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

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Majorana Fermions and Disclinations in Topological Crystalline Superconductors

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We prove a topological criterion for the existence of zero-energy Majorana bound-state on a disclination, a rotation symmetry breaking point defect, in 4-fold 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 is then to ask 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 (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 2d, 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' vector *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

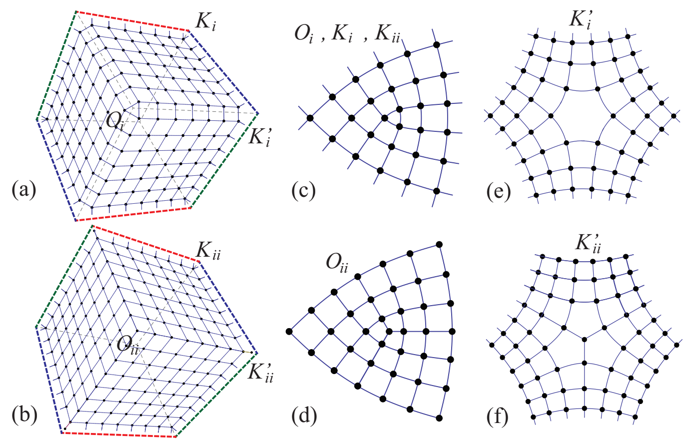

FIG. 1. (a), (b) 2D lattice configurations with three disclinations. Each of the three faces is a $L \times L$ square lattice. Periodic boundary conditions are taken on the six edges of the hollow cubes as indicated by matching colors/line styles. (c)-(f) Flattened, zoomed-in versions of the $\Omega = -90°$ (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.

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 Fig. 1c,d. The difference between the two primitive disclinations can be observed at the defect cores where 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 4-fold 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, with a particle hole constraint $\Xi H(\mathbf{k})\Xi^\dagger = -H(-\mathbf{k})$, where Ξ is a local, anti-unitary 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 $ch = \frac{i}{2\pi}\int_{BZ} d^2k \quad \epsilon^{ij}\mathrm{Tr}(\partial_{k_i}\mathcal{A}_j) \in \mathbb{Z}$ for $(\mathcal{A}_i)_{mn}(\mathbf{k}) = \langle u_m(\mathbf{k})|\partial_{k_i}|u_n(\mathbf{k})\rangle$ being the Berry connection of the negative-energy bands[31–33], (ii) the eigenvalues of the rotation operator $\hat{r}$ for all the negative energy states at the 4-fold symmetric momenta $\Pi = \Gamma, M(=(\pi,\pi))$ (iii) the spectrum of the C_2 rotation $\hat{r}^2$ at *one* of the *equivalent* 2-fold symmetric momenta $X = (\pi, 0)$ or $X' = (0,\pi)$. We label the bands at the symmetry points by their rotation eigenvalues following Ref. 34. 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 labelled by $\Pi_5, \Pi_6, \Pi_7, \Pi_8$ respectively; while at X, a band with $\hat{r}^2 = i, -i$ is labelled 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:

$$n_3 = \#X_3 - \#\Gamma_6 - \#\Gamma_8 \tag{1}$$

$$n_4 = \#X_4 - \#\Gamma_5 - \#\Gamma_7 \tag{2}$$

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

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

$$ch + n_6 + 2n_4 + 3n_7 \equiv 0 \mod 4. \tag{4}$$

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

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

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

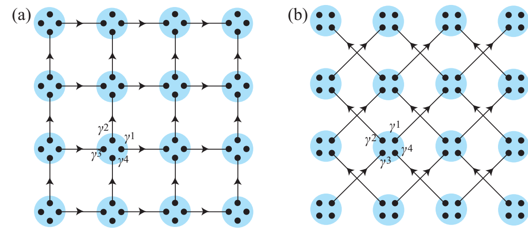

FIG. 2. C_4-symmetric tight binding models with four Majorana fermions (black dots) at each site. (a) H_b (b) H_c

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
$H_a^{(2;1)}$	$u_2 > \lvert u_1\rvert$	2	-1	0	0

TABLE I. Chern and rotation invariants for the chiral p_x+ip_y superconductor (6). The Hamiltonians are superscript labeled by their Chern and weak invariants $(ch;\nu)$.

