New Class of Topological Superconductors Protected by Magnetic Group Symmetries

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We study a new type of three-dimensional topological superconductor that exhibits Majorana zero modes (MZM) protected by a magnetic group symmetry, a combined antiunitary symmetry composed of a mirror reflection and time reversal. This new symmetry enhances the noninteracting topological classification of a superconducting vortex from Z_2 to Z, indicating that multiple MZMs can coexist at the end of one magnetic vortex of unit flux. Especially, we show that a vortex binding two MZMs can be realized on the (001) surface of a topological crystalline insulator SnTe with proximity induced BCS Cooper pairing, or in bulk superconductor $In_xSn_{1-x}Te$.

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Topological superconductors are superconductors that are fully gapped in the bulk and yet possess gapless boundary excitations at zero-dimensional [1–3] (0D), one-dimensional (1D), or two-dimensional [4–8] (2D) boundaries, called Majorana zero modes (MZM), respectively [9–11]. 0D MZMs have so far received the most attention [2,9,12–17]. The proposals of realizing these states include vortex bound states in $p+ip$ superconductors [1], vortex bound states on surfaces of a strong topological insulator (TI) with induced s-wave superconductivity [3] and the end states of a spin-orbital coupled quantum wire with proximity induced s-wave superconductivity and subject to a strong Zeeman field [12–16].

In the above proposals of 0D MZM, a *single* MZM exists, while any two Majorana modes will hybridize and open a gap. In the presence of two or more Majorana modes, perturbations in the form $\Delta H = i\gamma_a\gamma_b$ can be added, where γ_a denotes a Majorana fermion operator of species a. Such perturbations gap Majorana modes in pairs, giving Z_2 topological classification of 0D systems with no symmetry. The existence of multiple Majorana modes requires symmetry to forbid their hybridization. For example, with (spinful) time-reversal symmetry (TRS), a pair of MZMs can appear if they make a Kramers' pair [4–6]. Local and unitary symmetries in general enhance the classification to Z^k, where $2k$ is the number of *complex* eigenvalues of the symmetry operator [18–21]. The nontrivial phases in these classes require intrinsic or induced unconventional superconductivity, with sign changes in the pairing amplitude between different Fermi surfaces.

Here we propose a new class of 3D topological superconductors that have multiple MZMs bound to each magnetic vortex core of unit flux on certain surface terminations. The hybridization between MZMs is prohibited by a nonlocal magnetic group symmetry: a vertical mirror plane reflection followed by TRS, denoted by M_T. This is the generic symmetry of any superconductor that (i) has a mirror symmetric lattice, (ii) has mirror symmetric and TRS invariant Cooper pairing, and (iii) is subject to an external magnetic field and/or Zeeman field parallel to the mirror plane. Neither mirror reflection nor TRS is a symmetry as they both invert the magnetic or Zeeman field which is a pseudo-vector, but their combination leaves the field invariant. This symmetry was first identified by Tewari and Sau [22] as a "new TRS" in quasi-1D superconducting quantum wires with Zeeman field along the length, which can protect multiple MZMs, but is absent when inter subband Rashba coupling is included; in Ref. [23], a spin-orbital coupled quasi-1D optical lattice is proposed which has this exact symmetry and therefore hosts multiple MZMs. In this Letter, we prove that the topological classification protected by M_T is Z in general, and then we show that a $z=2$ state (having two protected MZMs at each vortex core) can be realized on the (001) plane of a topological crystalline insulator [24–26] (TCI) SnTe with induced or intrinsic s-wave superconductivity on the surface. We expect that this phase can be realized in a (001)-thin-film SnTe deposited on an BCS-superconducting substrate such as $NbSe_2$ or bulk superconductor $In_xSn_{1-x}Te$.

