with the assumption of the specularly reflecting surface,

$$\begin{aligned} t_{kp}^2 = &\quad \tilde{t}^2\delta(k_\parallel - p_\parallel)\delta(k_\perp - p_\perp)\frac{v_\perp(p)}{v(p)}\theta(v_\perp(p)) \\ r_{kp}^2 = &\quad \tilde{r}^2\delta(k_\parallel - p_\parallel)\delta(k_\perp + p_\perp)\frac{v_\perp(p)}{v(p)}\theta(v_\perp(p)) \end{aligned} \tag{2.9}$$

where θ is the step function. It should be noted here that if the angular dependences of the tunneling matrix elements were omitted, the coupling between two superconductors should vanish, and thus it would lead to unphysical results.

§3. Relation to Phenomenological Theory

Now let us briefly summarize the content of the phenomenological theory of Ref.4 to describe a $\mathcal{T}$-violating surface state. The properties of the bulk system are described by the free energy F. We assume that only a d-wave OP is present in the bulk system, and the coupling between Δ_d and Δ_s is repulsive, if the latter were present. Namely, a_d is negative below a critical temperature, while $a_s > 0$ for all T, and $\gamma_1 - \gamma_2 > 0$ and $\gamma_2 > 0$. An important point here is that positive γ_2 favors the relative phase between Δ_d and Δ_s, denoted as ϕ_{ds}, to be $\pm\pi/2$, i.e., the system would break $\mathcal{T}$ if both d and s- components coexist. We expect $\gamma_2 > 0$ for the following reason. The complex combination $d \pm is$, resulting from $\gamma_2 > 0$, would open a complete gap in the excitation spectrum, such that the system would gain more condensation energy. If $\phi_{ds} = 0$ or π ($(d \pm s)$-state), the nodes remain though their locations are shifted, and the gain of the condensation energy would be smaller.

The interface properties are described by F_I. In the presence of an interface, Δ_s can be induced by the reflection of Cooper pairs and by the proximity effect from Δ_0 in (L). These processes are possible because of the lowering of the symmetry (translational and point-group) in the presence of the interface. In usual cases ϕ_{ds} is determined by the bilinear coupling terms in F_I which induces the finite Δ_s. On the other hand, the γ_2 term favoring $\phi_{ds} = \pm\pi/2$ is biquadratic and it would not be dominant in the sense of GL theory. Then ϕ_{ds} takes a value 0 or π depending on the sign of t_d, t_s and g_{ds}. There is no $\mathcal{T}$-breaking in this case. Under certain conditions, however, a different relative phase is favored leading to a state which breaks $\mathcal{T}$. In Ref.4 it was argued based on the symmetry consideration that t_d and g_{ds} should vanish at $\theta = \pi/4$ and are small for θ close to $\pi/4$, while t_s remains always finite. Then, for $\theta \sim \pi/4$ ϕ_{ds} is determined by γ_2, and, thus, it is possible to have a locally $\mathcal{T}$-violating state near the interface.

We numerically calculate coefficients in F and F_I as functions of the doping rate δ and the temperature T. We take $t/J = 3$ throughout in this paper. First we solve the self-consistency equations for the uniform RVB state (the state where only χ_F and $\chi_B = \delta$ are finite), to get χ_F and the chemical potential, λ_F. By using them we calculate the coefficients in F and F_I. For the doping rate where the superconductivity is observed in real systems, i.e., $0 < \delta < 0.3$, only α_d can be negative and all other coefficients of F are positive definite[20]. This implies that we deal with a single d-wave component. We find indeed a positive γ_2 which favors the phase difference $\phi_{ds} = \pm\pi/2$. Hence, the above results are consistent with the assumptions of the previous purely phenomenological theory.

