Local Density of States of Quasi-Particles around a Vortex Core in a Square Superconducting Plate with a Random Impurity Potential

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Abstract. We have solved the Bogoliubov-de Gennes equation with a random impurity potential $V_{\text{imp}}(r)$ under an external magnetic field with the finite element method and obtained the local density of states and the order parameter around a vortex. From these results, we find two properties of a vortex structure in a dirty superconductor. First, the order parameter structure around the vortex is deformed by the impurity potential. Second, distributions of bound states is also deformed, but these deformations of the order parameter and bound states do not correspond with each other.

1. Introduction
Pinning of vortices in a superconductor is important for applications of superconductors. There were several theoretical studies on dirty superconductors. Roland et al. investigated vortices trapped in a superconductor with randomly distributed spherical impurities using the large-scale simulation of the time-dependent Ginzburg-Landau (TDGL) equations [1]. The TDGL simulation is very useful for investigating several vortices in a mesoscopic system. On the other hand, the TDGL simulation cannot describe properties on a scale of a vortex core radius, such as the attractive interaction between vortices [2] and discrete bound states around a vortex core. This is because in the TDGL simulation only a macroscopic wavefunction is considered. In order to investigate microscopic properties, we should solve the Bogoliubov-de Gennes (BdG) equation or the Gor’kov equation. Hang et al. investigated the impurity effect on a vortex core by using the BdG equation on a tight binding model with an impurity potential [3]. However, they only considered a $\delta$-function like impurity potential at a vortex core and did not consider spatially extended impurity potentials such as a nanorod.

In this paper, we show the superconducting order parameter and the local density of states (LDOS) of quasi-particles by solving the BdG equation with a random impurity potential for a square $s$-wave superconducting plate. We think that an amorphous superconductor is an example of our model.

Contents of this paper are as follows. In Section II, we explain the BdG equations with an impurity potential and our numerical method. In Section III, we show numerical results for order parameter and the LDOS in a square dirty superconducting plate. Section IV is devoted to the summary.
2. Method

In order to investigate structures of vortices in a dirty superconducting plate, we solve the BdG equations with an impurity potential \( V_{\text{imp}}(r) \),

\[
\begin{align*}
\left[ \frac{1}{2m} \left( -\nabla + \frac{e}{c} A \right)^2 - \mu + V_{\text{imp}}(r) \right] u_n(r) + \Delta(r) v_n(r) &= E_n u(r), \quad (1a) \\
- \left[ \frac{1}{2m} \left( -\nabla - \frac{e}{c} A \right)^2 - \mu + V_{\text{imp}}(r) \right] v_n(r) + \Delta^*(r) u_n(r) &= E_n v(r). \quad (1b)
\end{align*}
\]

Here, \( u_n(r) \), \( v_n(r) \) and \( E_n \) are the electron and hole components of \( n \)-th quasi-particle wave function and its eigen energy, respectively. \( \Delta(r) \) is the superconducting order parameter and obtained by the self-consistent equation,

\[
\Delta(r) = g \sum_{|E_n| < E_c} u_n(r) v_n^*(r) \left( 1 - 2f(E_n) \right) .
\]

Here, \( E_c \) is the cut-off energy, which is the Debye energy \( h\omega_0 \) in BCS theory. \( g \) is a magnitude of the attractive interaction between electrons and \( f(E_n) \) is the Fermi distribution function,

\[
f(E_n) = \frac{1}{1 + \exp(E_n/k_B T)}.
\]

Solving following Maxwell equation,

\[
\nabla \times (\nabla \times A(r) - H_0) = \frac{4\pi}{c} j(r),
\]

we obtain the magnetic vector potential \( A \). Here \( H_0 \) is a uniform applied magnetic field and \( j(r) \) is a current density, which is given by,

\[
\begin{align*}
 j(r) &= -\frac{e}{m} \sum_n \left[ f(E_n) u_n^*(r) \left( \frac{\hbar}{i} \nabla + \frac{e}{c} A(r) \right) u_n(r) + h.c. \right] \\
&\quad - \frac{e}{m} \sum_n \left[ (1 - f(E_n)) v_n(r) \left( \frac{\hbar}{i} \nabla + \frac{e}{c} A(r) \right) v_n^*(r) + h.c. \right]. \quad (5)
\end{align*}
\]

We take the London gauge as

\[
\nabla \cdot A(r) = 0, \quad A(r) \cdot \mathbf{n} = 0,
\]

where \( \mathbf{n} \) is a normal vector at edges of the superconducting plate. We impose the boundary condition of wave functions at the edges as

\[
\begin{align*}
u_n(r) &= 0, \\
v_n(r) &= 0.
\end{align*}
\]

We solve these equations self-consistently with a particle number conservation condition, by which we determine the chemical potential \( \mu \). The particle number conservation condition is given by

\[
N_e = \int d\mathbf{r} \sum_n \{ f(E_n)|u_n(r)|^2 + (1 - f(E_n))|v_n(r)|^2 \},
\]

where \( N_e \) is a total electron number.

