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Time-reversal symmetry breaking and gapped surface states due to spontaneous emergence of new order in *d*-wave nanoislands

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We solve the Bogoliubov-de Gennes equations self-consistently for the d-wave order parameter in nanoscale d-wave systems with [110] surfaces and show that spontaneous time-reversal symmetry (TRS) breaking occurs at low temperatures due to a spontaneously induced complex order parameter of extended s-wave symmetry. The Andreev surface bound states, which are protected by a one-dimensional (1D) topological invariant in the presence of TRS, are gapped by the emergence of this new order parameter. The extended s-wave order parameter is localized within a narrow region near the surfaces, which is consistent with the fact that topological protection of the gapless Andreev surface states is characterized by the 1D topological invariant. In this TRS-breaking phase, not only is the complex order parameter induced, but also the d-wave order parameter itself becomes complex. Furthermore, the disappearance of topological protection brings about novel vortex phenomena near the surfaces. We show that vortex-antivortex pairs are formed in the extended s-wave order parameter along the surfaces if the side length of a nanoisland or the width of an infinitely long nanoribbon is relatively large.

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Symmetry is at the heart of both high-energy and condensed matter physics. Symmetry breaking underlies not only mass in our universe, but also superconductivity in metals. Symmetry classifies topological materials [1]. Symmetry protects topological order, such as the Haldane phase in a spin-1 chain with time-reversal, parity, and translation symmetries [2].

Time-reversal symmetry (TRS) and topological phenomena associated with it are hot topics in condensed matter physics. Sato *et al.* have shown the bulk-edge correspondence between the zero-energy Andreev bound states on [110] surfaces of a high-T_c cuprate superconductor and a topological invariant protected by TRS [3]. The Andreev bound states are understood as arising from the sign-changing property of the $d_{x^2-y^2}$-wave order parameter [4,5]. From the topological point of view, such zero-energy surface states are robust as the bulk-edge correspondence ensures the existence of gapless surface states in a topologically nontrivial system [6,7]. In a 2D nodal d-wave superconductor, a 1D topological invariant as a function of momentum along the [110] surface can be defined, through which TRS provides topological protection of the Andreev bound states [3].

Gapless surface states can become gapped when the corresponding symmetry is broken. The surface states in a topological insulator acquire a gap as a result of spontaneous or nonspontaneous breaking of TRS [8,9]. An example of spontaneous TRS breaking is the anomalous Hall effect in tetradymite semiconductors, where the ferromagnetic order parameter induced by the Van Vleck type spin susceptibility results in the gapped surface states [9]. Splitting of the Andreev bound states due to spontaneously induced surface currents, i.e., spontaneous TRS breaking has been discussed by assuming the existence of a subdominant order parameter with relative phase $\pi/2$, which is stabilized on the [110] surface of a d-wave superconductor [5,10–12]. This has been a controversial topic in the past two decades owing to contradictory experimental results on high-T_c cuprates [13,14]. A recent experiment, however, has clearly detected a full gap in the excitation spectrum that is consistent with spontaneously broken TRS in a nanoscale $YBa_2Cu_3O_{7-\delta}$ island [13]. By introducing an intrinsic s-wave pairing interaction and controlling its strength in terms of the ratio of the bare bulk transition temperature to that of the d-wave order, Black-Schaffer *et al.* [15] have found that the resulting $d+is$ symmetry is consistent with the experimental findings of Ref. [13].

Vorontsov has proposed that films of a d-wave superconductor at low temperatures can exhibit unusual superconducting phases due to transverse confinement, with TRS or continuous translational symmetry broken spontaneously [16]. Recently, a theoretical study of d-wave superconducting nanoislands within the quasiclassical Eilenberger framework with no subdominant pairing channel has predicted spontaneous breaking of TRS at low temperatures, where staggered fractional vortices are formed along the surfaces, each containing the zero-energy Andreev bound states at its center [14]. The quasiclassical formulation, however, is limited in that it cannot resolve individual quasiparticle excitations and it is not a good approximation for high-T_c cuprates as it requires the coherence length to be much larger than $1/k_F$.

