

Excitation spectrum of Josephson vortices on surface superconductor

Takuto Kawakami¹, Yuki Nagai², Shunsuke Yoshizawa¹, Howon Kim³, Yukio Hasegawa³, Tomonobu Nakayama¹, Takashi Uchihashi¹, and Xiao Hu¹

¹ International Center for Material Nanoarchitectonics (WPI-MANA), National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba 305-0044, Japan, ²CCSE, Japan Atomic Energy Agency, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8587 Japan, ³The Institute for Solid State Physics, University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8587, Japan

E-mail: kawakami.takuto@nims.go.jp

Abstract. Motivated by recent discovery of superconductivity in monatomic In layer on silicon surfaces and scanning tunneling microscopy and spectroscopy (STM/STS) measurement, we study the excitation spectrum of vortex in a two-dimensional superconductor. According to the STM/STS measurements, the zero bias conductance (ZBC) for the vortices trapped at atomic steps has an anisotropic shape. In order to understand the experimental results, we study the local density of states (LDOS) as a function of strength of hopping integral at atomic steps. Our analysis is based on the self-consistent solution of the Bogoliubov-de Gennes equation coupled with a gap equation. The amplitude of the order parameter is restored at the vortex core and the phase winding becomes anisotropic with decreasing the hopping strength at atomic steps. The zero energy LDOS stretches along the step and the intensity decreases associated with the deformation of the order parameter. By comparing the theoretical results with experiments, we conclude Josephson vortices in 2D superconductivity have been observed.

1. Introduction

Experimental progress in observing the superconductivity in the monatomic layer on the silicon surface reconstruction [1, 2, 3] open new frontiers for exploring the two-dimensional superconductivity. One of the interesting points of this system is the existence of atomic steps of the silicon surface separating terraces. The atomic steps inherently interfere the electron motion between neighboring two-dimensional terraces. The observation of supercurrent thorough the atomic steps [2, 3] provides a scenario that this system behaves as Josephson junctions [2].

Very recently, the ZBC of the scanning tunneling spectroscopy (STS) measurement in the superconducting In monatomic layer on the Si(111)-($\sqrt{7}\times\sqrt{3}$) reconstruction has been reported as follows [4]. Under the magnetic field perpendicular to the surface, spots of ZBC appear both on the atomic steps and on the terrace region. The spots on the atomic steps have an elliptic shape with the longer axis parallel to the steps while those on the terrace are cylindrically symmetric. In addition, their aspect ratio differs depending on the atomic steps and the longer spots have smaller intensity.

The STS measurement images vortex shape through direct observation of quasiparticle excitation spectrum with high spatial resolution. The anisotropy of STS image should depend



on the strength of interterrace Josephson coupling. Nevertheless, most of the theoretical works for the Josephson vortex [5, 6, 7] are based on the London or Ginzburg-Landau theory, which do not include information of quasiparticles. In this paper, we study the excitation spectrum in this system by using Bogoliubov-de Gennes (BdG) theory. We investigate the spatial profile of order parameter and excitation spectrum of vortices in a self-consistent way and analyze the contribution of the quasiparticles. We conclude that the vortex image with strong anisotropic ZBC in STS measurements [4] can be considered as Josephson vortex in the surface superconductor.

2. Model and Formulation

We theoretically analyze the excitation spectrum of vortex core in terms of BdG theory. We use a two-dimensional tight-binding model with a square lattice. The BdG equation is described as

$$\sum_j \begin{pmatrix} \hat{K}_{i,j} & \hat{\Delta}_{i,j} \\ \hat{\Delta}_{j,i}^* & -\hat{K}_{i,j}^* \end{pmatrix} \begin{pmatrix} u_\gamma(\mathbf{r}_j) \\ v_\gamma(\mathbf{r}_j) \end{pmatrix} = E_\gamma \begin{pmatrix} u_\gamma(\mathbf{r}_i) \\ v_\gamma(\mathbf{r}_i) \end{pmatrix}. \quad (1)$$

The single particle part is $\hat{K}_{i,j} = -t_{ij} \exp \left[i(\pi/\Phi_0) \int_{\mathbf{r}_i}^{\mathbf{r}_j} \mathbf{A}(\mathbf{r}') \cdot d\mathbf{r}' \right] - \mu \delta_{ij}$, where t_{ij} is the hopping strength between the nearest neighbor atomic sites, \mathbf{A} is the vector potential due to the external field, and $\Phi_0 = h/2e$ is the flux quantum.

