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Topological Nonsymmorphic Crystalline Superconductors

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Topological superconductors possess a nodeless superconducting gap in the bulk and gapless zero energy modes, known as "Majorana zero modes", at the boundary of a finite system. In this work, we introduce a new class of topological superconductors, which are protected by nonsymmorphic crystalline symmetry and thus dubbed "topological nonsymmorphic crystalline superconductors". We construct an explicit Bogoliubov-de Gennes type of model for this superconducting phase in the D class and show how Majorana zero modes in this model are protected by glide plane symmetry. Furthermore, we generalize the classification of topological nonsymmorphic crystalline superconductors to the classes with time reversal symmetry, including the DIII and BDI classes, in two dimensions. Our theory provides a guidance to search for new topological superconducting materials with nonsymmorphic crystal structures.

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I. INTRODUCTION

The research on topological superconductors (TSCs) has attracted intensive interests due to its gapless boundary excitations, known as the "Majorana zero modes"[1–15], with intrinsically non-local nature and exotic exchange statistics, and aims in the potential applications in low-decoherence quantum information processing and topological quantum computations[16–19]. The search for new topological superconducting phases and materials is a substantial step for this goal.

The first classification of TSCs (and also other topological insulating phases) was achieved by Schnyder *et al.*[20] based on Altland-Zirnbauer symmetry class[21,22] for the systems with or without particle-hole symmetry (PHS), time reversal symmetry(TRS) and their combination, the so-called chiral symmetry. Later, it was realized that when additional symmetry exists in a system, new topological phases can be obtained, and the gapless edge/surface modes require the protection from additional symmetry. In particular, it has been shown that new topological insulating and superconducting phases emerge when the system has mirror symmetry and are dubbed "topological mirror insulators"[23–27] and "topological mirror superconductors"[25,28–30], respectively. Recent work has also revealed that nonsymmorphic symmetry, including glide plane symmetry and screw axis symmetry, can lead to new topological insulating phases, as well as topological semi-metal phases[31–35]. In this work, we are interested in the role of the nonsymmorphic crystalline symmetry, mainly glide plane symmetry, in the classification of TSCs. We focus on the following three questions: (1) are there any topologically non-trivial phases that are protected by glide plane symmetry? (2) What's the difference between glide plane symmetry and mirror symmetry in the classification of TSCs? (3) What's the relationship between this superconducting phase and other TSCs? Below, we will first discuss the role of glide plane symmetry in the classification of superconducting gap functions, which indicates the possibility of topological superconductors protected by glide plane symmetry, thus dubbed "topological nonsymmorphic crystalline superconductors (TNCSc)". We also construct an explicit tight-binding model in the D class with boundary Majorana zero modes and demonstrate that the existence of Majorana zero modes comes from nonsymmorphic symmetry of this model. Finally, we discuss the relationship between TNSCs and weak TSCs and generalize TNCSc to the classes DIII and BDI with time reversal symmetry for both spinless and spin-$\frac{1}{2}$ fermions.

II. NONSYMMORPHIC SYMMETRY AND SUPERCONDUCTING GAP FUNCTION

In this section, we will first consider the role of glide plane symmetry in the classification of superconducting gap functions. We start from a generic Bogoliubov-de Gennes (BdG) type of Hamiltonian of superconductors with nonsymmorphic symmetry in the normal states, which can be written in the momentum space as

$$H = \frac{1}{2}\sum_{\mathbf{k}}(c^\dagger_{\mathbf{k}}, c^T_{-\mathbf{k}})H_{BdG}\begin{pmatrix} c_{\mathbf{k}} \\ c^{\dagger T}_{-\mathbf{k}} \end{pmatrix}$$

with

$$H_{BdG} = \begin{pmatrix} h(\mathbf{k}) - \mu & \Delta(\mathbf{k}) \\ \Delta^\dagger(\mathbf{k}) & -h^*(-\mathbf{k}) + \mu \end{pmatrix}, \qquad (1)$$

where $h(\mathbf{k})$ is for single-particle Hamiltonian of normal states, μ is the chemical potential and Δ denotes the superconducting gap function. $c_{\mathbf{k}}$ is an annihilation operator with n components and we also use $c_{\mathbf{k},\alpha}$ ($\alpha = 1, ..., n$) to denote each component with $\alpha = \{s, l\}$ for spins s and orbitals(lattice sites) l. The superconducting gap function is related to annihilation operators by $\Delta_{\alpha,\beta}(\mathbf{k}) = V_0\langle c_{\mathbf{k},\beta}c_{-\mathbf{k},\alpha}\rangle$, where V_0 is the strength of attractive interactions. The BdG Hamiltonian satisfies the PHS $CH_{BdG}(\mathbf{k})C^{-1} = -H_{BdG}(-\mathbf{k})$ with the PHS operator $C = \tau_1 \times \mathbb{I}K$, where τ_1 is the first Pauli matrix acting on the Nambu space, $\mathbb{I}$ is an $n \times n$ unit matrix and K is complex conjugation. The PHS (or Fermi statistics) requires the constraint $\Delta(\mathbf{k}) = -\Delta^T(-\mathbf{k})$ for the gap function.

