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Quasiclassical Theory of Twin Boundaries in High-T_c Superconductors

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We investigate the electronic structure of twin boundaries in orthorhombically distorted high-T_c materials using the quasiclassical theory of superconductivity. At low temperatures we find a local instability to a time-reversal symmetry breaking state at the twin boundary. This state yields spontaneous currents along the twin boundary that are microscopically explained by the structure of the quasiparticle bound states. We calculate the local density of states and find a splitting in the zero-bias peak once the spontaneous currents set in. This splitting is measurable by STM techniques and is a unique signature of time-reversal breaking states at a twin boundary.

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A large number of experiments have convincingly demonstrated that Cooper pairs have basically $d_{x^2-y^2}$-wave symmetry in high-temperature superconductors [1]. In a strict sense this classification applies only to superconductors with perfectly tetragonal crystal symmetry where the $d_{x^2-y^2}$ represents a "relative angular momentum" of the Cooper pairs with reduced symmetry. On the other hand, there is a number of slightly orthorhombically distorted systems such as $YBa_2Cu_3O_7$ (YBCO) where the intrinsic crystal deformation removes the symmetrical distinction between this pairing state and a conventional s-wave type. We may interpret this also in the way that the orthorhombic distortion couples the two pairing channels [2,3]. Clear evidence for this kind of mixing has been found in recent c-axis Josephson experiments between YBCO and Pb [4]. These experiments established the presence of an s-wave component and the dominance of the $d_{x^2-y^2}$-wave symmetry.

An interesting aspect of the s-wave admixture due to orthorhombic distortion occurs in the vicinity of twin boundaries (TB) which separate the two degenerate orthorhombic lattice shapes (twins). It was suggested that the two order parameter components, s and d wave, could locally twist in a way that time-reversal symmetry $\mathcal{T}$ is broken. Various physical properties are connected with this effect. In Ref. [2] it was shown on the level of Ginzburg-Landau theory that the $\mathcal{T}$-violating state is accompanied by a spontaneous current flowing parallel to the twin boundary. Recently this system was studied by solving the Bogolubov–de Gennes equations [5,6] confirming the results of the Ginzburg-Landau description and discussing the local IV characteristics observable in a tunneling experiment. Time-reversal breaking surface states were also predicted [7] and experimentally found [8] at surfaces of YBCO.

In this paper, we study this type of system and its properties using the quasiclassical theory of superconductivity developed by Eilenberger [9]. We calculate the structure of the order parameter self-consistently at all temperatures. Our calculation includes the orthorhombic distortion in the form of anisotropic quasiparticle masses. In contrast to Ref. [5], the twin boundary has no extension and is not explicitly pair breaking. In the bulk this formulation gives a mixing between s- and d-wave pairing due to the orthorhombic distortion in agreement with the other methods. For the twin boundary we show that the time-reversal symmetry is indeed broken at low enough temperature. The lower symmetry is noticeable also in the energy levels of quasiparticle bound states at the TB. In the $\mathcal{T}$-invariant state there is a large density of bound states at zero energy. The breakdown of time-reversal symmetry in the TB leads to the splitting of this energy level, and this effect in the local density of states is observable by STM (scanning tunneling microscopy). The properties of these bound states lead also to a microscopic interpretation of the spontaneous current along the TB.

In YBCO the orthorhombic symmetry reduction is partially induced by lattice deformation and mainly due to the presence of CuO chains. The introduction of this orthorhombicity into the quasiclassical formulation is done by changing the single electron dispersion to

$$\varepsilon(\boldsymbol{k}) = \frac{\boldsymbol{k}^2}{2m} - \frac{c}{m} k_x k_y \,, \qquad (1)$$

where the (dimensionless) constant $-1 < c < 1$ parametrizes the distortion (the sign of c defines the two twin domains). Here the x and y axes correspond to the direction $[1\ 1\ 0]$ and $[1\ \ -1\ 0]$ of the tetragonal lattice. This leads to a noncylindrical Fermi surface (FS) with $k_{\mathrm{F}}(\theta) = \frac{k_{\mathrm{F0}}}{\sqrt{1-c\sin 2\theta}}$ where θ is the angle between $\boldsymbol{k}$ and the k_x direction and k_{F0} the Fermi wave vector of the undistorted system. We will neglect all effects of electron motion in c-axis direction. With this anisotropy the averaging over the FS has to be modified compared to the standard case,

$$\sum_{\boldsymbol{k}} \rightarrow N_0 \langle \cdots \rangle = N_0 \int_0^{2\pi} \frac{d\theta}{2\pi}\, n(\theta)\,. \qquad (2)$$

Here, N_0 is the normal density of states at the Fermi energy, and

$$n(\theta) = n_f \frac{\boldsymbol{k}_F^2(\theta)}{m|\boldsymbol{k}_F(\theta)\boldsymbol{v}_F(\theta)|} = n_f \frac{1}{1 - c\sin 2\theta}, \quad (3)$$

where n_f is a normalization factor. A realistic estimate for the parameter c is ~ 0.2; this is mainly due to the chains [10]. Besides this modification of the dispersion we will neglect all other effects related to the chains.

