2 = \Delta_0 c^3/(\pi N_0 (1+c^2)^{3/2})$.

The solution in eq.(3.10) and (3.11) are very similar to the bound state discussed in connection with magnetic impurities in conventional superconductors,\textsuperscript{15,16} and was noticed by Buchholtz and Zwicknagel.\textsuperscript{17} However, the important difference lies in the angular momentum structure of the above bound states. We can easily see that the for the electron-like state the particle wave functions couples with 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 can carry a circular current. In terms of the wavefunctions $u$ and $v$ the current is expressed as,

$$j_B(r) = \frac{e}{2m} \sum_{i,\sigma} \left[ f(\epsilon_i) u_{i\sigma}^* (r) \nabla u_{i\sigma} (r) + (1 - f(\epsilon_i)) v_{i\sigma} (r) \nabla v_{i\sigma}^* (r) - c.c \right]$$

where $\hat{e}_\theta$ is the unit vector of the $\theta$ component, $\epsilon = \Delta_0/\sqrt{1+c^2}$, and $f(\epsilon)$ is the Fermi distribution function. We immediately realize that this current disappears for low-temperatures exponentially, $\propto \exp(-\epsilon/k_BT)$, if $U$ is positive (repulsive). Basically no spontaneous current is caused by the bound states if consider the electron states, since the electron state corresponds to an anti-bound state due to the repulsive potential. On the other hand, considering the situation from the hole point of view the potential is attractive and the hole in a real bound state such that it carries circular current. We will discuss this point using the e-h transformation at the end of this section.

3.2 Contribution of the continuous spectrum

We turn now to the discussion of the continuous part of the quasiparticle spectrum. Analyzing Fig.2 we immediately see that these states are relevant for the formation of circular currents as they are occupied at low temperature. In order to discuss their contribution to the current we have to go beyond the discussion we used for the midgap states. A possible formulation can be based on the solution of the Lippmann-Schwinger equation for the scattering problem. Let us start with the construction of the out-going wave as

$$\psi^{(+)}_k(r) = \phi_k(r) + \int \text{d}y \hat{G}_k^0(r,r')U(r')\tau_3 \psi^{(+)}_k(r') = \phi_k(r) + \hat{G}_k^0(r,0) \frac{U\tau_3}{1 - \hat{G}_k^0(0,0)U\tau_3} \phi_k(0) \quad (3.15)$$
where $\tau_i$ denotes the $i$-th Pauli matrix and the function $\phi(x)$ is the solution of the B-dG equation without impurity given by

$$
\phi_k(r) = \begin{pmatrix} u^{(0)}_k(r) \\ v^{(0)}_k(r) \end{pmatrix} = \frac{1}{\sqrt{2VE_k(E_k + \xi_k)}} \begin{pmatrix} E_k + \xi_k \\ \Delta_k^* \end{pmatrix} e^{i k \cdot r} \tag{3.16}
$$

for the case $I_0 \neq 0$, $\Gamma_0 = 0$ and

$$
\phi_k(r) = \begin{pmatrix} u^{(0)}_k(r) \\ v^{(0)}_k(r) \end{pmatrix} = \frac{1}{\sqrt{2VE_k(E_k - \xi_k)}} \begin{pmatrix} \Delta_k \\ E_k - \xi_k \end{pmatrix} e^{i k \cdot r} \tag{3.17}
$$

for $I_0 = 0$, $\Gamma_0 \neq 0$. Note that each momentum $k$ corresponds to two values of the energy, $E_k = \pm \sqrt{\xi_k^2 + \Delta_0^2}$. The Green function entering eq. (3.15) is constructed from these solutions

$$
\hat{G}_k^0(r,r') = \sum_{k'} \frac{\phi_{k'}(r) \phi^*_k(r')}{E_k + i\delta - E_{k'}}
$$

$$= \frac{1}{\sqrt{V}} \sum_{k'} \left( \frac{E_k' + \xi_{k'}}{2E_{k'}} \frac{\Delta_{k'}}{2E_{k'}} \frac{\Delta_{k'}}{E_{k'} - \xi_{k'}} \right) e^{i k' \cdot (r-r')}
$$

