Boundary-obstructed topological high-$T_c$ superconductivity in iron pnictides

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Non-trivial topology and unconventional pairing are two central guiding principles in the contemporary search for and analysis of superconducting materials and heterostructure compounds. Previously, a topological superconductor has been predominantly conceived to result from a topologically non-trivial band subject to intrinsic or external superconducting proximity effect. Here, we propose a new class of topological superconductors which are uniquely induced by unconventional pairing. They exhibit a boundary-obstructed higher-order topological character and, depending on their dimensionality, feature unprecedentedly robust Majorana bound states or hinge modes protected by chiral symmetry. We predict the 112-family of iron pnictides, such as $\text{Ca}_{3-x}\text{La}_x\text{FeAs}_2$, to be a highly suited material candidate for our proposal, which can be tested by edge spectroscopy. Because of the boundary-obstruction, the topologically non-trivial feature of the 112 pnictides does not reveal itself for a bulk-only torus band analysis without boundaries, and as such had evaded previous investigations. Our proposal not only opens a new arena for highly stable Majorana modes in high-temperature superconductors, but also provides the smoking gun evidence for extended s-wave order in the iron pnictides.

Iron-based high temperature (high $T_c$) superconductors have recently appeared as an exciting platform to realize topological superconductivity at high temperatures$^{1-9}$. Due to an intrinsic superconducting proximity effect, the surfaces in these materials can host Majorana zero modes (MZMs), evidence of which has been observed in the vortex core of $\text{Fe}(\text{Te},\text{Se})$ and $(\text{Li}_{1-x}\text{Fe}_x)\text{OHFeSe}$ crystals$^{10-13}$. That is, a band inversion between the $d$ and the ligand $p$ orbitals is found, which then culminates with the superconducting proximity effect imposed by the particle-particle instability at the Fermi level. While this band inversion appears to be rather generic for the pnictides, current experimental evidence suggests that the topological superconducting phase necessitates significant tuning of Fermi level and chemical composition.

In unconventional high $T_c$ superconductors, the pairing symmetry is as essential as it can be difficult to directly identify it. In cuprates, only several years after their discovery, a $d$-wave pairing symmetry has been unambiguously proved by detecting the $\pi$ phase shift in corner junction interferometer experiments$^{14}$. In iron-based superconductors, the pairing symmetry has been subject of a long-lasting debate ever since their discovery a decade ago. An $s_{\pm}$-wave pairing, possessing a sign-reversed gap on hole and electron pockets in momentums space, has been proposed for iron-based superconductors with some indirect evidences in neutron scattering and scanning tunneling microscopy$^{15-21}$. So far, however, no decisive experiment has been proposed to distinguish $s_{\pm}$-wave from a sign-unchanged $s$-wave pairing because both states share the same $A_{1g}$ symmetry character. As we will show in this work, $s_{\pm}$-wave and $s$-wave, despite their identical symmetry character, can give rise to different topological phases, and thus, we claim that the topological aspects in iron-based high $T_c$ superconductors can shine a light on this outstanding problem.

Higher-order topological phases$^{22-26}$ are a new family of phases of matter with the defining property of hosting fractional charges or topological states at corners or hinges of the material. In 2D insulators, these phases manifest fractional corner charges protected by crystalline symmetries and are directly related to the positions of the Wannier centers of the occupied bands$^{25}$ or to the topology of its Wannier bands$^{22,23}$. In superconductors, despite the absence of a Wannier description, particle-hole and/or chiral symmetries can also protect the existence of corner-localized MZMs. Recently, several proposals have been put forward for the realization of HOTSC in 2D or 3D$^{22,27-41}$, some of which include certain iron-based superconductor compounds$^{27,28,36,40,41}$. Setting aside that the complete characterization of HOTSC by topological invariants is still missing, there is, in addition, a significant disconnect between the toy models studied in those works and actual material candidates.

