Symmetry reduction and boundary modes for Fe chains on an s-wave superconductor

Yu-Qin Chen 1,2, Yi-Ming Wu 1,2 and Xiong-Jun Liu 1,2

1 International Center for Quantum Materials and School of Physics, Peking University, Beijing 100871, People’s Republic of China
2 Collaborative Innovation Center of Quantum Matter, Beijing 100871, People’s Republic of China

E-mail: xiongjunliu@pku.edu.cn

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Abstract
We investigate the superconducting phases and boundary modes for a quasi-1D system formed by up to three Fe chains on an s-wave superconductor, motivated by a recent experiment. While the Rashba type spin–orbit coupling together with a magnetic ordering is necessary to drive the system to be of nontrivial topology, we show that the onsite $I \cdot \sigma$ spin–orbit term, inter-chain diagonal hopping couplings, and magnetic disorders in the Fe chains are crucial in determining the symmetry classes of superconducting phases, which can be topologically trivial or nontrivial in different parameter regimes. In general multiple low-energy Andreev bound states, as well as a single Majorana zero mode if the phase is topological, are obtained in the ends of Fe chains. The nontrivial symmetry reduction mechanism is uncovered to provide an understanding of the present results, and may explain the zero-bias peak observed in the experiment. The present study can be applied to generic multiple-chain system.

Keywords: topological superconductor, Majorana fermion, symmetry protected topological phase, spin–orbit coupling

(Some figures may appear in colour only in the online journal)

1. Introduction

The recent Princeton experimental realization of superconducting Fe chains with ferromagnetic ordering opened a new branch of research in searching for Majorana zero modes [1], which are non-Abelian quasiparticles [2–4] and have potential applications to fault-tolerant topological quantum computation [5–9]. Majorana zero mode exists in the vortex core of a two-dimensional (2D) $p + ip$-wave topological superconductor (SC) [10], and at the end of a 1D $p$-wave SC [11]. Theoretical proposals showed that topological SC can be obtained with heterostructures formed by conventional $s$-wave SC and topological insulators [12] or semiconductors with a Zeeman splitting [13–18]. Motivated by these proposals, suggestive signatures of MZMs have been detected in experiments using semiconducting nanowires/s-wave SC heterostructures [23–25] by measuring the zero-bias peak in the differential tunneling conductance spectra [19–22], while alternative theoretical interpretations are also available for such observed zero-bias peak [26, 27].

The recent Princeton experiment with Fe chains is motivated by, but different from, the earlier proposals of realizing 1D topological SC by adatoms with helical spin configurations on an $s$-wave SC [28]. It was interpreted in theory that such Fe chains may exhibit topological superconductivity since the Zeeman splitting, $s$-wave SC order, and Rashba spin–orbit interaction can be induced through the couplings between Fe atoms and SC substrate [1, 29]. In the experiment a spatially resolved zero-bias peak is observed in the end area of Fe chains by scanning tunneling microscopy (STM) [1]. On the other hand, the valence electrons of Fe atoms occupy the $d$-orbital states, which may lead to complicated phase diagram and boundary modes, including the Majorana zero modes and Andreev bound modes, for a three-chain system as considered in the experiment. It is interesting to ask the question: what generic underlying mechanism governs the phase diagram and boundary modes, and the energy spectra of the boundary modes?

In this work, we show the generic underlying mechanism for the superconducting phases and boundary modes in three Fe chains placed on an (Pb) $s$-wave SC (figures 1(a)–(c)). The onsite
\[ H_{\text{triple}} = -\mu_p \sum_\alpha \sum_\tau c_{\alpha \tau}^\dagger(r)c_{\alpha \tau}(r) \]

\[ + \sum_{\alpha \alpha', j, \sigma} \sum_{r, r'} t_{\alpha \alpha'}^{(j)}(r, r') c_{\alpha \sigma}(r)c_{\alpha' \sigma}(r') + \text{h.c.} \]

\[ + \sum_{\alpha, \alpha', \sigma, \sigma'} c_{\alpha \sigma}(r)J_{\alpha \sigma} c_{\alpha' \sigma}(r) \]

\[ + i \lambda_{\text{soa}} \sum_{\alpha, \alpha', r, \sigma, \sigma'} c_{\alpha \sigma}(r)\tilde{c}_{\alpha' \sigma}(r) + \text{h.c.} \]

