Atomic line defects in unconventional superconductors as a new route toward one dimensional topological superconductors

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Topological superconductors (TSCs) are correlated quantum states with simultaneous off-diagonal long-range order and nontrivial topological invariants. They produce gapless or zero energy boundary Majorana excitations with topologically protected phase coherence that are essential for fault-tolerant quantum computing. Candidate TSCs are very rare in nature. Here, we propose a novel route toward one-dimensional TSCs along an intrinsic atomic line defect in unconventional but topologically trivial s-wave or d-wave superconductors. We show that the inversion symmetry breaking along the line defect and the charge transfer resulting from the missing atoms lead to occupation of inipient impurity bands with Rashba spin-orbit coupling and innate superconductivity of mixed parities of s-wave and p-wave pairing. The time reversal invariant TSC emerges in a large part of the parameter space, as does the time reversal symmetry breaking TSC when magnetism develops, with robust Majorana zero modes at the both ends of the line defects. This new mechanism provides a natural explanation for the recent experimental discovery of zero-energy bound states at both ends of an atomic line defects in the monolayer Fe(Te,Se) superconductors, and pave the way for novel material realizations of the simplest and most robust 1D TSCs in unconventional superconductors with high transition temperatures.

Introduction

The simplest model for a TSC is the Kitaev chain of spinless (single-spin) fermions with p-wave pairing. The model does not have time-reversal invariance (TRI) and belongs to the topological class D.[8,9] The TSC phase has a nontrivial Z2 invariant and one Majorana zero mode (MZM) at each end of the open chain. To land at this 1D conductor, and a Zeeman field from a magnetic insulator or exchange thus relying on a hybrid structure of uncontrolled proximity- that nanowires with strong Rashba SOC are usually not SC, localized on both ends of the nanowire. The bottleneck is controversial whether the TSC has been realized with MZMs perconductors made advances,[13–15] but it remains ing Rashba nanowires proximity coupled to conventional su-

 trance. Majorana excitations with topologically protected phase coherence that are essential for

The idea was motivated by the recent experimental discovery of zero-energy bound states at both ends of an atomic line defect in monolayer high-Tc Fe-based superconductor Fe(Te,Se) grown on SrTiO3 substrates with Tc ~ 60 K.[17–19] We will use its atomic structure as an example, but the physics can be more generally applied to other suitable unconventional superconductors. The one-unit-cell Fe(Te,Se) monolayer contains three atomic layers (Fig. 1a), and the as-grown atomic line defect corresponds to the line of missing Te/Se atoms on the top layer above the Fe-plane. The missing atoms break inversion symmetry centered on the Fe atom below, giving rise to large Rashba SOC αR. To emphasize this property, we will refer to the latter as a Rashba atomic line defect (RALD). The second important consequence of the missing Te/Se atoms is the quenched p-d charge transfer along the RALD. Since each Fe2+ was supposed to transfer two electrons to Te2-/Se2−, there is an excess of one-electron per unit cell along the RALD. For the monolayer Fe(Fe,Se)16, an incept impurity band can arise and be occupied by up to one electron (Fig. 1b). In more general cases, there can be occupations of more impurity bands.[20] Let’s denote the impurity band dispersion as ε(k) where k is the 1D momentum. The inversion symmetry breaking implies that the superconductivity induced on the RALD has mixed parity involving both spin-singlet Δs(k) = Δs(−k) and spin-triplet Δp(k) = −Δp(−k) components,[21,22] but retains the time-reversal symmetry of the bulk SC state.

Effective 1D theory for RALD – While microscopic considerations will be given later, one can write down the effective 1D model for the RALD based on symmetry arguments. In the Nambu basis of the electron operators (f↓, f↑, f†↓, f†↑), the BdG Hamiltonian is given by

\[ H_{1D}(k) = \varepsilon_{k}(k) \tau_z + 2\alpha_{R} \sin k \sigma_{i} \tau_{y} + \Delta_{s}(k) \sigma_{i} \tau_{y} + \Delta_{p}(k) \tau_{y} \]

where \(\sigma_{i}\) and \(\tau_{i}\) are the Pauli matrices acting in the spin and particle-hole sectors respectively. Note that the odd-parity, spin-triplet pairing, i.e. the \(\Delta_{p}(k)\) term, does not arise in Rashba nanowires in proximity to s-wave superconductors.