In the following, we restrict our discussion to the s-wave and $d_{x^2-y^2}$-wave pairing channels. The pairing interaction is modeled as

$$V(\theta, \theta') = V_s + 2V_d \sin(2\theta)\sin(2\theta'), \quad (4)$$

where the angular dependence of the d-wave part follows from our choice of the coordinate frame. The coupling strengths $V_{s/d}$ are eliminated in favor of the bare critical temperatures $T_{cs/d}$ and the energy cutoff ω_c, the latter assumed to be the same for both channels. Then the coupling constants can be defined as $V_{s,d}^{-1} = \ln(T/T_{cs,d}) + \sum_{n>0}^{n<\omega_c/2\pi T}(n + 1/2)^{-1}$.

The bulk solution for the off-diagonal quasiclassical Green's function is $f_\omega(\theta) = \Delta(\theta)/\Omega(\theta)$, where $\Omega(\theta) = \sqrt{\omega^2 + |\Delta(\theta)|^2}$. The gap function is a linear combination of the s- and d-wave component, $\Delta(\theta) = \Delta_d \sin(2\theta) + \Delta_s$.

The self-consistent calculation leads to two coupled equations for the s- and d-wave component. In the case $c = 0$ we either find a one-component solution (i.e., the s- or the d-wave component vanishes), or both are finite and appear in the complex combination $d \pm is$; i.e., they have the relative phase $\phi = \pm\pi/2$ [11]. At $T = 0$ the complex phase occurs for $0.6 \lesssim T_{cs}/T_{cd} < 1.0$ (see the inset of Fig. 1).

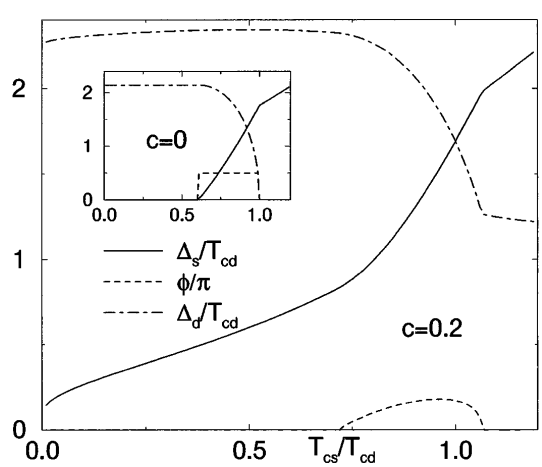

FIG. 1. Zero-temperature properties of an orthorhombic superconductor with mixed d and s pairing. For different magnitudes of the orthorhombic distortion $c = 0.2$ (main graph) and $c = 0$ (inset), the two order parameters and the relative phases are shown as a function of T_{cs}/T_{cd}.

An expansion in c immediately shows that the s and d components are coupled for $c \neq 0$ and a finite value of one of the components drives the other component to be nonzero. A nonvanishing c also leads to a renormalized onset temperature for superconductivity,

$$T_c(c) = \tfrac{1}{2}(T_{cs} + T_{cd}) + \tfrac{1}{2}\sqrt{(T_{cs} - T_{cd})^2 + 2\tilde{c}^2 T_{cs}T_{cd}}, \quad (5)$$

where $\tilde{c} = c\sum_{n=0}^{\omega_c/2\pi T_c} 1/(n + 1/2)$.

The numerical results for the two order parameters and their relative phase at $T = 0$ are shown in Fig. 1 as a function of T_{cs}/T_{cd}. They always coexist. In contrast to the case $c = 0$, the relative phase ϕ varies continuously and is different from zero in a narrow window of values of T_{cs}/T_{cd}. The region of broken time-reversal symmetry is shrinking with increasing $|c|$, in qualitative agreement with the Ginzburg-Landau approach.

In the following we will assume $T_{cs}/T_{cd} = 0.3$ (see Ref. [7]) and $c = 0.2$ which leads to $\Delta_s \sim 0.25\Delta_d$ and $\phi = 0$ or π (see Fig. 1); i.e., no bulk $\mathcal{T}$-violating state occurs in agreement with the present experimental status.

