

## Generic phase diagram for Weyl superconductivity in mirror-symmetric superconductors

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We study topological phase transitions in three-dimensional odd-parity or noncentrosymmetric superconductors with mirror symmetry when time-reversal symmetry is broken. We construct a generic phase diagram for Weyl superconductivity in the mirror-symmetric superconductors. It is shown that Weyl superconductivity generally emerges between the trivial and the topological crystalline superconductor phases. We demonstrate how a trajectory of the Weyl nodes determines the change in mirror Chern numbers in the topological phase transition. We also discuss a relationship between particle-hole symmetry and the trajectory of the Weyl nodes which realizes the topological crystalline superconductor phase.

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*Introduction.* Thanks to interplay of topology and crystal symmetries, novel topological phases have been suggested theoretically. Topological crystalline insulators [1–6] and topological semimetals [7–12] are understandable as a manifestation of their complex interplay. Recent works have shown that the interplay also produces intriguing superconductor (SC) phases, such as topological crystalline SCs [13–16] and nodal SCs [17–21]. For example, mirror symmetry enables topological phases in three-dimensional SCs [13,14], and  $\text{Cu}_x\text{Bi}_2\text{Se}_3$  [22,23] and  $\text{UPT}_3$  [24] are known as the candidates. Nowadays, various topological phases are proposed from systematic topological classification of the quantum matter based on the crystal symmetry [25–30].

Meanwhile, Weyl SCs [17,31–34] are three-dimensional SCs with point nodes which are stable without protection by crystal symmetries. The point nodes are called Weyl nodes. Weyl nodes are protected topologically by monopole charges related to Chern numbers and always exist in pairs with opposite monopole charges [35,36]. Hence, Weyl nodes cannot appear or vanish unless the pair creation or annihilation occurs. Because intrinsic particle-hole symmetry gives opposite monopole charges to Weyl nodes at  $\mathbf{k}$  and  $-\mathbf{k}$  [37], broken time-reversal symmetry is necessary for Weyl SCs, although Weyl semimetals are realizable in time-reversal invariant systems [35,38–42]. The candidates of Weyl SCs are  $\text{SrPtAs}$  [43,44], uranium-based compounds (including  $\text{UPT}_3$ ) [45–48],  $\text{PrOs}_4\text{Sb}_{12}$  [49–52],  $\text{Nb}_x\text{Bi}_2\text{Se}_3$  [53–55], and so on. It is also predicted that an external magnetic field induces a phase transition from a noncentrosymmetric line-node SC phase to a Weyl SC phase [56].

In this Rapid Communication, we focus on Weyl superconductivity in mirror-symmetric SCs breaking time-reversal symmetry. The Weyl SCs are difficult to predict from crystal symmetries as with Weyl semimetals since their Weyl nodes are located at general points. Meanwhile, the Weyl semimetal phase necessarily intervenes between trivial and topological insulator phases when Kramers degeneracy is absent [3,35,57,58]. The universal emergence of the Weyl semimetal phase has been used to search for candidate materials of the Weyl semimetals [41,59,60]. Therefore, it should

be useful to study Weyl SCs as an intermediate phase in order to search for candidate materials of the Weyl SCs. In this Rapid Communication, we show that the Weyl SC phase generally appears between trivial and topological crystalline SC phases in an odd-parity or a noncentrosymmetric SC as shown in Fig. 1. Also, we investigate how the system enters the topological crystalline SC phase through the Weyl SC phase. We show that trajectories of the Weyl nodes due to the change in the parameters determine the topological phase transition.

*Weyl SC phase between trivial and topological crystalline SC phases.* We start by introduction of a topological crystalline SC and a Weyl SC in order to discuss a topological phase transition between the two phases (see the Supplemental Material [61]). If a Bogoliubov–de Gennes (BdG) Hamiltonian without time-reversal symmetry has a mirror symmetry, the system can realize a topological crystalline SC phase [13,14,25,26,28]. When the normal state is mirror symmetric, the mirror symmetry is preserved in the BdG Hamiltonian if the gap function is mirror odd or even, i.e.,  $M \Delta(\mathbf{k}) M^t = \mp \Delta(\mathbf{k})$  on the mirror plane.  $M$  and  $\Delta(\mathbf{k})$  are mirror operations in the normal state and the gap function of the SC, respectively. The topological SC is characterized by a mirror Chern number [62]. The mirror Chern number  $\nu^{(\lambda)}$  is a Chern number defined in the mirror sector of the mirror eigenvalue  $\lambda = \pm i$  on the mirror plane. We denote the BdG Hamiltonian in the mirror sector of  $\lambda$  as  $\mathcal{H}_\lambda(\mathbf{k})$ . When the SC is gapped and some of mirror Chern numbers are nonzero, a topological crystalline SC is realized.

