Twin boundaries in *d*-wave superconductors

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Twin boundaries in orthorhombic *d*-wave superconductors are investigated numerically using the Bogoliubov–deGennes formalism within the context of an extended Hubbard model. The twin boundaries are represented by tetragonal regions of variable width, with a reduced chemical potential. For sufficiently large twin boundary width and change in chemical potential, an induced *s*-wave component may break time-reversal symmetry at a low temperature T^*. The temperature T^*, and the magnitude of the imaginary component, are found to depend strongly on electron density. The results are compared with recent tunneling measurements. [S0163-1829(97)51134-9]

In spite of mounting experimental evidence that the high-temperature superconductors have an order parameter with $d_{x^2-y^2}$ (*d*-wave) symmetry,[1] a number of experiments on both twinned and untwinned $YBa_2Cu_3O_{7-\delta}$ (YBCO) suggest the presence of an additional *s*-wave order parameter.[2,3] By symmetry, a small *s*-wave component always coexists with a predominantly *d*-wave order parameter in an orthorhombic superconductor such as YBCO, and changes its sign (relative to the *d*-wave component) across a twin boundary.[4] The experimental results can be understood either if the *s*-wave component of the order parameter breaks time-reversal ($\mathcal{T}$) symmetry near the twin boundary at low temperatures, as it can near surfaces,[5–10] or if there is far more of one kind of twin domain (i.e., twin boundaries form in groups).[11,12] Recent superconducting quantum interferrence device measurements on vortices trapped by twin boundaries in YBCO did not detect the fractional flux that would accompany local $\mathcal{T}$ violation.[13] In the present work, however, we present strong evidence that such a symmetry breaking could indeed occur in the vicinity of twin boundaries at low temperatures under certain conditions.

Sigrist *et al.*[7] have addressed the possibility of $\mathcal{T}$ violation near boundaries by considering the Ginzburg-Landau (GL) free energy for a homogeneous orthorhombic *d*-wave superconductor:

$$F_s = F_n + \alpha_d|d|^2 + \alpha_s|s|^2 + \beta_1|d|^4 + \beta_2|s|^4 + \beta_3|s|^2|d|^2 + \beta_4(s^{*2}d^2 + s^2d^{*2}) + \beta_5(s^*d + sd^*), \quad (1)$$

where *s* and *d* are the *s*-wave and *d*-wave components of a superconducting order parameter of the form $d + e^{i\theta}s$, with θ the relative phase between *s* and *d*. Only the lowest-order orthorhombic term is kept in the GL free energy since $s \ll d$ for small β_5. Assuming all the coefficients are positive (except α_d), the β_5 term favors $\theta = n\pi$ (*n* integer), while the β_4 term favors $\theta = \pi/2$. Thus, in a tetragonal superconductor there can be a continuous transition to a bulk $\mathcal{T}$-violating phase at a temperature T^* given by $\alpha_s(T^*) = [2\beta_4(T^*) - \beta_3(T^*)]d^2(T^*)$.[8] The coefficients of the GL free energy can be chosen such that $T^* \leqslant 0$ for a uniform system; the orthorhombic term further discourages a positive T^*. Yet the suppression of *d* near an inhomogeneity, or the presence of a tetragonal region within an orthorhombic system, could induce local $\mathcal{T}$ violation for a finite temperature $0 \leqslant T \leqslant T^*$. Furthermore, the associated imaginary *s*-wave component could be large relative to $|d|$, and would vary on a new length scale.[7] In contrast, an *s*-wave component nucleated solely through spatial variations of *d*, such as is found in magnetic vortices[14,15] or near impurities,[16] is usually small relative to $|d|$ (unless $\alpha_s \to 0$, which only occurs for densities just above a crossover to bulk *s*-wave superconductivity[17]) and varies on a length scale of the *d*-wave coherence length.

