Classification of Exceptional Nodal Topologies Protected by $\mathcal{PT}$ Symmetry

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Exceptional degeneracies, at which both eigenvalues and eigenvectors coalesce, and parity-time ($\mathcal{PT}$) symmetry, reflecting balanced gain and loss in photonic systems, are paramount concepts in non-Hermitian systems. We here complete the topological classification of exceptional nodal degeneracies protected by $\mathcal{PT}$ symmetry in up to three dimensions and provide simple example models whose exceptional nodal topologies include previously overlooked possibilities such as second-order knotted surfaces of arbitrary genus, third-order knots and fourth-order points.

I. INTRODUCTION

Parity-time ($\mathcal{PT}$) symmetric non-Hermitian (NH) descriptions were originally suggested as a fundamental amendment to the standard quantum mechanics motivated by their capacity of having real spectra [1, 2]. By now, NH models are instead recognized as effective descriptions with a remarkably wide range of applications [3], and $\mathcal{PT}$ symmetry is an ubiquitous feature of photonic experiments where it reflects a balance between gain and loss [4]. Exceptional point (EP) degeneracies at which both eigenvalues and eigenvectors coalesce is a central and uniquely NH feature associated with a rich phenomenology in these systems [5]. Recently, the merger between topological [6, 7] and NH physics has led to the burgeoning field of NH topological systems [8].

The topological properties of NH nodal band structures, consisting of EPs, are central topic within this field [8]. EPs are topologically distinguished from Hermitian degeneracies in that they are generic in the bulk of two-dimensional (2D) systems [9–12], giving closed (potentially knotted) lines of EPs in 3D [13–19]. In general, EPs of order $n$ ($n$EPs) require the tuning of $2n - 2$ real parameters, resulting in their absence for $n \geq 3$ in systems of 3D or lower. The inclusion of discrete symmetries can, however, relax this constraint and make symmetry-protected 2EPs generic already in one dimension (1D), while rings and surfaces of 2EPs are stabilized in 2D and 3D, respectively [20–25]. These EPs are associated with open Fermi arc degeneracies in the real part of the spectrum with telltale signatures in experiments [9]. Very recently, it was shown that physically relevant symmetries can also stabilize higher-order EPs, and explicit examples of models with point-like 3EPs in 2D were explored [26, 27].

Here, we show that $\mathcal{PT}$ symmetry protects a remarkably rich family of nodal EP topologies in 3D.

By explicit construction, we below provide a classification thereof, including possibilities such as knotted surfaces of arbitrary genus of 2EPs, knotted lines of 3EPs and point-like 4EPs, cf. Figure 1 and Table I. All structures are generic and stable in the sense that they are indeed protected by $\mathcal{PT}$ symmetry; small
perturbations can destroy the EP topologies only if they break $\mathcal{PT}$. This points to their experimental relevance mainly in photonic systems where the $\mathcal{PT}$ can be realized with great precision and system parameters may be tuned with excellent control [4].

| Exceptional Nodal Topologies | Without $\mathcal{PT}$ | With $\mathcal{PT}$ |
|------------------------------|------------------------|-------------------|
| $D = 1$                      |                         | 2EPs              |
| $D = 2$                      | 2EPs                   | Lines of 2EPs     |
| $D = 3$                      | Knots of 2EPs          | Surfaces of 2EPs  |
|                              |                        | Knots of 3EPs     |
|                              |                        | 4EPs              |

Table I. The impact of $\mathcal{PT}$ symmetry on the exceptional nodal topologies in systems of physically relevant dimensions.

III. EXCEPTIONAL NODAL SURFACES

$\mathcal{PT}$ symmetry preserving anti-Hermitian terms split ordinary Hermitian points to exceptional rings in two-band systems [20]. Generalizing this reasoning to higher dimensions, nodal lines split to exceptional surfaces when exposed to similar perturbations. To demonstrate this, we first show that $\mathcal{PT}$ symmetry-protected nodal torus knots are split into exceptional knotted tori. Consider the following $\mathcal{PT}$-symmetric Hermitian Hamiltonian [31],

$$H_{(p,q)} = \text{Re}[\zeta^p(k_x, k_y, k_z) + \xi^q(k_x, k_y, k_z)] \sigma^x + \text{Im}[\zeta^p(k_x, k_y, k_z) + \xi^q(k_x, k_y, k_z)] \sigma^z,$$

