Route to Topological Superconductivity via Magnetic Field Rotation

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The verification of topological superconductivity has become a major experimental challenge. Apart from the very few spin-triplet superconductors with $p$-wave pairing symmetry, another candidate system is a conventional, two-dimensional (2D) $s$-wave superconductor in a magnetic field with a sufficiently strong Rashba spin-orbit coupling. Typically, the required magnetic field to convert the superconductor into a topologically non-trivial state is however by far larger than the upper critical field $H_{c2}$, which excludes its realization. In this article, we argue that this problem can be overcome by rotating the magnetic field into the superconducting plane. We explore the character of the superconducting state upon changing the strength and the orientation of the magnetic field and show that a topological state, established for a sufficiently strong out-of-plane magnetic field, indeed extends to an in-plane field orientation. We present a three-band model applicable to the superconducting interface between LaAlO$_3$ and SrTiO$_3$, which should fulfil the necessary conditions to realize a topological superconductor.

While topologically non-trivial superconducting (SC) states have been established theoretically in numerous systems1–6, an experimental verification of such a state is still awaited. This is largely a consequence of the required conditions, which tend to counteract superconductivity itself. A topologically non-trivial state is generally described by a non-zero momentum space Berry phase $\gamma = 2\pi C$ with an integer $C$ whenever there is an energy gap separating occupied from unoccupied states1. The superconducting state can acquire a finite Berry phase through a chiral order parameter, and also via gapping a chiral normal-metal state upon entering a conventional SC state. Examples of the former case are selected spin-triplet states, e.g., the A-phase of superfluid $^3$He1 and most likely the superconducting phase of Sr$_2$RuO$_4$7,8. Very recently, a similar topological character was also proposed for the superconducting state in strongly underdoped cuprates9 in which a gap exists even along the nodal direction of a $d$-wave order parameter10. These proposals are built on states of matter, where the topological nature is an intrinsic property. The chiral order parameter however requires a very special pairing interaction; the $p$-wave states are rare in nature and pose considerable experimental challenges.

On the other hand, if the material provides a chiral band structure by itself, a conventional BCS superconductor with an $s$-wave order parameter can be topologically non-trivial as well. Most often discussed is an $s$-wave superconductor with a Rashba type spin-orbit coupling (SOC) in two dimensions5. On the two Fermi surface sheets generated by Rashba SOC the electron spins wind around in opposite directions (see Fig. 1 or e.g. ref. 11). Therefore, in order to reach a state with a finite overall Berry phase, an additional Zeeman field is needed which is strong enough to depopulate one of the SOC split bands. The topological character of the resulting SC state is equivalent to the quantum-Hall state. Such states are classified by a topological invariant, the so-called TKNN integer $C$ (after Thouless, Kohmoto, Nightingale, and Nijs)12. If the magnetic field is perpendicular to the plane of the 2D superconductor,
the minimal Zeeman splitting required to reach the topological phase is $\mu_B H_t = \sqrt{\epsilon_0^2 + \Delta^2}$, where $\epsilon_0$ measures the distance of the band energy at $k = 0$ to the Fermi energy, and $\Delta$ is the SC energy gap. The obstacle for realizing this topological state experimentally is to find a system which remains superconducting in the required high magnetic fields. Suggested model systems are, e.g., neutral ultra-cold atoms in an optical trap, or heterostructures where Cooper pairs are induced through the proximity effect. The problem of realizing the topological s-wave state has two distinct aspects: (i) $\mu_B H_t$ must be larger than $\Delta$. While the presence of the Rashba SOC allows in principle s-wave superconductivity in a Zeeman field larger than $\Delta$, the orbital critical field $H_{c2}^i$ is typically much smaller. (ii) The superconductor must have $\epsilon_0$ smaller than the Zeeman splitting. This requires a low band filling and, therefore, superconductivity must be stabilized by yet another band with larger filling. In this article, we address both of these aspects and demonstrate that the problems can be overcome in real solid-state systems.

A simple way to circumvent the orbital critical field $H_{c2}^i$ is to rotate the magnetic field into the plane of the 2D superconductor. The in-plane field however leads to an unusual type of pairing. In the presence of Rashba SOC, an in-plane magnetic field shifts the Fermi surfaces out of the Brillouin-zone center (cf. Fig. 1), and the electron pairs thereby acquire a finite center-of-mass momentum (COMM)\textsuperscript{15}. Edge states in an in-plane magnetic field have recently been investigated for s-wave superconductors, but with zero COMM\textsuperscript{15,17}. As we show here, the inclusion of a finite COMM in such a field geometry is indispensable for the discussion of topology. Specifically, we analyze the topological properties of an s-wave superconductor under rotation of the magnetic field within a fully self-consistent treatment of the SC order parameter. It is verified that the topological state reached in out-of-plane fields indeed persists to in-plane field orientations, if the COMM is appropriately chosen to minimize the free energy. For in-plane fields the energy gap closes, accompanied by a topological transition. Nevertheless, chiral edge modes remain even for a regime with a closed gap.