It is not clear, however, whether GL theory (which is strictly valid only near the bulk superconducting transition temperature) can reliably describe the low-temperature regime associated with $\mathcal{T}$ violation. In the present work, twin boundaries in *d*-wave superconductors are investigated numerically using Bogoliubov–deGennes theory. We employ an extended Hubbard model which gives rise to *d*-wave superconductivity in a restricted parameter regime.[18] Despite its simplicity, results obtained previously using this model[19,20] are consistent with those obtained within the context of a model better representing the high-T_c oxides,[17,21] and with experimental results.[22,23] Twin boundaries are modeled as tetragonal regions of varying widths and reduced chemical potential, in order to approximate the experimental observations that twin boundaries are oxygen-deficient (i.e. locally antiferromagnetically insulating) regions, generally 7–40 Å wide.[24]

The Hamiltonian for the extended Hubbard model is:

$$H = -\sum_{\langle ij\rangle\sigma} t_{ij}c^\dagger_{i\sigma}c_{j\sigma} - \mu\sum_{i\sigma} n_{i\sigma} - \sum_{i\sigma} \mu^I_i n_{i\sigma} - V_0\sum_i n_{i\uparrow}n_{i\downarrow} - \frac{V_1}{2}\sum_{\langle ij\rangle\sigma\sigma'} n_{i\sigma}n_{j\sigma'}, \quad (2)$$

where the sums are over spin and nearest-neighbors on the square lattice, t_{ij} is a direction-dependent hopping parameter used to model orthorhombicity, μ is the chemical potential, μ^I is a site-dependent impurity potential representing the depletion of the carrier density at the twin boundary, and V_0 and V_1 are on-site and nearest-neighbor interactions, respectively ($V > 0$ denotes attraction). Choosing the unit cell as shown in Fig. 1, we can exploit the translational invariance

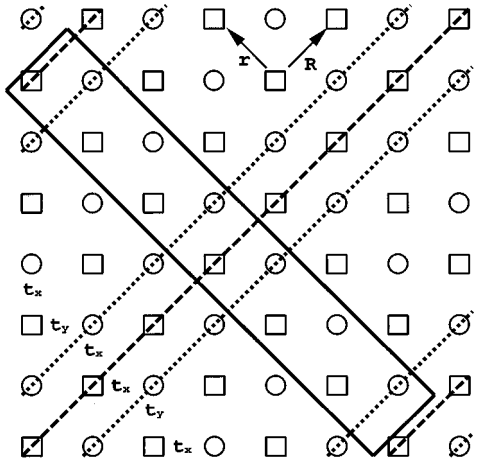

FIG. 1. The unit cell of the finite-size system for the BdG calculations is shown as a solid line superimposed on a square lattice. Long and short dashed lines represent twin boundaries of width 0 and $|\hat{r}|$, respectively. Basis points are labeled by circles and squares.

of the Hamiltonian in the (110) direction. With $\hat{R}\equiv\hat{x}+\hat{y}$ parallel and $\hat{r}\equiv-\hat{x}+\hat{y}$ perpendicular to the twin direction, we obtain the Bogoliubov-deGennes (BdG) equations:

$$\begin{pmatrix} \hat{\xi} & \hat{\Delta} \\ \hat{\Delta}^* & -\hat{\xi} \end{pmatrix} \begin{pmatrix} u_{n,k}(r_\alpha) \\ v_{n,-k}(r_\alpha) \end{pmatrix} = \varepsilon_{n,k} \begin{pmatrix} u_{n,k}(r_\alpha) \\ v_{n,-k}(r_\alpha) \end{pmatrix}, \tag{3}$$

such that

$$\hat{\xi}u_{n,k}(r_\alpha) = -\sum_{\hat{\delta}} t_\delta u_{n,k}(r_\alpha+\hat{\delta}) - [\mu+\mu^I(r_\alpha)]u_{n,k}(r_\alpha), \tag{4}$$

$$\hat{\Delta}u_{n,k}(r_\alpha) = \Delta_0(r_\alpha)u_{n,k}(r_\alpha) + \sum_{\hat{\delta}} \Delta_\delta(r_\alpha)u_{n,k}(r_\alpha+\hat{\delta}), \tag{5}$$

where the gap functions are defined by

$$\Delta_0(r_\alpha) \equiv V_0\langle c_\uparrow(r_\alpha)c_\downarrow(r_\alpha)\rangle; \tag{6}$$

$$\Delta_\delta(r_\alpha) \equiv V_1\langle c_\uparrow(r_\alpha+\hat{\delta})c_\downarrow(r_\alpha)\rangle. \tag{7}$$