Next, we consider how the nonsymmorphic symmetry yields constraint on the forms of single-particle Hamiltonian and superconducting gap functions in a nonsymmorphic crystal. Here we consider the glide plane symmetry, represented by $g = \{m|\tau\}$ where m is a mirror operator and τ is a non-primitive translation operator along a direction within the mirror plane. For single-particle Hamiltonian, the glide plane symmetry requires $D^\dagger_{\mathbf{k}}(g)h(\mathbf{k})D_{\mathbf{k}}(g) = h(g\mathbf{k})$, where $D_{\mathbf{k}}(g)$ is the representation matrix for glide plane symmetry at the momentum $\mathbf{k}$ and defined as $gc^\dagger_{\mathbf{k},\alpha}g^{-1} = \sum_\beta D^*_{\mathbf{k},\alpha\beta}(g)c^\dagger_{g\mathbf{k},\beta}$[36]. Here we emphasize that the representation matrix for glide plane symmetry takes the form $D_{\mathbf{k}}(g) = e^{i\mathbf{k}\cdot\tau}D(m)$, where $e^{i\mathbf{k}\cdot\tau}$ is a phase factor due to a non-primitive translation and $D(m)$ is the projective representation of mirror operator m. For the case with only glide plane symmetry, all the projective representations are one dimensional (1D) and equivalent to the conventional representations.

The symmetry of the gap function $\Delta(\mathbf{k})$ is determined by the Cooper pair wave functions, which transform as the direct product of the representation $D^\dagger_{\mathbf{k}}(g) \otimes D^*_{-\mathbf{k}}(g)$[36]. For the case with only glide plane symmetry, all the 1D representations can be labeled by $D_{\mathbf{k}}(g) = e^{i\mathbf{k}\cdot\tau}D(m) = \delta e^{i\mathbf{k}\cdot\tau}$ where $\delta = \pm i$ for spin-$\frac{1}{2}$ systems and $\delta = \pm 1$ for spinless systems. Thus, the gap function should transform as $D^\dagger_{\mathbf{k}}(g)\Delta(\mathbf{k})D^*_{-\mathbf{k}}(g) = \eta\Delta(g\mathbf{k})$, where $\eta = \pm$ applies for both the spin-$\frac{1}{2}$ and spinless systems and depends on the nature of superconducting gap functions[36]. We will show how to classify different superconducting gap functions based on glide plane symmetry explicitly for a model Hamiltonian in the next section.

We emphasize that the superconducting gap function may preserve ($\eta = +$) or spontaneously break ($\eta = -$) glide plane symmetry. Nevertheless, similar to the case of inversion symmetry[37,38] or mirror symmetry[29], one can always re-define a glide plane symmetry operation as $G_\eta(\mathbf{k}) = Diag[D_{\mathbf{k}}(g), \eta D^*_{-\mathbf{k}}(g)]$ for the BdG type of Hamiltonian, which satisfies the condition $G^{-1}_\eta(\mathbf{k})H_{BdG}(\mathbf{k})G_\eta(\mathbf{k}) = H_{BdG}(g\mathbf{k})$. In this way, we can regard the BdG Hamiltonian as a semiconductor Hamiltonian with additional PHS.

Due to the existence of the glide plane symmetry $G_\eta(\mathbf{k})$, the eigenstates $\psi(\mathbf{k})$ of the BdG Hamiltonian, $H_{BdG}\psi(\mathbf{k}) = E\psi(\mathbf{k})$, can also be chosen to be the eigenstate of $G_\eta(\mathbf{k})$, $G_\eta(\mathbf{k})\psi(\mathbf{k}) = \delta_\eta e^{i\mathbf{k}\cdot\tau}\psi(\mathbf{k})$, on the glide invariant plane (GIP) in the momentum space, $g\mathbf{k} = \mathbf{k}$ (mod $\mathbf{P}$), where $\mathbf{P}$ is a reciprocal lattice vector. Here δ_η is given by $\pm$ ($\pm i$) for the spinless (spin-$\frac{1}{2}$) systems and we call the eigenvalue $\delta_\eta e^{i\mathbf{k}\cdot\tau}$ as glide parity. Next, we look at the relationship of glide parities between one eigenstate $\psi(\mathbf{k})$ and its

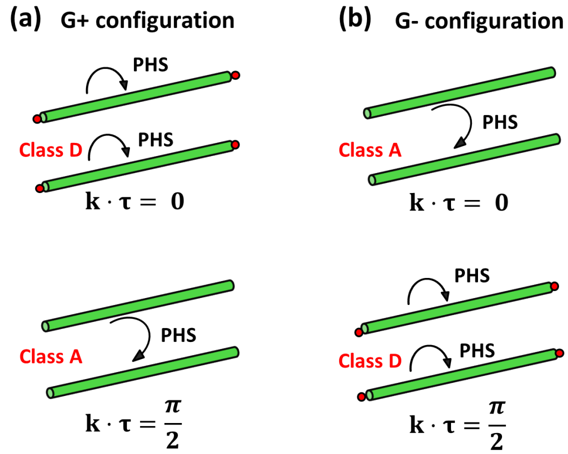

FIG. 1. (Color online). Two different configurations for $G_\pm(\mathbf{k})$. For $G_+(G_-)$, the Hamiltonian symmetry class is D(A) along $\mathbf{k}\cdot\tau = 0$ lines; while along $\mathbf{k}\cdot\tau = \frac{\pi}{2}$ lines, the Hamiltonian symmetry class is A(D). The red dots denote possible Majarona zero modes at ends of the lines.