In this paper, by solving the Bogoliubov-de Gennes (BdG) equations [17] self-consistently for the d-wave order parameter in $d_{x^2-y^2}$-wave nanoislands with [110] surfaces, we show that spontaneous TRS breaking occurs at low temperatures due to *spontaneous* emergence of a new complex order parameter. The spontaneous disappearance of topological protection is accompanied by this new order parameter that is induced only near the surfaces below a certain temperature, which is lower than the superconducting transition temperature T_c. This order parameter has extended s-wave symmetry, and it characterizes the energy gap of the split Andreev bound states on the surfaces, as schematically illustrated in Fig. 1(b) [18]. This is analogous to the gap opening on surfaces of a topological insulator originating from the spontaneously

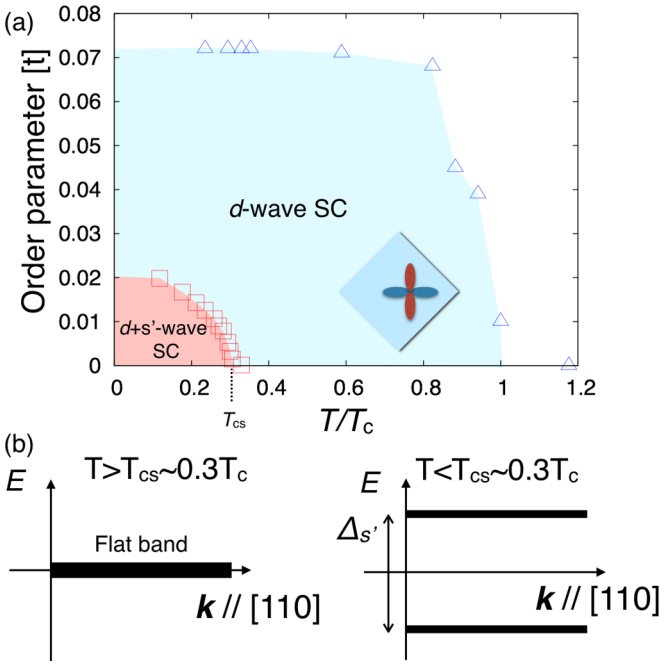

FIG. 1. (a) Temperature dependence of the order parameters in the d-wave nanoisland. The system size is $L_x \times L_y = 96 \times 96$ and the critical temperature is $T_c = 0.085t$. (b) Schematic illustration of the eigenvalues around zero energy. The zero-energy Andreev bound states on the [110] surface are gapped because of spontaneous time-reversal symmetry breaking. The gap size is characterized by the extended s-wave order parameter that is induced along the surfaces.

induced ferromagnetic order [9]. We find that the phase transition is of second order, similarly to the transition to the TRS-breaking state within the purely d-wave phase found by the quasiclassical Eilenberger approach [14]. Our approach beyond the quasiclassical theory allows us to accurately study the discrete spectrum of quasiparticle excitation, unraveling a close relation between the spontaneously induced order parameter and the surface excitation. The extended s-wave order parameter is localized within a narrow region along the surfaces: This is compatible with the fact that the topological protection is characterized by a 1D topological invariant defined along the surfaces. We also find that when the phase transition to this TRS-breaking phase occurs, the d-wave order parameter itself becomes complex.

To summarize, spontaneous disappearance of topological protection occurs in a $d_{x^2-y^2}$-wave nanoisland with [110] surfaces as a second-order phase transition, leading to the gapped surface excitation originating from the formation of extended s-wave Cooper pairs near the surfaces. This is an example of a spontaneously induced order parameter being behind the breaking of the symmetry that would otherwise protect the gapless surface states. Furthermore, the disappearance of topological protection brings about novel vortex phenomena near the surfaces. We show that vortex-antivortex pairs are formed along the surfaces of a $d_{x^2-y^2}$-wave nanoisland when the side length is relatively long. The phase winding occurs in the extended s-wave order parameter, where there is a 2π phase winding around each vortex or antivortex. It is shown in the Supplemental Material [18] that the disappearance of zero-energy surface states due to spontaneous TRS breaking can be understood in terms of the fundamental group [19] for homogeneous systems with spin-singlet pairing. The fundamental group corresponding to the ground-state manifold changes from $\pi_1(S^1) = \mathbb{Z}$ to $\pi_1(S^2) = 0$ as the TRS-breaking order emerges [18,20].