In the type-II limit, the magnetic field penetrates into the superconductor in the form of vortex lines along the field direction. We take the limit where vortex lines are far away from each other and can be considered isolated. Now we terminate the system on a surface perpendicular to the mirror plane. A terminated vortex line has the particle-hole symmetry (PHS) and the magnetic group symmetry M_T. Assume that the end of a vortex line hosts several MZMs close to each other. Their Hamiltonian can be written in the PHS symmetric basis (Majorana basis) as

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$$\hat{H} = i\sum_{a,b}\mathcal{H}_{ab}\gamma_a\gamma_b, \quad (1)$$

where $\mathcal{H}_{ab}$ is a real skew-symmetric matrix. A matrix representation of M_T is in general

$$M_T = K\mathcal{M}, \quad (2)$$

where $\mathcal{M}$ is a unitary matrix and K is complex conjugation. Physically, we have the following constraints on the form of M_T: (i) it must commute with PHS and (ii) $M_T^2 = M^2 \times T^2 = -1 \times (-1) = 1$, as both mirror reflection and time reversal square to -1 for a spinful fermion. (Here, M and T represent operators for mirror reflection and TRS, respectively, in the single fermion Hilbert space.) They require that $\mathcal{M}$ be real and symmetric. Hence, the eigenvalues of $\mathcal{M}$ can only be ± 1. If M_T is a symmetry of $\hat{H}$, we have

$$[i\mathcal{H}, K\mathcal{M}] = \{\mathcal{H}, \mathcal{M}\} = 0. \quad (3)$$

Equation (3), after straightforward algebraic work [27], leads to the result that there are exactly $|\mathrm{tr}(\mathcal{M})|$ eigenvalues of $\mathcal{H}$ fixed at zero. Since $|\mathrm{tr}(\mathcal{M})|$ is an integer, there can be an integer number of MZMs at each end of the vortex line, giving rise to a Z classification.

We have yet to determine the physical requirements, including band structure and the form of Cooper pairing, for a nontrivial superconductor that supports such vortices to appear. In this Letter, we do not provide a general answer to this question, but instead provide a realization for each nontrivial phase in a class of heterostructures made of conventional BCS superconductors and new materials called topological crystalline insulators (TCI) having mirror symmetry and TRS. In TCI, the surface states have multiple Dirac points protected by mirror symmetries, if the surface termination is perpendicular to the mirror plane. Rock-salt (Pb,Sn)Te is a TCI having four Dirac cones on the (001)-surface [28–30]: two along $k_y = 0$ (denoted by $\mathbf{D}_{1,3}$) and two others along $k_x = 0$ ($\mathbf{D}_{2,4}$), protected by mirror planes of $M_{1\bar{1}0}$ and M_{110}, respectively. At the vicinity of each Dirac point, the low energy effective theory is that of 2D massless Dirac fermions [Fig. 1(a)]. We then assume that a Cooper pairing induced on the surface states preserves all lattice symmetries and TRS. In reality, this surface superconductivity can be proximity induced by a conventional BCS superconductor. We prove that given the induced superconductivity in SnTe, any vortex line along $\{001\}$ has two MZMs protected by M_T. Fourfold symmetry that is specific to this system can be broken without changing the result. An extension of the discussion [27] applies to a general TCI with induced superconductivity, showing that there are exactly $|C_M|$ MZMs at the end of a vortex line protected by M_T, where C_M is the mirror Chern number of the TCI.

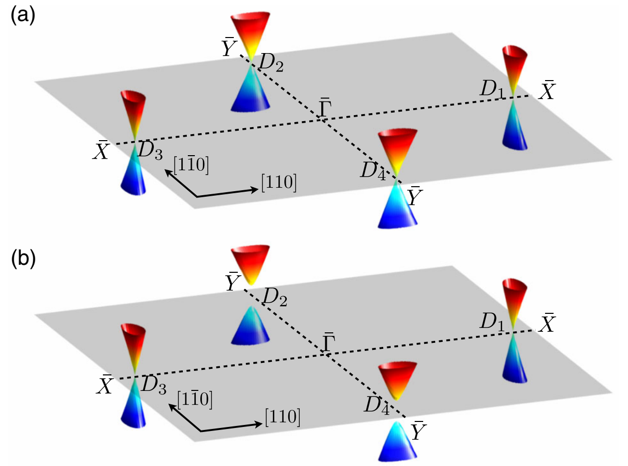

FIG. 1 (color online). (a) The dispersion of rocksalt SnTe (001)-surface bands, calculated using the model Eq. (12) with $t_1 = -1$, $t_2 = 0.5$, $m = 2.5$. (b) The dispersion of SnTe (001)-surface bands with rhombohedral distortion along the [111] direction, the strength of which is $\epsilon = 0.1$.

