Higher-Order Topological Lattice Defects in Iron-based Superconductors

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We show that lattice dislocations of topological iron-based superconductors such as FeTe$_{1-x}$Se$_x$, will intrinsically trap non-Abelian Majorana quasiparticles, in the absence of any external magnetic field. Our theory is motivated by the recent experimental observations of normal-state topology and surface magnetism that coexist with superconductivity in FeTe$_{1-x}$Se$_x$, the combination of which naturally evokes an emergent second-order topological superconductivity in a two-dimensional subsystem spanned by screw or edge dislocations. This exemplifies a new embedded higher-order topological phase in class D, where Majorana zero modes appear around the “corners” of a low-dimensional embedded subsystem, instead of those of the full crystal. A nested domain wall theory is developed to understand the origin of these defect Majorana zero modes. When the surface magnetism is absent, we further find that s$\pm$ pairing symmetry itself is capable of inducing a different type of class-DIII embedded higher-order topology with defect-bound Majorana Kramers pairs. We also provide detailed discussions on the real-world material candidates for our proposals, including FeTe$_{1-x}$Se$_x$, LiFeAs, $\beta$-PbBi$_2$ and heterostructures of bismuth, etc. Our work establishes lattice defects as a new venue to achieve high-temperature topological quantum information processing.

I. INTRODUCTION

Crystals of quantum materials are rarely perfect in the real world. While it appears natural to always suppress lattice disorders and pursue crystals of a higher purity, defectiveness in topological quantum materials often binds exotic massless quasiparticles that hold great promise for future electronics. A prototypical example is the famous Jackiw-Rebbi problem [1] and its condensed matter realization in polyacetylene [2], where zero-energy fermion modes are trapped by the domain wall defects of a one-dimensional (1D) dimerized atomic chain. Since then, gapless electronic or Majorana modes have been established in the defects of various topological phases, including weak and crystalline topological insulators (TIs) [3, 4], topological superconductors (TSCs) [5–11], and topological semimetals [12, 13], etc.

While gapless defects usually emerge as a result of bulk-state topologies, exceptions do exist. For example, a partial lattice dislocation can host helical electron modes irrespective of the underlying bulk topological physics, since the 2D stacking fault itself carries a nontrivial $\mathbb{Z}_2$ index. This provides an exemplar of “embedded topology” (ET), that even inside a trivial insulator or superconductor, a geometric subsystem such as lattice defects can carry its own emergent topological physics [14, 15]. Similar to bulk topologies, we expect that ETs can be further divided into finer categories based on their orders of topology [16–20]. Namely, an embedded nth-order topology (dubbed ET$_n$) can be defined by a $(d-n)$-dimensional gapless boundary of a d-dimensional system, which is further embedded in a D-dimensional bulk system with $D > d > n > 0$. However, demonstrations of ET in the literature have been limited to the 1st-order level, and a fundamental open question is whether and how a higher-order version of ET can in principle exists.

Meanwhile, 1D ET of vortex-line defects has been possibly established in the state-of-the-art experiments of topological iron-based superconductors (tFeSCs) such as FeTe$_{1-x}$Se$_x$ [21–23], (Li,Fe)OHFeSe [24], LiFeAs [25–27], etc. Notably, the topology of bulk tFeSCs only lies in their normal states, that a band inversion at Z point generates both a nontrivial $\mathbb{Z}_2$ electronic band topology and an accompanied helical Dirac surface [28]. Below the critical temperature $T_c$, an s-wave-like pairing gap is developed for both bulk and surface states, wiping out all normal-state topological physics around the Fermi energy. Despite the bulk triviality, 1D ET emerges along the field-induced vortex line defects, leading to vortex Majorana zero modes (MZMs) at the surface vortex cores. Interestingly, Majorana-like signals have also been observed in the atomic line defects of a FeTe$_{1-x}$Se$_x$ monolayer, which are likely caused by 1D ET of the line-shaped Se/Te atom vacancies [29–31]. However, it is still unclear whether lattice defects in bulk tFeSCs can evoke similar ET and ET-induced Majorana modes.

The main finding in this work is that screw or edge dislocations of bulk tFeSCs can naturally bind embedded second-order topology (i.e., ET$_2$), offering an unprecedented vortex-free mechanism to realize non-Abelian Majorana quasiparticles. While a screw or an edge dislocation appears one-dimensional, it is attached to a 2D cutting plane $P_c$ that only terminates at either another dislocation or the crystal boundary. It is the same 2D $P_c$ that harbors ET$_2$ in tFeSCs and further traps a sin-
ple MZM to each of its four geometric corners, i.e., the surface dislocation cores.

Our theory is completely based on the recent experimental observations of normal-state topology and intrinsic surface magnetism $\mathbf{M}$ of FeTe$_{1-x}$Se$_x$. Given that $\mathbf{M}$ is found to be around three times greater than the surface superconducting (SC) gap, our recipe for ET$_2$ in tFeSCs turns out to be surprisingly simple: it emerges once the dislocation Burgers vector $\mathbf{b} = (b_x, b_y, b_z)$ satisfies $b_z \equiv 1 \mod 2$. We derive this ET$_2$ condition through a nested domain wall analysis and further confirm the existence of both ET$_2$ and defect MZMs through lattice model simulations. Remarkably, this topological criterion is a natural outcome of a less recognized weak topological index of tFeSCs. Therefore, our recipe is directly applicable to other weak-index carrying topological materials such as $\beta$-Bi$_2$Pd, Bi, BiTe, etc. We also highlight that the above paradigm is independent of the explicit type of SC pairing symmetry. Nonetheless, when surface magnetism is locally absent, $s_\pm$-wave pairing symmetry is capable of inducing a distinct time-reversal-invariant (TRI) ET$_2$ phase in class DIII for dislocations with corner-localized Majorana Kramers pairs (MKPs). We also provide detailed discussions on real-world material candidates and experimental detection of ET$_2$.