(3)

where a $\sigma^y$-term is absent due to the symmetry. Here, $\zeta(k_x, k_y, k_z) = k_x + i k_y$, $\xi = k_z + i[M - (k_x^2 + k_y^2 + k_z^2)]$, $M \in \mathbb{R}$, $\sigma^i$ the Pauli matrices, and $k_i$ the lattice momentum components. Here, $p$ and $q$ are positive integers, and the corresponding nodal points form torus knots when $p$ and $q$ are relatively prime, and torus links otherwise. By adding a constant symmetry preserving anti-Hermitian term, resulting in the following Hamiltonian,

$$H = H_{(p,q)} + i \delta \sigma^y,$$

(4)

for $\delta \in \mathbb{R}$, the nodal knots are inflated to form second-order exceptional surfaces of knotted tori, displayed in Figs. 1(a), 2(a), and (b). This construction is however not restricted to torus knots, but is also applicable for the hyperbolic Turk’s head knots by following the construction in Ref. [17]. Details can be found in the online Supplemental Material [32].

Despite being topologically different, in the sense that the different knotted tori cannot be continuously deformed into each other, they are all different examples of embeddings of the regular torus into $\mathbb{R}^3$. Thus, the genus of a knotted torus is always 1— the genus is independent of the embedding. Since embeddings of 2D surfaces in 3D spaces are completely classified by the corresponding genus, we expect higher genus exceptional surfaces to appear as well. To this end, let us again consider the Hamiltonian in Eq. (4), and let $p = q = n$. The exceptional structure for $H$ consist of $n$ individually linked tori. When $\delta$ becomes large enough, the tori are merged together close to the origin of momentum space, and the exceptional structure attain the form of a sphere with $n$ handles, i.e., a genus $n$ surface. This is explicitly shown in Figs. 1(b) and 2(c) for $n = 2$ and $n = 3$, respectively, while higher genus examples are provided in the Supplemental Material [32]. Thus,
it is possible to obtain second-order exceptional surfaces with any genus. These surfaces are furthermore generic and stable, in the sense that they are protected by $\mathcal{PT}$ symmetry.

\section{Knotted Exceptional Lines of Order Three}

The plethora of exceptional nodal topologies protected by $\mathcal{PT}$ symmetry does not only contain second-order surfaces, but also higher-order degeneracies. Below, building on the recent examples on 3EPs (points) in two dimensions \cite{26, 27}, we exemplify this by explicit construction of a three-band model hosting knotted exceptional lines of order three. Consider the Hamiltonian given by

\begin{equation}
H_3 = \begin{pmatrix}
f_2 & 0 & \Lambda \\
\alpha & 0 & \beta \\
f_1 & -f_2 & \beta 
\end{pmatrix},
\end{equation}

where $f_1$ and $f_2$ are continuously differentiable functions of the lattice momentum components, and $\alpha, \beta, \Lambda \in \mathbb{R}$. The corresponding characteristic equation determining the eigenvalues reads,

\begin{equation}
f_1 (\alpha \Lambda - \beta f_2) + \lambda (f_2^2 + \Lambda f_2 + \beta f_1) - \lambda^3 = 0.
\end{equation}

To have third-order exceptional structures, all eigenvalues have to coalesce. This happens exactly when

\begin{equation}
f_1 (\alpha \Lambda - \beta f_2) = 0,
\end{equation}

\begin{equation}
(f_2^2 + \Lambda f_2 + \beta f_1) = 0.
\end{equation}

When $|\Lambda|$ is sufficiently large, the only solution becomes $f_1 = f_2 = 0$. Recalling the interpretation of a knot as the intersection of two implicitly defined surfaces, $f_1$ and $f_2$ can be defined such that their common zeros resemble any knot \cite{29, 30}. By choosing

\begin{equation}
f_1 = \text{Re} [\zeta^p(k_x, k_y, k_z) + \xi^q(k_x, k_y, k_z)],
\end{equation}

\begin{equation}
f_2 = \text{Im} [\zeta^p(k_x, k_y, k_z) + \xi^q(k_x, k_y, k_z)],
\end{equation}

with $\zeta$ and $\xi$ as above, the exceptional lines are torus knots \cite{28}, while an exceptional hyperbolic figure-eight knot is obtained when

\begin{equation}
f_1 = (k_y^2 - k_x^2)x^2 + R (8R^2 - 2x^2),
\end{equation}

\begin{equation}
f_2 = 2\sqrt{2} R k_y k_z + k_x (8R^2 - 2x^2),
\end{equation}

where $R^2 = x^2 - (k_x^2 + k_y^2 + k_z^2)$ \cite{33}. In Fig. 3, a sample of illustrations is provided, including examples from both of the cases above. The topology of the knots can be determined by computing knot invariant polynomials, such as the Alexander polynomial \cite{17, 34}. In the Supplemental Material \cite{32}, additional examples, including hyperbolic Turk’s head knots, are provided.