We consider the tight-binding model Hamiltonian $\mathcal{H} = \mathcal{H}_{\rm BCS} + \mathcal{H}_{\rm fab}$. Here the generalized Bardeen-Cooper-Schrieffer (BCS) Hamiltonian for d-wave superconductivity is $\mathcal{H}_{\rm BCS} = \sum_{ij,\sigma}(-t_{ij} - \mu)c^\dagger_{i\sigma}c_{j\sigma} + \sum_{ij}[\Delta_{ij}c^\dagger_{i\uparrow}c^\dagger_{j\downarrow} + {\rm H.c.}]$, where $c^\dagger_{i\sigma}$ creates the electron with spin σ at site i and μ denotes the chemical potential. The hopping is restricted within nearest-neighbor sites for simplicity. We use the unit system with $\hbar = k_B = 1$. The Hamiltonian for the fabrication potential $\mathcal{H}_{\rm fab}$ is written as $\mathcal{H}_{\rm fab} = \sum_{i,\sigma} V_i c^\dagger_{i\sigma}c_{i\sigma}$, where the potential $V_i = 0$ $(500t)$ inside (outside) the nanoisland. One can diagonalize $\mathcal{H}$ to solve the BdG equations expressed as

$$\sum_j \begin{pmatrix} [\hat{H}^{\rm N}]_{ij} & [\hat{\Delta}]_{ij} \\ [\hat{\Delta}^\dagger]_{ij} & -[\hat{H}^{\rm N*}]_{ij} \end{pmatrix} \begin{pmatrix} u_\gamma(\boldsymbol{r}_j) \\ v_\gamma(\boldsymbol{r}_j) \end{pmatrix} = E_\gamma \begin{pmatrix} u_\gamma(\boldsymbol{r}_i) \\ v_\gamma(\boldsymbol{r}_i) \end{pmatrix}. \quad (1)$$

Here $[\hat{H}^{\rm N}]_{ij} = -t_{ij} - (\mu - V_i)\delta_{ij}$ and $[\hat{\Delta}]_{ij} = V_{ij}\sum_{\gamma=1}^{2N} u_\gamma(\boldsymbol{r}_j)v^*_\gamma(\boldsymbol{r}_i)f(E_\gamma)$, where N is the number of lattice sites, V_{ij} denotes the pairing interaction, and $f(x)$ is the Fermi-Dirac distribution function. For the results presented below, the chemical potential is fixed to be $\mu = -1.5t$ and the pairing interaction is nonzero only between nearest-neighbor sites, $V_{ij} \equiv U = -2t$, so that the resulting order parameter is purely of the $d_{x^2-y^2}$-wave symmetry. The order parameter at site i is given in terms of the d-wave mean fields by

$$\Delta_{d,i} = (\Delta_{\hat{x},i} + \Delta_{-\hat{x},i} - \Delta_{\hat{y},i} - \Delta_{-\hat{y},i})/4 \quad (2)$$

with $\Delta_{\pm\hat{e},i} = \Delta(\boldsymbol{r}_i, \boldsymbol{r}_i \pm \hat{e})$, where $\hat{x}$ and $\hat{y}$ denote the unit vectors in the square lattice. Considering two-dimensional systems, we assume that the field penetration depth λ is infinity. We use pure d-wave mean fields with randomly-distributed phases as the initial guess for our self-consistent calculation.

The BdG equations (1) are solved self-consistently along with the d-wave gap equation with the use of the reduced-shifted-conjugate-gradient (RSCG) method [21]. The mean field $\langle c_i c_j \rangle$ can be expressed as $\langle c_i c_j \rangle = T\sum_{n=-n_c}^{n_c} \boldsymbol{e}(j)^{\rm T}\boldsymbol{x}(i,\omega_n)$, where $[\boldsymbol{e}(i)]_\gamma = \delta_{i\gamma}$ and n_c is the cutoff parameter for the Matsubara frequencies, $\omega_n = (2n + 1)\pi T$. The $2N$-dimensional vector $\boldsymbol{x}(i,\omega_n)$ is obtained by solving the linear equations defined by $(i\omega_n \hat{I} - \hat{H}_{\rm BdG})\boldsymbol{x}(i,\omega_n) = \boldsymbol{h}(i)$, with $[\boldsymbol{h}(i)]_\gamma = \delta_{i+N\gamma}$ and the BdG matrix $\hat{H}_{\rm BdG}$ on the left-hand side (LHS) of Eq. (1). These linear equations with different frequencies can be solved simultaneously by the RSCG method [21]. We use the maximum Matsubara frequency $\omega_c = 240\pi = \pi T(2n_c + 1)$. A criterion for the residual is set to 0.1, which is small enough to obtain accurate Green's functions [21].

