Spontaneous edge and corner currents in \( s + is \) superconductors

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The recently discovered so-called \( s + is \) superconducting state is a non-topological and non-chiral state in the modern classification scheme. It does not have topological surface states, and no spontaneous surface currents are expected in this class of materials. We present a microscopic study that demonstrates that \( s + is \) superconductors can have spontaneous boundary currents and spontaneous magnetic fields of a different kind. These arise at lower-dimensional boundaries: corners of two-dimensional samples and corners and edges of three-dimensional samples.

The most common type of superconductivity occurs where electrons form spin-singlet Cooper pairs. Such a superconductor spontaneously breaks local \( U(1) \) symmetry. Recent experiments reported the discovery of the so-called \( s + is \) superconductor Ba\(_1−x\)K\(_x\)Fe\(_2\)As\(_2\) [1–3]. The \( s + is \) superconductor [4–7] is a spin singlet superconductor, that spontaneously breaks an additional – time reversal – symmetry, so the total broken symmetry becomes \( U(1) \times \mathbb{Z}_2 \). The evidence of such states comes from spontaneous magnetic fields observed in the system’s bulk in muon spin relaxation experiments [4–6]. Previous theoretical studies, based on Ginzburg-Landau models, predicted such fields to arise due to certain types of defects, present in the bulk of an \( s + is \) superconductor [8–14].

Superconducting states that break time-reversal symmetry have been sought-after for decades. Previously, the research was almost exclusively focused on different kinds of superconductors with broken time-reversal symmetry (BTRS) \( U(1) \times \mathbb{Z}_2 \): the topological and chiral superconductors, such as \( p+ip \), although experimental observation of this state is still under debate. A hallmark of chiral superconductors that spontaneously break time-reversal symmetry, are surface currents producing magnetic fields near surfaces [15–18]. By contrast, by the standard symmetry and topology arguments, the \( s + is \) superconductors should not have surface currents. Namely, these are superconductors with Copper pairing in different bands, described by several complex fields \( |\Delta_\alpha|e^{i\theta_\alpha} \), which serve as order parameters. The time-reversal symmetry breaking is associated with a non-trivial phase difference locking between different bands \( \theta_\alpha - \theta_\beta \neq 0,\pi \), so that a time-reversal operation, i.e., complex conjugation of the order parameters brings the system into a different state, from which, one cannot rotate back to the original state by a gauge transformation. The standard argument for the existence of a surface current is: let us assume there is a spontaneous surface current in the superconductor. However, since there is no chirality in real space in a \( s + is \) state, flipping the sample does not change the chirality of the state and should not invert the current direction. Thus, one would conclude that the edge currents should be absent.

In this paper, we show that, nonetheless, non-topological, non-chiral BTRS superconducting states, such as \( s + is \) states, do have edge currents and edge magnetic fields. These fields and currents have dipolar structures and are allowed by symmetry. The spontaneous currents originate from the counterparts of non-topological boundary states recently reported in non-BTRS systems [19–22].

To answer the question of boundary effects, a fully microscopic theory is required. To this end, we obtain self-consistent solutions in a three-band Bogoliubov-de-Gennes model (BdG) with gauge field, describing a three-band \( s \)-wave superconductor. For a \( d \) dimensional hypercubic lattice defined on a domain \( \Omega \), it reads:

\[
H = \sum_{\alpha=1}^{3} \Psi_\alpha^\dagger H_\alpha \Psi_\alpha + \int_\Omega dr \frac{(\nabla \times A)^2}{2},
\]

where the Nambu spinors are defined as

\[
\Psi_\alpha = \left( c_{\alpha 1\uparrow}, \ldots, c_{\alpha N\uparrow}, c_{\alpha 1\downarrow}, \ldots, c_{\alpha N\downarrow} \right),
\]

\[
\Psi^\dagger_\alpha = \left( c_{\alpha 1\uparrow}^\dagger, \ldots, c_{\alpha N\uparrow}^\dagger, c_{\alpha 1\downarrow}^\dagger, \ldots, c_{\alpha N\downarrow}^\dagger \right)^T,
\]

and with \( H_\alpha \) being the \( \alpha \)-band’s Hamiltonian

\[
H_\alpha = \left( \begin{array}{cc} h_{\alpha\alpha} & \Delta_\alpha \\ \Delta_\alpha^\dagger & -h_{\alpha\alpha} \end{array} \right).
\]

\( (h_{\sigma\alpha})_{ij} = -\mu_\sigma \delta_{ij} - t_{\alpha ij} \), where the roman indices \( i, j \in \Omega \) label the position on a lattice with \( N \) lattice points. \( \sigma = \uparrow, \downarrow \) indicates the spin, while \( \alpha, \beta = 1, 2, 3 \) label the band component. \( \mu_\alpha \) is the chemical potential, and the hopping coefficient \( t_{\alpha ij} \) contains the Peierls phase as follows

\[
t_{\alpha ij} = t_{\alpha j} \delta_{i-j-1} e^{i q_j} \mathbf{A}(r) \cdot dr.
\]

