Inversion-protected Higher Order Topological Superconductivity in Monolayer WTe$_2$

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Monolayer WTe$_2$, a centrosymmetric transition metal dichalcogenide, has recently been established as a quantum spin Hall insulator and found superconducting upon gating. Here we show that generally a superconducting inversion-symmetric quantum spin Hall material whose normal state is "effectively gapped", such as gated monolayer WTe$_2$, can be an inversion-protected topological crystalline superconductor featuring possible "higher-order topology" if the superconductivity is parity-odd. Instead of edge states, we explicitly show how zero-dimensional boundary modes can emerge in such type of superconductor within a two-dimensional minimal model. We then study the pairing symmetry of superconducting WTe$_2$ with a microscopic model at mean-field level, and find two types of exotic pairings. First is a time-reversal symmetric odd-parity pairing favored by nearest-neighbor attractions. We numerically show that this self-consistently obtained paired state possesses a nontrivial bulk symmetry indicator, and hosts two Majorana Kramers pairs localizing at opposite corners. Even when on-site attractions dominate and favor the conventional pairing, we find that an intermediate in-plane field exceeding the Pauli limit stabilizes an unconventional equal-spin pairing aligning with the field. Our findings suggest gated monolayer WTe$_2$ is a playground for exotic odd-parity superconductivity, and possibly the first material realization for inversion-protected Majorana corner modes without utilizing proximity effect.

I. INTRODUCTION

Extensive experimental and theoretical effort has been devoted to transition metal dichalcogenides (TMD), a family of materials with chemical formula MX$_2$ (M = transition metal, X = S, Se, Te) known to host a rich variety of intriguing ground states, such as topological insulators and semimetals$^{1-6}$, charge density waves$^{7-13}$, and various types of possibly unconventional superconductivity$^{13-21}$. Moreover, tuning among these phases is possible by widely accessible experimental knobs, for example changing the thickness, pressure$^{10,22-25}$, electrostatic gating$^{13,16,26}$, and recently even the twist angle between monolayers$^{27,28}$. Recently, a centrosymmetric member of the TMD family, monolayer WTe$_2$, has been established$^{1-4,29,30}$ as a quantum spin Hall (QSH) insulator$^{31,32}$. Remarkably, in this same material, superconductivity at temperatures around 1 K was soon after reported under tunable electrostatic gating$^{20,21}$. We are thus motivated to understand the nature of this superconductivity given the prevailing expectation that inducing superconductivity in already topological materials is a promising route for achieving topological superconductors.

Theoretically a known necessary condition for two-dimensional (2D) time-reversal-invariant topological superconductors requires negative pairing order parameters on an odd number of Fermi surfaces that enclose the high symmetry points$^{33,34}$. The presence of the inversion symmetry, however, enforces two-fold degeneracy of the Fermi surfaces and thus sets up a "no-go" theorem to preclude this material from being topologically superconducting. Nonetheless, recent developments suggest that inversion symmetry can unexpectedly enrich the topological structure of a system$^{35-37}$, and enable new topological crystalline superconductors (TCsc) that are completely beyond the paradigm set by Ref. 33 and 34.

In particular, there exists a type of inversion-protected TCsc in dimension $d$ that has no protected Majorana boundary modes in $d-1$ dimension, yet is still topologically distinct from a trivial superconductor$^{36,37}$. Although the bulk-boundary correspondence has not been proven, this suggests the possibility that such inversion-protected TCsc belongs to the so-called "higher order topological phases"$^{38-48}$, and may host Majorana boundary modes in $d-2$ or lower dimension.

Here, we point out that the recipe for this exotic inversion-protected TCsc is surprisingly simple: (1) the normal state is an inversion-symmetric QSH material with Fermi pockets away from time-reversal invariant momenta (TRIMs), and (2) the superconductivity is parity-odd. Furthermore, we explicitly demonstrate how "higher-order" boundary modes can naturally emerge within a minimal model we build for such a TCsc in 2D. Given that gated monolayer WTe$_2$ readily satisfies criteria (1), unconventional superconductivity with odd parity becomes the last piece of the puzzle for an inversion-protected TCsc that could host exotic Majorana corner modes.

In fact, in WTe$_2$ there is ample reason to suspect that electron correlations might be strong, and odd-parity superconductivity is therefore plausible. First is the fact that the superconductivity reported in Refs. 20 and 21 apparently occurs at a low carrier density, while ab initio calculations do not reproduce the low-energy normal state band structure found by angle-resolved photoemission (ARPES) and scanning tunnelling microscopy (STM) studies unless one goes beyond the generalized-gradient approximation$^{12,49}$. Moreover, the reported in-plane upper critical field $H_c^2$ is few times higher than...
the Pauli limit $H_p^{\text{207, 21}}$. While an $H_p^{2}$ higher than the Bardeen-Cooper-Schrieffer theory prediction in centrosymmetric materials can occur when the normal state has a high spin-orbit scattering rate\(^{50}\) or when the g factor deviates from two\(^{21}\), another plausible origin is a spin-triplet (and thus odd-parity) paired state with spin aligning in the field direction.

In this work, we investigate the pairing symmetry and topological nature of the newly discovered two-dimensional superconductivity in gated monolayer WTe\(_2\), and propose this material to be a candidate for an inversion-protected higher-order topological superconductor. In section II, we investigate the the pairing symmetry in this material at mean-field level to obtain a phase diagram for various microscopic interactions. In section III, we first present a general recipe for an inversion-protected topological crystalline superconductor, and analytically show how higher-order boundary modes can emerge in such superconductor within a minimal model construction. We then numerically show that a self-consistently obtained odd-parity paired state in monolayer WTe\(_2\), which fulfills our recipe, indeed carries the expected $Z_2$ bulk indicator for such topological superconductor and hosts Majorana corner modes in a sample with open boundaries. In section IV, we study how symmetries of different paired states in the phase diagram change with an increasing in-plane magnetic field. Surprisingly, we find that while an intermediate field exceeding $H_p$ destroys even-parity pairings as expected, it stabilizes an equal-spin pairing aligning with the field. Finally in section V, we discuss about the robustness and possible experimental detections for the Majorana corner modes in WTe\(_2\), and also the difference between our minimal model for higher-order superconductor and the microscopic model for WTe\(_2\). To our knowledge, our material candidate provides the first realistic proposal of an inversion-symmetry-protected topological state in two dimension.

