Non-Hermitian spatial symmetries and their stabilized exceptional topological semimetals

W. B. Rui,¹,∗ Zhen Zheng,¹ Chenjie Wang,¹,‡ and Z. D. Wang¹,†

¹Department of Physics and HKU-UCAS Joint Institute for Theoretical and Computational Physics at Hong Kong, The University of Hong Kong, Pokfulam Road, Hong Kong, China

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Without the constraint imposed by Hermiticity, non-Hermitian systems enjoy greater freedom than Hermitian ones. While internal symmetries enriched by non-Hermiticity have been revealed, the interplay between spatial symmetries and non-Hermiticity remains to be explored. Here we study non-Hermitian spatial symmetries — a class of symmetries that have no counterparts in Hermitian systems — and study how exceptional semimetals can be stabilized by these symmetries.

Different from internal ones, spatial symmetries act non-locally in momentum space and enforce global constraints on quantities at different momentum locations. We derive general constraints on geometric and topological invariants imposed by non-Hermitian spatial symmetries, which differ from those by Hermitian spatial symmetries. With these constraints, we reveal that certain exceptional manifold is only compatible with and stabilized by non-Hermitian spatial symmetries but is intrinsically incompatible with Hermitian spatial symmetries. We illustrate our theory using two three-dimensional (3D) models, dubbed exceptional unconventional Weyl semimetal and exceptional triple-point semimetal, respectively. Experimental cold-atom realization of the former is also proposed.

Introduction. — Symmetry serves as a guiding principle in the study of topological phases. A hallmark is the classification of topological phases with internal symmetries [1–3] or spatial symmetries (i.e., topological crystalline phases) [3–17]. Recently, the study has been extended into the non-Hermitian regime [18–28]. A salient feature of non-Hermitian systems is the existence of exceptional points (EP) [29–31], at which the Hamiltonian is degenerate and the energy bands are degenerate. All EPs collectively form an exceptional manifold [32], such as exceptional ring [33–38], exceptional surface [38–40], and more complicated structure like knot/link/nexus [41–45]. Certain structure of the exceptional manifold, e.g., branching points where more than two exceptional lines meet, are generally unstable without symmetries.

Internal symmetries, although widely studied in non-Hermitian systems [46–54], seem playing little role in stabilizing the global structure of an exceptional manifold (assuming instability without symmetries). To stabilize these exceptional manifolds, it is then natural to resort to spatial symmetries. Like internal symmetries that are greatly ramified by non-Hermiticity [50–54], spatial symmetries also come in different classes, such as the Hermitian and non-Hermitian classes — see Eqs. (1) and (2) for definitions. So far, it is unclear whether and how different classes of spatial symmetries can stabilize the structure of exceptional manifold, and how they constrain topological properties of exceptional non-Hermitian systems.

In this work, we focus on non-Hermitian spatial symmetries and demonstrate how they characterize and stabilize 3D exceptional topological semimetals [33–43]. We first study general relations and constraints imposed by non-Hermitian spatial symmetries on geometric and topological quantities, including Wilson loops, Chern numbers and winding numbers. Next, we explore two models, the exceptional unconventional Weyl semimetal and the exceptional triple-point semimetal. The former involves non-Hermitian rotation while the latter involves multiple non-Hermitian spatial symmetries. Through these models, we show that certain exceptional manifold (e.g., Fig. 1(b)) is compatible with and can only be stabilized by non-Hermitian spatial symmetries, but it is intrinsically incompatible with Hermitian spatial symmetries due to constraints on topological quantities. This justifies the unique importance of non-Hermitian spatial symmetries. We also discuss possible realization of our models in cold-atomic systems.

Non-Hermitian spatial symmetries. — Consider a crystal or lattice system with lattice-translation symmetries, so that the Hamiltonian can be transformed into momentum space. If the system respects a crystalline symmetry, the Hamiltonian usually transforms as

$$\mathcal{G} \mathcal{H}(k) \mathcal{G}^{-1} = \mathcal{H}(gk),$$

(1)

where we take $\mathcal{G}$ to be unitary and $g$ transforms the crystal momentum $k$. In Hermitian systems, the above transformation is equivalent to

$$\mathcal{G} \mathcal{H}(k) \mathcal{G}^{-1} = \mathcal{H}(gk).$$

(2)

However, the equivalence no longer holds in non-Hermitian systems as $\mathcal{H}(gk) \neq \mathcal{H}(k)$. Accordingly, Eqs. (1) and (2) describe different classes of symmetries. Such ramification by non-Hermiticity is similar to that of non-spatial symmetries. The latter has been systematically studied, e.g. in Ref. [51], which shows that there are 38-fold symmetry classes, far beyond the celebrated Altland-Zirnbauer 10-fold classes in Hermitian systems. We will refer to those satisfying (1) as “Hermitian spatial
symmetries”, and those satisfying (2) as “non-Hermitian spatial symmetries”. Note that $G$ can also be anti-unitary. However, we focus on the unitary case below.

Let $|\Psi_{L,n}(k)\rangle$ and $|\Psi_{R,n}(k)\rangle$ be the left and right eigenvectors of the non-Hermitian Hamiltonian $H(k)$, respectively, where $n$ is the band index. The two vectors satisfy $H(k)|\Psi_{R,n}(k)\rangle = E_n(k)|\Psi_{R,n}(k)\rangle$ and $H^\dagger(k)|\Psi_{L,n}(k)\rangle = E^*_n(k)|\Psi_{L,n}(k)\rangle$. They are different in general and form a biorthonormal basis, satisfying $\langle \Psi_{L,m}(k)|\Psi_{R,n}(k)\rangle = \delta_{mn}$. If $H(k)$ admits a non-Hermitian spatial symmetry $G$ satisfying Eq. (2), one can show that

\begin{align}
H^\dagger(gk)G|\Psi_{R,n}(k)\rangle &= E_n(k)G|\Psi_{R,n}(k)\rangle, \\
H(gk)G|\Psi_{L,n}(k)\rangle &= E^*_n(k)G|\Psi_{L,n}(k)\rangle.
\end{align}

(3)

Accordingly, every right (left) eigensystem $\{|\Psi_{R,n}(k)\rangle, E_n(k)\}$ is mapped to a left (right) eigensystem $\{|G|\Psi_{R,n}(k)\rangle, E^*_n(k)\}$ at $gk$. As $G$ is invertible, this map is a one-to-one correspondence. On the other hand, a Hermitian symmetry $G$ maps right (left) eigensystem to right (left) eigensystem.

This correspondence also holds at EPs, where energy eigenvectors do not span the whole Hilbert space. Consider an EP at momentum $k_{\text{EP}}$. The Hamiltonian $H(k_{\text{EP}})$ can be transformed by an invertible matrix $P$ to a Jordan normal form $J(k_{\text{EP}})$,

$$P^{-1}H(k_{\text{EP}})P = J(k_{\text{EP}}).$$

(4)

For simplicity, we assume $J(k_{\text{EP}})$ is composed of a single Jordan block $J(k_{\text{EP}}) = E(k_{\text{EP}})I + N$, where $I$ is the identity matrix, and $N$ the nilpotent matrix defined by $N_{ij} = \delta_{i,j-1}$. In the presence of a non-Hermitian symmetry (2), it is straightforward to derive

$$\tilde{P}H(gk_{\text{EP}})\tilde{P}^{-1} = J^\dagger(k_{\text{EP}}),$$

(5)

where $\tilde{P} = P^\dagger G^\dagger$ is invertible. Comparing Eq. (4) with (5), we see that $H(gk_{\text{EP}})$ is brought to the same Jordan normal form as $H(k_{\text{EP}})$, up to Hermitian conjugation. Therefore, the exceptional manifold is symmetric under $G$ action. The Hermitian conjugate in (5) implies that $E(gk_{\text{EP}}) = E^*(k_{\text{EP}})$, similarly to normal eigenvalues.