II. EMBEDDED HIGHER-ORDER TOPOLOGY

Our focus in this work is dislocation-induced ET$_2$ in a 3D trivial superconducting system. The goal of this section is to identify a simple recipe for enabling ET$_2$ in symmetry class D, which, by definition, will carry unpaired MZMs bound to the corners of the dislocation cutting plane. This recipe, as will become clear in the coming sections, directly leads us to the prediction of defect bound MZMs in tFeSCs.

A. Condition for Class-D ET$_2$

Let us first provide some motivations for our recipe. To trap a 0D bound state in a 3D system, one can start from a 3D gapless quasiparticle (e.g. a massless Dirac fermion) and further constrain its degrees of freedom (d.o.f.) in all three spatial directions. This “dimensional reduction” procedure can be feasibly achieved by decorating the Dirac fermion with a hierarchical set of $\mathbb{Z}_2$ mass domains, with each domain effectively reducing the dimension of gapless state by one. For example, the 2D gapless surface of a 3D TI can be viewed as a domain wall bound state for a 3D massive Dirac fermion, with the TI bulk and the outside vaccum carrying opposite Dirac masses, respectively. A second SC/magnetism domain for the 2D surface Dirac fermion further reduces the gapless d.o.f. to 1D, leading to a 1D chiral Majorana domain-wall mode [32, 33]. To eventually achieve a 0D Majorana mode, it clearly requires a third $\mathbb{Z}_2$ domain.

We find that, under certain circumstances, lattice domains introduced by screw=edge dislocations can serve as mass domains and thus contribute the last piece of the jigsaw puzzle. This approach of understanding ET$_2$ is thus dubbed a nested domain wall construction.

Another key motivation is from the material side. Recent experimental breakthroughs have revealed hidden topological Dirac surface states for several high-Tc iron-based SCs. Among these tFeSC candidates, FeTe$_{1-x}$Se$_x$ is of particular interest to us, as it additionally harbors surface ferromagnetism that coexists with bulk superconductivity below its superconducting $T_c \sim 14.5$ K. Furthermore, screw dislocations for FeTe$_{1-x}$Se$_x$ can be generated in a highly controllable manner during the growth process. Therefore, it is natural to expect FeTe$_{1-x}$Se$_x$ to be a wonderful playground for the class D ET$_2$, and a possible recipe for ET$_2$ will be extremely helpful to diagnose the topological situation here.

We now derive the topological condition for ET$_2$ that is directly applicable to tFeSCs. Our starting point is a 3D TRI TI with bulk isotropic $s$-wave spin-singlet superconductivity. The normal-state topology is indicated by a strong $\mathbb{Z}_2$ topological index $\nu_0$ and a set of weak $\mathbb{Z}_2$ indices $\boldsymbol{\nu} = (\nu_1, \nu_2, \nu_3)$ [34]. In particular, $\nu_0 = 0$ ($\nu_0 = 1$) dictates an even (odd) number of Dirac surface states, while the values of weak indices $\nu_{1,2,3}$ decide the momentum-space locations of the surface states. The bulk $s$-wave SC, however, necessarily spoils the normal-state topology by introducing an isotropic SC gap $\delta_{SC}$ to all Dirac surfaces through a “self-proximity” effect. Motivated by FeTe$_{1-x}$Se$_x$, we further introduce surface magnetism $\delta_M$ to both top and bottom (001) surfaces of our TI system. The explicit type of magnetism is flexible as long as it can act as a mass term for Dirac surface state and further competes with the surface SC. Since the side surfaces are magnetism-free, when

$$|\delta_M| > |\delta_{SC}|,$$

a SC/magnetism domain emerges around the edges between top/bottom and side surfaces. This condition thus generates a 1D chiral Majorana mode around both top and bottom surfaces, i.e., a chiral Majorana hinge mode. We emphasize that the chiral Majorana hinge mode here is a result of 2D surface topology alone, that the top and bottom surfaces both feature a BdG Chern number of $|\mathcal{C}| = 1$, as will be discussed in Sec. III B. The 3D bulk topology will not be altered and thus remains trivial throughout the surface magnetism decoration.

Our last ingredient, the lattice dislocations, is intuitively a “gluing fault” when combining two identical copies of our setup. For example, a screw dislocation, as schematically shown in Fig. 1 (a), is formed when the left parts of the two crystals are combined perfectly, while the right parts mismatch with each other by a displacement vector $\mathbf{b}=(0,0,1)$, i.e., the Burgers vector. The cutting plane $P_c$ is highlighted by an orange boundary in Fig. 1 (a).

To explore the fate of chiral Majorana hinge modes
FIG. 1. Nested domain wall theory for class-D ET$_2$. (a) shows a single screw dislocation with a Burgers vector $\mathbf{b} = (0, 0, 1)$ along with other key ingredients for ET$_2$: weak electronic topology, bulk SC, and surface magnetism. In (b), we cut the crystal in halves following the orange cutting plane in (a), which leads to two disjoint magnetism-gapped top surfaces and two SC-gapped side surfaces. Further folding the top surfaces following the trajectory arrows leads to the “bilayer” configurations of Dirac surface states in (c). The competition between magnetism (M) ans SC leads to a pair of counterpropagating 1D Majorana modes once $\delta_M > \delta_{SC}$. In (d), we glue everything together to restore the crystal, and the introduction of a dislocation decorates the intersurface hopping between Dirac particles on the orange cutting plane with a phase factor of $e^{i\pi \mathbf{b} \cdot \mathbf{\nu}}$. This gaps out the Majorana modes in a nontrivial way shown in (e), which can be mapped to a 1D Jackiw-Rebbi domain wall problem and results in a localized Majorana zero mode at the surface dislocation core. We carry out a numerical simulation of a pair of screw dislocatons for FeTe$_{1-x}$Se$_x$ on a $28 \times 28 \times 28$ lattice. Four zero-energy modes are found and their spatial wavefunctions are found to localized around each dislocation core, as shown in (f).

