Time-reversal symmetry breaking surface states of d-wave superconductors induced by an additional order parameter with negative T_c

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(Received 31 May 2008; revised manuscript received 1 August 2008; published 29 September 2008)

Surface states of $d_{x^2-y^2}$-wave superconductors are studied using the Ginzburg-Landau (GL) theory. For a [110] surface it has been known that the time-reversal symmetry ($\mathcal{T}$) breaking surface state, $(d\pm is)$-wave state, can occur if the bare transition temperature of the s-wave order parameter (OP) is positive. We show that even if this bare T_c is negative, it is possible to break $\mathcal{T}$ because the coupling to the spontaneously generated magnetic field may induce the s-wave OP. The $\mathcal{T}$-breaking state is favored when the GL parameter κ is small.

DOI: 10.1103/PhysRevB.78.094519 PACS number(s): 74.20.De, 74.20.Rp

I. INTRODUCTION

Superconducting (SC) states of high-T_c cuprates are known to have $d_{x^2-y^2}$-wave symmetry.[1,2] Since the pair wave function of such an unconventional SC state has strong angular dependence, the effects of the presence of surfaces, impurities are different from those in conventional s-wave superconductors. For example, it is possible to break the time-reversal symmetry ($\mathcal{T}$) near a surface or a Josephson junction by inducing the second component of the SC order parameter (OP) (Refs. 2–14) with a nontrivial phase difference between the two OPs. In the case of a Josephson junction it may occur when the surface has [110] orientation, because the second SCOP induced by the tunneling process can have phase difference $\pm\pi/2$ leading to a $\mathcal{T}$-breaking state.[8,9] For a [110] surface faced to a vacuum the necessary condition to break $\mathcal{T}$ seems to be that the bare transition temperature (T_c) of the second OP is positive.[7,10–12,14]

In this paper we examine the possibility to have a $\mathcal{T}$-breaking surface state near the [110] surface of a $d_{x^2-y^2}$-wave superconductor when the bare T_c of the additional OP is negative, namely, the second OP will not occur in the bulk even at zero temperature. We take an s-wave SCOP as the second component, since $d_{x^2-y^2}$-wave and extended s-wave symmetries are natural candidates for superconducting states in the models with nearest-neighbor interactions (e.g., the t-J model). We will show that this kind of $\mathcal{T}$ violation is possible, and that both the SCOPs and the magnetic field (vector potential) should be treated self-consistently in order to describe this situation correctly. It also turns out that the $\mathcal{T}$ violation may occur for a relatively small GL parameter κ (i.e., of the order of 10), when T_c of the second OP is negative. Then the present mechanism may not be relevant to the $\mathcal{T}$ violation in hole-doped cuprates in which $\kappa\sim 100$. However, we expect the surface states of electron-doped cuprates may be described by the present theory, because some of the latter systems have much smaller κ values.[15,16]

II. GINZBURG-LANDAU EQUATION

We consider a superconductor with tetragonal symmetry and assume only a $d_{x^2-y^2}$-wave SCOP, Δ_d, is present in the bulk. An s-wave SCOP, Δ_s, is taken into account as a possible second component when Δ_d is suppressed near the surface. For such a system the Ginzburg-Landau (GL) free energy is given as[3]

$$\mathcal{F}=\int d\mathbf{r}\Bigg\{\sum_{\mu=d,s}\left[\alpha_\mu|\Delta_\mu|^2+\frac{\beta_\mu}{2}|\Delta_\mu|^4+K_\mu|\mathbf{D}\Delta_\mu|^2\right]+\gamma_1|\Delta_d|^2|\Delta_s|^2+\gamma_2[\Delta_d^2(\Delta_s^*)^2+(\Delta_d^*)^2\Delta_s^2] + K_{ds}[(D_x\Delta_d)(D_x\Delta_s)^*-(D_y\Delta_d)(D_y\Delta_s)^*+\text{c.c.}]+\frac{1}{8\pi}(\nabla\times\mathbf{A})^2\Bigg\}, \quad (1)$$