We have introduced the index α labeling the two basis points in the unit cell, the label k which is the Fourier inverse of R, and $\hat{\delta}=\hat{0},\hat{r},\hat{r}-\hat{R},-\hat{R}$ connecting nearest neighbors with different basis indices. Equations (3) are subject to the self-consistency requirements

$$\Delta_0(r_\alpha) = V_0\sum_{nk} u_{n,k}(r_\alpha)v^*_{n,-k}(r_\alpha)\tanh\left(\frac{\beta\varepsilon_{n,k}}{2}\right), \tag{8}$$

$$\Delta_\delta(r_\alpha) = \frac{V_1}{2}\sum_{nk\delta} [u_{n,k}(r_\alpha+\hat{\delta})v^*_{n,-k}(r_\alpha) + u_{n,k}(r_\alpha)v^*_{n,-k}(r_\alpha+\hat{\delta})]\tanh\left(\frac{\beta\varepsilon_{n,k}}{2}\right), \tag{9}$$

where the sum is over positive energy eigenvalues $\varepsilon_{n,k}$ only.

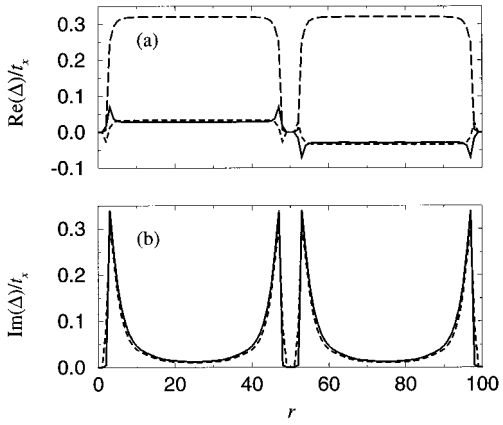

FIG. 2. The (a) real and (b) imaginary components of the d-wave, on-site, and extended s-wave gap functions (corresponding to long-dashed, short-dashed, and solid lines, respectively) are shown as a function of distance r perpendicular to the twin boundary. In (b), $\mathrm{Im}(\Delta_s)$ is multiplied by a factor of -10 to facilitate comparison with $\mathrm{Im}(\Delta_0)$. Results are obtained using $\mu=-t_x$, $\mu^I=-10t_x$, $T=0$, and twin width $4|\hat{r}|$. Twin boundaries are centered at positions $r=0$ (which is equivalent to $r=100$ by periodic boundary conditions) and $r=50$ in units of $|\hat{r}|$.

The orthorhombicity of YBCO is modeled by an anisotropy in the hopping parameters, reflecting the increased electronic mobility associated with the chains;[25] throughout the present work we use $t_y/t_x=1.5$, which approximates the observed a-b anisotropy in the magnetic penetration depth,[26] and $V_0=-V_1=-3t_x$. Twin boundaries of up to $4|\hat{r}|$ width (corresponding to approximately 22 Å) are investigated, with $t_y=t_x$ and $\mu^I\leqslant 0$ within the twin. The largest system studied is $100|\hat{r}|$ in length with 400 k states, or 80 000 sites; periodic boundary conditions are assumed throughout.

At a twin boundary of zero width and $\mu^I=0$, we find within the BdG theory that for all temperatures the dominant d-wave component of the order parameter is virtually unaffected. The extended and on-site s-wave components, whose bulk values are approximately 10% of Δ_d, go from their near-bulk values to zero, over a single lattice spacing r, reversing their sign relative to Δ_d on either side of the boundary. As the impurity strength is increased at low temperatures, however, the d-wave and s-wave components become increasingly perturbed from their bulk values over the coherence length $\xi_{d+s}(T)$, where $\xi_{d+s}(0)\approx|\hat{r}|$ in the present work. When the magnitude of the d-wave component in the twin boundary is suppressed to approximately half its bulk value, an additional imaginary s-wave component may be nucleated near the twin edge, breaking time-reversal symmetry. We have found no evidence for a phase transition to a bulk $\mathcal{T}$-violating state in a uniform system.