In order to understand the new class of superconductors we propose in this work, we need to develop a novel fused perspective on the current fields of unconventional superconductivity and higher-order topological states of matter. Specifically, we show that $s_{\pm}$-wave symmetry pairing, together with the topological properties in the 112-family of iron pnictides, drives the material into a HOTSC that hosts a Kramer pair of MZMs at each corner of each unit-layer. Different from previous proposals, the MZMs are particularly robust, as they do not depend on crystal symmetries, but are protected by chiral symmetry. The demonstration of high-order topology in this family of compounds will provide a “smoking-gun” evidence for $s_{\pm}$-wave pairing. Remarkably, the topological phase we find for this material has the property of being adiabatically connected to the trivial phase in the absence of boundaries, but, once boundaries are introduced, an edge-localized obstruction topologically separates it from the trivial phase. This property, referred to as boundary topological obstruction, was
originically identified in the minimal model for a higher-order topological insulator (HOTI) hosting a quantized quadrupole moment protected by reflection symmetries\textsuperscript{23,24}. In insulators, boundary topological obstructions have recently been explained in terms of the Wannier centers of the occupied bands\textsuperscript{42}. Here, we generalize the concept of boundary topological obstructions to superconductors – for which a Wannier description is absent – and identify the 112-family of iron pnictides as the first intrinsic material realization of boundary-obstructed HOTSCs. The existence of MZMs in boundary-obstructed HOTSCs is a clear signature of its nontrivial topology. Upon a phase transition into a trivial phase, the bulk remains gapped, only the edges become gapless, providing one-dimensional channels for the MZMs to hybridize as they disappear into the trivial phase.

The detection of MZMs in this material would be a decisive evidence for $s_{\pm}$-wave pairing in iron-based superconductors for the following reason: The 112-family of iron pnictides, including Ca$_{1-x}$La$_x$FeAs$_2$\textsuperscript{43} and (Ca,Pr)FeAs$_2$\textsuperscript{44}, with $T_c$ up to 47 K, are intrinsic topological insulator/high $T_c$ superconductor heterostructures\textsuperscript{45,46} with a staggered intercalation between zigzag chain-like As1 layers with the quantum spin Hall state and the superconducting Fe–As layers along the $c$ axis, as shown in Fig.1(a). The edge Dirac cones from the As1 layers are at two orthogonal (100) and (010) edges are in proximity to projections of bulk pockets around $\Gamma$ and $\mathbf{M}$ from adjacent FeAs layers, respectively. The $s_{\pm}$-wave pairing with opposite gap functions on pockets around $\Gamma$ and $\mathbf{M}$ points will create the Majorana Kramers pairs at corners, as demonstrated in Fig.1(c).

In what follows, we first investigate $s_{\pm}$ pairing in Ca$_{1-x}$La$_x$FeAs$_2$ and relate the bulk spectrum to that of its edges, which gives rise to the mechanism that realizes the corner MZMs. We then demonstrate that under $s_{\pm}$ pairing, the topological phase in this material is boundary-obstructed by showing that across the topological phase transition (TPT) between the topological and trivial phases, the energy gap only closes at the boundary of a slab configuration, while it remains open in the bulk. Finally, since the two phases are protected by chiral symmetry, we propose a new quantity, the edge winding number, as the invariant that captures the corresponding topological obstruction, and show that this invariant jumps by an integer across a TPT.

