Higher-order Weyl superconductors with anisotropic Weyl-point connectivity

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Weyl superconductors feature Weyl points at zero energy in the three-dimensional (3D) Brillouin zone and arc states that connect the projections of these Weyl points on the surface. We report that higher-order Weyl superconductors can be realized in odd-parity topological superconductors with time-reversal symmetry being broken by periodic driving. Different from conventional Weyl points, the higher-order Weyl points in the bulk separate 2D first- and second-order topological phases, while on the surface, their projections are connected not only by conventional surface Majorana arcs, but also by hinge Majorana arcs. We show that the Weyl-point connectivity via Majorana arcs is largely enriched by the underlying higher-order topology and becomes anisotropic with respect to surface orientations. We identify the anisotropic Weyl-point connectivity as a characteristic feature of higher-order Weyl materials. As each 2D subsystem can be singled out by fixing the periodic driving, we propose how the Majorana zero modes in the 2D higher-order topological phases can be detected and manipulated in experiments.

Introduction. —The particular excitations of topological semimetals and nodal superconductors emerge around gapless degeneracies and constitute one of the main research activities in the field of topological materials [1–6]. Typical examples are Weyl and Dirac semimetals or nodal superconductors whose low-energy physics around the gapless points can be described by Weyl or Dirac Hamiltonians [7–14]. Besides exotic quasiparticles in the bulk, the bulk topology of the systems also gives rise to fascinating topological boundary states.Conventionally, in an n-dimensional topological phase, the topological boundary states are constrained to (n − 1) dimensions.

Recently, inspired by higher-order topology [15–25], new topological phases, termed higher-order topological gapless phases, have attracted increasing interest [26–31]. In addition to gapless degeneracies in the n-dimensional bulk and conventional (n − 1)-dimensional boundary states, these topological systems feature also (n − d)-dimensional hinge or corner states with d ≥ 2. As an important member of gapless phases, Weyl superconductors must break time-reversal or inversion symmetry [10, 11, 32, 33]. Time-reversal-symmetry breaking is particularly important, as most reported first-order (conventional) Weyl superconductors are realized in this way [34–42]. However, so far, there has been no study on higher-order Weyl superconductors (HOWSCs) with broken time-reversal symmetry. An interesting fundamental question in HOWSCs concerns their boundary states, namely, how the connectivity of surface projected Weyl points by Majorana arcs, a characteristic feature of Weyl superconductors, is reshaped by the higher-order topology.

In this Letter, we show that HOWSCs with broken time-reversal symmetry can be realized by periodically driving a 2D second-order odd-parity topological superconductor. The periodic driving breaks time-reversal symmetry and offers an unprecedented way to extend the 2D superconductor to a third dimension with periodic boundary conditions. Weyl points can be generated in this dynamic process, which split the system into different regions of first- (FOTP) or second-order topological phases (SOTP), leading to a HOWSC. In sharp contrast to the surface Majorana arcs protected by a bulk Chern number in the FOTP regions, the hinge Majorana arcs in the SOTP regions, which are protected by inversion symmetry, depend strongly on the surface orientation due to the higher-order topology. This results in an intriguing and diverse recombination of surface and hinge Majorana arcs upon orientation change, leading to an anisotropic Weyl-point connectivity. By developing an effective boundary theory capable of describing both surface and hinge Majorana arcs, we thoroughly analyze this intricate Weyl-point connectivity of Majorana arcs in every surface orientation. Furthermore, both the FOTP and SOTP can be individually investigated as the periodic driving offers an advantage to single out each 2D slice of the system by fixing the driving parameters. We propose to control and detect the Majorana zero modes in the SOTP regions via circularly polarized light (CPL) in experiments.