We discuss the experimental realizability of a topological s-wave superconductor in a nearly in-plane magnetic field. As a candidate system, which can possibly fulfill the required conditions, we consider the metallic LaAlO$_3$-SrTiO$_3$ (LAO-STO) interface\textsuperscript{18,19}. For this system, several models are proposed for a topologically non-trivial superconducting state, which rely on an unconventional order parameter\textsuperscript{18-22}. Assuming instead an s-wave pairing state, we demonstrate that a multi-band model involving the titanium $t_{2g}$ orbitals allows for a topologically non-trivial superconductor in a realistic parameter regime for the LAO-STO interface. We suggest that it may be achieved with the currently used experimental setups.

Results

In order to investigate the magnetic-field dependence of an s-wave superconductor with Rashba SOC in transparently simple terms, we use a one-band tight-binding model on a square lattice in the $x$-$y$-plane at zero temperature. In our analysis of the topology upon rotating the magnetic field $H$ into the plane, we include the Zeeman coupling of the electrons to the magnetic field, but neglect the orbital coupling. This approximation is well justified for the nearly in-plane field orientation on which we focus here; but orbital effects are necessarily important for the superconducting state in an out-of-plane magnetic field.

The Rashba SOC and the Zeeman coupling to the magnetic field $H$ are combined into

![Figure 1. Energy bands $\xi^\pm_k$ (pink) and $\xi^-_k$ (blue) and Fermi surfaces with $\alpha > 0$ and magnetic field $|H| < H_t$. (a) For $H = 0$, the two bands touch at $k = 0$. (b,c) For $|H| > 0$, the band splitting at $k = 0$ is equal to the Zeeman splitting $2\mu_B|H|$. The centers of the shifted Fermi surfaces in (c) are at the momenta $q^+/2 = (q^+/2, 0)$ and $q^-/2 = (q^-/2, 0)$, respectively. Although $q^+ \approx -q^-$, their absolute values are in general different. In (c), the spins on the $k_x$-axis orient according to the magnetic field rather than according to the SOC, if $H > \alpha|\sin k_y|$. Note that the Fermi energy is somewhat larger than $|\epsilon_0|$ because of the SOC induced band splitting.](image-url)
\[\mathcal{H}_s = \sum_{k,s} \mathbf{h}_k \cdot \sigma \epsilon_k^s c_k^s c_{k-s}^s\]

with \(s = \pm 1\), the Bloch vector \(\mathbf{h}_k = \alpha g_{\mathbf{k}} + \mu H\), and \(g_{\mathbf{k}} = (\sin k_y - \sin k_x, 0)\); \(\sigma\) is the vector with the Pauli matrices as components. The strength of the Rashba SOC \(\alpha\) derives originally from the Dirac Hamiltonian, but may have other sources in multi-band systems (see section “Discussion”). Diagonalizing the kinetic energy together with \(\mathcal{H}_s\) gives the two chiral energy bands \(\epsilon_k^s = \epsilon_k \pm |\mathbf{h}_k|\) where \(\epsilon_k = -2t (\cos k_x + \cos k_y) - \mu\) with the nearest-neighbor hopping amplitude \(t\) and the chemical potential \(\mu\) (thus \(\epsilon_0 = -4t - \mu\)). In these bands, the spin is either parallel or antiparallel to \(\mathbf{h}_k\) and has a component which rotates either counter-clockwise or clockwise upon circulating the Fermi surfaces (see Fig. 1).