\textbf{Effective Model for As1 layers –} We start with the tight-binding model for the As1 layers. The nearest-neighbor hopping $t_{\sigma}$ is assumed to be undifferentiated between As atoms. The pairing state of CaFeAs$_2$ is expected to be dominantly determined by the Fermi surface from FeAs layers. Here we adopt a five-band model whose band structure fits well with those in DFT calculations [see Sec. I in the supplementary material (SM)]. Fig.2(a) displays the spin susceptibility. The peak around $(\pi, 0)$ is attributed to the Fermi surface nesting between the hole and electron pockets. Consequently, the dominant pairing is $s_{\pm}$-wave from the effective attractive electron-electron interactions mediated by spin fluctuations\textsuperscript{15}. Fig.2(b) shows the typical gap function of $s_{\pm}$ pairing from random phase approximation (RPA) calculations for CaFeAs$_2$, revealing a sign change in superconducting gaps between hole and electron pockets (see Sec. II in SM). The sign change and gap size can also be well described by a simple form factor $\cos k_x \times \cos k_y$ in one-Fe unit cell originating from the next-nearest neighbor antiferromagnetic exchange coupling\textsuperscript{16}. Unlike the $d$-wave state in cuprates, in which a sign change occurs in orthogonal directions, $s_{\pm}$ pairing with a sign change in momentum space is extremely difficult to be detected via Josephson interferometry. Although some evidence for the existence of sign change in pairing states have been provided in inelastic neutron scattering and scanning tunneling microscopy measurements\textsuperscript{15–21}, a decisive signature for $s_{\pm}$-pairing is still missing in iron pnictides. In the following, we show that $s_{\pm}$ pairing gives rise to a HOTSC phase in CaFeAs$_2$ with Majorana corner states, which can be regarded as the direct evidence for $s_{\pm}$-pairing.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Crystal structure and Fermi surfaces for (Ca,La)FeAs$_2$. (a) Crystal structure for (Ca,La)FeAs$_2$. (b) Lattice model for the As1 layers, where As1 atoms form a zigzag chain along $y$. (c) Fermi surfaces and pairing gap functions for (Ca,La)FeAs$_2$. The red and blue curves represent the Fermi surfaces from FeAs layers in the presence of $s_{\pm}$ pairing. The superconducting gaps possess a sign change between hole pockets around $\Gamma$ and electron pockets around $\mathbf{M}$. The orange curves are Fermi surfaces from As1 layers. The edge Dirac cones from As1 layers acquire a positive (negative) superconducting gap for the (100) edge (010) edge) in proximity to the bulk hole (electron) pockets around $\Gamma$ (M). There is a Majorana Kramers pair (gray circles) at each corner where two edges meet.}
\end{figure}
Here B and a semi-infinite system along x Sec. IV of SM. The edge states can be obtained by solving binding model. For the (100) edge, a distorted Dirac cone denoted by an effective Hamiltonian X nontrivial, leading to an intrinsic topological insulator/high Z superconductor heterostructure in CaFeAs. Spin susceptibility and (100) edge, (d) (010) edge.

The matrix elements in the Hamiltonian \( h(k) \) are provided in Sec. III in the SM. A band inversion occurs at the X point and it generates two gapless Dirac cones in the bulk dispersion along X-M path without spin-orbit coupling (SOC), protected by the screw axis along y\(^4\)\(^5\)\(^6\). Two small pockets appear around the X point derived from these cones, demonstrated by orange circles in Fig.1(c) and supported by ARPES experiments\(^8\)\(^9\). Further including SOC opens a gap in the Dirac cones and the As1 layers becomes Z\(_2\) topologically nontrivial, leading to an intrinsic topological insulator/high TC superconductor heterostructure in CaFeAs\(_2\). Around the X point, the bulk dispersion of As1 layers can be described by an effective Hamiltonian \( \mathcal{H}_{\text{eff}} = \sum_k \tilde{v}_k^\dagger \bar{h}_{\text{eff}}(k) \tilde{v}_k \) with basis \( \tilde{v}_k = (\tilde{c}_{X, k, -}^\dagger, \tilde{c}_{X, k, +}^\dagger, \tilde{c}_{Y, k, -}^\dagger, \tilde{c}_{Y, k, +}^\dagger) \), where "\( \tilde{\cdot} \)" denotes the eigenvalue of \( C_{2z} \) for eigenstates at the X point and

\[
\bar{h}_{\text{eff}}(k) = \epsilon_0(k) + M(k)\sigma_z - A_1 k_x s_0 \sigma_2 + A_2 k_y s_3 \sigma_1.
\]  

where \( \Delta_0 \) and \( \Delta_1 \) are the on-site pairing and pairing between the next nearest neighbor sites, respectively. The \( \Delta_1 \) term gives rise to the well-known \( s_+ \) pairing in iron based superconductors. Owing to the absence of spin-flip SOC terms, the Bogoliubov-de Gennes (BdG) tight-binding Hamiltonian \( \mathcal{H}_{\text{BdG}} = \mathcal{H}_0 + \mathcal{H}_{SC} \) can be written as two block diagonal parts \( \mathcal{H}_{\text{BdG}}^\dagger \) and \( \mathcal{H}_{\text{BdG}} \) (see Sec. V in SM). In each block, time reversal and particle-hole symmetries are absent but chiral symmetry is preserved, thus, each block belongs to class AIII in the ten fold classification.

