Odd-frequency Cooper pair amplitude around a vortex core in a chiral $p$-wave superconductor in the quantum limit

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Solving the Bogoliubov-de Gennes equation, we study the spatial structure of odd-frequency s-wave Cooper pair amplitudes at each quantized energy level of vortex bound states in chiral $p$-wave superconductors. For zero energy Majorana states, the odd-frequency s-wave pair amplitude has the same spatial structure as that of the local density of states even in atomic length scale. This relation also holds in finite energy bound states for single vortex winding anti-parallel to the chirality, but not for parallel vortex winding. The double winding vortex case is also studied.

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I. INTRODUCTION

Studies of spatial-variation in unconventional superconductors give valuable information to know characters of unconventional superconductivity. Among these studies, such as for ferromagnet/superconductor junctions, normal metal/superconductor interfaces, and vortex states, it has been shown that their low energy quasiparticle states are tightly related to the induced odd-frequency Cooper pair amplitude. Nowadays, it is accepted that the Andreev bound states and anomalous proximity effects are interpreted as the emergence of the odd-frequency Cooper pairs.

Since quasiparticles in superconducting states have to satisfy the anti-commutation relation, the pair potential must change its sign after a permutation of two quasiparticles is done. The minus sign comes from the combination of orbital components (odd or even parities), spin component (singlet or triplet) and Matsubara frequency (even or odd frequency). Conventional even-parity spin-singlet pairing and odd-parity spin-triplet pairing are classified to the even-frequency pairing. On the other hand, within the odd-frequency pairing, even-parity spin-triplet pairing and odd-parity spin-singlet pairing are also possible. Here, we study odd-frequency pair amplitudes induced around a vortex in even-frequency pairing superconductors. When spin-flip mechanism is absent for quasiparticles, an odd-frequency spin-singlet odd-parity (OSO) pair amplitude appears around vortex of even-frequency spin-singlet even-parity (ESE) superconductors, or an odd-frequency spin-triplet even-parity (OTE) pair amplitude appears around vortex of even-frequency spin-triplet odd-parity (ETO) superconductors. We discuss the latter case in this work.

Most of previous studies for odd-frequency pairing were based on quasiclassical Eilenberger theory which is valid in the limit $2(k_F\xi)^{-1} = \Delta/E_F \ll 1$ for superconducting gap $\Delta$ and Fermi energy $E_F$. $k_F$ is Fermi wave number and $\xi$ is superconducting coherence length. When the limit $\Delta/E_F \ll 1$ is not satisfied in the strong-coupling superconductors or we focus fine energy structures, low-energy bound states around a vortex core are quantized to Caroli-de Gennes-Matricon (CdGM) states with energy splitting of the order $\Delta^2/E_F$. The quantum nature associated with CdGM states has been directly observed through the STM-STS in an anisotropic superconductor and the quantum depletion of the particle density in Fermi gases. To study the quantum limit case within $\Delta \sim E_F$, we have to consider the eigen-states by solving the Bogoliubov-de Gennes (BdG) equation, without using the quasiclassical approximation.

Recently vortex bound states in chiral $p$-wave superconductors attract much attention, because Majorana state appears at exactly zero energy in the bound states. In a Majorana zero mode of the half quantum vortex, particle and hole states are equivalent each other, giving rise to the non-Abelian statistics of its host vortices. Note that in the case of an integer vortex state with Majorana zero modes, the statistics is non-trivial. On the other hand, the quasiclassical study in superfluid $^3$He and superconductors showed the relation between odd-frequency pair amplitudes and the local density of states (LDOS) in Majorana bound states. Most recently, the issue on the relation between Majorana zero modes and odd frequency pairing has been addressed in a quantum nanowire. The structures of bound states are distinguished by the direction of vortex winding, i.e., parallel or anti-parallel to the chirality of chiral $p$-wave superconductivity. Within the quasiclassical theory, it has been revealed that the zero energy DOS in the parallel (anti-parallel) vortex is fragile (robust) against nonmagnetic impurities, which is understandable with the odd-frequency pairing localized at the vortex. Hence, since the zero energy state has many facets, it is important to study how the odd-frequency pair amplitude is related to the bound states, including Majorana state, in chiral $p$-wave superconductors.