To emphasize that the knotted exceptional structures are indeed of order three, let us consider the eigenvectors, which are given by

\begin{equation}V_i = \left( -\frac{\Lambda}{f_2 - E_i}, \frac{\alpha \Lambda}{f_2 - E_i}, -\frac{\beta f_2 + \alpha \Lambda + \beta E_i}{(f_2 - E_i)}, 1 \right)^T, \end{equation}

where $E_i$ denotes the corresponding eigenvalue, and $i = 1, 2, 3$. Taking the difference $V_i - V_j$ for $i \neq j$, and letting $E_i \to E_j$, the eigenvectors indeed coalesce when the eigenvalues do, and hence, the degeneracies at $E_i = 0$ are exceptional of order three. They are furthermore stable towards symmetry-preserving perturbations, which follows by the stability of the models in Refs. \cite{16, 17}.
Here, $\Gamma$ constitute a representation of the Clifford algebra. The exceptional knot in (c) is a figure-eight knot, appearing when choosing $f_1$ and $f_2$ as in Eqs. (11) and (12), with $\epsilon = 1$.

### V. 4EPS IN PERTURBED DIRAC SEMIMETALS

Finally, we demonstrate the existence of 4EPs in $\mathcal{PT}$-symmetric four-band systems. Let us start with the Hamiltonian of a real Dirac semimetal,

$$H_D = k_x \Gamma^1 + k_y \Gamma^2 + k_z \Gamma^3,$$

(14)

where $\Gamma^1 = \sigma_1 \otimes \tau_0$, $\Gamma^2 = \sigma_2 \otimes \tau_2$ and $\Gamma^3 = \sigma_3 \otimes \tau_0$, together with $\Gamma^4 = \sigma_2 \otimes \tau_1$ and $\Gamma^5 = \sigma_2 \otimes \tau_3$ constitute a representation of the Clifford algebra. Here, $\sigma_i$ and $\tau_i$ denote the Pauli matrices. Anti-commuting $\Gamma^1, ..., \Gamma^4$ provides a complete basis of $4 \times 4$-matrices. Adding an anti-Hermitian term on the form $H_{AH} = i\delta_4 \Gamma^4 + \delta_5 \Gamma^6 + k_x \delta_{12} \Gamma^{12}$, to obtain

$$H = H_D + H_{AH},$$

(15)

with $\Gamma^6 = \Gamma^3 \Gamma^2$, $\Gamma^{12} = \Gamma^1 \Gamma^2 \Gamma^3$ and $\delta_4, \delta_5, \delta_{12} \in \mathbb{R}$, splits the Dirac node at energy $E = 0$ into eight 4EPs, all located at $E = 0$. Here, $A^{[\mu_1, ..., \mu_n]} = \frac{1}{n!} \epsilon_{\mu_1, ..., \mu_n} A^{\mu_1} \cdot ... \cdot A^{\mu_n}$ with $\epsilon_{\mu_1, ..., \mu_n}$ the Levi-Civita symbol. This can be seen by studying the characteristic polynomial, which attains the form of a depressed quartic. If such polynomials have four-fold degenerate solutions, they are necessarily located at $E = 0$. In Fig. 4, the maximum of the absolute values of all eigenvalues $E_1, ..., E_4$ are displayed as a density plot in the appropriate planes in momentum space. The 4EPs occur exactly when the maximum value is zero since then all eigenvalues necessarily coalesce at $E = 0$. The points are indeed exceptional since the dimensions of the eigenspaces at those points are one, indicating that the eigenvalues $E_1 = E_2 = E_3 = E_4 = 0$ share one eigenvector.

### VI. DISCUSSION

In this Letter, we provide a classification of exceptional nodal topologies protected by $\mathcal{PT}$ symmetry in 3D. Through explicit construction, we demonstrate the existence of several hitherto overlooked types of exceptional nodal degeneracies: knotted surfaces of arbitrary genus of 2EPs, knotted lines of 3EPs, and 4EPs, thus extending the already rich plethora of NH topological phases [8, 20–23, 35–43]. We note that higher-order EPs require tuning of more parameters than allowed by dimensional constraints, making the list of exceptional nodal topolo-
gies complete for physically relevant systems if additional tuning variables are not considered.