\[ + i \xi_R \sum_{\alpha, \alpha', r, \sigma, \sigma'} c_{\alpha \sigma}(r)\tilde{c}_{\alpha' \sigma}(r + a\hat{z}) + \text{h.c.} \]

\[ + \sum_{\alpha, \tau} |\Delta_\tau(r)| c_{\alpha \tau}(r)c_{\alpha \tau}(r) + \text{h.c.}, \]

where \( c_{\alpha \tau} (c_{\alpha \tau}^\dagger) \) is the annihilation (creation) operator for the \( d \)-orbital electron—with \( \alpha = \uparrow, \downarrow \) labeling the five orbital and spin states—\( \mu_p \) is the chemical potential, \( J \) is the Stoner-theory spin splitting energy with magnetization along the \( y \) direction, \( \lambda_{\text{soa}} \) is the onsite spin–orbit coefficient, \( t_R \) is the Rashba spin–orbit coefficient, and \( \Delta_\tau \) is the proximity induced \( s \)-wave SC order in the Fe chains. The coefficients \( t_{\alpha \alpha'}^{(j)}(r, r') \) represent the nearest-neighbor (for \( j = 1 \)), next-nearest-neighbor or diagonal (for \( j = 2 \)), and next-next-nearest-neighbor (for \( j = 3 \)) hopping couplings in the Slater–Koster approximation (figure 1(b)). The magnitudes of the parameters are adopted from the density function theory (DFT) calculation in [1], with \( t_{\alpha \alpha'}^{(1)}(r, r') = -0.1445 \) eV, \( t_{\alpha \alpha'}^{(2)}(r, r') = 0.5760 \) eV, and \( t_{\alpha \alpha'}^{(3)}(r, r') = -0.6702 \) eV. The spin splitting \( J = 2.7 \) eV is the largest energy scale in the above formula, which leads to the spin polarized bands in the Fermi energy. We note that the quantitative details of the parameters, including the magnitude of the spin-splitting \( J \), the superconducting order \( \Delta_\tau \), and the hopping parameters, do not affect the main results, which are governed by symmetries. The cases with different sets of parameter regimes will be considered. In the presence of the Rashba spin–orbit interaction induced by the interface hybridization between Fe \( d \)-orbital and Pb \( p \)-orbital states, the proximity induced \( s \)-wave SC might be driven into an effective \( p \)-wave topological SC, which can support Majorana zero modes at the Fe-chain ends [15–17].
3. Single Fe-chain case

Let us first consider the simplest situation with a single Fe Chain, which might be relevant for the experimental study at Basel [31]. This is equivalent to studying the Hamiltonian (1) without inter-chain couplings. Taking the lattice constant to be unit (a = 1), we get the single chain Hamiltonian $H_{\text{single}}(\lambda_{so}, k) = (2V_1 \cos k_z + 2V_2 \cos 3k_z - \mu_F)\sigma_z + 2t_0 \sin k_x k_y - J/2s x + \Delta s y \tau_y + \lambda_{so} \bar{J} \cdot \bar{s} \tau_z$, where $\sigma$ and $\tau$ represent Pauli matrices acting on the Nambu and real spin spaces respectively. $V_1$ and $V_2$ are matrices corresponding to hopping terms $t_0^{(1)}$ and $t_0^{(3)}$ respectively, given in tables 1 and 2 according to the Slater–Koster approximation [1, 48].

A key feature of the present system is that the symmetry class of the Hamiltonian depends on the onsite $\bar{J} \cdot \bar{s}$ term. In the absence of this onsite spin–orbit term, i.e. if $\lambda_{so} = 0$, we find that the Hamiltonian respects both a pseudo time-reversal (TR) symmetry $\Theta$ and charge conjugation symmetry $\mathcal{C}$ defined via $\Theta H_{\text{single}}(\lambda_{so} = 0, k)\Theta^{-1} = H_{\text{single}}(\lambda_{so} = 0, -k)$, and $\mathcal{C} H_{\text{single}}(\lambda_{so} = 0, k)\mathcal{C}^{-1} = -H_{\text{single}}(\lambda_{so} = 0, -k)$, with

$$\Theta = K x \tau_z, \quad \mathcal{C} = \tau_x, \quad \Theta^2 = \mathcal{C}^2 = 1. \quad (2)$$

Here $K$ is the complex conjugate. The above result implies that $H_{\text{single}}(\lambda_{so} = 0, k)$ belongs to the BDI symmetry class according to the ten-fold topological classification [32–38], which can protect integer number of Majorana zero modes at each end, i.e. those Majorana zero modes would not couple to each other forming regular Fermions [39–46] (see figure 2(a)). Note that the symmetries $\Theta, \mathcal{C}$ do not transform orbital states, implying that each orbital band at the Fermi energy contributes one Majorana zero mode. Thus the multiple Majorana zero modes correspond to the multiple orbital subbands crossing the Fermi energy.