The purpose of this paper is to clarify the relation between the CdGM states and the odd-frequency pairing. To capture the quantum limiting behaviors inside the core, we here utilize the BdG equation which is capable of describing the rapid oscillations of wave func-
tions in atomic length scale of $k_F^{-1}$ and exactly deals with the Majorana mode. The studies in the quantum regime have not been done with the quasiclassical theory\cite{10,11,34} because of the lack of the $k_F^{-1}$-scale physics. We also note that in previous works, such as Refs.\cite{1} 23, 24, 31 odd-frequency pairings have been discussed in connection with surface bound states. However, the vortex bound state which we consider here may exhibit distinct behaviors from surface one in the sense that each level of the CdGM states is well isolated in the scale of $\Delta^2/E_F$. In addition, the quasiparticle structure inside the core is determined by not only the bulk topology but also the vortex winding number $\pm 2$. Hence, we here unveil how the vortex winding number affects the odd-frequency pairing around the core.

**II. FORMULATION OF BOGOLIUBOV-DE GENNES EQUATION**

We consider a cylindrical system of isotropic chiral $p_+$ wave superconductor with radius $R = 200k_F^{-1}$ and two-dimensional isotropic Fermi surface\cite{23,24,31}. Therefore, the cylindrically symmetric order parameter with vortex winding $w \in \mathbb{Z}$ is given by

$$\Delta(r, k) = \Delta_+(r) e^{i\phi} + \Delta_-(r) e^{i(w+1)\phi},$$

(1)

at the position $r = r(\cos \theta, \sin \theta)$, where the pairing function is given by $Y_{\pm}(k) = (\xi_{kz} \pm ik_y)/\sqrt{2k_F}$ for relative momentum $k = (k_x, k_y)$. In the $p_+$-wave superconductor, the Cooper pair has internal angular momentum $L_z = 1$ along $z$-axis. In the right-hand side of Eq. (1), the first term is the dominant $p_+$-component with a vortex, and the second term of $p_-$ wave indicates the small induced component of opposite chirality around the vortex.

The eigen-energy $E_q$ and wave functions $u_q(r), v_q(r)$ of quasiparticles are calculated by the BdG equation\cite{23,24,31}

$$\begin{pmatrix} H_0(r) & \Pi(r) \\ -\Pi^*(r) & -H_0(r) \end{pmatrix} \begin{pmatrix} u_q(r) \\ v_q(r) \end{pmatrix} = E_q \begin{pmatrix} u_q(r) \\ v_q(r) \end{pmatrix},$$

(2)

where $H_0(r) = (\partial_z^2 + \partial_y^2)/2M - E_F$ with mass $M$, and $\Pi(r) = -\frac{i}{2} \sum_m \{ F^{(m)}, \Delta_m(r) \}$ with $m = \pm$ and $F^{(\pm)} = \mp i e^{\pm i\phi}(\partial_z \pm i r^{-1} \partial_y)/\sqrt{2k_F}$ in chiral $p$-wave superconductors. $k_F = (2M E_F)^{1/2}$. Throughout this letter, we use units $\hbar = k_B = 1$. For the cylindrical symmetric system, wave functions are given by

$$u_q(r) = \tilde{u}_q(r) e^{i\eta r}, \quad v_q(r) = \tilde{v}_q(r) e^{i(qy-w-1)r).}$$

(3)

The eigen-states are labeled by $q = (q_0, \nu)$, where $\nu$ assigns eigen-states of the BdG equation for real functions $\tilde{u}_q(r)$ and $\tilde{v}_q(r)$. To numerically solve the BdG equation, we utilize the Bessel function expansion method, where $\tilde{u}_q(r)$ and $\tilde{v}_q(r)$ are expanded in terms of the Bessel functions $J_q(r)$ as

$$\tilde{u}_q(r) = \sum_j C_j \varphi_j^{(q)}(r), \quad \tilde{v}_q(r) = \sum_j D_j \varphi_j^{(q)}(r),$$

