Existence of Majorana-Fermion Bound States on Disclinations and the Classification of Topological Crystalline Superconductors in Two Dimensions

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We prove a topological criterion for the existence of a zero-energy Majorana bound state on a disclination, a rotation symmetry breaking point defect, in fourfold symmetric topological crystalline superconductors (TCS) in two dimensions. We first establish a complete topological classification of TCS using the Chern invariant and three integral rotation invariants. By analytically and numerically studying disclinations, we algebraically deduce a $\mathbb{Z}_2$ index that identifies the parity of the number of Majorana zero modes at a disclination. Surprisingly, we also find weakly protected Majorana fermions bound at the corners of superconductors with trivial Chern and weak invariants.

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Symmetry protected topological insulators and superconductors have theoretically, and experimentally risen to prominence in the last half decade [1]. Recent developments in this field have moved on from the study of discrete symmetries such as time reversal and charge conjugation [2–4] to translational and point-group symmetries [5–15]. While spatial symmetries are not preserved as generically as, say, time reversal, they can still support robust topological states in clean crystalline systems. It is understood that the so-called strong topological invariants, which are protected no matter what spatial symmetries are broken, determine the appearance of disorder-insensitive gapless boundary states. Interestingly, it was found that weak invariants, which require an additional translation symmetry, support boundary states [16,17] and, more surprisingly, robust bound states on crystal dislocations [18–22]. A natural question to ask is then whether topological defects of the point-group rotational symmetry, i.e., disclinations, can also bind low-energy states in topological phases protected by point-group symmetry. A related problem has been studied in a different context in graphene [23–25]. In this Letter we address this question for 2D topological superconductors with point-group symmetry. Our main results are (i) a complete classification of 2D superconductors with C_4 symmetry, (ii) the derivation of a Z_2 index theorem that determines the existence of zero-energy Majorana bound states (MBS) [26,27] on disclinations and the corners of material samples, and (iii) a unique algebraic approach that can be used to prove generic index theorems.

Just as dislocations are local topological defects in the translational order of crystals, disclinations are topological defects in the discrete rotational order. In two dimensions, disclinations are point defects that can be constructed by removing or inserting material in certain angular sections with angles compatible with the crystalline symmetry (see Fig. 1) [28]. Dislocations are characterized by their Burgers vectors, i.e., the translation element acquired when a particle encircles the defect; disclinations are described by an element in the space group encoding the amount of rotation Ω and translation $\mathbf{T}$ one picks up traveling around the point defect. The translation piece $\mathbf{T}$ is not unique and depends on the enclosing path; however, for a C_4-symmetric lattice the evenness (type 0) or oddness (type 1) of the number of translations is unique. The C_4 symmetry thus yields a $\mathbb{Z}_2$ characteristic that distinguishes classical disclinations with the same Frank angle Ω. Examples are shown for $\Omega = -90°$ disclinations in Figs. 1(c) and 1(d). The difference between the two primitive disclinations can be observed at the defect cores where

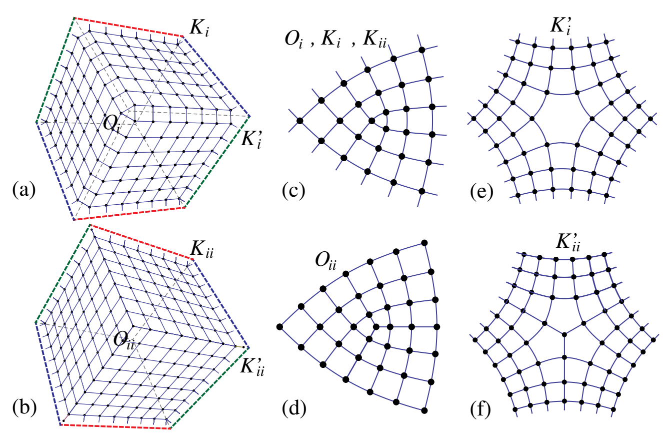

FIG. 1 (color online). (a),(b) 2D lattice configurations with three disclinations. Each of the three faces is a $L \times L$ square lattice. Periodic boundary conditions are taken on the six edges of the hollow cubes as indicated by matching colors and line styles. (c)–(f) Flattened, zoomed-in versions of the $\Omega = -90°$ (c),(d) and $\Omega = +180°$ (e),(f) disclinations at O, K, and K'. (c) Type-1 disclination centered at a triangular plaquette with an odd number of translations around its boundary. (d) Type-0 disclination centered at a trivalent vertex with an even number.