We consider the vortex lattice by using the periodic boundary condition

$$\begin{pmatrix} u_\gamma(\mathbf{r} + \mathbf{R}) \\ v_\gamma(\mathbf{r} + \mathbf{R}) \end{pmatrix} = e^{i\mathbf{k} \cdot \mathbf{R}} e^{i\hat{\sigma}_z \chi(\mathbf{r}, \mathbf{R})} \begin{pmatrix} u_\gamma(\mathbf{r}) \\ v_\gamma(\mathbf{r}) \end{pmatrix}, \quad (2)$$

where $\mathbf{R}(p_1, p_2) = \sum_\alpha p_\alpha \mathbf{a}_\alpha$ is the two-dimensional Bravais lattice vector and \mathbf{a}_α ($\alpha \in 1, 2$) is the primitive translation vector of the vortex lattice; \mathbf{k} is the Bloch vector satisfying $\mathbf{k} \cdot \mathbf{R} = 2\pi \sum_\alpha p_\alpha q_\alpha / N_\alpha$ with $p_\alpha, q_\alpha \in Z$ and the system size $N_\alpha |\mathbf{a}_\alpha|$ for \mathbf{a}_α -direction; and the condition $\chi(\mathbf{r}, \mathbf{R}) = \frac{n\pi}{2} [\mathbf{g}(\mathbf{R}) \cdot \mathbf{r} + p_1 p_2]$, where $\mathbf{r} = \sum_\alpha r_\alpha \hat{\mathbf{a}}_\alpha$, $\hat{\mathbf{a}}_\alpha = \mathbf{a}_\alpha / |\mathbf{a}_\alpha|$ and $\mathbf{g} = \sum_{\alpha\beta} \epsilon_{\alpha\beta} p_\alpha \hat{\mathbf{a}}_\beta$ [12, 10]. We use the symmetric gauge $\mathbf{A} = \frac{1}{2} \mathbf{H} \times \mathbf{r}$ which generate n vortices within the unit cell $\mathbf{a}_1 \times \mathbf{a}_2$.

For simplicity, we consider a straight terrace step with one atomic spacing and model it by modulating the hopping strength along the step $t_{ij} = t_s$ while keeping the hopping strength as a constant $t_{ij} = t$ elsewhere as shown in Fig. 1 (a), (b). In this work, we deal with square geometry including 192×192 atomic sites.

We obtain the following gap function and LDOS

$$\Delta(\mathbf{r}_i) = \delta_{ij} V \sum_\gamma u_\gamma(\mathbf{r}_i) v_\gamma(\mathbf{r}_j) f(E_\gamma) = \delta_{ij} V \int dE' \sum_\gamma u_\gamma(\mathbf{r}_i) v_\gamma(\mathbf{r}_j) f(E_\gamma) \delta(E' - E_\gamma), \quad (3)$$

$$\mathcal{N}(E, \mathbf{r}) = \sum_\gamma |u_\gamma(\mathbf{r})|^2 \delta(E - E_\gamma). \quad (4)$$

According to the Chebyshev-polynomial expansion scheme [8, 9, 11], we expand the Dirac delta function as

$$\delta(\omega - \omega') \sim \sum_{n=0}^{n_c} \frac{2T_n(\omega)T_n(\omega')}{\pi \sqrt{1 - \omega^2} (1 + \delta_{n,0})}, \quad (5)$$

where $T_n(\omega)$ is the n -th Chebyshev polynomial within the interval $\omega \in [-1, 1]$. Here, we rescale the Hamiltonian as $\hat{K}'_{i,j} = \hat{K}_{i,j}/a$ and $\hat{\Delta}'_{i,j} = \hat{\Delta}_{i,j}/a$ with parameters $a = 20t$ and set the cutoff constant $n_c = 1000$. In order to examine the origin of the behavior of the DOS in terms of quantized quasiparticle, we also calculate several dozen of eigenvalues and wave functions of quasiparticles by using shifted-invert Arnoldi algorithm [13].

