Model for vortex-core tunneling spectroscopy of chiral $p$-wave superconductors via odd-frequency pairing states

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The local density of states (LDOS) is studied theoretically in terms of the odd-frequency (odd-$\omega$) Cooper pairing induced around a vortex core. We find that a zero energy peak in the LDOS at the vortex center is robust against nonmagnetic impurities in a chiral $p$-wave superconductor owing to an odd-$\omega$ s-wave pair amplitude. We suggest how to discriminate a spin-triplet pairing symmetry and spatial chiral-domain structure by scanning tunneling spectroscopy via odd-$\omega$ pair amplitudes inside vortex cores.

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The unambiguous determination of Cooper pairing symmetry is of prime importance for understanding the pairing mechanism of unconventional superconductivity. In the last decade, the discovery of the ruthenate superconductor (SC) $\text{Sr}_2\text{RuO}_4$ has stimulated an enormous amount of studies, where a chiral superconductivity with time-reversal-symmetry breaking was indicated by muon-spin-rotation and polar Kerr effect experiments, and a spin-triplet state such as a $p$-wave one was suggested by Knight-shift measurements [1, 2]. Therefore, experiments based on new ideas are needed [4]. We suggest how to observe directly the spatial structure of chiral domains by scanning tunneling spectroscopy and surface Andreev bound states (SABS) [5]. The SABS origins from a sign change of the odd-frequency (odd-$\omega$) pairing state [8]. The odd-$\omega$ pairing state is characterized by a pair amplitude that is an odd function of the Matsubara frequency [9]. The origin of the generation of odd-$\omega$ pair amplitude is as follows. In inhomogeneous system, due to the breakdown of translational invariance, the pair potential acquires a spatial dependence which leads to coupling between the even- and odd-parity pairing states. The Fermi-Dirac statistics then dictates that the pair amplitude of opposite parity should be opposite in frequency [10]. Owing to an axial symmetry of a vortex, there exists a fundamental rule [11, 12] that relates the angular momentum of the odd-$\omega$ Cooper pair and the topology (winding number) of vortex. It is interesting and important to confirm experimentally the existence of odd-$\omega$ pair amplitudes subjected to the topological symmetry rule due to the vortex. Note that the SABS are also interpreted as a generation of the odd-$\omega$ pairing states [13].

In this Letter, we will show that nonmagnetic impurity scattering effect on the SABS can be used to detect the symmetry rule for the induced odd-$\omega$ pair amplitudes. We will study the odd-$\omega$ pairing amplitude and the local density of states (LDOS) around a vortex for spin-singlet s-wave and spin-triplet chiral $p$-wave SCs. The effect of nonmagnetic impurities serves as a probe of the symmetry rule and the pairing symmetry in candidates for a spin-triplet chiral SC such as $\text{Sr}_2\text{RuO}_4$. We will also point out how to observe spatial chiral-domain structure by scanning tunneling spectroscopy/ microscopy (STS/STM). The issue of chiral domains has been studied experimentally in $\text{Sr}_2\text{RuO}_4$ [14, 15]. However, a more direct observation by spatially resolved probe has not been performed. Therefore, it is interesting to propose an idea to observe directly the spatial structure of chiral domains. In the present theory, we point out that the proposed method for identifying a spin-triplet chiral $p$-wave state can be simultaneously used for detecting chiral domains.

We consider a spin-singlet s-wave and a spin-triplet chiral $p$-wave pairing state with a $d$-vector parallel to the $z$ axis [1]. In both cases, the quasiclassical Green’s function $\tilde{g}(\omega_n, r, \vec{k})$ is represented in a $2 \times 2$ matrix form as [16]

$$\tilde{g} = -i\pi \left( \begin{array}{cc} g & i\bar{f} \\ -i\bar{f} & -g \end{array} \right).$$

(1)

It follows the Eilenberger equation

$$-i\nu_F \cdot \nabla \tilde{g} = \left[ \omega_n \hat{\tau}_z - \hat{\Delta} - \hat{\Sigma}, \tilde{g} \right],$$