The real and imaginary parts of the various components of the order parameter are shown in Fig. 2 for a twin boundary with $\mu^I=-10t_x$, $\mu=-t_x$, $T=0$, and boundary width $W_T=4|\hat{r}|$. While all the components go to zero rapidly within the twin boundary, both the real and imaginary parts of the s-wave gap functions are enhanced near the twin edge. In the immediate vicinity of the twin boundary, the real s-wave components are perturbed from their bulk values over a short distance comparable to $\xi_{d+s}(0)$, reflecting the local nucleation of additional s-wave components through

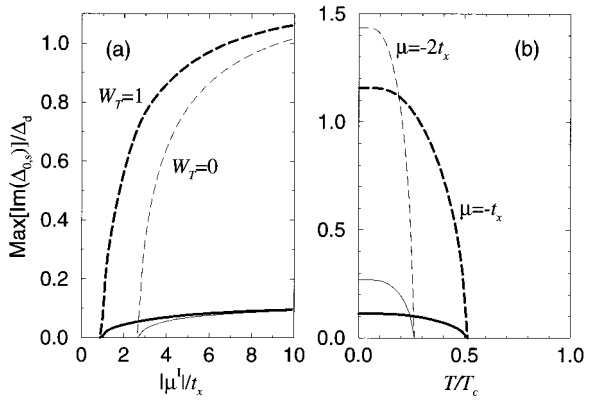

FIG. 3. The maximum value of the imaginary on-site (dashed lines) and extended s-wave (solid lines) components relative to the bulk value of the d-wave order parameter are shown as a function of (a) $|\mu^I|$ (note $\mu^I \leq 0$) and W_T at zero temperature and $\mu = -t_x$, and (b) T/T_c and μ. In (a) thin and bold lines correspond to twin boundary widths $W_T/|\hat{r}| = 0$ and 1, respectively. In (b), thin and bold lines denote results for $\mu = -2t_x$ and $\mu = -t_x$, and we have chosen $\mu^I = -100t_x$, and $W_T = 0$.

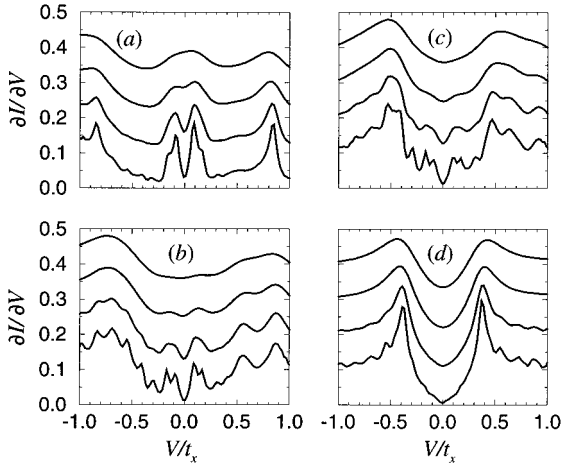

FIG. 4. A low-energy portion of the tunneling conductance near a twin boundary is shown as a function of energy, distance r from the twin edge where (a) through (c) correspond to $|\hat{r}|$ through $3|\hat{r}|$ while (d) illustrates the bulk, and temperatures $T = 0$ (lower), $T = 0.05T_c$ (offset 0.1), $T = 0.1T_c$ (offset 0.2), and $T = 0.15T_c$ (offset 0.3). Parameters are as in Fig. 2.

spatial variations of the dominant d-wave component. The presence of finite complex gap functions in the bulk, however, implies that the imaginary components vary over a different characteristic distance $\xi_{is}(0) \gg \xi_{d+s}(0)$. This longer length scale, as well as the comparable sizes of Im(Δ_0) near the twin edge and the bulk Δ_d, is consistent with the GL predictions[7] discussed above.

