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Topological crystalline superconductivity in locally noncentrosymmetric CeRh₂As₂

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Recent discovery of superconductivity in CeRh₂As₂ clarified an unusual *H*-*T* phase diagram with two superconducting phases [Khim *et al.* Science, **373**, 1012 (2021)]. The experimental observation has been interpreted based on the even-odd parity transition characteristic of locally noncentrosymmetric superconductors. Indeed, inversion symmetry is locally broken at the Ce site, and CeRh₂As₂ molds a class of exotic superconductors. The low-temperature and high-field superconducting phase is a candidate for the odd-parity pair-density-wave state, suggesting a possibility of topological superconductivity like spin-triplet superconductors. In this Letter, we first derive the formula expressing the \mathbb{Z}_2 invariant of glide symmetric and time-reversal symmetry-broken superconductors by the number of Fermi surfaces on a glide invariant line. Next, we conduct first-principles calculations for the electronic structure of CeRh₂As₂. Combining the results, we show that the field-induced oddparity superconducting phase of CeRh₂As₂ is a platform of topological crystalline superconductivity protected by nonsymmorphic glide symmetry and accompanied by boundary Majorana fermions.

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I. INTRODUCTION

For decades, symmetry breaking has been the most important concept to describe various phases of quantum matter such as magnetism, density waves, and superconductivity as well as critical phenomena in condensed matter physics [1]. Recently, topological science has shed light on other aspects [2-5]. Topological phase transitions without symmetry breaking have been uncovered, and topological insulators/superconductors are widely recognized as intriguing phases of matter. One of the exotic phenomena in topological materials is the appearance of gapless modes at boundaries and defects of the systems, though the topology is determined by only bulk information. Topological superconductors host Majorana fermions, which have been proposed for topological fault-tolerant quantum computation [6,7]. Such unique properties, attractive from the viewpoints of basic and applied science, triggered tremendous efforts for searching for topological superconductivity [8–45]. However, the realization of topological superconductivity is still under intensive debate.

By pioneering research [46-48], the topological phases were classified based on local symmetries, namely, timereversal, particle-hole, and chiral symmetries. It has later been recognized that symmetries unique to solids enrich the topological properties of materials. This idea led to the concept of topological crystalline insulators/superconductors (TCIs/TCSCs) [49–70]. However, major candidates of TC-SCs are odd-parity superconductors, as is the case for usual topological superconductors [3–5]. Unfortunately, the odd-parity superconductors are usually spin-triplet superconductors, which are rarely known in nature. On the other hand, superconductivity with exotic symmetry beyond the paradigm of standard classification theory [71] has recently attracted attention, and odd-parity superconductivity due to an ordinary spin-singlet pairing has been reported in CeRh₂As₂ [72]. This discovery may open a route to realize topological superconductivity.

This Letter was triggered by a recent experimental report of an unusual superconducting H-T phase diagram in a heavyfermion superconductor CeRh₂As₂ [72]. A high upper critical field much beyond the Pauli-Clogston-Chandrasekhar limit and the phase transition between two superconducting phases have been observed [Fig. 1(a)]. Thus, CeRh₂As₂ is a fascinating platform of multiple superconducting phases. Different from the previous examples, UPt₃ [73] and UTe₂ [74–77], the phase diagram was attributed to the locally noncentrosymmetric crystal structure [72] in accordance with a theoretical proposal [78]. Soon after the experimental report, theoretical works along this line were conducted [79–82].