We will now consider a TB, a boundary between two domains with the relative orientation of the crystal axes of 90°; see Fig. 2. The quasiclassical equations have to be solved along classical trajectories, which are characterized by a momentum direction on the Fermi surface $\boldsymbol{k}_F$ [9]. At the TB the k vectors with the same k_y component have to be matched. The reflection coefficient for a given $\boldsymbol{k}_F$ in the absence of a boundary potential is $R = (v_{Fx1} - v_{Fx2})^2/(v_{Fx1} + v_{Fx2})^2$. If we consider the energy dispersion given in Eq. (1) [$c = \mathrm{sgn}(x)|c|$], we find that $v_{Fx1} = v_{Fx2}$ for all scattering directions. Consequently, we have *no normal* reflection at the TB [6].

We solve the quasiclassical equations numerically in a self-consistent way for various temperatures for a single twin boundary. The calculation was simplified by applying the Schopohl-Maki transformation to the Eilenberger equations [12]. Consistent with experimental observations [1,4] we assumed that the d-wave component

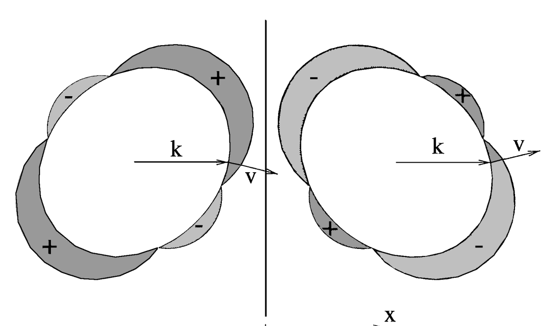

FIG. 2. Fermi surfaces and bulk gap (shaded region) on both sides of the TB. Fermi wave vectors $\boldsymbol{k}_F$ vectors and Fermi velocities $\boldsymbol{v}_F$ for a perpendicular trajectory are indicated by arrows. The parallel components of v_F for these trajectories on both sides of the TB have different signs.

is identical on both sides, whereas the s-wave component changes sign.

Results for two different temperatures are shown in Fig. 3. For the higher temperature $T = 0.1T_{cd}$ the relative phase jumps from 0 to π at the twin boundary and Δ_s goes to zero directly at the TB. On the other hand, for $T = 0.01T_{cd}$ we observe a local $\mathcal{T}$ violation where the relative phase changes continuously from 0 to π with a nonvanishing s-wave pairing component. The inset of the upper graph shows $|\Delta_s|^2$ at the TB as a function of temperature. It becomes finite for $T \lesssim 0.05$. A particular feature of local $\mathcal{T}$ violation is the appearance of spontaneous currents in the vicinity of the TB flowing in opposite directions on both sides. These spontaneous currents at $T = 0.01T_{cd}$ are shown in Fig. 3 (inset lower graph). Note that screening effects are not taken into account here.

The local density of states (LDOS) can be calculated by solving the Eilenberger equation for real energies. The results are given in Fig. 4. In the $\mathcal{T}$-invariant state a pronounced zero-energy peak occurs in the vicinity of the TB. In the $\mathcal{T}$-violating state, the zero-energy peak splits into two symmetric peaks. The separation of the peaks is proportional to $\Delta_s(0)$. The LDOS can be measured by scanning tunneling microscopy (STM). In particular, the splitting of the zero-energy peak would prove the existence of a time-reversal breaking state in YBCO [5]. The temperature at which the splitting occurs, $T \sim 0.05T_{cd} \sim O(5\ \mathrm{K})$, is well within reach of current low-temperature STM technology.

To investigate the microscopic nature of the gap feature in the LDOS and the spontaneous current it is useful to turn to an angle-resolved view of the problem. The zero-energy peak in the LDOS in the $\mathcal{T}$-invariant situation can be understood by considering classical trajectories with angles θ centered around 0, π, and $\pm\pi/2$ in a range $2\delta\theta = \arcsin(\Delta_s/\Delta_d)$. The corresponding Andreev (electron-hole) bound state for such angles is confined between two superconducting domains with a phase shift of π which leads to a zero-energy level [13]. On the other hand, broken time-reversal symmetry will generate phase shifts different from π leading to up- or down-shifted energy levels and the splitting of the zero-energy peak. Alternatively, this effect may also be seen as a driving mechanism: the large DOS of the zero-energy bound states at the Fermi energy gives rise to a local Fermi surface instability opening a (pseudo)gap.