In order to solve these equations, we use the two-dimensional finite element method (2D FEM). We divide a system into small triangular elements, where the vertex of the \( e \)-th elements are \((x_i^e, y_i^e)\) \((i = 1, 2, 3)\). Then, we define \( i \)-th area coordinate \( \zeta_i^e \) in the \( e \)-th element as

\[
\zeta_i^e = \frac{1}{2S_e} (a_i + b_i x + c_i y) \quad (i = 1, 2, 3),
\]

where \( S_e \) is an area of the \( e \)-th element and \( a_i, b_i \) and \( c_i \) are defined in Appendix. We expand \( u_n(r), v_n(r), \Delta(r), A(r) \) and \( V_{\text{imp}}(r) \) using area coordinates,

\[
\begin{align*}
 u_n(r) &= \sum_e \sum_i \zeta_i^e u_{n,i}^e, \\
v_n(r) &= \sum_e \sum_i \zeta_i^e v_{n,i}^e,
\end{align*}
\]

(12a)

and (12b)
\[ \Delta(r) = \sum_s \sum e \zeta^e \Delta^e, \quad (12c) \]
\[ A(r) = \sum_s \sum e \zeta^e A^e, \quad (12d) \]
\[ V_{\text{imp}}(r) = \sum_s \sum e \zeta^e V^e_{\text{imp},i}. \quad (12e) \]

The BdG equations (1a) and (1b) becomes as,
\[
\sum_j \left[ \frac{\hbar^2}{2m} \sum_{\alpha} K_{ij}^{\alpha \alpha} + \frac{e\hbar}{2mc} \sum_{i_1 \alpha} (j_{i_1,ij}^\alpha - j_{f_1,ij}^\alpha) A_{i_1,\alpha}^e + \frac{e^2}{2mc} \sum_{i_1 i_2 \alpha} l_{i_1 i_2 j}^e A_{i_1,\alpha}^e A_{i_2,\alpha}^e + \sum_{i_1} V_{\text{imp},i} l_{i_1 j}^e - \mu l_{ij}^e \right] u_{n,j}^e + \sum_{i_1} \Delta_{i_1}^e l_{i_1 j}^e v_{n,j}^e = E \sum_{j} l_{ij}^e u_{n,j}^e, \quad (13a) \]
\[
\sum_j \left[ -\frac{\hbar^2}{2m} \sum_{\alpha} K_{ij}^{\alpha \alpha} + \frac{e\hbar}{2mc} \sum_{i_1 \alpha} (j_{i_1,ij}^\alpha - j_{f_1,ij}^\alpha) A_{i_1,\alpha}^e - \frac{e^2}{2mc} \sum_{i_1 i_2 \alpha} l_{i_1 i_2 j}^e A_{i_1,\alpha}^e A_{i_2,\alpha}^e - \sum_{i_1} V_{\text{imp},i} l_{i_1 j}^e + \mu l_{ij}^e \right] v_{n,j}^e + \sum_{i_1} \Delta_{i_1}^e l_{i_1 j}^e u_{n,j}^e = E \sum_{j} l_{ij}^e v_{n,j}^e. \quad (13b) \]

Equation (4) becomes,
\[
\sum_{j} \left[ K_{ij}^{x x} + K_{ij}^{y y} + \frac{4\pi e^2}{mc^2} \sum_{i_1 i_2} l_{i_1 i_2 j}^e \sum_n \{ f(E_n) u_{n,i_1}^e u_{n,i_2}^e + (1 - f(E_n)) v_{n,i_1}^e v_{n,i_2}^e \} \right] A_{jx}^e
+ \sum_{j} \left[ K_{ij}^{y x} - K_{ij}^{x y} \right] A_{jy}^e
= -\hbar \omega_{ij}^e \sum_{i_1 i_2} \sum_n \{ f(E_n) u_{n,i_1}^e u_{n,i_2}^e + (1 - f(E_n)) v_{n,i_1}^e v_{n,i_2}^e \} (j_{i_1,i_2}^x - j_{i_1,i_2}^x), \quad (14a) \]
\[
\sum_{j} \left[ K_{ij}^{x x} + K_{ij}^{y y} + \frac{4\pi e^2}{mc^2} \sum_{i_1 i_2} l_{i_1 i_2 j}^e \sum_n \{ f(E_n) u_{n,i_1}^e u_{n,i_2}^e + (1 - f(E_n)) v_{n,i_1}^e v_{n,i_2}^e \} \right] A_{jy}^e
+ \sum_{j} \left[ K_{ij}^{y x} - K_{ij}^{x y} \right] A_{jx}^e
= \hbar \omega_{ij}^e \sum_{i_1 i_2} \sum_n \{ f(E_n) u_{n,i_1}^e u_{n,i_2}^e + (1 - f(E_n)) v_{n,i_1}^e v_{n,i_2}^e \} (j_{i_1,i_2}^y - j_{i_1,i_2}^y). \quad (14b) \]

