Theoretical analysis for spin-polarized local density of states in the vortex state of helical $p$-wave superconductors

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Abstract. Based on the quasi-classical Eilenberger theory, we calculate the site-dependence of order-parameter and spin-polarized local density of states (LDOS) in the vortex lattice state of helical $p$-wave superconductors. The spin-polarized LDOS is induced around the vortex core by the vorticity coupling to the chirality of up-spin pair or down-spin pair. In order to distinguish the $d$-vector symmetry, we investigate the magnetic field effect on the spatial structure of the spin-polarized LDOS.

1. Introduction
The spin-triplet superconductors have attracted great interest, since Majorana state is induced around the surface and vortex core. The ruthenate superconductor Sr$_2$RuO$_4$ is a leading candidate material for the spin-triplet superconductor. However, the detailed structure of $d$-vector in this material remains unclear. A lot of studies support that Sr$_2$RuO$_4$ is a spin-triplet chiral $p$-wave superconductor [1, 2]. On the other hand, the helical $p$-wave state also has been studied as another scenario [3, 4, 5, 6]. In addition, from the theoretical study employing the multi-orbital model of Sr$_2$RuO$_4$ [7], it is found that the condensation energy of chiral and helical $p$-wave states are very close. Therefore, we investigate behaviors of physical quantities depending on the difference between chiral and helical superconducting states, to distinguish the $d$-vector symmetry of Sr$_2$RuO$_4$ and other candidate materials for spin-triplet superconductors.

In the bulk state of chiral $p$-wave superconductor, time-reversal symmetry breaking state is realized by chirality of Cooper pair, i.e., orbital angular momentum $L_z = \pm 1$. According to the theoretical studies for the vortex state of chiral $p$-wave superconductors, the local density of states (LDOS) and the local NMR relaxation rate around the vortex core show the chirality dependent behaviors [8, 9, 10, 11, 12]. These chirality dependences of physical quantities are caused by the vorticity coupling to the chirality, depending on whether the chirality is parallel ($L_z = +1$) or anti-parallel ($L_z = -1$) to the vorticity ($W = +1$) [13, 14]. On the other hand, in the helical $p$-wave superconductor, a time-reversal-invariant state has a full pairing gap in the bulk. This is because the chirality $L_z = \pm 1$ are quenched with the degeneracy between up-spin and down-spin pairs. The order-parameter of up-spin (down-spin) pair $\Delta_{\uparrow\uparrow}(\Delta_{\downarrow\downarrow})$ has chirality $L_z = -1(+1)$ so that $L_z + S_z = 0$ [3]. $S_z = +1(-1)$ is the spin angular momentum of
up-spin (down-spin) pair. Therefore, the spin components of LDOS in the vortex state of helical \( p \)-wave superconductor show unique behaviors, reflecting the vorticity coupling to the chirality of \( \Delta_{\uparrow\uparrow}(L_z = -1) \) or \( \Delta_{\downarrow\downarrow}(L_z = +1) \) [15].

In the various superconductors, the scanning tunneling microscopy and spectroscopy (STM/STS) measurements can detect the site- and energy-dependence of LDOS in the vortex state [16, 17]. Recently, the STM/STS measurement in the vortex state of topological insulator-superconductor \( \text{Bi}_2\text{Te}_3/\text{NbSe}_2 \) heterostructure has also performed [18]. From the theoretical studies for the measurement, the existence of Majorana state is suggested at the inside of the vortex core [19, 20]. The spin-polarized Majorana state in the vortex core has been also examined by the spin-polarized STM/STS measurement [21]. The spin-polarized STM/STS measurement can selectively observe the spin-dependent tunnelling conductance. In addition, by solving the Bogoliubov-de Gennes equation [22], the spin-polarized Majorana state in the vortex state of \( \text{Cu}_x\text{Bi}_2\text{Si}_3 \) has been studied. Recently, we revealed that the spin-polarized LDOS appears in the vortex state of helical \( p \)-wave superconductors, and focused on the magnetic field \( H \)- and energy \( E \)-dependence of the spin-polarized LDOS [15]. We also confirmed the instability of the helical \( p \)-wave state at high fields.

In this paper, we focus on the spatial structure of the spin-polarized LDOS in the vortex lattice state of helical \( p \)-wave superconductor, and investigate the magnetic field effects on the spatial structure of the spin-polarized LDOS. We expect that these calculation results help to investigate the vortex state of helical \( p \)-wave superconductors and the spin-polarized Majorana state by the spin-polarized STM measurement.

