Spin-current induced around half-quantum vortices in chiral p-wave superconducting states

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Abstract. We study the electronic state around a half-quantum vortex (HQV) in a chiral p-wave superconductor based on a square lattice three band tight-binding model by means of the Bogoliubov-de Gennes theory. In particular, the spatial distribution of charge and spin currents are mainly discussed. This analysis shows that the spin current is strengthened between the neighboring HQVs, resulting in the energy cost for HQV formation.

1. Introduction
Non-integer quantum vortices are allowed in multicomponent superfluids or superconductors\cite{1}. In particular, a half-quantum vortex (HQV) expected in the chiral p-wave spin-triplet pairing superconducting state is an exciting topic due to Majorana fermion zero modes predicted at the vortex cores\cite{2}. A HQV is formed by a $\pi$-rotation of the superconducting phase and also a $\pi$-rotation of the d-vector around the vortex core. Thus the magnetic flux through HQV is one-half of the flux quantum. HQVs are topologically allowed in spin-triplet superconducting states, however, whether the energy of a HQV or a pair of HQVs is lower than that of an integer quantum vortex (IQV) is a question to be carefully considered, largely because the spin current accompanied by a HQV increases the energy of a system\cite{3}.

Stability conditions of HQVs have been analyzed mainly based on the phenomenological Ginzburg-Landau (GL) theory. These studies have predicted that HQVs are unstable unless the ratio of the spin fluid density to superfluid density $\rho_{sp}/\rho_s$ is sufficiently small\cite{3}, and unless the spin-orbit coupling is sufficiently small\cite{4, 5}. To argue these conditions in the systems of realistic materials, features of materials should be considered, for example, the anisotropy of the pairing interaction and the Fermi surface structure. Appropriate consideration of these features needs microscopic analyses in parallel with the GL theory.

In this paper, as a first step, we investigate the distribution of spin current around a HQV in a chiral p-wave equal spin pairing superconducting state in a square lattice three band tight-binding model with the pairing interaction between nearest-neighbor sites based on the Bogoliubov-de Gennes (BdG) theory. We also compare the electronic energy of a pair of HQVs with that of an IQV in our system. In this study, we suppose the system of a two-dimensional RuO$_2$ plane in Sr$_2$RuO$_4$, which is strongly believed that a chiral p-wave superconducting state is realized\cite{6}. The Fermi surfaces of Sr$_2$RuO$_4$ are formed by three band, $\alpha$, $\beta$ band, largely derived
from the $d_{yz}$ and $d_{zx}$ orbitals of Ru, and $\gamma$ band, from the $d_{xy}$ orbital of Ru.[6]. We consider all three bands and introduce the spin-orbit coupling to reproduce the Fermi surface of Sr$_2$RuO$_4$.

2. Model and Method
The Hamiltonian of a three band Hubbard model used in this study is given as[7]

$$\mathcal{H} = \mathcal{H}_{\alpha\beta} + \mathcal{H}_\gamma + \mathcal{H}_W + \mathcal{H}_{SO} + \mathcal{H}_\mu$$

$$\mathcal{H}_{\alpha\beta} = -\sum_{i\sigma} \left( t_{\alpha\beta_i} c_{\alpha\beta_i}^\dagger c_{\alpha\beta_i} + t_{\alpha\beta_i}^{\dagger} c_{\alpha\beta_i}^\dagger c_{\alpha\beta_i} + \text{H.c.} \right)$$

$$\mathcal{H}_\gamma = -\sum_{i\sigma} \left( t_{\gamma_i} c_{\gamma_i}^\dagger c_{\gamma_i} + t_{\gamma_i}^{\dagger} c_{\gamma_i}^\dagger c_{\gamma_i} + \text{H.c.} \right)$$

$$\mathcal{H}_W = -W \sum_{i\sigma\sigma'} \left( \sum_{m=1,2,3} n_{mi+\hat{x}} n_{mi+\hat{\sigma}} + \sum_{m=2,3} n_{mi+\hat{y}} n_{mi+\hat{\sigma}} \right)$$

$$\mathcal{H}_{SO} = -i \lambda \sum_{m=1,2,3} \sum_{\sigma\sigma'} \epsilon_{mm''\sigma'} c_{m\sigma}^\dagger \sigma_{\sigma\sigma'}^m c_{m''\sigma'}$$

$$\mathcal{H}_\mu = -\mu \sum_{m} \hat{n}_m - \delta \sum_{m} n_{3m}$$

where $m$ denotes the orbital number ($m=1, 2, 3$), and $\hat{x}$ ($\hat{y}$) denotes the difference of nearest-neighbor sites in the $x$ ($y$) direction. Numbers 1, 2, 3 correspond to $d_{yz}$, $d_{zx}$, $d_{xy}$ orbitals, respectively. Site symbol $i$ involves a two-dimensional position, i.e. $i = (i_x, i_y)$. Nearest-neighbor (next-nearest-neighbor) hopping amplitude in $d_{yz}$, $d_{zx}$ orbitals and $d_{xy}$ orbitals are denoted as $t_{\alpha\beta ij}$ ($t'_{\alpha\beta ij}$) and $t_{\gamma ij}$ ($t'_{\gamma ij}$), respectively. The uniform magnetic field is introduced in terms of the Peierls phase of the hopping term as

$$t_{\alpha\beta\gamma ij} = t_{\alpha\beta\gamma ij} \exp \left[ i \frac{\pi}{Q_0} \int_{r_i}^{r_j} \mathbf{A}(r) \cdot \mathbf{dr} \right] \quad \text{and} \quad t'_{\alpha\beta\gamma ij} = t'_{\alpha\beta\gamma ij} \exp \left[ i \frac{\pi}{Q_0} \int_{r_i}^{r_j} \mathbf{A}(r) \cdot \mathbf{dr} \right].$$

