Intertwined Weyl phases: higher-order topology meets unconventional Weyl fermions via crystalline symmetry

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We report intertwined Weyl phases, which come from superposing topological phases by crystalline symmetry. In the intertwined Weyl phases, an unconventional Weyl phase where Weyl points possess a higher charge (monopole charge>1) due to rotation symmetry, and a higher-order topological phase enforced by rotation symmetry, are superposed. The two phases are no longer separable, but intertwine with each other, resulting in the novel phase. Remarkably, the intertwining leads to a prominent characteristic feature of the intertwined Weyl phases: the change of Fermi-arc topology in a periodic pattern, i.e., the way how Fermi arcs connect to Weyl points changes drastically with respect to surface orientation, which exhibits a periodic pattern. Such a phenomenon is absent in any individual phase alone. Moreover, we elaborate on how to emulate the intertwined double-Weyl phase in cold atoms. Our theory is quite promising for generating new topological phases based on existing ones.

Introduction.—Weyl fermions, originally proposed in high-energy physics, were first discovered as quasiparticle excitations around linear twofold degenerate points in solid state materials [1–3]. Owing to fertile ground of electronic structures and crystalline symmetries, Weyl physics has been undergoing rapid development and tremendous enrichment in condensed matter physics [1–8]. In particular, crystalline symmetry is essential in the diversification of Weyl fermions, leading to the discovery of unconventional Weyl fermions, which possess a monopole charge higher than that of conventional charge±1 Weyl fermions [9–17]. For example, threefold Weyl fermions with charge ±2 can be stabilized by nonsymmorphic symmetry [9–12], and double(triple)-Weyl fermions with a quadratic(cubic) twofold degeneracy can be protected by rotation symmetry [13–17].

On the other hand, crystalline symmetries have deepened and widened the concept of topological phases of matter. Besides non-spatial symmetries (e.g. time-reversal symmetry), topological materials can be largely enriched by spatial crystalline symmetries [18–29]. Recently, higher-order topological phases, which feature anomalous boundary states due to crystalline symmetries, have been discovered [30–40]. In contrast to conventional bulk-boundary correspondence, i.e., a d-dimensional bulk topology corresponds to (d−1)-dimensional boundary states, the boundary states of higher-order topological phases are further restricted by crystalline symmetries and exhibit boundary states in a lower dimension, e.g., corner or hinge states. It was later realized that higher-order topology also applies to gapless systems, resulting in higher-order Dirac, Weyl, and nodal-line semimetals [41–51].

Though crystalline symmetries play a vital role in both unconventional Weyl materials with higher-charge Weyl fermions and topological crystalline materials with anomalous boundary states, the two topological phases seem unrelated. We are interested in whether these two phases by the same crystalline symmetry can be superposed to generate new topological phases, and if successful, what their topological features would be.

In this work, we discover intertwined Weyl phases, by superposing unconventional Weyl fermions and higher-order topology protected by the same rotation symmetry. The superposition is possible because rotation symmetry acts in a twofold way: the symmetry stabilizes unconventional Weyl points in the system, and furthermore, it enforces higher-order topology on the system. Strikingly, the two phases in superposition no longer act individually, but intertwine with each other, resulting in the intertwined Weyl phase. This new phase can be characterized by a prominent topological feature: the change of Fermi-arc topology in a periodic pattern, which comes from the intertwining. On the surface, the projections of unconventional Weyl points are connected by Fermi arcs, while the topology of these Fermi arcs are drastically changed by the higher-order topological phase, leading to the periodic change of Fermi-arc topology with respect to surface orientation. The period is determined by rotation symmetry, i.e., a 2n-fold rotation symmetry leads to a period of π/n. Specifically, we discuss intertwined double-Weyl phases, where double-Weyl fermions and higher-order topology are intertwined by a fourfold rotation symmetry. The topological phase is characterized by the periodic change of Fermi-arc topology with period π/2. The periodic behavior can be perfectly explained by the effective boundary Hamiltonian, in accordance with our theory. We show that intertwined
double-Weyl phases are realizable in cold-atom experiments, which can serve as a platform to verify our theory experimentally.

**Intertwining topological phases by crystalline symmetry.** We begin by showing how to intertwine topological phases by crystalline symmetry. The essential physics can be captured by the following simple but generic Hamiltonian in three-dimensional (3D) momentum space,

\[
H(k) = H_{\text{Weyl}} + m \Gamma_h
= k_x^2 \tau_3 \sigma_- + k_y^2 \tau_3 \sigma_+ + k_z \tau_3 \sigma_3 + m \Gamma_h,
\]

where \( k_\pm = k_x \pm i k_y \), \( \sigma_\pm = (\sigma_1 \pm i \sigma_2)/2 \), and \( \sigma_i \) and \( \tau_i \) (\( i = 1, 2, 3 \)) are Pauli matrices denoting (pseudo)spin and orbital degrees of freedom, respectively. \( H_{\text{Weyl}} \), responsible for generating unconventional Weyl points, is superposed with \( m \Gamma_h \), a term for introducing higher-order topology. \( m \) is a real constant, and \( \Gamma_h \) a 4 × 4 matrix. Each of the two parts is invariant under the 2n-fold rotation symmetry \( C_{2n} \) about the \( z \) axis, with \( 2n \leq 6 \) by lattice restriction (\( n \in \{2, 3 \} \)).