Realization of HOWSCs. —Our starting point is a 2D second-order odd-parity topological superconductor that respects time-reversal symmetry. Different from previous proposals for higher-order topological superconductors [43–65], we consider an inter-orbital s-wave pairing potential with a constant magnitude $\Delta_0$, which may be induced...
The Hamiltonian is invariant under time-reversal ($\mathcal{T}$) and particle-hole ($\mathcal{C}$) symmetry. The pairing interaction is of odd parity as indicated by $\mathcal{P}h_\Delta \mathcal{P}^{-1} = -h_\Delta$ with the inversion operator $\mathcal{P} = \sigma_z$. Correspondingly, the BdG Hamiltonian is symmetric under inversion $\mathcal{P}\mathcal{H}(\mathbf{k})\mathcal{P}^{-1} = \mathcal{H}(-\mathbf{k})$ with $\mathcal{P} = \tau_z\mathcal{P}$. Furthermore, spin rotation about the $z$ axis $J_z = \tau_z s_z$ is preserved. Due to the second-order topology, our model features two 0D Majorana Kramers pairs at a disk boundary in the horizontal direction, which are protected by time-reversal and inversion symmetries [Fig. 1(a)].

Next, we show that HOWSCs can be generated on the basis of the model (1) through periodic driving. For concreteness, we consider periodic driving in the form of CPL which is shed on the system in the $z$ direction and described by the vector potential $\mathbf{A}(t) = A_0(\cos(\omega t), \sin(\omega t + \phi), 0)$. $\phi$ characterizes the phase shift, $A_0$ the strength and $\omega$ the frequency. The CPL couples to the electrons/holes via the Peierls substitutions $\mathbf{k} \to \mathbf{k} \pm \epsilon\mathbf{A}(t)$. To proceed analytically and elucidate our main results, we employ Floquet theory and derive a static effective Hamiltonian [66]. The effective Hamiltonian is obtained on the basis of Eq. (1) and contains a non-trivial correction that preserves spin-rotation symmetry about the $z$ axis. We can find it as [66]

$$h(\mathbf{k}) = h_0(\mathbf{k}) + \gamma(\mathbf{k}) \cos \phi,$$

where $\gamma(\mathbf{k}) = (2mI/\omega)(v \sin k_x \sigma_x + v \sin k_y \sigma_y - \sigma_z^2/2m)$ and $h_0(\mathbf{k}) = \tau_z[(m(\mathbf{k}) + mI)\sigma_z + v \sin k_x \sigma_x + v \sin k_y \sigma_y - \mu] - \Delta_0 \tau_z \sigma_x$ with $I = e^2 A_0^2$ corresponding to the intensity of the light. The periodic driving breaks time-reversal symmetry. Increasing $I$ above a critical value, we observe that the Majorana zero modes at the disk boundary jump from the horizontal to vertical positions [Fig. 1(b)].

The model in Eq. (2) is periodic in the parameter $\phi$. We may regard it as an extra (third) dimension. Since at each $\phi$ time-reversal symmetry is broken, the 2D systems for fixed $\phi$ belong to class A and are characterized by a Chern number [67]. Strikingly, stacking these 2D systems along the $\phi$ direction gives a 3D Weyl superconductor with 16 Weyl points in the synthetic 3D Brillouin zone, as displayed in Fig. 1(c). These Weyl points can be grouped into four distinct sets.

In Fig. 1(d), we stack the 2D disks with different $\phi$, forming a 3D cylinder. The cylinder is finite in $x$ and $y$ directions but periodic in $\phi$ direction. As can be seen by the dimensions of the boundary states, the system splits into two kinds of topological phases: (i) FOTPs within each of the Weyl-point sets, with 2D surface states at the boundary (green belts); (ii) SOTPs between different Weyl-point sets, with 1D hinge states (red lines). As the Weyl points mediate between the FOTP and SOTPs, we coin the system a HOWSC.