(4)

where the normalization condition imposed on $u_q(r)$ and $v_q(r)$ reduces to $2\pi \sum_j (C_j^2 + D_j^2) = 1$. Here, we introduce the set of the orthogonal functions, $\varphi_j^{(q)}(r) = \sqrt{2}/R_j J_k^{(q)}(k, r), \delta_j^{(q)} = \alpha_j^{(q)} R_j$ is the $j$-th zero of $J_k^{(q)}(r)$. This reduces the BdG equation\cite{22} to a matrix eigenvalue problem\cite{35,36,39}.

For simplicity we assume that the pairing interaction $g_p$ works only for chiral $p$-wave components and that the quantization axis of spin is parallel to the $d$-vector of spin-triplet pairing. This implies a singular vortex state, accompanied by spin-degenerate Majorana zero modes\cite{27}. Although in the half quantum vortex with a non-Abelian Majorana mode the $d$-vector is transverse to the spin quantization axis, the low energy quasiparticles are commonly describable with the BdG equation\cite{22}. Here we treat Zeeman energy to be negligible at enough low fields. Then, the selfconsistent condition $\Delta_{\pm}(r)$ for chiral $p$-wave pair potentials is given with the imaginary part of the retarded Green’s function $F$ by

$$\Delta_{\pm}(r) = g_p \sum_{|E| < E_{\text{cut}}} F_{\pm, \text{triplet}}(r, E) f(E),$$

(5)

where $r$ denotes the center-of-mass coordinate. Here, $f(E)$ denotes the Fermi distribution function and even-frequency $p_+$-wave pair amplitudes are given by

$$F_{m, \uparrow\downarrow}(r, E) = \sum_q \lim_{\epsilon \to 0} \mathcal{P}_{12}^{(m)*} [u_q(r_1) v_q^* \delta(E - E_q),}$$

(6)

using $\mathcal{P}_{12}^{(m)}$ obtained from $\mathcal{P}^{(m)}$ with $r \rightarrow r_{12} = r_2 - r_1$. $F_{m, \uparrow\downarrow}$ is obtained from Eq. (6) with replacing $(u_q, v_q, E_q)$ to $(v_q^*, u_q, -E_q)$. It is found that for ETO superconductors without a magnetic Zeeman term, even-frequency spin-triplet $p_+$-wave pair amplitude $F_{\pm, \text{triplet}}(r, E)$ satisfies $F_{\pm, \text{triplet}}(r, E) = -F_{\pm, \text{triplet}}(r, -E)$ and $F_{\pm, \text{triplet}}(r, E) \equiv F_{\pm, \text{triplet}}(r, -E)$. The BdG equation\cite{22} with Eqs. (5) and (6) gives a closed set for the selfconsistent calculation of $\Delta_{\pm}(r)$ and wave functions of the eigen-states.

From the selfconsistent solutions, we calculate the LDOS with $u_q \equiv u_q(r)$ and $v_q \equiv v_q(r)$ as

$$N(r, E) = \sum_q \left[ |u_q|^2 \delta(E - E_q) + |v_q|^2 \delta(E + E_q) \right].$$

(7)

The odd-frequency spin-triplet $s$-wave pair amplitude is given by

$$F_{s, \uparrow\downarrow}(r, E) = \sum_q v_q^*(r) u_q(r) \delta(E - E_q)$$

$$F_{s, \downarrow\uparrow}(r, E) = \sum_q u_q(r) v_q^*(r) \delta(E + E_q).$$

(8)