Once the $\bar{J} \cdot \bar{s}$ term is switched on, the pseudo TR symmetry $\Theta$ defined in equation (2) is broken. The onsite spin–orbit term $H_{so} = \lambda_{so} \bar{J} \cdot \bar{s} \tau_z$ takes the following form

$$H_{so} = \frac{1}{2} \lambda_{so},$$

It can be verified that $\Theta H_{so}\Theta^{-1} = H_{so}$ and $\mathcal{C} H_{so}\mathcal{C}^{-1} = -H_{so}$. Thus the pseudo TR symmetry $\Theta$ defined in equation (2) is broken by the onsite $\bar{J} \cdot \bar{s}$ term. Only the charge conjugation symmetry keeps.

The symmetry reduction has an interesting interpretation. Note that the multiple d-orbital states can be equivalently treated as the degree of freedom of a ‘synthetic’ transverse dimension. Then the $\bar{J} \cdot \bar{s}$ and 1D Rashba terms render the spin–orbit couplings in the synthetic and physical dimensions, respectively, giving an effective 2D spin–orbit coupling. Together with the spin splitting J-term, the total Hamiltonian with such effective 2D spin–orbit coupling is complex, and does not commute with the complex conjugate operator, thus breaking the above $\Theta$ symmetry. Only the charge conjugation symmetry remains and the symmetry class of the system is reduced from BDI class to D class, with the topology being classified by a $Z_2$ invariant, calculated by $(-1)^\nu = \text{sgn}[\text{Tr}(H(k_z = 0)\tau_z)\text{Tr}(H(k_z = \pi)\tau_z)]$. The topologically nontrivial (trivial) phase corresponds to $\nu = 1(0)$. From figure 2(b) we can see that while in most of the system the phase is topological, there are small regions which are topologically trivial. In the topological phase, only a single Majorana zero mode is obtained in each end of the chain, with several ABSs coexisting. These ABSs originate from the mixing between Majorana zero modes obtained in figure 2(a) by the $\bar{J} \cdot \bar{s}$ symmetry-breaking term. In the trivial phase, only low-energy ABSs are obtained.

4. Triple Fe-chain case

Now we turn to the three Fe-chain model given in equation (1). We first consider the configuration (a). It will be shown that in this case the diagonal hopping couplings also become crucial in determining the phases. To see this effect clearly, we parameterize the three-chain Bloch Hamiltonian $H_{\text{triple}}(t^{(2)}_{\alpha\alpha^{*}}, k)$ as function of $t^{(2)}_{\alpha\alpha^{*}}$. It is interesting that a new set of TR ($\tilde{\Theta}$) and charge conjugation ($\tilde{\mathcal{C}}$) symmetries are found if $t^{(2)}_{\alpha\alpha^{*}} = 0$, satisfying $\tilde{\Theta} H_{\text{triple}}(t^{(2)}_{\alpha\alpha^{*}} = 0, k)\tilde{\Theta}^{-1} = H_{\text{triple}}(t^{(2)}_{\alpha\alpha^{*}} = 0, -k)$, and $\tilde{\mathcal{C}} H_{\text{triple}}(t^{(2)}_{\alpha\alpha^{*}} = 0, k)\tilde{\mathcal{C}}^{-1} = -H_{\text{triple}}(t^{(2)}_{\alpha\alpha^{*}} = 0, -k)$. Here $\tilde{\mathcal{C}} = \mathcal{C}$, while the pseudo TR symmetry reads...
\[
\hat{\Theta} = UU^T K_x \tau_z, \quad U = \frac{1}{\sqrt{2}} \begin{bmatrix}
1 & 0 & 0 & 0 & -i \\
0 & 1 & 0 & -i & 0 \\
0 & 0 & \sqrt{2} & 0 & 0 \\
0 & 1 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 & 1
\end{bmatrix}.
\]

Here \( U \) is a local unitary matrix acting on the five \( d \)-orbital bases \([d_x, d_y, d_z, d_{x^2-y^2}, d_{x^2+y^2}]\), and one can verify that \( \hat{\Theta}^2 = 1 \).

