Möbius topological superconductivity in UPt$_3$

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(Dated: June 30, 2017)

Intensive studies for more than three decades have elucidated multiple superconducting phases and odd-parity Cooper pairs in a heavy fermion superconductor UPt$_3$. We identify a time-reversal invariant superconducting phase of UPt$_3$ as a recently proposed topological nonsymmorphic superconductivity. Combining the band structure of UPt$_3$, order parameter of $E_{2u}$ representation allowed by $P6_3/mmc$ space group symmetry, and topological classification by $K$-theory, we demonstrate the nontrivial $Z_2$-invariant of three-dimensional DIII class enriched by glide symmetry. Correspondingly, double Majorana cone surface states appear at the surface Brillouin zone boundary. Furthermore, we show a variety of surface states and clarify the topological protection by crystal symmetry. Majorana arcs corresponding to tunable Weyl points appear in the time-reversal symmetry broken B-phase. Majorana cone protected by mirror Chern number and Majorana flat band by glide-winding number are also revealed.

I. INTRODUCTION

Unconventional superconductivity in strongly correlated electron systems is attracting renewed interest because it may be a platform of topological superconductivity accompanied by Majorana surface/edge/vortex/end states. Although previous studies focused on the proximity-induced topological superconductivity in s-wave superconductor (SC) heterostructures, natural s-wave SCs are mostly trivial from the viewpoint of topology. On the other hand, unconventional SCs may have topologically nontrivial properties originating from non-s-wave Cooper pairing. In particular, time-reversal symmetry (TRS) broken chiral SCs and odd-parity spin-triplet SCs are known to be candidates of topological superconductivity. However, from the viewpoint of materials science, evidences for chiral and/or odd-parity superconductivity have been reported for only a few materials, such as URu$_2$Si$_2$, SrPt$_2$A$_6$, Sr$_2$RuO$_4$, Cu$_2$Bi$_2$Se$_3$, and ferromagnetic heavy fermion SCs.

Superconductivity in UPt$_3$ has been discovered in 1980. Multiple superconducting phases illustrated in Fig. 1$^{11}$ are known to be candidates of topological superconductivity. However, after several theoretical proposals examined by experiments for more than three decades, the $E_{2u}$ representation has been regarded as the most reasonable symmetry of superconducting order parameter. In particular, the multiple phase diagram in the temperature-magnetic field plane is naturally reproduced by assuming a weak symmetry breaking term of hexagonal symmetry. Furthermore, a phase-sensitive measurement and the observation of spontaneous TRS breaking in the low-temperature and low-magnetic field B-phase, which was predicted in the $E_{2u}$-state, support the $E_{2u}$ symmetry of superconductivity. The order parameter of $E_{2u}$ symmetry represents odd-parity spin-triplet Cooper pairs. Therefore, topologically nontrivial superconductivity is expected in UPt$_3$.

![Crystal structure of UPt$_3$.](image.png)

FIG. 1. (Color online) Crystal structure of UPt$_3$. Uranium ions form AB stacked triangular lattice. 2D vectors, $e_i$, and $r_i$, are shown by arrows.

Furthermore, UPt$_3$ has an intriguing feature in the crystal structure, which is illustrated in Fig. 1. The symmetry of the crystal is represented by nonsymmorphic space group $P6_3/mmc$, glide and screw symmetries including a half translation along the c-axis are preserved in spite of broken mirror and rotation symmetries. Exotic properties ensured by glide and/or screw symmetry are one of the central topics in the modern condensed matter physics. This topic for SCs traces back to Norman’s work in 1995 for UPt$_3$, a counterexample of Blount’s theorem$^{10}$. The line nodal excitation predicted by Norman has been revisited by recent studies; group-theoretical proof$^{33,34}$, microscopic origin$^{12}$, and topological protection$^{35}$ have been elucidated, and they have been confirmed by a first principles-based calculation$^{36}$.

Recent developments in the theory of nonsymmorphic topological states of matter$^{37,38}$ have uncovered novel topological insulators and SCs enriched by glide and/or screw symmetry, which are distinct from those classified by existing topological periodic table for symmorphic systems$^{39}$. Since eigenvalues of glide and two-fold screw operators are $4\pi$-periodic, a Möbius structure appears in the wave function and changes the topologi-
Topological classification. Although such topological nonsymmorphic crystalline insulators have been proposed in KHgX (X = As, Sb, Bi)\cite{49,50} and CeNiSn\cite{51}, topological nonsymmorphic crystalline superconductor (TNSC) has not been identified in materials. In this paper we show the topological invariant specifying the TNSC by $K$-theory, and demonstrate its nontrivial value in UPt$_3$.

Multiband structures give rise to both intriguing and complicated aspects of many heavy fermion systems. However, the band structure of UPt$_3$ has been clarified to be rather simple\cite{27,52-54}. Fermi surfaces (FSs) are classified into the two classes. The FSs of one class enclose the $A$-point in the Brillouin zone (BZ) [band 1 and band 2 in Ref.\cite{54}], while those of the other class are centered on the $\Gamma$-point or $K$-point [bands 3, 4, and 5 in Ref.\cite{54}]. The two classes are not hybridized in the surface state on the (100)-direction where the glide symmetry is preserved. Therefore, we can separately study the topological invariants and surface states arising from the multiband FSs. The TNSC is attributed to the former FSs in Sec. V. The latter FSs are also accompanied by various topological surface states, for which we identify topological invariant in Sec. VI.

The paper is organized as follows. In Sec. II, we introduce a minimal two-sublattice model for nonsymmorphic superconductivity in UPt$_3$. In Sec. II.B, Dirac nodal lines protected by $P6_3/mmc$ space group symmetry are proved. In Sec. II.C, the order parameter of superconductivity in UPt$_3$ is explained. The calculated surface states on the glide invariant (100)-surface are shown in Sec. III. In Sec. IV, three-dimensional (3D) TNSC of DIII class is classified on the basis of the $K$-theory. In Sec. V, we show that the glide-$Z_2$ invariant characterizing the TNSC is nontrivial in UPt$_3$ $A$-phase. The underlying origin of the TNSC accompanied by double Majorana cone surface states is discussed. In Sec. VI, we characterize other topological surface states by low-dimensional topological invariants enriched by crystal mirror, glide, and rotation symmetries. Constraints on these topological invariants by nonsymmorphic space group symmetry are also revealed. Finally, a brief summary is given in Sec. VII. Ingredients giving rise to rich topological properties of UPt$_3$ are discussed.

II. MODEL

A. Nonsymmorphic two-sublattice model

We study the superconducting state in UPt$_3$ by analyzing the Bogoliubov-de Gennes (BdG) Hamiltonian for nonsymmorphic two-sublattice model\cite{52}:

$$\mathcal{H}_\text{BdG} = \sum_{k,m,s} \xi(k) c_{kms}^\dagger c_{kms} + \sum_{k,s} \left[ a(k) c_{ks}^\dagger c_{k2s} + \text{h.c.} \right] + \sum_{k,m,s,s'} \alpha_m g(k) \cdot s_{ss'} c_{kms}^\dagger c_{km's'} + \frac{1}{2} \sum_{k,m,m',s,s'} \left[ \Delta_{mm's's'}(k) c_{kms}^\dagger c_{km's'}^\dagger + \text{h.c.} \right],$$

(2.1)

where $k$, $m = 1, 2$, and $s = \uparrow, \downarrow$ are index of momentum, sublattice, and spin, respectively. The last term represents the gap function and others are normal part Hamiltonian. Taking into account the crystal structure of UPt$_3$ illustrated in Fig.\cite{figA} we adopt an intra-sublattice kinetic energy,

$$\xi(k) = 2t \sum_{i=1,2,3} \cos k_i \cdot e_i + 2t_z \cos k_z - \mu,$$

(2.2)

and an inter-sublattice hopping term,

$$a(k) = 2t' \cos \frac{k_z}{2} \sum_{i=1,2,3} e^{ik_i \cdot r_i},$$

(2.3)

with $k_\parallel = (k_x, k_y)$. The basis translation vectors in two dimension are $e_1 = (1,0)$, $e_2 = (-\frac{1}{2}, \frac{\sqrt{3}}{2})$, and $e_3 = (-\frac{1}{2}, -\frac{\sqrt{3}}{2})$. The interlayer neighboring vectors projected onto the basal plane are given by $r_1 = (\frac{1}{2}, 0)$, $r_2 = (\frac{1}{2}, \frac{1}{\sqrt{3}})$, and $r_3 = (0, -\frac{1}{\sqrt{3}})$. These 2D vectors are illustrated in Fig.\cite{figA}

Although the crystal point group symmetry is centrosymmetric $D_{6h}$, local point group symmetry at Uranium ions is $D_{3h}$ lacking inversion symmetry. Then, Kane-Mele spin-orbit coupling (SOC)\cite{55} with $g$-vector\cite{56}

$$g(k) = \hat{z} \sum_{i=1,2,3} \sin k_\parallel \cdot e_i,$$

(2.4)

is allowed by symmetry. The coupling constant has to be sublattice-dependent, $(\alpha_1, \alpha_2) = (\alpha, -\alpha)$, so as to preserve the global $D_{6h}$ point group symmetry\cite{55,57,58}.

Quantum oscillation measurements combined with band structure calculations\cite{27,49,50-54} have shown a pair of FSs centered at the $A$-point (A-FSs) on the BZ face. Interestingly, the paired bands are degenerate on the $A-L$ lines and form Dirac nodal lines\cite{52}. This has been experimentally observed by de Haas-van Alphen experiment\cite{52}. In the next subsection we show that the Dirac nodal lines are protected by the nonsymmorphic space group symmetry of $P6_3/mmc$ (No. 194)\cite{47,48}. Thus, the two A-FSs are naturally paired by the nonsymmorphic crystal symmetry. By choosing a parameter set $(t, t_z, t', \alpha, \mu) = (1, -4, 1, 2, 12)$ our two band model reproduces the paired A-FSs. In this paper we show that the peculiar band structure results in exotic superconductivity in terms of symmetry and topology.
First principles band structure calculations also predict three FSs centered on the \( \Gamma \)-point (\( \Gamma \)-FSs), and two FSs enclosing the \( K \)-point (\( K \)-FSs)\(^{27,39,52} \), although the existence of \( K \)-FSs is experimentally under debates\(^{54} \).

We show that a variety of topological surface states may arise from these bands. A parameter set \((t, t_x, t', \alpha, \mu) = (1, 4, 1, 0, 16)\) reproduces one of the \( \Gamma \)-FSs, while another set \((t, t_x, t', \alpha, \mu) = (1, -1, 0.4, 0.2, -5.2)\) is adopted for the \( K \)-FSs.

**B. Dirac nodal lines in space group \(P6_3/mmc\)**

The single particle states are four-fold degenerate on the \(A-L\) lines \([k = (0, k_y, \pi)]\) and symmetric lines. In addition to the usual Kramers degeneracy, the sublattice degree of freedom gives additional degeneracy. This feature is reproduced in the normal part Hamiltonian, because the inter-sublattice hopping vanishes on the BZ face \((k_z = \pi)\) and the SOC disappears on the \(A-L\) lines. Below we show that the existence of Dirac line nodes is ensured by the space group symmetry.