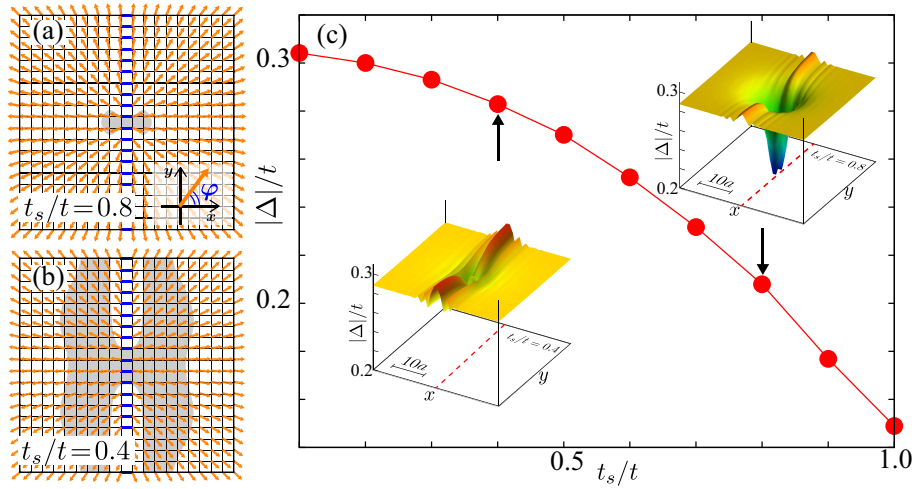


Figure 1. Spatial profile of order parameter. The direction of an arrow denotes the phase $\varphi(\mathbf{r})$ of order parameter on each atomic site for hopping strength $t_s/t = 0.8$ (a) and 0.4 (b). The thick (blue) bonds denote the junction where the hopping strength $t_{ij} = t_s < t$. In the shaded region, the phase gradient is relatively small. The main panel in (c) shows the amplitude $|\Delta(\mathbf{r})|$ of order parameter at the center of vortex. The left (right) inset shows the two-dimensional profile of the amplitude $|\Delta(\mathbf{r})|$ for $t_s/t = 0.4$ (0.8). Parameters are set as $\mu/t = -2.5$ and $V/t = 3.0$.

3. Results

Figures 1 (a), (b) show profiles of the phase $\varphi(\mathbf{r})$ of order parameter $\Delta = |\Delta(\mathbf{r})|\exp[i\varphi(\mathbf{r})]$ for hopping strength at terrace step $t_s/t = 0.8$ and 0.4 . For $t_s/t \sim 1$ (Fig. 1(a)), the profile is almost cylindrically symmetric. As the hopping strength at step t_s/t is reduced, the phase gradient along the step $\partial_y \varphi$ becomes smaller near the vortex core as shown in Fig. 1(b), which reduces the total kinetic energy. The amplitude of the order parameter for $t_s/t \sim 1$ is suppressed significantly at the vortex core $r \leq \xi$ ($\xi = v_F/\Delta_0$) (Fig. 1(c)). As the hopping strength at the step is reduced, the suppression of amplitude at vortex becomes weaker, and invisible for small hopping $t_s/t \ll 1$; simultaneously the healing length along the step becomes much larger than the vertical direction (see the insets in Fig. 1(c)). It is intriguing to observe that, as in inset of Figs. 1(c), the order parameter is enhanced at the terrace step with weak hopping strength, due to the interference of quasiparticles scattered by the step.

Figure 2 shows t_s -dependence of the quasiparticle eigenstates, which is obtained by using the self-consistent solution $\Delta(\mathbf{r})$ in Fig. 1. For $t_s/t \sim 1$, the vortex core bound state has mini gap $\delta E \sim \Delta^2/E_F$ [14]. With decreasing hopping t_s/t , the mini gap becomes larger as shown in Fig. 2(a). Figures 2(b) and (c) show the wave functions $u_{\gamma=1,2}(\mathbf{r})$ of the lowest and 2nd lowest energy states for $t_s/t = 0.8$ and 0.4 . The squared absolute value of wave function $|u_{\gamma}(\mathbf{r})|^2$ is proportional to the local density of states $\mathcal{N}(\pm E_{\gamma}, \mathbf{r})$. When the hopping strength is $t_s/t = 1$, $|u_{\gamma=1,2}(\mathbf{r})|$ exhibits four fold rotational symmetry originating from Fermi surface. As shown in Fig. 2(c), the tail of wave function approaches to the step for $t_s/t < 1$. This can be understood as follows. For $t_s/t < 1$, the phase gradient of order parameter in Fig. 2(b) becomes smaller on left and right region sandwiching the vortex core (see shaded region in Fig. 1(a) and (b)). Since the external magnetic field cannot be canceled by the phase gradient, low energy quasiparticles tend to avoid this region in order to save kinetic energy. Consequently, the low energy quasiparticle $u(\mathbf{r})$ is suppressed more strongly in this region with reduction of t_s/t , and the lowest energy wave function has elongated shape along y -direction. In particular, at the region close to the vortex $r \sim \xi$, the peak of the lowest energy wave function becomes elliptic and longer axis is