During the gluing process, it is helpful to fold the top surfaces of the two to-be-glued crystals as shown in Fig. 1 (b). Then the previous interfacial problem is now mapped to a 2D bilayer system in the $y$-$z$ plane, with each layer hosting a TI surface state. Distribution of $\delta_M$ and $\delta_{SC}$ are shown in Fig. 3 (c). The domain wall will bind a pair of counterpropagating chiral Majorana modes as denoted by the green and red arrows in Fig. 1 (c). Combining the two crystals is equivalent to introducing an interlayer coupling $t$ for only the bottom parts of the bilayer, i.e., the previous side surfaces, which will also couple the oppositely propagating Majorana modes and gap them out. However, the interlayer mass term for the Majorana fermions will obtain a phase factor $e^{i\pi \mathbf{b} \cdot \mathbf{\nu}}$, following the side Dirac surface states [3]. In the presence of a lattice dislocation, the cutting plane [i.e., orange region in Fig. 1 (c)] features a finite Burgers vector $\mathbf{b}$, while the purple region has a zero Burgers vector because of the perfect lattice matching. Assuming the dislocation at $y = 0$, we have

$$t(y) = \begin{cases} t_0 & y < 0, \\ t_0 e^{i\pi \mathbf{b} \cdot \mathbf{\nu}} & y > 0. \end{cases}$$

(2)

Crucially, when

$$\mathbf{b} \cdot \mathbf{\nu} = 1 \mod 2,$$

(3)

we have $t(y) = t_0 \text{sgn}(y)$. Namely, when Eq. (3) is fulfilled, the chiral Majorana pair at the SC/magnetism domain experiences an additional mass domain due to the dislocation-induced lattice mismatch. This exactly resembles a 1D Jackiw-Rebbi problem and further results in a 0D MZM localized around the defect core, as shown in in Fig. 1 (e), completing the final part of our nested domain wall construction. Similar nested domains will simultaneously show up for the dislocation core at the bottom surface, as well as the other two corners of the cutting plane. This is how both Eq. (1) and Eq. (3) together serves as a sufficient condition for the class-D ET$_2$ phase in superconducting TIs.

B. Boundary of ET$_2$ & Majorana Inflation

As mentioned earlier, a dislocation-induced cutting plane $P_c$ can terminate at either a crystal surface or another dislocation, leading to two seemingly different yet equivalent boundary conditions for ET$_2$. For example,
Finite size gap making the hinge to harbor a another zero mode. Numerically, we find that the defect a zero mode can only be spoiled while interacting with MZM merges with the hinge Majorana modes as shown in enclose a dislocation pair.

In Fig. 2 (a), the chiral Majorana hinge modes always feature a finite-size gap that is inversely proportional to the cylinder radius [35], as shown in Fig. 2 (b). This gap is a manifestation of the anti-periodic boundary condition to a periodic one with a $\pi$-flux insertion. Thus, despite their chiral Majorana dispersions, the hinges do not carry any zero-energy mode when they enclose a dislocation pair.

Because of this finite-size hinge gap, when the defect MZM merges with the hinge Majorana modes as shown in Fig. 2 (c), its zero-energy nature remains. This is because a zero mode can only be spoiled while interacting with another zero mode. Numerically, we find that the defect MZM eventually merges with the 1D chiral hinge mode, making the hinge to harbor a 1D zero-energy mode at $k = 0$, as schematically shown in Fig. 2 (d). Therefore, the corner-localized 0D MZMs of ET$_2$ can be inflated to 1D zero modes by simply changing the terminations of the cutting plane $P_c$.

III. MODEL

In this section, we provide a minimal lattice model for FeTe$_{1-x}$Se$_x$ to demonstrate the above ET$_2$ recipe. Bulk superconductivity and surface ferromagnetism (FM) are also included in our model setup. By analyzing the competition of SC and FM for the Dirac surface states, we map out a surface topological phase diagram to discuss when Eq. (1) will be fulfilled. This can be directly translated to a condition for ET$_2$ to emerge in FeTe$_{1-x}$Se$_x$, which we verify through explicit screw dislocation simulations for our minimal model.

A. Hamiltonian

Our minimal Bogoliubov-de Gennes (BdG) Hamiltonian for FeTe$_{1-x}$Se$_x$ is

$$\mathcal{H}_{\text{BdG}}(k) = \begin{pmatrix} \mathcal{H}_0(k) - \mu & \Delta(k) \\ \Delta^*(k) & -\mathcal{H}_0^*(k) - \mu \end{pmatrix},$$

where the normal-state Hamiltonian $\mathcal{H}_0 = v (\sin k_x \Gamma_1 - \sin k_y \Gamma_2 + \sin k_z \Gamma_3 + m(k) \Gamma_5)$. The $\Gamma$ matrices are $\Gamma_1 = \sigma_x \otimes s_x, \Gamma_2 = \sigma_x \otimes s_y, \Gamma_3 = \sigma_x \otimes s_z, \Gamma_4 = \sigma_y \otimes s_0, \Gamma_5 = \sigma_z \otimes s_0$, where $s_{0, x, y, z}$ and $\sigma_{x, y, z}$ are Pauli matrices for spin and orbital d.o.f., respectively. Here $m(k) = m_0 - m_1 (\cos k_x + \cos k_y) - m_2 \cos k_z$ and $\mu$ is the chemical potential. We choose $v = 1, m_0 = -4, m_1 = -2, m_2 = 1$ to ensure a single topological band inversion at $Z$ [36, 37], leading to $\nu_0 = 0$ and $\nu = (0,0,1)$. This well matches the low-energy topological band ordering of FeTe$_{1-x}$Se$_x$.

To introduce superconductivity, we adopt a spin-singlet extended s-wave pairing for our model, where the pairing matrix $\Delta(k) = [\Delta_0 + \Delta_1 (\cos k_x + \cos k_y)](i\sigma_0 \otimes s_y)$. Here $\Delta_0 (\Delta_1)$ is the on-site (nearest-neighbor) intra-orbital pairing strength.