First, we show the additional degeneracy in the absence of the SOC. In the SU(2) symmetric case, the two spin states are equivalent and naturally degenerate. Then, we can define the TRS, \(T = K\), and screw symmetry \(S_z^\alpha(k_z)\) in each spin sector, where \(K\) is the complex conjugate operator. At the BZ face, \(k_z = \pi\), we have \(S_z^\alpha(\pi) = i\sigma_y\) where \(\sigma_i\) is the Pauli matrix in the sublattice space. Because the combined magnetic-screw symmetry satisfies \([S_z^\alpha(\pi)T]^2 = -1\), the two-fold degeneracy in each spin sector is proved by familiar Kramers theorem. Taking into account the spin-degeneracy, we obtain four-fold degenerate bands on the entire BZ face.

The four-fold degeneracy is partly lifted by the SOC. However, the degeneracy of two spinful bands is protected on the \(A-L\) lines, that is proved as follows. The little group on the \(A-L\) lines includes the rotation symmetry \(I^\text{G}G^z(k_z)\), mirror symmetry \(M^{yz}\), and magnetic-inversion symmetry \(IT\). We here represent \(T = is_yK\), \(I = \sigma_x\), and \(M^{yz} = is_x\), respectively. The rotation symmetry is represented by \(G^z(k_z) = s_y\sigma_y\) at \(k_z = \pm \pi\) while \(G^z(k_z) = is_y\sigma_x\) at \(k_z = 0\). The non-symmorphic property of rotation symmetry is emphasized by denoting as \(IG^z(k_z)\). The symmetry operations satisfy the algebra

\[
\begin{align*}
&|IG^z(\pi)|^2 = -1, \quad (2.5) \\
&\{IG^z(\pi), IT\} = 0, \quad (2.6) \\
&\{IG^z(\pi), M^{yz}\} = 0. \quad (2.7)
\end{align*}
\]

The first relation ensures the sector decomposition to the \(\lambda = \pm i\eta\) eigenstates of rotation operator. Because the \(IT\) symmetry is preserved in each subsector, the Kramers theorem holds. The anti-commutation relation of two unitary symmetries, Eq. (2.7), shows that a Kramers pair in one subsector has to be degenerate with another Kramers pair in the other subsector. Therefore, the four-fold degeneracy on the \(A-L\) lines is protected by symmetry.

![FIG. 2. (Color online) FSs on the BZ face, \(k_z = \pi\). Thin red lines show the FSs in the presence of the SOC (\(\alpha = 1\)), while the thick black line is the overlapping FSs in the absence of the SOC (\(\alpha = 0\)). Dashed lines show the \(A-L\) lines in the first BZ. We set parameters \((t, t_x, t', \mu) = (1, -4, 1, 12)\) to reproduce the \(A\)-FSs.](image)

**C. Order parameter of \(E_{2u}\) representation**

The multiple superconducting phases in \(\text{UPt}_3\) have been reasonably attributed to two-component order parameters in the \(E_{2u}\) irreducible representation of \(D_{6h}\) point group\(^{29,37}\). The gap function is generally represented by

\[
\hat{\Delta}(k) = \eta_1\hat{\Gamma}_1^{E_{2u}} + \eta_2\hat{\Gamma}_2^{E_{2u}}. \quad (2.8)
\]

The two-component order parameters are parametrized as

\[
(\eta_1, \eta_2) = \Delta(1, i\eta)/\sqrt{1 + \eta^2}, \quad (2.9)
\]

with a real variable \(\eta\). The basis functions \(\hat{\Gamma}_1^{E_{2u}}\) and \(\hat{\Gamma}_2^{E_{2u}}\) are admixture of some harmonics. Adopting the neighboring Cooper pairs in the crystal lattice of \(\text{U}\) ions,
we obtain the basis functions
\[
\hat{\Gamma}_1^{E_{2u}} = \left[ \delta \{ p_x(k) s_x - p_y(k) s_y \} \sigma_0 
+ f_{(x^2-y^2)z}(k) s_z \sigma_2 - d_{yz}(k) s_z \sigma_y \right] i s_y, 
\]
\[
\hat{\Gamma}_2^{E_{2u}} = \left[ \delta \{ p_y(k) s_x + p_z(k) s_y \} \sigma_0 
+ f_{xyz}(k) s_z \sigma_2 - d_{xz}(k) s_z \sigma_y \right] i s_y, 
\]
which are composed of the \( p \)-wave, \( d \)-wave, and \( f \)-wave components given by
\[
p_x(k) = \sum_i e_i^x \sin k_{||} \cdot e_i, 
\]
\[
p_y(k) = \sum_i e_i^y \sin k_{||} \cdot e_i, 
\]
\[
d_{xz}(k) = -\sqrt{3} \sin k_z \frac{k_z}{2} \text{Im} \sum_i r^x_i e^{i k_{||} \cdot r_i}, 
\]
\[
d_{yz}(k) = -\sqrt{3} \sin k_z \frac{k_z}{2} \text{Im} \sum_i r^y_i e^{i k_{||} \cdot r_i}, 
\]
\[
f_{xyz}(k) = -\sqrt{3} \sin k_z \frac{k_z}{2} \text{Re} \sum_i r^x_i e^{i k_{||} \cdot r_i}, 
\]
\[
f_{(x^2-y^2)z}(k) = -\sqrt{3} \sin k_z \frac{k_z}{2} \text{Re} \sum_i r^y_i e^{i k_{||} \cdot r_i}. 
\]

Pauli matrix in the spin and sublattice space are denoted by \( s_i \) and \( \sigma_i \), respectively.

The purely \( f \)-wave state has been intensively investigated, and the phase diagram compatible with \( \text{UPt}_3 \) has been obtained\cite{26,27}. However, an admixture of a \( p \)-wave component is allowed by symmetry and it changes the gap structure and topological properties\cite{26,27}. Thus, we here take into account a small \( p \)-wave component with \( 0 < |\eta| \ll 1 \). The small \( p \)-wave component does not alter the phase diagram consistent with experiments. On the other hand, the dominantly \( p \)-wave state discussed in Ref. 39 would fail to reproduce the phase diagram.

Besides the \( p \)-wave component, a sublattice-singlet spin-triplet \( d \)-wave component accompanies the \( f \)-wave component as a result of the nonsymorphic crystal structure of \( \text{UPt}_3 \). The neighboring Cooper pairs on \( r_1 \) bonds give equivalent amplitude of \( d \)-wave and \( f \)-wave components in Eqs. (2.10) and (2.11). The \( d \)-wave order parameter plays a particularly important role on the superconducting gap at the BZ face, \( k_z = \pi \). Later we show that the TNSC is induced by the \( d \)-wave component.

Now we review the multiple superconducting phases in \( \text{UPt}_3 \). Three thermodynamically distinguished superconducting phases are illustrated in Fig. 3.\cite{21,23,26,27}. The A-, B-, and C-phases are characterized by the ratio of two-component order parameters \( \eta = \eta_2 / \eta_1 \) summarized in Table I. A pure imaginary ratio of \( \eta_1 \) and \( \eta_2 \) in the B-phase implies the chiral superconducting state which maximally gains the condensation energy. Owing to the \( p \)-wave component, the B-phase is non-unitary. It has been considered that the A- and C-phases are stabilized by weak symmetry breaking of hexagonal structure, possibly induced by weak antiferromagnetic order of 26,27,65,66. We here assume that the A-phase is the \( \Gamma_2 \) state (\( \eta = \infty \)), while the C-phase is the \( \Gamma_1 \) state (\( \eta = 0 \)), and assume non-negative \( \eta \geq 0 \) without loss of generality.

\[
\begin{array}{|c|c|}
\hline
\text{A-phase} & |\eta| = \infty \\
\text{B-phase} & 0 \leq |\eta| \leq \infty \\
\text{C-phase} & \eta = 0 \\
\hline
\end{array}
\]

TABLE I. Range of the parameter \( \eta \) in the A-, B-, and C-phases of \( \text{UPt}_3 \).\cite{26,27}.

Contrary to the experimental indications for the \( E_{2u} \)-pairing state mentioned before, a recent thermal conductivity measurement\cite{67} has been interpreted in terms of the \( E_{1u} \) symmetry of the orbital part of order parameter. However, this interpretation is not incompatible with the \( E_{2u} \) symmetry of total order parameter. For instance, the basis functions, Eqs. (2.10) and (2.11), include components \( p_x(k) s_x - p_y(k) s_y \) and \( p_y(k) s_x + p_z(k) s_y \), where the orbital part \( p_x(k) \) and \( p_y(k) \) belong to the \( E_{1u} \) symmetry. Although in Ref. 67, the superconducting state with TRS has been discussed along with a theoretical proposal\cite{26,27}, the spin part of order parameter can not be deduced from thermal conductivity measurements. Thus, we here assume the \( E_{2u} \)-pairing state.

For clarity of discussions for topological properties, we carry out the unitary transformation for the BdG Hamiltonian. When the model Eq. (2.7) is represented in the...
The BdG matrix $\hat{H}_{\text{BdG}}(k)$ in this form does not satisfy the periodicity compatible with the first BZ. To avoid this difficulty, we represent the BdG Hamiltonian by

$$\hat{H}_{\text{BdG}}(k) = U(k)\hat{\mathcal{H}}_{\text{BdG}}(k)U(k)\dagger,$$  

using the unitary matrix

$$U(k) = \begin{pmatrix} 1 & 0 \\ 0 & e^{ik}\tau \end{pmatrix} \otimes s_0 \otimes \tau_0. \quad (2.21)$$

By choosing the translation vector, $\tau = (0, -1/\sqrt{3}, \frac{1}{2})$, $\hat{H}_{\text{BdG}}(k)$ is periodic with respect to the translation $k \rightarrow k + K$ for any reciprocal lattice vector $K$. The transformed BdG Hamiltonian has the same form as Eq. (2.1), although the inter-sublattice components acquire the phase factor

$$a(k) \rightarrow \tilde{a}(k) = a(k)e^{-ik\cdot\tau}, \quad (2.22)$$

$$f_1(k) \rightarrow \tilde{f}_1(k) = f_1(k)e^{-ik\cdot\tau}, \quad (2.23)$$

$$d_1(k) \rightarrow \tilde{d}_1(k) = d_1(k)e^{-ik\cdot\tau}. \quad (2.24)$$

### III. TOPOLOGICAL SURFACE STATES

We calculate the energy spectrum of quasiparticles with surface normal to the (100)-axis, $E(k_{sd}) = E(k_x, k_z)$, because the nonsymmorphic glide symmetry is preserved there. Both glide and screw symmetry are broken in the other surface directions. Figures 4 and 5 show results for the $\Gamma$-FS and $A$-FSs, respectively. The black regions represent the zero energy surface states. It is revealed that a variety of zero energy surface states appear on the (100)-surface in the A-, B-, and C-phases. We clarify the topological protection of these surface states below. Indeed, all of the zero energy surface states are topologically protected. In Figs. 4 and 5, the topological surface states discussed in Secs. VI A - VI E are labeled by (V) and (A)-(E), respectively.

The most panels of Figs. 4 and 5 show the results for $\alpha = 0$ by neglecting the SOC. Most of the surface states are indeed robust against the SOC. Exceptionally, the surface states around $k_z = \pi$ are affected by the SOC, because the nodal bulk excitations may be induced by the SOC$^{35,38}$. For our choice of parameters, the bulk excitation gap remains finite at $k_z = \pi$ for $\alpha = 1$ although the gap may be suppressed for $\alpha = 2$. Thus, we show the surface states for $\alpha = 2$ in Fig. 5(f) for a comparison. The gapless bulk excitations which are not shown for $\alpha = 0$ [Fig. 5(c)] are observed around the surface BZ boundary.