$\lambda$ and $\delta$ stand for the the amplitude of the spin-orbit coupling and the energy difference between the $d_{yz}$ or $d_{zx}$ orbital and the $d_{xy}$ orbital. $\epsilon_{mm''\sigma'}$ and $\sigma$ in $\mathcal{H}_{SO}$ are the Levi-Civita symbol and the Pauli matrix, respectively. $\mu$ is the chemical potential. We set $t_{\alpha\beta} = 0.1t_{\alpha\beta}$, $t_{\gamma} = 0.7t_{\alpha\beta}$, $t'_\alpha = 0.3t_{\alpha\beta}$, $\lambda = 0.1t_{\alpha\beta}$, $\delta = 0.065t_{\alpha\beta}$, and $\mu = t_{\alpha\beta}$ then a filling $n \simeq 4$ to reproduce the Fermi surface topology of Sr$_2$RuO$_4$[7]. The third term in the Hamiltonian (1) represents nearest-neighbor attractive interactions, then $W > 0$. We introduce the BCS-type mean field using superconducting order parameters $\Delta_{mij\sigma} = W(\epsilon_{m\sigma} c_{m\sigma})$, which are corresponding to the chiral p-wave gap function written as $\Delta(k) = \sin k_x + i \sin k_y$ in wavenumber space. Total order parameter is defined as $\Delta_{ij\sigma} = \Delta_{ij\sigma} + \Delta_{ij\sigma} + \Delta_{ij\sigma}$. We assume here for simplicity the d-vector lies within the ab-plane despite that it is parallel to the c-axis in Sr$_2$RuO$_4$[6].

We numerically solve the Bogoliubov-de Gennes (BdG) and the gap equation derived from the Hamiltonian (1) and the superconducting order parameters self-consistently, with $W = 0.75t_{\alpha\beta}$. To make the Peierls phase compatible with vortex lattice symmetry, we need a magnetic unit cell with $2N \times N$ sites including two vortices[8]. In this case, by the appropriate choice of gauge, the order parameter $\Delta_{ij\sigma}$ has a translational symmetry with respect to the magnetic unit cell. A position of a vortex center is located just on a site if $N$ is odd, and in the middle of square plaquette surrounded by four sites if $N$ is even. Here we take $N = 15$ with periodic boundary condition.
3. Results and Discussion

Figure 1 shows the local density of states (LDOS) without magnetic field, i.e. in a uniform chiral p-wave system. The LDOS exhibits a nodeless (full gap) structure of the superconducting gap expected in the chiral p-wave superconductor. In Fig. 2, we present the spatial distributions of the amplitude of the superconducting order parameters around the cores of HQVs with the distributions of the up- and down-spin current. We define the average of the superconducting order parameters around a site \( \Delta_{j\sigma} = (\Delta_{jj+ix \sigma} + \Delta_{j-ixj \sigma} - i\Delta_{jj+iy \sigma} - i\Delta_{j-iyj \sigma})/4 \). We see that up-spin component and down-spin component form HQVs independently in Fig. 2 accompanied by the each spin current around the core of HQVs. We note here that the position of HQVs depend on the initial conditions for BdG calculations. The furrows of the superconducting order parameter parallel to the axial directions result from the (quasi-) one-dimensional property of \( d_{yz} \) and \( d_{zx} \) orbitals have the long coherent lengths in the each direction. The electronic energy of this system is calculated, \( E_{HQV} = -10.020 t_{\alpha \beta} \), while the energy of the system where an IQV is formed in our calculation \( E_{IQV} = -10.004 t_{\alpha \beta} \). The difference between the pair of HQV and IQV, \( \Delta E = |E_{HQV} - E_{IQV}|/E_{HQV} \sim 0.002 \), is fairly small, therefore, it is not suitable to discuss the energetic stability of HQVs within the present calculation framework, although the energy of HQVs is slightly lower than that of an IQV. Figure 3 shows the spatial distribution of the total charge and spin currents around the cores of HQVs. The charge current is weakened between the HQVs and is strengthened outside, while the spin current is strengthened between the HQVs and is weakened outside as prefigured from Fig 2. The free energy of spin current is represented as \( T_{sp} = J_{sp}^2 / (2\rho_{sp} \) \( (J_{sp} \) and \( \rho_{sp} \) are amplitude of spin current and spin current density), therefore, the enhance of spin current between the neighboring HQVs results in the energy cost for HQV formation.

4. Summary

We have investigated the distribution of spin current, which makes a HQV unstable, around a HQV in a chiral p-wave equal spin pairing superconducting state in a square lattice three band
Figure 2. Spatial distributions of the amplitude of the superconducting order parameters, $|\Delta_j^1|$ (a) and $|\Delta_j^2|$ (b), around the cores of HQVs. The amplitude is normalized by that in a system without magnetic field, $|\Delta^B_j|$. Blue vectors in the $z=0$ plane represent the up-spin (a) and down-spin (b) currents. Red dots indicate the cores of HQVs.

Figure 3. Distribution of the total charge (a) and spin (b) current around half quantum vortecies. Red dots indicate the cores of HQVs.

tight-binding model based on the Bogoliubov-de Gennes (BdG) theory. We confirmed that the spin current is strengthened between the HQVs and is weakened outside, therefore, the energy of a system tends to become high between HQVs.

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