Next we consider the interface terms F_I. By taking the angular dependences of t_{kp} and r_{kp} as in eq.(2.9), we get the the coefficients in F_I as functions of φ, i.e., the angle between the interface and the crystal a-axis of the right hand side. We can explicitly examine the following properties using the expressions of t_i and g_{ij} $(i, j = d, s)$:

$$\begin{aligned} t_s(\varphi \pm \pi/2) = &\quad t_s(\varphi), \quad t_d(\varphi \pm \pi/2) = -t_d(\varphi) \\ t_s(\varphi \pm \pi) = &\quad t_s(\varphi), \quad t_d(\varphi \pm \pi) = t_d(\varphi) \\ t_s(-\varphi) = &\quad t_s(\varphi), \quad t_d(-\varphi) = t_d(\varphi) \end{aligned} \tag{3.1}$$

and

$$\begin{aligned} g_{ii}(\varphi \pm \pi/2) = &\quad g_{ii}(\varphi), \quad g_{ds}(\varphi \pm \pi/2) = -g_{ds}(\varphi) \\ g_{ii}(\varphi \pm \pi) = &\quad g_{ii}(\varphi), \quad g_{ds}(\varphi \pm \pi) = g_{ds}(\varphi) \\ g_{ii}(-\varphi) = &\quad g_{ii}(\varphi), \quad g_{ds}(-\varphi) = g_{ds}(\varphi) \end{aligned} \tag{3.2}$$

where $i = d, s$. We have calculated t_i and g_{ij} numerically, as shown in Fig. 3, with a choice of parameters $\delta = 0.15$ and $T = 0.8T_c$ ($T_c \sim 0.108J$). The important point here is that t_s does not vanish for any value of φ. This property is robust for any doping δ and temperature T. Another point is that $|t_s|$ is much smaller than $|t_d|$ except very near $\varphi = \pi/4$. This can be explained as follows. The integrand in the expression of t_s has a factor $(\cos k_x + \cos k_y)$, while that of t_d has $(\cos k_x - \cos k_y)^2$. Since we are treating the square lattice system, the factor $(\cos k_x + \cos k_y)$ is small everywhere on the Fermi surface, for the doping rate as small as $\delta = 0.15$, while the factor $(\cos k_x - \cos k_y)^2$ can be large there. Hence $|t_d|$ can be much larger than $|t_s|$. (For $\varphi = \pi/4$, t_d has to vanish by symmetry. Then $|t_s|$ can be larger than $|t_d|$ if φ is close enough to $\pi/4$.)

§4. $\mathcal{T}$-breaking state and Surface Current

In this section we analyze the appearance of the $\mathcal{T}$-breaking state. For this purpose we minimize the total free energy, $F_{tot} = F + F_I$, with respect to the OP, Δ_s and Δ_d, and the vector potential $\vec{A}$. We use a coordinate system $(\tilde{x}, \tilde{y})$, with $\tilde{x}$ $(\tilde{y})$ being perpendicular (parallel) to the interface. Under the transformation from (x, y) to $(\tilde{x}, \tilde{y})$, only $\tilde{K}$ terms are changed, and it transforms to

$$\begin{aligned} &\tilde{K}\big[\cos 2\varphi\big\{(D_{\tilde{x}}\Delta_d)(D_{\tilde{x}}\Delta_s)^* - (D_{\tilde{y}}\Delta_d)(D_{\tilde{y}}\Delta_s)^*\big\} \\ &+ \sin 2\varphi\big\{(D_{\tilde{x}}\Delta_d)(D_{\tilde{y}}\Delta_s)^* + (D_{\tilde{y}}\Delta_d)(D_{\tilde{x}}\Delta_s)^*\big\}\big]. \end{aligned} \tag{4.1}$$

Since there is no spatial variation of the OP along $\tilde{y}$-direction, the GL equations are formally written as

$$\frac{\partial F}{\partial \Delta_i(\tilde{x})} = \partial_{\tilde{x}}\frac{\partial F}{\partial(\partial_{\tilde{x}}\Delta_i(\tilde{x}))} \quad (i = d, s) \tag{4.2}$$

and

$$\begin{aligned} J_{\tilde{x}} \equiv &\quad -\frac{\partial F}{\partial A_{\tilde{x}}} = 0, \\ J_{\tilde{y}} \equiv &\quad -\frac{\partial F}{\partial A_{\tilde{y}}} = -\frac{1}{4\pi}\partial_{\tilde{x}}B \end{aligned} \tag{4.3}$$