C_4 symmetry is violated at either a triangular plaquette or a trivalent vertex. The $\mathbb{Z}_2$ characteristic arises from the fact that there are two inequivalent fourfold rotation centers, vertex or plaquette, which can be extended to general C_n [29].

We will only consider fully gapped, translationally invariant superconductors in the mean-field limit which are described by Bogoliubov–de Gennes (BdG) Hamiltonians $H(\mathbf{k})$, in Bloch form defined on a square Brillouin zone (BZ), with a particle-hole constraint $\Xi H(\mathbf{k})\Xi^\dagger = -H(-\mathbf{k})$, where Ξ is a local, antiunitary operator. A point-group element r is represented by a unitary operator $\hat{r}$ that commutes with the full Hamiltonian, and satisfies $\hat{r}H(\mathbf{k})\hat{r}^\dagger = H(r\mathbf{k})$ for the Bloch Hamiltonian, and $\Xi\hat{r}\Xi^\dagger = \hat{r}$ for the particle-hole operator [30]. For the duration of our work we will focus on the Abelian point-group C_4 generated by $\pi/2$ rotations, which is a symmetry commonly shared by all layered perovskite superconductors. We use the half-integer spin rotation such that $\hat{r}^4 = (\hat{r}^2)^2 = -1$.

C_4-symmetric superconductors in two dimensions are classified by (i) the Chern invariant $\mathrm{Ch} = (i/2\pi)\int_{\mathrm{BZ}} d^2k\epsilon^{ij}\mathrm{Tr}(\partial_{k_i}\mathcal{A}_j) \in \mathbb{Z}$ with $(\mathcal{A}_i)_{mn}(\mathbf{k}) = \langle u_m(\mathbf{k})|\partial_{k_i}|u_n(\mathbf{k})\rangle$ being the Berry connection of the negative-energy bands [32–34], (ii) the eigenvalues of the rotation operator $\hat{r}$ for all the negative-energy states at the fourfold symmetric momenta $\Pi = \Gamma, M(=(\pi,\pi))$, and (iii) the spectrum of the C_2 rotation $\hat{r}^2$ at one of the equivalent twofold symmetric momenta $X = (\pi, 0)$ or $X' = (0, \pi)$. We label the bands at the symmetry points by their rotation eigenvalues following Ref. [35]. At $\Pi = \Gamma$, M, a band with $\hat{r} = e^{-i\pi/4}$, $e^{i\pi/4}$, $e^{3i\pi/4}$, $e^{-3i\pi/4}$ is labeled by Π_5, Π_6, Π_7, Π_8, respectively, while at X, a band with $\hat{r}^2 = i, -i$ is labeled by X_3, X_4, respectively. Let $\#\Pi_i$, $\#X_i$ be the number of appearances of Π_i, X_i within the negative-energy states. Only the differences of the eigenvalues between symmetry points carry topological information, and our convention uses the eigenvalues relative to the values at the Γ point. We define

$$n_3 = \#X_3 - \#\Gamma_6 - \#\Gamma_8, \quad (1)$$

$$n_4 = \#X_4 - \#\Gamma_5 - \#\Gamma_7, \quad (2)$$

$$n_i = \#M_i - \#\Gamma_i, \quad \text{for } i = 5, 6, 7, 8. \quad (3)$$

These are easy to understand as Γ_6, Γ_8 (Γ_5, Γ_7) both square to $+i(-i)$ and thus n_3, n_4 determine the difference in the C_2 eigenvalues at X and Γ while $n_{5,6,7,8}$ determine the C_4-eigenvalue differences between M and Γ. These integers obey $n_3 + n_4 = n_5 + n_6 + n_7 + n_8 = 0$ (from the constant number of negative-energy bands throughout the BZ) and $n_5 + n_6 = n_7 + n_8 = 0$ (from the particle-hole constraint). Following the work of Ref. [14], one can show that