Note that $e^{-i(w+1)\phi} F_{s, \downarrow\uparrow}(r, E)$ can be real, since $u_q(r)$ and $v_q(r)$ are obtained as a real function from Eq. (4).
with an appropriate U(1) phase of $\Delta_\pm$. Since ETO superconductors without a Zeeman field hold $F_{s,\uparrow\downarrow}(r, E) = F_{s,\uparrow\downarrow}(r, -E)$ and $F_{s,\uparrow\downarrow}(r, E) = F_{s,\downarrow\uparrow}(r, E)$, spin-singlet components in ETO superconductors, such as $F_{s,\uparrow\downarrow}(r, E) - F_{s,\downarrow\uparrow}(r, E)$, vanish. Equation (8) is scaled so that $\max(e^{-i(|w+1|\theta)}F_s(r, E = 0)) = \max(N(r, E = 0))$. In figures, the LDOS and pair amplitudes are normalized by these maximum values at $E \sim 0$.

III. NUMERICAL RESULTS

In our calculation, we set $g_\phi = 1.65$, $E_{\text{cut}} = 2.0E_F$, $T = 0$, so that $\Delta \sim 0.1E_F$ when $w = 0$. First, we consider two cases of the parallel ($w = 1$) and anti-parallel ($w = -1$) vortex state. The obtained pair potentials $|\Delta_\pm(r)|$ are shown in Fig. 1(a). Around the vortex core of $\Delta_+(r)$, the opposite chiral component $\Delta_-(r)$ is induced. The induced component for $w = 1$ is smaller than that for $w = -1$, since the winding of $\Delta_+(r)$, $w + 2 = 3$, is larger than $w + 2 = 1$ in the anti-parallel case.

We examine the relation of LDOS $N(r, E)$ and odd-frequency pair amplitude $F_{s,\text{triplet}}(r, E)$ near the vortex core, which are shown in Figs. 1(b) and 1(c) as a function of $r$ and $E$. There, we see the quantization of CdGM bound states on $E$, and the quantum oscillations of wave functions with respect to $r$. For parallel vortex winding, the LDOS $N(r, E)$ is not symmetric for $E \leftrightarrow -E$, since the low energy LDOS at $r = 0$ is finite only at positive energy as shown in the left panel of Fig. 1(b). On the other hand, the odd-frequency $F_{s,\text{triplet}}(r, E)$ is symmetric for $E \leftrightarrow -E$ and shows oscillation between positive and negative values as a function of $r$, as shown in the left panel of Fig. 1(c). It is seen from the right panels of Figs. 1(b) and 1(c) that for anti-parallel vortex winding, $F_{s,\text{triplet}}(r, E)$ has the spectral evolution similar to $N(r, E)$. Both are positive and symmetric for $E \leftrightarrow -E$ at $|E| < \Delta$.

To examine whether the odd-frequency pair amplitude has the spatial structure exactly same as the LDOS or not, we compare the profiles as a function of $r$ for each energy level. Figure 2(a) shows $N(r, E)$ and $F_{s,\text{triplet}}(r, E)$ for Majorana bound state at $E = 0$. Here, we confirmed that the relations $N(r, E = 0) \propto F_{s,\text{triplet}}(r, E = 0)$ and

$$F_{s,\text{triplet}}(r, E = 0) = 0,$$

at $\theta = 0$ in the fully quantum level of $k_F^{-1}$, by solving the BdG equation (2). This implies that the LDOS of the Majorana state consists of odd-frequency pairing amplitudes without including even-frequency ones. Substituting the Majorana condition $u_q(r) = v_q^*(r)$ into Eqs. (7) and (8) at $E = 0$, we obtain exactly