One of the main results of this paper is a signature of TNSC in UPt$_3$, that is indicated by the label (V) in Fig. 5(c). This surface state is robust against the SOC unless the bulk excitation gap is closed. According to the first principles band structure calculation, the band splitting by the SOC is tiny along the $A-H$ lines$^{27}$ and significantly decreased by the mass renormalization factor$^{62}$, $z \sim 1/100$ in UPt$_3$. Thus, it is reasonable to assume a small SOC leading to the gapped bulk excitations at the BZ face. This assumption is compatible with the recent field-angle-dependent thermal conductivity measurement which has shown nodal lines/points lying away from the BZ face$^{63}$.

In the next section, superconducting phases of 3D DIII class with additional glide symmetry are classified on the basis of the $K$-theory, and the topological invariants are derived. In Sec. VI we show that a surface state labeled by (V) is protected by the strong topological index characterizing the TNSC. The topological protection of other surface states is revealed in Sec. VI.

### IV. CLASSIFICATION OF CLASS DIII SUPERCONDUCTORS WITH Glide symmetry

Topological classification of TNSC is carried out for both glide-even and glide-odd superconducting states of DIII class. For simplicity, the cubic first BZ with volume $(2\pi)^3$ is assumed in this section. We do not rely on any specific model, and therefore, the results obtained in this section are valid for all the superconducting states preserving the glide symmetry and TRS.

#### A. Glide-even superconductor

First, we study glide-even superconducting states. The $\Gamma_2$-state (A-phase) of UPt$_3$ corresponds to this case. The symmetries for the BdG Hamiltonian are summarized as

$$C\mathcal{H}(k)C^{-1} = -\mathcal{H}(-k), \quad C = \tau_x K, \quad (4.1)$$

$$T\mathcal{H}(k)T^{-1} = \mathcal{H}(-k), \quad T = is_y K, \quad (4.2)$$

$$G(k)\mathcal{H}(k)G^{-1}(k) = \mathcal{H}(m_y k), \quad G(m_y k)G(k) = -e^{-ik_z}, \quad (4.3)$$

$$TG(k) = G(-k)T, \quad CG(k) = G(-k)C, \quad (4.4)$$

where $m_y k = (k_x, -k_y, k_z)$ is the momentum flipped by glide operation, and $K$ is the complex conjugate. The stable classification of bulk superconductors is given by the $K$-theory over the bulk 3D BZ torus with symmetries.
\[ \eta = 0 \] (a) \[ \eta = 0.7 \] (b) \[ \eta = 1 \] (c) \[ \eta = 1.5 \] (d) \[ \eta = \infty \] (e)

**FIG. 4.** (Color online) Energy of surface states on the (100)-surface. We impose open boundary condition along the [100]-direction and periodic boundary condition along the other directions. The lowest excitation energy of BdG quasiparticles \( \equiv \min |E(k_{sf})| \) as a function of the surface momentum \( k_{sf} = (k_y, k_z) \) is shown. Parameters \((t, t_z, t', \alpha, \mu, \Delta, \delta) = (1, 4, 1, 0, 16, 4, 0.02)\) are assumed so that the \( \Gamma \)-FS is reproduced. (a) C-phase (\( \eta = 0 \)), (b)-(d) B-phase (\( \eta = 0.7, 1, \) and 1.5), and (e) A-phase (\( \eta = \infty \)). Arrows with characters (A), (B), (C) and (E) indicate surface states clarified in Secs. VI A, VI B, VI C, and VI E, respectively. The green circles show the projections of Weyl point nodes.

\[ \alpha = 2, \eta = 1 \]

**FIG. 5.** (Color online) (a)-(e) Energy of surface states on the (100)-surface for parameters reproducing the paired A-FSs, \((t, t_z, t', \alpha, \mu, \Delta, \delta) = (1, -4, 1, 0, 12, 0.7, 0.04)\). (a) C-phase (\( \eta = 0 \)), (b)-(d) B-phase (\( \eta = 0.6, 1, \) and 2), and (e) A-phase (\( \eta = \infty \)). We choose \( \alpha = 2 \) in (f) while the other parameters are the same as (c). Comparison between (c) and (f) reveals the effect of the SOC. Arrows with characters (V), (A), and (C) indicate surface states discussed in Secs. VI A, VI B, and VI C, respectively. The green circles show the projections of Weyl point nodes.
From Ref. 42, the result is

\[ \mathbb{Z}_2 \oplus \mathbb{Z}_2 \oplus \mathbb{Z}_2 \oplus \mathbb{Z}_2. \]  \hspace{1cm} (4.5)

The bold style \( \mathbb{Z}_2 \) expresses an emergent topological phase which disappears if the glide symmetry is broken. Each underbrace represents the momentum dependence of generating Hamiltonian. For instance, \( \mathbb{Z}_2 \) means that the generating Hamiltonian of the \( \mathbb{Z}_2 \) phase can be \( k_y \)-independent, that is, the stacking of layered Hamiltonians \( H_y(k_x, k_z) \) in the \( xz \)-plane along the \( y \)-direction.

We focus on the gapless states on the surfaces preserving the glide symmetry, i.e. \( x = \text{constant} \). The classification of the surface gapless states is given by a similar \( K \)-theory over the surface 2D BZ torus under the same symmetries 4.1-4.3 with the \( k_x \)-direction excluded. The bulk-boundary correspondence holds if the glide symmetry, i.e. \( k_z = \pi \), the glide symmetry is reduced into the mirror symmetry

\[ G(k_x, k_y, \pi)H(k_x, k_y, \pi)G^{-1}(k_x, k_y, \pi) = H(k_x, -k_y, \pi), \] \hspace{1cm} (4.7)

\[ G(k_x, -k_y, \pi)G(k_x, k_y, \pi) = 1, \] \hspace{1cm} (4.8)

\[ TG(k_x, k_y, \pi) = G(-k_x, -k_y, \pi)T, \] \hspace{1cm} (4.9)

\[ CG(k_x, k_y, \pi) = G(-k_x, -k_y, \pi)C. \] \hspace{1cm} (4.10)

On the \( k_y = \Gamma_y \equiv 0, \pi \) lines, since the TRS and the particle-hole symmetry (PHS) commute with the glide symmetry, we can define \( \mathbb{Z}_2 \) invariant \( \nu(\Gamma_y, \pm) \in \{0, 1\} \) of one-dimensional (1D) class DIII SCs for each glide-subsectors \( G(k_x, \Gamma_y, \pi) = \pm 1 \),

\[ \nu(\Gamma_y, \pm) = \frac{i}{\pi} \int_0^{2\pi} dk_x \sum_n \left\langle u^{(f)}_{\pm, n}(k_x, \Gamma_y, \pi) \right| \partial_{k_x} \left| u^{(f)}_{\pm, n}(k_x, \Gamma_y, \pi) \right\rangle \quad (\text{mod 2}), \]

\( \Gamma_y = 0, \pi \),

where \( u^{(f)}_{\pm, n}(k_x, \Gamma_y, \pi) \) represents one of the Kramers pair of occupied states in the glide-subsector \( G(k_x, \Gamma_y, \pi) = \pm 1 \). Noticing that the combined symmetries \( TG(k_x, k_y, \pi) \) and \( CG(k_x, k_y, \pi) \),

\[ [TG(k_x, k_y, \pi)]H(k_x, k_y, \pi)[TG(k_x, k_y, \pi)]^{-1} \]
\[ = H(-k_x, k_y, \pi), \] \hspace{1cm} (4.11)

\[ TG(-k_x, k_y, \pi)TG(k_x, k_y, \pi) = -1, \] \hspace{1cm} (4.12)

\[ [CG(k_x, k_y, \pi)]H(k_x, k_y, \pi)[CG(k_x, k_y, \pi)]^{-1} \]
\[ = -H(-k_x, k_y, \pi), \] \hspace{1cm} (4.13)

\[ CG(-k_x, k_y, \pi)CG(k_x, k_y, \pi) = 1, \] \hspace{1cm} (4.14)

indicate the emergent class DIII symmetry for all \( k_y \), we have a constraint

\[ \nu(0, +) + \nu(0, -) = \nu(\pi, +) + \nu(\pi, -), \quad (\text{mod 2}). \] \hspace{1cm} (4.15)

Because of this emergent class DIII symmetry, all the surface states on the \( k_z = \pi \) plane show two-fold degeneracy. The three kinds of surface states may be generated by
Symmetries for the BdG Hamiltonian are which may be realized in the $\Gamma_1$-phase of UPt$_3$ respectively, with the positive glide eigenvalue $\nu_C$. Here, $\nu_C$ is denoted as glide-$Z_2$ invariant, $\nu_C \equiv \frac{Z_2}{(k_x, k_y, k_z)}$. It is given by

$$\nu_C = \nu(0, +)\nu(0, -) - \nu(\pi, +)\nu(\pi, -) \pmod{2}. \quad (4.19)$$

Later, we show that the glide-$Z_2$ invariant $\nu_C$ is nontrivial in the A-phase of UPt$_3$.

### B. Glide-odd superconductor

Next, we study glide-odd superconducting states, which may be realized in the $\Gamma_1$-state of UPt$_3$ (C-phase). Symmetries for the BdG Hamiltonian are

$$T\mathcal{H}(k)T^{-1} = \mathcal{H}(-k), \quad T = i\sigma_y K, \quad (4.20)$$

$$C\mathcal{H}(k)C^{-1} = -\mathcal{H}(-k), \quad C = \sigma_x K, \quad (4.21)$$

$$G(k)\mathcal{H}(k)G^{-1}(k) = \mathcal{H}(m_y k), \quad G(m_y k)G(k) = -e^{-ik_z}, \quad (4.22)$$

$$TG(k) = G(-k)T, \quad CG(k) = -G(-k)C. \quad (4.23)$$

From Ref. 42, the $K$-theory classification of the bulk reads

$$= \mathbb{Z} \oplus \mathbb{Z}_2 \oplus \mathbb{Z}_4 \oplus \mathbb{Z}_2 \oplus \mathbb{Z}_2 \oplus \mathbb{Z}_2. \quad (4.24)$$

The bold-style indices express emergent topological phases which requires the glide symmetry. From the bulk-boundary correspondence, it holds that

$$\left( \begin{array}{c} \text{The classification of surface states} \\ \text{on the } x = \text{constant surface} \end{array} \right) = \mathbb{Z} \oplus \mathbb{Z}_2 \oplus \mathbb{Z}_4. \quad (4.25)$$

The 3D $\mathbb{Z}_2$ index is the ordinary winding number $\mathbb{Z}_2$, $\mathbb{Z}_4$,

$$N := \frac{1}{48\pi^2} \int \text{tr}(\mathcal{H}^{-1} d\mathcal{H})^3, \quad \Gamma = iT C. \quad (4.26)$$

By imposing the glide symmetry, we have two $\mathbb{Z}_4$ invariants $\theta(\Gamma_y = 0, \pi) \in \{0, 1, 2, 3\}$ on the glide invariant $k_y = 0$ and $\pi$ planes$^{42}$,

$$\theta(\Gamma_y) := \frac{2i}{\pi} \left[ \int_0^{2\pi} dk_z \text{tr}\mathcal{A}^T(k_x, \Gamma_y, \pi) + \frac{1}{2} \int_0^\pi dk_z \int_0^{2\pi} dk_x \text{tr}\mathcal{F}_+(k_x, \Gamma_y, k_z) \right] \pmod{4}, \quad (4.27)$$

Here, $\mathcal{A}^T(k_x, \Gamma_y, \pi)$ and $\mathcal{F}_+(k_x, \Gamma_y, k_z)$ are the Berry connection of one of Kramers pair of occupied states and the Berry curvature of the occupied states, respectively, with the positive glide eigenvalue $G(k_x, \Gamma_y, \pi) = 1$. In modulo 2, $\theta(\Gamma_y)$ is recast into the $\mathbb{Z}_2$ invariant at $(k_x, \Gamma_y, k_z = 0)$ lines as follows:

$$\theta(\Gamma_y) := \frac{i}{\pi} \int_0^{2\pi} dk_x \text{tr}\mathcal{A}_+(k_x, \Gamma_y, 0) \pmod{2}. \quad (4.28)$$

by the Stokes’ theorem.