And the self-consistent equation becomes as,
\[
\sum_{i_1 i_2} l_{ij}^e \Delta_{ij}^e = g \sum_{i_1 i_2} u_{n,i_1}^e v_{n,i_2}^e (1 - 2f(E_n)). \quad (15) \]

A particle number conservation condition becomes as,
\[
N_e = \sum_{i,j} l_{ij}^e \sum_n \{ f(E_n) u_{n,i}^e u_{n,j}^e + (1 - f(E_n)) v_{n,i}^e v_{n,j}^e \}. \quad (16) \]

Coefficients, \( l_{ij}^e, l_{ijk}^e, l_{ijkr}^e, j_{ijr}^e, j_{ijr}^e, j_{ijr}^e, K_{ij}^{x x}, K_{ij}^{y y}, K_{ij}^{y x}, K_{ij}^{x y} \) and \( K_{ij}^{x y} \) are defined in Appendix.

We solve equations (14a)-(17) self-consistently. We consider a square superconducting plate with size \( L \times L \), which is shown in figure 1. We set parameters as follows; the energy gap \( \Delta_0 = 0.2 E_C \), the coherence length \( \xi_0 = L / 3 \), the Fermi wave vector \( k_F = 3.0 / \xi_0 \) and the Ginzburg-Landau parameter \( \kappa = 2.0 \) for a bulk superconductor at zero temperature.

In our simulation, first, we determine the total particle number \( N_e \) in a square superconducting plate for given \( k_F \). Next, we determine the BCS coupling constant \( g \) and the critical temperature \( T_C \) of a bulk
system for a given $\Delta_0$. Then, we solve the BdG equation self-consistently for given applied field and temperature with these parameters $N_e$, $g$, and $T_C$. When we get the self-consistent solution, $\{ u_n(r), v_n(r), E_n \}$, we can obtain the LDOS $N(r, E)$ as,

$$ N(r, E) = -\sum_n \{|u_n(r)|^2 f'(E_n - E) + |v_n(r)|^2 f'(E_n + E)|. $$

This expression is expanded by the area coordinate as,

$$ N(r, E) = -\sum_{ij} \sum_n \{u_n^e u_n^e \}, $$

where $f'(E) = \frac{\partial f}{\partial E}$.

3. Results and Discussion

In this section, we show the order parameter and the LDOS in a two-dimensional square dirty superconducting plate. We set the temperature $T = 0.1 / T_C$ and the magnetic field $H = 4.0 \Phi_0 / L^2$. First, we consider a clean system with $V_{imp}(r) = 0$. Figure 2 shows the distribution of amplitude of order parameter and figure 3 shows the phase $\theta$ of the order parameter $|\Delta|e^{i\theta}$. From these figures, we see there is a single quantized vortex at the center. This vortex has four-fold symmetry because of the square symmetry of the superconducting plate.

Figure 1. Our finite element model of a square superconducting plate.

Figure 2. Distribution of the order parameter with no impurity potential for $k_F \xi_0 = 3.0$.

Figure 3. Phase of the order parameter with no impurity potential for $k_F \xi_0 = 3.0$.

Second, we take a random impurity potential $V_{imp}(r)$ with $-0.5 < V_{imp}(r) / E_C < 0.5$, which is shown in figure 4. Figure 5(a) shows amplitude of order parameter and figure 5(b) shows phase of the order parameter. From these figures, we can see there is a single vortex which is trapped in a higher impurity potential region that is closed by a green line in figure 4(b). Comparing with non-impurity case, the vortex is deformed from the four-fold symmetric structure. Moreover, in the lower impurity potential area that is closed by a red line in figure 4(b), amplitude of the order parameter is higher in the red circle area in figure 5(a). On the other hand, in the higher impurity potential area which is closed by a blue line in figure 4(b), amplitude of the order parameter is lower in the blue circle area in figure 5(a).
Figure 4. Three dimensional plot (a) and contour plot (b) of distribution of a random impurity potential.

Figure 5. (a) Distributions of amplitude (a) and phase (b) of the order parameter with the random impurity potential.