partner $\tilde{\psi}(-\mathbf{k}) = C\psi(\mathbf{k})$ under PHS. Direct calculation gives $G_\eta(-\mathbf{k})\tilde{\psi}(-\mathbf{k}) = \eta\delta^*_\eta e^{-i\mathbf{k}\cdot\tau}\tilde{\psi}(-\mathbf{k})$ by using that $CG_\eta(\mathbf{k})C^{-1} = \eta G_\eta(-\mathbf{k})$[36]. Therefore, $\psi_{\mathbf{k}}$ and its particle-hole partner $\tilde{\psi}_{-\mathbf{k}}$ possess glide parity $\delta_\eta e^{i\mathbf{k}\cdot\tau}$ and $\eta\delta^*_\eta e^{-i\mathbf{k}\cdot\tau}$, respectively. This leads to the conclusion as depicted in Fig. 1. When the gap function satisfies $G_+(\mathbf{k})$ symmetry, for the spinless (spin-$\frac{1}{2}$) systems, $\psi_{\mathbf{k}}$ and its particle-hole partner $\tilde{\psi}_{-\mathbf{k}}$ share the same glide parity along the momentum line $\mathbf{k}\cdot\tau = 0$ ($\mathbf{k}\cdot\tau = \frac{\pi}{2}$) on the GIP, while they have opposite glide parities along the momentum line $\mathbf{k}\cdot\tau = \frac{\pi}{2}$ ($\mathbf{k}\cdot\tau = 0$) on the GIP. When the gap function satisfies $G_-(\mathbf{k})$ symmetry, we find an opposite behavior for the momentum lines $\mathbf{k}\cdot\tau = 0$ and $\mathbf{k}\cdot\tau = \frac{\pi}{2}$, compared to the case of $G_+(\mathbf{k})$ symmetry. We notice that the momentum line $\mathbf{k}\cdot\tau = \frac{\pi}{2}$ corresponds to the BZ boundary since 2τ is a primitive lattice vector of the system.

Here we emphasize different roles of glide plane symmetry and mirror symmetry for the BdG Hamiltonian of superconductivity. For the glide plane symmetry $g = \{m|\tau\}$ and the corresponding mirror symmetry m, the GIP and the mirror invariant plane are the same. As shown in Ref. 29, the PHS either preserves the subspace with a fixed mirror parity or transforms the subspace with one mirror parity to the other. In contrast, due to the additional phase factor from the non-primitive translation of glide plane symmetry, the behaviors of PHS acting on the glide parity subspaces are always opposite for the momentum lines $\mathbf{k}\cdot\tau = 0$ and $\mathbf{k}\cdot\tau = \frac{\pi}{2}$. This prevents us to define a topological invariant on the whole 2D GIP since two glide parity subspaces are always "connected" to each other. However, if we limit the glide parity subspace only on the momentum line $\mathbf{k}\cdot\tau = 0$ or $\mathbf{k}\cdot\tau = \frac{\pi}{2}$, the PHS will either preserve the glide parity subspace or transform the subspace with one glide parity to the other, similar to the case of mirror symmetry. This immediately suggests the possibility of defining topological invariants on the 1D momentum lines $\mathbf{k}\cdot\tau = 0$ or $\mathbf{k}\cdot\tau = \frac{\pi}{2}$ for superconductors with glide plane symmetry. Below, we will present explicitly a BdG type of model Hamiltonian with glide plane symmetry and show the existence of Majorana zero modes at the boundary. Then we will discuss bulk topological invariants and the corresponding topological classification.

III. MODEL HAMILTONIAN IN THE D CLASS

Our spinless fermion model with glide plane symmetry is based on a two dimensional (2D) rectangle lattice with two sets of equivalent sites, as shown by A and B sites in Fig. 2(a) and (b). The glide plane symmetry operator is given by $g_z = \{m_z|\tau = (\frac{a}{2}, 0, 0)\}$ with a reflection m_z along the z direction followed by a translation of $a/2$ along the x direction (a is a lattice constant), and relates the A sites to the B sites. The normal state Hamiltonian reads

$$h(\mathbf{k}) = \epsilon(\mathbf{k})\sigma_0 + t_3 cos(\frac{(k_x-\phi)a}{2})cos(\frac{k_x a}{2})\sigma_1 + t_3 cos(\frac{(k_x-\phi)a}{2})sin(\frac{k_x a}{2})\sigma_2 \quad (2)$$