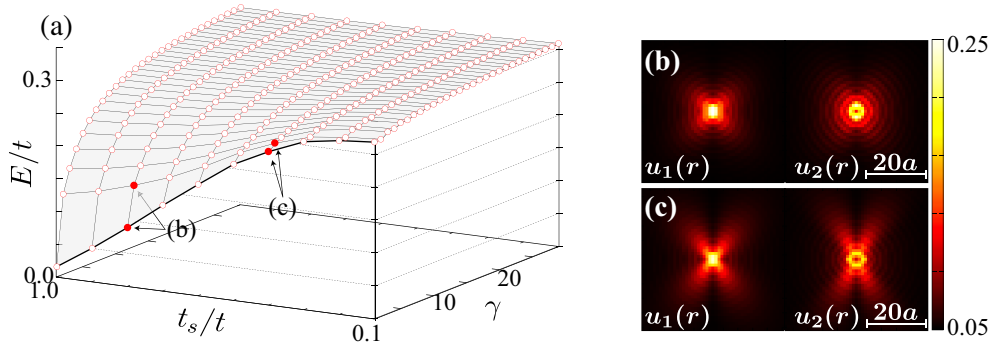


Figure 2. Eigen energy E of γ -th lowest eigenstates as a function of t_s/t (a) and the spatial profile of the wave function of lowest and second lowest eigenstates $|u_{\gamma=1,2}(\mathbf{r})|$ for $t_s/t=0.8$ (b) and for $t_s/t=0.4$ (c). The filled symbol in (a) denotes the eigenstate shown in (b) and (c).

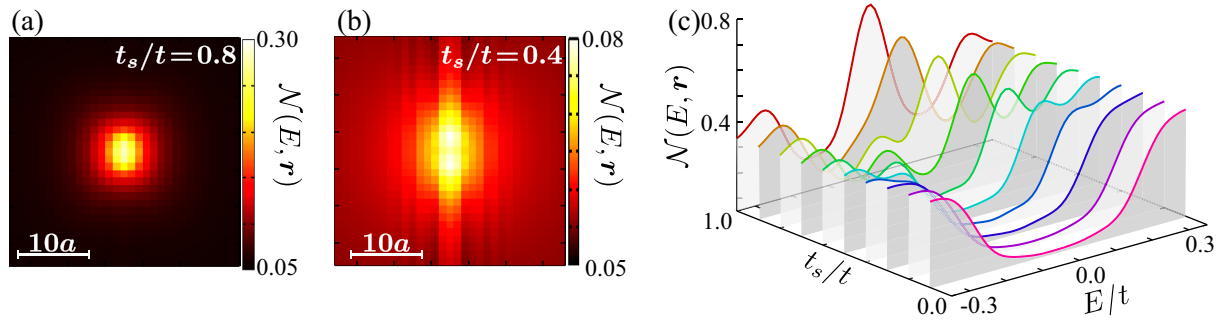


Figure 3. Two dimensional profile of the zero-energy density of states $\mathcal{N}(E=0, \mathbf{r})$ for hopping strength $t_s/t=0.8$ (a) and 0.4 (b), and the LDOS at the vortex center as a function of the energy and hopping t_s/t (c). We set the other parameters $\mu/t=-2.5$ and $V/t=3.0$.

y -direction.

Figures 3 (a), (b) show the zero-energy DOS (ZDOS) $\mathcal{N}(E=0, \mathbf{r})$ associated with the order parameter $\Delta(\mathbf{r})$ shown in Fig. 1. For $t_s/t \sim 1$, the ZDOS is cylindrically symmetric (Fig. 3 (a)) and becomes elliptic when the hopping strength reduces (Fig. 3 (b)) originating from the shape of elliptic peak of the lowest wave function $|u_1(\mathbf{r})|$. Figure 3 (c) shows the LDOS at the vortex center as a function of energy E and hopping integral t_s/t along the terrace step. The value of ZDOS decreases with reduction of t_s/t , and for small $t_s/t \ll 1$, the vortex shape cannot be distinguished as ZBC spots of STS signal. On the other hand, the mini gap at the vortex center increases with reduction of the t_s/t . This corresponds to excitation of $\gamma=1$ in Fig. 2(a). We suggest that the strength of Josephson coupling for the terrace step may be estimated by comparing the mini gap in STS at the vortex center with theoretical one shown in Fig. 3(c).

4. Summary

We have investigated the excitation spectrum at the vortex on atomic steps which has electron hopping strength t_s weaker than bulk t by using the Bogoliubov-de Gennes framework. The results are consistent with the experimental observations. We conclude that Josephson vortices have been observed at the step with weak coupling.

Acknowledgments

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