To define the mirror Chern number, we introduce Berry connection  $A^\lambda(\mathbf{k})$  and Berry curvature  $F^\lambda(\mathbf{k})$  in the mirror sector  $\mathcal{H}_\lambda(\mathbf{k})$  given by [13]

$$A^\lambda(\mathbf{k}) = i \sum_n \langle u_n^\lambda(\mathbf{k}) | \nabla_{\mathbf{k}} | u_n^\lambda(\mathbf{k}) \rangle, \quad (1)$$

$$F^\lambda(\mathbf{k}) = \nabla_{\mathbf{k}} \times A^\lambda(\mathbf{k}), \quad (2)$$

where  $|u_n^\lambda(\mathbf{k})\rangle$  is the  $n$ -th eigenstate of the BdG Hamiltonian with the mirror eigenvalue  $\lambda$ . The sum in  $A^\lambda(\mathbf{k})$  is taken over the negative energy states. For example, we take the mirror plane to be the  $xy$  plane. The mirror Chern number is then

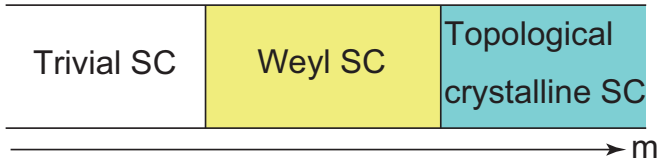


FIG. 1. A generic phase diagram for the Weyl SC and the topological crystalline SC in the absence of time-reversal symmetry.  $m$  is any parameter determining the phase, such as an external magnetic field, a chemical potential, pressure, etc.

given by

$$\nu^{(\lambda)}(k_z) = \frac{1}{2\pi} \int dk_x dk_y F_z^\lambda, \quad (3)$$

where  $F_z^\lambda$  is integrated over the mirror plane  $k_z = 0$  or  $\pi$ . As seen from Eq. (3), to change the mirror Chern number, the system needs a gap closing between the negative and the positive energy states with the same mirror eigenvalues. The properties of the mirror Chern numbers vary according to mirror parity of the gap function. In the mirror-odd (mirror-even) SC,  $\nu^{(+i)}$  and  $\nu^{(-i)}$  are independent (equal) because each mirror sector has (does not have) its own particle-hole symmetry [13,28].

Meanwhile, in Weyl SCs, the Weyl nodes are typically created at general points by accidental band touching between two nondegenerate states. The band touching and emergent nodes can be described by a two-band effective Hamiltonian if all the states in the SC are nondegenerate. From analysis of the two-band effective Hamiltonian, the Weyl nodes are allowed only in an odd-parity or a noncentrosymmetric SC [18,63,64]. To study the Weyl nodes in mirror-symmetric SCs, we also need to consider band touching on the mirror plane. Then, there are two types of band evolution after the band touching on the mirror plane in the three-dimensional SC, depending on the mirror eigenvalues of the two states [65]. If the two states have the same mirror eigenvalues, the band touching leads to pair creation of Weyl nodes (see the Supplemental Material [61]). The created Weyl nodes move symmetrically with respect to the mirror plane. In contrast, if the two states have opposite mirror eigenvalues, a line node appears on the mirror plane since the two bands do not hybridize (see the Supplemental Material [61]).

Hereafter, by using the above arguments, let us discuss a topological phase transition to realize topological crystalline SC phases in three-dimensional SCs. We set any tunable parameter  $m$ , which governs the topological phase transition in the mirror-symmetric SC without time-reversal symmetry. Below, we make the following assumptions: (i) All the bands are nondegenerate in the SC [66]. (ii) The mirror symmetries in the SC are invariant by a change in the parameter  $m$ . (iii) The SC becomes gapful all over the Brillouin zone within a finite range of the parameter  $m$ .