\(|i-j|=1\) if \( i \) and \( j \) are neighboring points in the hypercubic lattice. \( \mathbf{A}(r) \) is the vector potential defined on the domain \( \Omega \) and \( q \) the carriers charge. The gaps are complex fields \( \Delta_{\alpha\beta} = |\Delta_{\alpha\beta}|e^{i\theta_{\alpha\beta}} \) obtained through the self-consistency equation

\[
\Delta_{\alpha\beta} = \sum_{\beta=1}^{3} V_{\alpha\beta} \langle c_{\alpha\beta}^\dagger c_{\beta\beta} \rangle_\beta
\]
where $V_{\alpha\beta}$ is the matrix containing the intra-band $(V_{11}, V_{22}, V_{33})$ and inter-band couplings $(V_{12}, V_{13}, V_{23})$. The thermal average $\langle \cdot \rangle_\beta$ means it is performed over the eigenvalues of the Hamiltonian $H_\beta$. To ensure the Hamiltonian to be hermitian, we have $h_{\alpha\alpha} = h_{\alpha\alpha}^\dagger$ and $V = V^\dagger$. At each iteration for $\Delta_{\alpha\alpha}$, we compute the current density

$$J_{ij} = -i \sum_{\sigma = \pm, \alpha} (t_{\alpha ij} \langle c_{\alpha i\sigma} c_{\alpha j\sigma} \rangle - t_{\alpha ji} \langle c_{\alpha j\sigma} c_{\alpha i\sigma} \rangle),$$

which is then used, together with Maxwell’s equations to compute the vector potential. Our study is restricted to two-dimensional samples, which also give insights for three-dimensional systems which are translationally invariant along the $z$-direction. The gap fields $\Delta_{\alpha\alpha}$ are defined on the lattice sites. The vector potential $A(\mathbf{r})$ is discretized using a finite difference method, where $\Delta x = \Delta y = a$, where $a$ is the lattice length. Both the vector potential and current density components are defined on the links between lattice sites, and the magnetic field $B_z$ is defined on the plaquettes. Since the lattice length is set to unity, the magnetic flux through a plaquette equals the local magnetic field.

We solve self-consistently for the gaps and the vector potential. To compute $\Delta_{\alpha\alpha}$, we use Chebyshev polynomial expansion method [23–25], with polynomial up to order 700, which is sufficient in the considered temperature range. To calculate the vector potential, at each iteration, we perform a gradient descent step, adapting $A$ to the changing current density distribution. Then, we use the new vector potential to update all the hopping coefficients. We iterate this fully self-consistent procedure until the convergence criterion $|\Delta_{\alpha\alpha}^{(n+1)} - \Delta_{\alpha\alpha}^{(n)}|/|\Delta_{\alpha\alpha}^{(n)}| \leq 10^{-8}$, and $|A^{(n+1)} - A^{(n)}|/|A^{(n)}| \leq 10^{-8}$ is fulfilled; $n$ indicates, respectively, the self-consistent iteration number and the gradient descent step. In our study, we consider 2D square lattice samples of size $N_xN_y = 100 \times 100$. The solver is a custom CUDA implementation.

The parameters we use in all the numerical computations presented in this work are: $\mu_1 = \mu_2 = \mu_3 = 0.0$, $t = -1$ both along $x$ and $y$, $T = 0.44$ and $q = 0.5$. The intra and inter-band interactions are given by the coupling matrix

$$V_{\alpha\beta} = \begin{pmatrix} 1.92 & 1.0 & 1.0 \\ 1.0 & 1.95 & 1.0 \\ 1.0 & 1.0 & 1.9 \end{pmatrix}_{\alpha\beta}. \quad (7)$$

In $s + is$ superconductors, the inter-band couplings yield frustration. To fully minimize the energy, a phase difference of $\pi$ between each band would be preferred, which is not achievable in the three bands’ case. The $s + is$ state arises where the disparity of the coupling is not too significant so that there are two energetically equivalent interband phase-difference locking $\theta_\alpha - \theta_\beta \neq 0, \pi$.

We begin by analyzing the case of a squared sample. The resulting gaps absolute values and phase differences are shown in Figure 1.

Near the sample edges and corners, there is an enhancement in the superconducting gaps. The effect originates from the peculiarity of the density of states near the sample’s boundaries, and its range is set by the coherence length [20, 22]. Our solutions show a spontaneous magnetic field near sample corners shown in Figure 2. We find this effect in our model when there is a disparity in the couplings of different bands. In each corner,
the spontaneous magnetic field has a dipolar structure, and therefore it carries zero net flux through the whole system. The field configuration respects rotation symmetry. The origin of the spontaneous magnetic field can be understood as follows. Firstly, in an $s + is$ superconductor, the normal modes are a mixed linear combination of the gap amplitudes and phase difference [5]. That is, even a tiny variation of relative densities results in a variation of relative phases. This contrasts with ordinary multiband superconductors, where minor spatial variations of the gap amplitudes do not produce variations in the phase difference. Secondly, it is based on the existence of topological Skyrme-like terms in hydro-magneto-statics of multicomponent superconductors [26].

