Impurity effects in a vortex core in a chiral $p$-wave superconductor within the $t$-matrix approximation

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Abstract We study the effects of non-magnetic impurity scattering on the Andreev bound states (ABS) in an isolated vortex in a two-dimensional chiral $p$-wave superconductor numerically. We incorporate the impurity scattering effects into the quasiclassical Eilenberger formulation through the self-consistent $t$-matrix approximation. Within this scheme, we calculate the local density of states (LDOS) around two types of vortices: “parallel” (“anti-parallel”) vortex where the phase winding of the pair-potential coming from vorticity and that coming from chirality have the same (opposite) sign.

When the scattering phase-shift $\delta_0$ of each impurity is small, we find that impurities affect differently low energy quasiparticle spectrum around the two types of vortex in a way similar to that in the Born limit ($\delta_0 \to 0$). For a larger $\delta_0 (\leq \pi/2)$ however we find that ABS in the vortex is strongly suppressed by impurities for both types of vortex. We found that there are some correlations between the suppression of ABS near vortex cores and the low energy density of states due to impurity bands in the bulk.

1 Introduction

Quantized magnetic fluxes in type II superconductors are one of the most important phenomena in the superconductivity. They dominate various properties of superconductors under high field, and therefore to know their behavior has a significant meaning for industrial use of superconducting materials.
Recently, importance of topological phase of condensed matter is recognized and such materials are attracted very much by their novel features for both theoretical and applicational interests. In superconductors, the topological phase exhibits exact zero energy states localized on the surface or within vortices. Because this states are topologically protected, they can be tolerant against perturbations.

It is well known that within a vortex in clean superconductors, there are discrete low energy bound states known as Caroli-de Gennes-Matricon (CdGM) mode. The order of energy gap between CdGM states are represented by bulk’s order parameter amplitude $\Delta_b$ and Fermi energy $E_F$, and in topologically non-trivial superconductors, the energy lowest states of the CdGM mode is about $(1/2)\Delta_b^2/E_F$ contrary to the topological superconductors of which lowest energy level is exactly zero. In ordinary superconductors the energy spectrum of CdGM mode are almost continuous, for usually $E_F$ is much larger than $\Delta_b$. CdGM mode is also considered as a kind of Andreev bound states and the continuous energy spectrum is given well by this picture. Because $E_F \gg \Delta_b$, there are many nearly zero energy states in the vortex and these states are not protected by the topology even in topological superconductors. So it is not clear how tolerant toward the perturbations the zero energy states is, even if being protected itself.

Two-dimensional chiral $p$-wave superconductivity, which is believed to be realized in Sr$_2$RuO$_4$ and thin film superfluid $^3$He-A phase, is one of topological superconductivities and can have an exact zero energy state in its vortex. This order breaks the time reversal symmetry spontaneously and has two degenerate ground states, each of which corresponds to the internal angular momentum of its Cooper pair. It is considered that there are two types of isolated single vortex in this superconductor perpendicular to the plane. One is that whose winding of vorticity is the same as the winding of chirality of the Cooper pair (“parallel vortex”), and the other is opposite (“anti-parallel vortex”). The total angular momentum of the system $l_z$ is $\pm 2$ about the first one and 0 about the second one.

Within an isolated vortex in this system, it is theoretically predicted that in the anti-parallel vortices the effect of non-magnetic spatially-averaged impurities are dramatically suppressed compared to the parallel vortices. This effect was also reported in a similar system and some authors are trying to treat this robustness more generally as “odd-frequency pairing”. However, these studies have been done only in the Born limit, which corresponds to the situation where a lot of very weak scatterers exist randomly, and the scattering phase-shift of a single impurity potential $\delta_0$ is 0 in $t$-matrix formulation. Recently it is reported that the core-shrinkage effect of vortex in the two-dimensional $s$-wave or chiral $p$-wave superconductors are different between Born and unitary limit ($\delta_0 \rightarrow \pi/2$), and there may be another difference between them besides this effect. Because the phase-shift depends on the superconducting material and species of impurities in general (for example, see Ref.22), it is therefore not sufficient for adapting these theories to the real materials. In addition, because some authors have been reported a different result, we consider that the impurity effect on this system is still unclear.