**Wilson loop and Chern number.**— Many geometric and topological observables in Hermitian systems [55-58] can be generalized into non-Hermitian systems. For biorthonormal eigenstates, Wilson loops in non-Hermitian systems can be defined as [59, 60]:

$$W^\alpha_\gamma(k) = \exp\left[-\int_{k_0} dk A^\alpha_\gamma(k)\right],$$

(6)

where $\alpha = R, L$ (with $\bar{R} = L$ and $\bar{L} = R$), $L$ is a loop in momentum space with $k_0$ being a base point, and "exp" denotes that the integral is path-ordered. The non-Abelian Berry connection is defined as $A^\alpha_\gamma(k) = \langle \Psi_{\alpha,n}(k)|\partial_k|\Psi_{\beta,n}(k)\rangle$ for a set of bands that are separated from other bands along the loop $L$. The Wilson loop $W^\alpha_\gamma$ is invariant under a basis transformation (gauge transformation) only in the Abelian case (i.e., a single band). For multiple bands, one needs to consider the determinant

$$\det(W^\alpha_\gamma) = \exp(a^\alpha_\gamma + i\gamma^\alpha_\gamma),$$

(7)

where both $a^\alpha_\gamma$ and $\gamma^\alpha_\gamma$ are real. The phase $\gamma^\alpha_\gamma$ is the Berry phase. We show in the Supplemental Material (SM) [61] that

$$a^{LR}_{\alpha} = -a^{RL}_{\alpha}, \quad \gamma^{LR}_{\alpha} = \gamma^{RL}_{\alpha}. $$

(8)

With a non-Hermitian spatial symmetry in (2), the Wilson loop satisfies the following relation (see SM [61] for details)

$$W_{\gamma_{\alpha}} = S^\dagger_{\gamma,\alpha}(k_0)\bar{\gamma}^\alpha_\gamma S_{\gamma,\alpha}(k_0),$$

(9)

where $gL$ is the image of $L$ under $G$, and the sewing matrix $S^\alpha_\gamma(k) = \langle \Psi_{\alpha,n}(gk)|G|\Psi_{\mu,n}(k)\rangle$. Here, “$\bar{n}$” indexes the bands associated with the states $G|\Psi_{\mu,n}(k)\rangle$, which are not necessarily the same as those of $|\Psi_{\alpha,n}(k)\rangle$, and $W^\alpha_\gamma$ is the corresponding Wilson loop. Unitarity of $G$ leads to $S^\dagger_{\gamma,\alpha}(k)S_{\gamma,\alpha}(k) = I$. Taking the determinant on both sides of (9), we obtain

$$\bar{a}_{\gamma_{\alpha}} = a^\alpha_\gamma, \quad \bar{\gamma}_{\gamma_{\alpha}} = \gamma^\alpha_\gamma. $$

(10)

Instead, if $G$ is a Hermitian symmetry, we have $\bar{a}_{\gamma_{\alpha}} = a^\alpha_\gamma$ and $\bar{\gamma}_{\gamma_{\alpha}} = \gamma^\alpha_\gamma$.

Chern numbers can also be defined in non-Hermitian systems. The non-Abelian Berry curvature is defined as $B^\alpha_\gamma = i\nabla \times A^\alpha_\gamma + iA^\alpha_{\gamma\alpha} \times A^\alpha_\gamma$. Then, associated with every closed surface $\Sigma$ on which a set of energy bands are separate from others, the Chern number is given by

$$C_{\Sigma} = \frac{1}{2\pi} \text{Re} \int_{\Sigma} dS \cdot \text{tr}(B^\alpha_\gamma).$$

(11)

We show in SM [61] that $C_{\Sigma}$ is independent of $\alpha$ and that it takes integer values. Similarly to the Hermitian case, one can show that $C_{\Sigma} = C_{\bar{\Sigma}}$, where $\bar{\Sigma}$ is the image of $\Sigma$ under $G$, and $C_{\bar{\Sigma}}$ is associated with the bands of $G|\Psi_{R,n}(k)\rangle$.

**Exceptional manifold and winding number.**— In practice, the exceptional manifold can be found by studying the characteristic polynomial $\chi_{\text{ker}}(E) = \text{det}(H(k) - E)$. Without additional symmetry-protected degeneracy, $\chi_{\text{ker}}(E) \propto |E(k_{\text{EP}}) - E|^\mu$ near an EP at $k_{\text{EP}}$, where the order $\mu$ is equal to the size of Jordan block. Accordingly, at $E = E(k_{\text{EP}})$,

$$\chi_{k_{\text{EP}}}(E) = \frac{\partial \chi_{k_{\text{EP}}}(E)}{\partial E} = \cdots = \frac{\partial^{\mu-1} \chi_{k_{\text{EP}}}(E)}{\partial E^{\mu-1}} = 0.$$ 

(12)

Considering both $\chi$ and $E$ are complex, we have $2\mu$ equations and $D+2$ variables for $D$-dimensional systems. For
order-2 EPs in 3D systems, the number of variables is one more than that of equations, indicating that EPs generally form exceptional lines (ELs). Assuming a gap around such an EL, a winding number can be defined [22, 46]:

$$W(k_{\text{EP}}) = \frac{1}{2\pi i} \oint_{S^1} dk \cdot \nabla_k \log \det \left[ \mathcal{H}(k) - E(k_{\text{EP}}) \right],$$

where $S^1$ is a loop that encircles the EL and $k_{\text{EP}}$ is any point on the EL. The integral (13) needs an orientation on $S^1$ to be unambiguous. It can be done by first assigning an orientation to the EL, which then induces a orientation on $S^1$ through the right-hand rule. Changing the orientation of EL gives a minus sign to $W(k_{\text{EP}})$.

In the presence of spatial symmetry $\mathcal{G}$, we show in SM [61] that

$$W(gk_{\text{EP}}) = \zeta \sigma(gk_{\text{EP}}, k_{\text{EP}})\sigma(g)W(k_{\text{EP}}),$$

where $\zeta = +1$ if $\mathcal{G}$ is a Hermitian symmetry, and $\zeta = -1$ if $\mathcal{G}$ is a non-Hermitian symmetry. The factor $\sigma(gk_{\text{EP}}, k_{\text{EP}}) = 1$ if the orientations of the ELs at $k_{\text{EP}}$ and $gk_{\text{EP}}$ match under $\mathcal{G}$, and $\sigma(gk_{\text{EP}}, k_{\text{EP}}) = -1$ otherwise. The factor $\sigma(g) = 1$ or $-1$, if $\mathcal{G}$ preserves (e.g. rotation) or reverses (e.g. mirror reflection) the chirality of the momentum space, respectively.

**Exceptional unconventional Weyl semimetals.** With the above general results, we now study two models of exceptional topological semimetals. The first model is a non-Hermitian extension of unconventional Weyl semimetals, where the momentum space hosts monopoles of charge $\pm 2$. It is our main example to demonstrate how non-Hermitian spatial symmetries can stabilize exceptional manifolds in a different way from the Hermitian counterpart. We discuss a cold-atom realization of this model in SM [61]. The non-Hermiticity is introduced by the on-site atomic decay.

The momentum-space Hamiltonian of our model reads

$$\mathcal{H}^w(k) = \mathcal{H}^w_0(k) + H^w_1(k),$$

where all parameters $M_0, t_{\parallel}, t_z, A$ and $\lambda$ are real. The unperturbed Hamiltonian $\mathcal{H}^w_0$ respects a normal four-fold rotation symmetry $\mathcal{C}_{4z} = \sigma_3$, $\mathcal{C}_{4z}^* H^w_0(k) \mathcal{C}_{4z} = \mathcal{H}^w_0(-R_{4z}k)$ with $R_{4z}(k_x, k_y, k_z) = (k_y, -k_z, k_x)$. It has two Weyl points with monopole charge $\pm 2$, located at $K_{\pm} = (0, 0, \pm \arcsin(M_0 - 4t_{\parallel})/2t_z)$. The Weyl points are stabilized by the Hermitian $\mathcal{C}_{4z}$ symmetry [62], in the sense that they do not split into monopoles of charge $\pm 1$. With the non-Hermitian term $H^w_1$ included, $\mathcal{C}_{4z}$ is not respected as a Hermitian symmetry, because $[\mathcal{C}_{4z}, i\lambda \sigma_1] \neq 0$. However, as a non-Hermitian symmetry, $\mathcal{C}_{4z}$ is still preserved, which reads

$$\mathcal{C}_{4z} \mathcal{H}^w(k_x, k_y, k_z) \mathcal{C}_{4z}^{-1} = \mathcal{H}^w(k_y, -k_z, k_x).$$

Figure 1 (a) shows that the exceptional manifold of the model, and Fig. 1 (b) shows an enlargement around $K_{\pm}$. Each of the original Weyl points turns into four rotation-symmetric ELs that jointly terminate on rotation axis. All EPs including those on the rotation axis are of order 2. All winding number is $W(k_{\text{EP}}) = \pm 1$. We plot the real and imaginary parts of eigenenergies in the 2D $k_xk_y$ Brillouin zone (BZ) across $K_{\pm}$ ($\pm \delta k_z = 0$) in the right panel in Fig. 1 (b). The spectrum and EPs clearly exhibit a four-fold rotation symmetry. We note that EPs in the right panel of (b) are connected by bulk Fermi arcs [18], as shown by the white lines. The relations in (8) are explicitly verified for a family of loops in Fig. 1 (c).