Thus the Hamiltonian \( H_{\text{triple}}(t_{\alpha\sigma}^{(2)} = 0) \) belongs to a new BDI symmetry class characterized by \( \hat{\Theta} \) and \( \hat{C} \), and can support multiple Majorana zero modes. We note that, since the onsite \( \hat{t} \cdot \vec{s} \) term breaks the pseudo TR symmetry \( \Theta \) as defined in the single-chain model and leads to low-energy ABSs, in general there are both multiple Majorana zero modes and multiple ABSs in the present three-chain system, as shown numerically in figure 3(a). The ABSs are due to the couplings in Majorana zero modes induced by the \( \hat{t} \cdot \vec{s} \) spin-orbit term.

Similar as the result in the single-chain system, the diagonal hopping in configuration (a) (see table 3 [48]) can break the new pseudo TR symmetry by verifying that \( \hat{\Theta} H_{\text{triple}}(t_{\alpha\sigma}^{(2)} = 0) \hat{\Theta}^{-1} \approx H_{\text{triple}}(t_{\alpha\sigma}^{(2)} = 0) \) for \( t_{\alpha\sigma}^{(2)} \neq 0 \).

This implies that the symmetry class is again reduced from the new BDI class to the D class, and the topology is classified by the \( \mathbb{Z}_2 \) invariant. Therefore, the diagonal hopping terms can couple the remaining multiple Majorana zero modes, with only a single Majorana zero mode surviving if the total number of Majorana zero modes is odd for the case without diagonal hopping couplings. Conversely, if the number of Majorana zero modes for \( H_{\text{triple}}(t_{\alpha\sigma}^{(2)} = 0, k_x) \) is even, the diagonal hopping term drives the system into a trivial phase with only low-energy ABSs existing. We plot the phase diagram numerically in figure 3(b). It is clear that both topologically trivial and nontrivial phases are obtained in the large ranges of chemical potential, with each gap closing point separating a topological phase and a trivial phase. Due to the symmetry reduction mechanism, the multiple ABSs are generically obtained in the different parameter regimes. It is worthwhile to note that, while in general the phase diagram and boundary modes shown in figures A2(a) and (b) are complicated, they can be understood with the clear symmetry mechanisms uncovered here.

We emphasize that for the triple-chain case the symmetry-breaking mechanism requires the magnetization to be perpendicular to the Fe-chain stacking direction. This implies that for the second configuration (figure 1(b)), while the onsite spin-orbit term \( \hat{t} \cdot \vec{s} \) can break the first type of \( \Theta \) symmetry, the diagonal hopping term cannot break the second type \( \Theta \) symmetry since the averaging magnetization is parallel to the stacking \( \gamma \) direction. This can be verified by examining the diagonal hopping matrix in this configuration, as shown in table 4 [48]. By a straightforward calculation we find that this diagonal hopping term commutes with \( UU^T \) in the \( \hat{\Theta} \) operator.

To break the \( \Theta \) symmetry, a nonzero magnetization in the out-of-plane \( \sigma \) direction is required. In the realistic system, the symmetry breaking occurs when random magnetic disorder with magnetization \( \delta \hat{J}(\mathbf{r}) = \delta J^x \hat{c}(\mathbf{r}) \) along \( x \) axis is present, which satisfies \( \langle \delta J^x(\mathbf{r}) \rangle = 0 \) giving the disorder Hamiltonian

\[
V_{\text{dis}} = \sum_\mathbf{r} \sum_{\alpha,\sigma,\sigma'} c_{\alpha\sigma}(\mathbf{r}) \delta J^x(\mathbf{r}) s_{\alpha\sigma}(\mathbf{r}) c_{\alpha\sigma'}(\mathbf{r}).
\]

The inclusion of magnetic disorder in the configuration of figure 1(b) leads to the same phase diagram as shown in figure 3(b).