II. PAIRING SYMMETRY IN MONOLAYER WTe\(_2\)

A. The model

Monolayer WTe\(_2\) is stable in the $1T'$ structure, which is a buckled honeycomb lattice that is distorted into a rectangular lattice consisting of in-plane and buckled zigzag chains of W and Te atoms, respectively, see Fig. 1(a). This lattice is nonsymmorphic, with a two-fold screw rotation symmetry $C_{2\pi}$ and a glide mirror symmetry $M_x$ each with a half-unit-cell translation along the chain direction $\hat{x}$. The lattice also has inversion symmetry $\mathcal{I}_0$, which results from the product of the two symmetries.

To study the dominant pairing channels in gated monolayer WTe\(_2\), we start from a minimal tight-binding model previously obtained by other authors from a low-energy fit to \textit{ab initio} band structure calculations\(^{52,53}\). The Hamiltonian is written in a basis of spin $s$ and four Wannier orbitals described by a sublattice $\sigma = A, B$ and whether they transform as $d_{x^2-y^2}$ or $p_z$ orbitals ($l = d, p$), deriving from W and Te atoms respectively. Each degree of freedom is described by the corresponding Pauli matrices, $\hat{s}, \hat{\sigma}$, and $\hat{l}$, respectively.

The full normal state Hamiltonian is

$$H_0(k) = \delta_0 \otimes \left( \hat{h}_0(k) - \mu \right) + V_{soc}\hat{s}_z\hat{\sigma}_z\hat{l}_y.$$  \hspace{1cm} (1)

The $s_z$-preserving intrinsic spin-orbit coupling $V_{soc}$ is the lowest order term in $k$ that obeys time-reversal, screw rotation, and glide mirror symmetries, while the spin-degenerate part $\hat{h}_0(k)$ is a $4 \times 4$ matrix in the basis of $\hat{s} \otimes \hat{l}$,

$$\hat{h}_0(k) = \begin{pmatrix}
\varepsilon_d(k) & 0 & t^{AB}_d g_k & t^{AB}_p f_k \\
0 & \varepsilon_p(k) & -t^{AB}_d f_k & t^{AB}_p g_k \\
t^{AB}_d g_k & -t^{AB}_d f_k & \varepsilon_d(k) & 0 \\
t^{AB}_p g_k & t^{AB}_p f_k & 0 & \varepsilon_p(k)
\end{pmatrix}$$ \hspace{1cm} (2)

The momentum dependence is contained in the functions $\varepsilon_l(k) = \mu_l + 2t_l \cos(k_x) + 2t'_l \cos(2k_x)$, $f_k = 1 - e^{-ik_x}$, $g_k = (1 + e^{-ik_x})e^{ik_y}$. Finally, we continue to follow Ref. 53 in fixing the tight-binding parameters (in eV units) as: $\mu_d = 0.4935, \mu_p = -1.3265, t_d = -0.28, t'_d = 0.075, t_p = 0.93, t'_p = 0.075, t^{AB}_0 = 1.02, t^{AB}_d = 0.52, t^{AB}_p = 0.40, V_{soc} = 0.115$.

As a zeroth-order approximation to the gating effects, we set the overall chemical potential $\mu = 0.5$. The resulting Fermi surface consists of two electron pockets

![Fig. 1. Schematics for (a) the top view of the lattice of $1T'$-WTe\(_2\), and (b) the microscopic interactions considered in Eq. 3. In (a), the filled orange circles represent the W atoms, which locate on the $z = 0$ plane. The filled and hollow blue circles (grey triangles) represent the Te atoms above and below the $z = 0$ plane, which are (are not) associated with the Wannier orbital centers in the low-energy tight-binding description. The grey rectangle indicates a unit cell with lattice constants $a_x$ ($a_y$) in the $\hat{x}$ ($\hat{y}$) direction, the horizontal and vertical black lines show the screw rotation axis and the glide mirror plane respectively, and the black cross marks the inversion center. In (b), we omit the Te atoms (grey triangles) that do not contribute to the Wannier orbitals.](image)
centered along the Γ – X line [see Fig. 2 (a)], as observed by ARPES\textsuperscript{2}. We note that the spectrum of $H_0$ is at least two-fold degenerate for all $k$ since $H_0$ preserves time-reversal and inversion symmetries.

We add short-ranged density-density interactions that preserve the lattice symmetries up to nearest-neighbor unit cells [see Fig. 1(b)]:

$$H_{\text{int}} = \sum_{rr'} \sum_{\alpha' \sigma \beta'} \Gamma_{\alpha' \beta', \alpha \beta}(r, r') c_{r \sigma l}^\dagger c_{r' \beta l}^\dagger \left( V_{l l'}^{\dagger} [n_{B l}(r + \delta_l) + n_{B l}(r + \bar{x} + \delta_l)] n_{A l}(r) \right) + \text{H.c.}$$

where $l$ and indices are summed over, $n_{\sigma l}(r)$ is the electron density at $r$, and $n_{\sigma l}(r) = \sum_{\sigma} n_{\sigma l}(r)$. Here $V_{l l'}$ denotes the on-site interactions for orbital $l$, and $V_{l l'}^{\dagger} (V_{l l'}^\dagger)$ denotes the nearest-neighbor (next nearest-neighbor) interactions on the zigzag chains with intra- or inter-orbital characters for $l = l$ and $l' = l$, respectively. For simplicity, in the following we consider the case where $U_{l l'} = U$, $V_{l l'}^{\dagger} = V_{l l'} = V$.

| $\eta_{C_{xx}}$ | $\eta_{M_z}$ | Examples |
|----------------|-------------|----------|
| $A_g$ | $+$ | $+$ | $k_0 \otimes \sigma_0 \otimes l_0$ |
| $B_g$ | $-$ | $-$ | $k_0 \otimes \sigma_x \otimes l_z$ |
| $A_u$ | $+$ | $+$ | $k_x \tilde{s}_x \otimes \sigma_0 \otimes l_z$ |
| $B_u$ | $-$ | $-$ | $k_x \tilde{s}_x \otimes \sigma_0 \otimes l_z$ |

TABLE I. The parities of the irreducible representations under the $I\bar{T}$' lattice symmetry operations. The action of the symmetries on crystal momentum and internal indices and the used Nambu basis are shown in the text.