**Out-of-plane magnetic field.** For an out-of-plane magnetic field with \(H_z = H_t = 0\), the topological properties of the superconducting state are readily established (see e.g. Ref. 5). Its Hamiltonian
\[\mathcal{H} = \sum_{k} \mathbf{C}_k \mathbf{H}_k \mathbf{C}_k\]
is represented by the 4 \(\times\) 4 matrix
\[\mathbf{H}_k = \begin{pmatrix} \epsilon_k^0 + \mathbf{h}_k \cdot \sigma & i\sigma \Delta \\ -i\sigma \Delta & -\epsilon_k^0 + \mathbf{h}_k \cdot \sigma \end{pmatrix} \]
with \(\mathbf{C}_k = (c_{k,\up}, c_{k,\down}, c_{k,\up}^\dagger, c_{k,\down}^\dagger)\) and \(\sigma^0\) is the \(2 \times 2\) unit matrix; the pairing field \(\Delta\) is calculated self-consistently from Eq. (7) (with \(q = 0\)). The four eigenenergies \(E_{k,n}\) obtained from diagonalizing (2) are generally the solutions of a 4th order polynomial, but simplify to
\[E_{0,n} = \pm \sqrt{\epsilon_0^2 + \Delta^2} \pm \mu_B |\mathbf{H}|\]
for \(k_x = k_y = 0\), since \(g_{\mathbf{k}} = 0\). The number \(n\) labels the four combinations of the plus and minus signs. It follows that the energy gap closes at \(k = 0\) for \(\mu_B^2 H_z^2 = \epsilon_0^2 + \Delta^2 \equiv \mu_B^2 H_t^2\), which thereby allows for a topological transition\(^{26}\).

The topological character of the SC state is given by the TKNN number
\[C = \frac{\gamma}{2\pi} = \frac{1}{2nN} \sum_{\mathbf{k}} \Omega(\mathbf{k})\]
where
\[\Omega(\mathbf{k}) = i \sum_{n,\lambda} [\nabla_k \times (u_{n\lambda}(k) \nabla_k u_{n\lambda}(k))]_z\]
is the \(z\)-component of the Berry curvature\(^{32}\). The sum over \(n\) runs over the occupied bands \(E_{k,n} < 0\) and \(\lambda = 1, \ldots, 4\) labels the components of the eigenvectors \(u_{\lambda}(\mathbf{k})\) of the matrix \(\mathbf{H}_k\). The number \(C\) is integer valued, if the occupied energy levels are separated by a finite gap from the unoccupied levels. The value of \(C\) and therefore the topology of the quantum state changes when the energy gap closes at \([H_z] = H_t\).

For magnetic fields \([H_z] > H_t\), the energy gap opens again. This reopening of a gap, above the paramagnetic limiting field \(\mu_B|H_z| = \Delta\), is tied to the presence of SOC, which protects the spin-singlet pairing channel. (In the presence of SOC, the spin susceptibility \(\chi_S\) of the spin-singlet superconductor remains finite down to \(T = 0\). In particular, if \(\Delta \ll \alpha\), \(\chi_S\) is almost equal the Pauli susceptibility of the normal state. Therefore, the Clogston-Chandrasekhar paramagnetic limit \(H_{CC} = \Delta/\sqrt{2}\alpha\) does also not apply.)

Only the momenta \(\mathbf{k}\) for which \(\xi_k^+\) lie within a window \(\Delta\) below the Fermi energy contribute to \(C\). The sign of this contribution reflects the winding direction of the \(x\)-\(y\) components of the spin \((\hbar/2)(\epsilon_{k,\up}^s, \sigma \epsilon_{k,\down}^s, \epsilon_{k,\up}^s, \epsilon_{k,\down}^s)\) in momentum space (see Fig. 1). If \([H_z] < H_t\), the \(\mathbf{k}\)-integrated Berry curvatures in the vicinity of the two normal-state Fermi surfaces cancel exactly [Fig. 2(a)] and consequently \(C = 0\).

The topological state emerging for \([H_z] > H_t\) is of different nature in two distinct density regimes:

(A) small electron density (\(\mu < -2t\)): the condition \([H_z] > H_t\) leads to \(\xi_k^+ > \Delta\) for all \(\mathbf{k}\) and therefore the \(\xi_k^+\)-band is empty and does not contribute, i.e., the pink (positive) contributions to \(C\) in Fig. 2(a) vanish. Consequently, the superconducting state is characterized by \(C = \mp 1\), depending on the sign of \(H_t\). This situation is realized for small band fillings.

(B) densities near half-filling (\(|\mu| < 2t\)): in this regime, two separate topological transitions are possible. At a magnetic field \(\mu_B |H_z| = \sqrt{\epsilon_0^2 + 4t^2 + \Delta^2} < \mu_B H_t\), the character of the \(\xi_k^+\)-band changes from particle- to hole-like and thereby reverses the sign of \(\Omega(\mathbf{k})\) in the vicinity of the corresponding Fermi surface [Fig. 2(b)]. Therefore, a topological transition to \(C = \pm 2\) occurs, depending on the sign of \(H_z\), with both, the \(\xi_k^+\) and the \(\xi_k^-\)-band, partially occupied. A realization of this superconducting state close to half filling is however unlikely due to possibly competing orders. For an even
larger magnetic field $\mu_B H_0 > H_t$, the $\xi^+_k$-band is again lost, and $C$ changes to $= \pm 1$. The topological properties of both cases, (A) and (B), correspond to those described in ref. 4 in the context of spin-triplet superconductors.