Anisotropic Weyl-point connectivity.—In conventional Weyl superconductors, the surface Majorana arcs that connect the projections of the Weyl points in the surface via the proximity effect. The minimal Hamiltonian in momentum space can be written as $\mathcal{H} = \mathcal{H}_0 + h_\Delta$ with

$$\mathcal{H}_0 = m(\mathbf{k})\tau_z \sigma_z + v \sin k_x \sigma_x + v \sin k_y \sigma_y - e^2 \sigma_z/2m,$$

$$h_\Delta = \Delta_0 \tau_y s_y \sigma_x,$$

where $m(\mathbf{k}) = M_0 - 2m(\cos k_x + \cos k_y)$ and the Pauli matrices $\sigma$, $\tau$ act on spin, orbital, and Nambu spaces, respectively. $\mu$ is the chemical potential, $M_0$, $m$ and $v$ are material dependent parameters. The Hamiltonian is invariant under time-reversal ($\mathcal{T}$) and particle-hole ($\mathcal{C}$)
Brillouin zone are protected by a non-zero Chern number. Figure 2(a) shows the Chern number calculated in $k_x k_y$-planes for different $\phi$ in the HOWSC. It takes the nontrivial value of 2 or $-2$ inside each set of Weyl points (corresponding to the FOTP regions). In contrast, it vanishes between neighboring sets (corresponding to the SOTP regions). This can be understood from the fact that there is an equal number of Weyl points of opposite chirality in each Weyl-point set, rendering the Chern number non-zero only inside each set. Thus, the surface Majorana arcs in the FOTPs are protected by a Chern number, while the hinge Majorana arcs [68] in the SOTPs (corresponding to the FOTP regions). In contrast, it can always be observed, the hinge Majorana arcs depend sensitively on surface orientation. Thus, the Weyl-point connectivity is anisotropic.

**Effective boundary theory.**—For a better understanding of the orientation-dependent connectivity of the Majorana arcs, it is instructive to develop a boundary theory applicable to any surface orientation. To do so, we first derive two boundary states ($\Psi_{\uparrow \rightarrow}, \Psi_{\downarrow \rightarrow}$) for each $\phi$ in the absence of pairing interactions [66]. Using these boundary states as a basis, the resulting effective boundary Hamiltonian can be obtained as

$$h_{\text{eff}}(\theta) = \left( \begin{array}{c|c} |v^+|k_x - \mu & \Delta(\theta) \langle\psi|e^{i\theta} - e^{-i\theta}\rangle \\ \hline -\Delta(\theta)^* & |v^-|k_x + \mu \end{array} \right), \quad (3)$$

where $v^\pm = v(1 \pm 2m\mathcal{I}\cos\phi/\omega)$, $\theta$ is the angle between the boundary and $x$ direction, and $k_x$ is the momentum along the boundary (see Fig. 1 in the Supplemental Material [66]). The projected pairing potential $\Delta(\theta)$ is obtained as

$$\Delta(\theta) = \frac{i}{2} \mathcal{F} \Delta_0 \text{sgn}(v^-) \langle\psi|e^{i\theta} - e^{-i\theta}\rangle, \quad (4)$$

with $\text{sgn}(\cdot)$ being the sign function. The prefactor $\mathcal{F}$ stems from the overlap of the boundary state wavefunctions [66]. It is unity for $\cos\phi = 0$ but smaller than one in general. The eigenenergies are given by $E_{\text{eff}} = (|v^+| - |v^-|)k_x/2 + \{[(|v^+| + |v^-|)k_x/2 - \mu]^2 + (\Delta(\theta))^2\}^{1/2}$. The chemical potential $\mu$ can be absorbed in $k_x$ in the square root and the band gap is given by $2|\Delta(\theta)|$. For simplicity, we set $\mu$ to zero in the following discussion. Notably, Eq. (3) takes the form of a 1D Dirac Hamiltonian with a Dirac mass $\Delta(\theta)$. The mass gaps out the
boundary spectrum everywhere, except for isolated values of \( \theta \) where \( \Delta(\theta) = 0 \). This is the reason why the appearance of hinge Majorana arcs depends sensitively on the surface orientation in the SOTPs.