Stability of this exceptional semimetal comes at different levels. First, we compute the Chern number $C_5$ of one of the two bands on 2D slides $\Sigma = P_1$, $P_2$ and $P_3$, shown as pink planes Fig. 1 (a). We find that $C_{P_1} = 0$, $C_{P_2} = -2$, and $C_{P_3} = 0$, agreeing with the fact that original monopoles have charge $\pm 2$. It implies that, between $P_1$ and $P_2$ and between $P_2$ and $P_3$, there must exist regions that are energetically degenerate, making the system a semimetal. Second, we perform a perturbative analysis for the low-energy theory of $\mathcal{H}^w_0$ around $K_{\pm}$. We find that constant perturbations that respect the non-Hermitian $\mathcal{C}_{4z}$ symmetry are $i\lambda \sigma_1$ and $i\lambda \sigma_2$, which produce similar exceptional manifolds as in Fig. 1(a) (details are given in SM [61]). In fact, stability of the structure of this exceptional manifold — specifically, existence of the branching points on rotation axis — can be argued...
In order for ELs to terminate on the rotation axis, \( \eta \neq 0 \). In order for ELs to terminate on the rotation axis, \( \eta \neq 0 \) (14). In order for ELs to terminate on the rotation axis, \( \eta \neq 0 \) (a), a Hermitian symmetry at \( \eta = 0 \) (a), a Hermitian symmetry at \( \eta = 0 \) (a), and broken when \( 0 < \eta < 1 \) (b). The loops \( \mathcal{L} \) and \( g\mathcal{L} \) refer to the red and blue arrows in Fig. 1(a).

at a topological level, as we show below.

To give a comprehensive analysis, we consider a modified Hamiltonian

\[
\mathcal{H}^w(k) = \mathcal{H}_0^w(k) + i\lambda [(1 - \eta)\sigma_1 + \eta\sigma_3].
\]  

When \( \eta = 0 \), \( \mathcal{H}^w \) reduces to \( \mathcal{H}^u \). When \( \eta = 1 \), the non-Hermitian perturbation \( i\lambda\sigma_3 \) respects \( C_{4z} \) as a Hermitian symmetry. Accordingly, by tuning \( \eta \in [0, 1] \), we achieve a transition from a non-Hermitian \( C_{4z} \) to a Hermitian \( C_{4z} \).

When \( 0 < \eta < 1 \), \( C_{4z} \) is not respected either as Hermitian or non-Hermitian symmetry.

Figure 2 shows the evolution of the exceptional manifold as \( \eta \) varies. It exhibits a fourfold rotation symmetry both at \( \eta = 0 \) and \( \eta = 1 \). The key difference is that: there are exceptional branching points on the rotation axis at \( \eta = 0 \), while the whole axis is non-degenerate at \( \eta = 1 \). This difference can be explained by the constraint (14). In order for ELs to terminate on the rotation axis, the total winding number must vanish such that

\[
\sum_{n=0}^{3} W(g^n k_{\text{EP}}) = 0.
\]  

If \( C_{4z} \) is Hermitian, Eqs. (14) and (18) together lead to \( W(k_{\text{EP}}) = 0 \). In other words, the exceptional manifold in Fig. 2(a) is intrinsically incompatible with Hermitian symmetries. On the other hand, Eq. (18) is always satisfied for a non-Hermitian \( C_{4z} \) due to Eq. (14). Moreover, the exceptional branching points are indeed protected by the non-Hermitian \( C_{4z} \) (see an analysis in SM[61]).

Therefore, we conclude that non-Hermitian and Hermitian spatial symmetries may stabilize exceptional manifolds in very different manners.

We also visualize the difference in Wilson loops for non-Hermitian and Hermitian symmetries in Fig. 2. We consider a family of non-contractible loops \( \mathcal{L} : (t, -\pi, 0) \rightarrow (t, \pi, 0) \) (red arrow the lower panel of Fig. 1(a)) with \( t \in [0, \pi] \). Under \( C_{4z} \), \( \mathcal{L} \) is mapped to \( g\mathcal{L} : (\pi, t, 0) \rightarrow (-\pi, t, 0) \) (blue arrow in Fig. 1(a)). The quantities \( a^w_{\alpha\alpha}, \gamma_{\alpha\alpha}, a^{g}\gamma_{\alpha\alpha} \) and \( \gamma_{g\alpha} \) are plotted in Fig. 2 against the parameter \( t \), which agrees with Eqs. (8) and (10) \((C_{4z} \) maps each band to itself in our model, so all quantities in (10) are associated with the same band).

**Exceptional triple-point semimetals.**— Our second model involves multiple non-Hermitian spatial symmetries and appearance of higher-order EPs, i.e., multifold degeneracy with more than two eigenvectors coalescing to one. It is based on a Hermitian triple-point semimetal [63, 64], with the low-energy momentum-space Hamiltonian given by

\[
\mathcal{H}'(k) = \mathcal{H}_0'(k) + i\lambda\Lambda
\]

\[
= \begin{pmatrix}
\alpha k_x & \beta k_z & -\beta k_y \\
\beta k_z & -\alpha k_x & 0 \\
-\beta k_y & 0 & -\alpha k_x
\end{pmatrix} + i\lambda \begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & 1 \\
0 & 1 & 0
\end{pmatrix}.
\]  

Without the non-Hermitian term \( i\lambda\Lambda \), the triple point is stabilized by three symmetries: a fourfold rotation symmetry about the \( x \) axis \( (C_{4x}) \), a mirror symmetry about the \( xz \)-plane \( (M_{xz}) \), and a combined symmetry of space-inversion and time-reversal symmetry \( (PT) \). Such a triply degenerate point can be found in materials of space group No. 225 [65].

The full Hamiltonian \( \mathcal{H}'(k) \) respects \( C_{4x}, M_{xz} \) and \( PT \) all as non-Hermitian symmetries (see SM[61] for a detailed discussion). As shown in Fig. 3, the non-Hermitian term \( i\lambda\Lambda \) turns the triple point into an exceptional manifold, computed by the characteristic polynomial according to Eq. (12). We find that apart from order-2 ELs (green lines), there are four order-3 EPs (magenta points). Different from exceptional Weyl system, the triple point does not have a well-defined topological invariant like Chern number, because a fully gapped sphere surrounding it cannot be found. However, the stability of the exceptional manifold is perturbatively protected by the non-Hermitian symmetries, as we show in SM[61].
that $i\lambda A$ is the only symmetry-allowed term. The relation (14) is confirmed for both the orientation-preserving $C_4$ and orientation-reversing $M_{22}$ non-Hermitian spatial symmetries.

Conclusions. — We have studied non-Hermitian spatial symmetries and exceptional topological semimetals stabilized by them. We have derived the general constraints on band structure, geometric and topological quantities, imposed by non-Hermitian spatial symmetries. We have proposed two models to demonstrate how non-Hermitian spatial symmetries can stabilize exceptional topological phases, in a different way from Hermitian symmetries. In particular, we reveal that certain exceptional manifold is incompatible with Hermitian symmetries and can only be protected by the non-Hermitian symmetries. Cold-atom realization of the exceptional unconventional Weyl semimetal phase is also proposed.

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Supplemental Material for

“Non-Hermitian spatial symmetries and their stabilized exceptional topological semimetals”

W. B. Rui, Zhen Zheng, Chenjie Wang, and Z. D. Wang

In this Supplemental Material, we derive biorthogonal Wilson loops in non-Hermitian systems in Sec. I, reveal the relations and constraints on Wilson loop and Chern number under non-Hermitian symmetry in Sec. II, calculate the relation of winding numbers between symmetry-related exceptional lines in Sec. III, discuss the symmetries in exceptional unconventional Weyl semimetals in Sec. IV, discuss the symmetries in exceptional triple-point semimetals in Sec. V, and propose the experimental realization of exceptional unconventional Weyl semimetals in Sec. VI.

I. BIORTHOGONAL WILSON LOOPS IN NON-HERMITIAN SYSTEMS

In this section, we discuss some general properties of Wilson loop observables in non-Hermitian band theory. While only Abelian Wilson loops are used in the main text, here we consider general non-Abelian Wilson loops associated with $N$ bands. Recall that in Hermitian systems a Wilson line is defined as

$$\mathcal{W}_P = \exp \left[ - \int_{k_i}^{k_f} dk A(k) \right],$$

(1)

where $P$ is a path from $k_i$ to $k_f$ in the momentum space, $A(k)$ is the matrix-valued Berry connection, "\_\_" indicates that the integral is path-ordered, and the $N$ bands are separated from other bands along the path $P$. We will denote the path as $P: k_f \leftarrow k_i$. Given a set of orthonormal energy eigenstates $\langle \Psi_m(k) | \Psi_n(k) \rangle = \delta_{mn}$, the Berry connection is defined as $[A(k)]_{mn} = (\Psi_m(k) | \partial_k | \Psi_n(k) \rangle$. The orthonormality leads to $A_{mn}(k) = -A_{nm}(k)$, i.e., $A(k)$ is anti-Hermitian, which guarantees that $W_P$ is a unitary matrix. Under a unitary basis transformation $| \Psi_n(k) \rangle \rightarrow U(k) | \Psi_n(k) \rangle \equiv | \psi_n(k) \rangle$, the Berry connection and Wilson line transform as

$$A(k) \rightarrow A'(k) = U^\dagger(k) A(k) U(k) + U^\dagger(k) \partial_k U(k), \quad W_P \rightarrow W'_P = U^\dagger(k_f) W_P U(k_i).$$

(2)

We observe that $A(k)$ and $W_P$ resemble the gauge potential and Wilson line in $U(N)$ gauge theory respectively, and $U(k)$ resembles a gauge transformation. Note that the transformation $U(k)$ should preserve eigenenergy, so it is arbitrary only if the $N$ bands are fully degenerate along the path $P$. Considering a closed loop $L: k_0 \leftarrow k_0$, with $k_0$ being a base point, we can construct the following gauge invariant Wilson loop observable

$$e^{i \gamma_L} = \text{det}(W_L).$$

(3)

Note that gauge transformations (2) on $W_L$ cancel out for a closed loop $L$ after taking a determinant. The phase factor $e^{i \gamma_L}$ is also independent of the base point $k_0$ of $L$.