5. Minigap and tunneling spectra

With the existence of multiple ABSs in an end, it is important to determine the minigap, defined as the energy of the lowest ABSs \( E_{\text{mini}} = \min \{E_{\text{ABS}}\} \), of the real system. A sizable minigap...
Table 3. Diagonal hopping couplings for configuration (a) [48].

| \( \sqrt{2} J_l l_j^2 \) (eV) | \( d_{xy} \) | \( d_{xz} \) | \( d_{x^2-y^2} \) |
|-----------------------------|-----------|-----------|-----------------|
| \( d_{xy} \)               | 0.2158    | 0         | 0.3603          |
| \( d_{xz} \)               | 0.1138    | 0.3630    | 0.1971          |
| \( d_{x^2-y^2} \)          | –0.3603   | 0.2158    | –0.0629         |

Note: Here \( \tilde{J} = i + \alpha \tilde{c} + \alpha \tilde{c}' \).

| \( \sqrt{2} J_l l_j^2 \) (eV) | \( d_{sy} \) | \( d_{sz} \) | \( d_{s^2} \) | \( d_{s_d} \) |
|-----------------------------|-----------|-----------|-----------|-----------|
| \( d_{sy} \)               | 0.2158    | 0         | 0         | 0         |
| \( d_{sz} \)               | 0.1138    | 0.3630    | 0         | 0         |
| \( d_{s^2} \)              | –0.3603   | 0.2158    | –0.0629   |           |

Note: Here \( \tilde{J} = i + \alpha \tilde{c} + \alpha \tilde{c}' \),

is necessary to distinguish the topologically nontrivial phase from trivial phases by STM measurement. The eigenvalues of the boundary modes at the end can be calculated from the surface Green’s function through iteration methods [47], with the calculation being performed by transfer matrix method. The iteration will not end until the Majorana and ABS spectra are unchanged when increasing the length of Fe chains, in which case the finite size effect vanishes. For the present 1D system with next-nearest-neighbor hopping couplings, one can separate the Fe chains into many principle segments (PSs) along the \( z \) axis, with each PS containing \( q \geq 2 \) Fe atoms along the chain direction (the total Fe atom number in a PS is then \( 3q \)). For the case with magnetic disorder, one needs to take \( 3q \gg 1 \) so that the disorder averages to zero within each PS: \( \langle \delta J^i(r) \rangle_{PS} = 0 \). Then the Hamiltonian for each PS can be treated as identical. In this way the numerical error can be minimized. The Green’s function of the system is denoted by \( G_{n,n'}^{\alpha \alpha}(\omega) \), where \( n,n' \) are the PS indices and \( I, I' = 1, \ldots , q \) denote the \( q \) atomic layers in each PS. The surface Green’s function corresponds to \( n = n' = I = I' = 0 \), and can be solved through

\[
G_{00}(\omega) = \frac{1}{\omega - i\tilde{\delta}^+ - H_{00} - H_{0}T}.
\]

Here \( I \) is a \( 60q \times 60q \) unit matrix, \( H_{00} \) is the block Hamiltonian of the surface PS, and \( H_{0} \) represents the couplings between the surface PS and the next PS which include the hopping couplings and the Rashba spin–orbit term. The transfer matrix \( T \) is obtained by iteration:

\[
T(\omega) = t_0 + \sum_{n=1}^{N} \prod_{m=0}^{n-1} i\tilde{\delta}_m \Theta_m,
\]

where \( t_0 = (\omega - H_{00})^{-1}H_{01} \), \( \tilde{\Theta}_0 = (\omega - H_{00})^{-1}H_{10} \), \( a_m = (I - \tilde{\Theta}_{m-1})^{-1} \tilde{\Theta}_{m-1} \) with \( a_m = t_m \) or \( \tilde{\Theta}_m; N_c \) is a cut-off. The local density of states are then given by

\[
\rho(\omega; n, I) = \frac{1}{\pi} \text{Im} G_{n,n}^{\alpha \alpha}(\omega), \quad n = I = 0, \quad (7)
\]

which determines the spectra of the boundary modes. With the obtained surface Green’s function one can further calculate the tunneling spectra by considering a metallic tip coupled to the end area of the chains according to the following formalism [49]

\[
I = \frac{e}{\hbar} \int d\omega \text{ReTr} \left\{ [1 - G_{0}^{R} \Gamma^{L}]^{-1} \left[ \tanh \left( \frac{\omega - eV}{2} \right) G_{0}^{R} \Gamma^{L} 
- \tanh \left( \frac{\omega}{2} \right) \right] G_{1}^{A} \right\} \\
[1 - G_{0}^{A} \Gamma^{L}]^{-1} \right\}. \quad (8)
\]

Here \( f(\omega) \) is the Fermi distribution function, \( eV \) is bias, \( G_{0}^{R} \) is the retarded Green’s function numerically given by \( G_{0}^{R}(\omega) \); the advanced Green’s function \( G_{0}^{A}(\omega) = [G_{0}^{R}(\omega)]^*, \) and \( \Gamma^{R(A)} = \Gamma^{R(A)}(\omega - eV) \) represent the tunneling coupling functions which characterize the tunneling energy. For simplicity, one may consider a metallic Fe tip and the tunneling coupling occurs only at the three sites corresponding to \( (n,I) = (0,1) \). In the real calculation one may assume that the tunneling couplings do not change the spin or \( d \)-orbital states. The trace in equation (B.8) is performed in the position, \( d \)-orbital, and spin spaces. The tunneling conductance can be calculated via equation (B.8) numerically.