The periodic driving preserves inversion symmetry of the system. Thus, Eq. (3) obeys \( \mathcal{P} h_{\text{eff}}(\theta)\mathcal{P}^{-1} = h_{\text{eff}}(\theta + \pi) \) with \( \mathcal{P} = \sigma_x \), the projected inversion operator, enforcing a constraint on \( \Delta(\theta) \): \( \Delta(\theta + \pi) = -\Delta(\theta) \). Obviously, \( \Delta(\theta) \) changes sign when advancing from \( \theta \) to \( \theta + \pi \), leading to a gapless point along \( \theta \). The gapless point corresponds to the positions of a hinge Majorana arc. In this regard, the SOTP is protected by inversion symmetry. This result is not restricted to a specific geometry as long as inversion symmetry is preserved. From Eq. (4), we can determine the positions of the gapless points explicitly,

\[
\theta = \pi [1 - \text{sgn}(v^+ v^-)]/4 + n\pi, \quad n \in \{0, 1\}.
\]

When \( 2mI/\omega > 1 \), \( v^+ v^- \) changes sign at \( \phi = \phi_j \) with \( j \in \{1, 2, 3, 4\} \), \( \phi_1 = -\phi_3 = \pi - \arccos(\omega/2mI) \) and \( \phi_2 = -\phi_4 = \arccos(\omega/2mI) \). As a result, the positions in Eq. (5) switch from \( \{0, \pi\} \) to \( \{\pi/2, 3\pi/2\} \).

Facilitated by the boundary theory, we are now able to explain the anisotropic connectivity of the Majorana arcs obtained numerically in Fig. 2. First, for the (100) surface, \( k_y = k_y \) and \( \theta = 0 \). In this case, the vanishing of the mass \( \Delta(\theta) \) in Eq. (4) is determined by \( \text{sgn}(v^+ v^-) = +1 \), which gives \( \phi \in (\phi_1, \phi_2) \cup (\phi_3, \phi_4) \). Thus, the hinge Majorana arcs connect the Weyl-point sets \( \phi_1 \) and \( \phi_2 \) with \( \phi_3 \) and \( \phi_4 \) at \( k_y = 0 \), as shown by the vertical bars in Fig. 2(b). Second, for the (010) surface with \( k_x = k_x \) (\( \theta = \pi/2 \)), \( \Delta(\theta) \) vanishes at \( \text{sgn}(v^+ v^-) = -1 \), leading to \( \phi \in (\phi_4, \phi_1) \cup (\phi_2, \phi_3) \). In this orientation, the hinge Majorana arcs instead connect \( \phi_4 \) with \( \phi_1 \) and \( \phi_2 \) with \( \phi_3 \) at \( k_x = 0 \), as shown by the vertical bars in Fig. 2(c). In contrast, for the (110) surface with \( \theta = \pi/4 \), \( \Delta(\theta) \) is always non-zero for all \( \phi \) [Fig. 2(d)]. As a result, there are no hinge arcs connecting the Weyl points.

**Manipulating Majorana zero modes.**—The realization of detectable and tunable Majorana zero modes is one of the main research goals in Majorana physics [69–74]. As shown in Fig. 1, by varying \( \phi \) in the SOTPs, the positions of the Majorana zero modes at the boundary of the 2D disk are tunable. Besides this, we find that the Majorana zero modes have finite spin polarization which can also be controlled by tuning CPL.

To elucidate this manipulation, we calculate explicitly the wavefunctions of the Majorana zero modes and hence their spin polarizations. Starting with the boundary Hamiltonian Eq. (3), we first obtain the wavefunctions of the zero-energy modes. From these zero-energy modes, two Majorana zero modes can then be derived. Their wavefunctions in the Nambu and spin basis \( (\Psi_{\uparrow t}, \Psi_{\downarrow t}, \Psi_{\uparrow b}, \Psi_{\downarrow b}) \) can be written as \( \Phi_1 \propto (e^{i\theta}\text{sgn}(v^+)\sqrt{|v^-|}, -i\sqrt{|v^+|} e^{-i\theta}\text{sgn}(v^-)\sqrt{|v^-|}, i\sqrt{|v^+|} T, -|v^-| T)^T \) and \( \Phi_2 \propto (-ie^{i\theta}\text{sgn}(v^+)\sqrt{|v^-|}, \sqrt{|v^+|}, |v^-|, ie^{-i\theta}\text{sgn}(v^-)\sqrt{|v^-|})^T \).