(2)

which is supplemented by the normalization condition $g^2 + f\bar{f} = 1$. Here, $\omega_n = (2n + 1)\pi T$ is the Matsubara frequency, $\nu_F$ is the Fermi velocity, and $\hat{\tau} = (\hat{\tau}_x, \hat{\tau}_y, \hat{\tau}_z)$ are Pauli matrices in the particle-hole space. We use units in which $\hbar = k_B = 1$. $r$ denotes the center of mass of the Cooper pair, and $\vec{k}$ is the unit vector of the Fermi wave number ($\vec{k} = k_F/k_B$). The pair potential is expressed as $\hat{\Delta}(r, \vec{k}) = (\hat{\tau}_x + i\hat{\tau}_y)\Delta(r, \vec{k})/2 - (\hat{\tau}_y - i\hat{\tau}_x)\Delta^*(r, \vec{k})/2$. We incorporate the impurity scattering effect within the Born approximation. The impurity self energy is given as $\Sigma(\omega_n, r) = \Gamma \left( \langle \hat{\tau}_x + i\hat{\tau}_y \rangle \langle f(\omega_n, r, \vec{k}) \rangle - \langle \hat{\tau}_x - i\hat{\tau}_y \rangle \langle \bar{f}(\omega_n, r, \vec{k}) \rangle \right)$.
We consider a spin-singlet state with the quantum number of the angular momentum \(l\). The chiral \(p_x \pm ip_y\) wave is represented by \(\exp(\pm i\theta)\). The self-consistent equation for the pair potential is given by

\[
\Delta(r, \theta) = \Delta_+(r)e^{i\theta} + \Delta_-(r)e^{-i\theta},
\]

(3)

\[
\Delta_\pm(r) = \pi TV \sum_{|n_\omega|<\omega_c} \langle e^{\pm i\theta_0'f(i\omega_n, r, \theta')} \rangle,
\]

(4)

where \(V\) is the coupling constant (see Ref. \[16\] for details). We consider a spin-singlet \(s\)-wave state \((l = 0)\) and a spin-triplet chiral \(p\)-wave one \((l = 1)\) for the pair potential. The Fermi-surface average is \(\langle \cdots \rangle = \int_{0}^{2\pi} d\theta' \cdots / (2\pi)\). The pair amplitudes represented in the Matsubara frequency are

\[
F^{(l)}(i\omega_n, r, \theta) = F_+^{(l)}(i\omega_n, r)e^{i\theta} + F_-^{(l)}(i\omega_n, r)e^{-i\theta},
\]

(5)

\[
F_\pm^{(l)}(i\omega_n, r, \theta) = \langle e^{\mp i\theta_0'f(i\omega_n, r, \theta')} \rangle,
\]

(6)

with the quantum number of the angular momentum \(l\) = 0, 1, 2, \ldots, \(N\). The even-\(\omega\) and odd-\(\omega\) pair amplitudes satisfy

\[
F(i\omega_n, r, \theta') = f(-i\omega_n, r, \theta'), \quad \text{and} \quad f(i\omega_n, r, \theta') = -f(-i\omega_n, r, \theta'),
\]

respectively.

The Eilenberger equation is simplified by introducing the Riccati parameterization \[17\]. We numerically solve the resulting Riccati equations and the self-consistent equations for the impurity self energy and pair potential iteratively \[16\]. Throughout the paper we set the temperature \(T = 0.1T_c\), where \(T_c\) is the critical temperature in the absence of impurities. Using the self-consistently obtained pair potential, we determine the self energy by the analytical continuation with \(\omega_n \rightarrow E + i\delta\ \[18\]. The LDOS is then calculated as \(N(r, E) = N_F(\Re g_R(r))\). Here, \(N_F\) is the normal-state density of states at the Fermi level, \(g_R = g(i\omega_n \rightarrow E + i\delta)\), \(E\) means the quasi-particle energy, and \(\delta\) is an infinitesimal quantity. We select \(\delta = 0.06\Delta_0\) as a typical value, where \(\Delta_0\) is the bulk amplitude of the pair potential at \(T = 0\) and \(\Gamma = 0\).