To find the true ground state on the mean-field level, once self-consistency has been achieved, we calculate the thermodynamic potential given as [22,23]

$$\Omega_s = -T\sum_{\gamma=1}^{2N} \ln\left[1 + \exp\left(\frac{E_\gamma}{T}\right)\right] - \sum_{ij}\frac{|[\hat{\Delta}]_{ij}|^2}{U}. \quad (3)$$

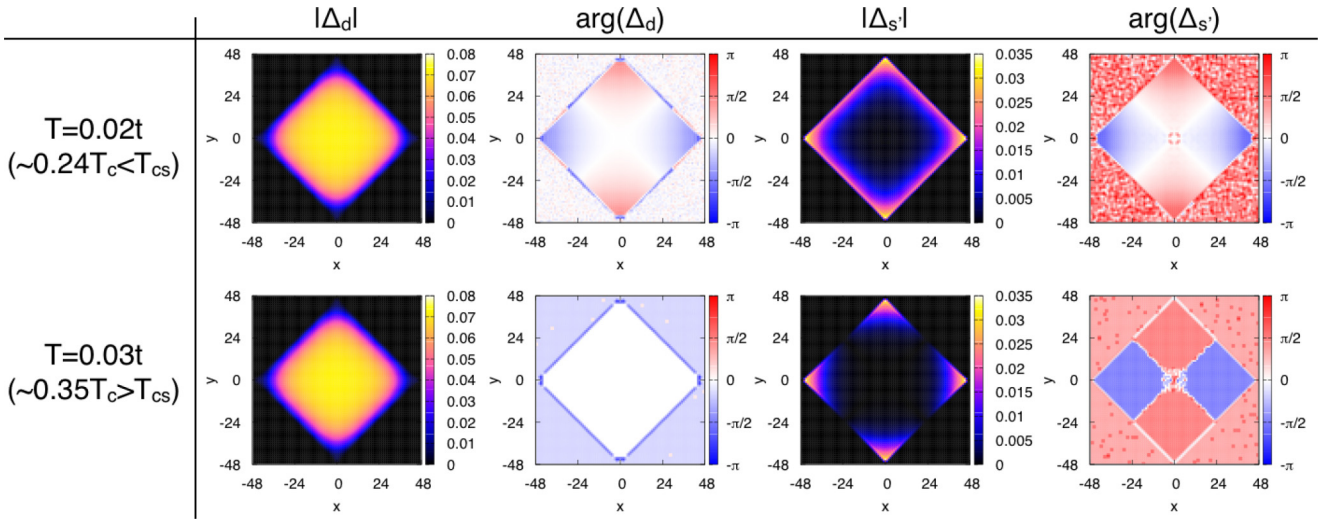

FIG. 2. d-wave and extended s-wave order parameters below and above T_{cs}. The system size is $L_x \times L_y = 96 \times 96$. To clearly present the spatial variation, $\arg(\Delta_{s'})$ has been shifted by $\pi/2$.

We obtain all the eigenvalues E_γ by means of the Sakurai-Sugiura (SS) method [24] after the self-consistent calculation [18]. The SS method allows us to extract the eigenpairs whose eigenvalues are located in a given domain on the complex plane from a generic matrix [25–27]. We find that at a certain temperature, the system goes through a second-order phase transition into a state where the extended s-wave order parameter defined by [28]

$$\Delta_{s',i} = (\Delta_{\hat{x},i} + \Delta_{-\hat{x},i} + \Delta_{\hat{y},i} + \Delta_{-\hat{y},i})/4 \tag{4}$$

becomes nonzero along the surfaces. This order parameter is complex and results in the state having gapped Andreev bound states and lower energy than that of the pure d-wave phase with gapless surface excitation. A complex order parameter produces currents and thus breaks TRS (see discussion in relation to topology in Sec. S6 [18]).