where $\mathbf{A}$ is the vector potential and $\mathbf{D}=\nabla-(2\pi i/\Phi_0)\mathbf{A}$ is the gauge-invariant gradient with $\Phi_0=hc/2e$ being the magnetic-flux quantum. Coefficients $\alpha_\mu(\propto T-T_{c\mu})$, β_μ, K_μ, γ_1, γ_2, and K_{ds} are real, and we assume $T_{cd}>0$, while T_{cs} can be both positive and negative. The γ_2 is one of the terms which determine the relative phase of OPs, $\phi_{ds}[\equiv\phi_d-\phi_s;\Delta_\mu=|\Delta_\mu|\exp(i\phi_\mu)]$. We take $\gamma_2>0$, because this choice would lead to the $(d\pm is)$-state ($\phi_{ds}=\pm\pi/2$) instead of the $(d\pm s)$-state ($\phi_{ds}=0,\pi$). In the former case the nodes of the d-wave state are removed and the more condensation energy can be gained. It is also to be noted that $\gamma_1\pm 2\gamma_2$ is positive in usual weak-coupling model, since two OPs compete each other. Now we rewrite $\mathcal{F}$ in the dimensionless unit[17] to see the parameter dependence of the model more clearly,

$$\mathcal{F}=\frac{H_c^2\xi_d^3}{4\pi}\int d\mathbf{r}\Bigg\{-|\eta_d|^2+\frac{1}{2}|\eta_d|^4+|\tilde{\mathbf{D}}\eta_d|^2+\tilde{\alpha}_s|\eta_s|^2+\frac{\tilde{\beta}_s}{2}|\eta_s|^4+\tilde{K}_s|\tilde{\mathbf{D}}\eta_s|^2+\tilde{\gamma}_1|\eta_d|^2|\eta_s|^2+\tilde{\gamma}_2[\eta_d^2(\eta_s^*)^2+(\eta_d^*)^2\eta_s^2]$$
$$+\tilde{K}_{ds}[(\tilde{D}_x\eta_d)(\tilde{D}_x\eta_s)^*-(\tilde{D}_y\eta_d)(\tilde{D}_y\eta_s)^*+\text{c.c.}]+(\nabla\times\mathbf{a})^2\Bigg\}, \tag{2}$$

where $\eta_\mu=\Delta_\mu/\Delta_0$ $(\mu=d,s)$ with $\Delta_0=\sqrt{|\alpha_d|/\beta_d}$ being the bulk d-wave OP. $\mathbf{r}$ was rescaled using the coherence length for the d-wave OP, $\xi_d(=\sqrt{K_d/|\alpha_d|})$, as $\mathbf{r}\to\mathbf{r}/\xi_d$, and $\tilde{\mathbf{D}}\equiv\nabla-i\mathbf{a}/\kappa$. Here $\mathbf{a}=\mathbf{A}/(\sqrt{2}H_c\xi_d)$, and the magnetic field is measured in units of $\sqrt{2}H_c$, where $H_c=\sqrt{4\pi\alpha_d^2/\beta_d}$ is the thermodynamic critical field. $\kappa=\lambda_d/\xi_d$ is the GL parameter with $\lambda_d=\phi_0/(2\sqrt{2}\pi H_c\xi_d)$ being the penetration depth for the bulk d-wave superconductor. The parameters in Eq. (2) are defined as $\tilde{\alpha}_s=\alpha_s/|\alpha_d|$, $\tilde{\beta}_s=\beta_s/\beta_d$, $\tilde{K}_s=K_s/K_d$, $\tilde{\gamma}_1=\gamma_1/\beta_d$, $\tilde{\gamma}_2=\gamma_2/\beta_d$, and $\tilde{K}_{ds}=K_{ds}/K_d$.