Noncentrosymmetric superconductivity in global inversion asymmetric systems have been investigated for several decades [9-13,43,44,83-92]. The concept was recently extended to locally noncentrosymmetric superconductivity, and unique superconducting phenomena have been uncovered [57,78,93-101]. The *H*-*T* phase diagram of CeRh₂As₂ is consistent with the prediction based on a two-sublattice Rashba model [78,100]. The similarity of phase diagrams between experiment [72] and theory [78,100] suggests that local inversion symmetry breaking plays an essential role in

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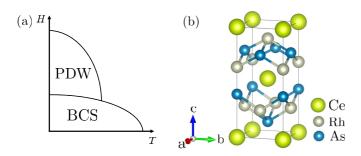


FIG. 1. (a) Schematic H-T phase diagram of CeRh₂As₂ [72]. The Bardeen-Cooper-Schrieffer state is assumed to be an even-parity superconducting phase, and the high-field phase is supposed to be the pair-density-wave (PDW) state, the main topic in this Letter. (b) Crystal structure of CeRh₂As₂ generated by VESTA [104].

CeRh₂As₂, and the superconducting phase in the high magnetic field region is the pair-density-wave (PDW) state. In the PDW state, the superconducting gap function changes sign depending on Ce layers [102]. The most crucial property of this phase is the odd-parity superconductivity despite dominant spin-singlet pairing. The odd parity is owing to the sign change of the gap function between the sublattices related by inversion symmetry [78]. Thus, the locally noncentrosymmetric crystal is a platform of odd-parity superconductivity without requiring rare spin-triplet pairing. It may be realized in CeRh₂As₂, making a candidate of the topological superconductor different from potential spin-triplet superconductors UPt₃ [56,62], UCoGe [63], and UTe₂ [103].

II. CRYSTAL STRUCTURE AND GLIDE SYMMETRY

CeRh₂As₂ crystallizes in the centrosymmetric tetragonal CaBe₂Ge₂-type structure [72] with stacking Ce layers and Rh₂As₂ layers [Fig. 1(b)]. Importantly, Rh₂As₂ layers at the top and bottom of the Ce layer have different compositions. Therefore, inversion symmetry is locally broken at the Ce sites, although the global inversion center exists in the middle of the two Ce sites in the unit cell. The space group is P4/nmm (No. 129) including one glide reflection and three screw rotations. Since the magnetic field parallel to the *c* axis destroys the three screw symmetries, only glide symmetry is respected in the field-induced phase, and we hereafter focus on the glide operation \hat{G} , which is $\{M_z | \mathbf{a}/2 + \mathbf{b}/2\}$ in Seitz notation. Here, \mathbf{a} and \mathbf{b} are the lattice vectors along the *a* and *b* axes, respectively.

In the Brillouin zone, glide symmetry is preserved in the two glide-invariant planes $k_z = 0, \pi$, and we can divide the Hilbert space into each Bloch state and glide sector:

$$\mathbb{V}_{k_{z}=0,\pi} = \bigoplus_{\mathbf{k} \in \mathrm{BZ}_{k_{z}=0,\pi}} \mathbb{V}_{\mathbf{k}}^{\mathfrak{g}^{+}} \oplus \mathbb{V}_{\mathbf{k}}^{\mathfrak{g}^{-}}.$$
 (1)

Here, $\mathbb{V}_{\mathbf{k}}$ is the Hilbert space consisting of Bloch states labeled by \mathbf{k} , and \mathfrak{g}^{\pm} are eigenvalues of the glide operation. Because the Hamiltonian preserves glide symmetry $[\hat{H}, \hat{G}] = 0$, we can label eigenstates of the Hamiltonian by glide eigenvalues as $|\mathbf{k}^{\mathfrak{g}^{\pm}}\rangle \in \mathbb{V}_{\mathbf{k}}^{\mathfrak{g}^{\pm}}$. To evaluate the eigenvalues in the spinful case, we focus on the following relation:

$$\hat{G}^2 = \{-E | \mathbf{a} + \mathbf{b}\}.$$
 (2)

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Owing to Eq. (2), any state $|\mathbf{k}\rangle$ in $\mathbb{V}_{k_z=0,\pi}$ satisfies

$$\hat{\boldsymbol{G}}^{2} \left| \mathbf{k} \right\rangle = -\exp\left[-i(k_{x} + k_{y})\right] \left| \mathbf{k} \right\rangle, \qquad (3)$$

and we conclude that the glide eigenvalues are

$$\mathfrak{g}^{\pm} = \pm i \exp\left[-\frac{i(k_x + k_y)}{2}\right].$$
 (4)