We emphasize again that our findings rely only on the presence of $\mathcal{PT}$ symmetry. Being arguably the most widely implemented symmetry in photonic experimental setups, make them highly relevant in optics [4]. It should be possible to experimentally simulate the models we present using single-photon interferometry as in Ref. [44]. We furthermore note that 2EPs, together with their bulk Fermi arcs, as well as the more exotic knotted lines of 2EPs and their concomitant Fermi-Seifert surfaces were both experimentally realized and observed shortly after being theoretically predicted [9, 44]. This suggests that topological phases of higher-order EPs are within experimental reach in several platforms and encourages the search for tailor-made setups where they can be realized.

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Note added: An independent work shows how symmetry-protected 4EPs may naturally be realized in three-dimensional correlated many-body systems [45].

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Figure 5. Exceptional knotted surfaces of order 2. (a) displays an inflated (4, 3) torus knot, obtained from the Hamiltonian in Eq. (4), with \( p = 4, q = 3, M = 1 \) and \( \delta = 0.35 \). In (b) and (c), an inflated figure-eight knot and inflated Borromean rings are shown, obtained by using Eqs. (A1) and (A2) in the Hamiltonian Eq. (4), with \( \delta = 0.15, \epsilon = 1 \) and \( N = 2, 3 \) respectively.

Appendix A: Supplementary Material for “Classification of Exceptional Nodal Topologies Protected by \( \mathcal{PT} \) Symmetry”

In this supplementary material, we provide details on our derivations and arguments presented in the main text, along with complementary figures.

1. Hyperbolic nodal knots

Here, we provide a short summary on how to construct functions whose common zeros represent hyperbolic Turk’s head knots. For further details, see Ref. 17.

In contrast to torus knots, which are described as zeros of a complex polynomial \([28]\), the Turk’s head knots are illustrated as the zeros of a real polynomial, constrained on \( S^3_{\epsilon} \) (the three-sphere of radius \( \epsilon \)) \([33]\). Explicitly, the polynomial is,

\[
F(x, y, z, t) = \left\{ z \left[ x^2 + y^2 + z^2 + t^2 \right] + x \left[ 8x^2 - 2 \left( x^2 + y^2 + z^2 + t^2 \right) \right], \sqrt{2}t x + y \left[ 8x^2 - (x^2 + y^2 + z^2 + t^2) \right] \right\},
\]

with

\[
F(x, y, z, t) = \left( z \left[ x^2 + y^2 + z^2 + t^2 \right] + x \left[ 8x^2 - 2 \left( x^2 + y^2 + z^2 + t^2 \right) \right] \right),
\]

where \( x, y, z, t \) denote coordinates on \( \mathbb{R}^4 \) and \( N \in \mathbb{N} \). Note that \( F : \mathbb{R}^4 \rightarrow \mathbb{R}^2 \). By finding the zeros, restricting them to \( S^3_{\epsilon} \), and introducing the lattice momentum appropriately, these knots can be realized as third-order exceptional degeneracies. In Figure 7, this is illustrated for different values of \( N \), with the lattice momentum introduced as,

\[
x = \epsilon^2 - (k_x^2 + k_y^2 + k_z^2), \quad y = k_x, \quad z = k_y, \quad t = k_z.
\]

Additionally, these hyperbolic knots can be inflated to form knotted surfaces, just as displayed for the torus knots in the main text. This is illustrated in Figure 5, along with a more complicated inflated torus knot.

2. Higher genus surfaces

As mentioned in the main text, the presented techniques can in principle be used to achieve second-order exceptional surfaces of arbitrary genus. Here, we present a few additional figures to strengthen this claim.
Figure 6. Higher genus exceptional surfaces of order 2 from the Hamiltonian Eq. (4). In all panels, \( M = 1 \). In (a), \( p = q = 4 \), and \( \delta = 1 \), giving a genus 4 surface. In (b), \( p = q = 6 \), and \( \delta = 2.5 \) resulting in a genus 6 surface. Lastly, (c) displays a genus 10 surface, obtained by choosing \( p = q = 10 \) and \( \delta = 30 \).