Finally, following the experimental observations of FeTe$_{1-x}$Se$_x$ in Ref. [38] and [39], we introduce uniform surface ferromagnetism to both top and bottom (001) surfaces in a finite-size slab geometry, with $N_z$ layers stacked along $\hat{z}$ direction. $\mathcal{H}_\text{FM} = f(z)[g_1 \sigma_0 + g_2 \sigma_3] \otimes (\mathbf{s} \cdot \mathbf{M})$ with $f(z) = \delta_{z,1} + \delta_{z, N_z}$ for a lattice layer index $z = 1, 2, ..., N_z$. Here $\delta_{z,i}$ is the Kronecker delta function, $\mathbf{M}$ denotes the surface magnetization, and $g_1 \pm g_2$ are the effective isotropic Landé g-factor for the two orbitals involved in our model. We take $g_1 = 0.5$ and $g_2 = 0.2$ in our numerical simulations throughout this work. More discussions on the experimental aspects of FeTe$_{1-x}$Se$_x$ and other candidate materials, can be found in Sec. V.
Energy $\mu$, $\Delta_0$ to that of $M_z$. Therefore, the effect of a general FM pairing gap from the $M_z$ face state will develop an $M_z$ pairing term from the $M_z$ face Hamiltonian reads,

$$\mathcal{H}_{\text{surf}} = v_F (k_x \tau_x s_y - k_y \tau_0 s_x) - \mu \tau_z s_0 + \Delta_0 \tau_y s_y + \Sigma_y \tau_0 s_y + \Sigma_z \tau_z s_z,$$

where $s$ and $\tau$ represent spin and particle-hole degree of freedom, respectively. $v_F$ is the surface Fermi velocity. Up to the first-order perturbation approximation, $\Sigma_y \approx g_1 M_y$ and $\Sigma_z \approx g_1 M_z$ are the Zeeman energies [36]. Notably, condition of Eq. (1) is primarily concerned with the gap structures at $\bar{\Gamma}$. We thus find that $E_F = \pm \sqrt{\mu^2 + \Delta_0^2} \pm \sqrt{\Sigma_{y}^2 + \Sigma_{z}^2}$. If we add back $\Sigma_y \approx g_1 M_y$, then the surface gap closing condition is $\mu^2 + \Delta_0^2 = \Sigma^2$ with $\Sigma = (\Sigma_x, \Sigma_y, \Sigma_z)$. It is then easy to check that the ET$_2$ condition of Eq. (1) now becomes

$$|\Sigma| > \sqrt{\mu^2 + \Delta_0^2},$$

which coincides with the condition for the Dirac surface states to carry a BdG Chern number $|c| = 1$. This non-trivial C accounts for the chiral Majorana hinge modes in Fig. 1 (c), a crucial step to complete the nested domain wall configuration for achieving ET$_2$. According to Eq. (3), a pair of screw or edge dislocations featuring an odd $b_z$ will span a 2D cutting plane with class D ET$_2$. Given the existence of such dislocations, Eq. (6) now serves as the ET$_2$ condition for FeTe$_{1-x}$Se$_x$.

On the other hand, a large in-plane $M_z$ is capable of inducing partial Fermi surface (PFS) in a superconducting TI [40, 41]. As shown in Fig. 3 (c) and (d), PFS occurs when some surface quasi-particle bands cross zero energy to form metal-like band patterns. While the formation of PFS is irrelevant to our target ET$_2$ physics, however, it can coexist with ET$_2$ and thus contributes an important part of our surface phase diagram. As an intuitive example, we consider $M = (0, M_y, 0)$ and find the dispersion of $\mathcal{H}_\text{surf}$ at $k_y = 0$ is $E_{\alpha\beta}(k_x) = \alpha \Sigma_y + \beta \sqrt{(v_F k_x - \alpha \mu)^2 + \Delta_0^2}$ with $\alpha, \beta = \pm 1$. For $\alpha \beta < 0$, $E_{\alpha\beta}$ has two zero-energy solutions at $k_x = k_x^{(\pm)}$ with

$$k_x^{(\pm)} = \frac{1}{v_F} (\alpha \mu \pm \sqrt{\Sigma_y^2 - \Delta_0^2}).$$

Therefore, when $|\Sigma_y| \geq |\Delta_0|$, $E_{++} = 0$ and $E_{--} = 0$ lead to four $k_x$ solutions that form two sets of partial Fermi surfaces. Thanks to the rotation symmetry of Dirac surface Hamiltonian, we expect this PFS condition to be generalized to

$$|\Sigma| \geq |\Delta_0| \quad \text{for} \quad M_z = 0,$$

where $\Sigma = g_1 M_y$. Combining Eq. (6) with Eq. (8), we conclude that with $|M_z| \ll M_y$, increasing $M_z$ will always first drive the formation of PFS ($M_y \approx |\Delta_0|$) before ET$_2$ phase is achieved ($M_y = \sqrt{\Delta_0^2 + \mu^2}$).

The above analytical results are in excellent agreement with our numerical surface topological phase diagram in Fig. 3 (a). This $M_y$-$M_z$ phase diagram is essentially an

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**FIG. 3.** Surface topological phase diagrams as a function of $(M_y, M_z)$ and $(M_z, \mu)$ are shown in (a) and (b). The darker the blue color is, the larger the surface energy gap is. The region colored in white has no energy gap, and could indicate the existence of either a surface topological phase transition or a partial Fermi surface (PFS). Note that ET$_2$ and PFS can coexist. (c) shows the surface spectrum of a PFS along $k_x$ with $(M_y, M_z) = (0.5, 0.05)$. An example of surface spectrum with coexisting ET$_2$ and PFS is shown in (d) with $(M_y, M_z) = (0.9, 0.05)$.