The intertwining can be induced by crystalline symmetry that superposes the two phases at the same time:

1. The bulk Weyl points with higher monopole charge are stabilized by rotation symmetry. Unconventional Weyl points with charge \( \pm n \) (\( n > 1 \)) can be generated by breaking time-reversal and/or inversion symmetry in \( H_{\text{Weyl}} \). After the substitution of \( (k_x, k_y) = (k \cos \theta, k \sin \theta) \) [see Fig. 1(a)], \( H_{\text{Weyl}} \) can be rewritten as

\[
\hat{C}_{2n} H_{\text{Weyl}}(\theta) \hat{C}_{2n}^{-1} = H_{\text{Weyl}}(R_{2n} \theta).
\]

Here, \( \hat{C}_{2n} = \tau_3 \sigma_3 \), and \( R_{2n} \theta = \theta + \pi/n \) acts in momentum space.

2. The higher-order topology is further enforced by rotation symmetry. The topological protection by symmetry can be explicitly demonstrated at the boundary. After projecting the Hamiltonian to the boundary subspace, we can get an effective Hamiltonian on the surface in the form of [52]

\[
h_{\text{surface}} = \sum_{i=0}^{n} a_i k_i^2 \sigma_3 + m(\theta) \gamma_{h},
\]

where \( a_i \) is a real coefficient, which may depend on \( k_x \), \( \theta \) is the surface orientation, and \( k_i \) the momentum parallel to the surface [see Fig. 1(a)]. The 1D Hamiltonian (3) for a fixed \( k_z \) is characterized by a \( Z \) topological invariant. The higher-order
term $m(\theta)\gamma_h$, originated from $m\Gamma_h$, is still rotation-symmetric $\hat{c}_{2n}m(\theta)\gamma_h\hat{c}_{2n}^{-1} = m(R_{2n}\theta)\gamma_h$, with the projected rotation operator $\hat{c}_{2n} = \sigma_3$. $\gamma_h$ shall anticommute with $\sigma_3$, so that it acts as a mass term in Eq. (3). Thus, we obtain

$$m(\theta) = -m(R_{2n}\theta) = -m(\theta + \pi/n).$$

(4)

It means $m(\theta)$ must have a zero value between $\theta$ and $\theta + \pi/n$, which leads to a gapless point in surface spectrum. Note that the same mechanism leads to higher-order topological insulators, where corner and hinge modes correspond to the position of gapless point protected by crystalline symmetry [39, 40].

The two topological phases in superposition no longer act individually, but intertwine with each other, as we discuss next. Thus, we refer to the resulting phase as “intertwined Weyl phase”, which is different from each of the individual phases.

**Change of Fermi-arc topology in a periodic pattern.**—

Without $m(\theta)$, the surface Hamiltonian (3) describes Fermi arcs in unconventional Weyl semimetals. The topology of Fermi arcs is isotropic, i.e., the way how Fermi arcs connect to Weyl points does not depend on surface orientation $\theta$. The higher-order topological term $m(\theta)$ drastically changes the topology of Fermi arcs in two aspects.

First, the gapless point enforced by the higher-order topological phase in Eq. (4) crucially affects the Fermi-arc topology. It determines whether the Fermi arcs can go through the higher-order phase region at an angle $\theta$. Thus, strikingly, the Fermi-arc topology changes with $\theta$, which is enforced by higher-order topology.

Second, $m(\theta)$ in Eq. (4) is antiperiodic. Remarkably, it becomes periodic in the surface spectrum $E_{\text{surface}} = \pm \sqrt{\sum_{l=0}^{n} a_l k_{l\parallel}^2 + m^2(\theta)}$, since the square of $m(\theta)$ obeys

$$m^2(\theta) = m^2(\theta + \pi/n),$$

(5)

which has a period of $\pi/n$.

The periodic function $m^2(\theta)$ indicates that the topology of Fermi arcs not only changes with the surface orientation $\theta$, but also in a periodic pattern. Such a phenomenon is absent in any individual phase alone, and thus, it constitutes the characteristic feature of intertwined Weyl phases.