$$\mathrm{Ch} + n_6 + 2n_4 + 3n_7 \equiv 0 \mod 4. \quad (4)$$

Hence C_4-symmetric topological crystalline superconductors are completely classified by four integral invariants $\chi_i \equiv (\mathrm{Ch}, n_4, n_6, n_7)$ that satisfy Eq. (4). Moreover the weak $\mathbb{Z}_2$ topological invariant is determined by the inversion eigenvalues at M and X,

$$\mathbf{G}_\nu = \nu(\mathbf{G}_1 + \mathbf{G}_2), \qquad \nu = (n_4 + n_6 - n_7) \mod 2, \quad (5)$$

where $\mathbf{G}_1$, $\mathbf{G}_2$ are the reciprocal lattice vectors.

The essential ingredient of our index-theorem proof is a collection of 2D C_4-symmetric superconductor models that "generate" all the topological classes characterized by the χ_i. Since the χ_i are four component vectors we need four Hamiltonians which have linearly independent χ_i. Combining the Hamiltonians via a direct sum combines the vectors with a vector sum, so any topological class χ_i can be produced. We choose two generators to be spinless, chiral $p_x + ip_y$ superconductors on a square lattice,

$$H_a = \Delta(\sin k_x\tau_x + \sin k_y\tau_y) + [u_1(\cos k_x + \cos k_y) + 2u_2\cos k_x\cos k_y]\tau_z, \quad (6)$$

where τ_a acts on Nambu space, Δ is the $p_x + ip_y$ pairing, and the first or second neighbor hoppings u_1, u_2 are kinetic energy terms that gap out the nodes of the pairing term at the points Γ, X, X', M. The particle-hole and rotation operators are given by $\Xi_a = \tau_x K$ and $\hat{r}_a = (\mathbb{1}_2 + i\tau_z)/\sqrt{2}$, where K is complex conjugation. The invariants χ_i depend on u_1 and u_2 and are summarized in Table I. Flipping the signs of both u_1 and u_2 inverts $\chi_i \to -\chi_i$.

The other independent generators also have chiral $p_x + ip_y$ pairing, but have different single-particle kinetic energy terms. They can be clearly represented as 2D generalizations of Kitaev's p-wave wire [31]. Figure 2 depicts two tight-binding limits of C_4-symmetric Majorana fermion models with four fermions per site and arrows which represent the Majorana ordering convention. The two Hamiltonians are $\hat{H}_b = it\sum_{\mathbf{x}}(\gamma^1_{\mathbf{x}}\gamma^3_{\mathbf{x}+e_1} + \gamma^2_{\mathbf{x}}\gamma^4_{\mathbf{x}+e_2})$ and $\hat{H}_c = it\sum_{\mathbf{x}}(\gamma^1_{\mathbf{x}}\gamma^3_{\mathbf{x}+e_1+e_2} + \gamma^2_{\mathbf{x}}\gamma^4_{\mathbf{x}-e_1+e_2})$, where the $\gamma^i_{\mathbf{x}}$'s are Majorana operators with $\gamma^{i\dagger}_{\mathbf{x}} = \gamma^i_{\mathbf{x}}$ and $\{\gamma^i_{\mathbf{x}}, \gamma^j_{\mathbf{y}}\} = 2\delta^{ij}\delta_{\mathbf{xy}}$. The C_4 rotation operator $\hat{r}_{bc} = \prod_{\mathbf{x}}\exp[-(\pi/4)\gamma^1_{\mathbf{x}}\gamma^2_{r\mathbf{x}}] \times \exp[-(\pi/4)\gamma^2_{\mathbf{x}}\gamma^3_{r\mathbf{x}}]\exp[-(\pi/4)\gamma^3_{\mathbf{x}}\gamma^4_{r\mathbf{x}}]$ gives $\hat{r}_{bc}(\gamma^1_{\mathbf{x}}, \gamma^2_{\mathbf{x}}, \gamma^3_{\mathbf{x}}, \gamma^4_{\mathbf{x}})\hat{r}^\dagger_{bc} = (\gamma^2_{r\mathbf{x}}, \gamma^3_{r\mathbf{x}}, \gamma^4_{r\mathbf{x}}, -\gamma^1_{r\mathbf{x}})$, where r is the C_4 rotation in real space. If we transform to complex fermions $c_{\mathbf{x}} = (\gamma^1_{\mathbf{x}} + i\gamma^3_{\mathbf{x}})/2$ and $d_{\mathbf{x}} = (\gamma^2_{\mathbf{x}} + i\gamma^4_{\mathbf{x}})/2$ then we find

