Spin currents and spontaneous magnetization at twin boundaries of noncentrosymmetric superconductors

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Twin boundaries are generic crystalline defects in noncentrosymmetric crystal structures. We study theoretically twin boundaries in time-reversal-symmetric noncentrosymmetric superconductors that admit parity-mixed Cooper pairing. Twin boundaries support spin currents as a consequence of this parity mixing. If the singlet and triplet components of the superconducting order parameter are of comparable magnitude, the superconducting state breaks spontaneously the bulk time-reversal symmetry locally near the twin boundary. By self-consistently evaluating the Bogoliubov-de Gennes equations and the gap functions, we find two distinct phases: First, time-reversal-symmetry breaking enhances the spin currents but does not lead to charge current. A secondary phase transition then triggers a spin magnetization and a finite charge current near the twin boundary.

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Initiated by the discovery of superconductivity in the noncentrosymmetric heavy-fermion compound CePt3Si, noncentrosymmetric superconductors (NCSC) have opened up new perspectives in the study of unconventional superconductivity.1–9 Due to the lack of inversion symmetry, these systems feature antisymmetric spin-orbit coupling that breaks completely the SU(2) spin-rotation symmetry. As a consequence, the superconducting condensate has no definite parity and can be viewed as a superposition of even- and odd-parity (spin-singlet and spin-triplet) Cooper pairs.5,7,13–15 The mixing ratio of even- and odd-parity components is a convenient tuning parameter to characterize the superconducting state of a NCSC. For example, quasi-two-dimensional (2D) superconductors of this kind have a $\mathbb{Z}_2$ topological attribute when fully gapped (symmetry class DIII in the classification of Ref. 11) because the phases with dominant even-parity pairing (odd-parity pairing) are topologically trivial (nontrivial). They are separated by a gap-closing topological phase transition.12 Akin to the helical electronic edge states of a 2D $\mathbb{Z}_2$ topological insulator, helical edge modes in the form of Andreev bound states transport a nonconserved spin current along the boundary of a NCSC with dominant odd-parity pairing.5,7,13–15 Andreev bound states are a specific signature of unconventional Cooper pairing and directly manifest themselves in tunneling spectroscopy measurements.8

Very generally, the topology of phases of matter can be probed at defects, such as boundaries, lattice dislocations, or vortices in a superconducting order parameter.16 In noncentrosymmetric materials, the crystal structure allows for another type of defect when two regions of space with the opposite inversion-symmetry breaking face each other in a single crystal. In fact, the formation of such twin domains, similar to the domains in ferroelectrics, is rather likely in the crystal growth processes. A first step towards understanding the superconducting state at twin boundaries of a noncentrosymmetric material has been undertaken in Ref. 6. It revealed that time-reversal symmetry (TRS) can be spontaneously broken at the twin boundary (TB) that can then host vortices enclosing fractional fluxes, which have been studied in the context of anomalous flux flow observed experimentally in some NCSC.17

In our study, we extend the phenomenology of the possible pairing states at the TB by self-consistently evaluating the Bogoliubov-de Gennes (BdG) equations and the gap functions. We find two distinct phases with broken TRS at the TB. In the first phase, the superposition of the two parity components turns complex. The spin currents, running along the TB for all ratios of parity mixing, are enhanced in this phase. Yet, contrary to naive expectations, no charge current flows despite the broken TRS. This changes with a secondary transition to a further phase that features both a nonvanishing magnetization and an orbital supercurrent along the TB. In our analysis, we clarify the relation between the bulk topological phase transition and the phase diagram of the states near the TB, as well as the nature and spatial profile of the spin and charge supercurrents in each phase.

We use a tight-binding model describing a 2D NCSC with Rashba spin-orbit coupling that includes spin-dependent nearest-neighbor pairing interactions which allow for the appearance of unconventional pairing channels. The electrons hop on a square lattice $\Lambda$ of $L_x \times L_y$ sites $r = (x,y) \in \Lambda$ that is spanned by the orthogonal unit vectors $a_i$, $i = x,y$. The corresponding Hamiltonian for the extended Hubbard model reads as10

$$H = -\sum_{r, i} \sum_{s} c_{r+a_i,s}^\dagger (t \delta_{\sigma} - \lambda_{r,a_i} \cdot \sigma) c_{r,s} + \sum_{r, i} \left[ J S_{r+a_i} \cdot S_{r} + D_{r,a_i} \cdot (S_{r+a_i} \times S_{r}) \right] + U \sum_{r} n_{r+a_i} n_{r},$$