Boundary-obstruction and phase transitions – To study the edge properties of the As1 layers, we consider a slab configuration for the above BdG Hamiltonian \( \mathcal{H}_{\text{BdG}}^\dagger \) with an open boundary along either \( x \) or \( y \) directions. With the on-site pairing term \( \Delta_0 \), the edge states from As1 layers open a gap, as shown in Fig.3 (a1) and (b1). Now we investigate the effect of \( s_\pm \) pairing on these edge states. At the (100) edge, the gap of edge states around \( \bar{\Gamma} \) monotonously increases with increasing \( \Delta_1 \), as shown in Fig.3 (a1) to (a3). For the (010) edge, however, the gap around \( \bar{X} \) exhibits a rather different behavior. Upon \( \Delta_1 \) increasing to \( 0.051 \) eV, the gap closes and a pair of gapless modes with linear dispersion appears [Fig. 3 (b2)]. Further increasing \( \Delta_1 \) reopens the gap, suggesting a TPT that separates a \( \Delta_0 \)-dominated phase from a \( \Delta_1 \)-dominated phase. Note that throughout this transition there is no gap closing in the bulk states (see Sec. VIII in SM). In fact, we show in Sec. VII of the SM that all the symmetry indicator invariants due to the \( C_{2z} \) and reflection symmetries in the lattice structure of \( \mathcal{H}_{\text{BdG}} \) identically vanish due to time-reversal symmetry, which is a necessary condition for the existence of boundary-obstructed phases.

To calculate the effective pairing at the edges, we first analytically obtain the wavefunctions of the edge states by solving \( \bar{h}_{\text{eff}} \) with open boundary conditions and then projecting the bulk pairing on the edge states\(^2\). The obtained pairings at the Dirac points on the (100) and (010) edges are

\[
\Delta_{\text{eff}}^{(100)} = \Delta_0 + 2\Delta_1 \frac{M_0}{B_1}, \quad \Delta_{\text{eff}}^{(010)} = \Delta_0 - 2\Delta_1 \frac{M_0}{B_2},
\]  

Below \( T_c \), the As1 layers become superconducting through the proximity effect to the adjacent FeAs layers. We model the superconducting pairing on As1 layers the same way as in FeAs layers and consider a spin-singlet intra-orbital pairing within the same sublattice. The corresponding pairing Hamiltonian reads

\[
\mathcal{H}_{SC} = \sum_{\alpha \sigma \nu} [\Delta_0 + 2\Delta_1 (\cos k_x + \cos k_y)] c_{\alpha \sigma}^\dagger(k) c_{\alpha \nu (-k)} + h.c.,
\]  

where \( \Delta_0 \) and \( \Delta_1 \) are the on-site pairing and pairing between the next nearest neighbor sites, respectively. The \( \Delta_1 \) term gives rise to the well-known \( s_\pm \)-wave pairing in iron based superconductors. Owing to the absence of spin-flip SOC terms, the Bogoliubov-de Gennes (BdG) tight-binding Hamiltonian \( \mathcal{H}_{\text{BdG}} = \mathcal{H}_0 + \mathcal{H}_{SC} \) can be written as two block diagonal parts \( \mathcal{H}_{\text{BdG}}^\dagger \) and \( \mathcal{H}_{\text{BdG}} \) (see Sec. V in SM). In each block, time reversal and particle-hole symmetries are absent but chiral symmetry is preserved, thus, each block belongs to class AIII in the ten fold classification.
We find that $\Delta_0$ provides the same pairing at the two edges while the $s_\pm$-wave pairing $\Delta_1$ provides an opposite pairing sign. This can be heuristically understood from Fig.1(e). The edge Dirac states appear around $\Gamma$ and $X$ for (100) and (010) edges; the momentum independent term proportional to $\Delta_0$ induces the same positive superconducting gap at both edges; the $s_\pm$-wave pairing, on the other hand, induces superconducting gaps with opposite signs as the corresponding Dirac cones are in proximity to the bulk superconducting gap around $\Gamma$ and $M$ at the (100) and (010) edges, respectively (see Fig.1(c)). At a fixed non-zero value of $\Delta_0$, with increasing $\Delta_1$, $\Delta_{\text{eff}}^{(100)}$ monotonously increases while $\Delta_{\text{eff}}^{(010)}$ first decreases to zero, followed by increasing in amplitude albeit with opposite sign, which is consistent with the aforementioned numerical calculations. The finite chemical potential at the edges with respect to Dirac points should be taken into consideration but their relative small values have a negligible effect on the effective pairing (see Sec. VI in SM).