Figure 7. Hyperbolic exceptional knots of order 3 of the Hamiltonian Eq. (5), when defining \( f_1 \) and \( f_2 \) in terms of the components of the polynomial \( F \), defined in Eqs. (A1) and (A2). For all panels, \( \alpha = 1 \), \( \beta = -1 \) and \( \Lambda = 100 \), while \( N = 3, 4, 5 \) in (a), (b) and (c) respectively. (a) displays Borromean rings, while (b) and (c) are more complicated hyperbolic knots in the family of Turk’s head knots.

This is done by using the Hamiltonian on the form,

\[
H_2 = \text{Re} \left[ \xi^p(k_x, k_y, k_z) + \xi^q(k_x, k_y, k_z) \right] \sigma^x + \text{Im} \left[ \xi^p(k_x, k_y, k_z) + \xi^q(k_x, k_y, k_z) \right] \sigma^z + i\delta \sigma^y, \tag{A4}
\]

taking \( p = q = n \), and \( \delta \in \mathbb{R} \). In Figure 6, we illustrate this for \( n = 4, 6, 10 \), giving exceptional surfaces of genus 4, 6 and 10 respectively.

### 3. Controlling topology of third-order exceptional lines

Consider an arbitrary real \( 3 \times 3 \) Hamiltonian,

\[
H_3 = \begin{pmatrix}
  a_1 & a_2 & a_3 \\
  a_4 & a_5 & a_6 \\
  a_7 & a_8 & a_9 \\
\end{pmatrix} \tag{A5}
\]

with all \( a_j \) being real-valued, continuously differentiable function of the lattice momentum components, \( j = 1, ..., 9 \). Since we are interested in when all the eigenvalues of \( H_3 \) coalesce, we can assume that \( H_3 \) is traceless and take \( a_3 = 0 \), \( a_1 = -a_9 \). The corresponding characteristic polynomial reads,

\[
\text{Ch}_{H_3}(\lambda) = a_2a_6a_7 + a_3a_4a_8 - a_1a_6a_8 + a_1a_2a_4 + \lambda \left( a_2a_4 + a_3a_7 + a_6a_8 - a_1^2 \right) - \lambda^3 \tag{A6}
\]
Triple eigenvalue degeneracies occur when,

\[ a_2a_6a_7 + a_3a_4a_8 - a_1a_6a_8 + a_4a_2a_4 = 0, \quad (A7) \]

\[ a_2a_4 + a_3a_7 + a_6a_8 - a_1^2 = 0. \quad (A8) \]

Taking \( a_2 = 0 \) gives us

\[ a_8(a_3a_4 - a_1a_6) = 0, \quad (A9) \]

\[ a_3a_7 + a_6a_8 - a_1^2 = 0. \quad (A10) \]

We note that Eq. (A9) is satisfied if either \( a_8 = 0 \) or \( a_3a_4 - a_1a_6 = 0 \). Inspired by Ref. 16, we let \( |a_3| \gg 0 \), and thus forcing \( a_8 = 0 \) in order to Eq. (A9) to hold. By furthermore letting \( a_1 = a_7 \), Eqs. (A9) and (A10) hold when \( a_1 = a_8 = 0 \). Recalling the constructions in Refs. 16 and 17, we note that by letting the common zeros of \( a_1 \) and \( a_8 \) represent knots, the resulting exceptional line will indeed be knotted. Let \( f_1 \) and \( f_2 \) denote such functions, define \( a_3 := f_2, a_8 = f_1 \), and let \( a_3 = \Lambda, a_4 = \alpha \) and \( a_6 = \beta \), with \( \alpha, \beta, \Lambda \in \mathbb{R} \), and \( |\Lambda| \gg 0 \). Then, the resulting Hamiltonian,

\[
H_3 = \begin{pmatrix}
  f_2 & 0 & \Lambda \\
  \alpha & 0 & \beta \\
  f_2 & f_1 & -f_2
\end{pmatrix}
\quad (A11)
\]

host third-order exceptional knots. Torus knots are obtained when, e.g., \( f_1 = \text{Re} \left[ \zeta^p(k_x, k_y, k_z) + \xi^q(k_x, k_y, k_z) \right] \) and \( f_2 = \text{Im} \left[ \zeta^p(k_x, k_y, k_z) + \xi^q(k_x, k_y, k_z) \right] \), as discussed in the main text, while hyperbolic Turk’s head knots are obtained by choosing \( f_1 \) and \( f_2 \) as the first and second components of the function \( F \) defined in Eqs. (A1) and (A2).