Figure 1(a) shows the temperature dependence of the two order parameters in a $d_{x^2-y^2}$-wave nanoisland with $L_x \times L_y = 96 \times 96$ lattice sites. The d-wave order parameter is defined by Eq. (2) at the center of the nanoisland. The extended s-wave order parameter, which we call s'-wave, is defined by the minimum eigenvalue of the converged BdG equations. The d-wave order parameter suddenly goes to zero at the critical temperature $T_c = 0.085t$, as the coherence length reaches the system size at this temperature. The second-order phase transition to the phase with nonzero s'-wave order parameter along the surfaces occurs at $T/T_c \sim 0.3$. We call this transition temperature T_{cs}. As can be seen in Fig. 2, TRS is broken below T_{cs}. The s'-wave order parameter is finite around corners of the nanoisland above T_{cs}, as it can be induced by a scatterer such as a nonmagnetic impurity in a d-wave superconductor [28]. This localized s'-wave order parameter becomes global at temperature T_{cs}, i.e., nonzero all along the surfaces [18]. Below T_{cs} the d-wave order parameter also becomes complex, while the BdG equations converge to a real d-wave order parameter above T_{cs} despite the complex initial guess. In terms of topology, a 1D order parameter should be induced at the TRS-breaking temperature T_{cs}, since the topology of nodal time-reversal-invariant superconductors is characterized by a 1D topological invariant [18]. The s'-wave order parameter is 1D in the sense that it is induced within a narrow region along the surfaces. This second-order phase transition can be probed by various kinds of surface-sensitive experiments such as scanning tunneling microscopy or point contact spectroscopy.

Figure 3 shows the eigenvalue distributions below and above T_{cs}. One can see that the spectrum is gapped below T_{cs}. In the zero-temperature limit, the thermodynamic potential reduces to

$$\Omega_s \sim -\sum_{\gamma=1}^{2N} E_\gamma \theta(E_\gamma) - \sum_{ij} \frac{|[\hat{\Delta}]_{ij}|^2}{U}, \tag{5}$$

which is equivalent to the internal energy. Here $\theta(x)$ is the Heaviside step function. Equation (5) clearly shows that the zero-energy eigenvalues of the Andreev bound states do not contribute to the minimization of the internal energy. The first term in Eq. (5) decreases when the flat band in a superconductor is gapped. The second term is usually small since the system satisfies the relation $|[\hat{\Delta}]_{ij}|^2/|U| < |[\hat{\Delta}]_{ij}|$.

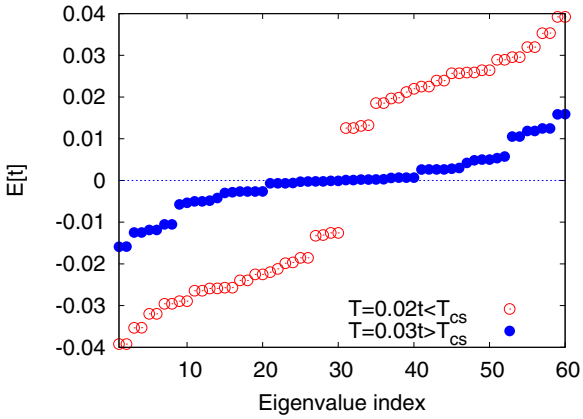

FIG. 3. Eigenvalue distribution below and above the time-reversal-symmetry breaking temperature T_{cs}. The parameters are the same as for Fig. 1.

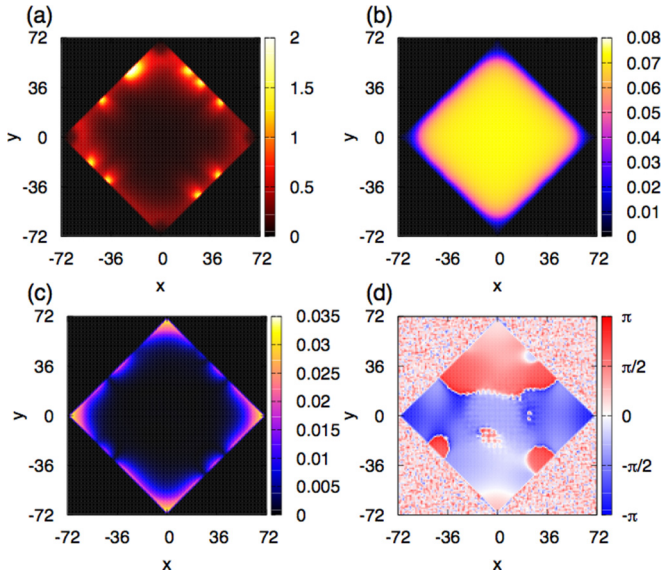

FIG. 4. Results for the larger d-wave nanoisland ($L_x \times L_y = 144 \times 144$) at temperature $T = 0.02t$: (a) zero-energy local density of states, (b) the amplitude of the d-wave order parameter, (c) the amplitude of the extended s-wave order parameter, (d) the phase of the extended s-wave order parameter.