A special characteristic feature of $s$-wave superconductivity in the presence of Rashba SOC is that the magnetic field induces an inter-band pairing contribution where a quasi-particle of the $\xi^+_k$-band is paired with one from the $\xi^-_k$-band at opposite momentum. This pairing contribution induces interior energy gaps above and below the Fermi energy (clearly visible e.g. in the spectra presented below, cf. ref. 24). A more detailed discussion of the relation between intra- and inter-band pairing is given in the Supplementary Informations.

In-plane magnetic field. For a finite in-plane magnetic-field component $H_\parallel$, the Fermi surfaces are shifted out of the Brillouin-zone center in opposite directions perpendicular to $H_\parallel$ [Fig. 1(c)], since $\xi^\pm = \xi^\mp$. The pairing of electrons with momenta $k$ and $-k$ is thereby suppressed. Instead, pairs are formed in which electrons have momenta $k$ and $k + q^\pm$, respectively, where the COMMs $q^\pm$ account for the Fermi surface shifts11,25–27 (see Supplementary Informations, Sec. B).

The SC ground state with an in-plane magnetic field component therefore contains in general two order parameters $\Delta^\pm_{q^\pm}$ and $\Delta_q^-$. These enter the generalized on-site pairing term as

$$\mathcal{H}_1 = \sum_{\mathbf{k},q} \left[ \Delta^+_{q^-} c_{-\mathbf{k}^+ q^-}^\dagger c_{\mathbf{k}^- q^+} + \Delta^-_{q^+} c_{-\mathbf{k}^- q^+}^\dagger c_{\mathbf{k}^+ q^-} \right],$$

where $\mathbf{q} = q^+, q^-$. The singlet order parameter for COMM $\mathbf{q}$ is calculated self-consistently from

$$\Delta_\mathbf{q} = \frac{V}{2N} \sum_{\mathbf{k}', q'} \left( c_{-\mathbf{k}'^- q'} c_{\mathbf{k}'^+ q'}^\dagger - c_{-\mathbf{k}'^+ q'} c_{\mathbf{k}'^- q'}^\dagger \right),$$

where $V$ is the strength of the pairing-interaction. With increasing in-plane magnetic-field strength $|\mathbf{H}_\parallel|$, the difference $|\mathbf{q}^+ - \mathbf{q}^-|$ grows. Such a finite COMM state is spatially non-uniform28 with lines of zero pair density, similar to the SC state proposed by Larkin and Ovchinnikov for a singlet superconductor in a strong Zeeman field29. Characteristic for this state is a mixing of intra- and inter-band pairing and the absence of a full energy gap (see Supplementary Informations)11,28.

For $|\mathbf{H}_\parallel| \neq 0$, the topological characterization is more involved. In situation (B), close to half-filling, both bands $\xi^+_k$ and $\xi^-_k$ are partially occupied and consequently two COMMs $\mathbf{q}^\pm$ appear. Therefore no full energy gap is present, which implies that $C$ is not an integer and therefore unsuitable to characterize the topology (nevertheless, edge modes may still occur, see Supplementary Informations). For this situation, the Berry curvature $\Omega(\mathbf{k})$ is finite within the window $\Delta$ below the Fermi energy. (a) In the topologically trivial state, (here: $\epsilon_0 = -0.7t$, $\mu_B H_0 = 0.3t$ and $\Delta$ is fixed to $0.1t$), the total Berry curvature integrates to zero over the Brillouin zone. (b) In the topological situation (B) (see main text, $\epsilon_0 = -4t$ and $\mu_B H_0 = 0.3t$), the Berry curvature integrates to $2\pi C = 4\pi$ over the Brillouin zone.