TABLE I. Chern and rotation invariants for the chiral $p_x + ip_y$ superconductor in Eq. (6). The Hamiltonians are superscript labeled by their Chern and weak invariants (Ch; ν).

H_a	Hopping strength	Ch	n_4	n_6	n_7
$H_a^{(1;0)}$	$u_1 > u_2 > 0$	1	-1	1	0
$H_a^{(1;1)}$	$-u_1 > u_2 > 0$	1	0	-1	0
$H_a^{(2;1)}$	$u_2 > \|u_1\|$	2	-1	0	0

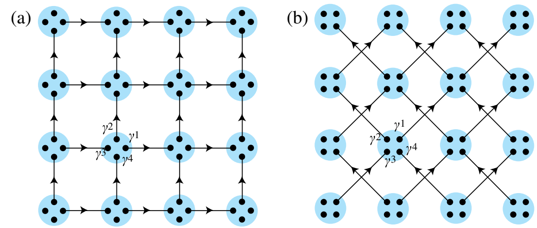

FIG. 2 (color online). C_4-symmetric tight binding models with four Majorana fermions (black dots) at each site. (a) H_b. (b) H_c.

$$H_b(\mathbf{k}) = t(\cos k_x\tau_z + \sin k_x\tau_y) \oplus t(\cos k_y\tau_z + \sin k_y\tau_y),$$
$$H_c(\mathbf{k}) = t(\cos(k_x + k_y)\tau_z + \sin(k_x + k_y)\tau_y)$$
$$\oplus\, t(\cos(k_x - k_y)\tau_z + \sin(k_y - k_x)\tau_y) \quad (7)$$

in the basis $\vec{\xi}_{\mathbf{k}} = (c_{-\mathbf{k}}, c^\dagger_{\mathbf{k}}, d_{-\mathbf{k}}, d^\dagger_{\mathbf{k}})^T$ and where the τ_i's act on Nambu space. The particle-hole and rotation operators are $\Xi_{bc} = (\mathbb{1}_2 \otimes \tau_x)K$ and $\hat{r}_{bc} = \sigma_+ \otimes \mathbb{1}_2 - i\sigma_- \otimes \tau_z$ where $\sigma_\pm = 1/2(\sigma_x \pm i\sigma_y)$ acts on the (c, d) space. The χ_i for H_b and H_c are shown in Table II and they complete the set of independent generators. Every C_4-symmetric superconductor has identical topological properties to direct sums of $H_a^{(1;0)}$, $H_a^{(1;1)}$, H_b and H_c. In particular the zero modes at disclinations in any C_4-symmetric superconductor can be determined this way.