on the basis $|A,\mathbf{k}\rangle$ and $|B,\mathbf{k}\rangle$, where $\epsilon(\mathbf{k}) = m_0 + t_1 cos(k_x a) + t_2 cos(k_y a)$, σ_0 is a 2×2 unit matrix, σ_i with $i = 1, 2, 3$ are Pauli matrices that describe the A and B sites and ϕ depends on the choice of orbitals[36]. Furthermore, the glide plane symmetry operator on such a basis is $D_{\mathbf{k}}(g) = e^{i\frac{k_x a}{2}}(cos(\frac{k_x a}{2})\sigma_1 + sin(\frac{k_x a}{2})\sigma_2)$. One can easily check that $D^2_{\mathbf{k}}(g) = e^{ik_x a}$ and $D^{-1}_{\mathbf{k}}(g)H(k_x, k_y)D_{\mathbf{k}}(g) = H(k_x, k_y)$.

As discussed above, the gap functions can be classified according to glide plane symmetry and when the glide plane symmetry for the BdG Hamiltonian is G_η, the gap function satisfies three conditions: $\Delta^T(\mathbf{k}) = -\Delta(-\mathbf{k})$ (PHS); $D^\dagger_{\mathbf{k}}(g)\Delta(\mathbf{k})D^*_{-\mathbf{k}}(g) = \eta\Delta(g\mathbf{k})$ (glide plane symmetry) and $\Delta(\mathbf{k}) = \Delta(\mathbf{k}+\mathbf{G})$[36]. The complete classificaiton of gap functions for this model Hamiltonian is discussed in the Supplemental Material[36]. Here we only consider two typical gap functions $\Delta_+ = \Delta_0 sin(k_y a)\sigma_0$ and $\Delta_- = \Delta_0 sin(k_y a)\sigma_3$ with the symmetries G_+ and G_-, respectively. We take the BdG Hamiltonian (Eq. 1) with the single-particle Hamiltonian (Eq. 2) and the gap function $\Delta_\pm$ and calculate energy dispersion of this Hamiltonian on a slab configuration. The slab is chosen to be infinite along the x direction and finite along the y direction, so that the glide plane symmetry g_z is still preserved. The energy dispersion is shown in Fig. 2 (c) for Δ_+ and (d) for Δ_-. In both cases, one can find two edge bands appearing in the bulk superconducting gap at one edge. However, these two edge bands cross at zero energy and give rise to Majorana zero modes at Γ for Δ_+ (Fig. 2(c)), but at X for Δ_- (Fig. 2(d)).

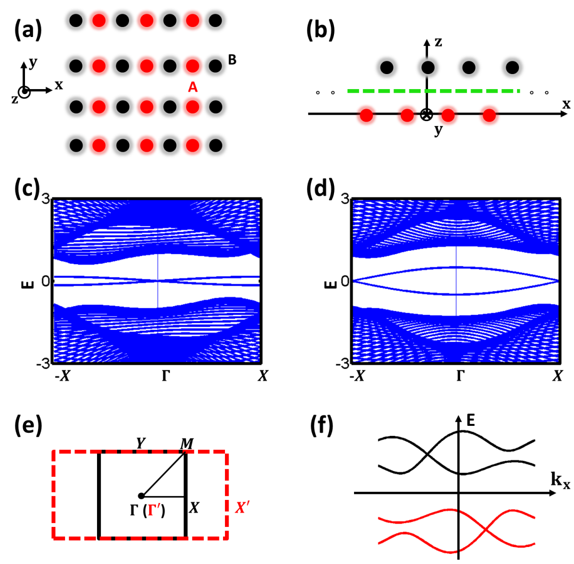

FIG. 2. (Color online). (a) and (b), Schematic plots of the lattice structure from top view and side view. They are 1D chains along y direction. There are two inequivalent atom sites, denoted as A(Red ball) and B(Black ball), respectively. A plane passing through the dashed green line is the glide plane. (c) Edge modes for G_+ configuration with Δ_+. (d) Edge modes for G_- configuration with Δ_-. (e) Brillouin zone(Black square) and extended Brillouin zone(Red dashed rectangle) defined by glide plane symmetry. (f) A general dispersion for a 1D chain with glide plane symmetry.