Figure 2. $z$-component of the Berry curvature $\Omega(\mathbf{k})$ for an out-of-plane magnetic field $H_z$ in the SC state. $\Omega(\mathbf{k})$ is finite within the window $\Delta$ below the Fermi energy. (a) In the topologically trivial state, (here: $\epsilon_0 = -0.7t$, $\mu_B H_0 = 0.3t$ and $\Delta$ is fixed to $0.1t$), the total Berry curvature integrates to zero over the Brillouin zone. (b) In the topological situation (B) (see main text, $\epsilon_0 = -4t$ and $\mu_B H_0 = 0.3t$), the Berry curvature integrates to $2\pi C = 4\pi$ over the Brillouin zone.
For such low densities, a large interaction strength $V$ is required to obtain a reasonably large order parameter. For each value of $|H|$, $q = (q, 0)$ is obtained by minimizing the free energy. The red circles indicate the magnetic field strength above which a finite COMM $q \neq 0$ is present.

Phase diagram and edge states. We start the analysis of the SC state with the discussion of the self-consistent solutions of the SC order parameter. Figure 3 shows the magnetic-field dependence of $\Delta_q$ for different angles $\theta$ of the field direction. The Rashba SOC ensures the presence of a finite in-plane spin component which allows for singlet pairing. Therefore the Zeeman coupling to a field in $z$-direction ($\theta = 0^\circ$ and $q = 0$) cannot wipe out superconductivity completely (pink curve) when orbital depairing is not included. A finite in-plane field component leads instead to a finite critical magnetic field $H_s(\theta)$, above which there are no solutions for $\Delta_q$.

An interesting result is the somewhat larger value for $\Delta_q$ in an in-plane magnetic field $|H| < H_s(\theta)$ than in an out-of-plane magnetic field of the same magnitude. Consequently, the magnetic field $H_s(\theta)$ at which the energy gap closes, grows with increasing angle $\theta$ and is maximal for an in-plane direction. Likewise, the field $H_s^+(\theta)$ above which the energy gap opens again and the topological state emerges, is maximal for $\theta = 90^\circ$, whereas $H_s^+(0^\circ) = H_s(0^\circ)$. The resulting phase diagram for different magnetic-field orientations is qualitatively drawn in Fig. 4. The topologically trivial SC state ($C = 0$) is bounded by the ellipse given by $H_s(\theta)$, which itself is within the slightly larger ellipse formed by $H_s^+(\theta)$. The white regime in between separates the state with $C = 0$ from the states with $C = \pm 1$. In this crossover region the energy gap is closed and $C$ is not an integer. A further topological transition occurs for the in-plane field orientation $\theta = 90^\circ$ and $|H| > H_s^+; if \theta$ sweeps through $90^\circ$, the out-of-plane field component $H_s$ changes sign and, accordingly, $C$ changes from $-1$ to $1$. As discussed above, the energy gap is closed as well along this transition line.

The importance of finite-COMM pairing for the topological properties of the SC state is illustrated using the energy spectra shown in Fig. 5. These spectra are calculated for a stripe geometry with open boundary conditions in $y$-direction, which allows for in-gap edge modes (drawn in red and green). We choose the in-plane magnetic-field component in the $y$-direction and thereby obtain a shift of the Fermi surfaces out of the Brillouin-zone center in $k_x$-direction. Therefore a COMM $q = (q, 0)$ ($q \geq 0$ for $H_s > 0$) has to be taken into account for pairing in the $\xi_{k_y}$-band. The free energy of the SC state is minimized for the smallest $q$ which is still large enough to avoid an indirect closing of the energy gap (see Fig. 5(a–c).
and Sec. B of the Supplementary Informations). The TKNN number $C$ thereby remains well defined up to the magnetic-field direction $\theta = 90^\circ$. For $\theta \rightarrow 90^\circ$ [Fig. 5(c)], the energy gap closes at two $k_x$-points, and a topological transition occurs. The magnetic field strength, above which a finite $q^-$ is required (dashed line in Fig. 4), depends on the angle $\theta$. In the limit $\theta \rightarrow 90^\circ$, it is necessarily smaller than $H_t$ and approaches $H_t$ for vanishing SOC. For every change in the field orientation the COMM $q^-$ has to be recalculated self-consistently. Since the calculations are performed on a finite lattice, $q^-$ evolves necessarily in discrete steps, determined by the system size, upon sweeping the angle $\theta$. Up to this unavoidable discreteness, the onset of a finite $q^-$ is a smooth transition, across which the energy gap evolves continuously.