To analyze the dominant pairing channel for given interactions $U$ and $V$, we first classify the symmetries of possible pairing gaps. The normal state preserves two nonsymmorphic symmetries $C_{2x} = e^{i k_x a_x/2} (-i \tilde{s}_x \otimes \sigma_x \otimes l_0)$, $k_y \rightarrow -k_y$, and $M_x = e^{i k_x a_x/2} (-i \tilde{s}_x \otimes \sigma_0 \otimes l_z)$, $k_x \rightarrow k_x$. The mean-field Bogoliubov-de Gennes Hamiltonian

$$H_{\text{BdG}}^{\text{BdG}} = \left( \begin{array}{cc} H_0(k) & \Delta(k) \\ \Delta^\dagger(k) & -T^\dagger H_0^\dagger(k)T \end{array} \right)$$

therefore obeys $g_k^{\text{BdG}} H_{\text{BdG}}^{\text{BdG}} (g_k^{\text{BdG}})^\dagger = H_k^{\text{BdG}}$, where $T = i s_y K$, $k \rightarrow -k$ is the time-reversal operation with $K$

the complex conjugation, and $g_k^{\text{BdG}} = \text{diag} [g_k, \eta_\eta g_k]$ describes how the two symmetries $g = C_{2z}, M_z$ act on the Nambu basis $[c_{k\uparrow}, c_{k\downarrow}, c_{k\uparrow}^\dagger, c_{k\downarrow}^\dagger]$. Thus, the pairing gaps transform as $g_k \Delta_k g_k^\dagger = \eta_\eta \Delta_k$, and we can classify all possible pairing gaps into four irreducible representations $A_g$, $B_g$, $A_u$, and $B_u$ according to their parities $\eta_\eta = \pm 1$ under the symmetry transformations $g$, see Table I.

Next, we determine which irreducible representation has the highest $T_c$ by solving the linearized gap equation\textsuperscript{54}

$$\Delta_{\alpha' \beta'}(k') = - \sum_{k'' k} \Gamma_{\alpha' \beta', \alpha \beta}(k', k') \times \chi_{\beta' \alpha', \alpha \beta}(k'', k, T) \Delta_{\alpha \beta}(k)$$

where Greek indices contain all the internal indices $(s, \sigma, l)$, and repeated indices are summed over. Here, the interaction $\Gamma_{\alpha' \beta', \alpha \beta}(k', k)$ is the Fourier transform of $\Gamma_{\alpha' \beta', \alpha \beta}(r, r')$ in Eq. (3), and $\chi_{\beta' \alpha', \alpha \beta}(k'', k, T)$ is the non-interacting static pairing susceptibility at temperature $T$. Solving Eq. (5) amounts to solving the eigenvalue problem of the effective interaction projected onto the Fermi surface

$$\tilde{\Gamma}(p', p) = -\sqrt{P_p} \Gamma(p', p) \sqrt{P_p}$$

where $P_p$ is the incoming (outgoing) momentum on the Fermi surface, and $P_p = (\sum_{n=1,2} p \cdot n) p \cdot n$ projects an electron-pair state to the two degenerate non-interacting bands $n$ on the Fermi surface at momenta $p$ and $-p$. The eigenvector $\psi(p)$ of $\tilde{\Gamma}$ with the most negative eigenvalue $\lambda$ is the solution to the gap equation Eq. (4) with the highest $T_c \propto \exp(-1/|\lambda|)$. We can then determine how $\psi(p)$ behaves under symmetries $C_{2x}$ and $M_z$ under different interactions and obtain the superconducting phase diagram of $H = H_0 + H_{\text{int}}$.

C. Phase diagram

In Fig. 2(b) we present this phase diagram as a function of $U$ and $V$. We find that while the on-site attraction favors the “trivial” representation $A_g$ with even parity under inversion as expected, the odd-parity representations $A_u$ and $B_u$ dominate over a large portion of the phase diagram where the attractive $V$ is the dominant pairing interaction. In particular, the degenerate $A_u$ and $B_u$ gaps at repulsive $U$ are equal-spin triplet in the out-of-plane $(\uparrow \uparrow \mp \downarrow \downarrow)$, and the $B_u$ gap at attractive $U$ has $s_z = 0 (\downarrow \downarrow \mp \downarrow \downarrow)$. This $SU(2)$ symmetry breaking is due to the intrinsic spin-orbit coupling $V_{\text{soc}}$.

To better understand the real-space structure of the pairing gap deep in each superconducting phase, we write down the mean-field Hamiltonian in Eq. (4) in real space and solve the self-consistency equations $\Delta_{\beta' \alpha'}(r, r') = -\sum_{\alpha \beta} \Gamma_{\alpha' \beta', \alpha \beta}(r, r') \langle c_{r' \beta} c_{r \alpha} \rangle$ by iteration. We consider the short-ranged attractions given in Eq. (3). We find the
FIG. 2. (a) The Fermi surface of $H_0$ with chemical potential $\mu = 0.5$, which consists of two pockets located at $k = \pm k_F, 0$ with $k_F \sim 1.2$. (b) Phase diagram obtained from solving the linearized gap equation. The two blue stars mark the representative points at which we study the field dependence in Fig. 5. The real space configurations of the dominant components in the self-consistent solutions with (c) $A_g$ and (d) $B_u$ symmetries. $\Delta_i \equiv |\Delta_{\nu,\nu'}(r, r')|$ for the bond with the $i$th largest gap magnitude. $\Delta_{1/2}$ in (c) denotes the magnitude for on-site gaps. The calculation for (c) and (d) is done on a system with 12 by 12 unit cells.

The dominant component in the $A_g$ gap to be the on-site pairings as expected, while the subdominant component is the spin-singlet nearest-neighbor pairing along the zigzag chains involving the $d$ orbitals, see Fig. 2(c). In contrast, the dominant contribution to the spin-triplet gap $B_u$ comes from the next-nearest-neighbor $d$-orbital pairing along the chains in the $\hat{x}$ direction, whereas the subdominant component is the staggered nearest-neighbor mixed-orbital pairing in the $\hat{y}$ direction, see Fig. 2(d).