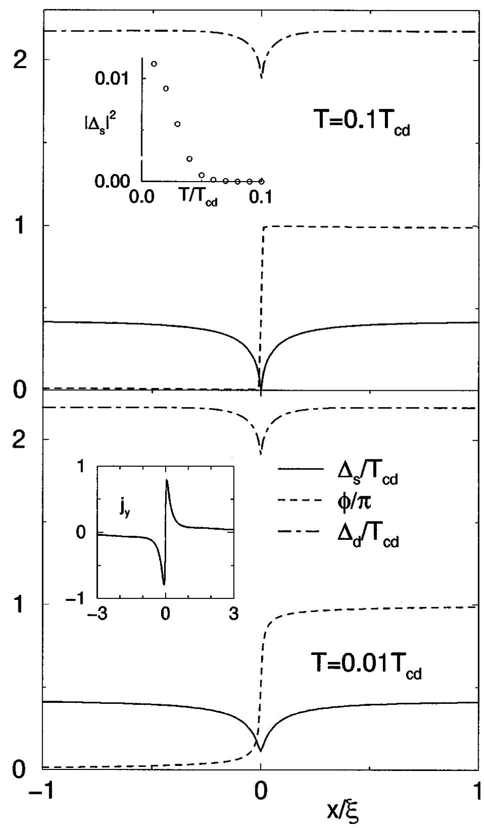

FIG. 3. Order parameters and relative phase in the vicinity of a twin boundary for $T_{cs}/T_{cd} = 0.3$ and $c = 0.2$. $\xi = v_F/2\pi T_{cd}$ is the coherence length. Upper graph: $\mathcal{T}$-invariant state of the TB for $T = 0.1T_{cd}$. The s component goes to zero at the TB. Lower graph: Locally $\mathcal{T}$-violating state for $T = 0.01T_{cd}$. The absolute value of the s component is finite for $x = 0$, and the relative phase changes smoothly from 0 to π. Inset upper graph: Modulus squared of (imaginary) s component as a function of temperature. Inset lower graph: Spontaneous current density in units of $10^{-1}eN_0T_{cd}v_F$.

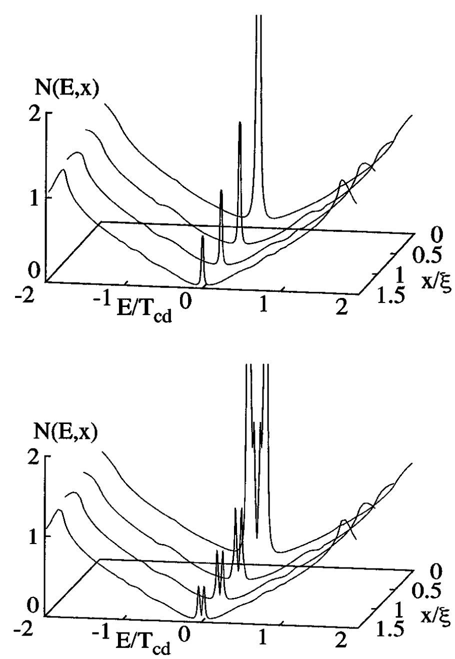

FIG. 4. Local density of states in the vicinity of a twin boundary for $T_{cs}/T_{cd} = 0.3$ and $c = 0.2$. The two graphs correspond to $T = 0.1T_{cd}$ (upper graph) and $T = 0.01T_{cd}$ (lower graph). In the $\mathcal{T}$-invariant state there is a large peak at zero energy. The peak splits symmetrically in the $\mathcal{T}$-violating state.

How does this splitting lead to spontaneous currents? Each state (bound or extended) carries a current parallel to $\boldsymbol{v}_{\mathrm{F}}(\boldsymbol{k})$. The phase gradient seen by these states leads to a shift in energy (bound states) or spectral weight (extended states). As a result left- and right-moving states are differently occupied. At $T = 0$ only the *right*-moving states of the bound states are occupied. On the other hand, because of the shift of the spectral weight the *left*-moving continuum states give the dominant contribution of the continuum states. They cancel the perpendicular current contribution of the bound states (as required by current conservation), leaving only a parallel component of the total current [14]. The sign of the parallel current is different on both sides of the TB due to the symmetry of the dispersion relation (the momenta and velocities for one of these states are indicated in Fig. 2).

In conclusion, we have studied the electronic structure of twin boundaries in orthorhombically distorted high-T_c superconductors. The orthorhombic distortion was introduced in the quasiclassical formalism of superconductivity, and the corresponding equations were solved self-consistently. In contrast to Ref. [5] we do not assume that the TB has a pair-breaking effect. At low temperatures, we found a localized $\mathcal{T}$-violating state at the TB. These localized states create spontaneous quasiparticle currents that flow in parallel to the TB. In addition, we find a splitting of the zero-bias anomaly in the local density of states. Using realistic parameters we estimate that this splitting could be observed around 5 K, i.e., using available low-temperature scanning tunneling microscopes. This splitting would be a unique signature of $\mathcal{T}$ violation in such systems.

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