Instead of a single set of eigenvectors at each $k$, a non-Hermitian system carries two sets of eigenvectors, the left and right eigenvectors, $\{| \Psi_{L,m}(k) \rangle \}$ and $\{| \Psi_{R,n}(k) \rangle \}$, respectively, which are not the same in general. We take the left and right eigenvectors to be biorthonormal, $\langle \Psi_{L,m}(k) | \Psi_{R,n}(k) \rangle = \langle \Psi_{R,n}(k) | \Psi_{L,m}(k) \rangle = \delta_{mn}$. We can define two types of Wilson lines:

$$W_P^{LR} = \exp \left[ - \int_{k_i}^{k_f} dk A^{LR}(k) \right], \quad W_P^{RL} = \exp \left[ - \int_{k_i}^{k_f} dk A^{RL}(k) \right],$$

(4)

where the Berry connection $A^{\alpha\beta}(k)$ is defined as $A^{\alpha\beta}_{nm}(k) = \langle \Psi_{\alpha,m}(k) | \partial_k | \Psi_{\beta,n}(k) \rangle$. Under a basis transformation $| \Psi_{L,n}(k) \rangle \rightarrow U(k) | \Psi_{L,n}(k) \rangle$ and $| \Psi_{R,n}(k) \rangle \rightarrow U(k) | \Psi_{R,n}(k) \rangle$, which preserves the biorthonormality, the transformations on $A^{\alpha\beta}(k)$ and $W_P^{\alpha\beta}$ are the same as in (2). Unlike in the Hermitian case, $W_P$ is not unitary in general. The biorthonormality of the left and right eigenvectors gives $A_{mn}^{RL} = -(A_{nm}^{LR})^*$, with which one can show the following relations

$$W_P^{\alpha\beta} = \left( W_P^{\alpha\beta} \right)^\dagger, \quad W_P^{\alpha\beta} \left( W_P^{\alpha\beta} \right)^\dagger = W_P^{\alpha\beta} W_P^{\alpha\beta} = I,$$

(5)
where \( \alpha \neq \beta \), \( \bar{P} \) is the inverse path of \( P \), and \( I \) is the \( N \times N \) identity matrix. If one considers a closed loop \( L \), then we have

\[
\det (W_{L}^{LR}) = e^{a_{c} + i\gamma c}, \quad \det (W_{L}^{RL}) = e^{-a_{c} - i\gamma c}, \quad \det (W_{L}^{IL}) = e^{-a_{c} + i\gamma c},
\]

(6)

where both \( a_{L} \) and \( \gamma_L \) are real numbers. We emphasize that while \( W_{L}^{\alpha\beta} \) is not unitary, the gauge transformation \( U(k) \) is still unitary. Shifting the phase \( \gamma_L \) by multiples of \( 2\pi \) corresponds to performing a large gauge transformation \( U(k) \) on the gauge potential \( A(k) \). Here, “large” corresponds to a nontrivial winding number from the loop \( L \) to \( U(N) \) matrices (more precisely, the diagonal \( U(1) \)).

The field strength is defined as \( F_{\mu\nu}^{\alpha\beta} = \partial_{\mu} A_{\nu}^{\alpha\beta} - \partial_{\nu} A_{\mu}^{\alpha\beta} + [A_{\mu}^{\alpha\beta}, A_{\nu}^{\alpha\beta}] \), where \( \mu, \nu \) are components of momentum \( k \).

The Berry curvature (or magnetic field) is defined as \( B^{\alpha\beta} = i \nabla \times A^{\alpha\beta} + i A^{\alpha\beta} \times A^{\alpha\beta} \) for 3D systems. We have the following relation

\[
e^{a_{c} + i\gamma c} = \det(W_{L}^{IL}) = \exp \left[ i \int_{\Sigma} d\mathbf{S} \cdot \text{tr} (B^{LR}) \right],
\]

(7)

where \( \Sigma \) is a surface with the boundary \( \partial \Sigma = L \), and taking determinant makes the path order irrelevant. This relation says that \( \det(W_{L}^{IL}) \) measures the total magnetic flux through the surface \( \Sigma \). For Eq. (7) to hold, it requires \( A^{LR} \) to be well defined everywhere on the surface \( \Sigma \). Note that \( \text{tr} (B^{LR}) \) is complex in general. For a boundaryless \( \Sigma \), the Chern number can be defined as

\[
C_{\Sigma} = \frac{1}{2\pi} \Re \int_{\Sigma} d\mathbf{S} \cdot \text{tr} (B^{LR}).
\]

(8)

The Berry curvature \( B^{RL} \) will give rise to the same \( C_{\Sigma} \). Like the Hermitian case, \( C_{\Sigma} \) must be integer. It follows from Eq. (7), that \( \gamma_L \) is defined up to multiples of \( 2\pi \), and that for boundaryless surface \( \gamma \partial \Sigma = \gamma_{0} = 0 \). Whether the imaginary part of the Berry curvature contains any topological information is unclear to us at this moment.

It is useful to have a discrete expression of \( W_{P}^{\alpha\beta} \) for numerical purpose. Let us discretize the path \( P : k_{f} \leftarrow k_{i} \) into \( M \) small segments, with the middle points being \( k_{1}, k_{2}, \ldots, k_{M-1} \) and \( \Delta k_{s} = k_{s+1} - k_{s} \) being infinitesimal. We take \( k_{0} \equiv k_{i} \) and \( k_{M} \equiv k_{f} \). Then, the Wilson line can be computed as

\[
W_{P}^{\alpha\beta} = \lim_{M \to \infty} e^{-\Delta k_{1} A^{\alpha\beta}(k_{1})} \cdots e^{-\Delta k_{M-1} A^{\alpha\beta}(k_{M-1})} e^{-\Delta k_{0} A^{\alpha\beta}(k_{0})}
\]

(9)

\[
= \lim_{M \to \infty} \prod_{s=0}^{M-1} \left[ I - \Delta k_{s} A^{\alpha\beta}(k_{s}) \right]
\]

\[
\equiv \lim_{M \to \infty} \prod_{s=0}^{M-1} W_{k_{s+1} \leftarrow k_{s}}^{\alpha\beta}
\]

where, in the second line, we have used the approximation \( \exp \left[ -\Delta k A^{\alpha\beta}(k) \right] = I - A^{\alpha\beta}(k)\Delta k + O(\Delta k^{2}) \). For the infinitesimal segment \( k_{s+1} \leftarrow k_{s} \), the Wilson line can be expressed as

\[
W_{k_{s+1} \leftarrow k_{s}}^{\alpha\beta} = \delta_{mn} - \Delta k_{s} A^{\alpha\beta}_{mn}(k_{s})
\]

(10)

\[
= \delta_{mn} - \langle \Psi_{\alpha,n}(k_{s+1})|\partial_{k}|\Psi_{\beta,n}(k_{s}) \rangle
\]

\[
= \delta_{mn} - \langle \Psi_{\alpha,n}(k_{s+1})|(|\Psi_{\beta,n}(k_{s+1})\rangle - |\Psi_{\beta,n}(k_{s})\rangle)
\]

where the biorthonormal condition is used to achieve the last line. This is a numerically friendly expression.