$$= G_{k,0}^0(r) \tau_0 + G_{k,3}^0(r) \tau_3 + G_{k,\theta}^0(r) \begin{pmatrix} 0 & e^{i\theta} \\
-e^{-i\theta} & 0 \end{pmatrix} \tag{3.18}
$$

where $r = |r - r'|$. The Green functions $G_{k,0}^0(r)$, $G_{k,3}^0(r)$ and $G_{k,\theta}^0(r)$ can be expressed analytically,

$$
G_{k,0}^0(r) = -\frac{2E_k \cdot \text{sgn}E_k N_0 \pi}{\sqrt{E_k^2 - \Delta_0^2}} \frac{1}{2} [H_0^{(1)}(k \text{sgn}E_k r) + H_0^{(2)}(k \text{sgn}E_k r)]
$$

$$
G_{k,3}^0(r) = -\frac{N_0 \pi}{V} [H_0^{(1)}(k \text{sgn}E_k r) - H_0^{(2)}(k \text{sgn}E_k r)]
$$

$$
G_{k,\theta}^0(r) = -\frac{iN_0 \Delta_0}{\sqrt{E_k^2 - \Delta_0^2}} \int dk k J_1(kr) \left\{ \frac{1}{k^2 - k_+^2 - i\delta \text{sgn}E_k} - \frac{1}{k^2 - k_-^2 + i\delta \text{sgn}E_k} \right\}
$$

$$= \frac{N_0 \Delta_0}{\sqrt{E_k^2 - \Delta_0^2}} \text{sgn} \pi \frac{1}{2} [J_1(k_+ r) + J_1(k_- r)]
$$

$$= -\frac{iN_0 \Delta_0}{\sqrt{E_k^2 - \Delta_0^2}} \Re \int dk k \left[ \frac{1}{k^2 - k_+^2} - \frac{1}{k^2 - k_-^2} \right] J_1(kr)
$$

$$= g_{1,k}(r) + ig_{2,k}(r) \tag{3.19}
$$

where $J_1(x)$ is the first kind Bessel function and $H_0^{(1)}(x)$ and $H_0^{(2)}(x)$ are Hankel functions. Moreover, the momenta $k_\pm$ are given by

$$
k_\pm = k_F \sqrt{1 \pm \frac{E_k^2 - \Delta_0^2}{\Delta_0^2}} \approx k_F \pm \frac{\sqrt{E_k^2 - \Delta_0^2}}{v_F}. \tag{3.20}
$$
where \( v_F = k_F/m \) is the Fermi velocity. The two momenta \( k_+ \) and \( k_- \) correspond to the more particle-like and more hole-like sections of the quasiparticle spectrum. The appearance of these two states together is a particular feature of the particle-hole mixing in the superconducting state and is related with the Andreev reflection. The last of these three Green functions will be important for the discussion of the circular current.

In (3.19) we decompose \( G_{k,0}(r) \) as \( g_{1,k}(r) \) and \( g_{2,k}(r) \) as it will be convenient for the later discussion. It is easy to see that \( g_{2,k}(r) \) is much smaller than \( g_{1,k}(r) \) for the states with \( |\sqrt{E_k^2 - \Delta_0}| \ll \epsilon_F \). Since these states will be dominant in the contribution to the currents, in particular, due to the enhanced density of states for energies just above the gap, we may safely neglect \( g_{2,k}(r) \).

The above Green function can now be used to define the T-matrix,

\[
\hat{T}(\epsilon) = \frac{U\tau_3}{1 - G_{k,0}(0,0)U\tau_3} = T_0\tau_0 + T_3\tau_3
\]

where the two components are given as,

\[
T_0 = -i\pi U^2 \rho(E_k) \frac{1}{1 + (\pi\rho(E_k)U)^2}
\]

\[
T_3 = \frac{U}{1 + (\pi\rho(E_k)U)^2}
\]

where \( \rho(E_k) = -\frac{1}{\pi} \text{Im} G_{k,0}(0) \). Note that \( T_0 \) is purely imaginary, while \( T_3 \) is real and vanishes in the unitary limit. This just reflects the fact that the scattering phase shift is \( \frac{\pi}{2} \) in this limit.