Usually the surface effect is described by the second-order surface GL free energy, $\mathcal{F}_{sf}=\int_{sf}dS\Sigma_{\mu,\nu=d,s}g_{\mu\nu}\eta_\mu^*\eta_\nu$, where integration is carried out on the surface. Using the symmetry argument we find $g_{ds}=g_{sd}=g_0\cos 2\theta$ where θ is the angle between the surface and the crystal a axis with g_0 being a constant. This term could also determine ϕ_{ds}, and it leads to the $(d\pm s)$-state in the case of a [100] surface ($\theta=0$), since the γ_2 term is higher order than the g_{ds} term. However, g_{ds} vanishes for a [110] surface ($\theta=45°$) which we consider in the following. The $g_{\mu\mu}$ term will represent the suppression of η_μ near the surface. Instead of using g_{dd} we impose the condition $\eta_d=0$ at the [110] surface, because the $d_{x^2-y^2}$-wave SCOP should vanish there. Since the s-wave SCOP is only little affected by the presence of the surface, we take $g_{ss}=0$. (In numerical calculations we have checked that taking small positive g_{ss} will not change the results qualitatively.) In order to consider the [110] surface we transform the coordinate system, $(x,y,z)\to(\tilde{x},\tilde{y},z)$. Here x (y) is parallel to the crystal a (b) axis (z is parallel to the surface), and $\tilde{x}$ and $\tilde{y}$ axes are perpendicular and parallel to the surface, respectively. (See Fig. 1.) In the free-energy density only the $\tilde{K}_{ds}$ term is changed under this transformation to

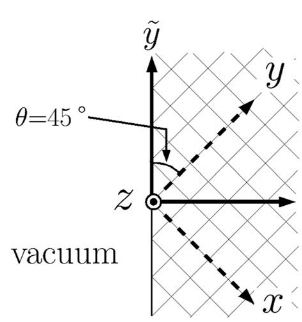

FIG. 1. Schematic of a [110] surface of a $d_{x^2-y^2}$-wave superconductor with tetragonal symmetry. x and y are parallel to the crystal a and b axes, respectively.

$$\frac{2\tilde{K}_{ds}}{\kappa}a_{\tilde{y}}\,\text{Im}(\eta_s^*\partial_{\tilde{x}}\eta_d-\eta_d\partial_{\tilde{x}}\eta_s^*), \tag{3}$$

where we have assumed that the system is uniform along the surface, and the gauge freedom was taken as $\mathbf{a}=a_{\tilde{y}}(\tilde{x})\mathbf{e}_{\tilde{y}}$.

The expression for the supercurrent is obtained by varying the electronic part of $\mathcal{F}$ (i.e., except the last term) with respect to $\mathbf{a}$. Since the surface is faced to the vacuum, the $\tilde{x}$ component, $J_{\tilde{x}}$, should obviously vanish. (We have numerically checked that $J_{\tilde{x}}$ actually vanishes.) The $\tilde{y}$ component, $J_{\tilde{y}}$, and that in the dimensionless unit, $j_{\tilde{y}}$, are given as

$$j_{\tilde{y}}=J_{\tilde{y}}\Bigg/\left(\frac{\sqrt{2}H_c c}{\xi_d}\right)$$
$$=-\frac{1}{4\pi}\Bigg[\frac{1}{\kappa^2}a_{\tilde{y}}(|\eta_d|^2+\tilde{K}_s|\eta_s|^2)+\frac{\tilde{K}_{ds}}{\kappa}\text{Im}(\eta_s^*\partial_{\tilde{x}}\eta_d-\eta_d\partial_{\tilde{x}}\eta_s^*)\Bigg]. \tag{4}$$

III. SURFACE STATE AND SPONTANEOUS CURRENT

We numerically solve the problem by employing the quasi-Newton method[18] to minimize the free energy $\mathcal{F}$ under the condition $\eta_d(\tilde{x}=0)=0$. We minimize $\mathcal{F}$ with respect to all variables, i.e., η_d, η_s, and $a_{\tilde{y}}$. Note that the Maxwell's equation is taken into account in this procedure, and we call this as "fully self-consistent calculation." For the sake of comparison we will also show the results by treating only η_d and η_s self-consistently.