To clarify impurity effects on the ABS in the vortex, in this paper we study both Born and unitary limit and the intermediate regime between them in a fully self-consistent way. We use Eilenberger’s quasiclassical theory with $t$-matrix formulation. The quasiclassical formulation is a kind of coarse-grained model of
Gor’kov theory (or Bogoliubov-de Gennes theory in the pure case) over the scale of the order of Fermi wavelength. This is because the quasiclassical theory is well suited to study real systems such as $^3$He and Sr$_2$RuO$_4$. We think that it is important to search for the novel phenomena that survive even in the quasiclassical regime, in order to find new phenomena related to topological superconductors accessible in experiments.

2 Model and Method

We consider two-dimensional chiral $p$-wave superconductors with isotropic circular Fermi surface in the type II limit, i.e. the ratio of the magnetic penetration depth to the coherence length is taken to be infinity. In the quasiclassical theory of superconductivity, the electronic structure of quasiparticles is described in terms of the quasiclassical Green function

$$\tilde{g}(i\omega, \vec{r}, \vec{k}) = \left( \begin{array}{cc} f & -f^\dagger \\ -f & -g \end{array} \right),$$

which is defined by Gor’kov Green function integrated over the magnitude of quasiparticle energy. Throughout this paper, we use the following dimensionless parameters:

$$\tilde{r} = r(\pi \xi_0)^{-1}, \quad \tilde{k} = k/k_F, \quad \tilde{T} = T/T_{c0},$$

$$\tilde{\Delta}(\tilde{r}, \tilde{k}) = \Delta(r, k)/\Delta_0, \quad \tilde{\omega} = \hbar \omega/\Delta_0, \quad \tilde{\epsilon} = \epsilon/\Delta_0,$$

where $\xi_0 = 2E_F(\pi k_F\Delta_0)^{-1}$ is the coherence length at zero temperature without impurities, $k_F$ is the Fermi wave number, $T_{c0}$ is the critical temperature without impurities and $\Delta_0$ is the amplitude of zero temperature order parameter in the bulk without impurities. The quasiclassical Green function (1) satisfies the Eilenberger equation

$$-i\vec{k} \cdot \nabla \tilde{g} = \left[ i\tilde{\omega} \tilde{\tau}_3 - \tilde{\Sigma} - \tilde{\Delta}, \tilde{g} \right],$$

and the normalized condition $\tilde{g}^2 = -\pi^2 \mathbf{1}$. Here $\tilde{\tau}_i$ $(i = 1, 2, 3)$ denote the Pauli matrices in the particle-hole space. The symbols $\tilde{\Sigma}$ and $\tilde{\Delta}$ denote, respectively, the impurity self-energy and the pair-potential.

Within the $t$-matrix approximation, the character of impurities is parametrized by the scattering rate in the normal state $\Gamma_n = \hbar(2\tau_n \Delta_0)^{-1}$ and the phase-shift of a single impurity $\delta_0$. The impurity self-energy

$$\tilde{\Sigma}(\tilde{r}) = \left( \begin{array}{cc} \Sigma_0(\tilde{r}) & \Sigma_{12}(\tilde{r}) \\ \Sigma_{21}(\tilde{r}) & -\Sigma_0(\tilde{r}) \end{array} \right)$$

is expressed in terms of $\tilde{g}$, $\Gamma_n$ and $\delta_0$ as

$$\tilde{\Sigma} = \pi^{-1}\Gamma_n \langle \tilde{g} \rangle / \cos^2 \delta_0 - \pi^{-2} \sin^2 \delta_0 (\langle \tilde{g} \rangle^2 - \langle f \rangle \langle f^\dagger \rangle).$$
The notation $\langle A \rangle$ denotes averaging $A$ over a Fermi surface, and in this case, it can be expressed as $\langle A \rangle = \int_0^{2\pi} d\alpha A(\alpha)/2\pi$ where $\vec{k} = (\cos \alpha, \sin \alpha)$.