The three invariants $\{N, \theta(0), \theta(\pi)\}$ are not independent, since there is a constraint

$$N + \theta(0) + \theta(\pi) = 0 \pmod{2}, \quad (4.29)$$

which can be understood as follows. On the $k_z = 0$ plane, the $\mathbb{Z}_2$ invariant $\nu = \theta(0) + \theta(\pi) \pmod{2}$ is equivalent to the 2D class DIII $\mathbb{Z}_2$ invariant. Since we can show that the existence of odd numbers of Majorana cones is al-
lowed only on the \( k_z = 0 \) plane, \( N \) (mod 2) is also equivalent to the \( \mathbb{Z}_2 \) invariant. Therefore, \( N = \nu \) (mod 2), which implies Eq. (4.29).

V. TOPOLOGICAL NONSYMMORPHIC SUPERCONDUCTIVITY IN A-PHASE

Now we go back to the superconductivity in UPt

Let’s focus on the surface zero mode at \( k_{sf} = (0, \pi) \) in the TRS invariant A-phase. Naturally, the A-FSS are considered in this section. The surface states labeled by (V) in Fig. 5(e) have the spectrum shown in Fig. 6. As we considered in this section. The surface states labeled by \( \nu_G \) for glide-even TNSCs, which has been introduced in Eq. (4.19).

![Double Majorana cone in the A-phase](image)

**FIG. 6.** (Color online) Double Majorana cone in the A-phase. Energy spectrum of (100)-surface states around \( k_{sf} = (0, \pi) \) is shown. Parameters are the same as Fig. 5(e) for the paired A-FSS.

The glide symmetry of \( P6_3/mmc \) space group is \( G^{xz} = \{M^{xz}, \bar{x}\} \) composed of mirror reflection and half translation along the \( z \)-axis. Thus, the nonsymorphic glide operator is intrinsically \( k_z \)-dependent. We have an operator for the normal part Hamiltonian, \( G^{xz}(k_z) = is_y \sigma_x V_\sigma(k_z) \), where

\[
V_\sigma(k_z) = \begin{pmatrix} 1 & 0 \\ 0 & e^{-ik_z} \end{pmatrix}_\sigma, \tag{5.1}
\]

acts in the sublattice space. The superconducting state preserves the glide symmetry in the TRS invariant A- and C-phases, although the glide symmetry is spontaneously broken in the B-phase. The glide operator in the Nambu space depends on the glide-parity of the superconducting state; \( G_{BdG}^{xz}(k_z) = G^{xz}(k_z)\tau_0 \) in the glide-even A-phase while \( G_{BdG}^{xz}(k_z) = G^{xz}(k_z)\tau_z \) in the glide-odd C-phase. Then, the BdG Hamiltonian respects the glide symmetry

\[
G_{BdG}^{xz}(k_z)\tilde{H}_{BdG}(k)G_{BdG}^{xz}(k_z)^{-1} = \tilde{H}_{BdG}(k_x, -k_y, k_z). \tag{5.2}
\]

The symmetries satisfy the algebra (4.1)–(4.4) and (4.20)–(4.23) in the A-phase and C-phase, respectively.

A. Glide-\( \mathbb{Z}_2 \) invariant

![Unfolded BZ (solid line) and folded BZ](image)

**FIG. 7.** (Color online) Unfolded BZ (solid line) and folded BZ (dashed line) projected onto a \( k_z = \) constant plane. The latter is compatible with the surface BZ. \( K_x = 2\pi \bar{x} \) and \( K_y = \frac{2\pi}{\sqrt{3}} \bar{y} \) are reciprocal lattice vectors of the folded BZ.

As we showed in Sec. IV A, only the 2D plane at \( k_z = \pi \) determines the topological properties of the glide-even A-phase. From Eq. (4.19), the glide-\( \mathbb{Z}_2 \) invariant \( \nu_G \) is given by the 1D \( \mathbb{Z}_2 \) invariant of DIII class, \( \nu(\Gamma_y, \pm) \). When we choose the rectangular BZ shown in Fig. 7, we have \( \Gamma_y = 0, \pi/\sqrt{3} \). For our choice of parameters, the FSSs do not cross a line \( k_y = \pi/\sqrt{3} \) on the BZ face. Therefore, \( \nu(\pi/\sqrt{3}, \pm) \) is trivial, and the glide-\( \mathbb{Z}_2 \) invariant is obtained by evaluating \( \nu(0, \pm) \). Below, we show that \( \nu(0, \pm) = 1 \), and thus, the glide-\( \mathbb{Z}_2 \) invariant is nontrivial.

First, the Hamiltonian is block-diagonalized by using the basis diagonal for \( G_{BdG}^{xz}(\pi) = s_y \sigma_y \tau_0 \),

\[
\tilde{H}_{BdG}(k_x, 0, \pi) = \tilde{H}_{1d}(k_x) \oplus \tilde{H}_{-1d}(k_x), \tag{5.3}
\]

on the 1D BZ \( k_x \in [-2\pi, 2\pi] \). The glide-subsector with eigenvalue \( \lambda_G = \pm 1 \) is obtained as,

\[
\tilde{H}_{\pm 1d}(k_x) = \begin{pmatrix} \tilde{H}_{\pm 0d}(k_x) & \Delta(k_x) \\ \Delta(k_x)^T & -\tilde{H}_{\pm 0d}(-k_x)^T \end{pmatrix}, \tag{5.4}
\]

with

\[
\tilde{H}_{\pm 0d}(k_x) = \begin{pmatrix} \xi_{\pm 0d}(k_x) & \mp \alpha g_{\pm 0d}(k_x) \\ \mp \alpha g_{\pm 0d}^*(k_x) & \xi_{\pm 0d}^*(k_x) \end{pmatrix}, \tag{5.5}
\]

\[
\Delta(k_x) = i\Delta \begin{pmatrix} \delta p_{\pm 0d}(k_x) & -\delta q_{\pm 0d}(k_x) \\ -\delta q_{\pm 0d}^*(k_x) & \delta p_{\pm 0d}^*(k_x) \end{pmatrix}. \tag{5.6}
\]
We defined \( p^{1d}_z(k_z) \equiv p_z(k_z, 0, \pi) = \sin k_z + \sin \frac{k_z}{\sqrt{3}} \) and \( d^{1d}_z(k_z) \equiv d_z(k_z, 0, \pi) = -\sqrt{3} \sin \frac{k_z}{\sqrt{3}} \). Thus, the glide-subsector is equivalent to the TRS invariant \( p \)-wave SC. It is easy to confirm that both TRS and PHS are preserved in each glide-subsector as expected from Sec. iva. In the A-phase we adopt time-reversal operator in the Nambu space \( T_{\text{BdG}} = i T \tau_2 \), since the gap function is chosen to be pure imaginary. Then, the commutation relation \([C, T_{\text{BdG}}] = 0\) is satisfied.

Although the inversion symmetry is broken in the glide-subsector by the SOC, we can adiabatically eliminate the SOC as \( \alpha \to 0 \), unless the SOC is large enough to suppress the superconducting gap. Then, the glide-subsector is reduced to the odd-parity spin-triplet SC, and the \( Z_2 \) invariant is obtained by counting the number of Fermi points \( N(\lambda_G) \) (per Kramers pairs) between the time-reversal invariant momentum, \( k_z = 0 \) and \( 2 \pi \). Since each glide-subsector represents a single band model with \( N(\pm 1) = 1 \), the nontrivial \( Z_2 \) invariant, \( \nu(0, \pm) = 1 \) (mod 2), is obtained from the formula \((-1)\nu(0, \pm) = (-1)^{N(\pm)}\).

Now we conclude that the glide-\( Z_2 \) invariant is nontrivial, namely, \( \nu_G = 1 \), because

\[
\left( \nu(0, +); \nu(0, -); \nu(\pi/\sqrt{3}, +); \nu(\pi/\sqrt{3}, -) \right) = (1, 1; 0, 0).
\]

(5.7)

This is the strong topological index characterizing the TNSC with even glide-parity.

It should be noticed that the paired FSs and the sublattice-singlet \( d \)-wave pairing are essential ingredients. Both of them are ensured by the nonsymmorphic space group symmetry (see Secs. 1Ba and 1Cc). The pseudospin degree of freedom in the glide-subsector corresponds to the pair of FSs. Although the \( f \)-wave component in the order parameter disappears on the glide invariant plane \( k_y = 0 \), the \( d \)-wave component induces the superconducting gap and gives rise to 1D \( Z_2 \) nontrivial superconductivity.

The topological surface state protected by the glide-\( Z_2 \) invariant should appear as a signature of the TNSC. Because the two glide-subsectors discussed above are TRS invariant and \( Z_2 \) nontrivial, two Majorana states per subsector, namely, four Majorana states in total, appear on the glide invariant \((100)\)-surface. Indeed, the double Majorana cone centered at \( k_{sf} = (0, \pi) \) (Fig. 6) is the characteristic topological surface states of the glide-even TNSC.

For confirmation, we show the topological indices of 1D Hamiltonian along the \( k = (k_x, 0, 0) \) and \( (k_x, 0, \pi) \) lines and 2D Hamiltonian on the \( k_z = 0 \) and \( \pi \) planes in Table II. For these low-dimensional Hamiltonian, the topological classification can be carried out without taking care of the nonsymmorphic property. The (anti-para)commutation relations of symmetry operators are summarized in Table III and accordingly the topological indices are obtained on the basis of the periodic table for symmorphic topological crystalline insulators and SCs.25

| \( k_z \) | \( (G_{\text{BdG}}^+)^2 \) | \( \eta \) | \( \eta_G \) | 1D invariant | 2D invariant |
|-----|-----------------|-----|-----|---------|---------|
| \( k_z \) | \( \pi \) | \( \pi \) | \( \pi \) | \( Z_2 \) | \( Z_2 \) |
| \( \eta = 0 \) | \( -1 \) | \( 1 \) | \( -1 \) | \( Z_2 \) | \( Z_2 \) |
| \( \eta = \infty \) | \( 1 \) | \( 1 \) | \( 1 \) | \( Z_2 \) | \( Z_2 \) |

TABLE II. Classification of 1D and 2D BdG Hamiltonian in the TRS invariant A- and C-phases. The low-dimensional Hamiltonian on the basal plane \((k_z = 0)\) and BZ face \((k_z = \pi)\) is classified. We show \((G_{\text{BdG}}^+)\), \(\eta\), and \(\eta_G\). (Anti-)commutation relations with time-reversal and particle-hole operators are represented as \(T_{\text{BdG}} G_{\text{BdG}}^+ = \eta \), \(G_{\text{BdG}}^+ T_{\text{BdG}} \), \(C G_{\text{BdG}}^+ = \eta G_{\text{BdG}}^+ C\). The right two columns show the 1D topological index on the \((k_y, k_z) = (0, 0)\) and \((0, \pi)\) lines and the 2D topological index on the \(k_z = 0\) and \(\pi\) planes.