Given the understanding about the real space configurations, we now attempt to understand the phase diagram in Fig. 2(a) within a simplified “two-patch” scheme, where we ignore the intra-pocket momentum-dependence and consider effectively two points located at $k = \pm k_F, 0$ instead of two pockets. Such simplification works well in small-pocket limit, and is similar in spirit to the Eliashberg formalism, where the momentum-dependence is assumed to be uniform within a pocket. Here we consider only the interactions responsible for the most dominant components in the self-consistency solutions with $A_g$ and $B_u$ symmetries [see the bonds with $\Delta_1$ in Fig. 2(b) and (c)], i.e. $U^d$ and $V^{dd}_2$ terms in Eq. (3).

Such interaction has a simple momentum dependence of $V(q) = U + V \cos(q_x)$, where we set $U^d = U$, $V^{dd}_2 = V$, and $q$ the momentum transfer. Thus the interaction matrix $\Gamma$ in Eq. (5) can be simplified into a $2 \times 2$ matrix in the basis of incoming and outgoing momenta running over $k'(\pm k_F, 0)$:

$$\Gamma = \begin{pmatrix} V(0) & V(2k_F) \\ V(-2k_F) & V(0) \end{pmatrix}. \quad (7)$$

The two eigenvalues $V(0) \pm V(2k_F)$ correspond to the parity-even and odd eigenvectors $(1, 1)$ and $(1, -1)$ respectively, and the eigenvector with the more negative eigenvalue corresponds to the dominant pairing gap. Evidently, repulsive $V$ forbids the parity-odd $A_u/B_u$ whereas repulsive $U$ forbids the parity-even $A_g$, given that $\cos(2k_F) < 0$. This is true for a wide range of $k_F$ values, including that from the model in Eq. (1). As for the cases where $U$ and $V$ are both attractive, the balance between $A_g$ and $B_u$ is tilted by the sign of the interaction with large momentum transfer $V(2k_F)$. To be precise, when the $2k_F$ component contributed by $V$ dominates over the momentum-independent $U$ ($V(2k_F) = U + V \cos(2k_F) > 0$), the odd-parity $B_u$ is favored over the even-parity $A_g$.

III. INVERSION-PROTECTED HIGHER-ORDER TOPOLOGICAL SUPERCONDUCTIVITY

In this section, we will show that this energetically favored odd-parity $B_u$ pairing, together with the normal-state WTe$_2$ being an inversion-symmetric QSH material, fulfill the recipe for building an inversion-protected TCsc with possible higher-order boundary modes. In subsection A, we will show how we arrive at the recipe for inversion-protected TCsc. Then in subsection B, to understand the link between such TCsc and higher-order topology, we will show analytically how zero-dimensional Majorana boundary modes emerge within an effective model for inversion-protected TCsc. Finally in subsection C, we will come back to the superconducting WTe$_2$ with $B_u$ pairing. Specifically, we will show that it is indeed such type of TCsc by calculating the corresponding symmetry indicator, and that it hosts two Majorana corner modes on opposite corners.

A. Recipe for a 2D inversion-protected TCsc

We conjecture a 2D inversion-protected TCsc in the presence of time-reversal symmetry by a $Z_4$ symmetry indicator

$$\kappa = \frac{1}{4} \sum_{k \in \text{TRIM}} \sum_n \xi_{kn} \mod 4 \quad (8)$$

inspired by indicators proposed for 3D systems$^{35,37}$, where $\xi_{k,n}$ are the parity eigenvalues of the occupied bands at the TRIMs $k$.$^{55}$ Application of this formula to superconductors requires extending the "normal" inversion operator $I_0$ to Nambu space. For odd-parity superconductors, which are defined by superconducting
pairing that satisfies $I_0 \Delta_k I_0^{-1} = -\Delta_{-k}$, the operator $I = \text{diag}(I_0, -I_0)$ defines the inversion symmetry for the BdG Hamiltonian. As for even-parity superconductors, the inversion operator for the BdG Hamiltonian has no minus sign, and the resulting $\kappa$ is always $0$.

For superconductors in the weak-coupling limit, the symmetry indicator $\kappa$ is related to the corresponding indicator $\kappa_N$ for the normal states as

$$\kappa = 2\kappa_N. \quad (9)$$

In turn, the normal state symmetry indicator $\kappa_N$ for inversion symmetry can be related to the normal state $Z_2$ index $\nu_N$ for time-reversal symmetry by

$$\nu_N = \kappa_N \mod 2 \quad (10)$$

for insulators, or for effectively gapped “topological metals” [see Supplementary Information A]. In this context, we define an effectively gapped “topological metal” to be a metal that is gapped at TRIMs allowing the definition of the indicator $\kappa_N$, and has the same number of filled bands at all TRIMs. This is expected to be the generic situation from doping or gating of a topological insulator as long as the Fermi surface does not circle a TRIM. Typically, such a doping would interfere with topological properties of the material such as transport. However, this can be avoided by introducing a gap at the Fermi surface through weak superconductivity, which cannot change the topological index defined at the TRIMs where the states are away from the Fermi energy.

Here we point out that these two relations in Eq. 9 and 10 among the topological invariants of the superconducting and normal states can be used to design inversion-protected TCsc. In particular, doping an inversion-symmetric quantum spin Hall insulator, assuming all band minima are away from TRIMs, will give rise to a topological metal with $\nu_N = 1$ and $\kappa_N = 1$ or $3$. When further gapped by weak odd-parity superconductivity, such a topological metal will become an inversion-protected TCsc with $\kappa = 2$, and hence our recipe.

Such a $\kappa = 2$ inversion-protected TCsc is particularly interesting. This is because while the $\kappa = 2$ state is topologically distinct from the $\kappa = 0$ state, both of these $\kappa'$s are even and therefore correspond to vanishing $Z_2$ index $\nu$ and the absence of Majorana edge modes. Nonetheless, the fact that $\kappa \neq 0$ suggests the possibility of some other type of protected boundary Majorana modes, and hence the possibility of higher order topological superconductors.

### B. Bulk-boundary correspondence

Whether a $\kappa = 2$ inversion-protected TCsc in 2D is bound to be a higher order topological superconductor, however, has not been rigorously proven to the best of our knowledge. Thus to gain more understanding about this bulk-boundary correspondence, in this subsection we will first present a minimal model for a $\kappa = 2$ TCsc in 2D, which can be tuned across phase boundaries to $\kappa = 3$ and 4 (trivial) phases. Then within this model, we will show analytically how zero-dimensional Majorana modes arise on the boundary of the $\kappa = 2$ phase when placed against the trivial phase.