**Exemplification of intertwined phases.**— The intertwined double-Weyl phase is generated by the fourfold rotation symmetry $C_4$, i.e., $n = 2$. The Weyl points carry a monopole charge of $\pm 2$, which emit two Fermi arcs on the surface. According to Eq. (5), the change of Fermi-arc topology is of period $\pi/2$. In Figs. 1(b, c, d), we show the topology of Fermi arcs in three representative orientations of $\theta = 0$, $\theta = \pi/4$, and $\theta = \pi/2$ in a full period of $[0, \pi/2]$, respectively. Clearly, by rotating surfaces, the Fermi-arc topology changes from Fig. 1(b) ($\theta = 0$) to Fig. 1(c) ($\theta = \pi/4$), and then returns to the initial topology in Fig. 1(d) ($\theta = \pi/2$).

A similar story applies to the intertwined triple-Weyl phase which is enforced by the sixfold rotation symmetry $C_6$, i.e., $n = 3$. Each triple-Weyl point emits three Fermi arcs on the surface, and the topology of Fermi arcs changes periodically with a period of $\pi/3$, as shown by Figs. 1(e, f, g) in a full period of $[0, \pi/3]$.

**Intertwined double-Weyl phase.**— We now apply our theory to the intertwined double-Weyl semimetals, which can be realized in cold-atom experiments or other artificial systems. The model Hamiltonian reads

$$H(k) = 2A(\cos k_y - \cos k_x)\gamma_3\sigma_1 + 2A\sin k_x \sin k_y \gamma_2 \sigma_2 + M(k)\gamma_3 \sigma_0 \sigma_3 + m\gamma_1 \sigma_1,$$

(6)

where $M(k) = M_0 - 2t(\cos k_x + \cos k_y + \cos k_z)$. The four double-Weyl points are located on the $k_z$ axis at $k_z = \pm k_{w1}$ and $k_z = \pm k_{w2}$, where $k_{w1(2)} = \arccos(\sqrt{(M + (\pm)\sqrt{c^2 + m^2})/2t})$ with $M = M_0 - 4t$. By series expansion around the Weyl points at $(0, 0, \pm k_{w1(2)})$, i.e., $(k_x, k_y, k_z) \rightarrow (\delta k_\cos \theta, \delta k_\sin \theta, \delta k_z)$, the form of the low energy model $H(k) = A\delta k_\cos^2 \gamma_3 \sigma_3 + A\delta k_\sin \sigma_0 \sigma_3 + C_\delta k_\cos \gamma_3 \sigma_3 + C_\delta k_\sin \gamma_\sigma_3 + m\gamma_1 \sigma_1$ is the same as Eq. (1). Double-Weyl points are generated by the $\epsilon$ term that breaks time-reversal symmetry. $\mu\gamma_1 \sigma_1$ corresponds to $m\Gamma_h$ in Eq. (1), responsible for the higher-order topology. The whole system is protected by the fourfold rotation symmetry $C_4 = \sigma_3 \gamma_3$. The Fermi arcs shown in Figs. 1(b)-(d) are numerically calculated by Eq. (6).

As shown in Fig. 2(a), the Chern number on $k_x$-$k_y$-plane against $k_z$ is plotted. Here, for simplicity and without loss of generality, we make $k_{w2} < k_{w1}$, for the chosen parameters as shown in Fig. 2. We can see that
the Chern number changes by 2 when passing a double-Weyl point. Thus, it is non-trivial between the upper pair \( k_x \in (k_{w2}, k_{w1}) \) and lower pair \( k_x \in (-k_{w1}, -k_{w2}) \) of Weyl points, but outside these two pairs, the Chern number is zero. This indicates that the Fermi arcs between upper or lower pairs of Weyl points are protected by the nontrivial Chern number.

**Effective boundary theory.**—To understand the periodic behavior of Fermi-arc topology, a boundary theory applicable to any surface orientation shall be developed. We can achieve this goal by firstly deriving two boundary states for each \( \theta \) in the absence of the higher-order term \( m\tau_1\sigma_1 \) in Eq. (6). The spinor part of two boundary states takes the form of \( \psi_1 \propto (e^{-2i\theta}, \sqrt{2} + 1, 0, 0) \) approximately in the region of \( k_z \in (-k_{w1}, k_{w1}) \), and \( \psi_2 \propto (0, 0, e^{-2i\theta}, \sqrt{2} + 1) \) in the region of \( k_z \in (-k_{w2}, k_{w2}) \). Note that the contribution from spatial part of the boundary states does not affect the main results, and is neglected for simplicity. By projecting the whole Hamiltonian into the subspace spanned by the boundary states, we can obtain the effective boundary Hamiltonian as [52]

\[
h_{\text{surf}} = -\frac{1}{\sqrt{2}} \left( (2k_{||}^2 - k_z^2)\sigma_3 - m \cos(2\theta)\sigma_1 \right),
\]  

up to a constant term of \(-1/\sqrt{2}e\sigma_0\), and \( k_z^2 = 2t \cos k_z - M \). Clearly, the boundary Hamiltonian is in the form of Eq. (3). The effective Hamiltonian is valid in the region where \( \psi_1 \) and \( \psi_2 \) overlap, i.e., \( k_z \in (-k_{w2}, k_{w2}) \) between the middle two Weyl points, where the Chern number is trivial.