Indeed, in the A-phase we have \( Z_2 \oplus Z_2 \) index for 1D Hamiltonian on the \( k = (k_x, 0, \pi) \) line, which are nothing but \( \nu(0, \pm) \). The \( Z_2 \) index of 2D Hamiltonian on the \( k_z = \pi \) plane is equivalent to the glide-\( Z_2 \) invariant discussed in this section. On the other hand, the \( k_z = \pi \) plane is trivial in the glide-odd C-phase, consistent with the absence of topological surface states in Fig. 5a.

B. Folded Brillouin zone

For the consistency with classification based on the \(K\)-theory in Sec. 1V we need to consider the folded Brillouin zone compatible with the surface BZ. To be specific, the translation symmetry along the \([010]\)-axis is partially broken on the \((100)\)-surface. The basic translation vectors on the surface are \((y, z) = (\sqrt{3} y, 0) \) and \((0, 1)\), and the reciprocal lattice vectors are \(K_y = \frac{2}{\sqrt{3}} \pi \hat{y}\) and \(K_z = 2 \pi \hat{z}\). Thus, the surface first BZ is a rectangle with \(k_y \in [-\pi/\sqrt{3}, \pi/\sqrt{3}]\) and \(k_z \in [-\pi, \pi]\). We have already adopted the bulk BZ compatible with the surface BZ. However, the periodicity with respect to \(K_y\) is lost in the BdG Hamiltonian. To satisfy the periodicity, we equate \(k\) with \(k + K_y\), and accordingly, adopt the folded BZ in Fig. 7.

The folded BdG Hamiltonian is transformed

\[
\tilde{H}_{\text{BdG}}(k) = U_{\text{sf}}(k) \left( \begin{array}{cc}
\tilde{H}_{\text{BdG}}(k) & 0 \\
0 & \tilde{H}_{\text{BdG}}(k + K_y)
\end{array} \right) U_{\text{sf}}(k)^T,
\]

by the unitary matrix

\[
U_{\text{sf}}(k) = \frac{1}{\sqrt{2}} \left( \begin{array}{cc}
1 & 0 \\
0 & e^{i k \tau'}
\end{array} \right) \left( \begin{array}{cc}
1 & 1 \\
1 & -1
\end{array} \right),
\]

with \(\tau' = (\frac{1}{2}, \sqrt{3}, 0)\). It is easy to check the periodicity of the folded BdG Hamiltonian, \(\tilde{H}_{\text{BdG}}(k + K_z) = \tilde{H}_{\text{BdG}}(k)\) with respect to \(K_z = 2 \pi \hat{x}\), \(K_y\), and \(K_z\). The glide symmetry is recast,

\[
\tilde{G}_{\text{BdG}}^{z^z}(k) \tilde{H}_{\text{BdG}}(k) \tilde{G}_{\text{BdG}}^{z^z}(k)^{-1} = \tilde{H}_{\text{BdG}}(k_x, k_y, k_z),
\]

(5.10)
Kramers degeneracy is ensured by the TRS. The Kramers structure typical of glide-even TNSC. At the spectrum in Fig. 9 is obtained. In Fig. 9(a), the surface states detached from bulk excitations show the Möbius structure typical of glide-even TNSC. At $k_{zf} = 0$, the Kramers degeneracy is ensured by the TRS. The Kramers pair is formed by $\pm i$ glide eigenstates since the TRS and PHS are also preserved, and $\nu_G = 1$.

C. Deformation to Möbius surface state

The glide-$Z_2$ invariant $\nu_G$ is the strong topological index specifying the gapped TNSC. However, the A-phase is actually gapless because of the point nodes of gap function at the poles of 3D FSs. Figure 8 shows the surface spectrum $E(0, k_z)$, and indeed, we observe gapless bulk excitations away from the surface BZ boundary $k_z = \pi$ in addition to the double Majorana cone at $k_z = \pi$. Therefore, UPt$_3$ A-phase does not realize the characteristic “Möbius surface state” of topological nonsymmetric insulators/superconductors.

However, the nontrivial glide-$Z_2$ invariant ensures that the gapped TNSC can be realized when the point nodes are removed by some perturbations preserving the symmetry. Then, we obtain the Möbius surface states with keeping the nontrivial glide-$Z_2$ invariant and the associated double Majorana cone. In other words, the double Majorana cone around $k_{zf} = (0, \pi)$ is regarded as a reminiscent of the Möbius surface states of glide-even TNSC.

A simple way is to deform the FS to be cylindrical so that the point nodes are removed. Then, the surface spectrum in Fig. 9 is obtained. In Fig. 9(a), the surface states detached from bulk excitations show the Möbius structure typical of glide-even TNSC. At $k_{zf} = 0$, the Kramers degeneracy is ensured by the TRS. The Kramers pair is formed by $\pm i$ glide eigenstates since the TRS and PHS are also preserved in the glide-subsector. When we look at the $k_{zf} = (k_y, 0)$ line, Fig. 9(b) shows two helical modes protected by the mirror Chern number $\nu^0_H = 4$, which is introduced in Sec. 4.13. The nontrivial relationship between the mirror Chern number and the glide-$Z_2$...
invariant will be shown elsewhere.24

D. Broken glide symmetry by crystal distortion

Strictly speaking, the symmetry of crystal structure in UPt$_3$ is still under debate, because a tiny crystal distortion has been indicated by a x-ray diffraction measurement.25 The distortion leads to layer dimerization that breaks the glide and screw symmetry. Then, the space group is reduced from nonsymmorphic $P6_3/mmc$ to symmorphic $P3m1$. If the crystal distortion actually occurs in UPt$_3$, the double Majorana cone protected by the glide-$Z_2$ invariant may be gapped.

![FIG. 10. (Color online) Energy spectrum on the (100)-surface in the presence of layer dimerization that breaks the glide symmetry. Parameters are the same as Fig. 8 while the intersublattice hybridization is replaced by Eq. (5.18) with $d = 0.2$. Surface states are highlighted by green lines.](image)

The layer dimerization makes the inter-sublattice hybridization asymmetric between the $+$ and $-$ directions. The asymmetry is taken into account by replacing,

$$a(k) = 2t' \cos \frac{k_z}{2} \sum_{i=1,2,3} e^{ik_i \cdot r_i},$$

$$\Rightarrow t' \left[ (1 + d)e^{ik_z/2} + (1 - d)e^{-ik_z/2} \right] \sum_{i=1,2,3} e^{ik_i \cdot r_i}. \quad (5.18)$$

The parameter $d$ represents the strength of the layer dimerization. For a finite $d$, the double Majorana cone at $k_{sd} = (0, \pi)$ indeed acquires mass term. In Fig. 10 we show the surface spectrum gapped at $k_{sd} = (0, \pi)$. In the figure, a strong layer dimerization $d = 0.2$ is assumed in order to visualize the effect of glide symmetry breaking. In reality, the parameter $d$ is expected to be tiny even if it is finite, because the crystal distortion reported is small.26 Therefore, the gap in the double Majorana cone may be tiny, and a fingerprint of topological glide-$Z_2$ superconductivity will appear even in the symmorphic $P3m1$ structure.

VI. OTHER TOPOLOGICAL SURFACE STATES

In contrast to toy models, the model specific for the real material shows rich topological properties. In Figs. 11 and 12 we have observed a variety of surface states other than the double Majorana cone discussed in Sec. V. In this section, we clarify the topological invariant protecting the surface states. In addition to the glide symmetry, we take the mirror symmetry into account. The Weyl charge, mirror Chern number, glide winding number, and rotation winding number are discussed below.

A. Chiral Majorana arc in Weyl B-phase

The TRS broken B-phase identified as a Weyl superconducting state hosts surface Majorana arcs, analogous to Fermi arcs in Weyl semimetals.73–79 The existence of Majorana arcs is ensured by the topological Weyl charge

$$q_i = \frac{1}{2\pi} \oint_S \langle \mathbf{F} \rangle(k), \quad (6.1)$$

which is nothing but the monopole of Berry flux,

$$F_i(k) = -ie^{ijk} \sum_{E_n(k) < 0} \partial_{k_j} \langle u_n(k) | \partial_{k_k} u_n(k) \rangle. \quad (6.2)$$

A wave function and energy of Bogoliubov quasiparticles are denoted by $| u_n(k) \rangle$ and $E_n(k)$, respectively. A nontrivial Weyl charge protects the Weyl point node in the bulk excitation spectrum. Indeed, the B-phase of UPt$_3$ is a point nodal SC compatible with Blount’s theorem when the $p$-wave and $d$-wave order parameters are appropriately taken into account.20,21 Although the purely $f$-wave state has a nodal line at $k_z = 0$, it is an accidental node removed by symmetry-preserving perturbation. In accordance with the bulk-boundary correspondence, the Majorana arcs appear on the surface and terminate at the projection of Weyl point nodes illustrated by green circles in Figs. 11 and 12.

Interestingly, the position of Weyl nodes is tunable. In the $E_{2u}$ scenario for UPt$_3$, the parameter $\eta$ smoothly changes from $\infty$ to 0 in the B-phase by decreasing the temperature and/or increasing the magnetic field (see Fig. 3 and Table I). Then, the pair creation, pair annihilation, and coalescence of Weyl nodes occur as a consequence of the $p$-$f$ mixing in the order parameter. Accordingly, the projection of Weyl nodes moves as illustrated in Figs. 12(b)-(d) and 12(b)-(d). The Majorana arcs follow the Weyl nodes.

In the generic $E_{2u}$-state studied in this paper, the Weyl nodes are purely protected by topology, and any crystal symmetry is not needed. Therefore, the positions of Weyl nodes are not constrained by any symmetry. Although the Weyl nodes are pinned at the poles of FS in the purely $f$-wave $E_{2u}$-state, that is an accidental result. In another candidate of Weyl SC URu$_2$Si$_2$, the
3D $d_{xz} \pm id_{yz}$-wave superconductivity has been revealed by experiments. Then, the Weyl nodes are pinned and the traveling of Weyl nodes does not occur, in contrast to UPt$_3$.

![Fig. 11](image_url)

**FIG. 11.** (Color online) Energy spectrum on the (100)-surface in the B-phase ($\eta = 0.6$). Surface and bulk quasiparticle states on slices of BZ at $k_z =$ constant planes are shown. The surface states are emphasized by green lines. The $k_z$-dependent Chern number is shown in each panel. (a)-(e) Parameters are the same as Fig. 6(b). (f) $\nu = 1$ while the others are the same as (e). The surface states are almost two-fold degenerate in (d) and (f) and four-fold degenerate in (e). Comparison of (e) and (f) reveals that the four-fold degeneracy in the absence of the SOC is lifted by the SOC.