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Each band is given by the product of the signs of $\Delta$ and $\pm\Delta$ where $s(k) = \prod\sgn(k_s)$, and $N(k) = 2\prod\sgn(k_s) - \cos k_s$. Thus, an odd number of Fermi points with negative momentum or energy and are energetically unfavorable [25] and thus not included in the 1D model.

The 1D model in Eq. (1) is invariant under the time-reversal operation $\mathcal{T} = i\sigma_y \mathcal{K}$ where $\mathcal{K}$ is the operator for complex conjugation. Besides time-reversal symmetry breaking TSC, there is a class (DIII) of TSC that are time-reversal invariant (TRI) and referred to as TRI TSC [9, 23, 24, 26]. Realizations of TRI TSC have been proposed theoretically for nanowires proximity coupled to iron-based and copper-based superconductors [27, 28]. TRI superconductors in 1D can be classified by a $Z_2$ invariant $N$ of the corresponding BdG Hamiltonian [6]. $N$ can be calculated from the expectations of the time-reversed pairing function [25, 26] $\delta_{nk} = n(k)\Delta^*_n(k)$ for each band $n$. For our 1D model in Eq. (1), the pairing function $\Delta_k = i\sigma_y \Delta_s(k) + i\sigma_y \delta_{p}(k)$. The 1D TRI topological invariant is given by the product of the signs of $\delta_{nk}$, i.e. $N = \prod\sgn(\delta_{nk})$, where $s = (n, k_F)$ runs over all the Fermi points between 0 and $\pi$. Thus, an odd number of Fermi points with negative time-reversed pairing functions corresponds to a nontrivial $(N = -1)$ $Z_2$ number and a TRI TSC, with four degenerate MZMs in the energy spectrum (Fig. 1c), pairwise localized at both ends of the open chain (Fig. 1e). The Kramers pair of MZMs (blue and red dots) are protected by time-reversal symmetry that forbids intra-pair scattering, while the inter-pair scattering is exponentially suppressed by the length of the 1D chain [30]. The dependence of the zero-bias conductance on the length of the RALD has indeed been observed in monolayer FeTe(Se) [16].

**Topological phase diagram for RALD** – For simplicity, but without loss of generality, we consider $\varepsilon_{l}(k) = -2t\cos k - \mu$ and nearest neighbor pairing gap functions $\Delta_{s}(k) = 2\Delta_{s}\cos k$, $\Delta_{p}(k) = 2\Delta_{p}\sin k$. The onsite pairing is ignored since it is suppressed in unconventional superconductors due to the strong Coulomb repulsion. Evaluating the topological invariant, we obtain

$$N = \sgn[(\Delta_{s}\cos k_{+} + \Delta_{p}\sin k_{+})(\Delta_{s}\cos k_{-} - \Delta_{p}\sin k_{-})].$$

The sign of $N$ thus determines the topological phase diagram (Fig. 1f) of the RALD in the $\mu/t - \Delta_{p}/\Delta_{s}$ plane, where the TRI TSC with $N = -1$ occupies a significant part of the phase space. The phase boundaries determined by the $Z_2$ number are further confirmed by performing the Zak phase calculations [29, 51]. There are a few remarkable characteristics of the phase diagram. First of all, in the limit $\Delta_{p}/\Delta_{s} \rightarrow \pm\infty$, the 1D chain is always a TRI TSC analytically connected to two Kitaev $p$-wave chains coupled by the TRI Rashba SOC. For finite $\Delta_{p}/\Delta_{s}$, the phase boundaries correspond to two gap-closing lines. Along the $\mu = 0$ axis (Fig. 1f), the impurity band is half-filled with $k_z$ shifted from $\pi$ by an amount $\pm \alpha_{R}/t$, where the spin-singlet gap function $\Delta_{s}(k)$ is near its minimum and smaller than the spin-triplet $\Delta_{p}(k)$ near its maximum, except for the region close to the origin. This leads to the striking results that the entire line corresponds to TSC except for the gapless critical point at $\alpha_{R}/t$. This highlights the robustness of TRI TSC resulting from the mixed parity pairing along the RALD and that the nontrivial topological invariant $N$ produced by predominantly $s$-wave and $p$-wave pairing functions amounts to analytically indistinguishable TSCs. At nonzero $\mu/t$ and sweeping $\Delta_{p}/\Delta_{s}$, the in-phase and antiphase TSCs are separated by a region of topologically trivial SC state.