The pair-potential has the matrix form of

$$\tilde{\Delta}(\vec{r}, \vec{k}) = \begin{pmatrix} 0 & \tilde{\Delta}(\vec{r}, \vec{k}) \\ -\tilde{\Delta}^*(\vec{r}, \vec{k}) & 0 \end{pmatrix},$$

where $\tilde{\Delta}(\vec{r}, \vec{k})$ satisfies the gap equation

$$\tilde{\Delta}(\vec{r}, \vec{k}) = \lambda \tilde{T}^\nu \frac{\hat{\omega}_k}{\pi} \sum_n \left\langle f(\vec{r}, \alpha') e^{\pm i(\alpha - \alpha')} \right\rangle_{\alpha'}.$$  

Here $\hat{\omega}_k = (2n + 1)e^{\pi \hat{T}}/\hbar$ is the Matsubara frequency, $\lambda$ is the (dimensionless) coupling constant that satisfies $\frac{1}{\lambda} = \ln \tilde{T} + \sum_{n=1}^{\infty} \frac{1}{n+1/2}$ and $\gamma \approx 0.5772$ is the Euler constant, which comes from the equation $k_B T_e = e^\gamma \Lambda_0/\pi$. The symbol $\hat{\omega}_k$ is a cut-off frequency.

In the absence of external magnetic fields, the chiral $p$-wave superconductors have two-fold degenerate thermodynamic states with the pair-potential $\Delta(\vec{k}) \propto \exp(\pm i\alpha)$; Each state has the Cooper pairs with internal angular momentum $\pm h$. In the chiral $p$-wave states with a single vortex with positive vorticity at $\vec{r} = 0$, the pair-potential $\Delta(\vec{r}, \vec{k})$ has the asymptotic form $e^{i(\phi + \alpha)}$ far away from vortex center. In the intermediate regime with finite $\vec{r}$ around the single vortex, both Cooper pairs with $\pm h$ coexist. Taking account of two-dimensional rotational symmetry around $\vec{r} = 0$, we can write the pair-potentials generally in the forms

$$\tilde{\Delta}^{(p)}(\vec{r}, \vec{k}) = \tilde{\Delta}^{(p)}_c(\vec{r}) e^{i(\phi + \alpha)} + \tilde{\Delta}^{(p)}_a(\vec{r}) e^{i(3\phi - \alpha)}$$

for a parallel vortex (where the angular momentum is $l_z = 2$) and

$$\tilde{\Delta}^{(a)}(\vec{r}, \vec{k}) = \tilde{\Delta}^{(a)}_c(\vec{r}) e^{i(\phi - \alpha)} + \tilde{\Delta}^{(a)}_a(\vec{r}) e^{i(-\phi + \alpha)}$$

for anti-parallel vortex (where the angular momentum is $l_z = 0$). The subscripts $+$ and $-$ describe dominant and induced components of pair-potential; The latter vanishes far away from the vortex center.

We numerically calculate the quasiclassical Green’s functions $\tilde{g}$ around the isolated vortex in a self-consistent way through a successive iteration of the Eilenberger equation, the Dyson equation and the gap equation.

We solve eq. (2) with use of Ricatti-transformation. Equation (2) is solved on the line (so called “quasiclassical trajectory”) with a constant $h = \vec{r} \cdot (\vec{z} \times \vec{k})$. Note that $h$ can be regarded as the impact parameter, which is the quasiparticle angular momentum divided by the Fermi momentum.

We adopt the classical fourth-order Runge-Kutta method to solve (2). We denote by $x = \vec{r} \cdot \vec{k}$ the spatial coordinate along the trajectory. For the initial value at cut-off $x = \pm x_c$, we use bulk solution. We set $x_c = 100$ when calculate pair-potential in the gap equation. We set the cut-off frequency $\hat{\omega}_k = 10$ as the same value in the earlier studies. 