To characterize the topological nature of the TPT, let us focus on the blocks $H_{\text{BdG}}^{\perp}$ and $H_{\text{BdG}}^{\parallel}$, each of which belongs to class AIII. Hamiltonians in this class are topologically characterized by the 1D winding number [10], defined by $\nu_1 = \frac{i}{2\pi} \int_{BZ} dk \partial^2 \text{Tr} \left[ q_k^{-1} \partial_q q_k \right]$. Here the unitary $q_k$ matrix is the off-diagonal part of the so-called $Q$ matrix, given by $Q_k = 1 - 2F_k = \begin{pmatrix} 0 & q_k^\dagger \\ q_k & 0 \end{pmatrix}$ within the eigenbasis of chiral symmetry, where $F_k$ is the projection operator of the Hamiltonian for a slab model $H_{\text{BdG, slab}}^{\perp}$ with $N$ lattice sites. We first consider the winding number on a slab configuration with open boundary along the (010) direction. The total winding number $\nu_1$ is zero across the TPT (see Sec. VIII in SM). Motivated by the fact that the bands close at the (010) edges of the slab during the TPT, we define a site-resolved winding number by projecting the total winding number $\nu_1$ into the lattice site basis as

$$\nu_1^{\gamma} = \frac{i}{2\pi} \sum_{\gamma} \int_{BZ} dk [q_k^{-1} \partial_k q_k]_{\gamma, \gamma},$$

such that $\nu_1 = \sum_{i=1}^N \nu_1^i$. Here, $i$ is the index for lattice site and $\gamma$ denotes the sublattice or orbital index (details are given Sec. VIII in SM). This site-resolved winding number resembles the site-resolved polarization defined in Ref. 24 to calculate the edge-localized dipole moments in insulators, including the boundary-obstructed quadrupole topological insulator[25]. The dependence of $\nu_1^\gamma$ on the site $i$ for the HOTSC and trivial phases is displayed by the blue and red curves in Fig.4(a). For both curves, one can see that the contribution to the winding number mainly comes from edges, with the opposite edges having opposite contributions. We also notice that the profile of $\nu_1^\gamma$ near one edge (see the zoom-in Fig.4(a)) has a substantial difference between the HOTSC and trivial phases. We define the edge winding number $\nu_1^{T}$ and $\nu_1^{B}$ for the top and bottom edges, respectively, by summing $\nu_1^i$ for the upper half part ($i = 1, ..., N/2$) and lower half part ($i = N/2 + 1, ..., N$) of the slab and examine the winding number change $|\Delta \nu_1^{T/B}|$ between two phases for the upper and lower half parts as a function of the lattice size $N$. As shown in Fig.4(b), we find that the winding number change $|\Delta \nu_1^{T}|$ approaches 1 in the thermodynamic limit ($N \to \infty$). Thus, the edge winding number $\nu_1^{T/B}$ characterizes the different topologies across the TPT in our new class of superconductor.