**B. Surface Topological Phase Diagram: Condition of ET$_2$ & Partial Fermi Surface**

The first step to realize class-D ET$_2$ is to identify the concrete condition to achieve Eq. (1) for our system by studying the competition between magnetism and superconductivity on the (001) surfaces. Note that the (001) Dirac surface state is localized around $\bar{\Gamma}$, the center of the surface Brillouin zone (BZ). As a result, the surface state will develop an isotropic pairing gap from the self-proximity effect [37], irrespective of the $s_\pm$ nature of $\Delta(k)$. In fact, the $s_\pm$ pairing will only play a role for ET$_2$ when the surface magnetism is absent (i.e., for symmetry class DIII), which will be discussed in Sec. IV. For the purpose of FeTe$_{1-x}$Se$_x$ and its class D ET$_2$ physics, we can simplify the pairing term to an on-site $s$-wave type by setting $\Delta_0 = 0$.

We further remark that the surface Dirac fermion has a continuous rotation symmetry around the z-axis in the low-energy limit. Therefore, the effect of a general FM configuration $M = (M_x, M_y, M_z)$ is always equivalent to that of $M' = (0, M_z, M_y)$ up to a coordinate transformation, where $M_z = \sqrt{M_x^2 + M_y^2}$. Without loss of generality, we thus consider $M = (0, M_y, M_z)$, and the

\[
H_{\text{surf}} = v_F (k_x \tau_x s_y - k_y \tau_0 s_x) - \mu \tau_z s_0 + \Delta_0 \tau_y s_y + \Sigma_y \tau_0 s_y + \Sigma_z \tau_z s_z,
\]

where $s$ and $\tau$ represent spin and particle-hole degree of freedom, respectively. $v_F$ is the surface Fermi velocity. Up to the first-order perturbation approximation, $\Sigma_y \approx g_1 M_y$ and $\Sigma_z \approx g_1 M_z$ are the Zeeman energies [36]. Notably, condition of Eq. (1) is primarily concerned with the gap structures at $\bar{\Gamma}$. We thus find that $E_F = \pm \sqrt{\mu^2 + \Delta_0^2} \pm \sqrt{\Sigma_y^2 + \Sigma_z^2}$. If we add back $\Sigma_y \approx g_1 M_y$, then the surface gap closing condition is $\mu^2 + \Delta_0^2 = \Sigma^2$ with $\Sigma = (\Sigma_x, \Sigma_y, \Sigma_z)$. It is then easy to check that the ET$_2$ condition of Eq. (1) now becomes

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which coincides with the condition for the Dirac surface states to carry a BdG Chern number $|c| = 1$. This non-trivial C accounts for the chiral Majorana hinge modes in Fig. 1 (c), a crucial step to complete the nested domain wall configuration for achieving ET$_2$. According to Eq. (3), a pair of screw or edge dislocations featuring an odd $b_z$ will span a 2D cutting plane with class D ET$_2$. Given the existence of such dislocations, Eq. (6) now serves as the ET$_2$ condition for FeTe$_{1-x}$Se$_x$.

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\[
k_x^{(\pm)} = \frac{1}{v_F} (\alpha \mu \pm \sqrt{\Sigma_y^2 - \Delta_0^2}).
\]

Therefore, when $|\Sigma_y| \geq |\Delta_0|$, $E_{++} = 0$ and $E_{--} = 0$ lead to four $k_x$ solutions that form two sets of partial Fermi surfaces. Thanks to the rotation symmetry of Dirac surface Hamiltonian, we expect this PFS condition to be generalized to

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The above analytical results are in excellent agreement with our numerical surface topological phase diagram in Fig. 3 (a). This $M_y$-$M_z$ phase diagram is essentially an
energy-gap mapping of surface BdG spectrum for Eq. (4) in a thick slab geometry along $\hat{z}$ direction, where we take $\mu = \Delta_0 = 0.2$. The color in this logarithmic plot is a measure of the energy gap of the lowest BdG band, and in particular, regions colored in white feature a vanishing BdG gap, i.e., either a topological phase transition or a PFS phase. Clearly, our analytical condition of ET$_2$ (black dashed line) in Eq. (6) matches perfectly with the numerical finding in Fig. 3 (a). In addition, Eq. (8) predicts a critical $M_z^{\text{crit}} = \Sigma_L^{(c)}/g_L = \Delta_0/g_L = 0.4$, also agreeing with numerically-mapped boundary of PFS phase at $M_z = 0$. As shown in Fig. 3 (a), PFS survives until $M_z$ reaches a critical value of $\sim 0.4$, and it is generally absent when $M_z > M_||$. Importantly, PFS coexists with ET$_2$ most of the time in the phase diagram. So we expect that in a large $M_||$ system, observation of PFS will serve as a promising indicator for ET$_2$ in the system.

In Fig. 3 (b), we further study the effect of chemical potential $\mu$ on the formation of ET$_2$. For a small $\mu$, the topological phase boundary separating ET$_2$ and trivial phase is well captured by the dashed guideline predicted by Eq. (6). Notably, the phase boundary undergoes a sudden turn at $\mu \sim 0.7$ and starts to deviate from the analytical results. This is because the bulk-band physics is getting more involved as $\mu$ grows, and thus our effective surface theory is no longer expected to faithfully describe the phase boundary of ET$_2$.

C. Defect Majorana Zero Modes

To confirm the ET$_2$ phase, we consider to place our minimal model for FeTe$_{1-x}$Se$_x$ on a $28 \times 28 \times 28$ lattice. Periodic boundary conditions are considered for both $x$ and $y$ directions of the lattice cube to eliminate possible unwanted hinge modes in our simulations. Out-of-plane FM are considered for both the top and bottom layers of the lattice cube, following $H_{FM}$. We further decorate our lattice system with a pair of screw dislocations with a Burgers vector $b = (0,0,1)$. The dislocation pair spans a 2D cutting plane $P_c$ that is parallel to the $y-z$ plane. In principle, one can consider a pair of edge dislocations instead, as along as their Burgers vectors satisfy

$$b_z \equiv 1 \mod 2. \quad (9)$$

As the FM is gradually turned on, the (001) surface gaps close and reopen in our cubic geometry following Fig. 3 (a), after which four zero-energy modes show up in the energy spectrum. In Fig. 1 (f), we visualize the spatial distribution of the zero-mode wavefunctions in the cubic geometry and find each of the four surface dislocation cores is trapping one of the zero modes. These dislocation-bound Majorana zero modes are exactly the defining boundary signature of ET$_2$ in our system.