First let us consider the case of $\tilde{\alpha}_s<0$ (i.e., $T<T_{cs}$). In this case, we would get finite η_s if η_d were absent. However, for $T_{cd}>T_{cs}$ the stability condition for η_s in the bulk is given as, $\tilde{\alpha}_s+(\tilde{\gamma}_1-2\tilde{\gamma}_2)|\eta_d|^2<0$, so the transition temperature of η_s is lower than the bare one, T_{cs}, and η_s would be totally suppressed if $T_{cd}\gg T_{cs}$. Near the surface or impurities the situation can be different. There η_s may be finite because the dominant SCOP, η_d, is suppressed. In Fig. 2 the spatial variations of the SCOPs near the surface are shown. η_s gets finite near the surface while η_d is suppressed. The relative phase ϕ_{ds} will be determined by $\tilde{\gamma}_2$ and $\tilde{K}_{ds}$ terms, and the former favors $\phi_{ds}=\pm\pi/2$ as mentioned. From Eq. (3) we see that the $\tilde{K}_{ds}$ term also favors $\phi_{ds}=\pm\pi/2$, and $a_{\tilde{y}}$ will be spontaneously generated. (We take η_d to be real and $a_{\tilde{y}}=0$ in the bulk, i.e., $\tilde{x}\to\infty$.) Numerical calculations show that η_d is real for all $\tilde{x}$, and that $\phi_{ds}=\pm\pi/2$ where η_s is finite. This indicates that a $\mathcal{T}$-violating $(d+is)$-wave surface state with a

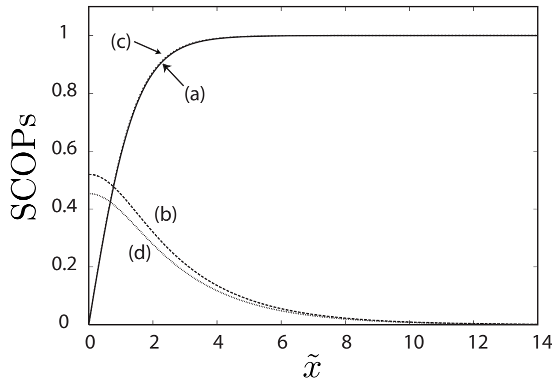

FIG. 2. Spatial variations of SCOPs for $\tilde{\alpha}_s=-0.2$, $\tilde{\beta}_s=0.2$, $\tilde{K}_s=0.5$, $\tilde{\gamma}_1=0.5$, $\tilde{\gamma}_2=0.1$, $\tilde{K}_{ds}=0.3$, and $\kappa=16$. Note that all SCOPs are normalized by the bulk d-wave OP, and $\tilde{x}=0$ corresponds to the surface faced to the vacuum. (a) Re η_d and (b) Im η_s in the fully self-consistent calculation. (c) Re η_d and (d) Im η_s in the simplified one without treating $a_{\tilde{y}}$ self-consistently.

spontaneous magnetic field b_z $(=\partial_{\tilde{x}}a_{\tilde{y}})$ and a supercurrent $j_{\tilde{y}}$ occurs near the surface. The spatial distributions of b_z and $j_{\tilde{y}}$ are presented in Fig. 3.

In order to see the role played by the vector potential, we investigate the same problem by setting $a_{\tilde{y}}=0$ everywhere. Namely we treat only SCOPs self-consistently. When $a_{\tilde{y}}$ is set to zero, the spontaneous current $j_{\tilde{y}}$ has contributions from only the spatial variations of SCOPs [i.e., the last line of Eq. (4)], and we calculate the magnetic field from $j_{\tilde{y}}$ using Maxwell's equation, $j_{\tilde{y}}(\tilde{x})=-\frac{1}{4\pi}\frac{\partial b_z(\tilde{x})}{\partial\tilde{x}}$. For $\tilde{\alpha}_s<0$, the results for the SCOPs look similar as in the fully self-consistent calculations. The $\mathcal{T}$-breaking $(d+is)$-state occurs as shown in Fig. 2. On the contrary, the behaviors of b_z and $j_{\tilde{y}}$ are different in that $j_{\tilde{y}}$ always has the same sign, and that b_z is a monotonous function of $\tilde{x}$. These results are not correct even qualitatively as well as in a quantitative sense. Integration of the Maxwell's equation with the boundary condition $b_z(\pm\infty)=0$ leads to $\int_{-\infty}^{\infty}d\tilde{x}j_{\tilde{y}}(\tilde{x})=0$, implying that the averaged current should vanish.[9] This is the case for the fully self-consistent calculation but not in the case where the magnetic field is not treated self-consistently, because of the absence of the screening effect in the latter.