**Incipient TSC from RALD in 2D** – We next go beyond the effective 1D model, and show that this mechanism for TRI TSCs can be applied directly to a RALD embedded in the 2D system such as the monolayer FeTe(Se). The electronic structure of monolayer FeTe$_{1-x}$Se$_x$ as a function of $x$ has been studied by angle-resolved photoelectron spectroscopy (ARPES) [19]. For $x > 0.4$, there are two fully occupied $d_{z^2}$ bands and one unoccupied, predominantly $p_z$ band just above the Fermi level near the zone center $\Gamma$ point. The electrostatic potential due to the missing negatively charged Te/Se ions pushes the $p_z$ band to cross the Fermi level to accommodate the excess electrons localized along the RALD. Since the

[Fig. 1: a. Schematics of the monolayer FeTe(Se) lattice structure with the atomic line defects of missing Te atoms along the (1,1) direction. The blue and green balls represent Te/Se atoms below and above the Fe plane respectively. Silver balls represent the Fe atoms. b. A simple example of the electronic structure for the TRI TSC ($N = -1$). The red open and solid circles are the Fermi points with positive and negative pairing, respectively. c. The energy spectrum of an 1D TRI TSC with open boundaries, with four zero-energy modes (blue and red dots) inside the SC gap. One blue and one red form a Kramers pair, localized at the ends of the chain as illustrated in e. Each of them provides a zero-energy peak in the LDOS spectrum in d, f. Topological phase diagram for the effective 1D theory of the RALD. ]
FIG. 2: Schematics the Fe(Te,Se) lattice structure with the RALD in the (1,1) direction for the Hamiltonian construction. a. Hopping and pairing parameters defined in the bulk \( H_b \) and the RALD \( H_{ef} \). b. Coupling parameters between the bulk and the RALD defined in \( H_f \). c-f. The leading processes generated in the 2nd order perturbation expansion. c. \( t_1c_1'f_{11} \) and \( \Delta_{11}c_{11}f_{11} \) induce onsite pairing \( \Delta_{11}c_{11}f_{11} \). d. \( t_1c_{11}'f_{11} \) and \( \Delta_{11}c_{11}f_{11} \) induce extend s-wave pairing \( \Delta_{11}c_{11}f_{11} \). e. \( \alpha c_{11}f_{11} \) and \( \Delta_{11}c_{11}f_{11} \) induce p-wave pairing \( \Delta_{p,11}c_{11}f_{11} \). f. \( t_1c_{11}'f_{11} \) and \( \alpha f_{11}'c_{11} \) induce Rashba coupling \( \alpha f_{11}'c_{11} \).

additional two nearly overlapping electron pockets give even number of degenerate pairs of Fermi points, the condition for the nontrivial topological invariant \( N \) will not be affected by the electron bands. The model can be further simplified by considering a single impurity band around the \( \Gamma \) point. We will use the spinors \( c_i = (c_{i\uparrow}, c_{i\downarrow})^T \) for the electrons in the bulk and \( f_i = (f_{i\uparrow}, f_{i\downarrow})^T \) for the electrons on the RALD. The total Hamiltonian can be written as \( H = H_e + H_f + H_{ef} \), with

\[
H_e = \sum_{ij} -t_{ij} (c_{i\uparrow} \sigma c_{j\downarrow} + c_{i\downarrow} \sigma c_{j\uparrow}) + \Delta_{ij} (c_{i\uparrow} c_{j\downarrow} + c_{i\downarrow} c_{j\uparrow}) + h.c. \tag{3}
\]

where \( i, j \) run over the 2D bulk Fe lattice except the line defect. We include the 1st and 2nd nearest neighbor hopping \( t_1 \) and \( t_2 \) and the 1st and 2nd nearest neighbor spin-singlet pairing \( \Delta_1 \) and \( \Delta_2 \) in the extended s-wave channel, respectively. \( H_f \) is written on the 1D Fe lattice sites along the Rashba line defect,

\[
H_f = \sum_{i,j \in \Gamma} -t_2' c_{i\uparrow} f_{j\downarrow} + \Delta_2 f_{i\downarrow} c_{j\uparrow} + h.c. \tag{4}
\]