Let us now rewrite the outgoing wave solution of the Lippmann-Schwinger equation. We restrict to the case where \( I_0 = 0 \) and \( I_0' \neq 0 \) since the other case gives finally the same contribution to the current.

\[
\psi_{k}^{(+)}(r) = \begin{pmatrix} u_k(r) \\ v_k(r) \end{pmatrix} = \frac{1}{\sqrt{2VE_k(E_k - \xi_k)}} \begin{pmatrix} \Delta_k \\ E_k - \xi_k \end{pmatrix} e^{ikr}
\]

\[
+ \frac{1}{\sqrt{2VE_k(E_k - \xi_k)}} \begin{pmatrix} (S_0(r) + S_3(r))\Delta_k \\ (S_0(r) - S_3(r))(E_k - \xi_k) \end{pmatrix} e^{i\theta}
\]

\[
+ \frac{G_{k,0}(r)}{\sqrt{2VE_k(E_k - \xi_k)}} \begin{pmatrix} (T_0 - T_3)(E_k - \xi_k)e^{i\theta} \\ (T_0 + T_3)\Delta_k e^{-i\theta} \end{pmatrix}
\]

with \( S_0(r) = G_{k,0}(r)T_0 + G_{k,3}(r)T_3 \) and \( S_3(r) = G_{k,0}(r)T_3 + G_{k,3}(r)T_0 \). We use now this solution to calculate the current according to eq.(3.14). Also in the present case only the angular component is finite which we decompose into two parts \( j_\theta(r) = j_1(r) + j_2(r) \). The product of the third term in eq.(3.24) and its derivative leads to
\[
j_1(r) = \frac{e}{mV} \sum_{k,E_k>0} \frac{|G^\theta_{k,0}(r)|^2}{r} (|T_0|^2 + |T_3|^2)
\]
\[
\approx \frac{e}{m} \int_{E_k>0} \frac{dkk}{2\pi} \frac{\pi^2 N_0^2 \Delta_0^2}{4(E_k^2 - \Delta_0^2)} \frac{(J_1(k_+ r) + J_1(k_- r))^2}{r} (|T_0|^2 + |T_3|^2)
\]
where we used that \(k_\pm \approx k_F\) and \(g_2 \ll g_1\) in eq.(3.19). Next we consider the contribution coming from the product of the first and the third term in eq.(3.24), again neglecting the contribution of \(g_2\),
\[
j_2(r) = \frac{e}{m|T_0|} \int \frac{dkk}{2\pi} \frac{g_{1,k}(r)}{E_k} \frac{J_1(kr)}{r} - c.c.
\]
\[
\approx \frac{e}{m|T_0|} \int_{E_k>0} \frac{dkk}{2\pi} \frac{\pi N_0 \Delta_0^2 T_0}{2\sqrt{E_k^2 - \Delta_0^2}} \frac{(J_1(k_+ r) + J_1(k_- r))J_1(kr)}{E_k r} - c.c.
\]
Note that the expression of the current the Fermi distribution function does not appear and the only temperature dependence enters only via \(\Delta_0\). In the unitary limit \((U \to \infty)\) \(T_3\) vanishes and the total circular current which comes from the continue parts reduces to rather simple form
\[
j_\theta(r) = \frac{e}{mr} \int \frac{dkk \Delta_0^2}{2\pi E_k} \left[ \frac{1}{16} \left\{ J_1(k_+ r) + J_1(k_- r) \right\}^2 - \frac{1}{2} (J_1(k_+ r) + J_1(k_- r))J_1(kr) \right]
\]
The main contribution of this integral comes from the states at the gap edge with the wave vector close to \(k_F\). In this form it is easy to analyze the long-distance behavior of \(j_\theta(r)\), i.e. \(r \gg 1/k_F\).
\[
j_\theta(r) \approx -\frac{7e\Delta_0}{8\pi v_F r^2} \left[ 1 + e^{-2\Delta_0/\nu_F} \right] \cos^2(k_F r - 3\pi/4)
\]
where \(v_F\) is Fermi velocity and both components of the current show the same \(r\)-dependence. We observe two distinct contributions showing Friedel-type oscillations, one is exponentially fast decaying and the other follows the power-law \(1/r^2\) (Fig.3). The latter is a particular result of the fact that the current is carried by the quasiparticles belonging to the continuum spectrum. This term does not fit well with the solution of the GL theory where we found an exponential decay behavior including also the flow of counter currents. While the power-law behavior may be appropriate in an intermediate length regime the GL treatment suggests that it should not apply for long distances. Definitely the long-range extension of the circular current should be inhibited by the Meissner effect which yields screening counter currents living on the length scale \(\lambda\), the London penetration depth. This effect is not included in our discussion here, as it was omitted in the analysis of the GL theory. A further more serious omission is, however, the self-consistency of the pair potential \(\Delta\). In the GL theory the reaction of the superconductor to the impurity was the admixture of superconducting
phase with opposite chirality, i.e. locally the state \( \mathbf{d}(\mathbf{k}) = \mathbf{z}(k_x - ik_y) \) is admixed to the bulk state \( \mathbf{d}(\mathbf{k}) = \mathbf{z}(k_x + ik_y) \).