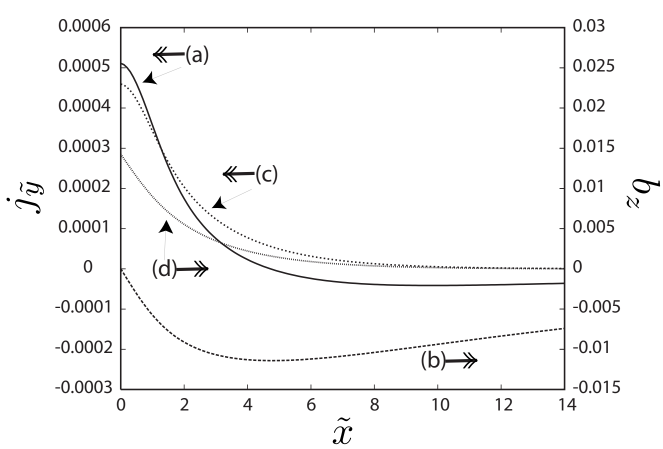

FIG. 3. Spatial variations of b_z and $j_{\tilde{y}}$. Parameters used are the same as in Fig. 2. (a) $j_{\tilde{y}}$ and (b) b_z in the fully self-consistent calculation. (c) $j_{\tilde{y}}$ and (d) b_z in the simplified one without treating $a_{\tilde{y}}$ self-consistently. Note b_z and j_y are in the dimensionless unit.

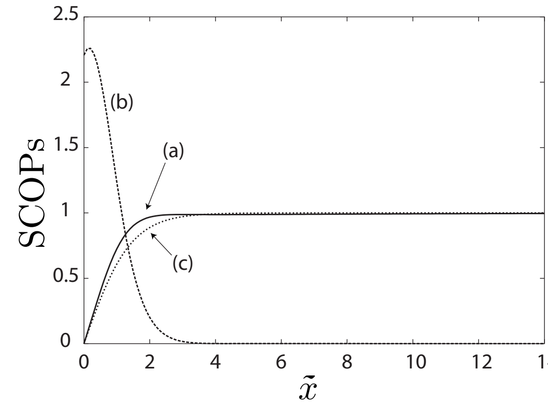

FIG. 4. Spatial variations of SCOPs for $\tilde{\alpha}_s=0.01$, $\tilde{\beta}_s=0.01$, $\tilde{K}_s=0.04$, $\tilde{\gamma}_1=0.5$, $\tilde{\gamma}_2=0.1$, $\tilde{K}_{ds}=1.0$, and $\kappa=16$. (a) Re η_d and (b) Im η_s in the fully self-consistent calculation. (c) Re η_d in the simplified one without treating $a_{\tilde{y}}$ self-consistently.