Here the number of Majorana arcs is verified by calculating the Chern number of effective 2D models on $k_z =$ constant planes,

$$\nu(k_z) = \frac{1}{2\pi} \int \text{d}k_{\parallel} F_z(k), \tag{6.3}$$

that is, a $k_z$-dependent Chern number of class A. The Chern number indicates the number of chiral surface modes. In Weyl SCs, the Chern number may change at a gapless $k_z =$ constant plane hosting Weyl nodes. Therefore, the zero energy surface states form arcs terminating at the projection of Weyl nodes. For parameters reproducing the $A$-FSs, the Chern number changes $\nu(k_z) = 0 \rightarrow 4 \rightarrow 8 \rightarrow -4$ with increasing $k_z$ from 0 to $\pi$, while $\nu(k_z) = 0 \rightarrow 4 \rightarrow 0$ for the $\Gamma$-FS. The bulk-boundary correspondence is confirmed by showing the surface spectrum on the $k_z =$ constant lines in Fig. 11. The number of chiral modes coincides with the $k_z$-dependent Chern number. We also observe the sign reversal of chirality in accordance with the sign change of the Chern number.

Finally, we discuss the Weyl superconducting phase in the phase diagram illustrated in Fig. 3. Because the TRS has to be broken in Weyl SCs, the $A$- and $C$-phases are non-Weyl superconducting states. Furthermore, the B-phase in the vicinity of the $A$-$B$ and $B$-$C$ phase boundaries are also non-Weyl state because the gap closing is required for the topological transition. Therefore, the transition from the non-Weyl state to the Weyl state occurs in the B-phase. The shaded region in Fig. 3 schematically illustrates the Weyl superconducting phase.

### B. Majorana cone and mirror Chern number

Next we discuss the surface state around $k_{sf} = (0, 0)$, which is observed in all the $A$-, $B$-, and $C$-phases (Fig. 4). In the TRS broken B-phase, the spectrum resembles a tilted Majorana cone as shown in Fig. 12 although the cone is not tilted in the $A$- and $C$-phases. Naturally, the $\Gamma$-FS and $K$-FS are considered in this subsection.

![Fig. 12](image_url)

**FIG. 12.** (Color online) Tilted Majorana cone at $k_{sf} = (0, 0)$ in the B-phase ($\eta = 0.5$). Parameters are $(t, t_z, t', \alpha, \mu, \Delta, \delta) = (1, 4, 1, 0, 16, 4, 0.02)$ reproducing a $\Gamma$-FS.

We may understand the topological protection by implementing the crystal mirror reflection symmetry with respect to the $xy$-plane. Mirror reflection operator for the normal part Hamiltonian is,

$$M^{xy}(k_z) = is_z V_\sigma(k_z). \tag{6.4}$$

The mirror reflection symmetry is equivalent to the product of inversion symmetry and screw symmetry, that
is, $M^{xy}(k_z) = IS^z(k_z)$. The nonsymmetric screw symmetry $S^z = \{ R_{z\pi/2} \}$ involves half translation along the $z$-axis, and therefore, the screw operator $S^z(k_z)$ is $k_z$-dependent. Thus, the mirror operator is also $k_z$-dependent, and we have $M^{xy}(\pi) = iS^x_S \sigma_z$ while $M^{xy}(0) = iS^x$. This momentum dependence of $M^{xy}(k_z)$ may yield the unusual line node in nonsymmetric odd-parity SCs, a counterexample of Blount’s theorem.

The normal part Hamiltonian is invariant under the mirror reflection symmetry

$$M^{xy}(k_z) \tilde{H}_0(k) M^{xy}(k_z)^{-1} = \tilde{H}_0(k_z, k_y, -k_z),$$

and the order parameter is mirror-odd irrespective of $\eta$, $M^{xy}(k_z) \tilde{\Delta}(k) M^{xy}(-k_z)^T = -\tilde{\Delta}(k_x, k_y, -k_z)$. (6.6)

Thus, the BdG Hamiltonian respects mirror reflection symmetry,

$$M^{xy}_{BdG}(k_z) \tilde{H}_{BdG}(k) M^{xy}_{BdG}(k_z)^{-1} = \tilde{H}_{BdG}(k_z, k_y, -k_z),$$

by defining the operator in the Nambu space,

$$M^{xy}_{BdG}(k_z) = \begin{pmatrix} M^{xy}(k_z) & 0 \\ 0 & -M^{xy}(-k_z)^* \end{pmatrix} \tau.$$ \hspace{1cm} (6.8)

According to the $K$-theory for topological crystalline insulators and SCs, the effective 2D Hamiltonian at mirror invariant planes, namely, $k_z = 0$ and $\pi$, is specified by a topological index of class D, $Z \oplus Z$, in the TRS broken B-phase. This is ensured by the algebra $[M_{BdG}^{xy}(\pi)]^2 = [M_{BdG}^{xy}(0)]^2 = -1$ and $\{M_{BdG}^{xy}(0), C\} = \{M_{BdG}^{xy}(\pi), C\} = 0$. One of the two integer topological invariants is nothing but the Chern number $\nu(k_z)$ introduced in Sec. 5.1A. The other is the mirror Chern number, $\nu_{BdG}^{\Gamma}$, which is defined below by using the mirror reflection symmetry. In the TRS invariant A- and C-phases, the Chern number must be zero, and the mirror Chern number is naturally the $Z$ topological index of class DII appearing in Ref. 48.

The commutation relation,

$$[M_{BdG}^{xy}(\Gamma_z), \tilde{H}_{BdG}(k_z, \Gamma_z)] = 0,$$

ensures that the BdG Hamiltonian is block-diagonalized on mirror invariant planes on the basis diagonalizing $M_{BdG}^{xy}(\Gamma_z)$. In other words, the BdG Hamiltonian is decomposed into two mirror-subsectors with mirror eigenvalues $\pm i$,

$$\tilde{H}_{BdG}(k_z, \Gamma_z) = \tilde{H}_{\pm i}^{\Gamma_z}(k_z) \oplus \tilde{H}_{\mp i}^{\Gamma_z}(k_z).$$ \hspace{1cm} (6.10)

The PHS is preserved in the mirror-subsector, because of $[M_{BdG}^{xy}(\Gamma_z)]^2 = -1$ and $\{M_{BdG}^{xy}(\Gamma_z), C\} = 0$. On the other hand, the TRS is not preserved even in the TRS invariant A- and C-phases since $[M_{BdG}^{xy}(\Gamma_z), T] = 0$. Thus, the symmetry of the mirror-subsector is class D irrespective of $\eta$, and the Chern number of mirror-subsector Hamiltonian given by

$$\nu_{BdG}^{\pm i} = \frac{1}{2\pi} \int d\mathbf{k}_z F^\pm_{\pm i}(\mathbf{k}_z),$$ \hspace{1cm} (6.11)

may be nontrivial. Here, $F^\pm_{\pm i}(\mathbf{k}_z)$ is the Berry curvature of $\tilde{H}_{\pm i}^{\Gamma_z}(k_z)$. The mirror Chern number is defined by

$$\nu_{M}^{\Gamma_z} = \nu_{\pm i}^{\mp i} - \nu_{\mp i}^{\pm i},$$ \hspace{1cm} (6.12)

while the total Chern number is given by $\nu(\Gamma_z) = \nu_{\pm i}^{\pm i} + \nu_{\mp i}^{\mp i}$.

1. Mirror Chern number at $k_z = 0$

Later we show that the mirror Chern number at $k_z = \pi$ has to vanish owing to the constraint by glide symmetry. On the other hand, the mirror Chern number may be nontrivial at $k_z = 0$, and the surface states around $k_z = 0$ are indeed protected by the mirror Chern number. Because we have $M^{xy}_{BdG}(0) = iS^x \sigma_0$, the mirror-subsector Hamiltonian $\tilde{H}_{\mp i}^{\Gamma_z}(k_z)$ is equivalent to the spin sector for $s = \uparrow, \downarrow$, respectively. Thus, we obtain

$$\tilde{H}_{\mp i}^{0}(k_z) = \begin{pmatrix} \hat{h}_{\pm i}(k_z) & \hat{\Delta}_{\pm i}(k_z) \\ \hat{\Delta}_{\pm i}^*(k_z) & -\hat{h}_{\mp i}(-k_z)^T \end{pmatrix},$$ \hspace{1cm} (6.13)

with

$$\hat{h}_{\pm i}(k_z) = \begin{pmatrix} \varepsilon(k_z) \pm \alpha g(k_z) \\ \alpha g(k_z) \hat{a}(k_z)^* \end{pmatrix},$$ \hspace{1cm} (6.14)

and

$$\hat{\Delta}_{\pm i}(k_z) = - \eta \mp \Delta_p \hat{p}_z(k_z) \pm ip_y(k_z) \sigma_0.$$ \hspace{1cm} (6.15)

We denoted $A(k_z) = A(k_z, 0)$ and $\Delta_p = \delta \Delta / \sqrt{1 + \eta^2}$. It turns out that the mirror-subsector Hamiltonian is equivalent to the BdG Hamiltonian of a two-band chiral $p$-wave SC. In our model for the $\Gamma$-FS, only one band crosses the Fermi level, and we obtain $\nu_{BdG}^{\pm i} = \pm 1$. The sign of Chern number is opposite between the two mirror-subsectors because of the opposite chirality of $p$-wave order parameter [see Eq. (6.15)]. Therefore, the total Chern number of the 2D BdG Hamiltonian is zero, $\nu(0) = \nu_{\mp i}^{\pm i} + \nu_{\pm i}^{\mp i} = 0$, even in the TRS broken B-phase. On the other hand, the mirror Chern number is nontrivial,

$$\nu_{M}^{0} = 2.$$ \hspace{1cm} (6.16)

We now understand that the (tilted-) Majorana cone in Fig. 12 is the topological surface states ensured by the bulk-boundary correspondence. Since the chirality of Majorana modes corresponding to $\nu_{BdG}^{\pm i} = \pm 1$ is opposite between two mirror-subsectors, the (tilted) helical mode appears at $k_z = 0$, and the helical mode is gapped at $k_z \neq 0$, implying the Majorana cone.

Finally, we comment on the multiband effect. Although Eq. (6.10) is obtained for a hole $\Gamma$-FS, we obtain $\nu_{M}^{0} = -2$ for a electron $\Gamma$-FS consistent with UPt$_3$-Sb$_2$-Sb. Because the mirror Chern number is additive, we will obtain the mirror Chern number $\nu_{M}^{\pm i} = -6$.
from three $\Gamma$-FSs. Then, the surface states form a (tilted) Majorana cone at $k_{sf} = (0, 0)$ and two cones away from the $\Gamma$-point, $k_{sf} = (\pm k_0^0, 0)$. Although the $K$-FSs have also been predicted by band structure calculations,\textsuperscript{39,52} the existence of them is still under debate\textsuperscript{53,55}. The $K$-FSs also give nontrivial mirror Chern number $\nu_0^M = -8$ if they exist. Then, the mirror Chern number is $\nu_0^M = -14$ by taking into account all the FSs. In any case, $\nu_0^M \in 4\mathbb{Z} + 2$ indicates the existence of Majorana cone at $k_{sf} = (0, 0)$.