III. SYMMETRY OF SUPERCONDUCTIVITY

Superconductivity is classified by the point group D_{4h} , which has 8 one-dimensional (1D) irreducible representations and 2 two-dimensional (2D) ones. Many Ce-based heavy-fermion systems undergo spin-singlet superconductivity, which is also expected in CeRh₂As₂ at H = 0. Thus, the low-field superconducting phase is supposed to be evenparity, either of A_{1g} , A_{2g} , B_{1g} , B_{2g} , or E_g state. Accordingly, the high-field phase is an odd-parity A_{1u} , A_{2u} , B_{1u} , B_{2u} , or E_u state when the PDW state is assumed. Hereafter, we focus on 1D odd-parity representations because the E_u state is unlikely in CeRh₂As₂ [72].

IV. \mathbb{Z}_2 INVARIANTS

Let us discuss the \mathbb{Z}_2 topological invariants protected by glide symmetry. By definition, the PDW state is glide-odd superconductivity in which the superconducting gap function obeys the following relation:

$$\mathcal{G}(\mathbf{k})\Delta(\mathbf{k})\mathcal{G}^{\top}(-\mathbf{k}) = -\Delta(M_{z}\mathbf{k}).$$
(5)

Here, $\mathcal{G}(\mathbf{k})$ is the representation matrix of the glide operation \hat{G} in the Hilbert space $\mathbb{V}_{\mathbf{k}}$, $M_z \mathbf{k} \equiv (k_x, k_y, -k_z)$, and $\Delta(\mathbf{k})$ represents the gap function.

In the following, we focus on the glide invariant planes in the Brillouin zone $k_z = 0, \pi$. From Eq. (5), the particle-hole operation \hat{C} and glide operation \hat{G} anticommutes $\{\hat{C}, \hat{G}\} =$ 0, and from Eq. (4), the glide eigenvalues become pure imaginary $\pm i$ in the restricted Hilbert space on $k_x + k_y = 0$. Combining these results, we show that the particle-hole symmetry is closed in each glide sector:

$$\hat{G}\hat{C} |\mathbf{k}^{\mathfrak{g}^{\pm}}\rangle = -\hat{C}(\pm i) |\mathbf{k}^{\mathfrak{g}^{\pm}}\rangle = (\pm i)\hat{C} |\mathbf{k}^{\mathfrak{g}^{\pm}}\rangle.$$
(6)

As the time-reversal symmetry is broken under the magnetic field, each glide sector on the line is classified into 1D class D superconductivity. This class is specified by the topological invariant \mathbb{Z}_2 , which is given by the integral of the Berry connection as introduced in Ref. [60]:

$$\nu^{\mathfrak{g}^{\pm}} = \frac{1}{\pi} \int_{\Gamma_1}^{\Gamma_2} dk_i \,\mathcal{A}_i^{\mathfrak{g}^{\pm}}(\mathbf{k}) \quad (\text{mod } 2), \tag{7}$$

where $\mathcal{A}_{i}^{\mathfrak{g}^{\pm}}(\mathbf{k})$ are *i*th components of the Berry connection of each glide sector given by $i \sum_{\text{occ.}} \langle \psi_{\mathbf{k}}^{\mathfrak{g}^{\pm}} | \partial_{k_{i}} | \psi_{\mathbf{k}}^{\mathfrak{g}^{\pm}} \rangle$. Here, $| \psi_{\mathbf{k}}^{\mathfrak{g}^{\pm}} \rangle$ are the occupied eigenstates of the Bogoliubov–de Gennes (BdG) Hamiltonian in each glide sector with the glide eigenvalue \mathfrak{g}^{\pm} . The time-reversal invariant momenta (TRIM) are $\Gamma_{1} = (0, 0, 0)$ (Γ point) or $(0, 0, \pi)$ (Z point) and $\Gamma_{2} = (\pi, -\pi, 0)$ (M point) or $(\pi, -\pi, \pi)$ (A point), depending on $k_{z} = 0$ or π .