where $c_{r,s}^\dagger$ creates an electron with spin $s = (\uparrow, \downarrow)$ at site $r \in \Lambda$. The antisymmetric spin-orbit coupling is a Rashba term of strength $\alpha_{r}$ parametrized by $\lambda_{r,a_i} = \alpha_{r}(\hat{z} \times a_i)$, $i = x,y$, where $\hat{z}$ is the unit vector normal to the plane of the lattice. The vector $\sigma = (\sigma^+, \sigma^-, \sigma^z)$ denotes the three Pauli matrices and $\delta_{\sigma}$ the $2 \times 2$ unit matrix. We define the electron density
yielding the highest transition temperature is the one with gapless helical edge states exist at the boundary of a 2D crystal structure also allows for a Dzyaloshinsky-Moriya-type spin-spin interaction of strength $D_{\pi}$ which is parametrized as $D_{r,a} = D_{\pi}(a \times a_i)$, $i = x, y$.

Let us illustrate the mean-field decoupling for a translational invariant system ($\alpha_r \equiv a$, $D_r \equiv D$, $\forall r$), assuming periodic boundary conditions in both the $a_i$ and $a_r$ directions. The Rashba-type spin-orbit interaction breaks the SU(2) spin-rotation symmetry and induces a splitting of the electron bands, with each band exhibiting a specific spin structure in momentum space. At the same time, it allows the gap function to be of mixed parity. The BdG mean-field Hamiltonian reads as $H_{\text{BdG}} = \sum_k c_k^\dagger \mathcal{H}_{\text{BdG}} c_k$, with the four-component notation $c_k = (c_k^\uparrow, c_k^\downarrow, c_k^{-\uparrow}, c_k^{-\downarrow})$, $k$ representing the 2D momentum in the Brillouin zone, and

$$\mathcal{H}_{\text{BdG}} = \begin{pmatrix} \Delta_k & \mathbf{g}_k \\ \mathbf{g}_k^\dagger & -\Delta_k \end{pmatrix}. \quad (2a)$$

The kinetic part of the Hamiltonian is given by

$$\mathcal{H}_{\text{kin}} := -2[a_x \sin(k_x) - a_y \sin(k_y)].$$

with $\mathbf{g}_k := 2[a_x \sin(k_x) - a_y \sin(k_y)]$. We can decompose the superconducting gap function $\Delta_k = (\sigma^x)(\Delta_k^0 + \Delta_k^{(e)})$ in a scalar even-parity spin-singlet part $\Delta_k^0$ and a vector odd-parity spin-triplet part $\Delta_k^{(e)}$. The assumption of an extended s-wave pairing in the former and p-wave pairing in the latter yields the momentum dependencies

$$\Delta_k^0 = \Delta_k^0 [\cos(k_x) + \cos(k_y)] + \Delta_0^0, \quad (2c)$$

$$\Delta_k^{(e)} = \Delta_k^{(e)} [\sin(k_x) - \sin(k_y)]0$$

of the order parameters. Note that the p-wave pairing state yielding the highest transition temperature is the one with $\Delta_k^{(e)} \propto \mathbf{g}_k$. This allows us to simultaneously diagonalize the gap function and the kinetic part of the Hamiltonian $\mathcal{H}_{\text{kin}}$ by going to the basis of $\mathbf{g}_k$.

We now turn to the electronic properties of the system with TB. For that, we equip the Rashba spin-orbit coupling and the Dzyaloshinsky-Moriya interaction in Hamiltonian (1) with the spatial dependencies

$$\alpha_r = \alpha \sgn(x - L_x/2), \quad D_r = D \sgn(x - L_x/2), \quad (3)$$

respectively. This models a TB located at $x = L_x/2$ and separates two regions of the superconductor that have the opposite sign of the Rashba and Dzyaloshinsky-Moriya coupling [see Fig. 1(a)]. Open and periodic boundary conditions are used in the $a_i$ and $a_r$ directions, respectively. The relative U(1) phase between $\Delta_k^{(e)}$ and $\Delta_p$ has to change by $\pi$ across the TB. The way the superconducting condensate accommodates this phase twist decisively determines the physics at the TB.

If $\Delta_k^{(o)}$ is the dominant component of the order parameter, gapless helical edge states exist at the boundary of a 2D topological superconductor, as dictated by the nontrivial $Z_2$ topological index. Localized modes within the bulk spectral gap also exist at the TB, although they would not be endowed with topological protection, for the $Z_2$ topological sector of the Hamiltonian is the same on either side. In order to identify the existence and spin polarization of the localized modes at TB, we calculated the spectral function

$$A_{\pm, k}(E) = -\frac{1}{\pi} \text{Im} \mathcal{G}_{\pm, k}(E), \quad (4)$$

where $\mathcal{G}_{\pm, k}(E)$ is the Green’s function at position $x$ and momentum $k_y$. Figures 1(b) and 1(c) show the spectral function for up-spin quasiparticles on the immediate left of the TB. We observe that the left- and right-going modes have opposite spin polarization at high energies and that this spin-momentum locking is lifted with the appearance of a hybridization gap near zero energy.