First, we investigate a topological phase transition in odd-parity SCs. The positive and the negative energy bands at  $k$  are symmetric with respect to zero energy due to the particle-hole and inversion symmetries. To see the topological phase transition, we consider the SC gapful and trivial when  $m < m_1$ . If the mirror Chern number becomes nonzero while we change

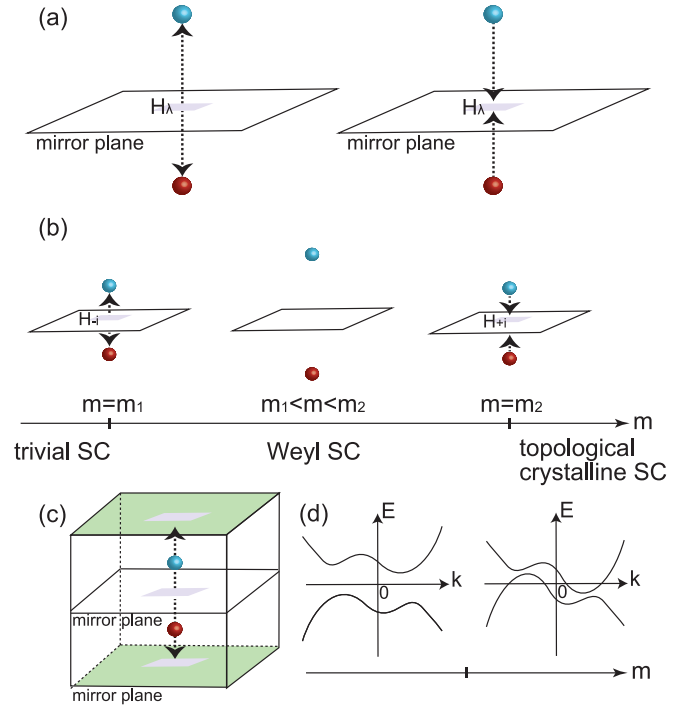


FIG. 2. (a) The pair creation and annihilation of Weyl nodes in the mirror sector  $\mathcal{H}_\lambda$ . The two colors of the Weyl nodes correspond to opposite monopole charges. Because of the gap closing on the mirror plane, the mirror Chern number  $\nu^{(\lambda)}$  changes by  $\pm 1$ . (b) and (c) Examples of a trajectory formed by one pair of Weyl nodes between trivial and topological crystalline SC phases. (d) Schematic of the band evolution near zero energy in the absence of inversion and time-reversal symmetries. The maximum energy of the hole bands can exceed zero energy.

the parameter  $m$ , a gap closes between two states with the same mirror eigenvalues on the corresponding mirror plane. Now, let us assume that the gap closes at  $m = m_1$  in the mirror sector  $\mathcal{H}_\lambda$ . The gap closing not only changes the mirror Chern number  $\nu^{(\lambda)}$ , but also leads to pair creation of Weyl nodes [Fig. 2(a)]. As  $m > m_1$  is increased, the Weyl nodes move in the Brillouin zone until the pair annihilation. Consequently, the SC is in the Weyl SC phase. Furthermore, we assume that the SC becomes gapped again after a further change in  $m$  annihilates all the Weyl nodes at  $m = m_2$ . Whether the gapful SC phase in  $m > m_2$  is trivial or topological is determined by the trajectory of the Weyl nodes in the Brillouin zone. To elucidate a relationship between the trajectory and the topological phase transition, suppose that one pair of Weyl nodes is created at  $m = m_1$  in the  $\mathcal{H}_{-i}$  sector on a mirror plane. Then, the SC system enters the Weyl SC phase with nonzero  $\nu^{(-i)}$ . If the Weyl nodes return to the  $\mathcal{H}_{-i}$  sector on the same mirror plane at  $m = m_2$ , the mirror Chern number  $\nu^{(-i)}$  becomes zero. Thus, the SC phase in  $m > m_2$  is trivial. As another example, suppose that the Weyl nodes are pair annihilated at  $m = m_2$  in the  $\mathcal{H}_{+i}$  sector on the same mirror plane as illustrated in Fig. 2(b). Then, the pair annihilation changes  $\nu^{(+i)}$ , whereas  $\nu^{(-i)}$  remains nonzero. As a result, topological crystalline SC phase is realized. In this trajectory, the Chern number  $\nu = \nu^{(+i)} + \nu^{(-i)}$  on the mirror plane is zero in the topological crystalline SC phase. Hence, mirror symmetry is essential for the topological phase transition. Moreover, the

Weyl nodes can vanish on another mirror plane. The trajectory also realizes a topological crystalline SC phase with nonzero Chern numbers in addition to nonzero mirror Chern numbers [Fig. 2(c)]. Generally, there can be more than one pair of Weyl nodes and several mirror planes, and pair creation and annihilation may not occur on the mirror plane. However, changes in mirror Chern numbers accompany pair creation or annihilation on the mirror plane. In this way, the generic topological phase transition can be understood from the trajectories formed by all the Weyl nodes. As a result, the Weyl SC phase can be regarded as an intermediate nodal state between the gapful SC phases with different mirror Chern numbers.