### 3.3 Electron-hole transformation

As mentioned above the repulsive impurity potential problem considered from the electron-hole converted point of view corresponds to a problem with attractive potential. This can be easily seen by applying electron-hole transformation which means that we replace

\[
\begin{align*}
    h_{0,e}(\mathbf{r}) & = -h_{0,h}(\mathbf{r}), \\
    \Delta_{e}(\mathbf{r}, \mathbf{r}') & = -\Delta_{e}^{*}(\mathbf{r}, \mathbf{r}') \\
    (u_{e,i}, v_{e,i}) & = (v_{h,i}, u_{h,i})
\end{align*}
\]

Here the subscripts \( e \) and \( h \) denote the problem in the electron or hole perspective, respectively. It is important to notice that the transformation of the gap is actually an inversion of the Cooper pair angular momentum, \( \mathbf{d}(\mathbf{k}) = \mathbf{z}(k_x + ik_y) \rightarrow \mathbf{z}(k_x - ik_y) \). The solution for the so generated attractive impurity problem gives the same current as the original repulsive case.

\[
\begin{align*}
    j_{h}(\mathbf{r}) & = \frac{e}{2m} \sum_{i,\sigma} [f(\epsilon_{i})u_{hi,\sigma}^{*} \nabla u_{hi,\sigma} + (1 - f(\epsilon_{i}))v_{hi,\sigma} \nabla v_{hi,\sigma}^{*} - c.c] \\
    & = j_{e}(\mathbf{r})
\end{align*}
\]

(3.30)

The main difference between the repulsive and the attractive one is the contribution of the bound state solution to the spontaneous current at the zero temperature. In the hole perspective, using the bound state solutions (3.10) and (3.11), the contribution of the bound state is given as

\[
\begin{align*}
    j_{B}(\mathbf{r}) & = -\hat{e}_{y} \frac{8e\Delta_{0} \pi N_{0}c}{m\sqrt{1+c^{2}}} (1 - f(\epsilon)) \frac{f_{2}(k_{F}r)^{2}}{r}.
\end{align*}
\]

(3.31)

which is non-vanishing. The continuum part compensates for this change, but has basically the same structure as eq.(3.28) with slightly different coefficients. Therefore, the sign of the impurity potential does not change the spontaneous circular current, but only the view point.

### 4. Discussion

We have considered a superconducting state whose Cooper pairs have a finite angular momentum, a chiral state. Clearly the total angular momentum of the system should be zero in the ground state or in thermodynamic equilibrium in the absence of an external magnetic field. Nevertheless, in the vicinity of an impurity the intrinsic angular momentum becomes visible in form of a circular current. In the Bogolyubov-de Gennes formulation we have seen that these circular currents originate mainly from quasiparticle scattering states belonging to the continuous part of the spectrum, while the quasi particle bound state at the impurity plays in this respect a minor role. This calculation has been done without taking self-consistence into account. Thus the order parameter is uniform.
and does not get a feedback from the modified quasi-particle spectrum. As a consequence the quasiparticle states, a hybridization of electron- and hole-like states of different angular momentum yield a finite total angular momentum if we do not include the edge of the system. The edge introduces chiral quasiparticle modes and a spontaneous surface current. In our solution of the B-dG problem the impurity potential leads to a shift of the electron concentration and some amount of charge is transferred to the edge modes which have zero-energy states. This in turn leads to a change of the edge currents and to a compensating change of angular momentum. In our solution this is connected with the circular current which decays like $r^{-2}$. Thus the total angular momentum of a finite system is not changed even in the non-self-consistent solution of the B-dG equations.