where \( \mu, \alpha, \beta, \gamma \) and \( \Delta \) are the local potential, Rashba SOC, hopping and pairing. Note that \( t_2' \ll t_1 \) and \( \Delta_2 \ll \Delta_1 \) due to the missing Te/Se atoms that were otherwise strong facilitators of such second nearest neighbor processes [32]. The vector \( \hat{d}_{ij} = \frac{r_{ij}}{|r_{ij}|} \) is the unit vector connecting sites \( i \) and \( j \). Finally, the Rashba line defect couples to the bulk according to

\[
H_{ef} = \sum_{i,j \in \Gamma} [t_1 c_{i\uparrow} \sigma c_{j\downarrow} + \Delta_{12} f_{i\downarrow} c_{j\uparrow} + h.c.]
- t_2 \sum_{i,j} c_{i\uparrow} c_{j\downarrow} + \sum_{i,j} f_{i\downarrow} c_{j\uparrow} + h.c. \tag{5}
\]

where, in addition to the couplings by the nearest and second nearest neighbor hopping and pairing terms that appeared in \( H_e \), the nearest neighbor Rashba SOC \( \alpha_1 \) is also included to capture the effects of inversion symmetry breaking. It is instructive to illustrate that integrating out the bulk states represented by \( c_i \) and \( c_i' \) produces essentially the effective 1D Hamiltonian in Eq. (1). The mechanism for inducing the pairing states of mixed parity can be understood from the processes (Fig. 2c-e) involved in the 2nd order perturbation expansion. For example, the combination of \( \Delta_{12} f_{i\downarrow} c_{j\uparrow} \) and \( t_2 c_{i\downarrow} f_{j\uparrow} \) in Eq. (5) induces pairing along the RALD described by \( t_3 \Delta_{b} G_{s} f_{i\downarrow} c_{j\uparrow} f_{j\uparrow} \) where the equal-time correlator \( G_{s} f_{i\downarrow} c_{j\uparrow} f_{j\uparrow} \). Processes of this type (Fig. 2c,d) give rise to the induced spin-singlet, even parity pairing with onsite (controlled by \( t_1 \Delta_1 \) and \( t_2 \Delta_2 \), nearest neighbor extend s-wave (controlled by \( t_1 \Delta_1 \)), and further neighbor even parity pairing terms along the chain. This part is similar to the proximity-effect superconductivity. Remarkably, due to the inversion symmetry breaking, the Rashba SOC combined with s-wave pairing between the RALD and the bulk superconductors produce odd-parity, spin-triplet pairing in real space. For example, \( -i\alpha_1 f_{i\downarrow} c_{j\uparrow} \) with \( \Delta_{12} f_{i\downarrow} c_{j\uparrow} \) in Eq. (5) generates \( -i\alpha_1 \Delta_{b} G_{s} f_{i\downarrow} c_{j\uparrow} f_{j\uparrow} \). The processes of this type (Fig. 2e) give rise to the TRI spin-triplet, odd-parity pairing \( \Delta_{p} (e^{i\delta} f_{i\downarrow} c_{j\downarrow} + e^{i\delta} f_{i\downarrow} c_{j\downarrow}) \) with \( \Delta_{p,1} \sim \alpha_1 \Delta_{1} \) for the nearest neighbor p-wave and further neighbor odd-parity higher harmonics.