Second, we comment on a topological phase transition between trivial and topological crystalline SC phases in non-centrosymmetric SCs. Because the BdG Hamiltonian breaks both time-reversal and inversion symmetries, the maximum energy of the hole bands may be larger than zero [67–69], depending on the parameter  $m$  [Fig. 2(d)]. Hence, Weyl nodes formed by the electron and the hole bands can deviate from zero energy in general. Then, the mirror Chern numbers in Eq. (3) are not available for characterization of the topological phase because the Berry connection is defined by negative states. However, we can use the mirror Chern numbers by replacing the sum of the negative states with that of the hole bands in Eq. (1) even if the maximum energy of the hole bands exceeds zero energy. The reason is that the mirror Chern number defined by the hole bands is unchanged as long as the gap survives between the hole and the electron bands. Therefore, our theory about trajectories of Weyl nodes is also applicable to the topological phase transition in the mirror-symmetric SCs breaking inversion symmetry.

Finally, we show that the mirror parity of the gap function restricts the trajectories to realize a topological crystalline SC phase. There is no such restriction on the trajectory in time-reversal breaking Weyl semimetals since the mirror parity is related to particle-hole symmetry [13,27,28]. In the following, we clarify the possible trajectories and the behavior of the gap closing, which depend on the mirror parity of the gap function.

We begin with a SC with a mirror-odd gap function. Since  $\nu^{(+i)}$  and  $\nu^{(-i)}$  are independent, the topological crystalline SC phase is realizable from the trajectory as shown in Fig. 2(b). Moreover, when inversion symmetry is present, a gap closing occurs on the mirror plane between the positive and the negative energy states with the same mirror eigenvalues due to particle-hole symmetry in each of the mirror sectors (see the Supplemental Material [61]). Namely, the gap closing in the SC necessarily leads to pair creation of Weyl nodes. Next, we consider a topological phase transition in a SC with a mirror-even gap function. Then,  $\nu^{(+i)}$  is always equal to  $\nu^{(-i)}$ , unlike the mirror-odd SC. Thus, pair creation or annihilation in the  $\mathcal{H}_{+i}$  sector coincides with that in the  $\mathcal{H}_{-i}$  sector. Hence, if the two pairs of the Weyl nodes emerge from the mirror plane and they return to the same mirror plane, the gapful SC becomes topologically trivial again. In order to reach the nontrivial phase, the Weyl nodes need to vanish away from the mirror plane where they have emerged. Additionally, the gap on the mirror plane can close between the two states with opposite mirror eigenvalues since each of the mirror sectors does not keep particle-hole symmetry. The gap closing then yields a nodal line on the mirror plane.

*Model calculation.* To demonstrate our theory, we study a SC modeled on a cubic lattice with mirror symmetry. As an example, we consider a BdG Hamiltonian written by  $H = \frac{1}{2} \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}}$  with  $\Psi_{\mathbf{k}}^{\dagger} = (c_{\mathbf{k}\uparrow}^{\dagger}, c_{\mathbf{k}\downarrow}^{\dagger}, c_{-\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow})$  and

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} \xi_{\mathbf{k}} - Bs_z & \Delta(\mathbf{k}) \\ \Delta^{\dagger}(\mathbf{k}) & -\xi_{\mathbf{k}} + Bs_z \end{pmatrix}. \quad (4)$$

Here,  $\xi_{\mathbf{k}} = 2t_x \cos k_x + 2t_y \cos k_y + 2t_z \cos k_z - \mu$  is a kinetic energy, and  $\Delta(\mathbf{k}) = i\mathbf{d} \cdot \mathbf{s}s_y$  is a gap function with  $\mathbf{d} = \Delta(\sin k_x, \sin k_y, \sin k_z)$  and  $\mathbf{s} = (s_x, s_y, s_z)$  Pauli matrices acting on the spin space.  $B$  is an external magnetic field breaking time-reversal symmetry. The eigenvalues are

$$E(\mathbf{k}) = \pm \left[ \xi_{\mathbf{k}}^2 + B^2 + \sum_i d_i^2 \pm 2B\sqrt{\xi_{\mathbf{k}}^2 + d_z^2} \right]^{1/2}. \quad (5)$$

We note that this model describes an odd-parity SC. This model without the magnetic field is studied as a time-reversal invariant topological SC [70].