3 Results and Discussion

Figures 1 and 2 show LDOS of the vortex core at $\tilde{T} = 0.1$, $\Gamma_n = 0.3$ in the Born limit ($\delta_0 \to 0$) and unitary limit ($\delta_0 \to \pi/2$) respectively. In the Born limit, there is a sharp peak at zero energy at the center of anti-parallel vortex ($l_z = 0$) but the peak is suppressed for the parallel vortex ($l_z = 2$). This result implies that low energy bound states (vortex ABS) in the anti-parallel vortex ($l_z = 0$) is more robust against impurities than those in the parallel vortex ($l_z = 2$). This behavior is consistent with earlier results.\cite{13,14,15,16}

On the other hand, in the unitary limit the zero energy peak is severely suppressed even in the anti-parallel vortex ($l_z = 0$) as well as the parallel vortex ($l_z = 2$).

We quantify the effects of impurities on vortex ABS by the peak value of LDOS at the vortex center $N(\tilde{r} = 0, \tilde{\epsilon} = 0)/N_0$, which is shown in fig. 3. The peak is suppressed more severely when $\delta_0$ approaches from the Born limit to the unitary limit.

For fig. 3(d), the peak of anti-parallel vortices ($l_z = 0$) is however suppressed even in the Born limit. We will discuss this behavior later.

In the following, we discuss the results shown in figs. 1-3, considering the impurity effects on quasiparticle density of states in the bulk chiral $p$-wave superconductors.
Both temperature and the non-magnetic impurities cause pair-breaking effect in chiral $p$-wave superconductors. As a result, the modulus of the pair-potential in the bulk $\Delta_b$ is suppressed regardless of the type of impurities when $T$ is high and $\Gamma_n$ is large. The reduction of $\Delta_b$ makes vortex ABS more extended spatially and lower the peak of LDOS near vortex core, regardless of the value of $\delta_0$.

Even when $\Delta_b$ is not so small (i.e., $T$ is sufficiently low and $\Gamma_n$ is sufficiently small), there exist quasiparticles with energy smaller than $\Delta_b$, which stem from impurity bands. Following the standard calculation of impurity effects in the spatially uniform unconventional weak-coupling superconductors\cite{28}, we can obtain the band edge of the impurity band. When the $\delta_0$ is increasing toward $\pi/2$, the energy of the band edge decreases as shown in fig. 4, and it becomes zero (i.e., the impurity band has a finite density of states at the Fermi level) when $\delta_0$ exceeds a critical value $\delta_c$. The value of $\delta_c$ is given as a solution of the equation

$$\delta_c = \arccos \frac{\Gamma_n}{|\Delta_b(\Gamma_n, \delta_c)|}$$

under the assumption that $\Delta_b$ is monotonically decreasing of $\delta_0$.

At the energy where the impurity band has the finite density of states, there is a resonance between the localized wave functions near vortex cores and wave functions spatially extended outside vortex and thus we can naturally understand the reason why the spectra of vortex ABS are heavily broadened.
Fig. 4 (color online) The edge of the impurity band in the bulk.

The suppression at the Born limit in fig. 3(d) is also understood in this point of view. For this parameter, the edge value of impurity band is finite but very small as in fig. 4. The narrow gap is insufficient to inhibit resonance between inner and outer states, and the peak is broadened even at the Born limit.

When $\Delta_0$ is not so small and $\delta_0$ is smaller than but not too close to $\delta_c$, quasi-particles with energy lower than the band edge of impurity band predominate the vortex ABS. Considering the impurity scattering between vortex ABS only, we see that the impurity effects on the vortex ABS strongly depend on the type of vortex.

We indicate $\delta_c$ by the arrows in fig. 3(a)-(d). We can see in fig. 3(a)-(c) that $\delta_c$ moderately well matches the crossover phase-shift from the regime (with smaller $\delta_0$) where the impurity effects depend strongly on the type of vortices to the regime (with larger $\delta_0$) where the vortex ABS on both types of vortices are heavily suppressed. This result is consistent with our argument in the above.

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