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

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

that "generate" all the topological classes characterized by the χ_i. Since χ_i is a four component vector we need four Hamiltonians which have linearly independent χ_i. Combining the Hamiltonians via 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:

$$\begin{aligned} H_a = {} & \Delta(\sin k_x\tau_x + \sin k_y\tau_y) \\ & +[u_1(\cos k_x + \cos k_y) + 2u_2\cos k_x\cos k_y]\tau_z \end{aligned} \tag{6}$$

where τ_a acts on Nambu-space, Δ is the $p_x + ip_y$ pairing and the first/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[35]. Fig. 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 $\hat{H}_b = it\sum_{\mathbf{x}}\left(\gamma^1_{\mathbf{x}}\gamma^3_{\mathbf{x}+e_1} + \gamma^2_{\mathbf{x}}\gamma^4_{\mathbf{x}+e_2}\right)$ and $\hat{H}_c = it\sum_{\mathbf{x}}\left(\gamma^1_{\mathbf{x}}\gamma^3_{\mathbf{x}+e_1+e_2} + \gamma^2_{\mathbf{x}}\gamma^4_{\mathbf{x}-e_1+e_2}\right)$, where $\gamma^i_{\mathbf{x}}$'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 $\hat{r}_{bc} = \prod_{\mathbf{x}} \exp(-\frac{\pi}{4}\gamma^1_{\mathbf{x}}\gamma^2_{r\mathbf{x}}) \exp(-\frac{\pi}{4}\gamma^2_{\mathbf{x}}\gamma^3_{r\mathbf{x}}) \exp(-\frac{\pi}{4}\gamma^3_{\mathbf{x}}\gamma^4_{r\mathbf{x}})$ gives $\hat{r}_{bc}(\gamma^1_{\mathbf{x}}, \gamma^2_{\mathbf{x}}, \gamma^3_{\mathbf{x}}, \gamma^4_{\mathbf{x}})\hat{r}^\dagger_{bc} = (\gamma^2_{r\mathbf{x}}, \gamma^3_{r\mathbf{x}}, \gamma^4_{r\mathbf{x}}, -\gamma^4_{r\mathbf{x}})$, 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

$$\begin{aligned} H_b(\mathbf{k}) &= t(\cos k_x\tau_z + \sin k_x\tau_y) \oplus t(\cos k_y\tau_z + \sin k_y\tau_y) \\ H_c(\mathbf{k}) &= t(\cos(k_x+k_y)\tau_z + \sin(k_x+k_y)\tau_y) \\ &\quad \oplus t(\cos(k_x-k_y)\tau_z + \sin(k_y-k_x)\tau_y) \end{aligned} \tag{7}$$

in the basis $\vec{\xi}_{\mathbf{k}} = (c_{-\mathbf{k}}, c^\dagger_{\mathbf{k}}, d_{-\mathbf{k}}, d^\dagger_{\mathbf{k}})^T$ and where 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 $(\Omega, \mathbf{T})$ 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 Fig. 1a,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 Fig.1c,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* $\hat{r}'(s) = e^{is(2\pi+\Omega)\tau_z/2}$, parameterized 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 Fig. 3a,b.

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 MBS to escape or enter the disclination core. This implies that, just as for the boundary modes of the topological p-wave wire[35], we can determine the parity of the zero-mode bound states pictorially in the tightly-bound limit. The MBSs of H_b and H_c at type-0 and type-1 $-90°$ disclinations are shown in Fig. 3c,d, where the MBSs are simply un-bonded 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.