In addition to the glide \mathbb{Z}_2 invariants $\nu^{\mathfrak{g}^{\pm}}$, we can define the Chern number *C* as well as two Zak phases γ and γ' on the



lines $k_x + k_y = \pi$ and 0, respectively. However, they are not independent of each other. Actually, $\gamma' = \nu^{\mathfrak{g}^+} + \nu^{\mathfrak{g}^-}$ holds, and later, we will show $\gamma = 0$. Thus, the topology of the PDW state for $k_z = 0$, π can be characterized by identifying $\nu^{\mathfrak{g}^\pm}$ and *C* (denoted by $\nu_{0,\pi}^{\mathfrak{g}^\pm}$ and $C_{0,\pi}$ for each k_z). Furthermore, the Chern number satisfies the relation

$$C = \gamma' - \gamma \pmod{2},\tag{8}$$

$$= \nu^{\mathfrak{g}^+} + \nu^{\mathfrak{g}^-} \pmod{2}. \tag{9}$$

Therefore, only one of $\nu^{\mathfrak{g}^{\pm}}$ is a strong topological index in accordance with *K*-theory classification for the strong indices $\mathbb{Z} \oplus \mathbb{Z}_2$ [60]. In this Letter, we discuss $\nu^{\mathfrak{g}^{\pm}}$ and *C* modulo two in CeRh₂As₂ since they do not rely on the details of the order parameter, as we see below. They are determined only by the topology of the Fermi surfaces and do not require the full calculation of the symmetry indicators [64–70].

Next, to simplify the expression in Eq. (7), we pay attention to the following relation:

$$\hat{I}\hat{G} = \hat{G}\hat{I}\{E|\mathbf{a} + \mathbf{b}\},\tag{10}$$

where \hat{I} is the space inversion operation. As $\{E | \mathbf{a} + \mathbf{b}\}$ is reduced to merely a phase factor $\exp[-i(k_x + k_y)]$, \hat{I} and \hat{G} commute in the Hilbert space $\mathbb{V}_{k_x+k_y=0,k_z=0,\pi}$. Therefore, the space inversion parity is well defined in the glide sector, and each glide sector corresponds to a 1D class D odd-parity superconductor. We can use the Fermi surface formula for odd-parity superconductors [31,32], by which the \mathbb{Z}_2 invariant is evaluated based on the topology of Fermi surfaces. As a consequence, we finally get the conclusion that $v^{\mathfrak{g}^{\pm}}$ is nontrivial (trivial) when the number of Fermi surfaces between Γ_1 and Γ_2 is odd (even):

$$\nu_0^{\mathfrak{g}^{\pm}} = \# \mathrm{FS}_{\Gamma \to M}^{\pm} \pmod{2}, \tag{11}$$

$$\nu_{\pi}^{\mathfrak{g}^{\pm}} = \# \mathrm{FS}_{Z \to A}^{\pm} \pmod{2}. \tag{12}$$

In a similar way, we can relate γ to the number of Fermi surfaces. Because the BdG Hamiltonian on the line $k_x + k_y = \pi$ can be regarded as a 1D odd-parity superconductor, the Fermi surface formula [31,32] reads

$$\gamma_{0,\pi} = \# FS_{\Gamma_1 \to \Gamma_2} \pmod{2}. \tag{13}$$

Here, $\Gamma_1 = X$, R and $\Gamma_2 = X'$, R' for $k_z = 0$, π , respectively. The fourfold rotation symmetry C_4^z forces the occupation numbers of electrons at Γ_1 and Γ_2 to be equal. Therefore, the electron bands must cross the Fermi level even times between Γ_1 and Γ_2 , leading to $\gamma_{0,\pi} = 0$.