TSC in s-wave dominated region – Now we present the results directly obtained from diagonalizing the 2D Hamiltonian \( H \) in Eqs. (3,5). Throughout the main text, we use \( t_2 \) as the energy unit and set to unity. We first set \( \alpha_1 = 0 \) and discuss the s-wave dominated region. To illustrate the incipient impurity band, the length of the defect line \( L_D \) is first set to be equal to \( L_{1,1} \), the dimension of the 2D system along the (1,1) direction. Periodic boundary condition in the (1,1) direction and open boundary condition in the perpendicular (1,-1) direction are applied. Since we stick to the momentum coordinates of the 2D bulk system, the Brillouin Zone of the RALD is from \(-\pi \) to \( \pi \) along the \( \Gamma \) direction, therefore, we use the number \( k \) to label the momentum \( k \) along the RALD. The normal state energy dispersions versus the momentum \( k \) in the (1,1) direction (Fig. 3a) show the incipient impurity bands (red lines) localized on the line defect that cross the Fermi level. The two bands are split by Rashba SOC \( \alpha_2 \) along the RALD. Therefore, if the SC pairing gap function of the impurity bands satisfies the \( Z_2 \) nontrivial condition in Eq. (2), a TRI one-dimensional TSC emerges on the RALD. When the dominant pairing is the even-parity s-wave channel, the condition simply requires a node of the pairing gap function located in between the two Fermi points. We thus calculate the induced spin-singlet pairing order parameter \( P_+ = i\sigma f_i c_i \) along the embedded line defect with \( L_D = 250 \pm 500 \sqrt{2} \) and \( L_{1,1} = 10 \sqrt{2} \). The pairing function is a mixing of even-parity harmonics (Fig. 3b) and displays a node at \( k^* \approx 0.28\pi \) in between the Fermi points and materializes the TSC. The energy spectrum obtained for the entire 2D sample contains two Kramers pairs of two MZMs (Fig. 3c) inside the SC
gap, which are localized at the ends of the RALD and manifested as the zero-energy peaks in the local density of states (LDOS). The Kramers pairs of MZMs are protected by the time-reversal symmetry. The tunneling conductance should be quantized to $4e^2/h$ \cite{28}.

TSC in p-wave dominated region – A crucial part of topological phase diagram (Fig. 1f) is the p-wave dominated region. Indeed, an incipient TRI TSC with dominant odd-parity pairing can emerge from the RALD embedded in the bulk s-wave superconductor. To this end, we set $\alpha_1 = 0.5$ and $t_1 = \Delta_2 = 0$, such that the induced even parity pairing is suppressed in the perturbative diagrams (Fig. 2c,d) discussed above. Two nearly degenerate impurity bands crossing the Fermi level are obtained (Fig. 3d) at $\alpha_2 = 0$, i.e. without a bare Rashba SOC along the line defect. In the SC state, the induced equal-spin triplet pairing order parameter $P_k = \frac{i\sigma_z}{2}P_{s}(k)$ is calculated on the embedded line defect. Fig. 3e shows that the induced pairing function is a mixing of odd-parity harmonics dominated by the near-neighbor $p$-wave pairing. The energy spectrum of the entire 2D sample contains two Kramers pairs of two MZMs inside the SC gap. They are spatially localized at the ends of the RALD and manifested as the zero-energy peaks in the LDOS. Indeed, this odd-parity TRI TSC is a realization of two Kitaev $p$-wave chains that reinstate the time-reversal symmetry. A crucial point is that the topological $Z_2$ invariant $N$ in Eq. (2) is non-trivial irrespective of a nonzero, band-splitting, Rashba SOC $\alpha_2$ that couples the two Kitaev chains without breaking time-reversal symmetry. In this sense, the odd-parity TRI TSC is a much more robust topological state.

TSC in general regions of mixed parity – In the most general cases, which are relevant to real materials such as Fe(Te,Se), the nonzero $\alpha_1 \Delta_1$ will induce odd-parity pairing and $t_1 \Delta_1$ and $t_2 \Delta_2$ even-parity pairing (Fig. 2c,e), such that the SC state on the RALD is in the regime of mixed parity, yet the TRI TSC emerges over a large region of the phase space. The 2D lattice calculations for the general set of parameters show the incipient impurity bands crossing the Fermi level (red lines in Fig. 4a). For generality, we have also considered the case where the bulk bands are partially filled giving rise to multiple impurity bands crossing the Fermi level. The impurity bands are split by the dynamically generated Rashba SOC along the line defects. For bulk $s$-wave pairing $\Delta_1 = 0.1$ and $\Delta_2 = 0$, the induced mixed parity pairing order parameter can be written as $P_k = i\sigma_zP_{s}(k) + \frac{\alpha_1}{\sqrt{2}}\sigma_yP_{c}(k)$. Fig. 4b shows that the even ($P_s$) and odd ($P_c$) parity pairing order parameters are of comparable magnitudes, composed of close neighbor s-wave and p-wave components and their higher order harmonics. Remarkably, close to the momenta of the split Fermi points, the odd-parity is at the maximum and dominate over the even-parity pairing amplitude, such that the topological $Z_2$ invar-
an even parity pairing to become strong enough and cause the SC gap to close and reopen, leading to a topological phase transition to the trivial SC phase. The energy spectrum of the 2D lattice shows four MZMs inside the SC gap and spatially localized at the ends of the line defects. These results are in good agreement with the recent experimental observation of the zero-energy bound states at the atomic line defects in monolayer Fe(Te,Se)\cite{16}.