We will now determine the properties of disclinations for each generator. A disclination configuration is specified by the pair $(\mathbf{\Omega}, \mathbf{T})$ mentioned earlier. The MBS of the chiral superconductors H_a (with pairing and hopping parameters $2u_2/\Delta = \pm u_1/\Delta = 1$) are studied numerically using periodic lattice models with three disclinations. We took three adjacent faces of a cube and glued the parallel sides [see Figs. 1(a) and 1(b)]. Two $-90°$ disclinations are located at the points O and K and a $+180°$ disclination is located at K'. We use two lattice configurations that differ in the choice of a type-0 or type-1 disclination at O [see Figs. 1(c) and 1(d)]. The superconducting phase is chosen so that it smoothly winds around the defects, but there are two inequivalent ways of specifying the defect lattice due to the double covering of the rotation group. The smooth winding around the disclination involves either the rotation $\hat{r}(s) = e^{is\Omega\tau_z/2}$ or $\hat{r}'(s) = e^{is(2\pi+\Omega)\tau_z/2}$, parametrized by $s \in [0, 1]$. We choose $\hat{r}(s)$ and thus the phase smoothly winds by $\pi/2$ around O, K and $-\pi$ around K'. Note, if we choose $\hat{r}'(s)$ then the C_4 operator would be $-\hat{r}$ instead which changes $n_6 \leftrightarrow -n_7$. We find that only $H_a^{(1;1)}$ supports an odd number of MBS and even then only for type-1 disclinations. The results are summarized in Table III and we show the zero-mode wave functions at the disclinations at O and K in Figs. 3(a) and 3(b).

TABLE II. Chern and rotation invariants of models in Fig. 2.

TB model	Ch	n_4	n_6	n_7
H_b	0	1	-1	1
H_c	0	2	0	0

TABLE III. Parity of the number of zero modes at a $-90°$ disclination for the chiral superconductors $H_a^{(1;0)}$, $H_a^{(1;1)}$ in Eq. (6) with smooth rotation $\hat{r}(s) = e^{is\Omega\tau_z/2}$ and the tight binding models H_b, H_c in Fig. 2.

$-90°$ disclination	$H_a^{(1;0)}$	$H_a^{(1;1)}$	H_b	H_c
Type-0	0	0	1	1
Type-1	0	1	0	1

For H_b, H_c we use the fact that the parity of the number of MBS at the defect is insensitive to all perturbations that do not violate the energy gap or rotation symmetry away from the point defect since there is no low-energy channel for a single Majorana bound state to escape or enter the disclination core. This implies that, just as for the boundary modes of the topological p-wave wire [31], we can determine the parity of the zero-mode bound states pictorially in the tightly bound limit. The MBS of H_b and H_c at type-0 and type-1 $-90°$ disclinations are shown in Figs. 3(c) and 3(d), where the MBS are simply unbonded Majorana fermions represented by thick red dots. We find that H_b has a zero mode for type 0, and H_c has zero modes for both types. This is summarized in Table III.

We are now in a position to determine the index theorem since any C_4-symmetric BdG Hamiltonian can be

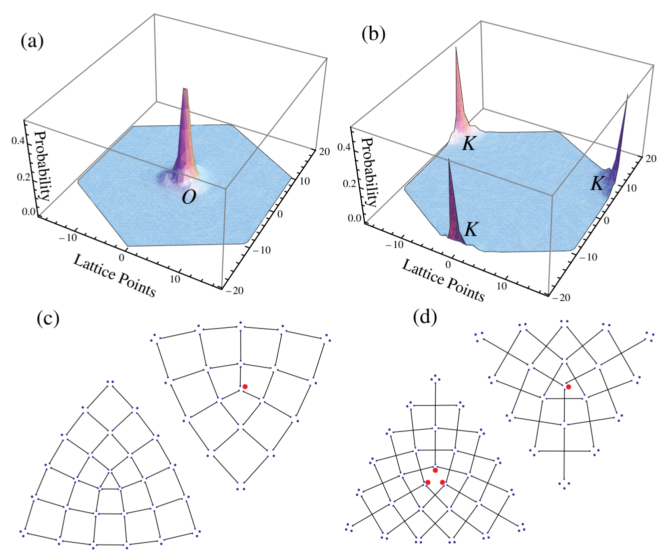

FIG. 3 (color online). (a),(b) Exponentially localized probability density of the Majorana zero mode at disclinations O and K, plotted on a torus geometry where parallel sides on the hexagonal domain are identified. Compare with 3D lattice in Fig. 1. (c) Tight binding model H_b with (left) type-1 and (right) type-0 disclinations. (d) H_c with (left) type-1 (right) type-0 disclinations. Thick red dots in disclination cores are unpaired Majorana bound states.