#### 1. Minimal model for an inversion-protected TCsc

Our eight-band minimal model $\mathcal{H} = \sum \mathcal{H}(k)$

$$\mathcal{H}(k) = \epsilon_0 \hat{\tau}_z \otimes \hat{s}_0 \otimes \hat{\rho}_0 + [m_0 + m_1 (\cos k_x + \cos k_y)] \hat{\tau}_z \otimes \hat{s}_0 \otimes \hat{\rho}_z + v \sin k_x \hat{\tau}_0 \otimes \hat{s}_z \otimes \hat{\rho}_x + v \sin k_y \hat{\tau}_0 \otimes \hat{s}_0 \otimes \hat{\rho}_y + \Delta \sin k_x \hat{\tau}_z \otimes \hat{s}_z \otimes \hat{\rho}_0 + \Delta \sin k_y \hat{\tau}_y \otimes \hat{s}_0 \otimes \hat{\rho}_z \quad (11)$$

consists of a regularized Bernevig-Hughes-Zhang (BHZ) like model for a QSH state with odd-parity pairing. Here $\hat{\tau}, \hat{s}, \hat{\rho}$ are Pauli matrices for particle and hole, spin $s = \uparrow, \downarrow$, and orbital $\rho = s, p...$. This model $\mathcal{H}$ is invariant under time reversal operation $\Theta = i\sigma_y \mathcal{K}$, $\mathbf{k} \rightarrow -\mathbf{k}$, particle-hole transformation $\mathcal{P} = \hat{\tau}_0 \mathcal{K}$, $\mathbf{k} \rightarrow -\mathbf{k}$, and the inversion operation defined for odd-parity superconductors $I = \hat{\tau}_z \otimes \hat{\rho}_z$, $\mathbf{k} \rightarrow -\mathbf{k}$.

This minimal model exhibits two bulk topological transitions in the parameter space of $\epsilon_0, m_0$, and $m_1$: one is from the inversion symmetry indicator $\kappa = 2$ to $\kappa = 3$, and the other from $\kappa = 3$ to $\kappa = 4$. In particular, we can tune through different phases by tuning $m_1$ at a fixed $m_0$ and $\epsilon_0 \geq 0$ as follows

$$\kappa = 4(0) : \quad -(m_0 - \epsilon_0) < 2m_1 < m_0 - \epsilon_0$$
$$\kappa = 3 : \quad -(m_0 + \epsilon_0) < 2m_1 < -(m_0 - \epsilon_0)$$
$$\kappa = 2 : \quad 2m_1 < -(m_0 + \epsilon_0), \quad (12)$$

where all band inversions occur at $\Gamma$. Taking the topologically trivial $\kappa = 4$ phase as the reference point, the spectrum first undergoes a single band inversion to enter the $\kappa = 3$ phase, then follows another band inversion to enter the $\kappa = 2$ phase.

#### 2. Edge modes in a three-domain geometry

To understand what kind of boundary modes a $\kappa = 2$ phase can host when placed against a trivial phase, we first study the edge modes in a geometry of concentric rings with three domains along the radial direction $r$: $\kappa = 2$ phase for $r < R_a$, $\kappa = 3$ phase for $R_a < r < R_b$, and $\kappa = 4$ phase for $r > R_b$ [see Fig. 3 (a)]. Since $\kappa$ is defined modulo 4, the phase $\kappa = 4 \equiv 0$ on the outside is the trivial phase. Given that all band inversions in $\mathcal{H}$ happen at $\Gamma$, it is more convenient to realize this geometry by working with the $k \cdot p$ model $\mathcal{H}_T(k)$ around $\Gamma$ written in the polar coordinate $(r, \theta)$. We focus on the $v \ll \Delta$
helical edge modes per domain wall [see Supplementary Information B]:

\[ \psi^{s/1}_{23}(r, \theta) = e^{-\frac{1}{2}i|r-R_a|} e^{i\theta} \begin{pmatrix} e^{\mp i\frac{\pi}{2}} & 0 \\ \pm i e^{\pm i\frac{\pi}{4}} & 0 \end{pmatrix}, \]  

(15)

and

\[ \psi^{s/1}_{34}(r, \theta) = e^{-\frac{1}{2}i|r-R_b|} e^{i\theta} \begin{pmatrix} 0 \\ e^{\pm i\frac{\pi}{2}} & 0 \end{pmatrix}, \]  

(16)

where \( l \) is the orbital angular momentum taking half integers. Given that \( \psi^{s}_{23/34}(r, \theta) \) obeys Majorana condition up to an overall phase and that the spin-up modes \( \psi^{s}_{23/34} \) and spin-down modes \( \psi^{s}_{23/34} \) propagate along the domain walls in opposite directions [see Supplementary Information C], we have arrived at one pair of helical Majorana edge modes per domain wall [see Fig. 3 (a)].

3. Majorana corner modes in a \( \kappa = 2 \) phase

We are now ready to study the boundary modes between a \( \kappa = 2 \) and a \( \kappa = 4 \) phase. In the following we will shrink the \( \kappa = 3 \) domain by bringing \( R_a \to R_b \), and see if there exists any symmetry-allowed perturbation that gaps out the edge modes \( \psi^{s}_{23} \) and \( \psi^{s}_{34} \) at the two domain walls.

We first write down the rotational invariant perturbations \( \mathcal{H}'_{\text{rot}}(r, \theta) \) up to linear order, and project them onto the edge modes from the two domain walls [see Supplementary Information D]. We find that \( \mathcal{H}'_{\text{rot}}(r, \theta) \) only couples edge modes propagating in the same direction, i.e. \( \psi^{s}_{23} \) and \( \psi^{s}_{34} \). The two pairs of helical edge modes therefore remain gapless in the presence of rotational invariant perturbations.