Eventually, Fig. 5 also shows the evolution of the in-gap edge modes (green and red lines) under the rotation of the magnetic field. (Note that for $\theta > 0$, the direction of the in-plane field component relative to the boundary is important. If there is a field component parallel to the boundary (in $x$-direction), the edge-mode disperses in $y$-direction as well. Since the dispersion in $y$-direction is quantized through the edges, the edge modes acquire an energy gap around the Fermi energy (also observed for the edge modes in chiral $p$-wave superconductors$^{4,17}$). This mesoscopic energy gap is of the size of the normal-state level spacing around $E_F$ and vanishes like $1/M$ in the thermodynamic limit, where $M$ is the number of lattice sites in $y$-direction.) Starting from $\theta = 0^\circ$, the energy difference $|\xi_k^+ - \xi_+|^2$ grows for increasing $\theta$ and thus the dispersion of the two opposite edge modes becomes asymmetric [Fig. 5(b)]. Upon approaching $\theta = 90^\circ$, the energy gap closes at two $k_x$ points [Fig. 5(c)]. Consequently, $q$ must be chosen to ensure that these closing points are located at the Fermi energy in order to prevent the energy bands above and below from overlapping. In this situation, the two edge modes are degenerate. Indeed, the two modes carry edge currents flowing in the same direction opposite to the flow of the bulk current. These modes are similar to the edge modes found for $p$-wave superconductors in an in-plane magnetic field$^{17,31,32}$, except for the presence of a finite COMM pairing due to the Rashba SOC.

Figure 5(d,e) illustrate the gap closing and the emergence of edge modes in the regime $H_z(90^\circ) \leq H_y \leq H_t^+(90^\circ)$. At $H_y = H_t(90^\circ)$, the energy gap closes at $k_x = 0$ [Fig. 5(d)]. However, the minimum of the $\xi_k^+$-band is at a momentum $k_x < 0$ and somewhat below the Fermi energy (indicated by the left black arrow), whereas the maximum of its mirrored hole-band is at a momentum $k_x > 0$ somewhat above the Fermi energy (right black arrow). Thus, the $\xi_k^+$-band and its mirrored hole band $-\xi_{-k+q^-}$
overlap indirectly. Superconductivity nevertheless persists because of the gain of condensation energy from the $\xi^+_k$-band. In the regime $H_y = H_y^c(\theta) < H_c^f$, a direct gap opens again around $k_x = 0$ with two gap-crossing edge modes, although they are no longer protected by topology [Fig. 5(e)].

For magnetic fields $H_y > H_y^c$, all states of the $\xi^+_k$-band are above the Fermi energy. In this regime an infinitesimally small out-of-plane magnetic-field component $H_z$ is sufficient to remove the two gap-closing points and ensure well defined TKNN numbers $C = \pm 1$. Eventually, superconductivity breaks down at $H_y = H_y^c(\theta)$: Above this critical magnetic field, the two gap-closing points move into the continuum of the energy bands above and below the Fermi energy. The upper and lower bands therefore overlap and the self-consistent solution for the SC order parameter is lost. Although $H_y^c(\theta)$ depends only weakly on the SOC strength $\alpha$, the critical magnetic field $H_y^c(\theta)$ grows with increasing $\alpha$. In order to obtain $H_y(90^\circ) > H_y^c(90^\circ)$, it is required that $\alpha > \muBH_y$. 

Figure 5. Energy spectra $E_n(k_x)$ for a stripe geometry with $600 \times 100$ sites, open boundary conditions and in-plane magnetic field component in $y$-direction, and parameters $V$, $\alpha$, and $n$ as in Fig. 3. (a–c) The evolution of the edge modes (green line: upper edge, red line: lower edge) upon rotating the magnetic field is shown for (a) $\theta = 0$, (b) $\theta = 45^\circ$, (c) $\theta = 90^\circ$, and $\muBH_y = 0.3t$. The self-consistently calculated order parameters $\Delta_{0}^e$ and COMMs $q^e$ are (a) $\Delta_{0}(0) = 0.11t$, (b) $\Delta_{0.02r}(0) = 0.12t$, and (c) $\Delta_{0.14r}(0) = 0.14t$. (d,e) illustrate the crossover regime $H_y(90^\circ) \leq H_y \leq H_y^c(90^\circ)$: (d) $\muBH_y = \muBH_y(90^\circ) = 0.23t$ and $\Delta_{0.12r}(0) = 0.21t$, and (e) $\muBH_y = 0.24t < \muBH_y(90^\circ)$ and $\Delta_{0.12r}(0) = 0.20t$. The black arrows in (d) indicate the partial occupation of states originating from the $\xi^+_k$-band. The opacity of each point encodes the weight with which the corresponding state contributes to the density of states.
Discussion

How can the above topologically non-trivial SC state be realized in a solid-state system? We infer that an ideal candidate system would consist of several partially filled energy bands with a sizable Rashba SOC. Such a model was proposed e.g. to describe the physics of the conducting interface between LaAlO$_3$ and SrTiO$_3$.