## II. WILSON LOOP AND CHERN NUMBER WITH NON-HermitIAN SYMMETRY

Here we discuss Wilson loops and Chern number in the presence of a unitary non-Hermitian spatial symmetry \( G \), which maps momentum \( k \) to \( gk \). Again, consider \( N \) bands that are separated from other bands on the paths, loops or surfaces under consideration. Let \( \{|\Psi_{L,n}(k)\rangle\} \) and \( \{|\Psi_{R,n}(k)\rangle\} \) be the biorthonormal left and right eigenvectors of \( H(k) \). As discussed in the main text, \( \bar{G}|\Psi_{R,n}(k)\rangle \) and \( G|\Psi_{L,n}(k)\rangle \) are the left and right eigenstates of \( H(gk) \) with
eigenenergy being \( E_\tilde{n}(g k) = E_n(k)^* \), where \( \tilde{n} \) is the corresponding band index. We note that the set of degenerate bands indexed by \( \tilde{n} \) is not necessarily the same as those indexed by \( n \). We expand \( \mathcal{G}|\Psi_{R,n}(k)\rangle \) and \( \mathcal{G}|\Psi_{L,n}(k)\rangle \) in the energy eigenstates \( \{|\Psi_{L,\tilde{n}}(g k)\rangle\} \) and \( \{|\Psi_{R,\tilde{n}}(g k)\rangle\} \):

\[
\mathcal{G}|\Psi_{R,n}(k)\rangle = \sum_{\tilde{n}} |\Psi_{L,\tilde{n}}(g k)\rangle S_{g,R}^{\tilde{n}n}(k),
\]

\[
\mathcal{G}|\Psi_{L,n}(k)\rangle = \sum_{\tilde{n}} |\Psi_{R,\tilde{n}}(g k)\rangle S_{g,L}^{\tilde{n}n}(k).
\]

where the sewing matrices are given by \( S_{g,\alpha}^{\tilde{n}n}(k) = \langle \Psi_{\alpha,\tilde{n}}(g k)|\Psi_{\alpha,n}(k)\rangle \), with \( \alpha = L, R \). Due to the unitarity of \( \mathcal{G} \), \( \mathcal{G}^\dagger \mathcal{G} = 1 \), the sewing matrix \( S_{g,\alpha}(k) \) satisfies the following relation

\[
S_{g,\alpha}(k)S_{g,\alpha}^\dagger(k) = S_{g,\alpha}(k)S_{g,\alpha}^\dagger(k) = 1,
\]

for any \( \alpha \) and \( k \), where we have introduced the notation \( \tilde{L} = R, \tilde{R} = L \), and \( I \) is the \( N \times N \) identity matrix.

To investigate how the non-Hermitian symmetry relates different Wilson lines, we use the discrete expression Eq. (9). The Wilson line on the infinitesimal segment \( k_{s+1} \rightarrow k_s \) satisfies the following relation

\[
\mathcal{W}_{k_{s+1} \rightarrow k_s}^{\alpha\tilde{\alpha}} = \langle \Psi_{\alpha,\tilde{n}}(g k_{s+1})|\Psi_{\alpha,n}(g k_s)\rangle S_{g,\alpha}(k_s) = \left[S_{g,\alpha}(k_{s+1}) S_{g,\alpha}^\dagger(g k_{s+1} \rightarrow g k_s) S_{g,\alpha}(k_s) \right]_{mn},
\]

where \( \mathcal{W}_{k_{s+1} \rightarrow k_s}^{\alpha\tilde{\alpha}} \) denotes the Wilson line associated with the bands indexed by \( \tilde{n} \). It can be more compactly written as \( \mathcal{W}_{k_{s+1} \rightarrow k_s}^{\alpha\tilde{\alpha}} = S_{g,\alpha}^\dagger(k_{s+1})G_{g,k_s}^{\alpha\tilde{\alpha}}S_{g,\alpha}(k_s) \). Inserting this relation into (9) for a general path \( P : k_f \leftarrow k_i \) and using (12), we immediately obtain

\[
\mathcal{W}_P^{\alpha\tilde{\alpha}} = S_{g,\alpha}(k_f)S_{g,\alpha}^\dagger(k_i).
\]

where \( gP : g k_f \leftarrow g k_i \) is the image of the path \( P \) under the action of \( \mathcal{G} \).

Considering Wilson observables on a closed loop \( \mathcal{L} : k_0 \leftarrow k_0 \), we have

\[
e^{a_{g\mathcal{L}} + i\gamma_{g\mathcal{L}}} = \det \left(W^L_{\mathcal{L}} \right) = \det \left(S_{g,\alpha}(k_0)S_{g,R}(k_0)\right) = \det \left(\tilde{W}^R_{g\mathcal{L}}\right) = e^{-a_{g\mathcal{L}} - i\gamma_{g\mathcal{L}}}
\]

Accordingly,

\[
\bar{a}_{g\mathcal{L}} = -a_{g\mathcal{L}}, \quad \hat{\gamma}_{g\mathcal{L}} = \gamma_{g\mathcal{L}}.
\]

Note that the bands indexed by \( n \) and \( \tilde{n} \) may be the same (which is the case in the exceptional unconventional Weyl semimetal example), so are the quantities in the above relations. Taking the loop \( \mathcal{L} \) to be infinitesimally small, we immediately have that the Berry curvature satisfies

\[
\text{tr} \left(B^{\alpha\tilde{\alpha}}(k)\right) = \sigma(g) \text{tr} \left(\tilde{B}^{\alpha\tilde{\alpha}}(g k)\right)^*.
\]

where \( \sigma(g) = 1 \) or \(-1\) denotes if \( \mathcal{G} \) is orientation-preserving or orientation-reversing. This further leads to that the Chern numbers satisfy \( C_{g\Sigma} = C_{\Sigma} \), for any boundaryless surface \( \Sigma \). If \( \Sigma \) is \( g \Sigma \) are homotopy equivalent up to orientation (i.e., can be continuously deformed to each other without sweeping through degenerate regions), we must have \( C_{g\Sigma} = \sigma(g)C_{\Sigma} \). Combining the two relations, we have \( C_{\Sigma} = 0 \) if \( \sigma(g) = -1 \).

III. RELATION BETWEEN \( W(k_{EP}) \) AND \( W(gk_{EP}) \)

Here we prove the relation Eq. (14) in the main text. First consider the case that \( \mathcal{G} \) is a non-Hermitian symmetry. According to the definition Eq. (13) in the main text, the winding numbers \( W(k_{EP}) \) and \( W(gk_{EP}) \) are given by

\[
W(k_{EP}) = \oint_{S^3} \frac{dk}{2\pi i} \cdot \nabla_k \log \det [\mathcal{H}(k) - E(k_{EP})]
\]

\[
W(gk_{EP}) = \oint_{S^3} \frac{dk}{2\pi i} \cdot \nabla_k \log \det [\mathcal{H}(k) - E(gk_{EP})]
\]
where $S_1^a$ is a loop encircling the exceptional line at $k_{EP}$ and $S_1^b$ is a loop encircling the exceptional line at $gk_{EP}$. Let us perform a change of variable $k = gk'$. Then,

$$W(gk_{EP}) = \oint_{S_1^a} \frac{d(gk')}{2\pi i} \cdot \nabla_{gk'} \log \det [\mathcal{H}(gk') - E(gk_{EP})]$$

$$= \oint_{S_1^b} \frac{dk'}{2\pi i} \cdot \nabla_{k'} \log \det [G\mathcal{H}^\dagger(k')G^{-1} - E^*(k_{EP})]$$

$$= \oint_{S_1^a} \frac{dk'}{2\pi i} \cdot \nabla_{k'} \log \det [\mathcal{H}^\dagger(k') - E^*(k_{EP})]$$

$$= -\sigma(S_1^a, S_1^b)W(k_{EP}), \quad (20)$$

where $S_1^a$ is a loop encircling the exceptional line at $k_{EP}$ such that it is mapped to $S_1^b$ under the action of the spatial symmetry $G$. In the second line, we have used Eq. (2) in the main text for non-Hermitian spatial symmetry and the relation $E(gk_{EP}) = E^*(k_{EP})$. The transformation matrix $g$ in $d(gk')$ cancels that in $\nabla_{gk'}$. In the last line, the minus sign follows from the Hermitian conjugation. The factor $\sigma(S_1^a, S_1^b)$ is real. The non-Hermitian term $i\lambda \sigma_3$ can be absorbed by $M(k)$. For two-band models, it suffices to employ Pauli matrices for discussion. Under the $C_{4z}$ rotation operation, the Pauli matrices transform as

$$C_{4z} \sigma_1 C_{4z}^{-1} = -\sigma_1, \quad C_{4z} \sigma_2 C_{4z}^{-1} = -\sigma_2, \quad C_{4z} \sigma_3 C_{4z}^{-1} = +\sigma_3. \quad (24)$$

It can be seen $\sigma_3$ is the only Hermitian symmetry-allowed term. A Hermitian $\lambda \sigma_3$ term can be absorbed by $M(k_x, k_y)$ in the model Hamiltonian of Eq. (22).

Next, we focus on non-Hermitian symmetry-allowed constant terms denoted by $i\lambda \sigma$. Here $\lambda$ is real. The non-Hermitian $C_{4z}$ symmetry allowed terms are

$$C_{4z}(i\lambda \sigma)C_{4z}^{-1} = (i\lambda \sigma)^\dagger: \quad \sigma = \sigma_1, \quad \sigma_2. \quad (25)$$

Thus, apart from $i\lambda \sigma_1$ discussed in the main text, $i\lambda \sigma_2$ is also a non-Hermitian $C_{4z}$ symmetry allowed non-Hermitian term. As shown in Fig. 1 (a), this term has a same effect as $i\lambda \sigma_1$ in the main text.