We turn now to the central issue, the analysis of TRS breaking phase at the TB. TRS breaking is signaled by the following two quantities: (i) the relative U(1) phase

$$\varphi := \arg\Delta_k^{(e)} = -\arg\Delta_p = \Delta_\pi \mp \arg\Delta_k^{(e)}$$

of the singlet component of the superconducting order parameter in the bulk on the left and right sides of the TB and (ii) the spin magnetization $M = n_1 - n_2$ at the TB. To understand the relevance of (i), we have to ask how the condensate can account for the $\pi$ shift in the relative U(1) phase between $\Delta_k^{(e)}$ and $\Delta_p$ across the TB. The two values of $\varphi$ compatible with TRS are $\varphi = 0$ and $\pi$. In the former case for $|\Delta_k^{(e)}| \gg |\Delta_p^{(o)}|$ and it is energetically favorable that $\Delta_p$ changes the sign being zero at
magnetic order at the TB as a function of onsite repulsion ratio. Continuous lines separate phases of (A) TRS singlet dominated from the values 0 and \( \pi \) near the TB, and (D) TRS triplet dominated superconductivity. The color scale indicates the spin magnetization near the TB that becomes nonzero in phase (C) via a secondary phase transition in the phase with broken TRS. Dashed lines encircle the region in parameter space where the bulk superconducting gap \( \Delta \) is high. In this case, the relative \( U(1) \) breaking \( \phi \) is spontaneously broken at the TB. This is also signaled by the spin magnetization (blue line) near the TB in the TRS broken phase. Parameters are \( J = 1.3, D = 2.1, V = 1.2, U = 0.87 \), such that \( \Delta_s/\Delta_p = 0.5 \) (Ref. 19).

Finally, let us study how the spontaneous TRS breaking manifests itself in the context of a (spin) Hall response at the TB. Spin currents are generically expected at edges and TB in noncentrosymmetric materials. We define the spin current of polarization \( i = x, y, z \) that runs in the y direction:

\[
J_y^{\text{spin-}i}(x) := \text{Tr} \sum_{k_y} c_{y,x}^\dagger \left( i \gamma_i \hat{T} L_{k_y,x} \right) \sigma^y c_{y,x},
\]

where the trace is taken over all states below zero energy. Figure 3(a) shows the spin currents \( J_x^{\text{spin-}x} \) and \( J_y^{\text{spin-}c} \) as a function of position \( x \) inside the phase B of phase diagram 2(a). Each of them has opposite signs on either side of the TB. The component \( J_y^{\text{spin-}z} \) vanishes in the bulk and is much smaller than \( J_y^{\text{spin-}c} \) at the TB (not shown). The component \( J_y^{\text{spin-}c} \) corresponds to the usual spin current, present at the sample edge as well as at the TB. The component \( J_y^{\text{spin-}x} \) is finite also in the bulk and increases at the boundary. However, its bulk contribution should not be interpreted as a physically measurable spin current. The phase C of phase diagram 2(a) is characterized by a finite magnetization \( M \) shown in Fig. 3(b). This magnetization appears together with an orbital supercurrent that runs in opposite directions on the immediate left and right of the TB [Fig. 3(b)]. This may be considered as a spontaneous spin Hall effect, for the supercurrent is a response to introducing an imbalance of the spin occupation on the spin current.

In summary, we studied the interface states between twin domains in a mixed-parity superconductor near a topological phase transition connecting a topologically trivial on a nontrivial phase. A sequence of two phases localized around the twin boundary appears. The primary phase breaks TRS and is, consequently, twofold degenerate, but does not show any magnetism. The secondary phase introduces magnetism through spin polarization along the \( z \) axis and a supercurrent parallel to the TB. This phase breaks the reflection symmetry for a mirror plane perpendicular to the TB including the spin current.
adding a further twofold degeneracy. The appearance of the spin polarization and the supercurrent is connected through the presence of spin current at the TB analogous to the spin Hall effect.\textsuperscript{25}

In closing, we note that the mechanism for TRS breaking that we discussed in this work is not limited to twin boundaries in NCSCs. It can also be of relevance to tunable devices with interface superconductivity such as SrTiO$_3$/LaAlO$_3$,\textsuperscript{26} where the Rashba spin-orbit coupling is not uniform in space.\textsuperscript{26} A similar phenomenology might apply to other ordering phenomena, such as the spontaneous generation of the quantum spin Hall effect in graphenelike materials.\textsuperscript{27} In this case, TRS may be broken at the boundary between regions of opposite spin Hall conductivity, spontaneously generating a charge Hall effect.

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