This paper is organized as follows. After the introduction, we explain formulation of the Eilenberger equation in the vortex lattice state and the spin-resolved LDOS in section 2. In section 3, we study the site-dependence of order-parameter and spin-polarized LDOS. In section 4, we show magnetic field effect on the spatial structure of the spin-polarized LDOS around the vortex core. The last section is devoted to the summary.

2. Formulation of Eilenberger theory
We calculate the spatial structure of the vortex lattice state by the quasi-classical Eilenberger theory. The quasi-classical theory is valid when \( k_F\xi \) is sufficiently larger than 1. \( k_F \) is the Fermi wave number and \( \xi \) is the coherence length. The quasi-classical condition is well satisfied for \( \text{Sr}_2\text{RuO}_4 \) [1, 2] and most superconductors.

We assume the helical \( p \)-wave pairing symmetry on the cylindrical Fermi surface, \( \mathbf{k} = (k_x, k_y) = k_F(\cos \theta_k, \sin \theta_k) \), and the Fermi velocity \( v_F = \frac{v_{F0} \mathbf{k}}{k_F} \). The hat \( \hat{\cdot} \) indicates the 2x2 matrix in spin space and the check \( \check{\cdot} \) is for the 4x4 matrix in particle-hole and spin spaces.

We obtain quasi-classical Green’s functions \( \hat{g}(i\omega_n, \mathbf{r}, \mathbf{k}) \) in the vortex lattice state by solving the Riccati equation derived from Eilenberger equation [23, 24, 15]

\[
-iv \cdot \nabla \hat{g}(i\omega_n, \mathbf{r}, \mathbf{k}) = \frac{1}{2}[(i\omega_n - v \cdot A)\sigma_z - \hat{\Delta}(\mathbf{r}, \mathbf{k}), \hat{g}(i\omega_n, \mathbf{r}, \mathbf{k})]
\]  

in the clean limit, where \( v = \frac{v_F}{v_{F0}} \), \( \mathbf{r} \) is the center-of-mass coordinate of the Cooper pair, \( \sigma_z \) is the Pauli matrix, and \( \omega_n \) is Matsubara frequency. The quasi-classical Green’s function and order parameter are defined by

\[
\hat{g}(i\omega_n, \mathbf{r}, \mathbf{k}) = -i\pi \begin{pmatrix} \check{g}(i\omega_n, \mathbf{r}, \mathbf{k}) & if(i\omega_n, \mathbf{r}, \mathbf{k}) \\ -if(i\omega_n, \mathbf{r}, \mathbf{k}) & -\check{g}(i\omega_n, \mathbf{r}, \mathbf{k}) \end{pmatrix},
\]

\[
\hat{\Delta}(\mathbf{r}, \mathbf{k}) = \begin{pmatrix} 0 & \check{\Delta}(\mathbf{r}, \mathbf{k}) \\ -\check{\Delta}^\dagger(\mathbf{r}, \mathbf{k}) & 0 \end{pmatrix}
\]
where $g^2 = -\pi^2 \hbar^2 \frac{1}{M}$. The matrix elements of $\hat{g}$ and $\hat{A}$ are defined by $g_{\sigma \sigma'}(i\omega_n, \mathbf{r}, \mathbf{k}) = [g_0(i\omega_n, \mathbf{r}, \mathbf{k})^\dagger + \sum_{j=1}^3 \delta_{\mathbf{r}, \mathbf{j}} g_0(i\omega_n, \mathbf{r}, \mathbf{k}) \hat{\sigma}^j_{\sigma \sigma'}]$ and $\Delta_{\sigma \sigma'}(\mathbf{r}, \mathbf{k}) = [i \sum_{j=1}^3 \delta_{\mathbf{r}, \mathbf{j}} (d_\mu(\mathbf{r}, \mathbf{k}) \hat{\sigma}^j_\mu)_{\sigma \sigma'}]$ where $\sigma, \sigma' = \uparrow$(up-spin) or $\downarrow$(down-spin), and $d_\mu$ is $\mu$-component of $d$-vector. On the other hand, to consider the order-parameter $\Delta_{\pm \sigma \sigma'}(\mathbf{r})$ about pairing function $\phi_{p \pm}(\mathbf{k}) = k_{\pm} \pm i k_y$ for $p_{\pm}$-state, the matrix elements of order-parameter are also defined by

$$\Delta_{\sigma \sigma'}(\mathbf{r}, \mathbf{k}) = \Delta_{+ \sigma \sigma'}(\mathbf{r}) \phi_{\mathbf{p} \uparrow}(\mathbf{k}) + \Delta_{- \sigma \sigma'}(\mathbf{r}) \phi_{\mathbf{p} \downarrow}(\mathbf{k}).$$  \hspace{1cm} (4)