$$N(r, E = 0) \propto e^{-i(|w+1|\theta)}F_{s,\text{triplet}}(r, E = 0).$$

In the zero-energy state for $w = 1$, $N(r, E = 0) = F_{s,\text{triplet}}(r, E = 0) = 0$ at the vortex center $r = 0$, because both $u_q(r)$ with $q_\theta = 1$ and $v_q(r)$ with $q_\theta - w - 1 = -1$ have non-zero winding. For anti-parallel winding $w = -1$, since $q_\theta = 0$ both for $u$ and $v$, $N(r, E = 0)$ and $F_{s,\text{triplet}}(r, E = 0)$ have peak at $r = 0$. The difference by the vortex winding direction is due to the angular momentum of CdGM vortex bound states.
The relation of the LDOS and the odd-frequency pair amplitude was studied by the quasiclassical theory for surface bound states in superfluid $^3$He and superconductors. However, since the rapid oscillation of the length order $k_F^{-1}$ is factorized out by the quasiclassical approximation, the theory discusses spatial variations only in the length scale of superconducting coherence length. This corresponds to the behavior of envelope function of the oscillating behavior in Fig. 3(b). Note that the STM-STS with a 0.1nm spatial resolution at low temperatures has succeeded in unveiling quantum limiting behaviors of a vortex core, whose microscopic structures are well understandable with the BdG theory but not with the quasiclassical theory.

Next, we study bound states at $E \neq 0$ in Figs. 2(b) and 2(c). In the parallel vortex winding case (left panels), the second lowest energy state at $E = 0.019E_F$ has $q_0 = 0$ for $u$ and $q_0 - w - 1 = -2$ for $v$. Thus, $N(r, E) \sim |v|^2$ has a sharp peak at the vortex center $r = 0$ and the odd-frequency pair amplitude $F_{s,\text{triplet}}(r, E) \sim uv \propto e^{i2\phi}$ vanishes at $r = 0$. In Figs. 2(b) and 2(c), $F_{s,\text{triplet}}(r, E)$ also shows oscillation between positive and negative values at $r > 0$, implying $N(r, E) \neq F_{s,\text{triplet}}(r, E)$. The third lowest energy state at $E = 0.032E_F$ has $q_0 = -1$ for $u$ and $q_0 - w - 1 = -3$ for $v$. Also in this state, we see that $N(r, E) \neq F_{s,\text{triplet}}(r, E)$. For the even-frequency pairing amplitude, we see that $F_{\text{triplet}}(r, E) \neq F_{\text{triplet}}(r, E)$. For the anti-parallel $w = -1$, as shown in the right panels of Figs. 2(b) and 2(c), the second lowest energy state at $E = 0.016E_F$ has $q_0 = 1$ both for $u$ and $v$. The third lowest energy state at $E = 0.029E_F$ has $q_0 = 2$ for $u$ and $v$. Even in these cases, we find that $N(r, E) \propto e^{-i(w+1)\phi} F_{s,\text{triplet}}(r, E)$ approximately holds, that is, the relation in Eq. (10) can be extended to a finite $E$. This comes from the symmetric LDOS structure for $E \leftrightarrow -E$ and the $\theta$-dependent structure $uv \propto \phi$ when $w = -1$, since the BdG equation holds the particle-hole symmetry, $(u, v) \leftrightarrow (u^*, v^*)$ for $E \leftrightarrow -E$. We also see that $F_{s,\text{triplet}}(r, E) \sim F_{s,\text{triplet}}(r, E)$, but there are small deviations between them.

To study the differences due to vortex winding directions in other energy states, in Fig. 3(a), we present the $E$-dependence of $N(r, E)$ and $e^{-i(w+1)\theta} F_{s,\text{triplet}}(r, E)$ at $r = 2k_F^{-1}$. We find $e^{-i(w+1)\theta} F_{s,\text{triplet}}(r, E) \neq N(r, E)$ for parallel vortex winding, except for $E = 0$. Only at $E = 0$, $e^{-i(w+1)\theta} F_{s,\text{triplet}}(r, E)$ has the same peak structure as that of $N(r, E)$, while it has negative value at $E \neq 0$. In the anti-parallel vortex winding case, we confirm $e^{-i(w+1)\theta} F_{s,\text{triplet}}(r, E) \sim N(r, E)$ for any bound states with $|E| < |\Delta|$. For the scattering state at $|E| > |\Delta|$, however, this relation does not hold.