The underlying physical reason of different positions of Majorana zero modes for these two cases comes from the relation between glide plane symmetry and PHS discussed in the last section. Let's take the case of the gap function Δ_+ with G_+ symmetry as an example. The state $\psi_{\mathbf{k}}$ and its particle-hole partner $\tilde{\psi}_{-\mathbf{k}}$ share the same glide parity at Γ ($k_x = 0$), and thus it is possible for them to be the same state. Since PHS changes the energy E of $\psi_{\mathbf{k}}$ to $-E$ of $\tilde{\psi}_{-\mathbf{k}}$, the eigen energy must be zero once they are the same state. This analysis also suggests that two Majorana zero modes at Γ must belong to different glide parity subspace, and thus no coupling is allowed between them to open a gap. In contrast, the glide parities for $\psi_{\mathbf{k}}$ and $\tilde{\psi}_{-\mathbf{k}}$ are opposite at X ($k_x = \frac{\pi}{a}$). Thus, these two states must be different at X and PHS can not require their energies to be zero. This analysis can also be applied to Δ_- with G_- symmetry and leads to the opposite conclusion. Another intuitive picture to prove non-trivial properties of 1D edge modes in Fig. 2 (c) and (d) is to consider a general one dimensional superconductor with glide plane symmetry. As shown in Ref. 32–34, due to the glide plane symmetry, all the bands must appear in pairs, as shown schematically by two black lines (two bands with opposite glide parities) in Fig. 2 (f). Furthermore, the PHS of superconductivity requires two additional hole bands at the negative energy, as shown by two red lines in Fig. 2 (f). Therefore, there must be even number of pairs of bands for a 1D nonsymmorphic superconductor. A single pair of bands shown in Fig. 2 (c) and (d) can only exist at the 1D boundary of a 2D system. This gives the "no-go" theorem for nonsymmorphic superconductors[39].

IV. BULK TOPOLOGICAL INVARIANTS AND THE EXTENDED BRILLOUIN ZONE

The above analysis has shown that two momentum lines $\mathbf{k}\cdot\tau=0$ and $\mathbf{k}\cdot\tau=\frac{\pi}{2}$ play the essential role in the classification of TSCs in nonsymmorphic crystals. We can view the bulk Hamiltonian on $\mathbf{k}\cdot\tau=0$ or $\mathbf{k}\cdot\tau=\frac{\pi}{2}$ as a 1D Hamiltonian. For the case of Δ_+ with the G_+ symmetry, the Hamiltonian H_{BdG} (Eq. 1) has PHS along the line $\mathbf{k}\cdot\tau=0$ for each glide parity subspace, thus belonging to the D class, while it has no PHS along the line $\mathbf{k}\cdot\tau=\frac{\pi}{2}$ for each glide parity subspace, as shown in Fig. 1 (a). Since two glide parity subspaces are decoupled, one $\mathbb{Z}_2$ topological invariant of the D class can be defined on the line $\mathbf{k}\cdot\tau=0$ in the glide parity subspace for a 1D Hamiltonian. In contrast, for the case of Δ_- with the G_- symmetry, one $\mathbb{Z}_2$ topological invariant can be defined on the line $\mathbf{k}\cdot\tau=\frac{\pi}{2}$. In our example, we can re-write the BdG Hamiltonian with the eigenstates of $G_\pm$ as a basis and one can see immediately for the case with the G_+ (G_-) symmetry, the Hamiltonian is exactly equivalent to the 1D Kitaev model of p-wave superconductors[40] in each glide parity subspace when $k_x=0$ ($k_x=\frac{\pi}{a}$)[36].