Length, temperature, and magnetic field are, respectively, measured in unit of $\xi_0$, $T_c$, and $B_0$. Here, $\xi_0 = h v_F 0 / 2 \pi k_B T_c$ is the coherence length, $T_c$ is superconducting transition temperature at a zero field. The energy $E$, pair potential $\Delta$ and $\omega_n$ are normalized by $\pi k_B T_c$. In the following, we set $\hbar = k_B = 1$. In this work, all calculations are performed at a $T/T_c = 0.5$.

As magnetic fields are applied to the $\hat{z}$ direction, the vector potential is set by $A(\mathbf{r}) = \frac{1}{2} \mathbf{H} \times \mathbf{r} + \mathbf{a}(\mathbf{r})$ in the symmetric gauge, where $\mathbf{H} = (0, 0, H)$ is a average flux density, and $\mathbf{a}(\mathbf{r})$ is related to the internal magnetic field $B(\mathbf{r}) = (0, 0, B(\mathbf{r})) = \mathbf{H} + \nabla \times \mathbf{a}(\mathbf{r})$. The unit cell is arranged to be square vortex lattice [1].

In order to obtain the spatial structure of the quasi-classical Green’s functions and the order-parameter $\Delta(\mathbf{r})$ selfconsistently, we calculate $\Delta(\mathbf{r})$ by the gap equation

$$\hat{\Delta}(\mathbf{r}) = g N_0 T \sum_{|i\omega_n| \leq \omega_{\text{cut}}} \langle \phi_{p \pm}(\mathbf{k}) \hat{f}(i\omega_n, \mathbf{r}, \mathbf{k}) \rangle_k,$$  \hspace{1cm} (5)

where $(g N_0)^{-1} = \ln T + 2T \sum_{0 < \omega_n \leq \omega_{\text{cut}}} \omega_n^{-1}$, $(\cdots)_k$ indicates Fermi surface average, and we set $\omega_{\text{cut}} = 20 \pi k_B T_c$. In equation (5), $p$-wave pairing interaction is isotropic in spin space. We use the current equation $\nabla \times (\nabla \times \mathbf{A}) = -\frac{2T}{\kappa T} \sum_{0 < \omega_n} \langle \mathbf{v} \mathbf{I} \mathbf{m}(g_0) \rangle_k$ with the Ginzburg-Landau parameter $\kappa = B_0 / \pi k_B T_c \sqrt{8N_0}$ for the selfconsistent calculation of the vector potential. In the calculations, we set $\kappa = 2.7$ appropriate to $\text{Sr}_2\text{RuO}_4$ as a candidate superconductor for the chiral or helical state. Equations (1)-(5) for $\omega_n$ are calculated selfconsistently until the order-parameter converges. From this calculation, we obtain the results of $A(\mathbf{r})$, $\Delta(\mathbf{r})$ and the quasi-classical Green’s functions of $\omega_n$ in the vortex lattice state.

$d$-vector in the helical $p$-wave superconductors is defined by $d(\mathbf{k}) \propto k_x \hat{x} + k_y \hat{y} = \phi_{p \pm}(\mathbf{k}) \mathbf{d}_{\pm}$ at a zero field $H = 0$, with $\mathbf{d}_{\pm}(\mathbf{k}) = \frac{1}{2} (1, \pm i, 0)$. Thus, when we iterate calculations of equations (1)-(5), as an initial value we set to be $d(\mathbf{r}, \mathbf{k}) = d(\mathbf{r}) (k_x \hat{x} + k_y \hat{y})$ where $d(\mathbf{r})$ is Abrikosov vortex lattice solution.