IV. $s_{\pm}$-WAVE PAIRING & CLASS DIII ET$_2$

For tFeSC candidates such as FeTe$_{1-x}$Se$_x$ and LiFeAs, the bulk $s_{\pm}$ pairing as described by $\Delta(k)$ is supported by experimental observations [42–44]. In particular, $\Delta_1 \neq 0$ is crucial for enabling a relative $\pi$-phase difference for the local superconductivity orders of the $\Gamma$ and $M$ pockets. As we have discussed, in the above ET$_2$ recipe, it is the competition between SC and FM, rather than the explicit SC pairing type, that is crucial for enabling the Majorana dislocation bound states. In this section, we show that $s_{\pm}$ pairing is indeed important for achieving a new class of time-reversal-invariant ET$_2$ in symmetry class DIII, but only when the surface FM is absent.

Our new recipe for class DIII ET$_2$ is motivated by the deep connection between hinge Majorana modes and ET$_2$, as revealed in the nested domain wall picture. Even in the absence of surface FM, a bulk $s_{\pm}$ pairing itself is capable of inducing a pairing mass domain for Dirac fermions living on the top (bottom) and side surfaces. As a result, the inter-surface hinge will harbor a pair of 1D helical Majorana modes that respect time-reversal symmetry [37]. As shown in Fig. 4, we can now follow a “cut and glue” procedure to reveal the dislocation physics. Similar to the steps we carried out in Sec. II, cutting the crystal now yields two pairs of helical Majorana modes trapped to the top hinges of the two smaller crystals [as:}

![Figure 4](image-url)

FIG. 4. Time-reversal-invariant ET$_2$ phase driven by an extended $s$-wave pairing with $(\Delta_0, \Delta_1) = (-0.85, 0.5)$. (a) and (b) illustrate a nested domain wall construction similar to that in Fig. 1. Two pairs of helical Majorana modes now show up, the gluing of which leads to a Kramers pair of Majorana bound states at each dislocation core. (c) shows the energy spectrum of a $36 \times 36 \times 20$ lattice with a pair of dislocation lines with eight Majorana zero modes. By plotting the spatial wavefunction distribution of these Majorana modes in (d), we numerically confirm that each dislocation core binds one Majorana Kramers pair.
shown in Fig. 4 (a) and (b)], as well as another two pairs bound to the bottom hinges. When gluing the crystal back together, a dislocation will introduce a z-phase domain to the inter-hinge binding term following Eq. (2), which will now trap a Kramers pair of Majorana zero modes around each of the surface dislocation core.

We now provide a lattice simulation to verify the existence of class DIII ET2 with our minimal model of FeTe1−xSex in Eq. 4. We adopt the same model parameters of Fig. 1 (f), with no surface FM assumed and an additional update of $\Delta_0 = -0.85$ and $\Delta_1 = 0.5$ to emphasize the effect of $s_\pm$ pairing. Note that the $s_\pm$ condition for tFeSCs with $\Delta(\Gamma)\Delta(M) < 0$ is generally achieved when $|\Delta_0| < 2|\Delta_1|$. The energy spectrum for the system is calculated for a $36 \times 36 \times 20$ lattice geometry, with a pair of screw dislocations placed in the $y$-$z$ plane. As shown in Fig. 4 (c), eight Majorana modes (orange circles) show up in the energy spectrum that are well separated from other higher-energy states. The small energy splitting for the Majorana modes is due to the finite-size effect of the cubic geometry. By plotting the Majorana wavefunctions in the real space, we find in Fig. 4 (d) that each surface dislocation core now harbors a pair of Majorana modes, which unambiguously demonstrates the existence of class DIII ET2 trapped by the lattice dislocations.

V. MATERIAL CANDIDATES

In this section, we will discuss material candidates that can harbor ET2 physics in both class D and class DIII. We will focus on the tFeSCs, especially FeTe1−xSex and LiFeAs, and further discuss their experimental relevance. However, ET2 is not a privilege of tFeSCs and can in principle exist in other superconducting systems as well. We will discuss $\beta$-PdBi2 as such an example.

A. FeTe1−xSex

As highlighted in Sec. II and Sec. III, FeTe1−xSex naturally combines all necessary ingredients of our class D ET2 recipe and manifests itself as perhaps the most promising platform for defect MZMs. Thanks to the recent extensive experimental studies on both the normal-state topology and high-temperature superconductivity of FeTe1−xSex [28, 45, 46], we are capable of discussing its ET2 possibility in a quantitative manner.

Evidence of surface magnetism in FeTe1−xSex has been experimentally established by a variety of measurement approaches. For example, an angle-resolved photoemission spectroscopy (ARPES) study in Ref. [38] reveals a direct surface gap of $\sim 8$ meV exactly at the surface Dirac point, in additional to the surface SC gap at the Fermi level. The spoiling of the Kramers degeneracy of Dirac surface state happens even above the superconducting transition temperature $T_c$, directly implying the breaking of time-reversal symmetry. Even though other more complex scenarios such as time-reversal-broken superconductivity is in principle possible [47, 48], a most straightforward interpretation of this magnetic gap would be the development of out-of-plane FM order on the surface. Similar evidence of surface FM has also been detected by the nanoscale quantum sensing of magnetic flux by nitrogen vacancy (NV) centers [39], where the magnetization is reported to feature an in-plane component as well.