Zeeman effect and time-reversal symmetry breaking TSC – There is the possibility of incipient local magnetism along the RALD. For the monolayer Fe(Te,Se), although the initial STM studies find no evidence of magnetism\cite{16}, the line of missing Te/Se atoms may cause the Fe atoms underneath to become magnetic. In the presence of incipient ferromagnetism, the RALD becomes analogous to the Rashba quantum wires \cite{19} and magnetic chains \cite{23}. The effective 1D model $H_{1D}$ in Eq. (1) is augmented by the Zeeman field $\hbar \sigma_z \tau_z$. Without time-reversal symmetry, the 1D TSC is classified by a different $Z_2$ topological invariant $N_\mu$, which can be calculated in terms of the Pfaffians of the BdG Hamiltonian in the Majorana basis at $k = 0$ and $k = \pi$ \cite{25,33}. We obtain,

$$N_\mu = \text{sgn}[\langle h^2 - (\mu + 2\tau)^2 - 4\Delta^2 \rangle^2 - 2\tau^2 - 4\Delta^2]| \langle h^2 - (\mu + 2\tau)^2 - 4\Delta^2 \rangle^2 |],$$

and $N_\mu = -1$ corresponds to a nontrivial TSC. Note the odd-parity pairing $\Delta_\mu$ does not enter the $Z_2$ invariant. Thus, a time reversal symmetry breaking TSC requires the Zeeman field to satisfy the condition $\hbar^2 \in [(|\mu| - 2\tau)^2 + 4\Delta^2, (|\mu| + 2\tau)^2 + 4\Delta^2]$. Thus, the TSC is difficult to arise if the incipient impurity band is nearly particle-hole symmetric ($\mu \approx 0$), but more easily achieved when $\mu$ is close to the band top or bottom. Such a 1D TSC supports a single MZM at each end of the RALD.

Summary and conclusion – We have demonstrated that incipient time-reversal invariant topological superconductors of mixed parity can emerge along intrinsic Rashba atomic line defects in unconventional superconductors. They hold two Kramers pairs of MZMs inside the SC gap at both ends of the chain that are robust and protected by time reversal symmetry. The new mechanism relies on the inversion symmetry breaking induced by the missing atoms that produces strong Rashba SOC, which together with the coupling to the extended s-wave superconductor in the bulk, induces incipient odd-parity spin-triplet pairing along the RALD and a nontrivial topological invariant in a large part of the parameter space. We showed that this mechanism provides a natural explanation for the zero-energy bound states discovered at the ends of the atomic line defect in monolayer Fe(Te,Se) high-Tc superconductor. In the supplemental section, the mechanism is shown to be applicable to a RALD in an unconventional $d$-wave superconductor\cite{28}. Our findings open a new direction towards realizations of embedded 1D topological superconductors with Majorana end states in unconventional superconductors with high transition temperatures.

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A. Real space local pairing and quasiparticle pairing

It is known that the Rashba SOC transforms the real space $s$-wave local pairing into effective $p$-wave pairing in the quasiparticle sector $[1-4]$. In this section, we provide the transformations between local pairings and quasiparticle momentum space pairings for all translation invariant pairing potentials in 1D. Note, however, that the mechanism introduced in the main text of generating mixed parity pairing in real space is new and beyond this transformation, which is only possible by real space coupling of the RALD to the bulk superconductor on the atomic scale.