The numerical results in the experimentally relevant parameter regimes are shown in figure 4, where (a) and (b) show the minigap as functions, respectively, of the ratio \( \eta = 4 \sqrt{2} J_{l l}^{(2)} J_{l l}^{(1)} / J_{l l}^{(1)} \) between the diagonal and nearest-neighbor hopping strengths with fixed \( J_{l l}^{(1)} \), and of the amplitude of the random magnetic disorder \( \delta J_{\max}^{l} \). The physical regime corresponds to \( \eta = 1 \) under the Slater–Koster approximation [48]. The coefficient of the onsite spin–orbit coupling \( I \cdot \sigma \) is fixed with \( \lambda_{c} = 60 \text{ meV} \) [1], which may determine the minigap of the system if \( \eta = \delta J_{\max}^{l} \) is large. Figures 4(a) and (b) show that the minigap in a topologically trivial regime increases with, respectively, the diagonal hopping coupling and disorder strength, but is typically a few \( \mu \text{ eV} \) for \( \eta \sim 1 \) and \( \delta J_{\max}^{l} < 30 \text{ meV} \). The local density of states are shown in figure 4(c), which reflects that no Majorana zero modes but low-energy ABSs exist in the trivial phase. However, from figure 4(d) we can see that when the tunneling energy is over the minigap, the tunneling spectra manifest a zero-bias peak, which brings about challenges to distinguish the topological phase from trivial phase by STM measurement. The more precise measurement is necessary to identify the Majorana zero modes [50].
6. Discussion and conclusion

A couple of issues are worth mentioning. Firstly, the configurations we consider are straight and parallel Fe chains within a single (xz or yz) plane. In the more general case the chains may be staggered or not in-plane due to the complexity of the Fe–Pb interface. A staggered and not-in-plane configuration can generically bring about additional hopping couplings,
which contribute to the symmetry reduction from the second type of BDI class to D class. Moreover, it was shown that the strong coupling between the Fe atoms and the substrate Pb atoms can strongly renormalize the Fermi velocities of the Fe bands [51, 52]. This effect is essentially because the transverse wave functions (penetrating into the substrate SC) of Fe electrons have strong dependence on the momentum \( k_z \) due to the interface couplings, which greatly suppresses the dependence of energies on \( k_z \). Nonetheless, if the interface couplings between Fe and Pb atoms do not break the pseudo TR symmetries \( \Theta \) and \( \tilde{\Theta} \) defined in the present work, the main results predicted here shall not be affected by the renormalization of Fermi velocities. A more detailed study of this effect shall be given in future work. Finally, we note that within the current model, the inclusion of more Fe chains gives results fully similar to the case with three Fe chains. The reason is because the hopping couplings in a system with more Fe chains are similar to those in the one with three chains, and we consider the Rashba type spin–orbit coupling only along a single (\( z \)) direction. On the other hand, for a many-chain system which is indeed a 2D system, and if we consider 2D Rashba spin–orbit coupling, one shall obtain 2D topological SC classified by Chern numbers. In particular, the orbital degree of freedom in such a case may lead to 2D topological SCs with high Chern numbers.

In summary, we have studied the superconducting phases and boundary modes in multiple Fe chains placed on an s-wave SC. We uncovered a nontrivial symmetry reduction mechanism with two different types of BDI classes (characterized by \( Z \) invariant) reduced to D classes (with \( Z_2 \) invariant) by the relevant couplings in Fe chains. From this mechanism one can show that in general multiple low-energy ABSs exist in each end of the system, while a single Majorana zero mode also survives if the phase is topological and separated from the ABSs by a small minigap. Both the Majorana zero modes and low-energy ABSs may contribute to zero bias peak in the tunneling measurements when the tunneling energy is greater than the minigap of the system. Our results on one hand show that the seemingly complicated phase diagram and boundary modes can be understood with clear symmetry reduction mechanisms; on the other hand suggest that more experimental efforts besides the zero-bias peak measurement are necessary and encouraged to confirm the existence of Majorana zero modes.