It should be noted that even though the non-Hermitian term $i\lambda \sigma_3$ does not respect non-Hermitian $C_{4z}$ symmetry, it respects the Hermitian $C_{4z}$ symmetry. The symmetry relation is given by

$$C_{4z}(i\lambda \sigma_3)C_{4z}^{-1} \neq (i\lambda \sigma_3)^\dagger, \quad C_{4z}(i\lambda \sigma_3)C_{4z}^{-1} = (i\lambda \sigma_3). \quad (26)$$

IV. SYMMETRIES IN EXCEPTIONAL UNCONVENTIONAL WEYL SEMIMETALS

In this section, we discuss the symmetries and symmetry-allowed non-Hermitian terms in the example of exceptional unconventional Weyl semimetals. Without the non-Hermitian term, the Hamiltonian reads

$$\mathcal{H}(k) = 2A(\cos k_x - \cos k_y)\sigma_1 + 2A \sin k_x \sin k_y \sigma_2 + [M(k_x, k_y) - 2t_z \cos k_z]\sigma_3. \quad (22)$$

where $M(k_x, k_y) = M_0 - 2t_1(\cos k_x + \cos k_y)$. The Hamiltonian respects the fourfold rotation symmetry about the $k_z$ axis,

$$C_{4z} \mathcal{H}(k) C_{4z}^{-1} = \mathcal{H}(R_{4z}k): \quad C_{4z} = \sigma_3, \quad \text{and} \quad R_{4z}(k_x, k_y, k_z) = (k_y, -k_x, k_z). \quad (23)$$

We will analyze all symmetry-allowed constant perturbations to $\mathcal{H}(k)$. For two-band models, it suffices to employ Pauli matrices for discussion. Under the $C_{4z}$ rotation operation, the Pauli matrices transform as

$$C_{4z} \sigma_1 C_{4z}^{-1} = -\sigma_1, \quad C_{4z} \sigma_2 C_{4z}^{-1} = -\sigma_2, \quad C_{4z} \sigma_3 C_{4z}^{-1} = +\sigma_3. \quad (24)$$

It can be seen $\sigma_3$ is the only Hermitian symmetry-allowed term. A Hermitian $\lambda \sigma_3$ term can be absorbed by $M(k_x, k_y)$ in the model Hamiltonian of Eq. (22).

Next, we focus on non-Hermitian symmetry-allowed constant terms denoted by $i\lambda \sigma$. Here $\lambda$ is real. The non-Hermitian $C_{4z}$ symmetry allowed terms are

$$C_{4z}(i\lambda \sigma)C_{4z}^{-1} = (i\lambda \sigma)^\dagger: \quad \sigma = \sigma_1, \quad \sigma_2. \quad (25)$$

Thus, apart from $i\lambda \sigma_1$ discussed in the main text, $i\lambda \sigma_2$ is also a non-Hermitian $C_{4z}$ symmetry allowed non-Hermitian term. As shown in Fig. 1 (a), this term has a same effect as $i\lambda \sigma_1$ in the main text.

It should be noted that even though the non-Hermitian term $i\lambda \sigma_3$ does not respect non-Hermitian $C_{4z}$ symmetry, it respects the Hermitian $C_{4z}$ symmetry. The symmetry relation is given by

$$C_{4z}(i\lambda \sigma_3)C_{4z}^{-1} \neq (i\lambda \sigma_3)^\dagger, \quad C_{4z}(i\lambda \sigma_3)C_{4z}^{-1} = (i\lambda \sigma_3). \quad (26)$$
Figure 1. (a) The exceptional structure from the non-Hermitian $i\lambda \sigma_2$, which respects the non-Hermitian $C_{4z}$ symmetry. It is equivalent to $i\lambda \sigma_1$ discussed in the main text. The lower panel shows the contour plots of the real and imaginary parts at $\delta k_z = 0$. (b) The non-Hermitian term $i\lambda \sigma_3$ turns the unconventional Weyl points to exceptional rings. This term breaks the non-Hermitian $C_{4z}$ symmetry, but it respects the Hermitian $C_{4z}$ symmetry. The lower panel shows the contour plots at $\delta k_x = 0$. The parameters are the same as the main text.

As shown in Fig. 1 (b), this non-Hermitian term turns a Weyl point into an exceptional ring. It can also be explained by the effective theory around the original Weyl points. After the inclusion of $i\lambda \sigma_3$, the effective Hamiltonian becomes

$$H_{\text{eff}}(\mathbf{K}+\delta \mathbf{k}) \approx (\delta k_y^2-\delta k_x^2)\sigma_1 + 2\delta k_x\delta k_y\sigma_2 + \delta k_z\sigma_3 + i\lambda\sigma_3$$

(27)

Around the original Weyl point, i.e., $\delta k_z = 0$, the exceptional structure is determined by $(\delta k_y^2-\delta k_x^2)^2 + (2\delta k_x\delta k_y)^2 - \lambda^2 = 0$. This yields $\delta k_x^2 + \delta k_y^2 = |\lambda|$, which is a ring. The exceptional structure is also symmetric with respect to $C_{4z}$ symmetry, as shown in Fig. 1 (b). This can be seen by the two exceptional points encircled by $\tilde{S}^1$ and $S^1$, their corresponding winding number satisfies Hermitian symmetry relation.

Finally, we show in detail the transition from system with the non-Hermitian $C_{4z}$ symmetry to that with Hermitian $C_{4z}$, by introducing a $\delta H = i\lambda[(1-\eta)\sigma_1 + \eta\sigma_3]$ term,

$$H_{\text{w'}}(\mathbf{k}) = H_{\text{w}}(\mathbf{k}) + i\lambda[(1-\eta)\sigma_1 + \eta\sigma_3].$$

(28)

At $\eta = 0$, the system respects the non-Hermitian $C_{4z}$ symmetry, while at $\eta = 1$, the system respects the Hermitian $C_4$ symmetry. In between, i.e., $0 < \eta < 1$, both Hermitian and non-Hermitian symmetries are broken. The evolution of exceptional manifolds against $\eta$ is shown in Fig. 2. Clearly, for both Hermitian and non-Hermitian symmetries, the exceptional structure preserves the $C_{4z}$ symmetry. While in between, the exceptional structure is not $C_{4z}$-symmetric.

Figure 2. The detail of evolution of exceptional manifold against $\eta$, in the transition between non-Hermitian $C_{4z}$ symmetry and Hermitian $C_{4z}$ symmetry.

The exceptional manifold at $\eta = 0$ is explicitly protected by the non-Hermitian $C_{4z}$ symmetry. This can be seen by introducing a small $\eta$ to break the symmetry. To be concrete, we focus on how the termination point $\mathbf{K}_j$ joined by ELs, as shown by red circle in Fig. 2, is broken by the perturbation. The perturbed Hamiltonian around the termination point $\mathbf{K}_j = (0,0,\lambda)$ can be approximated by

$$H_{\text{eff}}(\mathbf{K}_j+\delta \mathbf{k}) \approx (\delta k_y^2-\delta k_x^2)\sigma_1 + 2\delta k_x\delta k_y\sigma_2 + (\lambda + \delta k_z)\sigma_3 + i\lambda\sigma_1 + i\varepsilon\sigma_3.$$  

(29)
Here $\varepsilon = 0^+$. Using the characteristic polynomial, we find the exceptional manifold is determined by
\[
(\delta k_x^2 + \delta k_y^2)^2 + (\delta k_z + \lambda)^2 - (\varepsilon^2 + \lambda^2) = 0,
\]
\[
\lambda(\delta k_x^2 - \delta k_y^2) - \varepsilon(\delta k_z + \lambda) = 0. \tag{30}
\]
We find that the symmetry breaking term $\varepsilon$, if non-vanishing, breaks the termination point $K_j$, joined by ELs. This can be seen by the second equation above. For $\varepsilon = 0$, when the non-Hermitian symmetry is respected, on the $k_z$ axis, $\delta k_x^2 - \delta k_y^2 = 0$ yields just one point, i.e., $\delta k_x = \delta k_y = 0$, which respects the symmetry. However, for non-zero $\varepsilon$, on the $k_z$ axis, $\delta k_x = \delta k_y = 0$ as required by the $C_{4z}$ symmetry can no longer be achieved any more. Thus, the ELs can not join the termination point on the $k_z$ axis.