The $E$-dependences of odd-frequency $F_{s,\text{triplet}}(r, E)$ and even-frequency $F_{s,\text{triplet}}(r, E)$ are compared in Fig. 3(b). From the symmetry relation for $E \leftrightarrow -E$, $F_{s,\text{triplet}}(r, E)$ is the even- (odd-) function of the real energy $E$. For anti-parallel vortex winding, we see that $F_{s,\text{triplet}}(r, E) \sim F_{s,\text{triplet}}(r, E)$. However, this is not satisfied for parallel vortex winding.
domain wall between outer $p_+$ and inner $p_-$ regions at $r \sim 19k_F^{-1}$ as in Fig. 1(c). Thus, while the low energy bound states for $w = -2$ appear far from the vortex center, they reduce to the bound states at the domain wall. The quasiparticle bound at the domain wall has similar structure to surface Majorana state in chiral $p$-wave superconductors. It is seen from Fig. 1(d) that the relations $e^{-i(w+1)\theta} \mathcal{F}_{s, \text{triplet}}(r, E) \propto N(r, E)$ and $\mathcal{F}_{s, \text{triplet}}(r, E) \sim \mathcal{F}_{s, \text{bound}}(r, E)$ approximately hold in the low energy, while there are small deviations. This is similar behavior to that of $w = -1$ in Fig. 2.

The LDOS $N(r, E)$, which we present in Figs. 1-4, is detectable through a STM-STS experiment. Since it is demonstrated in Figs. 2 and 3 and Eq. (10) that the odd-frequency pairing amplitude, $\mathcal{F}_{s, \text{triplet}}(r, E)$, traces the spatial shape of the zero energy LDOS, the characteristic behaviors may be unveiled by using superconducting STM. The local Josephson current between the superconductor and the superconducting STM tip is allowed only when the symmetry of local pair amplitudes in the superconductor is matched with that of the superconducting STM tip. Hence, the sharp peak of the odd-frequency $s$-wave pair amplitude around the vortex core is responsible to the local Josephson coupling with a superconducting STM tip with the same symmetry. For the anti-parallel vortex state, as shown in Fig. 3(a), the STM experiments with an odd-frequency $s$-wave superconducting tip may observe the spatial variation similar to the LDOS. As shown in Eq. (11), however, the zero energy DOS does not contribute to even-frequency pair amplitudes, $\mathcal{F}_{s, \text{triplet}}(r, E = 0)$, which is not responsible to a STM with an even-frequency chiral $p$-wave superconducting tip. This might potentially be a signature of the odd-frequency pairing.

Before closing, we discuss candidates materials of chiral $p$-wave superconductor and superfluid. One of the experimentally accessible superconductor is Sr$_2$RuO$_4$, where surface Andreev bound state specific to chiral $p$-wave symmetry has been observed. Recently, there have been proposed several heterostructures topologically equivalent to chiral $p$-wave superconductor, e.g., topological insulator/spin-singlet $s$-wave superconductor heterostructures with strong spin-orbit coupling. The chiral superfluidity in Fermi gases near $p$-wave Feshbach resonances and spin-orbit coupled Fermi gases are also promising candidate systems.

We hope our theoretical prediction will be experimentally verified in these systems.

IV. SUMMARY

In summary, we have examined the relation of the odd-frequency $s$-wave pair amplitude $\mathcal{F}_{s, \text{triplet}}(r, E)$ and LDOS $N(r, E)$ for the quantum limit of CdGM vortex bound states in chiral $p$-wave superconductors, based on the BdG equation. The relation of Eq. (10) holds in the Majorana zero modes of a single winding vortex. Further, we have confirmed that $\mathcal{F}_{s, \text{triplet}}(r, E)$ and $N(r, E)$ for the bound states have the same spatial structures even in finite $E$ at the core of the vortex with $w = -1$, and approximately at chiral domain wall of the $w = -2$ vortex. These spatial structures of the odd-frequency pair amplitude give valuable information, when we identify the odd-frequency pair amplitude in future experiments and discuss the associated anomalous interference phenomena.

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