Earlier experimental studies [45] further reveals a surface superconducting order of $\Delta_0 \sim 2$ meV and a chemical potential of $\mu \sim 4.4$ meV, in addition to $\Sigma_\pm \sim 4$ meV. Considering the condition in Eq. (6), ET2 phase can be achieved with either (i) a slight electron doping to reduce $\mu$, or (ii) an enhancement of surface FM. Notably, engineering surface FM could be more experimentally accessible. For example, neutron scattering measurements have revealed that a single interstitial Fe impurity can induce magnetic Friedel-like oscillation involving $> 50$ neighboring Fe sites [49]. As a result, an interstitial Fe impurity on the surface is capable of generating a local magnetic patch with $\Sigma_\pm \sim 10$ meV [50], which is large enough to enable ET2. Although interstitial Fe impurities could naturally exist during sample growth, they can also be deposited to the sample surface as adatoms [51]. This provides us a highly controlled approach to enhance surface FM of general tFeSCs.

Remarkably, for FeTe1−xSex films epitaxially grown with pulsed laser deposition (PLD), formation of screw dislocations can be feasibly controlled by simply tuning the deposition rate [52]. In particular, samples grown at a low deposition rate generally feature spiral-like surface morphology that encodes a screw dislocation with a Burgers vector of $b = (0, 0, 1)$. This thus contributes the last key ingredient for materializing dislocation-bound MZMs in FeTe1−xSex at zero magnetic field.

B. Other Fe-based Superconductors

Besides FeTe1−xSex, evidences of Dirac surface states and vortex Majorana modes have also been found in other tFeSCs such as LiFeAs [25–27] and (Li,Fe)OHFeSe [24]. We first note that the topological band physics in (Li,Fe)OHFeSe is mainly attributed to the band inversion at $\Gamma$, thus leaving the system with zero weak indices. We therefore do not expect (Li,Fe)OHFeSe to carry ET2 physics proposed in this work. A similar conclusion could be reached for CaKFe1A2S4, whose

| Probe          | Mag. Type | Orientation | Surf. Gap |
|---------------|-----------|-------------|-----------|
| ARPES         | FM        | 2           | $\sim 8$ meV |
| NV Center     | FM        | 2           | N/A       |

TABLE I. Summary of experiments on the surface magnetism in FeTe1−xSex with ARPES [38, 53] and NV center [39].
normal-state band inversion also happens at $\Gamma$ due to a band folding effect [54].

The band structure of LiFeAs resembles that of FeTe$_{1-x}$Se$_x$ and features a weak-index vector $\nu = (0, 0, 1)$. While we are not aware of any surface magnetism for LiFeAs, evidence of $s_\pm$ pairing has been reported in earlier ARPES measurements [55]. This would make LiFeAs a good platform to host class DIII ET$_2$ and the associated defect Majorana Kramers pairs.

### C. $\beta$-PdBi$_2$, Bismuth, and Beyond

Just like FeTe$_{1-x}$Se$_x$, $\beta$-PdBi$_2$ [56] features both a single band inversion at $Z$ and intrinsic SC with a transition temperature of $T_c = 5.3$ K. By evaporating Cr atoms on Bi-terminated surface of $\beta$-PdBi$_2$, scanning tunneling microscopy (STM) technique can organize Cr atoms into a magnetic lattice that competes with SC on the surface [57]. In particular, both FM and anti-FM can be achieved by simply adjusting the lattice constant of the Cr adatoms. Therefore, we expect our ET$_2$ results on FeTe$_{1-x}$Se$_x$ to be directly applicable to $\beta$-PdBi$_2$ as well.

ET$_2$ can also be achieved in an extrinsic manner by assembling all the necessary elements together in a heterostructure. For example, candidates of weak-topological insulators carrying $Z_2$ indices $(\nu_0, \nu_1, \nu_2, \nu_3) = (0, 0, 0, 1)$ have been experimentally established in a plethora of Bi-related materials, including BiTe [58], Bi$_2$Te$_3$ [59], Bi$_3$I$_4$ [60], and ZrTe$_5$ [61] etc. While these candidates are non-superconducting, one can design an ABC “trilayer” structure by growing a thin film of the above weak TIs on some superconducting substrates and further deposit another ferromagnetic layer on top. When a lattice screw dislocation with $b = (0, 0, 1)$ occurs, the defect MZM should appear when Eq. (1) is satisfied.

We further note that a similar structure has been successfully fabricated for Bi(111) grown on a Nb(110) substrate, of which a ferromagnetic Fe cluster is placed on top [62]. Notably, the topological nature of Bi is disputable because of the tiny energy gap at $L$ point, and Bi is believed to be either a higher-order topological insulator with trivial $Z_2$ indices, or a strong topological insulator with $(\nu_0, \nu_1, \nu_2, \nu_3) = (1, 1, 1, 1)$. Interestingly, the latter scenario is recently supported by the observation of helical electron modes bound to a screw dislocation via an STM study [63]. These experimental progresses have together established Bi as another promising platform for defect MZMs.

### VI. EXPERIMENTAL DETECTION

Signatures of ET$_2$ for above material candidates can be feasibly revealed by mapping out the local density of states (LDOS) around lattice dislocations in experiments with the state-of-the-art STM technique. In this section, we numerically simulate the LDOS signals of dislocation-trapped MZMs for our minimal Hamiltonian in Eq. 4 using the iterative Green function method [64]. The geometry we considered involves an in-plane $20 \times 40$ lattice with a pair of screw dislocations embedded in the $y$-$z$ plane, sitting symmetrically around the $z$-axis at $(x, y) = (10, 20)$. The spatial distance of the dislocations is denoted as $\delta r_d$. After sufficient iteration steps, the LDOS on the top (001) surface is $D(r, E) = -\frac{1}{4}\text{Im}[G_{\text{surf}}(r, E)]$, where $G_{\text{surf}}(r, E)$ is the surface Green function. This simulated LDOS signal can be directly compared with ultra-low-temperature STM data in future experiments.