More insights about this system can be obtained from the view of the extended Brillouin zone (BZ)[41], which has been widely used in the field of iron pnictide superconductors. For nonsymmorphic crystals, all the eigenstates of the Hamiltonian can be labeled by the eigenvalues of glide operators, defined as $G_\eta\psi(\tilde{\mathbf{k}})=e^{i\tilde{\mathbf{k}}\cdot\tau}\psi(\tilde{\mathbf{k}})$, in which $\tilde{\mathbf{k}}$ is called "pseudocrystal momentum"[41] and defines the extended BZ. For our model, the glide plane symmetry operation only involves translation by $\frac{a}{2}$ along the x direction, and thus the extended BZ for $\tilde{k}_x$ is doubled along the x direction ($\tilde{k}_x\in[-\frac{2\pi}{a},\frac{2\pi}{a}]$), compared to the conventional BZ for k_x, as shown in Fig. 2 (e). Since we have $G_\eta\psi(\mathbf{k})=\delta_\eta e^{i\mathbf{k}\cdot\tau}\psi(\mathbf{k})$, this suggests that the pseudocrystal momentum $\tilde{\mathbf{k}}$ is related to momentum $\mathbf{k}$ by $\tilde{\mathbf{k}}=\mathbf{k}$ when $\delta_\eta=+$ and $\tilde{\mathbf{k}}=\mathbf{k}+\mathbf{Q}$ with $\mathbf{Q}\cdot\tau=\pm\pi$ when $\delta_\eta=-$. Here the sign of $\mathbf{Q}\cdot\tau$ is determined by keeping $\tilde{k}_x$ in the region $[-\frac{2\pi}{a},\frac{2\pi}{a}]$ and k_y in the region $[-\frac{\pi}{a},\frac{\pi}{a}]$. As a result, the BdG Hamiltonian can also be rewritten as $H^{ex}_{BdG}(\tilde{\mathbf{k}})=H_{BdG,+}(\mathbf{k})=H_{BdG,+}(\tilde{\mathbf{k}})$ for $\tilde{k}_x\in[-\frac{\pi}{a},\frac{\pi}{a}]$ and $H^{ex}_{BdG}(\tilde{\mathbf{k}})=H_{BdG,-}(\mathbf{k})=H_{BdG,-}(\tilde{\mathbf{k}}-\mathbf{Q})$ for $\tilde{k}_x\in[\frac{\pi}{a},\frac{2\pi}{a}]$ and $\tilde{k}_x\in[-\frac{2\pi}{a},-\frac{\pi}{a}]$ in the extended BZ. Here $H_{BdG,\pm}$ is the BdG Hamiltonian in the subspace with glide parity $\pm e^{i\mathbf{k}\cdot\tau}$. For our model Hamiltonian, $H_{BdG,\pm}$ corresponds to the two by two Hamiltonian defined in the Supplemental Material[36]. For the case of Δ_+, the form of H^{ex}_{BdG} is given by $H^{ex}_{BdG}(\tilde{\mathbf{k}})=-(\epsilon(\tilde{\mathbf{k}})-\mu+t_3cos(\frac{\tilde{k}_xa}{2})cos(\frac{\phi a}{2}))\tau_3+t_3sin(\frac{\tilde{k}_xa}{2})sin(\frac{\phi a}{2})\tau_0+\Delta_0sin(k_ya)\tau_1$, where $\epsilon(\tilde{\mathbf{k}})=m_0+t_1cos(\tilde{k}_xa)+t_2cos(k_ya)$. We notice that if we take the hopping parameters t_1 and t_3 along the x direction to be zero, this Hamiltonian exactly corresponds to the 1D Kitaev chain with one Majorana zero mode at the open boundary[40]. With the hopping along the x direction, all the 1D Kitaev chains are coupled along the x direction, so Majorana zero modes at the end of the chains couple to each other and expand into a band. This corresponds to the weak TSCs[42,43], which is in analogy to weak topological insulators[44]. The PHS requires $E(\tilde{\mathbf{k}})=-E(-\tilde{\mathbf{k}})$ for the band of Majorana zero modes. Therefore, zero energy states can only appear for $\tilde{k}_x=0$ and $\tilde{k}_x=\frac{2\pi}{a}$ ($\tilde{k}_x$ is periodic in $\frac{4\pi}{a}$), which both correspond to $k_x=0$ in the conventional BZ. In contrast, for the case of Δ_-, the gap function comes from the so-called η pairing for two electrons with the momenta $\tilde{\mathbf{k}}$ and $\mathbf{Q}-\tilde{\mathbf{k}}$ to form a Cooper pair[36,45–49] ($\mathbf{Q}=(\frac{2\pi}{a},0)$ for our model). In this case, the PHS requires $E(\tilde{\mathbf{k}})=-E(\mathbf{Q}-\tilde{\mathbf{k}})$ for the Majorana band, leading to the zero energy states at $\tilde{k}_x=\pm\frac{\pi}{a}$. This analysis based on the extended BZ is consistent with our previous results and show explicitly the relationship between TNSCs and weak TSCs.

V. DISCUSSION AND CONCLUSION

The above results for TNCSc can be directly generalized to the systems with spin-$\frac{1}{2}$ and with additional time reversal (TR) symmetry. For spin-$\frac{1}{2}$ systems, since δ_η in the glide parity is given by $\pm i$, there is an additional minus sign when considering how the glide parity of an eigenstate of the BdG Hamiltonian transforms under PHS. This leads to the consequence that the $\mathbb{Z}_2$ topological invariant can be defined at $\mathbf{k}\cdot\tau=\frac{\pi}{2}$ ($\mathbf{k}\cdot\tau=0$) for the systems with the G_+ (G_-) symmetry. According to the standard topological classification, TR symmetry can change the symmetry class from the D class to BDI for spinless systems and $DIII$ for spin-$\frac{1}{2}$ systems. To see how it affects the classification of TNCSc, we consider an example of a spin-$\frac{1}{2}$ system in the $DIII$ class with the G_+ symmetry. If we take a state $\psi(\mathbf{k})$ with glide parity $\delta e^{i\mathbf{k}\cdot\tau}$ where $\delta=i$, the glide parity of its PHS partner has been shown to be $\delta^*e^{-i\mathbf{k}\cdot\tau}$ and the glide parity of its TR partner is also $\delta^*e^{-i\mathbf{k}\cdot\tau}$, where $\Theta G_+(\mathbf{k})\Theta^{-1}=G_+(-\mathbf{k})$ is used and TR operator is $\Theta=\begin{pmatrix}\Theta_e & 0\\ 0 & \Theta_e^{\dagger T}\end{pmatrix}$ with $\Theta_e=i\sigma_0s_2K$ and s_2 the second Pauli matrix acting on spin space. One can see that chiral symmetry $\Pi=C\times\Theta$ exists in each glide parity subspace for any momentum. In addition, at the momentum line $\mathbf{k}\cdot\tau=\frac{\pi}{2}$, PHS and TRS also exist in each glide parity subspace. Therefore, the symmetry class is DIII for the momentum line $\mathbf{k}\cdot\tau=\frac{\pi}{2}$ and AIII for other momentum lines ($\mathbf{k}\cdot\tau\neq\frac{\pi}{2}$) in each glide parity subspace. This leads to $\mathbb{Z}_2\oplus\mathbb{Z}_2$ classification at $\mathbf{k}\cdot\tau=\frac{\pi}{2}$, $\mathbb{Z}$ classification at $\mathbf{k}\cdot\tau=0$ and $\mathbb{Z}\oplus\mathbb{Z}$ classification at other momentum lines for the whole BdG Hamiltonian[20,36], in sharp contrast to the $\mathbb{Z}\times\mathbb{Z}$ classification of topological mirror superconductors in the