For simplicity, the bare Hamiltonian for an 1D wire is approximated by the continuum model in the spinor basis $(f_\uparrow(x), f_\downarrow(x))$,

$$\hat{H}_{\text{wire}} = \int dx f_\uparrow(x)\left(-\frac{\partial^2}{2m} - \mu - i\alpha\sigma_y \partial_x + h\sigma_z\right)f(x) \quad (S1)$$

Besides the Rashba coupling $\alpha$, the Zeeman coupling $h$ is also included. After Fourier transformation,

$$\hat{H}_{\text{wire}} = \sum_k f_k^\dagger \left(\frac{k^2}{2m} - \mu + \alpha k\sigma_y + h\sigma_z\right)f_k. \quad (S2)$$

We can diagonalize the above Hamiltonian by a unitary transformation,

$$\begin{bmatrix} f_k^\dagger \\ f_\bar{k}^\dagger \end{bmatrix} = U \begin{bmatrix} \psi_{k+} \\ \psi_{k-} \end{bmatrix} \quad (S3)$$

where the unitary matrix $U$ is given by

$$U = \begin{bmatrix} \cos \theta_k & \sin \theta_k e^{i\phi_k} \\ -\sin \theta_k e^{-i\phi_k} & \cos \theta_k \end{bmatrix} \quad (S4)$$

with $\tan 2\theta_k = \alpha k/h$ and $\phi_k = \frac{\pi}{2}$. The diagonalized Hamiltonian becomes

$$\hat{H}_{\text{wire}} = \sum_k \begin{bmatrix} \psi_{k+}^\dagger & \psi_{k-}^\dagger \end{bmatrix} \begin{bmatrix} E_k^+ & 0 \\ 0 & E_k^- \end{bmatrix} \begin{bmatrix} \psi_{k+} \\ \psi_{k-} \end{bmatrix}$$

where $E_k^\pm = \frac{k^2}{2m} - \mu \pm e_k$ and $e_k = \sqrt{\alpha^2 k^2 + h^2}$. Due to Pauli-exclusion principle, there are only four possible pairing terms, one spin singlet and three spin triplets.

The spin singlet channel with inversion even pairing functions $g(k) = g(-k)$ transforms according to

$$g(k)(f_{k\uparrow}f_{\bar{k}\downarrow} - f_{k\downarrow}f_{\bar{k}\uparrow}) = \frac{g(k)\alpha k}{e_k}\left(\psi_{k+}\psi_{\bar{k}+} + \psi_{k-}\psi_{\bar{k}-}\right)$$

$$+ g(k)\frac{2h}{e_k}\psi_{k+}\psi_{\bar{k}-}. \quad (S5)$$

The intra-FS pairing $(k_+, \bar{k}_\pm)$ becomes an effective $p$-wave pairing under the Rashba SOC rotation.

The $S_z = 0$ triplet channel with inversion odd function $d_2(k) = -d_2(-k)$ is transformed as

$$d_2(k)(f_{k\uparrow}f_{\bar{k}\downarrow} + f_{k\downarrow}f_{\bar{k}\uparrow}) = d_2(k)(\psi_{k+}\psi_{\bar{k}-} + \psi_{k-}\psi_{\bar{k}+}). \quad (S6)$$
This clearly involves an inter-band or inter-FS pairing that either carries a finite pair-momentum or at finite energy.

The equal-spin $S_z = 1$ triplet channel with inversion odd function $d_1(k) = -d_1(-k)$ is transformed as

$$
d_1(k)f_{k\uparrow}f_{\bar{k}\downarrow} = d_1(k)\frac{i\alpha k}{2\epsilon_k}(\psi_{k\downarrow}\psi_{\bar{k}\uparrow} - \psi_{k\uparrow}\psi_{\bar{k}\downarrow})$$

$$+ d_1(k)(\frac{1 + h/e_k}{2}\psi_{k\downarrow}\psi_{\bar{k}\downarrow} + \frac{1 - h/e_k}{2}\psi_{k\uparrow}\psi_{\bar{k}\uparrow}) \tag{S7}
$$

The $S_z = -1$ triplet channel with inversion odd function $d_3(k) = -d_3(-k)$ is transformed as

$$
d_3(k)f_{k\uparrow}f_{\bar{k}\downarrow} = d_3(k)\frac{i\alpha k}{2\epsilon_k}(\psi_{k\downarrow}\psi_{\bar{k}\uparrow} - \psi_{k\uparrow}\psi_{\bar{k}\downarrow})$$

$$+ d_3(k)(\frac{1 - h/e_k}{2}\psi_{k\downarrow}\psi_{\bar{k}\downarrow} + \frac{1 + h/e_k}{2}\psi_{k\uparrow}\psi_{\bar{k}\uparrow}) \tag{S8}
$$