The hopping matrix elements for the three bands: $\Delta_0$, $\Delta_{SO}$, and $\Delta_2$, which is close to the Fermi energy $E_F$, require the presence of at least two bands at $\Delta_0$ given by $E = \Delta_0 \pm \sqrt{\Delta_0^2 + \Delta_{SO}^2}$, where $\Delta_{SO}$ is the spin-orbit coupling parameter.

In order to ensure $\epsilon_0 = 0$ (red dashed line), the Fermi energy should be at the degeneracy point of the upper, Rashba-like doublet. The parameters are here: $t_{yz}^x/t_{xz}^x = 0.1$, $\Delta_0 = t$, $\Delta_{SO} = \Delta_2 = 0.2t$.

### Figure 6.
Band structure of the three-band model for $k_z = 0$. In order to ensure $\epsilon_0 = 0$ (red dashed line), the Fermi energy should be at the degeneracy point of the upper, Rashba-like doublet. The parameters are here: $t_{yz}^x/t_{xz}^x = 0.1$, $\Delta_0 = t$, $\Delta_{SO} = \Delta_2 = 0.2t$.

The condition $\mu_\mu \mathbf{H} > \sqrt{\epsilon_0^2 + \Delta_0^2}$ for $C \neq 0$ implies that the lower limit for the Zeeman splitting is given by $\Delta_0$. The corresponding magnetic field is typically larger than the upper critical field $H_{c2}$ above which orbital depairing destroys superconductivity. Therefore the topological state is not accessible with a magnetic field oriented along the $z$-axis. The topological state can be reached only for a nearly in-plane field orientation with $H_x < H_{c2}$ but $\mathbf{H} > H_{c2}^\perp$. This excludes the situation (B) with a close to half-filled band, because of the presence of two different COMMs $q^\pm$ as discussed above. The alternative situation, on the other hand, requires that $\mu_\mu \mathbf{H} > |\epsilon_0|$ which is close to the Fermi energy $E_F$ in a one-band model. For a band filling large enough to allow for a SC state (for a reasonable interaction strength $V$), $E_F$ for this partially filled band must be at least several meV. The magnetic field required to overcome this energy would be far too large for experimental realizations.

In a multi-band setup, $\epsilon_0$ refers to the energy of the degeneracy point of a spin-orbit coupled doublet hosting the possibly topological state (see Fig. 6), relative to $E_F$. The necessity of stabilizing a superconducting state with $\epsilon_0 = 0$ requires the presence of at least two bands at $E_F$. A lower band provides the electron density for a sufficient gain of condensation energy in the superconducting state, whereas a second band has a minimum close enough to the Fermi energy so that it can be emptied or partially filled through an external control parameter.

A model which implements these features, and additionally also a strong Rashba-like SOC, recently emerged from the theoretical description of the LAO-STO interface. At this interface, the intrinsic electrostatic potential in LAO induces a nearly 2D electron liquid, which resides mainly in the titanium 3$d_{xy}$ orbitals of the first TiO$_2$ layer. The band-structure of this oxide interface provides a prototype for a class of similar interface systems that we introduce here by constructing a tight-binding Hamiltonian $\mathcal{H} = \mathcal{H}^0 + \mathcal{H}_{SO} + \mathcal{H}_C$ for the three $t_{2g}$ bands $d_{xy}$, $d_{xz}$, and $d_{yz}$ following refs 33,34. The free kinetic energy is given by

$$\mathcal{H}^0 = \sum_{k} \mathbf{C}_k^T \left[ \begin{array}{ccc} \epsilon_k^{xy} & 0 & 0 \\ 0 & \epsilon_k^{xz} & 0 \\ 0 & 0 & \epsilon_k^{yz} - \Delta_0 \end{array} \right] \otimes \sigma^0 \mathbf{C}_k,$$

where $\sigma^0$ is the 2 $\times$ 2 unity matrix and $\mathbf{C}_k^T = \{ \epsilon_k^{xy}, \epsilon_k^{xz}, \epsilon_k^{yz}, c_{k1}^{x}, c_{k1}^{y}, c_{k2}^{x}, c_{k2}^{y} \}$. The hopping matrix elements $t_k^{xy} = t_k^{yz}$ for the $d_x$ band are identical in the $x$- and $y$-direction, whereas they are different for the $d_{xz}$ and $d_{yz}$ bands: $t_k^{xz} = t_k^{yz} \gg t_k^{xy} = t_k^{yz}$. Furthermore, the in-plane $d_{xy}$ orbital is lowered in energy by $\Delta_0$ relative to the out-of-plane $d_{xz}$ and $d_{yz}$ orbitals because of the symmetry breaking interface.