First, we consider the surface states in the normal state. At Dirac point $\mathbf{D}_1$, the effective Hamiltonian is in general given by $\hat{h}_1 = \sum_{|\mathbf{q}|<\Lambda,\tau,\tau'=\uparrow,\downarrow} h_1^{\tau\tau'}(\mathbf{q}) f_{1\tau}^\dagger(\mathbf{q}) f_{1\tau'}(\mathbf{q})$, where $f_{1\tau}(\mathbf{q})$ is the annihilation operator at $\mathbf{k} = \mathbf{D}_1 + \mathbf{q}$ with pseudospin τ, denoting each state of the degenerate doublet at $\mathbf{D}_1$. The form of $h_1(\mathbf{q})$ is fixed by choosing the representation of the little group at $\mathbf{D}_1$ [31] to be $M_{1\bar{1}0} = i\sigma_y$ and $C_{2T} = K\sigma_x$, where $C_{2T} = C_2 * T$ is a twofold rotation followed by TRS. Using the symmetry constraint $[C_{2T}, \hat{h}_1] = [M_{1\bar{1}0}, \hat{h}_1] = 0$, we have,

$$h_1(\mathbf{q}) = v_0 q_x \sigma_0 + v_1 q_x \sigma_y + v_2 q_y \sigma_x \quad (4)$$

up to the first order of $|\mathbf{q}|$. Here the sign of v_1 is determined by the sign of C_M, while other parameters are related to details of the system. Using C_4 symmetry, we can fix the gauge for Dirac cones centered at $D_{2,3,4}$: $f_{2,3,4}(C_4\mathbf{q}) \equiv C_4 f_{1,2,3}(\mathbf{q}) C_4^{-1}$, where $C_4\mathbf{q}$ is $\mathbf{q}$ rotated by $\pi/2$, by which we have

$$h_1(\mathbf{q}) = h_2(C_4\mathbf{q}) = h_3(C_2\mathbf{q}) = h_4(C_4^{-1}\mathbf{q}). \quad (5)$$

In Table I, we list how $f_{i\tau}$ transforms under $C_{4v} \otimes T$, the full symmetry group of the (001) plane.

Next, we consider the Cooper pairing on the surface that does not break any lattice symmetry or TRS, such as that induced by a conventional BCS superconductor. A generic expression of a Cooper pairing with zero momentum is $\hat{\Delta} = \sum_{\mathbf{q}} f_1^T(\mathbf{q}) \Delta_X f_3(-\mathbf{q}) + f_2^T(\mathbf{q}) \Delta_Y f_4(-\mathbf{q}) + \mathrm{H.c.} + O(|\mathbf{q}|)$. Here we note that, since $f_{1,2,3,4}(\mathbf{q})$ carry momentum around $\mathbf{D}_{1,2,3,4}$, other intercone pairings and intracone pairings are not allowed, as both lead to pairs of finite total momentum. Using Table I, we find the only possible form of $\Delta_{X,Y}$ that preserves all symmetries is

TABLE I. Transformation of operators under C_{4v} and TRS.

	f_1	f_2	f_3	f_4
$M_{1\bar{1}0}$	$(i\sigma_y)f_1$	$(-i\sigma_y)f_4$	$(-i\sigma_y)f_3$	$(-i\sigma_y)f_2$
M_{110}	$(-i\sigma_y)f_3$	$(i\sigma_y)f_2$	$(-i\sigma_y)f_1$	$(-i\sigma_y)f_4$
T	$-\sigma_x f_3$	$-\sigma_x f_4$	$\sigma_x f_1$	$\sigma_x f_2$
C_4	f_2	f_3	f_4	$-f_1$

$$\Delta_X = \Delta_Y = \Delta_0 \sigma_x, \tag{6}$$

where Δ_0 is a real number representing the pairing amplitude. Combining Eqs. (4)–(6), we obtain the BdG Hamiltonian as

$$\begin{aligned}\hat{H}_0 &= \sum_{|\mathbf{q}|<\Lambda} \Big\{ \sum_i f_i^\dagger(\mathbf{q}) h_i(\mathbf{q}) f_i(\mathbf{q}) \\ &\quad + \Delta_0 [f_1^T(\mathbf{q})\sigma_x f_3(-\mathbf{q}) + f_2^T(\mathbf{q})\sigma_x f_4(-\mathbf{q}) + \mathrm{H.c.}] \Big\} \\ &= \sum_{\mathbf{r}} \Big\{ \sum_i f_i^\dagger(\mathbf{r}) h_i(-i\nabla) f_i(\mathbf{r}) \\ &\quad + \Delta_0 [f_1^T(\mathbf{r})\sigma_x f_3(-\mathbf{r}) + f_2^T(\mathbf{r})\sigma_x f_4(-\mathbf{r}) + \mathrm{H.c.}], \end{aligned} \tag{7}$$