### B. Topological invariants for effective 1D models

In this section, we provide a detailed calculation of the topological invariants for the effective 1D model with time-reversal symmetry (class $DIII$) and without time-reversal symmetry (class $D$) [5-3]. For TRI TSC, Ref. [4] introduced a simple equation using the effective pairing at the Fermi surface in the weak pairing limit. For our 1D model, the pairing function of mixed parity is defined as

$$\Delta_k = i\sigma_z\Delta_x(k) + i\sigma_0\Delta_p(k) \tag{S9}
$$

$$\Delta_x(k) = 2\Delta_x \cos k$$

$$\Delta_p(k) = 2\Delta_p \sin k$$

The effective pairing function $\delta_{nk}$ for each band $n$ at momentum $k$ is defined in terms of each eigenstate $|n,k\rangle$ as

$$\delta_{nk} = \langle n,k|\mathcal{T}\Delta^\dagger|n,k\rangle \tag{S10}
$$

where $\mathcal{T} = i\sigma_x\mathcal{K}$ is the time-reversal operator with $\mathcal{K}$ representing complex conjugation. The TRI topological invariant in 1D is given by a product

$$N = \Pi_s[\text{sgn}(\delta_s)] \tag{S11}
$$

where $s$ runs over all the Fermi points between 0 and $\pi$. For the 1D effective model in Eq. (1), we obtain

$$N = \text{sgn}[(\Delta_x \cos k + \Delta_p \sin k)(\Delta_x \cos k - \Delta_p \sin k)] \tag{S12}
$$

where $k_s$ are the two Fermi points between $k = 0$ and $k = \pi$ of the Rashba-split bands.

For the case with time-reversal breaking by the Zeeman field $h$, we need to write the BdG Hamiltonian in the Majorana basis. The fermion operator is related to the Majorana operators by

$$\gamma_{i\alpha\sigma} = f_{i\alpha\sigma} + f^\dagger_{i\alpha\sigma} \tag{S13}
$$

$$\gamma_{i\bar{\sigma}} = -i(f_{i\bar{\sigma}} - f^\dagger_{i\bar{\sigma}}) \tag{S14}
$$

### C. TSC from RALD in unconventional $d$-wave superconductors

In this section, we extend the idea to other unconventional superconductors with $d$-wave pairing. Owing to electron-electron correlation, $d$-wave superconductors are another large class of unconventional superconductors such as the cuprates. Since there is no difference between an extend $s$-wave and a $d$-wave superconductor in 1D, the pairing structure
along the line defect is essentially the same as that described the 1D effective Hamiltonian in Eq. (1).

We performed a similar calculation on a \( d \)-wave superconductor on the square lattice with a RALD along the \( x \) direction. The pairing symmetry is assumed to be \( d_{x^2-y^2} \), i.e. with nearest neighbor pairing \( \Delta_x = -\Delta_y = \Delta \). The model Hamiltonian can be written down as follows

\[
H_d = -t \sum_{\langle ij \rangle} c_i^\dagger c_j - i\alpha c_i^\dagger (\sigma \times \hat{d}_{ij}) c_j + \Delta_{ij} (c_i^\dagger c_j^\dagger + h.c.)
- \mu_0 \sum_i c_i^\dagger c_i - \mu_d \sum_{i \in l, \sigma} c_i^\dagger c_i, \tag{S18}
\]

where the line defect is denoted by the vector \( l \). It is important to note that the mechanism of induced pairing on the line defect discussed in the main text applies to the \( d \)-wave case as well and gives rise to pairing of mixed parity in real space. This is different than the case of a quasi-1D quantum wire proximity coupled to a \( d \)-wave superconductor where the pairing in the quantum wire in real space only has even parity spin-singlet pairing \([10]\). The energy dispersion (Fig. S1a) shows, as before, the incipient Rashba split impurity bands (red line) formed below the bulk bands that cross the Fermi level. Switching on the \( d \)-wave pairing potential in the bulk induces a pairing state of mixed parity along the RALD and realizes a TRI topological superconductor. There are two Kramers pairs of MZMs inside the SC gap (Fig. S1b). The zero-energy LDOS map (Fig. S1c) shows that the MZMs are well localized at both ends of the embedded line defects, where the LDOS spectrum displays a zero-energy conductance peak (Fig. S1d).

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