Next we consider the rotational-breaking perturbations. Here we focus on the lowest order terms \( \mathcal{H}' \), which have no spatial dependence. After projecting all the symmetry-allowed terms onto the edge modes \( \psi^{s}_{23}(r, \theta) \) and \( \psi^{s}_{34}(r, \theta) \) we find that there are only two non-vanishing terms that are hermitian and couple components in the edge modes that are counter-propagating

\[ \mathcal{H}'_a = \hat{\tau}_x \otimes \hat{\delta}_x \otimes \hat{\rho}_y \]

\[ \mathcal{H}'_b = \hat{\tau}_y \otimes \hat{\delta}_y \otimes \hat{\rho}_x. \]  

(17)

Both of these terms are pairing terms that are odd under inversion, i.e. \( [\mathcal{H}', I] = 0 \), where \( I \) is the inversion operator for odd-parity superconductors defined earlier. Moreover, their corresponding amplitudes after projection \( \mathcal{H}'_{a,b}(\theta) = \int dr \psi^{s}_{23}(r, \theta) \mathcal{H}'_{a,b} \psi_{34}(r, \theta) \) have an angular dependence of \( \mathcal{H}'_a(\theta) \propto i \sin \theta \) and \( \mathcal{H}'_b(\theta) \propto i \cos \theta \), respectively.
with Bu pairing satisfies the recipe for an inversion-protected topological superconductor is given by the sum of these eigenvalues divided by 4.

C. Higher-order topological superconductivity in WTe$_2$

We now turn back to superconductivity in monolayer WTe$_2$. It is now clear that the superconducting WTe$_2$ with Bu pairing satisfies the recipe for an inversion-protected topological superconductor. To be specific, the ungated WTe$_2$ as a QSH insulator is known to have the $Z_2$ index for a time-reversal topological insulator $\nu_N = 1$. Given the presence of inversion, we study the corresponding $Z_4$ indicator characterizing an inversion-protected topological crystalline insulator and find it to be $\kappa_N = 1$ due to the single band inversion in the Brillouin zone. When lightly gated, we emphasize that WTe$_2$ becomes an ‘effectively gapped topological metal’ since the two Fermi pockets are away from TRIMs. $\kappa_N$ is thus still well-defined and remains 1 for the lightly gated WTe$_2$ since the spectrum remains gapped and unchanged at all TRIMs. This topologically non-trivial normal state thus dictates the superconducting state to have $\kappa = 2$ (see Eq. 9), which we verified by explicitly calculating Eq. 8 for $H_{\text{BdG}}^k$ given in Eq. 4 and 1 with $\Delta$ being the self-consistently obtained Bu pairing [see Table II].

Next, we will show that WTe$_2$ as a TCsc with $\kappa = 2$ indeed hosts higher-order Majorana boundary modes. In Fig. 4 we numerically demonstrate the existence of w-band renormalization in the Brillouin zone. In this section, we study how superconducting states of different symmetries evolve under an in-plane magnetic field. Specifically, we solve the gap equations

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline
\textbf{\(\nu_N\)} & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
\hline
\textbf{\(\kappa\)} & - & - & + & - & + & + & + & + \\
\hline
\textbf{\(\kappa\)} & - & - & + & + & + & + & + & + \\
\hline
\textbf{\(\kappa\)} & - & - & + & - & + & + & + & + \\
\hline
\end{tabular}
\caption{The inversion eigenvalues $p_{\nu_N}$ of all the occupied BdG bands $\nu = 1, \cdots, 8$, ordered with increasing energy, at each of the time-reversal invariant momentum $k = (0, 0), (\pi, 0), (0, \pi)$ and $(\pi, \pi)$. The indicator $\kappa$ for inversion-protected topological superconductors is given by the sum of these eigenvalues divided by 4.}
\end{table}
order transition becomes a crossover as the direction of field rotates away from $\vec{z}$ since both $C_{2x}$ and $M_z$ symmetries are generally broken.

V. SUMMARY AND DISCUSSION

We point out that the newly discovered superconductivity in gated monolayer WTe$_2$, a superconducting quantum-spin-Hall material, can be an inversion-protected topological crystalline superconductor with “higher-order topology” if the pairing is parity-odd. Note that this is in contrast to the conventional wisdom that the presence of inversion and time-reversal symmetry is disadvantageous for superconductors being topological due to the spin-degenerate bands. We thus investigate the pairing symmetry of the gated monolayer WTe$_2$ at mean-field level in the absence and presence of an in-plane magnetic field to indicate qualitatively the short-ranged interactions that support odd-parity pairings.

We find that the time-reversal-symmetric odd-parity pairing that is energetically favored by the considered nearest-neighbor attractions is an inversion-protected topological crystalline superconductor characterized by a $Z_2$ indicator $\kappa = 2$. Although this paired state is not a traditional two-dimensional topological superconductor hosting Majorana edge modes, as has been previously sought in superconducting quantum-spin-Hall materials, it features Majorana corner states, verified by our calculation on a finite lattice. While the normal-state model we adopt from Ref. 53 fits well to ab initio results, Ref. 60 has pointed out that more spin-orbit coupling terms are required to have a better fit to the experimentally data on WTe$_2$. We nonetheless expect our phase diagram for pairing symmetry to change only quantitatively, and thus the existence of Majorana corner modes.

We expect that these Majorana corner modes cannot be removed without closing the bulk gap if we preserve inversion symmetry. When the inversion symmetry is broken, while the Majorana modes are no longer protected by the two-dimensional bulk topology, they are still protected by the gaps on the one-dimensional edges. In this case the paired state becomes the so-called “extrinsic” higher-order topological superconductor. We thus expect these Majorana corner modes can in principle be identified experimentally by scanning tunneling microscopy.

We emphasize that this material in fact satisfies our general recipe for inversion-protected topological crystalline superconductors featuring “higher-order” Majorana boundary modes, which we find by performing a symmetry indicator analysis and by establishing the bulk-boundary correspondence within a minimal model for this type of superconductor in two dimension. Although material prediction for topological superconductors is in general difficult due to the presence of interac-

FIG. 5. The pairing symmetries and the order parameter magnitudes of the dominant equal-spin ($\Delta^0_{ss}$) and opposite-spin ($\Delta^0_{ss'}$) components in the self-consistent solutions as a function of an in-plane field $h_x$. We consider two representative points [see blue stars in Fig. 2(b)] with on-site interactions being (a) $U = -0.2$ and (b) $U = -1$ at a fixed nearest-neighbor interaction $V = -0.4$. The blue and yellow background colors represent the pairing symmetries $A_g$ and $B_u''$ respectively. For the $A_g$ pairs, the opposite-spin component results from spin-singlet paired states. As for the $B_u''$ pairs, the opposite- and equal-spin components result from spin-triplet states $|\uparrow\downarrow + \downarrow\uparrow\rangle$ and $|\uparrow\uparrow + \downarrow\downarrow\rangle$ respectively.