where in the second line we have defined $f_i(\mathbf{r}) \equiv (1/\sqrt{N})\sum_{|\mathbf{q}|<\lambda} f_i(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}}$ in real space. Since $f_i(\mathbf{q})$ has momentum, $\mathbf{D}_i + \mathbf{q}$, $f_i(\mathbf{r})$ represents the slowly oscillating part of the wave function. The energy dispersion of Eq. (7) is

$$E(\mathbf{q}) = \pm\sqrt{\left(v_0 q_y - \mu \pm \sqrt{v_1^2 q_x^2 + v_2^2 q_y^2}\right)^2 + \Delta_0^2}, \tag{8}$$

where each band is fourfold degenerate. Equation (8) shows that the bulk is a fully gapped superconducting state for any parameter set with $\Delta_0 \neq 0$. A superconducting vortex is created by replacing the constant pairing amplitude Δ_0 with a spatially varying function having winding number $+1$ (the case of -1 can be similarly discussed). Here we take

$$\Delta_0 \to \Delta(r) e^{i\theta} \tag{9}$$

written in polar coordinates, where $\Delta(r)$ is a monotonic real function of r that satisfies $\Delta(0) = 0$ and $\Delta(\infty) = \Delta_0$. The vortex bound state(s) can be found by diagonalizing Eq. (7) after the substitution of Eq. (9). As we have mentioned, all parameters except the sign of v_1 can be adiabatically changed, so here we take $v_0 = \mu = 0$ and $-v_2 = v_1 \equiv v$ without changing the topological class of the vortex. For these parameters, the bound state problem can be solved analytically. There are four MZMs, given by

$$\begin{aligned}\gamma_1 &= \sum_{\mathbf{r}} (f_{1\downarrow}(\mathbf{r}) \pm f_{3\downarrow}(\mathbf{r}) + \mathrm{H.c.}) e^{-\int_0^r |\Delta(r')| dr'}, \\ \gamma_2 &= \sum_{\mathbf{r}} (e^{i\pi/4} f_{2\downarrow}(\mathbf{r}) \pm e^{i\pi/4} f_{4\downarrow}(\mathbf{r}) + \mathrm{H.c.}) e^{-\int_0^r |\Delta(r')| dr'}, \\ \gamma_3 &= \sum_{\mathbf{r}} (i f_{3\downarrow}(\mathbf{r}) \mp i f_{1\downarrow}(\mathbf{r}) + \mathrm{H.c.}) e^{-\int_0^r |\Delta(r')| dr'}, \\ \gamma_4 &= \sum_{\mathbf{r}} (e^{i3\pi/4} f_{4\downarrow}(\mathbf{r}) \mp e^{i3\pi/4} f_{2\downarrow}(\mathbf{r}) + \mathrm{H.c.}) e^{-\int_0^r |\Delta(r')| dr'}, \end{aligned} \tag{10}$$

where the upper or lower sign is taken if $\mathrm{sgn}[v_1\Delta_0] = +/-$ and the normalization factors are omitted. $M_T \equiv M_{xz} \times T$ is a symmetry of the system with vortex, and using Table I, we obtain the matrix representation of $M_T = K\mathcal{M}$ in the basis furnished by $\gamma_{1,2,3,4}$:

$$\mathcal{M} = \mathrm{sgn}[v_1\Delta_0] \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \tag{11}$$

Since $\mathrm{tr}(\mathcal{M}_T) = 2\mathrm{sgn}[v_1\Delta_0]$, there are two MZMs that are topologically protected by M_T. Although $\mathcal{M}_T$ is evaluated using the explicit forms of bound state solutions, its trace is a good quantum number invariant under any adiabatic change of parameters. While we have four MZMs given in Eq. (10), only two are protected. This is because one can write down a perturbation $\Delta\hat{H} = i\lambda(\gamma_1\gamma_2 + \gamma_2\gamma_3 + \gamma_3\gamma_4 + \gamma_4\gamma_1)$ that preserves M_T and gaps two out of the four MZMs. This perturbation does not break the fourfold rotation symmetry either, which means that C_4 symmetry here does not lead to additional degeneracy. A more detailed study in Ref. [27] shows that when the size of the vortex is far greater than the lattice constant, the above perturbation is very small and the other two modes will hence be very close to the zero energy.