### Table 5. Nearest-neighbor hopping coupling in \( y' \) direction.

| \( t_{ij}^{(1)} \) (eV) | \( d_{xy} \) | \( d_{xz} \) | \( d_{z^2} \) | \( d_{y^2-x^2} \) |
|---------------------|----------------|----------------|----------------|----------------|
| \( d_{xy} \)        | 0.5760         | 0             | 0             | 0             |
| \( d_{xz} \)        | 0              | −0.1445       | 0             | 0             |
| \( d_{z^2} \)       | 0              | 0             | −0.2759       | 0             |
| \( d_{y^2-x^2} \)   | 0              | 0             | 0             | 0.5760        |

Note: Here \( \vec{j} = \vec{i} + a\vec{e}_y \).

### Table 6. Next-next-nearest-neighbor hopping coupling in \( y' \) direction [48].

| \( 25t_{ij}^{(2)} \) (eV) | \( d_{xy} \) | \( d_{xz} \) | \( d_{z^2} \) | \( d_{y^2-x^2} \) |
|---------------------|----------------|----------------|----------------|----------------|
| \( d_{xy} \)        | 0.5760         | 0             | 0             | 0             |
| \( d_{xz} \)        | 0              | −0.1445       | 0             | 0             |
| \( d_{z^2} \)       | 0              | 0             | −0.2759       | 0             |
| \( d_{y^2-x^2} \)   | 0              | 0             | 0             | 0.5760        |

Note: Here \( \vec{j} = \vec{i} + 2a\vec{e}_y \).

### Appendix A. Phase diagram and boundary modes with different \( J \) values

With the Slater–Koster basis, the Hamiltonian for the triple chain system is given by equation (1) in the main text. The transverse hopping coefficients between neighboring sites and next-next-nearest neighboring sites are shown in tables 5 and 6 respectively. In the main text we study the phase diagram and boundary modes with Stoner-theory spin splitting energy \( J = 2.7 \) eV. Here we present the results with smaller \( J \) couplings. Figure A1 and A2 show the phase diagrams and boundary modes for \( J = 2.0 \) eV and \( J = 1.5 \) eV respectively.

The two figures show that the phase diagrams and boundary modes are similar to those with \( J = 2.7 \) eV, as presented in the main text. The main difference is that with a smaller \( J \), the topological gap is enhanced. This is reasonable, since the strength of the effective \( p \)-wave pairing driven by spin–orbit coupling is larger for a smaller \( J \).

### Appendix B. Calculation of boundary modes

To avoid finite size effects, the eigenvalues of the boundary modes at an end can be calculated with surface Green’s function through iteration methods [47]. In this approach, one can separate the Fe chains into many principle segments (PSs) along the \( z \) axis, with each PS containing \( q \) Fe atoms along the chain direction (the total Fe atom number in a PS is then \( 3q \)). The Green’s function of the system is denoted by \( G_{nm}^{i\prime j\prime}(q) \), where \( n, n' \) are the PS indices and \( i, i' (=1,...,q) \) denote the \( q \) atomic layers in each PS. For the present 1D system with next-next-nearest-neighbor hopping couplings, we take that \( q \geq 2 \), and then the couplings occur only within each PS and between nearest-neighbor PSs. To apply the iteration methods, the whole system should retain the translational symmetry in units of PSs, for which we shall consider the following cases. First, for the case without magnetic disorder, we can take that \( q = 2 \), which allows for a fast iteration process. Secondly, in the case with magnetic disorder, one needs to take \( 3q \gg 1 \) so that the disorder averages to zero within each PS: \( \langle \delta \rho (\vec{r}) \rangle _{PS} = 0 \). Then the Hamiltonian for each PS can still...
be treated as identical. In this way the numerical error can be minimized.

The Green’s function satisfies
\[ \sum_m (\omega + \imath \delta^+ - H_{nm}) G_{nm}(\omega) = \delta_{nm}, \]
(B.1)