DIII class[28]. This classification leads to the existence of edge flat bands in the DIII class for TNCSc (See Supplemental materials[36]). The spinless and spin-$\frac{1}{2}$ TNCSc in classes D, DIII and BDI are also studied in the Supplemental Material[36]. Nonsymmorphic symmetry is known to exist in several classes of superconducting materials, including iron pnictide superconductors[50–56], BiS_2-based layered superconductors[57–65], and heavy fermion superconductors[51,66], *e.g.* UPt_3[67], UBe_{13}[68]. Our topological classification of TNCSc can be directly applied to these systems to search for realistic topological superconducting materials.

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Note added. - After finishing this paper, we notice a paper on arxiv[69], which concerns possible topological superconducting phases in monolayer FeSe and potential relation to nonsymmorphic symmetry. We also notice another recent paper on arxiv[70] about topological classification of TNCSc based on the twisted equivariant K-theory.

1 S. Ryu and Y. Hatsugai, Physical review letters **89**, 077002 (2002).
2 L. Fu and C. L. Kane, Physical review letters **100**, 096407 (2008).
3 R. Roy, arXiv preprint arXiv:0803.2868(2008).
4 X.-L. Qi, T. L. Hughes, S. Raghu, and S.-C. Zhang, Physical review letters **102**, 187001 (2009).
5 F. Wilczek, Nature Physics **5**, 614 (2009).
6 K. Law, P. A. Lee, and T. Ng, Physical review letters **103**, 237001 (2009).
7 R. M. Lutchyn, J. D. Sau, and S. D. Sarma, Physical review letters **105**, 077001 (2010).
8 M. Z. Hasan and C. L. Kane, Reviews of Modern Physics **82**, 3045 (2010).
9 X.-L. Qi and S.-C. Zhang, Reviews of Modern Physics **83**, 1057 (2011).
10 J. Alicea, Reports on Progress in Physics **75**, 076501 (2012).
11 M. Leijnse and K. Flensberg, Semiconductor Science and Technology **27**, 124003 (2012).
12 V. Mourik, K. Zuo, S. Frolov, S. Plissard, E. Bakkers, and L. Kouwenhoven, Science **336**, 1003 (2012).
13 L. P. Rokhinson, X. Liu, and J. K. Furdyna, Nature Physics **8**, 795 (2012).
14 A. Das, Y. Ronen, Y. Most, Y. Oreg, M. Heiblum, and H. Shtrikman, Nature Physics **8**, 887 (2012).
15 C. W. J. Beenakker, Annual Review of Condensed Matter Physics **4**, 113 (2013).
16 D. A. Ivanov, Physical review letters **86**, 268 (2001).
17 G. Moore and N. Read, Nuclear Physics B **360**, 362 (1991).
18 C. Nayak, S. H. Simon, A. Stern, M. Freedman, and S. D. Sarma, Reviews of Modern Physics **80**, 1083 (2008).
19 J. Alicea, Y. Oreg, G. Refael, F. von Oppen, and M. P. Fisher, Nature Physics **7**, 412 (2011).
20 A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. Ludwig, Physical Review B **78**, 195125 (2008).
21 M. R. Zirnbauer, Journal of Mathematical Physics **37**, 4986 (1996).
22 A. Altland and M. R. Zirnbauer, Physical Review B **55**, 1142 (1997).
23 J. C. Teo, L. Fu, and C. Kane, Physical Review B **78**, 045426 (2008).
24 T. H. Hsieh, H. Lin, J. Liu, W. Duan, A. Bansil, and L. Fu, Nature communications **3**, 982 (2012).
25 K. Shiozaki and M. Sato, Physical Review B **90**, 165114 (2014).
26 Q.-Z. Wang, S.-C. Wu, C. Felser, B. Yan, and C.-X. Liu, Physical Review B **91**, 165435 (2015).
27 Y. Sun, Q.-Z. Wang, S.-C. Wu, C. Felser, C.-X. Liu, and B. Yan, arXiv preprint arXiv:1503.01006(2015).
28 F. Zhang, C. Kane, and E. Mele, Physical Review Letters **111**, 056403 (2013).
29 Y. Ueno, A. Yamakage, Y. Tanaka, and M. Sato, Physical Review Letters **111**, 087002 (2013).
30 C.-K. Chiu, H. Yao, and S. Ryu, Physical Review B **88**, 075142 (2013).
31 S. A. Parameswaran, A. M. Turner, D. P. Arovas, and A. Vishwanath, Nature Physics **9**, 299 (2013).
32 C.-X. Liu, R.-X. Zhang, and B. K. VanLeeuwen, Physical Review B **90**, 085304 (2014).
33 C. Fang and L. Fu, Physical Review B **91**, 161105 (2015).
34 K. Shiozaki, M. Sato, and K. Gomi, Physical Review B **91**, 155120 (2015).
35 C. Fang, Y. Chen, H.-Y. Kee, and L. Fu, arXiv preprint arXiv:1506.03449(2015).
36 Q.-Z. Wang and C.-X. Liu see Supplemental Material for details.
37 L. Fu and E. Berg, Physical review letters **105**, 097001 (2010).
38 S. A. Yang, H. Pan, and F. Zhang, Physical review letters **113**, 046401 (2014).
39 C. Wu, B. A. Bernevig, and S.-C. Zhang, Physical review letters **96**, 106401 (2006).
40 A. Y. Kitaev, Physics-Uspekhi **44**, 131 (2001).
41 P. A. Lee and X.-G. Wen, Physical Review B **78**, 144517 (2008).
42 J. C. Teo and C. L. Kane, Physical Review B **82**, 115120 (2010).
43 T. L. Hughes, H. Yao, and X.-L. Qi, Physical Review B **90**, 235123 (2014).