Next, we calculate $\hat{g}(E \pm i \eta, \mathbf{r}, \mathbf{k})$ for real energy $E$ by solving Eilenberger equation (1) with $i \omega_n \rightarrow E \pm i \eta$, using the selfconsistently obtained spatial structure of $\mathbf{A}(\mathbf{r})$ and $\Delta(\mathbf{r})$. $\eta$ is a small parameter as a smearing factor. We typically use $\eta = 0.01$. The spin-resolved LDOS $N_\sigma(E, \mathbf{r})$ is given by

$$N_\sigma(E, \mathbf{r}) = \langle \text{Re} \{ [\hat{g}(E + i\eta, \mathbf{r}, \mathbf{k})]_{\sigma \sigma} \} \rangle_k.$$  \hspace{1cm} (6)

We define the LDOS as $N(E, \mathbf{r}) = N_\uparrow(E, \mathbf{r}) + N_\downarrow(E, \mathbf{r})$, and spin-polarized LDOS as $M(E, \mathbf{r}) = N_\uparrow(E, \mathbf{r}) - N_\downarrow(E, \mathbf{r})$.

3. Site-dependence of order-parameter and spin-polarized LDOS

As shown in figure 1(a), we present the $r$-dependence of the order-parameter amplitudes at low $H$ on a line between NNN vortices within $0 < r < 0.5 a_x$. $a_x$ is distance between NNN vortices. Vortex center is at $r = 0$, and farthest site $r = 0.5 a_x$ from the vortex center is the midpoint between NNN vortex. We present $|\Delta_{\pm \sigma \sigma'}(\mathbf{r})|$ given by equation (4). In
the vortex state of helical $p$-wave superconductor, up-spin pair is described by $\Delta_{\updownarrow\updownarrow}(r, k) = \Delta_{-\updownarrow\updownarrow}(r)\phi_{p_+}(k) + \Delta_{-\updownarrow\downarrow}(r)\phi_{p_-}(k)$ with small component $\Delta_{+\updownarrow\updownarrow}(r)$ induced around the vortex core as shown in figure 1(a). The chirality of main component $\Delta_{-\updownarrow\updownarrow}(r)$ is $L_z = -1$. This is anti-parallel to vorticity $W = +1$ as $L_z + W = 0$. From the previous studies for the chiral $p$-wave superconductor [13, 14], the anti-parallel vortex state ($L_z + W = 0$) has larger amplitude of the order-parameter, compared with the parallel vortex state ($L_z + W = +2$). On the other hand, down-spin pair is described by $\Delta_{\updownarrow\uparrow}(r, k) = \Delta_{+\updownarrow\uparrow}(r)\phi_{p_+}(k) + \Delta_{-\updownarrow\downarrow}(r)\phi_{p_-}(k)$ with small induced $\Delta_{-\updownarrow\downarrow}(r)$. This corresponds to the anti-parallel vortex state $L_z + W = +2$, since the chirality of the main component $\Delta_{+\updownarrow\updownarrow}$ is $L_z = +1$. Therefore, $|\Delta_{-\updownarrow\updownarrow}(r)|$ is larger than $|\Delta_{+\updownarrow\updownarrow}(r)|$ at every position, reflecting the vorticity coupling to the chirality of $\Delta_{\updownarrow\updownarrow}(L_z = -1)$ or $\Delta_{\downarrow\uparrow}(L_z = +1)$.

In addition, we show the $r$-dependence of the zero-energy spin-polarized LDOS $M(E = 0, r)$ around the vortex core within $0 < r < 0.1a_x$ in figure 1(b). The spin-polarization of LDOS is induced by the vorticity coupling to the chirality of each spin-component of order-parameter, and $M(E = 0, r)$ has large amplitude near vortex center. Since the zero energy states localized inside the vortex core in the chiral and helical superconductors correspond to Majorana zero energy mode, figure 1(b) shows that the spin-polarized Majorana state is induced in the helical $p$-wave superconductors. This state is another type of spin-polarized Majorana state than that supposed in the vortex state of Bi$_2$Te$_3$/NbSe$_2$ [20] or Cu$_x$Bi$_2$Se$_3$ [22]. In the theoretical studies based on the Bogoliubov de-Gennes equation [20, 22], vortex states were investigated in the topological superconductivity induced by Rashba spin-orbit coupling.