Now, the normal state has a mirror symmetry with respect to the  $xy$  plane, and the mirror operation is given by  $M_z = -is_z$ . Thus, the gap function is mirror odd because  $M_z \Delta(k_x, k_y, k_z) M_z^{\dagger} = -\Delta(k_x, k_y, -k_z)$ . The BdG Hamiltonian also has a mirror symmetry described by  $\tilde{M}_z = \text{diag}(M_z, M_z)$ . Therefore, the mirror Chern numbers  $\nu^{(\pm i)}(k_z)$  can be defined on the planes  $k_z = 0$  and  $\pi$  in this model.

On the mirror planes, the Hamiltonian can be block diagonalized in the diagonal basis of  $\tilde{M}_z$ . Each mirror sector of the eigenvalues  $\pm i$  is described by

$$\mathcal{H}_{\pm i}(\mathbf{k}) = \pm \Delta \sin k_x \tau_x - \Delta \sin k_y \tau_y + [\xi_{\mathbf{k}} \pm B] \tau_z, \quad (6)$$

where  $\tau_{x,y,z}$  are Pauli matrices. According to Eq. (6), the mirror Chern numbers change when  $\xi_{\mathbf{k}} \pm B = 0$  on the mirror planes.

Figures 3(a) and 3(b) show phase diagrams in this model with  $\Delta = 0.3t_z$  and  $0.1t_z$ , respectively. Both of the phase diagrams are obtained when  $\mu = 0.25t_z$  and  $B = 0.05t_z$ . For example, we see the topological phase transition along the  $t_y = t_x$  line represented by the arrow in the phase diagram of Fig. 3(a). The band evolution is shown in Fig. 3(c). When  $t_y = 0.425t_z$ , the pair creation happens at  $\mathbf{k} = (\pi, \pi, 0)$  in the  $\mathcal{H}_{-i}$  sector. The Weyl nodes move along the line  $\mathbf{k} = (\pi, \pi, k_z)$  as  $t_y = t_x$  becomes larger. Eventually, the Weyl nodes are pair annihilated at  $\mathbf{k} = (\pi, \pi, 0)$  in the  $\mathcal{H}_{+i}$  sector when  $t_y = 0.45t_z$ . The trajectory is identical to that in Fig. 2(b), realizing the topological crystalline SC phase.

Moreover, we see a topological phase transition for  $\Delta = 0.1t_z$ . We also consider band evolution along the  $t_y = t_x$  line in Fig. 3(b). When  $t_y = 0.37t_z$ , four Weyl nodes emerge at points on the  $\mathbf{k} = (\pi, \pi, k_z)$  line but not on the mirror plane. When we increase  $t_y = t_x$ , the one pair vanishes in the  $\mathcal{H}_{-i}$  sector, and then the other pair does in the  $\mathcal{H}_{+i}$  sector. This trajectory also realizes a topological crystalline SC phase because the two pairs vanish in the different mirror sectors. Therefore, in both cases, the SC system enters the topological crystalline SC phase via the Weyl SC phase, which is consistent with our theory.

In the Weyl and the topological crystalline SC phases, Majorana states appear on the surface [13,27,28,31–33]. We show evolutions of the surface states of this model by changing