Below, we conduct first-principles calculations for CeRh₂As₂ and evaluate the \mathbb{Z}_2 invariants. The first-principles calculations are carried out at the zero magnetic field, where all the electronic bands are doubly degenerate $|\mathbf{k}^{g^{\pm}}\rangle$ and $\hat{I}\hat{\Theta} |\mathbf{k}^{g^{\pm}}\rangle$ because of the inversion symmetry \hat{I} and time-reversal symmetry $\hat{\Theta}$. The relation

$$\hat{G}\hat{I}\hat{\Theta}|\mathbf{k}^{\mathfrak{g}^{\pm}}\rangle = \hat{I}\hat{\Theta}\hat{G}|\mathbf{k}^{\mathfrak{g}^{\pm}}\rangle = \mathfrak{g}^{\mp}\hat{I}\hat{\Theta}|\mathbf{k}^{\mathfrak{g}^{\pm}}\rangle, \qquad (14)$$

reveals that the degenerate states belong to different glide sectors. Consequently, the numbers of Fermi surfaces are equivalent between the two glide sectors and coincide with the number of spinful bands crossing the Fermi level $\#FS^+_{\Gamma_1 \to \Gamma_2} =$

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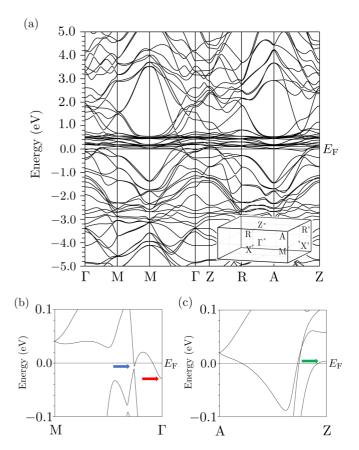


FIG. 2. Electronic band structure of CeRh₂As₂ with spin-orbit coupling calculated by WIEN2k. (a) The whole bands along symmetric lines. The heavy bands of Ce 4*f* electrons are seen near the Fermi level. (b) Enlarged view along the M- Γ line. The bands cross the Fermi level three times. (c) Enlarged view along the *A*-*Z* line. The bands cross the Fermi level four times.

 $\#FS_{\Gamma_1 \to \Gamma_2}^- \equiv \#FS_{\Gamma_1 \to \Gamma_2}$. The magnetic field does not alter the \mathbb{Z}_2 invariants and Chern number modulo two unless it causes the Lifshitz transition. We will discuss the effect of possible Lifshitz transitions later.

V. BAND STRUCTURE OF CeRh₂As₂

We carry out density functional theory (DFT) for electronic structure calculations using the WIEN2k package [106]. The crystallographic parameters are experimentally obtained values [72]. We employ the full-potential linearized augmented plane wave + local orbitals method within the generalized gradient approximation with the spin-orbit coupling. Details of the band calculations, density of states, and orbital weights for each atom are given in the Supplemental Material [107]. Figure 2(a) shows the band structure of CeRh₂As₂, revealing the heavy bands of $\operatorname{Ce} 4f$ electrons near the Fermi level. The main contribution to the density of states at the Fermi level comes from the Ce4f orbitals [107]. We show the Fermi surfaces in Fig. 3. The Ce4f electrons with hybridization to Rh $4d_{x^2-y^2}$ electrons mainly constitute the Fermi surface except for the pink pockets near the A point [Fig. 3(d)]. The largest Fermi surface [Fig. 3(c)] is quasi-2D, supporting the field-induced PDW state [78]. In the experiments, the Kondo

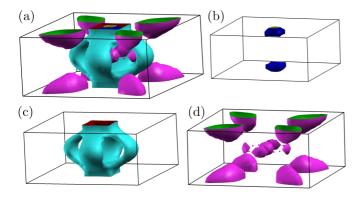


FIG. 3. (a) Fermi surfaces of $CeRh_2As_2$. Each Fermi surface is shown in (b)–(d). The Fermi surfaces other than the pockets around the *A* point in (d) are mainly constituted by Ce4f electrons. The figures are generated by XCRYSDEN software [105].

effect was observed [72,108], and the electronic specific heat coefficient γ was \sim 1000 mJ/mol K², which support the presence of heavy-fermion bands in CeRh₂As₂. Therefore, our result seems to be consistent with experiments.