V. SYMMETRIES IN EXCEPTIONAL TRIPLE-POINT SEMIMETALS

Without the non-Hermitian term, the original triple-point semimetal Hamiltonian reads,
\[
\mathcal{H}_0'(k) = \begin{pmatrix}
\alpha k_x & \beta k_z & -\beta k_y \\
\beta k_z & -\alpha k_x & 0 \\
-\beta k_y & 0 & -\alpha k_x
\end{pmatrix}. \tag{31}
\]
This Hamiltonian is invariant under fourfold rotation symmetry about $x$ axis, mirror symmetry about $xz$ plane, and the combination of space-inversion and time-reversal symmetry
\[
C_{4z}\mathcal{H}_0'(k)C_{4z}^{-1} = \mathcal{H}_0'(R_{4z}k), \\
\mathcal{M}_{xz}\mathcal{H}_0'(k)\mathcal{M}_{xz}^{-1} = \mathcal{H}_0'(M_{xz}k), \\
\mathcal{PT}\mathcal{H}_0'(k)(\mathcal{PT})^{-1} = \mathcal{H}_0'(k). \tag{32-34}
\]
The symmetry operators are
\[
C_{4z} = \begin{pmatrix}
-1 & 0 & 0 \\
0 & 0 & 1 \\
0 & -1 & 0
\end{pmatrix}, \quad R_{4x} : (k_x, k_y, k_z) \rightarrow (k_x, -k_z, k_y), \\
M_{xz} = \begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & -1
\end{pmatrix}, \quad M_{xz} : (k_x, k_y, k_z) \rightarrow (k_x, -k_y, k_z), \\
\mathcal{PT} = \begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix} \mathcal{K}, \quad \mathcal{PT} : (k_x, k_y, k_z) \rightarrow (k_x, k_y, k_z). \tag{35-37}
\]
Here $\mathcal{K}$ is the complex conjugation operation.

In order to discuss symmetry-allowed terms, we employ the $3 \times 3$ Gell-Mann matrices in the following form,
\[
\Lambda_1 = \begin{pmatrix}
0 & 1 & 0 \\
1 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}, \quad \Lambda_2 = \begin{pmatrix}
0 & -i & 0 \\
i & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}, \quad \Lambda_3 = \begin{pmatrix}
1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & 0
\end{pmatrix}, \quad \Lambda_4 = \begin{pmatrix}
0 & 0 & 1 \\
0 & 0 & 0 \\
0 & 1 & 0
\end{pmatrix}, \tag{38}
\]
\[
\Lambda_5 = \begin{pmatrix}
0 & 0 & -i \\
0 & 0 & 0 \\
i & 0 & 0
\end{pmatrix}, \quad \Lambda_6 = \begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & 1 \\
0 & 1 & 0
\end{pmatrix}, \quad \Lambda_7 = \begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & -i \\
i & 0 & 0
\end{pmatrix}, \quad \Lambda_8 = \begin{pmatrix}
1 & 0 & 0 \\
0 & \frac{1}{\sqrt{3}} & 0 \\
0 & 0 & -\frac{2}{\sqrt{3}}
\end{pmatrix}. \tag{39}
\]
We investigate how the Gell-Mann matrices transform under each symmetry operation as follows.

(1) Under $C_{4z}$ operation, the Gell-Mann matrices can be separated into 3 groups, which reads
\[
\{C_{4z}\Lambda_1C_{4z}^{-1} = \Lambda_4, \quad C_{4z}\Lambda_2C_{4z}^{-1} = -\Lambda_1\}, \quad \{C_{4z}\Lambda_3C_{4z}^{-1} = \Lambda_5, \quad C_{4z}\Lambda_5C_{4z}^{-1} = -\Lambda_2\}, \\
\{C_{4z}\Lambda_3C_{4z}^{-1} = \frac{1}{2}(\Lambda_3 + \sqrt{3}\Lambda_8), \quad C_{4z}\Lambda_3C_{4z}^{-1} = \frac{1}{2}(\sqrt{3}\Lambda_3 - \Lambda_8)\}, \\
\{C_{4z}\Lambda_6C_{4z}^{-1} = -\Lambda_6\}, \quad \{C_{4z}\Lambda_7C_{4z}^{-1} = \Lambda_7\}. \tag{40}
\]
(2) Under $M_{xz}$ operation, the Gell-Mann matrices transforms as
\[
\{M_{xz}\Lambda_1M^{-1}_{xz} = \Lambda_1, \ M_{xz}\Lambda_2M^{-1}_{xz} = \Lambda_2, \ M_{xz}\Lambda_3M^{-1}_{xz} = \Lambda_3, \ M_{xz}\Lambda_8M^{-1}_{xz} = \Lambda_8\},
\]
\[
\{M_{xz}\Lambda_4M^{-1}_{xz} = -\Lambda_4, \ M_{xz}\Lambda_5M^{-1}_{xz} = -\Lambda_5, \ M_{xz}\Lambda_6M^{-1}_{xz} = -\Lambda_6, \ M_{xz}\Lambda_7M^{-1}_{xz} = -\Lambda_7\}. \quad (41)
\]

(3) Under $\mathcal{PT}$ operation, the Gell-Mann matrices transforms as
\[
\{\mathcal{PT}\Lambda_1(\mathcal{PT})^{-1} = \Lambda_1, \ \mathcal{PT}\Lambda_3(\mathcal{PT})^{-1} = \Lambda_3, \ \mathcal{PT}\Lambda_4(\mathcal{PT})^{-1} = \Lambda_4, \ \mathcal{PT}\Lambda_6(\mathcal{PT})^{-1} = \Lambda_6, \ \mathcal{PT}\Lambda_8(\mathcal{PT})^{-1} = \Lambda_8\},
\]
\[
\{\mathcal{PT}\Lambda_2(\mathcal{PT})^{-1} = -\Lambda_2, \ \mathcal{PT}\Lambda_5(\mathcal{PT})^{-1} = -\Lambda_5, \ \mathcal{PT}\Lambda_7(\mathcal{PT})^{-1} = -\Lambda_7\}. \quad (42)
\]

**Hermitian symmetry-allowed terms**: Before discussing the non-Hermitian symmetries, we first investigate conventional Hermitian symmetries. We focus on the Hermitian constant terms denoted as $\lambda\Lambda$ that are invariant under the symmetry operation.

The $C_{4x}$ symmetry-allowed terms are
\[
C_{4x}(\lambda\Lambda)(k)C_{4x}^{-1} = (\lambda\Lambda) : \quad \Lambda = \left(\sqrt{3}\Lambda_3 + \Lambda_8\right), \Lambda_7. \quad (43)
\]

The $M_{xz}$ symmetry-allowed terms are
\[
M_{xz}(\lambda\Lambda)M_{xz}^{-1} = (\lambda\Lambda) : \quad \Lambda = \Lambda_1, \Lambda_2, \Lambda_3, \Lambda_8. \quad (44)
\]

The $\mathcal{PT}$ symmetry-allowed terms are
\[
\mathcal{PT}(\lambda\Lambda)(\mathcal{PT})^{-1} = (\lambda\Lambda) : \quad \Lambda = \Lambda_1, \Lambda_3, \Lambda_4, \Lambda_6, \Lambda_8. \quad (45)
\]

By comparing Eqs. (43), (44), and (45), we can find just one term that respects all the symmetries.
\[
\Lambda = \left(\sqrt{3}\Lambda_3 + \Lambda_8\right). \quad (46)
\]

Such a term, however, just shifts the location of the triple point on $k_x$ axis. This can be seen by expressing the Hamiltonian in terms of Gell-Mann matrices,
\[
\mathcal{H}_0(k) = \begin{pmatrix}
\alpha k_x & \beta k_x & -\beta k_y \\
\beta k_x & -\alpha k_x & 0 \\
-\beta k_y & 0 & -\alpha k_x
\end{pmatrix} = -\frac{1}{3}\alpha k_x I + \frac{\alpha}{\sqrt{3}} k_x \left(\sqrt{3}\Lambda_3 + \Lambda_8\right) - \beta k_y \Lambda_4 + \beta k_z \Lambda_1. \quad (47)
\]

After the inclusion of symmetry-allowed term, the Hamiltonian becomes
\[
\mathcal{H}_0(k) + \lambda\Lambda = -\frac{1}{3}\alpha k_x I + \frac{\alpha}{\sqrt{3}} (k_x + \lambda) \left(\sqrt{3}\Lambda_3 + \Lambda_8\right) - \beta k_y \Lambda_4 + \beta k_z \Lambda_1. \quad (48)
\]

Thus, the Hermitian symmetry-allowed term just shifts the location of the triple point in momentum space.

**Non-Hermitian symmetry-allowed terms**: We now turn to the non-Hermitian spatial symmetries. Consider the symmetry-allowed non-Hermitian terms in the form of $(i\lambda\Lambda)$, with $\lambda$ real and $\Lambda$ Hermitian. Note that the following relation
\[
(i\lambda\Lambda)^\dagger = -i\lambda\Lambda, \quad (49)
\]
will be used together with symmetry operations in Eqs. (40), (41), and (42).