When $\delta r_d$ is much greater than the Majorana localization length $l_{\text{MZM}} \sim 3$, the hybridization between neighboring defect MZMs is negligible, as shown in Fig. 5 (a). We then expect each dislocation to carry a sharp LDOS peak at the zero bias, as numerically confirmed in Fig. 5 (b). Moving away from the dislocation core, the peak intensity gradually drops to zero without any further splitting, implying the existence of a single zero-energy mode. Meanwhile, we carry out a similar simulation with $\delta r_d \sim O(l_{\text{MZM}})$, where the defect MZMs hybridize strongly [Fig. 5 (c)]. We similarly check the LDOS data near the bottom dislocation core and find the absence of any zero-bias peak in Fig. 5 (d). Instead, a double-peak structure emerges, indicating the annihilation of the dislocation MZMs. As for FeTe$_{1-x}$Se$_x$, we expect $l_{\text{MZM}}$ to be of the order of the superconducting coherence length $\xi_{\text{SC}} \sim 5$ nm, similar to that of vortex MZMs [22]. This sets a crucial length scale for $\delta r_d$, that only when $\delta r_d \gg \xi_{\text{SC}}$ will a clear experimental Majorana signal be expected.

We now remark on several phenomenological distinctions between defect and vortex MZMs. First, a quantum vortex always traps Caroli-de Gennes-Matricon (CdGM) states inside the SC gap, which can introduce Majorana-like signals near the zero energy and further complicates interpretations of experimental data. As for ET$_2$, however, we do expect the dislocation core to carry fewer or even no subgap states besides the defect MZMs, as shown in our numerical simulations. This “cleanliness” of Majorana signal of ET$_2$ can significantly enhance the unambiguity of future experiments on relevant topics. In addition, while a vortex Majorana wavefunction is usually circular symmetric [8], our defect MZM found to be

| Materials        | Scing Tc | $Z_2$ Index | Bound State |
|------------------|----------|-------------|-------------|
| FeTe$_{0.55}$Se$_{0.45}$ | 14.5 K   | (1;0,0,1)   | MZM         |
| LiFeAs           | 17 K     | (1;0,0,1)   | MKP         |
| (Li, Fe)OHFeSe   | 41 K     | (1;0,0,0)   | N/A         |
| $\beta$-PdBi$_2$ | 5.3 K    | (1;0,0,1)   | MZM         |

TABLE II. Candidate materials for ET$_2$ phases. Candidates with a defect MZM/MKP can realize an ET$_2$ of class D/DIII. (Li,Fe)OHFeSe is not expected to carry any ET$_2$ physics.
anisotropic, since the screw dislocations explicitly break in-plane mirror symmetries of the lattice. This feature is clearly revealed in the surface LDOS plot of Fig. 5 (a), which should be accessible via STM measurements.

Because of the known inhomogeneity of FeTe$_{1-x}$Se$_x$ samples, it is likely that local magnetic and non-magnetic patches, instead of a uniform FM order, will appear on a real-world sample surface [53]. Nonetheless, our prediction of defect MZM still holds once the dislocation core overlaps with the FM patch, which can be feasibly assembled by moving Fe adatoms. We further notice that applying a $\hat{z}$-directional magnetic field can facilitates the creation of ET$_2$ phase by enhancing the magnetic gap, at the price of introducing additional SC vortex physics. While our defect MZM is immune to an applied magnetic field, Ref. [50] predicts that the field-induced SC vortices living inside the magnetic patch do not harbor any vortex MZMs, and are thus dubbed “empty vortices”. With such an external magnetic field, we thus expect the defect MZM to contribute the only zero-bias peak signal to a STM scanning inside a local FM patch, and it will be further surrounded by a set of “satellite” empty vortices with no MZM signal. This unique phenomenon, if being observed, will serve as a rather compelling experimental evidence for ET$_2$.

VII. CONCLUSIONS AND DISCUSSIONS

To summarize, we introduce the concept of embedded higher-order topology and provide two concrete recipes for its realization in real-world materials. Even in topologically trivial s-wave superconductors, ET$_2$ offers unprecedented opportunity to rethink the role of lattice defects and further exploit them to trap non-Abelian Majorana zero modes. Topological Fe-based superconductors, in particular FeTe$_{1-x}$Se$_x$, are found to be an ideal venue to realize ET$_2$, while other weak-index-carrying material systems such as $\beta$-PdBi$_2$ are also promising candidates for our recipes. Given that remarkable capabilities of manipulating both the screw dislocations and surface magnetism have been reported in the literature of FeTe$_{1-x}$Se$_x$, we believe that our theoretical proposal of ET$_2$ will soon be experimentally realizable.

We further note that the ET$_2$ uncovered in this work is “extrinsic”, in the sense that the defect MZMs cannot be characterized by a 2D “bulk” topological invariant of the defect cutting plane. An interesting future direction to explore is the possibility of crystalline-symmetry-protected “intrinsic” ET$_2$. While a screw dislocation necessarily breaks the majority types of lattice symmetries, edge dislocations or even partial dislocations are probably better geometric subsystems to consider for this purpose [65]. Meanwhile, a generalization of ET$_2$ to non-superconducting systems should also be straightforward, and we do expect an ET$_2$ phase in class AII or BDI to carry fractional-charge-carrying zero modes that are stabilized by chiral symmetry.

Finally, motivated by the recent theoretical proposal of boundary-obstructed topological phases [66, 67], we conjecture the existence of defect-obstructed topological phase (DOTP) as a new class of topological matter. Namely, two phases that are both bulk and boundary topological equivalent can be defect obstructed, if the subsystem energy gap of a lattice or order-parameter defect must close while connecting the two phases. For example, the vortex topological phase transition of a doped s-wave superconducting TI described in Ref. [11] could separate...
two phases that are defect (i.e., vortex) obstructed. Both phases, living before and after the vortex transition, are bulk topologically trivial. However, a topological vortex phase does feature a different 1D BdG Wannier orbital configuration from that of a trivial phase, a feature that is revealed only when a 1D vortex line is inserted in the bulk system. The DOTP is clearly deeply connected to the embedded (higher-order) topological physics. We believe that a description of DOTP based on the topological quantum chemistry language is necessary to advance our understanding of subsystem topologies and possibly lead us to a novel simple mathematical diagnostic approach for both ET and ET$_2$. We will leave this interesting direction to future works.

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