**Majorana corner states** – In the $\Delta_1$ dominated phase, the (100) and (010) edges have the opposite superconducting gaps, belonging to topologically distinct phases. As a con-

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FIG. 3: Evolution of band structures for (100) edge (a) and (010) edge (b) as a function of the $s_\pm$ pairing $\Delta_1$. The plots in each column are generated with the same parameters and the adopted parameters in three columns (from left to right) are: $\Delta_1 = 0$, $\Delta_1 = 51$ meV and $\Delta_1 = 100$ meV with a fixed $\Delta_0 = 5$ meV. The color code shows the average position of each state. The blue and red circles denote the left (top) and right (bottom) localized edge states at the (100) ((010)) edges, respectively. The green circles represent extended bulk states.
FIG. 4: Edge winding number and energy and spatial pattern for MZMs. (a) Site-resolved winding numbers for the (010) edge with \( N = 150 \) unit cells along \( y \) in the two topologically distinct phases. (b) Winding number difference \( \Delta \nu_7^i \) as a function of the lattice size \( N \). (c) Energy of the MZMs as a function of the lattice size for a square geometry. The inset shows a typical energy spectra for the full lattice. (d) The probability density functions of the MZMs for a square geometry with eight MZMs (each corner hosts a Kramers pair of MZM) with 65 \( \times \) 65 lattice sites.

sequence, MZMs are expected to occur at the corners where they meet. We adopted the Hamiltonian \( \mathcal{H}_{BdG} \) with both open boundary conditions along \( x \) and \( y \) directions, and performed calculations with several lattice sizes. There are eight mid-gap states and their energies are zero up to finite-size effects. We examine the energy splitting due to the hybridization of the MZMs at different corners by plotting the energies \( E_M \) of mid-gaps states as a function of lattice size in Fig.4(c). The linear relationship between \( \log_{10}(E_m) \) and lattice size suggests that \( E_M \) goes to zero in the thermodynamic limit, compatible with the existence of zero-energy states exponentially localized at the corners of the lattice, as shown in Fig.4(d). At each corner, there are two zero-energy states forming a Majorana Kramers pair. The appearance of MZMs at the corners supports our prediction of a HOTSC phase with boundary-obstruction in CaFeAs\(_2\).

Discussion – As the 112-family of iron pnictides is 3D and the interlayer coupling is relatively weak, the helical Majorana states, localized at the hinges between (100) and (010) surfaces, have a weak dispersion along \( k_z \). MZMs can also appear at corners/hinges between non-orthogonal surfaces, as long as the corresponding surface states have the opposite effective superconducting gap in proximity to the bulk \( s_\pm \) pairing. Therefore, the \( s_\pm \) pairing is directly manifested by the appearance of MZMs at hinges, protected by chiral symmetry and irrespective of crystalline symmetries. The MZMs we find are robust against impurities and disorders in real material scenarios that always break crystalline symmetries. The detection of hinge MZMs in CaFeAs\(_2\) hence provides a “smoking-gun” evidence for the \( s_\pm \) pairing in iron pnictides. As the Fermi level only crosses the lower part of edge Dirac cones for edges in As1 layers within a wide electron-doping range, the MZMs can survive in electron-doped compounds Ca\(_{1-x}\)La\(_x\)FeAs\(_2\), providing a new high-temperature platform for MZMs without fine-tuning. In experiments, MZMs at the corner can directly be detected by local spectroscopy on As1 layers on the (001) surface, while transport measurements can likewise provide evidence for hinge MZMs.

Conclusion – We propose the 112 family of iron pnictides as the first material realization of boundary-obstructed topological superconductivity, owing to their intrinsic \( s_\pm \) pairing and effective topological insulator/high-\( T_c \) superconductor heterostructure profile. The edge topological obstruction, independent of crystalline symmetries and uniquely characterized by the edge winding number, provides a robust platform for the realization of MZMs, which en passant also constitutes decisive evidence for \( s_\pm \)-wave pairing in the 112 pnictides.

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Author contributions X.W., C.L. and J.H. conceived this project. W.A.B. posited this system as a boundary-obstructed topological phase. X.W., W.A.B. and Y.L. performed the numerical calculations and C.L., X.W., W.A.B., R.T. and J.H. performed the analysis. All the authors participated in the discussion and writing of the manuscript.

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