The non-Hermitian $C_{4x}$ symmetry-allowed terms are
\[
C_{4x}(i\lambda\Lambda)C_{4x}^{-1} = (i\lambda\Lambda)^\dagger : \quad \Lambda = \left(\Lambda_3 - \sqrt{3}\Lambda_8\right), \Lambda_6. \quad (50)
\]

The non-Hermitian $M_{xz}$ symmetry-allowed terms are
\[
M_{xz}(i\lambda\Lambda)M_{xz} = (i\lambda\Lambda)^\dagger : \quad \Lambda = \Lambda_4, \Lambda_5, \Lambda_6, \Lambda_7. \quad (51)
\]

The non-Hermitian $\mathcal{PT}$ symmetry-allowed terms are
\[
\mathcal{PT}(i\lambda\Lambda)(\mathcal{PT})^{-1} = (i\lambda\Lambda)^\dagger : \quad \Lambda = \Lambda_1, \Lambda_3, \Lambda_4, \Lambda_6, \Lambda_8. \quad (52)
\]
By comparing Eqs. (50), (51), and (52), there is only one non-Hermitian symmetry allowed term, namely,

$$\Lambda = \Lambda_6.$$  

(53)

With the inclusion of this term, the full Hamiltonian becomes

$$\mathcal{H}^t(k) = \mathcal{H}_0^t + i\lambda \Lambda_6$$  

(54)

$$= \begin{pmatrix} \alpha k_x & \beta k_z & -\beta k_y \\ \beta k_z & -\alpha k_x & 0 \\ -\beta k_y & 0 & -\alpha k_x \end{pmatrix} + i\lambda \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$  

(55)

which satisfies all the non-Hermitian symmetries

$$C_{4x} \mathcal{H}^t(k) C_{4x}^{-1} = \mathcal{H}^t(R_{4x} k) \dagger,$$  

(56)

$$M_{xz} \mathcal{H}^t(k) M_{xz}^{-1} = \mathcal{H}^t(M_{xz} k) \dagger,$$  

(57)

$$PT \mathcal{H}^t(k) (PT)^{-1} = \mathcal{H}^t(k) \dagger.$$  

(58)

VI. EXPERIMENTAL REALIZATION IN COLD ATOMS

Here we present the scheme details for realizing the model Hamiltonian in the main text using cold atoms, as shown in Fig. 3. We choose two atomic internal states as pseudo-spins, and load the atoms trapped in a two-dimensional optical lattice. We consider the following Hamiltonian composed of three parts,

$$H = H_1 + H_2 + H_3.$$  

(59)

Figure 3. Illustration of the setups for the model Hamiltonian. The $A_1$ and $t_{3,0}$ terms are generated via optical fields (61). The $A_2$ terms originate from the natural nearest-neighbor hopping by making the operator transformation (71). The $\lambda$ term is introduced by the on-site atomic decay.

The first part of Hamiltonian (59) describes the spin-orbit coupling [1],

$$H_1 = \int dr M(r) \psi_{\uparrow}(r) \psi_{\downarrow}(r) + H.c.$$  

(60)

It is generated by three optical fields that couple the two pseudo-spins,

$$M(r) = M_1(r) + M_2(r) + M_3(r),$$  

(61)

whose spatial modulations are prepared as

$$M_1(r) = i M_1 \sin(k_L x) \sin(k_L y),$$  

(62)

$$M_2(r) = M_2 \cos(k_L x) \cos(3k_L y) - \cos(3k_L x) \cos(k_L y),$$  

(63)

$$M_3(r) = M_3 \cos(2k_L x) \cos(2k_L y).$$  

(64)
Here \( k_L = \pi/d \) and \( d \) denotes the optical lattice constant. \( M_{1,2,3} \) denotes the corresponding field strength. We expand the Hamiltonian in terms of Wannier wave-function \( W(r) \). The field modes \( M_{1,2,3}(r) \) give rise to the following results: (i) Due to the odd parity of \( M_1(r) \) in the \( x-y \) plane, the on-site and nearest-neighbor coupling terms introduced by \( M_1(r) \) vanish, leaving the next-nearest-neighbor term dominant. (ii) As the system is homogeneous in the \( x-y \) plane, the on-site coupling term introduced by \( M_2(r) \) vanishes [2], leaving the nearest-neighbor term dominant. (iii) \( M_3(r) \) does not introduce nonlocal coupling because of the orthogonality of \( W(r) \) on different sites. Based on the aforementioned results, \( H_1 \) in the tight-binding approximation is expressed as

\[
H_1 = \sum_j (-1)^{j_x+j_y} \left[ i M_1 (-c_{j+\hat{e}_x}^\dagger c_{j} + c_{j+\hat{e}_x}^\dagger c_{j-\hat{e}_x} + c_{j+\hat{e}_y}^\dagger c_{j} + c_{j+\hat{e}_y}^\dagger c_{j-\hat{e}_y}) + M_2 (c_{j+\hat{e}_x} c_{j} + c_{j-\hat{e}_x} c_{j} - c_{j+\hat{e}_y} c_{j} - c_{j-\hat{e}_y} c_{j}) + M_3 c_{j+\hat{e}_x} c_{j+\hat{e}_y} \right] + H.c. \tag{65}
\]

where \( \hat{e}_{x,y} \) denotes the unit vector and \( j_x \) and \( j_y \) respectively denote the \( x \)- and \( y \)-directional index of the \( j \)-th site, and

\[
M_1 = \int M_1 \sin(k_L x) \sin(k_L y) W^*(r + d\hat{e}_x + d\hat{e}_y) W(r) \, dr \tag{66}
\]

\[
M_2 = \int M_2 \cos(k_L x) \cos(3k_L y) - \cos(3k_L x) \cos(k_L y) W^*(r + d\hat{e}_x) W(r) \, dr \tag{67}
\]

\[
M_3 = \int M_3 \cos(2k_L x) \cos(2k_L y) |W(r)|^2 \, dr \tag{68}
\]

The second part of Hamiltonian (59) describes the natural nearest-neighbor hopping,

\[
H_2 = -\sum_{j,\nu} J (c_{j+\hat{e}_x,\nu}^\dagger c_{j,\nu} + c_{j+\hat{e}_y,\nu}^\dagger c_{j,\nu} + H.c.) \tag{69}
\]

where \( J \) is the hopping magnitude.

The last part of Hamiltonian (59) describes the on-site atomic decay,

\[
H_3 = i\lambda \sigma_3 . \tag{70}
\]

A recent advance in cold atoms [3] shows the experimental feasibility for engineering spin-dependent decays using the auxiliary level transition.

We make the following transformation,

\[
c_{j+} \to (-1)^{j_x} c_{j+}, \quad c_{j-} \to (-1)^{j_x} c_{j-} . \tag{71}
\]

Under Eq.(71), the factor \((-1)^{j_x+j_y} \) in \( H_1 \) is eliminated and \( H_1 \) is rewritten as

\[
H_1 = \sum_j \left[ i M_1 (c_{j+\hat{e}_x+\hat{e}_y}^\dagger c_{j} + c_{j+\hat{e}_x+\hat{e}_y} c_{j} - c_{j+\hat{e}_x+\hat{e}_y+\hat{e}_x}^\dagger c_{j+\hat{e}_y} - c_{j+\hat{e}_x+\hat{e}_y+\hat{e}_y} c_{j+\hat{e}_x}^\dagger c_{j+\hat{e}_y}^\dagger) - M_2 (c_{j+\hat{e}_x}^\dagger c_{j+\hat{e}_y} + c_{j-\hat{e}_x}^\dagger c_{j+\hat{e}_y} + c_{j+\hat{e}_x} c_{j} + c_{j-\hat{e}_x} c_{j}) + M_3 c_{j+\hat{e}_y} c_{j+\hat{e}_y} \right] + H.c. \tag{72}
\]

\( H_2 \) is transformed to

\[
H_2 = -\sum_j \sum_{\nu\nu'} J[\sigma_z]_{\nu\nu'} (-c_{j+\hat{e}_x,\nu}^\dagger c_{j,\nu} + c_{j+\hat{e}_y,\nu}^\dagger c_{j,\nu} + H.c.) . \tag{73}
\]

\( H_2 \) remains unchanged under Eq.(71). We make the following denotation

\[
2M_1 \equiv A_1 , \quad -J \equiv A_2 , \quad M_2 \equiv t_\parallel , \tag{74}
\]

and assign the strength \( M_3 \) with a tunable cyclical parameter \( \theta \) [4],

\[
M_3 = M_0 - 2t_\theta \cos(\theta) . \tag{75}
\]
Then the model Hamiltonian (59) is given as

\[ H(k) = 2A_2 [\cos(k_y d) - \cos(k_x d)] \sigma_3 + 2A_1 \sin(k_x d) \sin(k_y d) \sigma_2 \\
+ [M_0 - 2t || \cos(k_x d) - 2t || \cos(k_y d) - 2t \theta \cos(\theta)] \sigma_1 + i \lambda \sigma_3. \]  

(76)

which is illustrated in FIG.3. By tuning \( A_2 = A_1 = A \), and after recognizing \( \theta \) as \( k_z \) and making the transformation \( \sigma_3 \leftrightarrow \sigma_1 \), one can find that Eq.(76) is identical to the model Hamiltonian (15) in the main text.

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