As shown in Fig. 3, the size of the imaginary s-wave component nucleated near the twin boundary is extremely sensitive to the temperature, impurity strength, and the width of the twin boundary. At zero temperature, Fig. 3(a), a $\mathcal{T}$-violating state first appears for $\mu^I \approx -2.7t_x$ at all electron densities for an impurity line (i.e., $W_T = 0$). As the impurity strength continues to increase, the perturbation of the d-wave component, and the maximum values of the imaginary s-wave components, begin to saturate. For $W_T > 0$, however, a lower impurity strength can give rise to $\mathcal{T}$ violation at zero temperature, since the d-wave component is already suppressed by approximately 20% in a locally tetragonal region (with $t_x = t_y$) even for $\mu^I = 0$. Increasing W_T beyond approximately $3|\hat{r}|$ has no further effect. This result, valid for all electron densities, is also consistent with the GL prediction[7] that local tetragonal symmetry could favor a time-reversal breaking state at low temperature.

The growth of all the s-wave components with decreasing chemical potential reflects the impending instability of the system against bulk dominant s-wave superconductivity at slightly lower electron densities.[17,18] As the temperature is increased at finite μ^I, the imaginary component decreases to zero as $\sqrt{1 - T/T^*}$; the transition temperature T^* is strongly density-dependent, scaling roughly with Δ_d. The same T^* is obtained for wider twin boundaries at a given density, though the magnitudes of the imaginary s-wave components increases with increasing W_T.

The spatial variation of the s-wave component's phase relative to Δ_d implied by Fig. 2 leads to currents which flow parallel to the twin surface and in opposite directions on either side of the twin boundary. The strong impurity potential therefore mimics a line of temperature-dependent magnetic flux passing through the twin boundary and oriented parallel to the c axis. As shown by the differential conductance in Fig. 4

$$\frac{\partial I(r)}{\partial V} \propto -\sum_{nk} \left[|u_{n,k}(r)|^2 f'(V - \varepsilon_{n,k}) + |v_{n,k}(r)|^2 f'(V + \varepsilon_{n,k}) \right], \tag{10}$$

where f' is the voltage derivative of a Fermi function, this effective field splits the low-energy band of virtual-bound states associated with Andreev reflections at the twin surface.[27] Alternatively, the presence of two low-energy quasiparticle peaks in the tunneling conductance at low temperatures reflects the existence of a physical gap in the excitation spectrum, proportional to the magnitude of the total complex s-wave component. The zero-temperature maximum peak-to-peak separation, found in Fig. 4(a) to be approximately $0.2t_x \sim 2$ meV (where t_x is estimated from $T_c = 0.51t_x \approx 60$ K at this carrier concentration $\langle n \rangle \approx 0.75$), grows with increasing $|V_0|$ and $|\mu^I|$ but diminishes with increasing temperature and distance from the twin boundary. While the tunneling conductance exhibits low-temperature features that are no doubt finite-size effects, it is evident that the low-energy band splits at a temperature $0.1T_c \approx 6$ K which is considerably lower than the $T^* \sim 0.5T_c$ estimated from Fig. 3(b). A comparable splitting of the zero-energy peak has been recently observed[6] in tunneling spectra of YBCO surfaces, and has been interpreted[10] as a clear signature of $\mathcal{T}$ violation.

In summary, we have found evidence for time-reversal symmetry breaking near twin boundaries in a d-wave orthorhombic superconductor at low temperatures $T < T^* < T_c$, where T^*/T_c scales approximately with the size of the bulk

d-wave gap. The magnitudes of the imaginary *s*-wave components associated with the $\mathcal{T}$ violation depend strongly on the chemical potential and depletion of the carrier density in the twin boundary. These *s*-wave gap functions could be responsible for the finite Josephson currents observed in c-axis tunnel junctions to heavily-twinned YBCO.[3] As a consequence of the time-reversal breaking, the low-energy quasiparticle peak in the tunneling conductance (related to the zero-bias anomaly in tunneling spectroscopy) is predicted to split in the vicinity of the twin edge.

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