[44] L. Fu, C. L. Kane, and E. J. Mele, Physical Review Letters **98**, 106803 (2007).
[45] C. N. Yang, Physical review letters **63**, 2144 (1989).
[46] J. Hu and N. Hao, Physical Review X **2**, 021009 (2012).
[47] J. Hu, N. Hao, and X. Wu, arXiv preprint arXiv:1303.2624(2013).
[48] N. Hao and J. Hu, Physical Review B **89**, 045144 (2014).
[49] Y. Wang, T. Berlijn, P. Hirschfeld, D. Scalapino, and T. Maier, Physical review letters **114**, 107002 (2015).
[50] Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, Journal of the American Chemical Society **130**, 3296 (2008).
[51] G. Stewart, Reviews of Modern Physics **83**, 1589 (2011).
[52] E. Dagotto, Reviews of Modern Physics **85**, 849 (2013).
[53] V. Cvetkovic and O. Vafek, Physical Review B **88**, 134510 (2013).
[54] W. Qing-Yan, L. Zhi, Z. Wen-Hao, Z. Zuo-Cheng, Z. Jin-Song, L. Wei, D. Hao, O. Yun-Bo, D. Peng, C. Kai, et al., Chinese Physics Letters **29**, 037402 (2012).
[55] S. He, J. He, W. Zhang, L. Zhao, D. Liu, X. Liu, D. Mou, Y.-B. Ou, Q.-Y. Wang, Z. Li, et al., Nature materials **12**, 605 (2013).
[56] S. Tan, Y. Zhang, M. Xia, Z. Ye, F. Chen, X. Xie, R. Peng, D. Xu, Q. Fan, H. Xu, et al., Nature materials **12**, 634 (2013).
[57] Y. Mizuguchi, H. Fujihisa, Y. Gotoh, K. Suzuki, H. Usui, K. Kuroki, S. Demura, Y. Takano, H. Izawa, and O. Miura, Physical Review B **86**, 220510 (2012).
[58] Y. Mizuguchi, S. Demura, K. Deguchi, Y. Takano, H. Fujihisa, Y. Gotoh, H. Izawa, and O. Miura, Journal of the Physical Society of Japan **81**, 114725 (2012).
[59] H. Usui, K. Suzuki, and K. Kuroki, Physical Review B **86**, 220501 (2012).
[60] D. Yazici, K. Huang, B. White, I. Jeon, V. Burnett, A. Friedman, I. Lum, M. Nallaiyan, S. Spagna, and M. Maple, Physical Review B **87**, 174512 (2013).
[61] R. Jha, A. Kumar, S. K. Singh, and V. Awana, Journal of superconductivity and novel magnetism **26**, 499 (2013).
[62] J. Xing, S. Li, X. Ding, H. Yang, and H.-H. Wen, Physical Review B **86**, 214518 (2012).
[63] Y. Yang, W.-S. Wang, Y.-Y. Xiang, Z.-Z. Li, and Q.-H. Wang, Physical Review B **88**, 094519 (2013).
[64] X. Lin, X. Ni, B. Chen, X. Xu, X. Yang, J. Dai, Y. Li, X. Yang, Y. Luo, Q. Tao, et al., Physical Review B **87**, 020504 (2013).
[65] C.-L. Dai, Y. Yang, W.-S. Wang, and Q.-H. Wang, Physical Review B **91**, 024512 (2015).
[66] G. Stewart, Reviews of Modern Physics **56**, 755 (1984).
[67] R. Joynt and L. Taillefer, Reviews of Modern Physics **74**, 235 (2002).
[68] H. Ott, H. Rudigier, Z. Fisk, and J. Smith, Physical review letters **50**, 1595 (1983).
[69] N. Hao and S.-Q. Shen, arXiv preprint arXiv:1506.07345(2015).
[70] K. Shiozaki, M. Sato, and K. Gomi, arXiv preprint arXiv:1511.01463(2015).