smoothly deformed into a unique composition $[H] \simeq m_1[H_a^{(1;0)}] \oplus m_2[H_a^{(1;1)}] \oplus m_3[H_b] \oplus m_4[H_c]$ up to topologically trivial bands far from the Fermi level. The direct sum implies taking m_i decoupled copies (m_i are integers), and $m_i < 0$ means a copy with the negative and positive energy states switched. To finish the derivation of the topological Z_2 index we need to carry out some simple algebraic manipulations. First, we see that since H_c only has $n_4(=2)$ nonzero and has zero modes for both disclination types the index gets a contribution of $1/2(n_4)$ mod 2. Next we can take $2H_a^{(1;0)} \oplus 2H_a^{(1;1)} \oplus H_c$ which has $\chi_i = (4, 0, 0, 0)$ and bound states for both types. This implies the index receives a contribution of $1/4(\mathrm{Ch})$ mod 2. Using these two pieces we can go back to $H_a^{(1;0)}$, which does not have any zero modes, and determine the equation $[1/2(n_4) + 1/4(\mathrm{Ch}) + k(n_6)] \bmod 2 = 0$ which upon substitution gives $k = 1/4$. To determine the contribution of n_7 we consider $H_a^{(1;0)} \oplus H_a^{(1;1)} \oplus H_b$ with $\chi_i = (2, 0, -1, 1)$. This model has bound states on both types of disclinations so we use $[1/2(n_4) + (1/4)(\mathrm{Ch}) + (1/4)n_6 + jn_7] \bmod 2 = 1$ to find $j = 3/4$. So far we were careful to choose all the Hamiltonian combinations above to have a vanishing weak invariant as it also contributes to the index. We can see this by taking $H_a^{(1;1)}$ which yields $1/4[\mathrm{Ch} + n_6 + 2n_4 + 3n_7] \bmod 2 = 0$, yet has a bound state on type-1 disclinations. This bound state, however, arises from a different mechanism, and comes from the interplay of the nonzero weak invariant and the oddness of the translation $\mathbf{T}$ around a type-1 disclination. Thus, we have determined the existence conditions for an odd number of MBS at a $-90°$ disclination. A $+90°$ disclination carries identical Majorana bound state parity since a $\pm 90°$ dipole of disclinations (of the same type) combines into a dislocation with an even Burgers vector and thus even overall Majorana bound state parity. Combining disclinations gives $(\Omega_1, \mathbf{T}_1) + (\Omega_2, \mathbf{T}_2) = (\Omega_1 + \Omega_2, \mathbf{T}_1 + r(\Omega_1)\mathbf{T}_2)$; e.g., fusing two $\Omega = \pi/2$ disclinations yields an $\Omega = \pi$ disclination. This implies that for generic C_4 disclinations with Frank angle Ω the topological index is

$$\Theta \equiv \left[\frac{1}{2\pi}\mathbf{T} \cdot \mathbf{G}_\nu + \frac{\Omega}{2\pi}(\mathrm{Ch} + n_6 + 2n_4 + 3n_7)\right] \bmod 2, \tag{8}$$

where $\mathbf{G}_\nu$ is the weak $\mathbb{Z}_2$ invariant (see the Supplementary Material for more detail [36]). The first term resembles the topological index for MBS at a dislocation, with the Burgers vector $\mathbf{B}$ replaced by $\mathbf{T}$ [18–20]. It vanishes for type-0 disclinations and equals $n_4 + n_6 + n_7$ (mod 2) for type-1 disclinations. The second term of Eq. (8) is an integer because of the constraint (4) and can distinguish Chern numbers which are even or odd multiples of 4, e.g., Ch = 4 or 8.