2. Vanishing mirror Chern number at $k_z = \pi$

We here show that the mirror Chern number at $k_z = \pi$ must be trivial owing to the glide symmetry, namely,

$$\nu_0^M = 0. \quad (6.17)$$

First, we consider the glide invariant A- and C-phases. The glide symmetry is also preserved in the mirror-subsectors at $k_z = \pi$ because of $[M^T_{BG}(\pi), G^T_{BG}(\pi)] = 0$, although $[M_{BG}^z(0), G^z_{BG}(0)] = 0$ indicates the broken glide-symmetry in the mirror-subsectors at $k_z = 0$. Then, we can prove the relation for Berry curvature,

$$F^z_{x,z}(k_x, k_y) = -F^z_{x,z}(k_x, -k_y). \quad (6.18)$$

Integration over the $(k_x, k_y)$ plane ends up vanishing Chern number, $\nu^z_{x \pm} = 0$, and thus, the mirror Chern number also vanishes. In the B-phase, the glide symmetry is spontaneously broken. However, considering the magnetic-glide symmetry $TG^z_{BG}(\pi)$, we can show the relation

$$F^z_{x,z}(k_x, k_y) = F^z_{x,z}(-k_x, k_y),$$

which leads to $\nu^z_{x} = \nu^z_{-x}$. Therefore, the mirror Chern number at $k_z = \pi$ vanishes in the B-phase as well.

The trivial mirror Chern number is confirmed in our model as follows. Using the mirror reflection operator $M^T_{BG}(\pi) = i\pi \sigma_z 7_0$, we obtain the mirror-subsector Hamiltonian respecting the PHS,

$$\hat{H}^T_{x,z}(k_{\|}) = \left( \begin{array}{c c} \hat{h}^T_{\pm}(k_{\|}) & \Delta_{x \pm}(k_{\|})^T \\ \Delta_{z \pm}(k_{\|}) & -\hat{h}^T_{\pm}(k_{\|})^T \end{array} \right). \quad (6.20)$$

The normal part is given by

$$\hat{h}^T_{\pm}(k_{\|}) = [\varepsilon(k_{\|}) \pm \alpha g(k_{\|})] \sigma_0. \quad (6.21)$$

For instance, the order parameter is

$$\Delta_{x \pm}(k_{\|}) = \Delta_{\mp} \times \left( \begin{array}{c c} \mp \delta [p_x(k_{\|}) \pm i p_y(k_{\|})] & \tilde{f}^{(x^2-y^2)z}(k_{\|}) \pm i \tilde{d}_{yz}(k_{\|}) \\ \tilde{f}^{(x^2-y^2)z}(k_{\|})^* & \pm \delta [p_x(k_{\|}) \pm i p_y(k_{\|})]^* \end{array} \right),$$

in the C-phase. When the $d + f$-wave component is dominant as we assume in this paper, the $p$-wave component can be adiabatically reduced to zero without closing the gap. Then, it turns out that the Chern number of mirror-subsectors is trivial because the phase winding of $\tilde{f}^{(x^2-y^2)z}(k_{\|}) \pm i \tilde{d}_{yz}(k_{\|})$ along the FS is zero. Even when the $p$-wave component is dominant, the Chern number vanishes because the chirality of gap function $p_x(k_{\|}) \pm i p_y(k_{\|})$ is opposite between the pseudopotential up and down Cooper pairs. Thus, we obtain $\nu^z_{\pm} = 0$ and $\nu^z_M = 0$ in the C-phase. It is straightforward to show $\nu^z_{\pm} = 0$ in the A-phase as well. In the B-phase we have obtained the nontrivial Chern number $\nu(\pi) = -4$ for the A-FSs. However, the mirror Chern number remains trivial, because $\nu^z_{\pm} = -2$. We have numerically confirmed Eq. (6.17) in the entire A-, B- and C-phases for all the FSs.

C. Majorana flat band and glide winding number

As shown in Figs. 4(d) and (e) and Figs. 5(d) and (e), the zero energy surface flat band appears in the A-phase and in a “half” of the B-phase ($|\eta| > 1$). We here show that the flat band is topologically protected by the glide winding number. Below we first demonstrate the topological protection in the A-phase, and later investigate the B-phase.

1. A-phase

Let’s consider the glide invariant plane $k_z = 0$ in the A-phase. The glide winding number is defined for 1D models $\hat{H}_{BG}(k_x, 0, k_z)$ parametrized by $k_z$. The 1D models do not respect TRS and PHS unless $(0, 0, k_z)$ is a time-reversal invariant momentum. On the other hand, the combined chiral symmetry, $\Gamma = i T_{BRG} C$, is preserved. Thus, the winding number of 1D AIH class can be defined. However, it is obtained to be zero.

The nontrivial winding number is obtained by implementing the glide symmetry, which has been represented by Eq. (5.22). The glide symmetry ensures the sector decomposition,

$$\hat{H}_{BG}(k_x, 0, k_z) = \hat{H}_{\Lambda+}(k_x, k_z) \oplus \hat{H}_{\Lambda-}(k_x, k_z),$$

for eigenvalues $\lambda_{\pm} = \pm ie^{-ik_z}/2$ of the glide operator. The chiral symmetry is preserved in the glide-subsector Hamiltonian $\hat{H}_{\Lambda\pm}(k_x, k_z)$ because $[\Gamma, G^z_{BG}(k_z)] = 0$ in the A-phase. Now we have two winding numbers of AIH class, $\omega_{G}(+\kappa, z)$ and $\omega_{G}(-\kappa, z)$, which correspond to the $\mathbb{Z} \oplus \mathbb{Z}$ topological index of 1D AIH class with $U_+$ crystal symmetry.\textsuperscript{88}

We here estimate the winding numbers by analyzing the original BdG Hamiltonian $\hat{H}_{BG}(k)$, instead of $\hat{H}_{BG}(k)$. The periodicity along the $k_z$-axis is satisfied in $\hat{H}_{BG}(k)$, and the unitary transformation $\hat{U}(2\pi x)$ does not alter the winding number, since $[\Gamma, \hat{U}(k)] = 0$. The glide operator for the original BdG Hamiltonian $\hat{H}_{BG}(k)$ is $G^z_{BG} = i \sigma_x \tau z e^{-ik_z}/2$ in the A-phase while $G^z_{BG} = i \sigma_x \tau z e^{-ik_x}/2$ in the C-phase.
In the A-phase, the glide-subsectors of $\hat{H}_{\text{BdG}}(k)$ are,

\[
\hat{H}_{\pm}(k_x, k_z) = e^{ik_x}(k_x)\sigma_0\tau_z \mp e^{ik_x}(k_x)\sigma_z\tau_x + \alpha g(k_x)\sigma_y\tau_0 \\
- \Delta\delta p_x(k_x)\sigma_0\tau_x \mp \Delta d_x(k_x)\sigma_y\tau_y.
\]

(6.24)

The chiral symmetry is confirmed by the poles of FSs (per Kramers pairs) is odd. The nontrivial glide-winding number is nontrivial. Thus, we obtain the off-diagonal form

\[
U_{\Gamma_s}\hat{H}_{\pm}(k_x, k_z)U_{\Gamma_s}^\dagger = \begin{pmatrix}
0 & \hat{q}_\pm(k_x, k_z) \\
\hat{q}_\pm(k_x, k_z) & 0
\end{pmatrix},
\]

(6.25)

by choosing the basis diagonalizing the chiral operator. From Eq. (6.24), we obtain

\[
q_\pm(k_x, k_z) = e^{ik_x}(k_x)\sigma_z \mp ia^{k_x}(k_x)\sigma_0 + \Delta\delta p_x(k_x)\sigma_0 + [\alpha g(k_x) \mp \Delta d_x(k_x)\sigma_y],
\]

(6.26)

for the $\lambda_\pm$ glide-subsector, respectively. We used abbreviations, $A^{\pm}(k_x) = A(k_x, 0, k_z)$.

Now the winding number of glide-subsectors given by

\[
\omega_G(\pm, k_z) = \frac{1}{4\pi i} \int_{0}^{4\pi} dk_y \text{Tr} \left[ \hat{q}_\pm(k_x, k_z)^{-1} \partial_{k_y} \hat{q}_\pm(k_x, k_z) - \hat{q}_\pm(k_x, k_z)^{-1} \partial_{k_y} \hat{q}_\pm(k_x, k_z) \right],
\]

(6.27)

is calculated. By adiabatically reducing $\alpha g(k_x) \to 0$ and $d_x(k_x) \to 0$ without closing the excitation gap, we obtain the winding number as

\[
\omega_G(\pm, k_z) = \begin{cases}
\mp 1 & \varepsilon(0, k_z) + a(0, k_z) > 0 > \varepsilon(0, k_z) - a(0, k_z) \\
0 & \text{[otherwise]}
\end{cases}
\]

(6.28)

for $t > 0$, $t' > 0$ and $\Delta\delta > 0$. This means that the $\lambda_\pm$ glide-subsectors of $\hat{H}_{\text{BdG}}(k)$ [and equivalently the subsectors of the periodic BdG Hamiltonian $\hat{H}_{\text{BdG}}(k)$] are topologically characterized by the glide-winding number $\omega_G(\pm, k_z) = \mp 1$, when the condition $\varepsilon(0, k_z) + a(0, k_z) > 0 > \varepsilon(0, k_z) - a(0, k_z)$ is satisfied. This condition is equivalent to the number of FSs (per Kramers pairs) is odd.

In Figs. 4(e) and 4(e), the flat band appears on the $k_y = 0$ line of surface BZ where only one FS is projected. The nontrivial glide-winding number demonstrated above protects this Majorana flat band. The zero energy states are two-fold degenerate in accordance with the bulk-boundary correspondence. One comes from the $\lambda_+ = e^{-ik_x/2}$ glide-subsector and the other comes from the $\lambda_- = -e^{-ik_x/2}$ glide-subsector. Note that the flat band is robust against the multiband effect. We find that the glide-winding number of $K$-FSs is zero. Taking into account three $\Gamma$-FSs, we will have glide-winding number $\omega_G(\pm, 0) = \mp 3$, or $\mp 1$, or $\pm 1$, or $\pm 3$ depending on the sign of order parameter. In any case, the glide-winding number is nontrivial.

2. B-phase

The glide-subsector is no longer well-defined in the B-phase, because the glide symmetry is spontaneously broken. However, the glide-winding number is well-defined by the magnetic-glide symmetry $G^0_{\text{BdG}} T$ preserved in the B-phase. Then, the glide-winding number is given by

\[
\omega_G(k_z) = \frac{i}{4\pi} \int_{0}^{2\pi} dk_y \text{Tr} \left[ \Gamma_G \hat{H}_{\text{BdG}}(k_x, 0, k_z)^{-1} \times \partial_{k_y} \hat{H}_{\text{BdG}}(k_x, 0, k_z) \right],
\]

(6.29)

where $\Gamma_G = e^{i\sigma_0 \frac{\partial}{\partial k_x}} G^0_{\text{BdG}}(k_z) T_{\text{BdG}} C$ is the glide-chiral operator with $\Gamma_G^2 = 1$. In the A-phase, Eq. (6.29) is reduced to

\[
\omega_G(k_z) = \omega_G(+, k_z) - \omega_G(-, k_z).
\]

(6.30)

Thus, we obtain $\omega_G(k_z) = -2$ in the A-phase. The nontrivial glide-winding number is robust as long as the gap is finite. Therefore, the Majorana flat band appears in the B-phase under the condition (6.28), when the parameter $|\eta|$ is large [see Fig. 13(a)]. When $|\eta|$ is decreased from infinity, the pair creation of Weyl nodes occurs in the bulk BZ on the $k_y = 0$ plane. Then, a part of the Majorana flat band disappears in between the pair of projected Weyl points [see Fig. 13(b)]. Therefore, the projected Weyl points are end points not only of the Majorana arc but also of the Majorana flat band. This feature has been shown in Figs. 4(d) and 5(d).