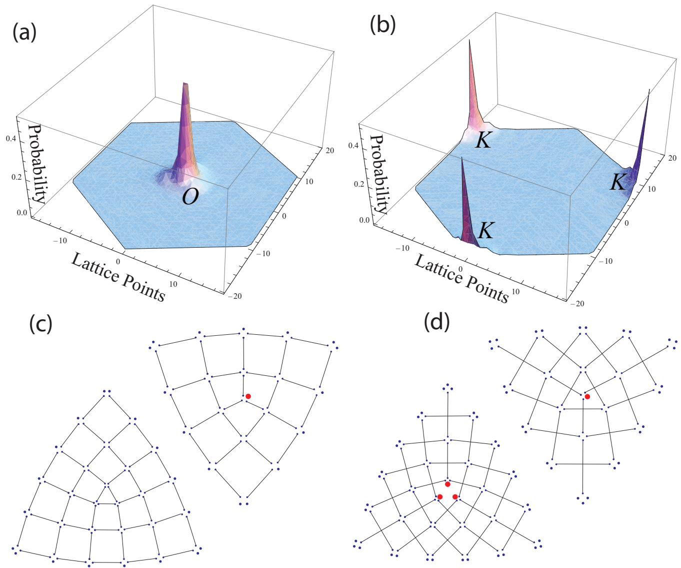

FIG. 3. (a,b) Exponentially localized probability density of the Majorana zero mode at disclinations O and K, plotted on a torus geometry where parallel sides on the hexagonal domain are identified. Compare with 3d lattice in Fig. 1. (c) Tight binding model H_b with (left) type-1 and (right) type-0 disclinations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

$-90°$ 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

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 (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.

We are now in a position to determine the index theorem since any C_4-symmetric BdG hamiltonian can be 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 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 $n_4(=2)$ non-zero 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 $1/4(ch)$ 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 $[1/2(n_4)+1/4(ch)+k(n_6)]$ mod $2=0$ 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 $[1/2(n_4)+(1/4)(ch)+(1/4)n_6+jn_7]$ mod $2=1$ 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 $1/4[ch+n_6+2n_4+3n_7]$ mod $2=0$, 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 non-zero 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 MBSs at a $-90°$ disclination. A $+90°$ disclination carries identical MBS parity since a $\pm 90°$ dipole of disclinations (of the same Type) combine into a dislocation with even Burgers' vector and thus *even* overall MBS 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:

$$\Theta \equiv \left[\frac{1}{2\pi}\mathbf{T}\cdot\mathbf{G}_\nu + \frac{\Omega}{2\pi}\left(ch+n_6+2n_4+3n_7\right)\right] \mod 2 \qquad (8)$$

where $\mathbf{G}_\nu$ is the weak $\mathbb{Z}_2$ invariant. The first term resembles the topological index for MBSs at a dislocation, with 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's. The second term of (8) is an integer because of the constraint (4) and can distinguish Chern numbers which are even or odd multiples of four *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 Fig. 3c,d). For Fig. 3c we see the boundary links carry one unbound Majorana each, and the corners contain two whereas in Fig. 3d the links carry two and the corners carry three. Since there is only one disclination, the parity of MBSs 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 MBSs (mod 2) on an edge with length $\mathbf{T}$, while $(ch+n_6+2n_4+3n_7)/4$ counts the Berry phase due to continuous rotation and the number of MBSs at a 90° corner. The index (8) therefore not only gives information about the disclination core, but also 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 MBSs in the form of corner states even in a defect and vortex free system.

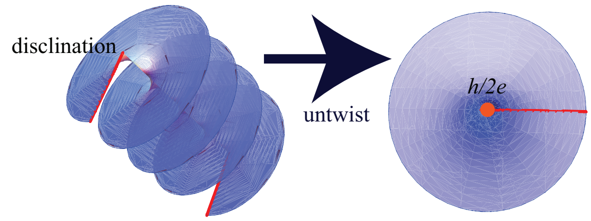

FIG. 4. Untwisting a $-90°$ disclination of the four layer p_x+ip_y continuum model H_4 into a single layer p_x+ip_y model with a quantum vortex.

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 $h_\phi=e^{i\phi\tau_z/2}h_0e^{-i\phi\tau_z/2}$, $h_0(\mathbf{k})=|\Delta|k_x\tau_z+|\Delta|k_y\tau_y+(m-\varepsilon k^2)\tau_z$. 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 MBS[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 $\chi_i=(ch,n_4,n_6,n_7)$ and a Z_2 index Θ determines the appearance of zero-energy MBSs at disclinations and sample corners. Although the index theorem relies on C_4 symmetry, MBS 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 MBSs 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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