self-consistently as above, but with an additional term $H_{\text{field}} = h_x \hat{s}_x \otimes \hat{s}_0 \otimes \hat{l}_0$ added to Eq. (1) for interactions $(U, V) = (-0.2, -0.4)$ and $(U, V) = (-1, -0.4)$, which support $B_u$ and $A_g$ states respectively in the absence of field. In Fig. 5, we show how the pairing symmetry and the equal-spin and opposite-spin gap magnitudes $\Delta^0_{ss} = \max(|\Delta_{ss'}|)$ on the dominant bands evolve with the field strength. For the case where $V$ dominates [Fig. 5(a)], we find that the predominantly spin-triplet $B_u$ gap survives beyond several times the Pauli limit $H_{\text{Pauli}}$ by rotating the spin direction from $|s_z = 0\rangle$ to $|s_x = 1\rangle$ to align with the field (dubbed $B_u''$). In contrast, for the case where $U$ dominates [see Fig. 5(b)], we find that the $A_g$ gap is killed by the field slightly below the Pauli limit as expected due to the predominant on-site components. Surprisingly, however, the $B_u''$ gap emerges upon the disappearance of the $A_g$ gap. This $B_u''$ gap stabilized by an intermediate in-plane field has a similar spatial configuration as Fig. 2 (c), but with a different spin structure $|s_x = 1\rangle$. At $U = -1$, the $A_g$ paired state undergoes a first-order transition to the $B_u''$ state accompanied with a change of $C_{2\pi}$-parity from even to odd, while the field $H_x$ explicitly breaks the mirror symmetry. In contrast, at $U = -0.2$ the $B_u$ undergoes a crossover to $B_u''$ where the spin direction of the paired state rotates without any symmetry change or discontinuity in the gap magnitude. The first
tions, our recipe provides general and useful guidelines for searching for or designing more realistic systems hosting “higher-order” topological superconductivity protected by inversion symmetry.

Even when on-site attractions dominate and the conventional pairing is favored as expected, we surprisingly find that an intermediate in-plane field beyond the Pauli limit not only destroys the spin-singlet pairs, but instead stabilizes an equal-spin triplet paired state aligning in the field direction. This is consistent with the in-plane critical field exceeding the Pauli limit reported by recent experiments. More importantly, although inversion symmetry is broken by the field, we expect such equal-spin pairing to be an extrinsic higher-order topological superconductor with single Majorana modes (instead of Majorana Kramer’s pairs) on opposite corners so long as the field magnitude is smaller than the gap on the edges.

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**Note added—** After posting this work we became aware of Ref. 62, which mainly discussed the formulation of symmetry indicators for inversion-protected TCsc in any d dimension. Their d = 2 case agrees with our conjecture in Eq. 8.

**Supplementary Information**

A. **Relation between the Z\(_4\) indicator and Z\(_2\) index for topological ‘metals’**

In this subsection, we explain why Eq. (10) in the main text holds for topological ‘metals’ that are ‘effectively gapped’. We first review the insulator case presented in Ref. 35. Consider an insulator with both time-reversal and inversion symmetries. The Z\(_2\) index \(\nu\) for time-reversal topological insulators can be calculated simply by

\[
(-1)\nu = \prod_{k \in \text{TRIM}} \prod_{m=1}^{n_k/2} \xi_{km},
\]

where \(\xi_{km}\) is the parity of the filled band \(m\) at a time-reversal invariant momentum (TRIM). Here \(n_k\) is the total number of filled bands at \(k\), and \(n_k = n\) is independent of \(k\) for insulators. Only half of the bands enter the product since the system is two-fold degenerate. When \((-1)^{\nu} = 1\) (0), the system is topological (trivial). As shown in Ref. 35, we can also express this index directly as

\[
\nu_N = \sum_{k \in \text{TRIM}} \frac{n_k^-}{2},
\]

where \(n_k^\pm\) is the number of occupied bands with parity \(\pm 1\).

Due to the presence of inversion symmetry, one can also calculate the \(Z_4\) symmetry indicator \(\kappa\) for inversion-protected topological crystalline insulators given by

\[
\kappa_N = \frac{1}{4} \sum_{k \in \text{TRIM}} \sum_{m=1}^{n_k} \xi_{km} = \sum_{k \in \text{TRIM}} \frac{n_k^+}{4} - \sum_{k \in \text{TRIM}} \frac{n_k^-}{2}.
\]

Here we have used the fact that \(\sum_{m=1}^{n_k} \xi_{km} = n_k^+ - n_k^- = n_k - 2n_k^\pm\). Now it is clear that

\[
(-1)^{\nu_N} = (-1)^{\kappa_N}
\]

if \(\alpha \equiv \sum_{k \in \text{TRIM}} \frac{n_k^\pm}{2}\) is even.

For insulators, \(\alpha = n(\text{number of TRIMs})/4\), where \(n\) is even due to the two-fold degeneracy. Eq. 22 thus is not guaranteed for 1D insulators, but holds for both 3D and 2D insulators, where the numbers of TRIMs are 8 and 4, respectively. As for metals with Fermi pockets enclosing any TRIM, \(n_k \neq n\) is different for different TRIMs in general, and thus \(\alpha\) is not guaranteed even. Nonetheless, for metals whose Fermi pockets are away from TRIMs, \(n_k = n\) is still \(k\)-independent, and thus Eq. 22 still holds in 2D and 3D.

B. **Edge modes in the three-domain geometry**

In this subsection, we show how we obtain the Majorana edge modes \(\psi_{23}^\dagger(r, \theta)\) and \(\psi_{34}^\dagger(r, \theta)\) in the three-domain geometry. Consider the domain wall between the \(\kappa = 2\) and \(\kappa = 3\) phases. The Hamiltonian \(\mathcal{H}_s^r\) in Eq. 13 becomes block diagonal after taking the limit \(v \rightarrow 0\), and it is clear from Eq. 14 that only the block with \(m_+(r)\) terms experiences a sign-changing mass term and is thus expected to trap a zero-energy eigenstate \(\psi_{23}^\dagger(r, \theta)\) localized at \(r = R_3\). In the following, we solve for the asymptotic for \(m_+(r, \theta)\). This 2 \times 2 block (represented by Pauli matrix \(\tau\)) with \(m_+(r)\) term for the spin-up sector is given by

\[
h_+^\dagger = m_+(r)\sigma_x + \Delta(-i\sigma_r)(\cos \theta \sigma_x + \sin \theta \sigma_y) = m_+(r)\sigma_x + \Delta(-i\sigma_r)e^{i\sigma_x \theta}.
\]