The angular positions \( \theta \) are either \( \{0, \pi\} \) or \( \{\pi/2, 3\pi/2\} \), depending on \( \phi \), as we have shown before. The spin polarization of the Majorana zero modes can be calculated as \( \langle \hat{S}_j \rangle = \langle \Phi_j | \hat{s} | \Phi_j \rangle \), where \( j \in \{1, 2\} \) and \( \hat{s} = \hbar(\tau_0 + \tau_z)/2 \) [75]. We find that the two Majorana zero modes have always opposite spins in \( x \)- and \( y \)-directions. Thus, they together yield vanishing \( \langle \hat{S}_z \rangle = 0 \) at the boundary. In contrast, for the \( z \)-component, we find an identical spin polarization for all the Majorana zero modes,

\[
\langle \hat{S}_z \rangle = \frac{\hbar}{2} |v^-|, \quad \forall \theta.
\]

which is independent of \( \theta \).

A phase diagram for the spin polarization of the Majorana zero modes with respect to the phase shift \( \phi \) and intensity \( I \) is plotted in Fig. 3(a). In contrast to the positions of the Majorana zero modes, the spin polarization depends continuously on the phase shift \( \phi \). The spin polarization splits into spin-up and spin-down regions with the border at \( \phi = \pi/2 \), because the correction \( \gamma(\mathbf{k}) \cos \phi \) in Eq. (2) induced by the CPL vanishes and time-reversal symmetry is restored at the border. \( \langle \hat{S}_z \rangle \) is an odd function of \( \phi - \pi/2 \). In the vicinity of \( \phi = \pi/2 \), it grows linearly with increasing \( \phi \). \( \langle \hat{S}_z \rangle \approx (2\hbar mI/\omega)(\phi - \pi/2) \). The spin polarization approaches its maximal value in regions where \( v^+ \) or \( v^- \) becomes zero. These regions actually separate different SOTPs, as indicated by solid lines in Fig. 3(a). Four representative cases in the diagram...
marked by (I-IV) are shown in Fig. 3(b). We can see that for the phase shift $\phi$ at I and II, the Majorana zero modes are spin-down polarized, while at III and IV, they are spin-up polarized. We note that the spin polarization is measurable by spin-polarized scanning tunneling spectroscopy [74]. This indicates that the Majorana zero modes in our system can be manipulated and detected at the same time.

Conclusions and discussions.—We have proposed to realize time–several symmetry broken HOWSCs in second-order topological superconductors with odd-parity pairing potential by periodic driving. We have revealed an important characteristic feature of higher-order Weyl materials, namely, the anisotropic Weyl-point connectivity of the surface and hinge Majorana arcs. We have further shown the possibility to detect and manipulate the Majorana zero states by CPL.

To generate Weyl points and realize the position switching of Majorana zero modes, the frequency and intensity of CPL need to satisfy $2m\omega/\omega > 1$. For typical values $m \approx 50$ eVÅ$^{2}$ (e.g., for inverted Hg(Cd)Te quantum wells [76]) and $\omega \approx 0.1$ eV, an experimentally feasible intensity of $cA_{0} = \sqrt{\omega} \geq 0.032$ Å$^{-1}$ is sufficient for our propose. Finally, we remark that the conclusion drawn in the present work is fundamental to generic higher-order Weyl materials, including not only superconductors and semimetals, but also artificial systems. Explicitly, the model in Eq. (2) and related physics could also be simulated by superconducting quantum circuits consisting of multiple qubits [77].

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