The spin-orbit coupling on the Ti atoms is described by $\mathcal{H}_{SO} = \Delta_{SO} \sum_k \mathbf{C}_k^T \mathbf{L} \otimes \sigma \mathbf{C}_k$, where the angular momentum operator $\mathbf{L}$ for $l = 2$ is represented in the $\{ d_{xz}, d_{yz}, d_{xy} \}$ basis. This term intermixes the $t_{2g}$ orbitals and generates three doublets; the upper two doublets are split by $2\Delta_{SO}$ (see Fig. 6). In
addition, the deformation of the $t_{2g}$ orbitals due to the interface potential leads to a hybridization of the $d_{xz}$, $d_{yz}$ orbitals with the $d_{xy}$ orbital, parameterized by

$$\mathcal{H}^c = i\Delta_s \sum_k \left[ \begin{array}{ccc} 0 & 0 & -\sin k_x \\
0 & 0 & \sin k_y \\
\sin k_x & -\sin k_y & 0 \end{array} \right] \otimes \sigma^0 C_k.$$

The $k$-dependence in $\mathcal{H}^c$ splits the three otherwise doubly degenerate doublets. For small momenta $k_x$ and $k_y$, this splitting acts on the lowest and the highest doublet exactly like a Rashba term in a one-band model. This source of an effective Rashba-like band splitting can be several orders of magnitude larger than the splitting through the relativistic term and thereby is able to explain qualitatively the spin splitting observed at the LAO-STO interface. Further, if the Fermi energy is tuned to $\Delta_s + \Delta SO$ by an external gate voltage, $\epsilon_0 \approx 0$ is fulfilled for the highest doublet (see Fig. 6). The SC state can be stabilized by the two lower doublets, whereas the highest generates a non-trivial topological number $C = \pm 1$.

This three-band model is likely the minimal model which fulfills the requirements discussed above for the realization of topological $s$-wave superconductivity in a solid. Various interface systems with a similar setup are conceivable, however, the formation of a topological SC state is viable only in a restricted parameter range: The Rashba-like band splitting, which is controlled by the parameter $\alpha$ in the one-band model, is replaced in the three-band model by $\alpha_R = 2\Delta SO/\Delta S$. Above which $C \neq 0$ is possible, varies little with $\alpha_R$, the magnetic field range $H_{c1} - H_{c2}$ vanishes when $\alpha_R$ approaches zero. To ensure a wide magnetic field range for the topological state, the parameter $\alpha_R$ should therefore be larger than the Zeeman splitting and thus also larger than the SC energy gap.

In the following we estimate that the above criteria are indeed satisfied in the candidate system LAO-STO. The interface superconducts below a critical temperature of about 300 mK and exhibits an energy gap $\Delta$ of about 40 meV with most likely $s$-wave symmetry. The Rashba parameter $\alpha_R$ was experimentally estimated to be in the range 20–100 meV, which is compatible with $\alpha_R$ determined from the three-band model using $\Delta_s$, $\Delta SO$, and $\Delta_s$ from the band-structure calculations of ref. 34. Assuming that $\epsilon_0$ can be adjusted to zero by a suitable gate voltage, the necessary Zeeman splitting $\mu_0|H| > \Delta$ is far smaller than $\alpha_R$ and corresponds to a magnetic field $H_{c1} \approx 600 \text{ mT}$ (the in-plane $H_{c1}$ might be somewhat larger). While the measured out-of-plane critical field is $H_{c2}(0) \approx 200 \text{ mT}$ and therefore smaller than $H_{c1}$, the observed in-plane critical field is $H_{c1}(90^\circ) \gtrsim 1T > H_{c2}(90^\circ)$.

The other important parameter defining $H_{c1}$ is $\epsilon_0$, which is controlled by the electron density $n$ at the interface. The electron density can be tuned between $1 \times 10^{-13} \text{ cm}^{-1}$ and $6 \times 10^{-13} \text{ cm}^{-1}$ due to the interface potential leading to a hybridization of the $d_{xz}$, $d_{yz}$ orbitals with the $d_{xy}$ orbital, parameterized by

$$\mathcal{H}^c = i\Delta_s \sum_k \left[ \begin{array}{ccc} 0 & 0 & -\sin k_x \\
0 & 0 & \sin k_y \\
\sin k_x & -\sin k_y & 0 \end{array} \right] \otimes \sigma^0 C_k.$$
Rotation.

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