Thus, the gapped phase can become the ground state. In a $d_{x^2-y^2}$-wave nanoisland, the flat band is spontaneously split as the extended s-wave order parameter emerges globally along the surfaces below T_{cs}. We propose that our findings are rather universal and that an unconventional superconductor with gapless surface states such as p_x-wave superconductors [3] can have a new symmetry-breaking phase with a second order phase transition.

We find the appearance of vortex-antivortex pairs in relatively large nanoislands. In a larger system with $L_x \times L_y = 144 \times 144$ sites, the TRS-breaking temperature T_{cs} is almost the same as that in the smaller system shown in Fig. 1(a). In Fig. 4 we present (a) the zero-energy local density of states, (b) $|\Delta_{d,i}|$, (c) $|\Delta_{s',i}|$, and (d) the phase of $\Delta_{s',i}$ for the $L_x \times L_y = 144 \times 144$ nanoisland. There are zero-energy bound states on the surfaces as can be seen in Fig. 4(a). The zero-energy local density of states has been calculated using the eigenfunctions obtained by the SS method, with the Lorentzian smoothing width $\eta = 0.01t$ [18]. It can be seen in Fig. 4(b) that the d-wave order parameter is similar to that in the smaller system shown in Fig. 2. Contrary to Fig. 2, however, the s'-wave order parameter in Fig. 4(c) vanishes at the positions that have zero-energy bound states. One can see in Fig. 4(d) that a phase singularity occurs in the s'-wave order parameter at each of these positions. Thus, these zero-energy bound states are the Andreev bound states in a vortex or an antivortex in the induced s'-wave order parameter. Vortices and antivortices can appear in spontaneous TRS-broken systems and in the work of Ref. [14], fractional vortex-antivortex chains along the surfaces were found in the d-wave order parameter. In contrast, our TRS-broken phase has *integer* vortex-antivortex pairs in the induced extended s-wave order parameter, since its phase as shown in Fig. 4(d) winds from $-\pi$ to π or vice versa. We note that the positions of vortex-antivortex pairs depend on the initial randomly-distributed phase of the d-wave order parameter. We have confirmed that such vortex-antivortex pairs appear in a larger system for $L_x \times L_y = 192 \times 192$.

Although we have focused on the chemical potential $\mu = -1.5t$ and the d-wave pairing interaction $U = -2t$ in presenting our results, we have found the second-order phase transition to the spontaneous TRS-broken phase with the induced s'-wave order for a wide range of μ and U. To address the question as to whether spontaneous TRS breaking happens only in nanoislands due to quantum confinement or it is a generic feature of the [110] surface, we have also performed self-consistent calculation for nanoribbons, which have infinitely long [110] surfaces but a finite width in the perpendicular direction. We have found that the second-order phase transition to the TRS-broken phase where the s'-wave order is induced along the surface is generic to [110] surfaces and also occurs in nanoribbons. For $\mu = -1.5t$ and $U = -2t$, vortex-antivortex pairs appear when the width of a nanoribbon or the side length of a nanoisland is roughly eight times or larger than the coherence length. Detailed studies of nanoribbons will be presented in a future publication.

In conclusion, we have shown by solving the BdG equations self-consistently for nanoscale d-wave systems that spontaneous emergence of new order results in gapping of the zero-energy surface states by breaking the underlying symmetry. We have found that not only is the induced order parameter complex, but also the d-wave order parameter itself becomes complex in the phase with broken TRS. The gapped surface states on [110] surfaces in the TRS-broken phase of a d-wave superconductor can be detected by surface-sensitive probes, and the Andreev bound states in vortex-antivortex pairs in the induced extended s-wave condensate can be distinguished from the gapless surface states in the TRS-preserving phase by measuring the concurrent magnetic field with nanoscale SQUIDs [14,29].

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