An enhancement of the LDOS in the presence of odd-\(\omega\) pairing can be understood by means of the normalization condition. Since \(\tilde{f}\) with \(E = 0\) is given by \(\tilde{f} = -f^*\) for odd-\(\omega\) pairing state \[8\], one can show that generally \(N(E = 0)/N_F > 1\) owing to \(g^2 = 1 + |f|^2 > 1\). This means that the emergence of odd-\(\omega\) pairing is a physical reason for a zero energy peak (ZEP) in the LDOS.

In circular coordinates \(r = (r, \phi)\), we consider an axially-symmetric vortex situated at \(r = 0\), the vorticity of which is perpendicular to the two-dimensional system. The axial symmetry requires \(\Delta \rightarrow \Delta \exp(i\alpha\phi)\) with an integer \(N\) for a rotational transformation \(\phi \rightarrow \phi + \alpha\) and \(\theta \rightarrow \theta + \alpha\ \[11\,12\,16\]. The pair potential that satisfies this constraint is

\[
\Delta(r, \theta) = \tilde{\Delta}(r)e^{im\phi},
\]

(7)

for a spin-singlet \(s\)-wave vortex, and

\[
\Delta(r, \theta) = \tilde{\Delta}_+(r)e^{m\phi} + \tilde{\Delta}_-(r)e^{-m\phi},
\]

(8)

for a spin-triplet chiral \(p\)-wave vortex. Here, \(m\) is the winding number of a vortex. We have assumed the \(p\)-wave state in bulk for the chiral \(p\)-wave vortex, namely \(\Delta_+(r \rightarrow \infty) = 0\) and \(\Delta_- (r \rightarrow \infty) \neq 0\). Due to the same constraint from axial symmetry, the pair amplitudes satisfy

\[
F_\pm^{(l)}(i\omega_n, r, \phi) = \tilde{F}_\pm^{(l)}(i\omega_n, r)e^{i(m \mp l)\phi},
\]

(9)

for the spin-singlet \(s\)-wave vortex, and

\[
F_\pm^{(l)}(i\omega_n, r, \phi) = \tilde{F}_\pm^{(l)}(i\omega_n, r)e^{i(m - l\mp l)\phi},
\]

(10)

for the spin-triplet chiral \(p\)-wave (\(p_\pm\)-wave) vortex. Note that if a pair amplitude has a finite phase proportional to \(\phi\), the amplitude inevitably becomes zero at \(r = 0\) where \(\phi\) is undefined.

First let us discuss the spin-singlet \(s\)-wave vortex \((l = 0)\) in the presence of impurity scattering. The spatial dependences of odd-\(\omega\) pair amplitudes \((\omega_n = 0)\) are plotted in Fig. 1(a). There, the distance \(r\) from the vortex center is normalized by the coherence length \(\xi_0 = v_F/\Delta_0\). In the case of winding number \(m = 1\), only the \(p_-\)-wave pair amplitude with odd-\(\omega\) is induced at the vortex center. It is because only the phase of the \(p_+\)-wave pair amplitude \(F_{++}^{(1)}\) is zero in Eq. \[9\] for \(m = 1\). As a result, the LDOS at the vortex center has the ZEP as shown in Fig. 1(b), reflecting the VABS that originates from the induced odd-\(\omega\) pair amplitude \[8\,10\]. The magnitude of the odd-\(\omega\) pair amplitude is suppressed with the increase of \(\Gamma\). Accordingly, the height of the ZEP decreases with increasing \(\Gamma\) [Fig. 1(b)]. Actually, a collapse of the ZEP upon doping impurities in an \(s\)-wave SC was observed experimentally \[19\]. Here, the induced odd-\(\omega\) pair amplitude is the \(p_\pm\)-wave (i.e., non-\(s\)-wave), and therefore Anderson’s theorem for non-magnetic impurities \[20\] is not applicable. As a
result, the odd-ω pair amplitude, namely the ZEP, is sensitive to impurity scattering.