Here $I$ is a $60q \times 60q$ unit matrix, and the segment Hamiltonian $H_{nm}$ can be obtained based on the original triple Fe-chain Hamiltonian. According to the above analysis we know that $H_{00} = H_{11} = ...$ and $H_{01} = H_{12} = ...$. From the equation (B.1) we have that
\[ G_{00}(\omega) = \tilde{t}_0 G_{-2,0}(\omega) + \tilde{t}_0 G_{n+2,0}(\omega), \]
(B.2)

where $t_0 = (\omega + i\delta^+ - H_{00})^{-1} H_{01}^{-1}$, $\tilde{t}_0 = (\omega + i\delta^+ - H_{00})^{-1} H_{01}$. Repeating this process one can get
\[ G_{00}(\omega) = t_1 G_{n-2,0}(\omega) + \tilde{t}_1 G_{n+2,0}(\omega), \]
(B.3)

where $t_1$ and $\tilde{t}_1$ can be derived through $t_m = (I - t_{m-1})^{-1} t_m - (I - t_{m-1})^{-1} I_{m-1}$ and $\tilde{t}_m = (I - t_{m-1} - \tilde{t}_{m-1} - \tilde{t}_{m-1})^{-1} t_{m-1}$ respectively. From the above relations we further obtain that
\[ G_{10}(\omega) = \left[ t_0 + \prod_{n=1}^{N-1} t_n \right] G_{00} + \tilde{t}_0 G_{n+1,0} \approx TG_{00}. \]
(B.4)
Here we have chosen a cut-off $N_c$ for the iteration, which is determined by the criterion that $n_1+n_{l+1} < \epsilon$ with $\epsilon$ being a small number. The transfer matrix $T$ reads

$$T(\omega) = t_0 + \sum_{n=1}^{N} \prod_{m=0}^{n-1} t_0 t_m.$$  \hspace{1cm} (B.5)

On the other hand, from equation (B.1) we have $(\omega + i\delta - H_{00})G_{00}(\omega) = I + H_0 G_{10}$. Together with the equation (B.4) we finally reach

$$G_{00}(\omega) = \frac{I}{\omega + i\delta - H_{00} - H_{01} T}.$$  \hspace{1cm} (B.6)

The surface Green’s function corresponds to $n = n' = l = l' = 0$. The local density of states are then obtained by

$$\rho(\omega; n, l) = -\frac{1}{\pi} \text{Im}[G_{n,l}(\omega)], \quad n = l = 0,$$  \hspace{1cm} (B.7)

with which one can determine the spectra of the boundary modes. With the obtained surface Green’s function one can further calculate the tunneling conductance by considering the tunneling coupling between a metallic tip and the end area of the chains according to the following formalism [49]

$$I = \frac{e}{h} \int d\omega 2\text{ReTr}\left\{1 - G_0^R(\omega) \Gamma R(\omega - eV)\right\}^{-1}$$

$$\times \left[\tanh\left(\frac{\omega - eV}{2}\right) G_0^R(\omega) \Gamma A(\omega - eV)$$

$$- \tanh\left(\frac{\omega}{2}\right) G_0^R(\omega) \Gamma A(\omega - eV)$$

$$+ 2(f(\omega - eV) - f(\omega)) G_0^R(\omega) \Gamma A(\omega - eV)\right\}.$$  \hspace{1cm} (B.8)

Here $f(\omega)$ is the Fermi distribution function, $eV$ is bias, $G_0^R$ is the retarded Green’s function and is given in equation (B.1), the advanced Green’s function $G_0^A(\omega) = [G_0^R(\omega)]^*$, and $\Gamma_{RA}$ represent the tunneling coupling functions and characterize the tunneling energy. For simplicity, one may consider a metallic tip and the tunneling coupling occurs only at the three sites corresponding to $(n, l) = (0, 1)$. $\Gamma_{RA}$ take the following forms

$$\Gamma_{RA} = \sum_{n', l'} |n', l'| (n, l; n', l') \int d\omega \frac{N(\omega)}{\omega - \epsilon - i\delta}.$$  \hspace{1cm} (B.9)

where $\Upsilon$ relates to the coupling matrix between the metallic tip and the Fe chains and $N(\epsilon)$ is the density of states in the tip. In the real calculation one may assume that the tunneling couplings do not change the spin or $d$-orbital states. The trace in equation (B.8) is performed in the position, $d$-orbital, and spin spaces. The tunneling conductance can be calculated via equation (B.8) numerically. In figure B1 the minigap versus the diagonal hopping coupling strength is shown with spin splitting energy $J = 2.0$ eV and 1.5 eV.

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Figure B1. Minigap as a function of $\eta$ for the trivial phase (a) with $\lambda_{Qo} = 60$ meV, $J = 2.0$ eV and $\mu = -2.16$ eV. (b) with $\lambda_{Qo} = 60$ meV, $J = 1.5$ eV and $\mu = -1.95$ eV.
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