Let us consider, for example, a Ginzburg-Landau model for a two-dimensional three-band superconductor. The expression for magnetic field $B_z$ can be written by expressing the vector potential as a function of the supercurrent and taking the curl. For a three-band superconductor with standard gradient terms, the expression reads [27]

$$B_z = -\epsilon_{ij} \partial_i \left( \frac{J_j}{e|\Psi|^2} \right) - \frac{i\epsilon_{ij}}{e|\Psi|^2} \left( \Psi^\dagger \partial_i \Psi \partial_j \Psi^\dagger \Psi \right. + \left. \Psi \partial_i \Psi \partial_j \Psi^\dagger \Psi \right).$$  \hspace{1cm} (8)

Where $\Psi = (\psi_1, \psi_2, \psi_3)$ is a vector made of three components of the order parameters corresponding to different bands, with modulus $|\Psi|^2 = \Psi^\dagger \Psi$. $J_i$ is the $i$-th spatial component of the current density and $\epsilon_{ij}$ is the 2d version of the Levi-Civita symbol. The first term in Equation 8 is the standard contribution, generic for London’s hydro-magneto-statics. The second term is specific for three-band superconductors and describes currents originating from the cross-gradients of the relative phases and relative amplitudes of the gaps in different bands. It has the form of $\mathbb{C}P^2$ skyrmionic topological charge density [27]

$$Q(\Psi) = \int_{R^2} \frac{i\epsilon_{ij}}{2\pi|\Psi|^2} \left( |\Psi|^2 \partial_i \Psi \partial_j \Psi + \Psi^\dagger \partial_i \Psi \partial_j \Psi^\dagger \Psi \right) \mathrm{d}^2 x.$$  \hspace{1cm} (9)

Note that the second term is identically zero if there is no disparity in variations of the gaps in different bands. Near the surfaces and corners, Friedel oscillations of the density of states produce disparities in the gap amplitudes of the different bands [20, 22]. However, when the gradients of these quantities are collinear, the second term in Equation 8 remains zero and, thus, one does not see any currents at the edge of a two dimensional or surface of a three dimensional isotropic $s + is$ superconductor.

In our two-dimensional microscopic solutions, we find that the spatial profile of the gaps in the corners has non-collinear gradients in the amplitude and phase difference, and therefore, generates spontaneous currents. Similar effects should be present on the edges and vertexes of a three-dimensional superconductor.

Let us consider now how the spontaneous magnetic field $B_z$ varies as $T$ changes. Figure 3 displays its maximum value for temperatures in the range $T \in [0.36, 0.44]$ for a square superconducting sample. The result in Figure 3 suggests that the presence of spontaneous magnetic signatures is not a universally detectable property of three-band superconductors breaking time-reversal symmetry, but it may be easiest to detect at elevated temperatures.

For a square geometry, the flux in each corner locally adds up to zero, which may compromise the detection process due to the resolution in scanning SQUID probes. To make the effect more observable, one may break the spatial symmetry by considering different shapes.

By cleaving a corner of a square, one obtains the geometry with five corners shown in Figure 4, where the color gray indicates the vacuum. In which case, the total flux is still zero. However, the corner states inherently depend on the corner angle, and the resulting flux fractionalization pattern becomes different: now there are well-separated corners with non-zero local flux. In this configuration, we notice how the magnetic field (left panel) maintains the same spatial profile of Figure 2 in the 90-degrees corner but substantially changes near the diagonal edge. The magnetic flux in the lower left and upper right corners of the sample is of the order of $10^{-4}$ flux quanta and does not have a locally dipolar structure, making it easier to detect.

In conclusion, we have shown that in a superconductor,
with broken time-reversal symmetry, there are spontaneous boundary currents. This superconducting state is non-chiral and non-topological within the common classification framework. By the standard symmetry and topology arguments, it should not possess edge currents. Nonetheless, we showed that spontaneous currents and spontaneous magnetic fields of a different origin arise. This occurs at lower-dimensional boundaries: near the corners in the two-dimensional case and on the edges of three-dimensional samples. The origin of these fields is the existence of surface states [20, 22, 28] and the mixing of gap amplitude and phase difference modes [5] in $s+i{s}$ superconductors.

In our example, we find that, the spontaneous fields are sufficiently strong and can be detected by scanning SQUID techniques [29], scanning Hall [30] or single-atom magnetic resonance [31]. Observation of this field should allow to infer the properties of $s+i{s}$ multiband superconductors, such as Ba$_{1-x}$K$_x$Fe$_2$As$_2$ [1]. Since the spontaneous fields originate from the interband phase-difference gradients, they are expected to persist and thus to serve as a probe of the $Z_2$ bosonic metal phase [32, 33], that was recently reported in Ba$_{1-x}$K$_x$Fe$_2$As$_2$ at $x \approx 0.8$ [3].

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