Clearly, the periodic change of Fermi-arc topology, shown in Fig. 1, is caused by the higher-order term \( m \cos(2\theta) \). The period is \( \pi/2 \), as determined by \( m^2 \cos^2(2\theta) \) in the spectrum, in accordance with the general theory of Eq. (5). Within a single period, the higher-order topology enforces the appearance of gapless point [Eq. (4)], which is located at \( m \cos(2\theta) = 0 \). The gapless point drastically changes the topology of Fermi arcs, because it determines whether the arcs can enter the region of \( k_z \in (-k_{w2}, k_{w2}) \) between the middle two Weyl points or not. Figures 1 (b)-(d) show three representative orientations in a full period of \( \theta \in [0, \pi/2] \). The Fermi arcs cannot go through the region between middle two Weyl points at \( \theta = 0 \). After rotating to \( \theta = \pi/4 \) at the gapless point, the Fermi arcs are allowed to go through. Finally, at \( \theta = \pi/2 \), the Fermi arcs return to their initial topology, completing one period.

**Experimental realization.**—Owing to technical advances, cold atoms have been widely applied in quantum simulations of topological matter [53–56], and now are also readily available for realizing the intertwined double-Weyl semimetal described by Eq. (6). Here we present the realization proposal using fermionic atoms. We choose two hyperfine states as the pseudo-spins \( \uparrow, \downarrow \) for the \( \sigma \) degrees of freedom. For our model Hamiltonian, which requires two extra degrees of freedom, we consider the atomic gases loaded in a 2D bilayer optical lattice. Couplings between opposite pseudo-spins are processed via laser fields of modes \( M_{1,2,3}(r) \). The on-site energy offset is prepared as \( \Gamma_\lambda(\phi) \) which not only depends on the layer index but also is manually controlled by the parameter \( \phi \).

![Fig. 3. Illustration of experimental setup. The atoms are confined in a bilayer optical lattice. Couplings between opposite pseudo-spins are processed via laser fields of modes \( M_{1,2,3}(r) \). The on-site energy offset is prepared as \( \Gamma_\lambda(\phi) \) which not only depends on the layer index but also is manually controlled by the parameter \( \phi \).](image)

In order to engineer the intra-layer spin-flipped hopping, we use laser fields of three modes \( M_{1,2,3}(r) \) to couple the pseudo-spins. The spatial modulations of the field modes are prepared as \( M_1(r) = iM_1 \sin(k_L x) \sin(k_L y) \), \( M_2(r) = M_2 \cos(k_L x) \cos(3k_L y) \cos(k_L z) \), and \( M_3(r) = -M_3 \cos(3k_L x) \cos(k_L y) \cos(k_L z) \), where \( k_L = \pi/d \) and \( d \) denotes the lattice constant. Due to the odd parity of \( M_1(r) \) in the \( xy \)-plane [58], the on-site and nearest-neighbor (NN) couplings vanish, while the next-NN coupling dominates, resulting in \( \sin k_x \sin k_y \sigma_1 \). Due to the crystal symmetry, the combination of \( M_2(r) \) and \( M_3(r) \) leads to the NN coupling (\( \cos k_x - \cos k_y \sigma_1 \)). After making operator transformations, all the intra-layer terms host opposite sign for different layers. Furthermore, the higher-order topological term \( \tau_1\sigma_1 \) is naturally introduced by the inter-layer hopping. The details of the realization proposal are shown in Supplemental Material [52].

**Conclusions and discussions.**—We have found that by superposing higher-order topology and unconventional Weyl fermions, intertwined Weyl phases can be generated. The intertwining between two kinds of topological phases in superposition is induced by crystalline symmetry. The intertwined topological phase is different from any of the individual phases, and exhibits its
own characteristic topological features. In intertwined Weyl phases, we have revealed the change of Fermi-arc topology in a periodic pattern as their characteristic feature. We have proposed a feasible cold-atom experiment to verify our theory and to realize the intertwined Weyl phases.

Finally, we note that our theory could serve as a guiding principle to generate new topological phases based on existing ones. A direct application would be to investigate the intertwining between topological semimetal phases with emergent particles other than Weyl fermions and topological crystalline phases, that are protected by the same symmetry [25–28, 59, 60]. Our theory may find applications not only in condensed matter and cold-atom systems, but also in other artificial periodic systems such as photonic crystals and electric circuit arrays.

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