We have so far assumed that the Fermi level is inside the bulk gap of the 3D system, making it sufficient to consider only the surface electrons. This assumption is impractical for experimentally realizing and measuring the MZMs because when the Fermi level is inside the bulk gap, the proximity-induced SC decays exponentially fast away from the interface, leaving too small a superconducting gap on the open surface for measurements. Therefore, we must find out if the above results hold when the Fermi level is inside the conduction or valence bands. Generically, a vortex line undergoes a quantum phase transition at some critical chemical potential μ_c inside the bulk bands, at which the MZMs localized at the two ends extend into the bulk of the line and hybridize [32–34]. Below we numerically confirm this picture in 3D SnTe.

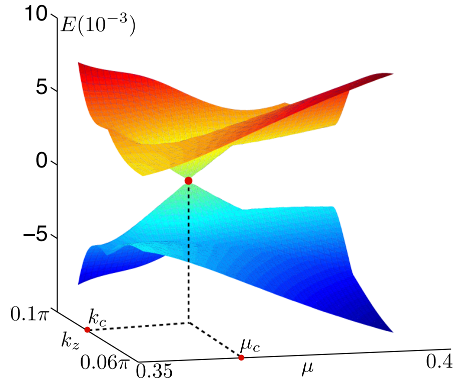

FIG. 2 (color online). The dispersion of the lowest bands in the vortex line as a function of k_z and chemical potential μ close to the critical point where the band gap closes at (k_c, μ_c). Because of PHS, there is another band crossing at $(-k_c, \mu_c)$.

We develop a 3D tight-binding model to describe the normal state of the TCI

$$\begin{aligned} H(\mathbf{k}) = & [m - t_1(\cos 2k_x + \cos 2k_y + \cos 2k_z)]\Sigma_{z0} \\ & + t_2[\sin k_x(\cos k_y + \cos k_z)\Sigma_{xx} \\ & + \sin k_y(\cos k_x + \cos k_z)\Sigma_{xy} \\ & + \sin k_z(\cos k_x + \cos k_y)\Sigma_{xz}], \end{aligned} \tag{12}$$

where $\Sigma_{ij} \equiv \sigma_i \otimes \sigma_j$ and the parameters are chosen as $\{m, t_1, t_2\} = \{2.5, -1.0, 0.5\}$. The model has cubic symmetry and TRS, and the BZ of this model is that of an fcc lattice (same as the real material); the symmetry group generators are given by the following matrices: $C_{4z} = \sigma_0 \otimes e^{i\sigma_z \pi/4}$, $C_{4x} = \sigma_0 \otimes e^{i\sigma_x \pi/4}$, $P = \Sigma_{z0}$, and $T = K(i\Sigma_{0y})$. The model gives the correct topological surface states as shown in Fig. 1. An onsite s-wave pairing with a vortex line is given by $\Delta(\mathbf{r}) = \Delta(\sqrt{x^2 + y^2})e^{i\theta}(i\Sigma_{02})$. We take the simplest form of $\Delta(r)$: $\Delta(r) = 0$ for $r < r_0$ and $\Delta(r) = \Delta_0$ for $r \geq r_0$. We solve the eigenvalue problem of a vortex line with periodic boundary along the z axis, and plot the energy spectrum against increasing chemical potential in Fig. 2. The result shows that the phase transition happens at critical chemical potential $\mu_c > \mu_b$, where μ_b is the minimum of the conduction band. (In the particular parameter set we choose to calculate Fig. 2, $\mu_c \approx 0.38$ and $\mu_b \approx 0.23$.) We note that there are two gap closings at μ_c with $k_z = \pm k_c$, in contrast to just one closing in Ref. [32], because here the transition is between a vortex line having two MZMs and one having none.