Next we consider the case of $\tilde{\alpha}_s>0$, i.e., $T>T_{cs}$. Note that T_{cs} may be negative, in which case η_s will not occur in the bulk at $T=0$ even when η_d is absent. The results for the SCOPs are depicted in Fig. 4. (Here the GL parameter is taken to be $\kappa=16$.) It is seen that finite Im(η_s) is obtained, though we naively expect $\eta_s=0$. This is because the $\tilde{K}_{ds}$ term couples $\partial_{\tilde{x}}$ Re(η_d) bilinearly to $a_{\tilde{y}}$ Im(η_s). It may induce the state with Im$(\eta_s)\neq 0$ and $b_z\neq 0$, but the state with $\eta_s=0$ and $b_z=0$ may also be a self-consistent solution. Numerical calculations show that the former one has the lower energy, and thus the time-reversal symmetry is violated spontaneously. Here $|\tilde{\alpha}_s|$, $\tilde{\beta}_s$, and $\tilde{K}_s$ were taken to be much smaller than those in Fig. 2. Otherwise the $\mathcal{T}$ violation will not occur, because these terms cost the energy for $\tilde{\alpha}_s>0$ and the energy gain is solely coming from the $\tilde{K}_{ds}$ term. The spatial variations of b_z and $j_{\tilde{y}}$ are shown in Fig. 5.

In the case of $\tilde{\alpha}_s>0$, the results with or without treating the vector potential self-consistently are completely different. If we do not take into account the $a_{\tilde{y}}$ term, η_s will never

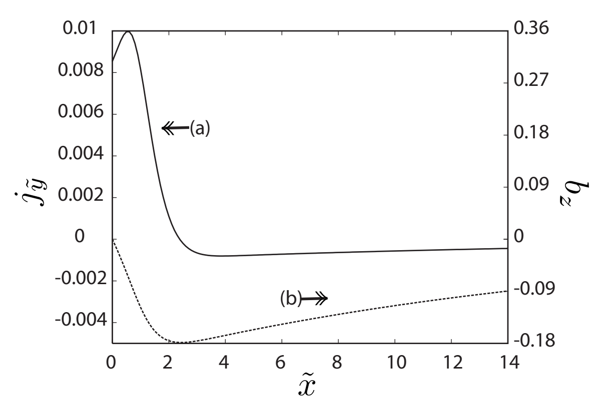

FIG. 5. Spatial variations of b_z and $j_{\tilde{y}}$. Parameters used are the same as in Fig. 4. (a) $j_{\tilde{y}}$ and (b) b_z in the fully self-consistent calculation.

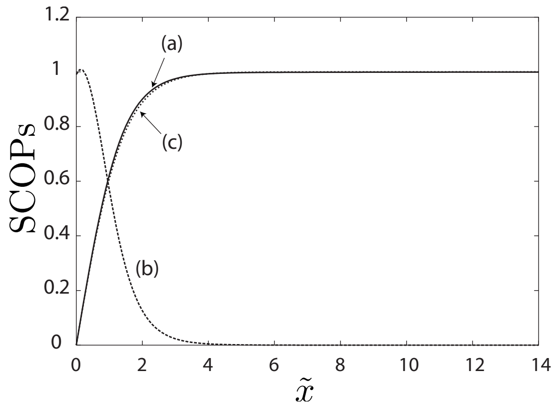

FIG. 6. Spatial variations of SCOPs. Parameters used are the same as in Fig. 4 except $\kappa=19$. (a) Re η_d and (b) Im η_s in the fully self-consistent calculation. (c) Re η_d in the simplified one without treating $a_{\tilde{y}}$ self-consistently.

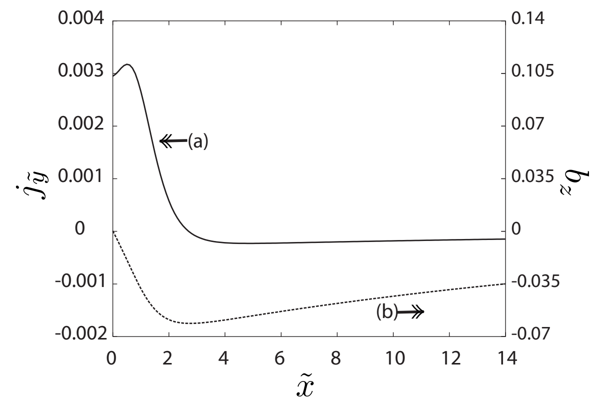

FIG. 7. Spatial variations of b_z and $j_{\tilde{y}}$. Parameters used are the same as in Fig. 6. (a) $j_{\tilde{y}}$ and (b) b_z in the fully self-consistent calculation.

appear, since there is no mechanism to derive finite η_s. Thus neither the spontaneous current nor the spontaneous field can occur. It implies that the $\mathcal{T}$-violation near the surface cannot be described in this kind of simplified treatment for the superconductors in which the second SCOP has negative T_c.