The clear difference between two states can be understood in terms of the symmetry of the odd-ω pair amplitude. Due to the phase factor in Eq. (10), the odd-ω pair amplitude induced at the vortex center is inevitably s-wave (l = 0) for the antiparallel vortex (m = 1) and d-wave (l = 2) for the parallel one (m = −1) as mentioned above. According to Anderson’s theorem [20], an s-wave pair amplitude is robust against non-magnetic impurities, while a d-wave pair amplitude is sensitive to such impurities (see the inset in Fig. 5).

The VABS (corresponding to the SABS in Ref. [13]) originates from an odd-ω pair amplitude [13], and it is reflected in the ZEP [8]. Hence, the ZEP is robust against the increase of Γ because of the d-wave (i.e., non-s-wave) pair amplitude. Accordingly, measurements of the ZEP under the influence of impurities correspond to observations of the symmetry of those odd-ω pair amplitudes as illustrated in Fig. 4. In order to visualize the striking difference between the antiparallel and parallel vortex states, we show in Fig. 5 the zero energy LDOS at the vortex center as a function of Γ. In the inset of Fig. 5 it is found that the odd-ω s-wave pair amplitude (circle) is likely to follow the Abrikosov-Gorkov (AG) law [22], while the odd-ω d-wave one (triangle) decays more rapidly with increasing Γ. The decrease of the odd-ω s-wave component is involved with the fact that the odd-ω component is generated through the coupling to the bulk even-ω p-wave pair potential which is sensitive to Γ.

The above results have a significant implication to identification of pairing symmetry in chiral SCs such as Sr$_2$RuO$_4$. In chiral superconductivity, the pair potential is composed of two degenerate components. As a result, degenerate chiral states, such as $p_x + ip_y$ and $p_x - ip_y$, form a domain structure in a chiral SC under field cooling condition with high-speed cooling rate [14]. Under magnetic fields the antiparallel vortex is known to be energetically favorable [23], and therefore the antiparallel vortex state, namely one of two chiral states, dominates in a sample under field cooling condition with slow cooling rate. In the case of high-speed cooling, a domain structure remains as a mixture of antiparallel- and parallel-vortex domains. If a SC is a spin-triplet chiral...
p-wave one, such a difference in the chiral state between slow and high-speed coolings is observable via the ZEP at vortex cores shown in Fig. 4. In addition, through a distribution of those two different vortex states, the existence of a chiral domain structure can be observed by STM at zero-bias under high-speed cooling with a spatial resolution of the order of inter-vortex distance. On the other hand, for any spin-singlet pairing state such as a chiral d-wave one [e.g., \( p_{z}(p_{z} \pm ip_{y}) \)], the induced odd-\( \omega \) pair amplitudes are inevitably spin-singlet odd-parity ones \([8]\) and the odd-\( \omega \) s-wave (= even-parity) pair amplitude is never induced. In Sr\(_{2}\)RuO\(_{4}\), the ZEP at a vortex core has been observed \([24]\), and samples with different impurity scattering rate could be prepared \([22]\). Therefore, an experimental setup proposed here may provide strong evidence for spin-triplet chiral p-wave superconductivity.

In conclusion, we have studied the odd-\( \omega \) pair amplitudes and the LDOS around a single vortex in s-wave and chiral p-wave SCs. For the antiparallel and parallel chiral p-wave vortices, we have found that the odd-\( \omega \) s-wave and d-wave pair amplitudes are inevitably induced at the vortex center, respectively. The robustness of the ZEP at the vortex core against non-magnetic impurities originates from this odd-\( \omega \) s-wave pair amplitude. Those odd-\( \omega \) pair amplitudes can be observed by STS/STM, serving as a probe of a spin-triplet pairing and of a spatial distribution of the chiral domains.

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