For a more physical understanding we can refer to the outer boundaries of regions surrounding a single disclination [see Figs. 3(c) and 3(d)]. For Fig. 3(c) we see the boundary links carry one unbound Majorana each, and the corners contain two whereas in Fig. 3(d) the links carry two and the corners carry three. Since there is only one disclination, the parity of MBS on the boundary will match the parity in the disclination core. We can clearly see that the two terms that comprise Θ represent the edge and corner contributions to the index, respectively. $\mathbf{T} \cdot \mathbf{G}_\nu/2\pi$ counts the number of MBS (mod 2) on an edge with length $\mathbf{T}$, while $(\mathrm{Ch} + n_6 + 2n_4 + 3n_7)/4$ counts the Berry phase due to continuous rotation and the number of MBS at a 90° corner. The index (8) therefore not only gives information about the disclination core, but also about the defect-free system boundary. In particular, even a system such as H_c, with vanishing Chern and weak $\mathbb{Z}_2$ invariants (which thus does not carry topologically protected edge modes) binds Majorana fermions at corners since $\Theta \equiv 1$. This implies that the rotation eigenvalues determine the existence of MBS in the form of corner states even in a defect and vortex free system.

Θ can also be illustrated in a continuum system on a disk geometry with a disclination at the origin. Take four copies of a spinless, continuum $p_x + ip_y$ superconductor with each copy rotated by $\pi/2$ relative to the previous: $H_4 = h_0 \oplus h_{\pi/2} \oplus h_\pi \oplus h_{3\pi/2}$ for $h_\phi = e^{i\phi\tau_z/2} h_0 e^{-i\phi\tau_z/2}$, $h_0(\mathbf{k}) = |\Delta|k_x\tau_z + |\Delta|k_y\tau_y + (m - \varepsilon k^2)\tau_z$. H_4 has the C_4 symmetry $\hat{r}_4$ which sends $h_0 \to h_{\pi/2}$, $h_{\pi/2} \to h_\pi$, $h_\pi \to h_{3\pi/2}$, $h_{3\pi/2} \to -h_0$. A $-90°$ disclination is represented by the helix in Fig. 4, where the top and bottom layers are glued along the branch cut (red line) with antiperiodic boundary conditions since $\hat{r}_4^4 = -1$. The disclination helix can be continuously untwisted to form a single copy of a $p_x + ip_y$ model with a π-flux vortex replacing the disclination at the origin that binds a Majorana bound state [26]. This is consistent with the index theorem (8) since Ch = 4, $n_4 = \mathbf{T} = 0$ for continuum models, and also $n_6 = n_7 = 0$ since momentum space can be compactified into a sphere $\mathbb{S}^2 = \mathbb{R}^2 \cup \{\infty\}$ and the rotation spectra at the fixed points $k = 0$ and ∞ are identical.

We have shown that topological crystalline superconductors in two dimensions with C_4 rotation symmetry are classified by four integers $\chi_i = (\mathrm{Ch}, n_4, n_6, n_7)$ and a Z_2

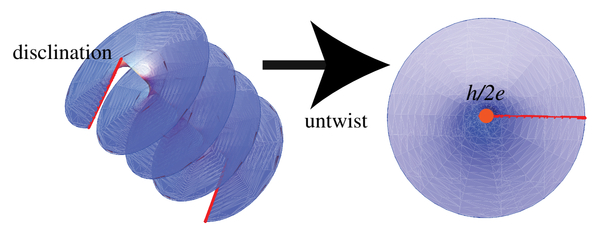

FIG. 4 (color online). Untwisting a $-90°$ disclination of the four layer $p_x + ip_y$ continuum model H_4 into a single layer $p_x + ip_y$ model with a quantum vortex.

index Θ determines the appearance of zero-energy MBS at disclinations and sample corners. Although the index theorem relies on C_4 symmetry, a Majorana bound state cannot escape without a low energy delocalized channel and thus is robust against any rotation breaking perturbation that does not close the bulk energy gap around the defect. The MBS at the corners of a sample, however, are sensitive to C_4 breaking perturbations, but could be observed in clean systems.

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[36] See Supplementary Material http://link.aps.org/supplemental/10.1103/PhysRevLett.111.047006 for more detail.