In order to see the dependence on κ we show the results for a larger κ ($\kappa=19$) in Fig. 6 and 7. It is seen that $|\eta_s|$, $|b_z|$, and $|j_{\tilde{y}}|$ are much smaller than those for $\kappa=16$. This κ dependence can be understood as follows. η_d is suppressed in the region near the surface ($\tilde{x}\lesssim\xi_d$), and η_s and $a_{\tilde{y}}$ would be finite there if $\mathcal{T}$ is broken. On the other hand the magnetic field b_z would be finite in the region $\tilde{x}\lesssim\lambda_d$. When κ is large, the loss of energy due to finite b_z in the large region ($\xi_d \lesssim\tilde{x}\lesssim\lambda_d$) overwhelms the energy gain coming from the $\tilde{K}_{ds}$ term which acts only in the small region $\tilde{x}\lesssim\xi_d$. Thus for large κ the $\mathcal{T}$ violation is not favored. If the larger value of $\tilde{K}_{ds}$ is taken, the $\mathcal{T}$-breaking state can occur for larger κ. But the natural assumption seems to be $K_{ds}\leq K_d$ ($\tilde{K}_{ds}\leq 1$), so that the $\mathcal{T}$ violation may occur for κ of the order of 10. (On the contrary the $\mathcal{T}$ violation may occur for much larger κ in the case of $\tilde{\alpha}_s<0$, because the energy can be gained by not only $\tilde{K}_{ds}$ but also $\tilde{\alpha}_s$ term.) It implies that the present mechanism may not be relevant to hole-doped cuprates in which $\kappa\sim 100$, but it may describe the surface states of electron-doped cuprates which have smaller κ.

If we assume $H_c=1$ T, the maximum values of $|B_z|$ and $|J_{\tilde{y}}|$ are 2.5×10^{-1} T and 3.7×10 A/cm^2, respectively, for $\kappa=16$. For $\kappa=19$ they are 8.6×10^{-2} T and 1.2×10 A/cm^2, respectively. These values rapidly decrease as κ increases, and the $\mathcal{T}$-breaking state disappears as κ exceeds 19 for the parameters used here. If we compare these values with experiments, it should be noted that surface roughness will reduce $|B_z|$ and $|J_{\tilde{y}}|$, because $\mathcal{T}$ violation is most favored in the case of $\theta=45°$.[12] (When $\theta\neq 45°$, g_{ds} will be finite and the $\mathcal{T}$ violation is not favored.)

IV. SUMMARY

We have examined the role played by the vector potential concerning the occurrence of surface states with spontaneously broken $\mathcal{T}$ in $d_{x^2-y^2}$-wave superconductors. It has been known that the $\mathcal{T}$-breaking state may naturally appear if the bare T_c of the additional OP is positive. For the Josephson junction composed of $d_{x^2-y^2}$-wave and other superconductors, tunneling may induce second component of SCOP and thus $\mathcal{T}$ may be broken. In these cases the $\mathcal{T}$-breaking states may be described without treating the vector potential self-consistently. In this paper it was shown that the surface state of a $d_{x^2-y^2}$-wave superconductor may break $\mathcal{T}$ even when the bare T_c of the second SCOP is negative. However, to describe this situation correctly not only the SCOPs but also the vector potential must be treated on an equal footing. In the present mechanism the $\mathcal{T}$ violation may occur for rather small values of the GL parameter κ ($\lesssim 20$), so that it may not be relevant to hole-doped cuprates. We expect that the present theory may be used to describe the surface states of electron-doped high-T_c cuprates, because their κ are much smaller than those of hole-doped systems.

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