Hereafter, we proceed with discussions based on DFT calculations. The formulas in Eqs. (11) and (12) of \mathbb{Z}_2 invariants are universal, and we can judge whether CeRh₂As₂ is TCSC when the topology of Fermi surfaces is determined. Although we keep in mind the spin-singlet pairing dominant PDW state, essential properties for the Fermi surface formula are the odd-parity and glide-odd nature of the PDW state. These properties are ensured by the negative character of the inversion operation and the glide operation for A_{1u} , A_{2u} , B_{1u} , and B_{2u} states regardless of whether the spin-singlet component or the spin-triplet component is dominant. Therefore, our formula also applies to spin-triplet dominant states, such as proposed in Ref. [79]. Since the magnitude of the spin-triplet channel affects the physical properties such as the paramagnetic effect and the local density of states [97], and these quantities can be measured in principle, further theoretical and experimental efforts are desired to clarify the detail of the high-field phase. However, the following results are not affected by the details.

VI. TCSC IN CeRh₂As₂

We now show the \mathbb{Z}_2 invariants. First, we discuss the topology on a glide-invariant plane $k_7 = 0$. Focusing on the Γ -M line [Fig. 2(b)], we notice that bands cross the Fermi level three times. Therefore, both $v_0^{\mathfrak{g}^{\pm}}$ are nontrivial, revealing the TCSC. The TCSC is robust against the Zeeman splitting. In CeRh₂As₂, the PDW state is observed under the magnetic field between 4 and 14 T [72], in which the Zeeman splitting energy is estimated as 2-8 meV when we assume a probably overestimated g factor g = 10. At the Γ point (red arrow), the conduction band is \sim 30 meV below the Fermi level, and thus, the occupation number does not change. Although the crossing points indicated by the blue arrow may be lifted, it does not influence the \mathbb{Z}_2 invariants according to the formula in Eq. (11). Therefore, the number of Fermi surfaces modulo two remains the same under the magnetic field, and the \mathbb{Z}_2 invariants $v_0^{\mathfrak{g}^{\pm}}$ are nontrivial in the PDW state.

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TABLE I. \mathbb{Z}_2 topological invariants and Chern number of CeRh₂As₂ in the PDW state based on first-principles calculations. A possibility of a Weyl superconducting state is shown. In the high-field region, one of the Zeeman split bands is supposed to cause a Lifshitz transition at the Z point.

	$(\nu_0^{\mathfrak{g}^+}, \nu_0^{\mathfrak{g}^-}, C_0)$	$(\nu_{\pi}^{\mathfrak{g}^+}, \nu_{\pi}^{\mathfrak{g}^-}, C_{\pi})$	Weyl SC
Low field	(1, 1, even)	(0, 0, even)	×
High field	(1, 1, even)	(1, 0, odd) or $(0, 1, odd)$	0

Next, we discuss the other glide-invariant plane $k_z = \pi$. On the Z-A line [Fig. 2(c)], bands cross the Fermi level four times, and accordingly, $v_{\pi}^{g^{\pm}}$ are trivial. However, a hole band (green arrow) is shallow, and the energy at the Z point is estimated to be ~4 meV. Therefore, the Lifshitz transition may occur under the magnetic field, and the \mathbb{Z}_2 invariants may become nontrivial. The \mathbb{Z}_2 topological invariants of CeRh₂As₂ are summarized in Table I based on the band structure calculation. We assume that one of the Zeeman split bands undergoes the Lifshitz transition at the Z point in the high-field region. Then the Chern number as well as a \mathbb{Z}_2 invariant is nontrivial. Because the Chern number is well-defined on any constant k_z plane, the difference in C_0 and C_{π} indicates a Weyl superconducting state as in UPt₃ [109].