The zero-energy eigenstate is then given by \(h_+^\dagger \psi_{23} = 0\), but we can obtain the edge state more conveniently by solving the zero-energy mode for a rotated Hamiltonian...
\[ \hat{h}_+ \phi = 0, \text{ where } \hat{h}_+ = \hat{\tau}_x \hat{U}_\theta \hat{h}_+ \hat{U}_\theta, \text{ and } \hat{U}_\theta = e^{i\tau_z \theta / 2} \text{ is a unitary transformation. After some algebra, we find that} \]
\[ \hat{h}_+ (r) = \hat{\tau}_x [m_+ (r) \hat{\tau}_+ + \Delta (-i \partial_r) \hat{\tau}_0] \]
\[ = -im_+ (r) \hat{\tau}_y + \Delta (-i \partial_r) \hat{\tau}_0. \tag{24} \]

Now \( \hat{h}_+ \) is \( \theta \)-independent, and we can thus write its zero-energy eigenstate as \( \phi \) with angular dependence \( L \) orbital part of the angular momentum has the form \( L \).

Recall that the edge modes are given by \( \tilde{\phi} \) and \( \Delta \). We thus find the energy correction arising from the boundary, obeys \( \hat{r}_\theta \xi = a \xi \). For simplicity, we take \( m_+ (r) = \text{sgn}(r - R_\alpha) \) and \( \Delta > 0 \). Then by solving the differential equation for \( f(r) \) and requiring that \( f(r) \) localized at the boundary \( r = R_\alpha \), we find that \( a = 1 \) and \( \phi (r) = e^{-1/\Delta r |r - R_\alpha|} (1, 0, i, 0)^T \). Together with the fact that the orbital part of the angular momentum has the form \( L_z = -i \partial_\theta \), we can then obtain the zero-mode for \( \hat{h}_+ (r, \theta) \) with angular dependence.

\[ \psi_{23} (r, \theta) = U_\theta^\dagger \phi (r) = e^{-\frac{i \pi |r - R_\alpha|}{2}} e^{i \theta} \begin{pmatrix} e^{-i \frac{\pi}{2}} \\ 0 \\ e^{i \frac{\pi}{2}} \\ 0 \end{pmatrix}. \tag{25} \]

\[ \mathcal{H}_\theta^{1/2} (r, \theta) = \begin{pmatrix} 0 & -i \Delta \frac{\pi \mu}{r} k_\theta & 0 & 0 \\ 0 & 0 & 0 & i \Delta \frac{\pi \mu}{r} k_\theta \\ i \Delta \frac{\pi \mu}{r} k_\theta & 0 & 0 & 0 \\ -i \Delta \frac{\pi \mu}{r} k_\theta & 0 & 0 & 0 \end{pmatrix}. \tag{26} \]

Recall that the edge modes are given by

\[ \psi_{23}^{1/2} (r, \theta) = e^{-\frac{i \pi |r - R_\alpha|}{2}} e^{i \theta} \begin{pmatrix} e^{i \frac{\pi}{2}} \\ 0 \\ \pm ie^{\pm i \frac{\pi}{2}} \\ 0 \end{pmatrix}, \tag{27} \]

and

\[ \psi_{34}^{1/2} (r, \theta) = e^{-\frac{i \pi |r - R_\alpha|}{2}} e^{i \theta} \begin{pmatrix} 0 \\ e^{i \frac{\pi}{2}} \\ 0 \\ \mp ie^{\mp i \frac{\pi}{2}} \end{pmatrix}. \tag{28} \]

where \( l \) is the orbital angular momentum taking half integers. We thus find the energy correction arising from rotational motion in \( \theta \) to be

\[ \langle \mathcal{H}_\theta^{1/2} \rangle_{j, \pm} = (\psi_j^\dagger)^\theta \mathcal{H}_\theta^\theta \psi_j^\dagger \propto 2l \]

\[ \langle \mathcal{H}_\theta^{1/2} \rangle_{j, \pm} = (\psi_j^\dagger)^\theta \mathcal{H}_\theta^\theta \psi_j^\dagger \propto -2l, \tag{29} \]

where \( j = 23, 34 \) denotes the two domain walls. We therefore conclude that the spin-up and spin-down modes are right- and left-movers respectively for both domain walls, which amounts to one pair of helical edge modes per domain wall [see Fig. 3 (a)] in the main text.

**D. Rotational invariant perturbations**

In this subsection, we write down the general form of rotational invariant perturbations \( \mathcal{H}_\theta^{\text{rot}} (\mathbf{k}) \) and its projection on to the edge modes \( \psi_{23} \) and \( \psi_{34} \). The rotational operator is given by \( C_\theta = e^{-i J_\theta \theta / 2}, k_\pm \to e^{\pm i \theta} k_\pm \), where the angular momentum has the form \( J_\theta = \hat{\tau}_z \otimes \hat{s}_z \otimes \hat{s}_y / 2 \), and \( k_\pm = k_x \pm i k_y \). The perturbations that preserve time-reversal symmetry \( \Theta \), particle-hole symmetry \( \mathcal{P} \), inversion symmetry for odd-parity pairing \( \mathcal{I} \), and also obey \( C_\theta H_\theta^{\text{rot}} (\mathbf{k}) C_\theta^\dagger = H_\theta^{\text{rot}} (\mathbf{k}) \) have the general form of

Note that the Majorana condition \( \Xi_{23} = \psi_{23} \) is satisfied up to an overall phase. \( \psi_{23} (r, \theta) \) and \( \psi_{34}^{1/2} (r, \theta) \) can be obtained in a similar way.
Here, $H'_{\text{rot}}(k)$ is written in the basis of $\hat{\tau} \otimes \hat{s} \otimes \hat{\rho}$, and $m_{1/2}, D_0, A, B,$ and $C$ are free parameters.

Since the edge modes with the same spin (opposite spins in order to create a gap) have free parameters.

opposite spins in order to create a gap. However, it is obvious from Eq. 30 that there exists no spin-flipping terms that are allowed by the symmetries considered. The edge modes $\psi_{23}^*$ and $\psi_{34}^*$ thus remain gapless in the presence of rotational invariant perturbations.

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