On the other hand, the GL formulation leads to a canceling of the angular momentum basically within the short length scale $\xi$. Thus the feedback of the superconducting condensate leads to a strong screening and the impurity and edge problem are decoupled from each other. Thus the above connection has to be considered as artificial. This type of screening was recently also discussed in detail by Kusama and Ohashi in connection with Bloch’s theorem.

While it is difficult to include this screening effect in an analytical way into the B-dG formulation, we can see this property very conveniently in the GL theory where around the impurity the $\eta_-$ component appears in addition to the bulk phase corresponding to $\eta_+$. This admixed order parameter has a phase winding and introduces vorticity yielding a counter flowing current. Since this order parameter decays towards the bulk the vorticity does not constitute a real vortex and no magnetic flux exists. The $\eta_-$ component disappears over a length comparable to the coherence length and with it counter currents which within this length completely compensate the angular momentum introduced by the impurity scattering states. Overall seen there is no net magnetic moment or magnetic flux. Consequently, the circular currents at the impurity are not easy to observe. Magnetometers would need a resolution higher than coherence length. One such probe is provided by spin polarized muons in zero magnetic field and has recently successfully lead to the observation of intrinsic magnetism in the superconducting state of Sr$_2$RuO$_4$.

Recently, Goryo and Ishikawa have proposed an experiment which has some similarity to the impurity problem treated here. Their analysis is based on a topological argument that the chiral p-wave state introduces an effective Chern-Simons term into the Ginzburg-Landau theory, which couples the vector potential with the scalar potential. A charge inserted into the superconductor should generate a circular current similar to a Hall current. There is clear analogies between the two studies in various aspects and it is certain worthwhile to investigate the connections more carefully. In particular, the argument about the vanishing angular momentum should apply for the Hall current of the Chern-Simon term as well in a finite system, since the external magnetic field is absent.

The physics associated with the chiral quasiparticle states around the impurity as well as at
the surface can be discussed in terms of Andreev bound states as they were investigated first by Buchholtz and Zwicknagel for $p$-wave states and in a related form for $d$-wave states by Hu and many others later. In the case of $d$-wave superconductivity, however, the topological argument discussed in Ref. does not apply and the zero-energy states at surfaces and impurities are not chiral. Nevertheless, they have other important implications.

The topological aspect is connected with the presence of an internal angular momentum of the Cooper pair of the type $p_x \pm ip_y, L_z = \pm 1$. Thus, similar physics is expected in other $\mathcal{T}$-violating superconducting states of the same or similar topology (angular momentum). To these belong the two $d$-wave states $d_{x^2-y^2} \pm id_{xy}$ with $L_z = \pm 2$ and $d_{xz} \pm id_{zy}$ with $L_z = \pm 1$. On the other hand, the $\mathcal{T}$-violating state $d_{x^2-y^2} \pm is$ is often discussed in connection with high-temperature superconductors does not belong to this class as it does not have an angular momentum. Consequently, we do not find a simple circular current around impurities in this case, in contrast to all other case mentioned above. The current pattern in this case is more complicated and will be discussed elsewhere.

§5. Acknowledgement

We would like to thank A. Furusaki, R. Heeb and T. Tamaribuchi for helpful discussions. This work was supported by Grant-in-Aid for Scientific Research from Ministry of Education. This work is supported by the Grant-in-Aid for Scientific Research (10740169) and (10640341), and one of the authors (Y.O) has been supported by a C.O.E. fellowship from the Ministry of Education, Science, Sports and Culture of Japan.
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Figure caption

- Fig.1 Circular current around the impurity derived from the GL theory. We take the value $\kappa = 7$, and the length is renormalized by the penetration depth $\lambda$ and the current by $4\pi S\kappa^2$. The expression of (2.8) (solid line) is not valid in short distance and the current should be 0 for $r \to 0$. We omit this in our graph as the length scales are rather different.

- Fig.2 Schematic view of the solutions of the B-dG equation. Circles (diamond) correspond to the continuous (bound) states. The solutions in the first and the third (the second and the forth) quadrants are particle (hole) like states.

- Fig.3 Current around the impurity from eq.(3.27). We renormalize the energy by $\Delta_0$, and the length by the coherence length $\xi = v_F/\Delta_0$, and the current by $e/(2m)$. 