**Figure 1.** (a) $r$-dependence of the order-parameter amplitudes $|\Delta_{-\updownarrow\downarrow}(r)|$, $|\Delta_{+\updownarrow\uparrow}(r)|$, $|\Delta_{-\updownarrow\updownarrow}(r)|$ and $|\Delta_{+\updownarrow\updownarrow}(r)|$. $H/H_c2 \geq 0.18$. (b) $r$-dependence of the spin-resolved LDOS $N_{\sigma}(E = 0, r)$ and spin-polarized LDOS $M(E = 0, r)$. $H/H_c2 \geq 0.18$. $r$ axis is along the next-nearest-neighbor (NNN) direction from the vortex center. $a_x$ is NNN intervortex distance. The inset shows distribution of $M(E = 0, r)$. Brighter region has larger $M(E = 0, r)$.

4. Magnetic field effect on the spatial structure of spin-polarized LDOS

In figures 2, we present the spatial structure of the zero-energy spin-resolved LDOS $N_{\sigma}(E = 0, r)$, LDOS $N(E = 0, r)$ and spin-polarized LDOS $M(E = 0, r)$ along a line between NNN vortices within $0 < r < 0.1a_x$ at some magnetic fields. Here we study lower field range to avoid instability of helical state at high fields [15]. At a very low field $H/H_c2 = 0.02$, $N_{\sigma}(E = 0, r)$ shows sharp peak at the vortex center $r = 0$. $N_{\uparrow}(E = 0, r)$ and $N_{\downarrow}(E = 0, r)$ show different behavior in the range $0.12 < H/H_c2 < 0.24$. There, with increasing $H$, the peak at the vortex center decreases in $N_{\uparrow}(E = 0, r)$ in figure 2(a), but the magnetic field effect on $N_{\downarrow}(E = 0, r)$ is small in figure 2(b). Therefore, the spatial structure of LDOS $N(E = 0, r)$ in figure 2(c) are similar to $N_{\uparrow}(E = 0, r)$. Since $N_{\uparrow}(E = 0, r)$ is smaller than $N_{\downarrow}(E = 0, r)$ at every position in the field range considered.
in figure 2, $M(E = 0, \mathbf{r})$ is positive value in figure 2(d). We note that the magnetic field effect on the spatial structure of $M(E = 0, \mathbf{r})$ shows a unique behavior. At $H/H_c^2 \simeq 0.02$ and 0.12, $M(E = 0, \mathbf{r})$ monotonically decreasing as a function of $r$. On the other hand, at $H/H_c^2 \simeq 0.18$ and 0.24, $M(E = 0, \mathbf{r})$ shows convex behavior as a function of $r$. These unique behaviors of the helical state are expected to be examined by spin-polarized STM measurement.

Figure 2. $r$-dependence of spin-resolved LDOS (a) $N_\uparrow(E = 0, r)$, (b) $N_\uparrow(E = 0, r)$, (c) LDOS $N(E = 0, r)$, and (d) spin-polarized LDOS $M(E = 0, r)$ at magnetic fields $H/H_c^2 \simeq 0.02, 0.12, 0.18, \text{and } 0.24$ along the NNN direction within $0 < a_x < 0.1$.

5. Summary
We studied the spatial structure of the helical $p$-wave superconductors in the vortex lattice state by solving the quasi-classical Eilenberger equation. In the helical state, up-spin pairing order-parameter $\Delta_{\uparrow\uparrow}$ has larger amplitude compared to that of down-spin pairing $\Delta_{\downarrow\downarrow}$ by the contribution of coupling between vorticity and chirality. Therefore, spin-resolved zero-energy LDOS shows the differences between $N_\uparrow(E = 0, \mathbf{r})$ and $N_\downarrow(E = 0, \mathbf{r})$, inducing finite spin-polarized LDOS $M(E = 0, \mathbf{r})$ around a vortex. The zero-energy state in the $p$-wave pairing is spin-polarized Majorana state localizing in a vortex core. We study how the spatial structure of $M(E = 0, \mathbf{r})$ is affected by the magnitudes of magnetic fields in the vortex states. At very low field, $M(E = 0, \mathbf{r})$ has a sharp peak at a vortex center. With increasing magnetic fields, the peak height decrease, and $M(E = 0, \mathbf{r} = 0)$ becomes local minimum at the vortex center. The spin-polarized Majorana state $M(E = 0, \mathbf{r})$ may be a key features to identify the helical $p$-wave state. We hope that the spin-polarized STM measurements will be performed to observe $M(E = 0, \mathbf{r})$ around vortices in candidate superconductors of helical $p$-wave state.

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