Topological exceptional surfaces in non-Hermitian systems with parity-time and parity-particle-hole symmetries

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We study topological band degeneracy in non-Hermitian systems with parity-time (PT) and parity-particle-hole (CP) symmetries. In d-dimensional non-Hermitian systems, it is shown that (d - 1)-dimensional exceptional surfaces can appear from band degeneracy thanks to PT or CP symmetry. We investigate topological stability and zero-gap quasiparticles for the exceptional surfaces due to the band degeneracy. We also demonstrate the band degeneracy by using lattice models of a topological semimetal and a superconductor.

I. INTRODUCTION

Since the discovery of topological insulators\textsuperscript{1,2}, many topological gapped phases have been suggested theoretically from systematic topological classification of quantum matter\textsuperscript{3}. This idea of the classification is generalized to gapless phases\textsuperscript{4-6}. Topologically gapped and gapless phases are related because some topological gapless phases necessarily intervene between trivial and topological gapped phases\textsuperscript{7,8}. Furthermore, crystal symmetries play an important role in topological phases. For example, parity (P) symmetry enables different topological phases\textsuperscript{9-26}.

Recent works have studied novel gapped topological phases in two- and three-dimensional non-Hermitian systems\textsuperscript{27-38}, while one-dimensional non-Hermitian nontrivial phases have been mainly investigated\textsuperscript{39-46}. Interestingly, time-reversal (T) and particle-hole (C) symmetries are unified in non-Hermitian systems\textsuperscript{23,30,32,47}, which provides new topological phases\textsuperscript{30,32,33}. Particle-hole symmetry can be seen in various non-Hermitian topological systems\textsuperscript{32,40,44,45,48-53}. Non-Hermiticity also yields intriguing topological phenomena such as topological insulator lasers\textsuperscript{54,55} and anomalous edge states\textsuperscript{56-58}.

As non-Hermitian topological gapless structures, exceptional points emerge from band degeneracy in two-dimensional systems\textsuperscript{56-58}. The exceptional points appear between normal and Chern insulator phases in non-Hermitian systems\textsuperscript{29,31,33}. In three-dimensional systems, exceptional lines are realizable in the momentum space\textsuperscript{59,60}. In addition to topological phases, such non-Hermitian band touchings give zero-gap quasiparticles\textsuperscript{61-66,69,70}. For instance, the zero-gap states form lines called bulk Fermi arcs in the two-dimensional momentum space\textsuperscript{61-66}. Moreover, when non-Hermitian systems have parity-time (PT) symmetry, exceptional points and lines can emerge in the one-dimensional\textsuperscript{60,65,71} and the two-dimensional bands\textsuperscript{72-74}, respectively. Hence, it is beneficial to reveal a relationship between band degeneracy and symmetry through non-Hermitian topology in general dimension.

In this paper, we study band degeneracy such as exceptional lines and exceptional surfaces in non-Hermitian systems when parity-time (PT) or parity-particle-hole (CP) symmetry is present. In particular, we investigate the cases of (PT)\textsuperscript{2} = 1 and (CP)\textsuperscript{2} = 1. We elucidate generic conditions to realize exceptional surfaces, and characterize them topologically. It is shown that new zero-gap quasiparticle states accompany topological exceptional surfaces. To confirm our theory, we investigate non-Hermitian lattice models of a nodal-line semimetal and an even-parity superconductor.

This paper is organized as follows. In Sec. II we construct effective models to describe exceptional surfaces in non-Hermitian systems. In Sec. III we discuss general topological properties of exceptional surfaces. We study lattice models to show exceptional surfaces in Sec. IV. Our conclusion is given in Sec. V.

II. BAND DEGENERACY IN NON-HERMITIAN SYSTEMS

In this section, we study general conditions to realize exceptional points, lines and surfaces. We investigate accidental band degeneracy between two states in non-Hermitian systems. Therefore, we consider a two-band non-Hermitian effective model.

A. General two-band effective Hamiltonian

Firstly, we introduce topological theory of band degeneracy in non-Hermitian systems without symmetry. When two states are nondegenerate, energy eigenvalues can be described by a 2 × 2 matrix which represents the subspace of the two states\textsuperscript{29,56,57}. We apply the theory to non-Hermitian bands with PT and CP symmetries in the next subsection. The generic effective Hamiltonian at wavevector $k$ is

$$H(k) = (a_0 + ia_1)\sigma_0 + b_0 \cdot \sigma + ib_1 \cdot \sigma,$$

(1)
where $\sigma_0$ and $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are the identity matrix and Pauli matrices, respectively. Here, $a_{0,1}$ and $b_{0,1} = (b_{i,x}, b_{i,y}, b_{i,z})$ are real. The energy eigenvalues are

$$E_{\pm}(k) = a_0 + ia_1 \pm \sqrt{b_0 \cdot b_0 - b_1 \cdot b_1 + 2ib_0 \cdot b_1}. \quad (2)$$