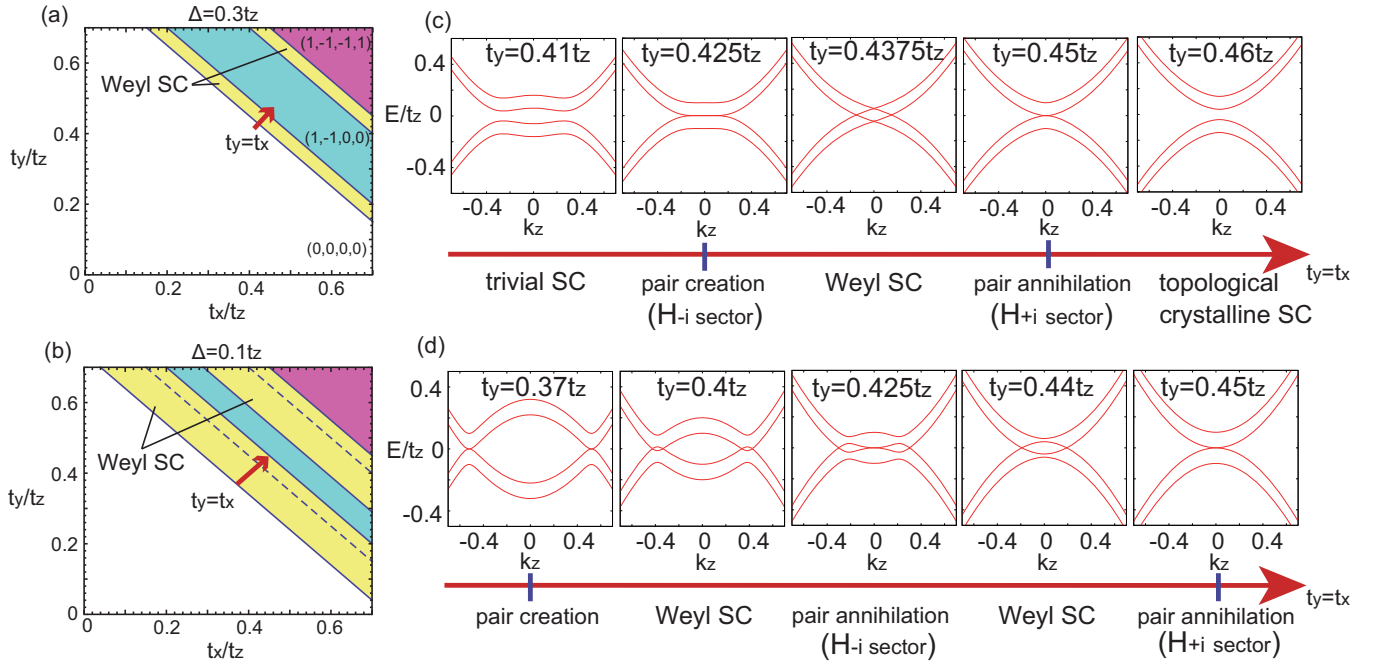


FIG. 3. (a) The phase diagram with  $\mu = 0.25t_z$ ,  $B = 0.05t_z$ , and  $\Delta = 0.3t_z$ . The blue and the purple regions are SC phases with the nonzero mirror Chern numbers  $[\nu^{(+i)}(0), \nu^{(-i)}(0), \nu^{(+i)}(\pi), \nu^{(-i)}(\pi)] = (1, -1, 0, 0)$  and  $(1, -1, -1, 1)$ , respectively. The yellow regions are Weyl SC phases. (b) The same as in (a) with  $\mu = 0.25t_z$ ,  $B = 0.05t_z$ , and  $\Delta = 0.1t_z$ . The dashed lines represent the parameters where a pair annihilation happens on the mirror plane whereas the system remains in the Weyl SC phase. (c) and (d) Band evolutions of the SC on the line  $\mathbf{k} = (\pi, \pi, k_z)$  along the arrows in (a) and (b). The arrows in the phase diagrams indicate the line  $t_y = t_x$ . (c) The mirror Chern number  $\nu^{(-i)}(0)[\nu^{(+i)}(0)]$  change at  $t_y = 0.425t_z(0.45t_z)$ . The Weyl node at  $\pm k_z (k_z > 0)$  has monopole charge  $\pm 1$ . (d) The pair creation happens at  $t_y = 0.37t_z$ . The Weyl nodes at  $k_z^1$  and  $k_z^2 (k_z^1 > k_z^2 > 0)$  have monopole charges  $-1$  and  $+1$ .

the parameters in the same way as the bulk states in the Supplemental Material [61].

**Conclusion and discussion.** In the present Rapid Communication, we have investigated Weyl superconductivity in mirror-symmetric superconductors without time-reversal symmetry. We have shown that Weyl superconductivity universally emerges between the trivial and the topological crystalline superconductor phases in odd-parity or noncentrosymmetric superconductors. We have also discussed a relationship between the Weyl nodes and the topological phase transition. It is shown that trajectories of the Weyl nodes determine the topological phase after the pair annihilation.

Our generic results are applicable to various unconventional superconductors breaking time-reversal symmetry because many crystals have mirror symmetry. Thus, the theory is

useful for prediction of Weyl and topological crystalline superconductors in addition to theoretical construction of the topological phase diagram. For example, recent papers have shown that an external magnetic field moves Weyl nodes in the Brillouin zone [17,56]. As shown in our model calculation, changing shapes of Fermi surfaces in the normal state can also induce the topological phase transition, which is expected by doping and pressure. Hence, the topological phase transition predicted in this Rapid Communication can be realized by controlling these parameters experimentally.

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