From these results, CeRh₂As₂ is shown to be a platform of TCSC. We would like to stress that the glide \mathbb{Z}_2 invariants are nontrivial at least on the $k_z = 0$ plane. Therefore, boundary Majorana states appear at the ($\overline{1}10$) surface preserving glide symmetry, which is generated by $\mathbf{a} + \mathbf{b}$ and \mathbf{c} .

VII. MODEL STUDY

To demonstrate the emergence of Majorana surface states, we conducted numerical calculations based on a tight-binding model. We construct the tight-binding model and set parameters [110] so that $\#FS_{\Gamma_1 \rightarrow \Gamma_2}^{\pm}$ are odd (even) at $k_z = 0$ ($k_z = \pi$), consistent with first-principles calculations. In the spectrum for $k_z = 0$ (Fig. 4), we recognize the stable Majorana surface states for both A_{2u} representation (s + p-wave state) and B_{2u} representation ($d_{x^2-y^2} + p$ -wave state). We also verified the Majorana states for the A_{1u} and B_{1u} representations, while the surface states are gapped on the other glide-invariant plane

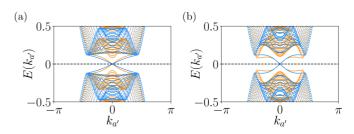


FIG. 4. ($\overline{1}10$) and ($1\overline{1}0$) surface states of (a) A_{2u} and (b) B_{2u} superconducting states at one of the glide-invariant planes, $k_z = 0$. The orange (blue) color represents the glide-even (odd) sector. The axis $k_{a'}$ corresponds to $k_x + k_y$, and Majorana surface states appear at $k_{a'} = 0$.

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 $k_z = \pi$ (see the Supplemental Material [110]). All results are consistent with the topological invariants discussed above.

VIII. SUMMARY AND CONCLUSIONS

In this Letter, we theoretically investigated the electronic structure and topological superconductivity in a recently discovered heavy-fermion superconductor CeRh₂As₂. First, using group theory, we clarified the algebra of symmetry operations in the Bloch representation and decomposed the Hilbert space on the glide-invariant planes $k_{z} = 0, \pi$ into the glide sectors. Supposing the PDW state in the high-field superconducting phase as proposed, based on these results, we derived the Fermi surface formula of \mathbb{Z}_2 invariants specifying the TCSC protected by nonsymmorphic glide symmetry. Second, we conducted first-principles calculations for the electronic structure of CeRh₂As₂. Evaluating the \mathbb{Z}_2 invariants, we found the TCSC due to heavy-fermion bands of $\operatorname{Ce} 4f$ electrons hybridizing with conduction electrons. The emergence of Majorana fermions at the surface preserving glide symmetry was demonstrated based on the tight-binding model. This Letter proposes CeRh₂As₂ as a class of topological superconductors in the following two senses: (1) The topological superconductivity requires neither spin-triplet pairing nor topological band structures. (2) The

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topological structure is protected by nonsymmorphic symmetry, which does not have a counterpart in continuous systems.

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Note added. Recently, two different groups independently reported the results of the electronic structure calculation of CeRh₂As₂ using the pseudopotential and full potential method [81,82]. Their results are consistent with our results and support our conclusion. In Ref. [81], the authors discuss the Lifshitz transition and orbital order using VASP. In Ref. [82], combining $\mathbf{k} \cdot \mathbf{p}$ theory and DFT calculation, the dominance of the Rashba type spin-orbit coupling around the Dirac line and the origin of the large critical field are discussed.

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