Next, we discuss LDOS around the vortex in superconductors with and without the impurity potential. In figure 6, we show the LDOS \( N(r, E) \) around the vortex without impurity potentials for \( E/E_C = 0.35(a), 0.3(b), 0.25(c), 0.23(d), 0.2(e), 0.15(f), 0.1(g), 0.0(h), -0.1(i), -0.15(j), -0.2(k), -0.23(l), -0.25(m), -0.3(n) \) and \(-0.35(o)\). We can see a bound state around \( E/E_C \sim 0.2 \) for the electron part \( (E > 0) \) and a bound state around \( E/E_C \sim -0.2 \) for the hole part \( (E < 0) \). They have four-fold symmetry, which comes from the square boundary of the superconductor. Other states are scattering or extended states. They have four-fold symmetry too. In figure 7, we show the LDOS \( N(r, E) \) around the vortex with the impurity potential for same energies as those in figure 6. Also, we can see a bound state for electron part around \( E/E_C \sim 0.23 \) and a bound state for hole part around \( E/E_C \sim -0.23 \). These bound states are deformed from those for the pure superconductor. They are elongated from right-lower corner to left-upper corner. The direction of the deformation is different from that for the vortex core structure in the order parameter distribution. In figure 8, we compare deformations of the order parameter and the bound states. The vortex core structure is elongated along the red dotted line, but the bound state around \( E/E_C \sim 0.23 \) is elongated along the green dotted line. The red (green) line connects higher (lower) potential region around the vortex, respectively. Therefore, we can say, the vortex core is extended toward higher potential regions and the bound state is extended toward lower potential regions. These features are explained as follows. In higher potential region, the electron number becomes low and superconductivity becomes weak. Then the vortex is attracted to such regions. The bound state is an eigen state of a quasi-particle and therefore it is attracted to lower potential regions.

We think these features are general. Therefore, the STS experiment on the bound states around the vortex cannot always observe the real vortex core structure.
Figure 6. Distribution of LDOS around the vortex without the impurity potential.
Figure 7. Distribution of LDOS around the vortex with the impurity potential.

Figure 8. Distribution of order parameter (a) and the bound state at $E/E_c = 0.23$ (b). Red (green) dotted lines show directions of extension of the order parameter (the bound state), respectively.
4. Summary

We have investigated the vortex structure and bound states around the vortex in the dirty superconducting square plate, solving the BdG equations with the finite element method.

We have found the vortex core structure is deformed and extended to higher potential regions. However, the bound state is extended to lower potential regions. These results mean that forms of the vortex core and the bound state do not always match. In the future, we will clarify this point using a simple impurity potential.

In this study, we set $k_F \xi_0 = E_F/\Delta_0 = 3.0$. So, we have only two bound states. Deformation of the bound state may depend on relation between its eigen-energy and the height of the impurity potential. Therefore, our conclusion may depend on the value of $k_F \xi_0$. In the future, we will also investigate $k_F \xi_0$ dependence of the bound state structure.

Appendix

The vertex of an elements are $(x_i, y_i)$ ($i = 1, 2, 3$). $a_i$ in equation (11) is defined as

$$a_i = x_j y_k - y_j x_k, \quad (A \cdot 1)$$

and $b_i$ is defined as

$$b_i = y_j - y_k, \quad (A \cdot 2)$$

and $c_i$ is defined as

$$c_i = x_k - x_j, \quad (A \cdot 3)$$

where $i, j$ and $k$ are 1, 2 and 3, following a cyclic order.

Coefficients, $I_{ij}^e$, $I_{ijk}^e$, $I_{i jk}^e$, $J_{ij}^\alpha$, $K_{ij}^{\alpha \alpha}$ and $K_{ij}^{\alpha \beta}$ are integrals of product of area coordinates and defined as

$$I_{ij}^e = \int_{A_e} \xi_i^e \xi_j^e \, d\Omega, \quad (A \cdot 4)$$

$$I_{ijk}^e = \int_{A_e} \xi_i^e \xi_j^e \xi_k^e \, d\Omega, \quad (A \cdot 5)$$

$$I_{ijk}^e = \int_{A_e} \xi_i^e \xi_j^e \xi_k^e \xi_l^e \, d\Omega, \quad (A \cdot 6)$$

$$J_{ij}^\alpha = \int_{A_e} \frac{\partial \xi_i^e}{\partial \alpha} \xi_j^e \, d\Omega, \quad (A \cdot 7)$$

$$J_{ij}^\alpha = \int_{A_e} \frac{\partial \xi_j^e}{\partial \alpha} \xi_i^e \, d\Omega, \quad (A \cdot 8)$$

$$K_{ij}^{\alpha \alpha} = \int_{A_e} \frac{\partial \xi_i^e}{\partial \alpha} \frac{\partial \xi_j^e}{\partial \alpha} \, d\Omega, \quad (A \cdot 9)$$

$$K_{ij}^{\alpha \beta} = \int_{A_e} \frac{\partial \xi_i^e}{\partial \alpha} \frac{\partial \xi_j^e}{\partial \beta} \, d\Omega, \quad (A \cdot 10)$$

Here, $\int_{A_e} \ldots \, d\Omega$ means an area integration over $e$-th element and $\alpha, \beta = x$ or $y$.

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