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 complex component, are found to depend strongly on electron density. The results are compared with recent tunneling measurements.

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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\(_2\)Cu\(_3\)O\(_{7−\delta}\) (YBCO) suggest the presence of an additional \( s \)-wave order parameter.\[2\] 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.\[3\] The experimental results can be understood either if the \( s \)-wave component of the order parameter breaks time-reversal (\( T \)) symmetry near the twin boundary at low temperatures, as it can near surfaces,\[4\] or if there is far more of one kind of twin domain (i.e. twin boundaries form in groups).\[5\] Recent SQUID measurements on vortices trapped by twin boundaries in YBCO did not detect the fractional flux that would accompany local \( T \)-violation.\[6\] 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 \( T \)-violation near boundaries by considering the Ginzburg-Landau (GL) free energy for a homogeneous orthorhombic \( d \)-wave superconductor:

\[
F_s = F_n + \alpha_d |d|^2 + \alpha_s |s|^2 + \beta_1 |d|^4 + \beta_2 |s|^4 + \beta_3 |s|^2 |d|^2 + \beta_4 (s^2 d^2 + s^2 d^2) + \beta_5 (s^2 d + s d^2),
\]

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 \( \theta \) 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 \( \beta_5 \). Assuming all the coefficients are positive (except \( \alpha_d \)), the \( \beta_5 \) term favors \( \theta = n\pi \) (\( n \) integer), while the \( \beta_4 \) term favors \( \theta = \pi/2 \). Thus, in a tetragonal superconductor there can be a continuous transition to a bulk \( T \)-violating phase at a temperature \( T^* \) given by \( \alpha_d (T^*) = [2\beta_2 (T^*) + \beta_3 (T^*)] |d|^2 (T^*) \). The coefficients of the GL free energy can be chosen such that \( T^* \leq 0 \) 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 \( T \)-violation for a finite temperature \( 0 \leq T \leq T^* \).

Furthermore, the associated complex \( s \)-wave component could be large relative to \( |d| \), and would vary on a new length scale.\[8\] In contrast, an \( s \)-wave component nucleated solely through spatial variations of \( d \), such as is found in magnetic vortices,\[9\] or near impurities, is usually small relative to \( |d| \) (unless \( \alpha_d \rightarrow 0 \), which only occurs for densities just above a crossover to bulk \( s \)-wave superconductivity\[10\] 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 \( T \)-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.\[11\] Despite its simplicity, results obtained previously using this model\[12\] are consistent with those obtained within the context of a model better representing the high-\( T_c \) oxides,\[13\] and with experimental results.\[14\] 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\( \AA \).\[15\]

The Hamiltonian for the extended Hubbard model is:

\[
H = - \sum_{(ij)\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i\sigma} n_{i\sigma} - \sum_{i\sigma} \mu_i n_{i\sigma} - V_0 \sum_i n_{i\uparrow} n_{i\downarrow} - \frac{V_1}{2} \sum_{(ij)\sigma\sigma'} n_{i\sigma} n_{j\sigma'},
\]

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, \( \mu \) is the chemical potential, \( \mu_i \) 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 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:

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

such that

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

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

where the gap functions are defined by

$$\Delta_0(r_\alpha) \equiv V_0 \langle c_\uparrow(r_\alpha) c_\downarrow(r_\alpha) \rangle;$$

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

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

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

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

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

The orthorhombicity of YBCO is modeled by an anisotropy in the hopping parameters, reflecting the increased electronic mobility associated with the chains; anisotropy in the hopping parameters, reflecting the in-

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 $\Delta_d$, go from their near-bulk values to zero, over a single lattice spacing $r$, reversing their sign relative to $\Delta_d$ 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 complex $s$-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 $T$-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 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 $\xi_s(0) \gg \xi_{d+s}(0)$. This longer length scale, as well as the comparable sizes of $\text{Im}(\Delta_0)$ near the twin edge and the bulk $\Delta_d$, is consistent with the GL prediction discussed above.

![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.](image-url)
As shown in Fig. 3, the size of the complex 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 $T$-violating state first appears for $\mu^{\dagger} \approx -2.7t_x$ 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 $T$-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 $\mu^{\dagger} = 0$. 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 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. As the temperature is increased at finite $\mu^{\dagger}$, the complex component decreases to zero as $\sqrt{1 - T/T_c}$; the transition temperature $T^*$ is strongly density-dependent, scaling roughly with $\Delta_d$. The same $T^*$ is obtained for wider twin boundaries at a given density, though the magnitudes of the complex $s$-wave components increases with increasing $W_T$.

The spatial variation of the s-wave component’s phase relative to $\Delta_d$ 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,

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

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. 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. 2, to be approximately $0.2t_x \sim 2\text{meV}$ (where $t_x$ is estimated from $T_c = 0.51t_x \approx 60\text{K}$ at this carrier concentration $<n> \approx 0.75$), grows with increasing $|V_0|$ and $|\mu^{\dagger}|$ 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 $0.17T_c \approx 6\text{K}$ which is considerably lower than the $T^* \sim 0.5T_c$ estimated from Fig. 3. A comparable splitting of the zero-energy peak has been
recently observed in tunneling spectra of YBCO surfaces, and has been interpreted as a clear signature of $T$-violation.

![Graph](image)

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 $|r|$ through $3|r|$ 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.

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 complex $s$-wave components associated with the $T$-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. As a consequence of the time-reversal breaking, the low energy quasiparticle peak in the tunneling conductance (related to the zero-bias anomaly in STS) is predicted to split in the vicinity of the twin edge.

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