FIG. 13. (Color online) Illustration of the Majorana flat band (a) in the A-phase and non-Weyl B-phase ($\eta > \eta_c$), (b) in the Weyl B-phase ($\eta_c > \eta > 1$), and (c) at the critical point ($\eta = 1$). Thick solid (purple) lines show the Majorana flat band. Thin lines illustrate the projection of a $\Gamma$-FS onto the (100)-surface BZ. The closed (blue) circles indicate projections of Weyl point nodes, (a), (b), and (c) correspond to the numerical results in Figs. 4(e), (d), and (c), respectively.

At $|\eta| = 1$, a pair of Weyl nodes is annihilated on the $k = (k_x, 0, 0)$ line, and other Weyl nodes coalesce on the poles of FSs. Then, the Majorana flat band completely disappears [Fig. 13(c)]. The fate of the Majorana
flat band in the B-phase is schematically illustrated in Fig. 13 and shown in Figs. 4 and 5 by the numerical diagonalization of the BdG Hamiltonian.

D. Symmetry constraint on winding numbers

The crystal symmetries preserved on the (100)-surface are as follows.

- Mirror symmetry \( M^{xy} \).
- Glide symmetry \( G^{xz} \).
- \( \pi \)-rotation symmetry \( R^\pi \).

The \( \pi \)-rotation is given by the product of mirror and glide operations.

In addition to the glide-winding number studied in Sec. VIC we can define the mirror-winding number \( \omega^M \) and the rotation-winding number \( \omega^R \) in the same manner. They are given by

\[
\omega^M_{\Gamma}(k_y) = \frac{i}{4\pi} \int_0^{4\pi} dk_x \text{Tr} \left[ \Gamma_M(\Gamma_z) \tilde{H}_{\text{BdG}}(k_x, k_y, \Gamma_z)^{-1} \times \partial_{k_z} \tilde{H}_{\text{BdG}}(k_x, k_y, \Gamma_z) \right],
\]

and

\[
\omega^R_{\Gamma}(k_y) = \frac{i}{4\pi} \int_0^{4\pi} dk_x \text{Tr} \left[ \Gamma_R \tilde{H}_{\text{BdG}}(k_x, 0, \Gamma_z)^{-1} \times \partial_{k_z} \tilde{H}_{\text{BdG}}(k_x, 0, \Gamma_z) \right].
\]

\( \Gamma_M(\Gamma_z) = e^{i\theta} M^{xy}(\Gamma_z) \Gamma \) and \( \Gamma_R = e^{i\theta'} R_{\text{BdG}} \Gamma \) are mirror-chiral operator and rotation-chiral operator, respectively. The phase factors \( e^{i\theta} \) and \( e^{i\theta'} \) are chosen so that \( \Gamma_M(\Gamma_z)^2 = \Gamma_R^2 = 1 \). The mirror-winding number is defined on the mirror invariant planes at \( k_z = \Gamma_z = 0, \pi \) and \( k_y \)-dependent. On the other hand, the rotation-winding number is defined on the rotation invariant lines. The mirror-winding number is defined only in the TRS invariant A- and C-phases, since the mirror-chiral symmetry is broken in the TRS broken B-phase.

From the algebra of symmetry operations we can prove that most of the winding numbers vanish. The proof relies on the fact that the winding number disappears when any unitary symmetry preserved on the surface anti-commutes with the chiral operator, \( \{ U, \Gamma_V \} = 0 \). This fact, \( \omega_V = 0 \), is understood by

\[
\omega_V = \frac{i}{4\pi} \int_0^{4\pi} dk_x \text{Tr} \left[ U \Gamma_V \tilde{H}_{1D}(k_x)^{-1} \partial_{k_z} \tilde{H}_{1D}(k_x) U^\dagger \right] = \frac{i}{4\pi} \int_0^{4\pi} dk_x \text{Tr} \left[ -\Gamma_V \tilde{H}_{1D}(k_x)^{-1} \partial_{k_z} \tilde{H}_{1D}(k_x) \right] = -\omega_V.
\]

Furthermore, the TRS has to satisfy \( \{ T, \Gamma_V \} = 0 \) when the winding number is nontrivial. All of the mirror, glide, and rotation symmetries are preserved at the rotation invariant lines in the A- and C-phases, although the glide and rotation symmetries are spontaneously broken in the B-phase. Thus, we obtain some constraints on the winding numbers at \( k_{sf} = (0, 0) \) and \( (0, \pi) \) in the A- and C-phases.

| \( \Gamma \) | \( c(M^{xy}, \Gamma_M) \) | \( c(G^{xz}, \Gamma_M) \) | \( c(R^\pi, \Gamma_M) \) | \( c(T, \Gamma_M) \) |
|---|---|---|---|---|
| A-phase | 0 | -1 | -1 | +1 | -1 |
| \( \pi \) | -1 | +1 | -1 | -1 |
| C-phase | 0 | -1 | +1 | -1 | -1 |
| \( \pi \) | -1 | -1 | +1 | -1 | -1 |

TABLE III. Commutation (anti-commutation) relations of the mirror-chiral operator \( \Gamma_M \) with the crystal symmetry and time-reversal operators represented by \( +1 \) (\(-1\)).

| \( \Gamma \) | \( c(M^{xy}, \Gamma_G) \) | \( c(G^{xz}, \Gamma_G) \) | \( c(R^\pi, \Gamma_G) \) | \( c(T, \Gamma_G) \) |
|---|---|---|---|---|
| A-phase | 0 | +1 | -1 | -1 | -1 |
| \( \pi \) | -1 | +1 | -1 | -1 |
| C-phase | 0 | +1 | +1 | -1 | +1 |
| \( \pi \) | -1 | -1 | +1 | -1 | +1 |

TABLE IV. Commutation (anti-commutation) relations of the glide-chiral operator \( \Gamma_G \) with the crystal symmetry and time-reversal operators.

| \( \Gamma \) | \( c(M^{xy}, \Gamma_R) \) | \( c(G^{xz}, \Gamma_R) \) | \( c(R^\pi, \Gamma_R) \) | \( c(T, \Gamma_R) \) |
|---|---|---|---|---|
| A-phase | 0 | +1 | -1 | -1 | -1 |
| \( \pi \) | -1 | +1 | -1 | -1 |
| C-phase | 0 | +1 | +1 | -1 | +1 |
| \( \pi \) | -1 | -1 | +1 | -1 | +1 |

TABLE V. Commutation (anti-commutation) relations of the rotation-chiral operator \( \Gamma_R \) with the crystal symmetry and time-reversal operators.

The commutation (anti-commutation) relations between crystal symmetry operators \( M^{xy}, G^{xz}, R^\pi \) and chiral operators \( \Gamma_M, \Gamma_G, \) and \( \Gamma_R \) are summarized in Tables III, IV, and V. From these algebra, we find that only \( \omega_{\Gamma}(0) \) and \( \omega^R_\Gamma \) may be nontrivial. Interestingly, all the winding numbers at \( k_z = \pi \) vanish as a consequence of the nonsymmorphic glide symmetry. The mirror-winding number at \( k_z = 0 \) also vanishes in both A- and C-phases. Furthermore, we see that the rotation-winding number \( \omega^R_\Gamma \) disappears in the A-phase, while the glide-winding number \( \omega_{\Gamma}(0) \) disappears in the C-phase. These symmetry constraints are consistent with our numerical calculations summarized in Table VI and also consistent with recently obtained general rules for winding numbers.

In addition to the glide-winding number \( \omega_{\Gamma}(0) \) discussed in Sec. VIC, we may have a nontrivial rotation-winding number, which is introduced below for completeness. Combining the \( \pi \)-rotation symmetry with TRS, we define the magnetic \( \pi \)-rotation symmetry by
### VII. SUMMARY AND DISCUSSIONS

We investigated topologically nontrivial superconducting phases in UPt$_3$. Taking into account the FSs reported by first principles band structure calculation and quantum oscillation experiments, we have calculated the topological invariants specifying the superconducting states and demonstrated topological surface states.

Among a variety of topological properties in UPt$_3$, the most intriguing result is the nontrivial glide-Z$_2$ invariant in the TRS invariant A-phase. By using the $K$-theory for topological nonsymmorphic insulators/superconductors, we showed that the glide-Z$_2$ invariant is the strong topological index specifying the 3D glide-even superconductivity of class DIII. Although UPt$_3$ is a gapless SC in the bulk, the glide-Z$_2$ invariant is well-defined and nontrivial. Thus, the UPt$_3$ A-phase can be reduced to a 3D gapped TNSC with keeping double Majorana cone surface states, when the point nodes are removed by some perturbations. By these findings, UPt$_3$ is identified as a 3D gapless TNSC. At our best knowledge, this is the first proposal for the material realization of emergent topological superconductivity enriched by nonsymmorphic space group symmetry.

Not only the A-phase but also the B- and C-phases have been identified as symmetry-enriched topological superconducting states. Combining the crystal symmetries of UPt$_3$ with the TRS and PHS, we find topological invariants and surface states as follows.

- Double Majorana cone protected by the glide-Z$_2$ invariant in the A-phase
- Chiral Majorana arcs in the Weyl B-phase
- Majorana cone protected by the mirror Chern number in the A-, B-, and C-phases
- Majorana flat band protected by the glide-winding number in the A-phase and “half” of the B-phase

It has been proved that the other mirror Chern number and winding numbers must be trivial because of the constraints by symmetry.

From the results obtained in this paper, we notice rich topological properties of superconducting UPt$_3$. Underlying origins of such topological superconducting phases are as follows. (1) Spin-triplet odd-parity superconductivity, which is often a platform of topological SC. (2) 2D $E_{2u}$ representation, which allows multiple superconducting phases distinguished by symmetry. (3) Nonsymmorphic space group symmetry $P6_3/mmc$, which gives rise to following features distinct from symmmorphic systems,

1. Classification of topological insulators and SCs changes, and allows emergent topological phases.
2. Dirac nodal lines yield the paired FSs which correspond to the pseudospin degree of freedom in glide-subsectors.
3. The sublattice-singlet $d$-wave pairing naturally admixes with the $f$-wave pairing, and leads to the nontrivial glide-$Z_2$ invariant.

4. Most mirror Chern numbers and winding numbers are forced to be zero, and do not support topological surface states.

Thus, an old heavy fermion superconductor UPt$_3$ is a precious platform of topological superconductivity enriched by non-symmetric space group symmetry.

ACKNOWLEDGMENTS

The authors are grateful to A. Daido, S. Kobayashi, M. Sato, and S. Sumita for fruitful discussions. This work was supported by Grant-in Aid for Scientific Research on Innovative Areas “J-Physics” (JP15H05884) and “Topological Materials Science” (JP16H00991) from JSPS of Japan, and by JSPS KAKENHI Grant Numbers JP15K05164 and JP15H05745. K.S. is supported by JSPS Postdoctoral Fellowship for Research Abroad.
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