Now we discuss the effect of the spontaneous rhombohedral distortion of SnTe at low temperatures, which has attracted theoretical and experimental attention [25,31,35]. The lattice distortion is equivalent to a small strain tensor $\varepsilon_{xy} = \varepsilon_{yz} = \varepsilon_{xz} = \varepsilon$, which breaks both C_2 and $M_{1\bar{1}0}$. It opens gaps at two Dirac points along the $\bar{\Gamma}\bar{Y}$ direction, leaving the other two gapless, as $M_{1\bar{1}0}$ is preserved. The strain gaps at $D_{2,4}$ can also be observed in our TB model adding a perturbation (one could verify that it transforms the same way as the strain tensor under the point group) $\epsilon[(\cos 2k_x - \cos 2k_y)\sin 2k_z + (\cos 2k_y - \cos 2k_z)\sin 2k_x + (\cos 2k_z - \cos 2k_x)\sin 2k_y]\Sigma_{y0}$ [see Fig. 1(b)]. However, this effect does not entail any topological transition in the vortex line. This is because the two MZMs at each end are protected by $M_T \equiv M_{1\bar{1}0} \times T$, unbroken by the strain.

Based on the theory, we design a simple TCI-SC heterostructure to realize the nontrivial state with $z = 2$. A thin-film SnTe is deposited on the top of a conventional superconductor such as $NbSe_2$. The Fermi level in the thin film is tuned through gating to a value inside but near the edge of the conduction or valence band ($\mu_b < |\mu| < \mu_c$). When the Fermi level is in the bulk bands, the proximity-induced SC pairings on the bottom layer of SnTe extend to the bulk with a power law decay. Therefore, on the top layer the SC pairing is still finite, and the whole thin film has an induced pairing that preserves all lattice symmetries and TRS. According to our theory, an isolated magnetic vortex in the thin film can bind exactly two MZMs on the top surface, which may be observed through tunneling measurements. Following a discussion similar to that presented in Ref. [36], we expect a zero bias conductance peak of intensity $4e^2/h$, if the tip is correctly located at the vortex. While the intrinsic rhombohedral strain as discussed above cannot open a gap between the MZMs, an applied strain which also breaks $M_{1\bar{1}0}$ can break the double degeneracy, making the vortex line fully gapped, and the peak splits into two at nonzero voltages with intensity $2e^2/h$ each. The vortex bound MZMs may also be realized in superconducting $In_xSn_{1-x}Te$, if the bulk superconducting gap is *trivial*, in contrast to some theoretical proposals. The proposed nontrivial odd parity pairing in the bulk leads to 2D Majorana modes, while here we have shown that even if the bulk gap is trivial, two MZMs can still be observed at vortex lines that are parallel to the mirror planes of the crystal, given that the Fermi energy is in the inverted regime at the edge of the bulk bands.

For the general case of a noninteracting TCI with mirror Chern number C_m, we can similarly prove that a vortex line parallel to the mirror plane can bind exactly C_m MZMs at each end. If an interaction, i.e., a four-Majorana term, is added to the system, the Z classification of a vortex line reduces to Z_8 without breaking any symmetry. If $C_m = \pm 4$, the noninteracting ground state is fourfold degenerate, but a four-Majorana interaction, in the form $\lambda\gamma_1\gamma_2\gamma_3\gamma_4$ lifts the degeneracy down to twofold. If $C_m = \pm 8$, the noninteracting ground state is 16-fold degenerate, but a four-Majorana interaction that breaks the SO(8) symmetry (rotation symmetry in the flavor space) renders the many-body ground state nondegenerate [37].

Finally, we discuss limitations of the theory. It presumes mirror symmetry in zero field, which is equivalent to the pure limit, because exact mirror symmetry is broken by any type of impurities. However, randomly distributed impurities may preserve mirror symmetry "on average" [38]. For this reason, the theory also applies in the case of many impurities if the size of the vortex is much larger than the average spacing of impurities, as long as the impurity intensity is much weaker than the superconducting gap. We also require the vortices to be sufficiently separated from each other such that the size of the Majorana fermions is much smaller than their average spacing. In our discussion, the magnetic field only supplies the vortex while the Zeeman field is ignored. The Zeeman field preserves M_T and hence does not hybridize the MZMs, but we require that its strength not exceed the superconducting gap.

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[27] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.112.106401 for (i) a proof that the number of MZMs equal the trace of $\mathcal{M}$, (ii) generalization of the results to systems whose normal state has a general mirror Chern number and (iii) a short discussion of why the other two vortex bound states, not protected by $M * T$, may also have close to zero energy, when large-momentum scattering is suppressed and the vortex size is much larger than the lattice constant.
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