If the two states become degenerate, i.e., $E_+ = E_-$, the bands satisfy

$$b_0 \cdot b_0 - b_1 \cdot b_1 = 0, \quad b_0 \cdot b_1 = 0. \quad (3)$$

Therefore, we have the two conditions for band degeneracy. To satisfy these conditions, the system needs two tunable parameters. In general, structures of band degeneracy are determined by difference between the number of parameters and that of conditions for band degeneracy. In $d$-dimensional non-Hermitian systems, since we have $d$ components of the wavevector, band degeneracy with $(d - 2)$-dimensional surface is realizable if $d \geq 2$ [Figs. 1(a) and (b)]. The band degeneracy can be characterized by a half-integer topological invariant. Note that the conditions in Eq. (3) are unchanged by only unitary crystal symmetry because this symmetry equally acts on $b_0 \cdot \sigma$ and $b_1 \cdot \sigma$ in Eq. (1). Thus, we consider anti-unitary symmetries $PT$ and $CP$.

**B. Exceptional surfaces in $PT$- and $CP$-symmetric non-Hermitian systems**

We construct an effective model to clarify conditions of band degeneracy in non-Hermitian systems with $PT$ or $CP$ symmetry. Firstly, we consider $PT$ symmetry which imposes $(PT)H(k)(PT)^{-1} = H(k)$ on the Hamiltonian in Eq. (1). Because this symmetry is anti-unitary, it can be generally represented as $PT = UK$, where $U$ is a unitary matrix and $K$ is complex conjugation. From $(PT)^2 = 1$, we can set $U = \sigma_0$ by choosing a proper basis. Then, the effective Hamiltonian is

$$H(k) = a_0\sigma_0 + b_{0,x}\sigma_x + b_{0,z}\sigma_z + ib_{1,y}\sigma_y. \quad (4)$$

The energy eigenvalues are

$$E_{\pm}(k) = a_0 \pm \sqrt{b_0 \cdot b_0 - b_1 \cdot b_1}. \quad (5)$$

Hence, $PT$ symmetry automatically leads to $b_0 \cdot b_1 = 0$ in Eq. (3). In other words, band degeneracy happens if $b_0 \cdot b_0 - b_1 \cdot b_1 = 0$ is satisfied in the momentum space. The number of conditions for band degeneracy is reduced to one. As a result, $(d - 1)$-dimensional exceptional surfaces can emerge in the $d$-dimensional non-Hermitian systems when $d \geq 1$. Thus, as shown in Figs. 1(c) and (d), we can obtain exceptional lines and surfaces in two- and three-dimensional non-Hermitian systems with $PT$ symmetry, respectively.

In the presence of the $PT$ symmetry, energy eigenvalues can be real. From Eq. (5), we have two real energy eigenvalues in the momentum space for $b_0 \cdot b_0 > b_1 \cdot b_1$. Meanwhile, the eigenvalues become complex in the region $b_0 \cdot b_0 < b_1 \cdot b_1$. Therefore, we can see that the number of real eigenvalues changes on the exceptional surface when $PT$ symmetry is present.

Secondly, let us consider $CP$ symmetry described by $(CP)H(k)(CP)^{-1} = -H(k)$. $CP$ symmetry is also anti-unitary. When $CP = K$ is chosen in a proper basis, we obtain

$$H(k) = ia_1\sigma_0 + b_{0,y}\sigma_y + ib_{1,x}\sigma_x + ib_{1,z}\sigma_z. \quad (6)$$

Therefore, $CP$ symmetry also gives $b_0 \cdot b_1 = 0$. Hence, we can also obtain $(d - 1)$-dimensional exceptional surfaces in the $d$-dimensional $CP$-symmetric systems. Moreover, it is found that the number of purely imaginary eigenvalues changes on the exceptional surface in the $CP$-symmetric system.

**III. TOPOLOGICAL PROPERTIES OF EXCEPTIONAL SURFACES**

Here, we characterize exceptional surfaces topologically when non-Hermitian systems have $PT$ or $CP$ symmetry. We also reveal topological properties associated with the exceptional surfaces. For simplicity, we assume that the exceptional surfaces exist at zero energy without loss of generality because the origin of the energy can be shifted. In this section, we refer to $(d - 1)$-dimensional exceptional surfaces just as exceptional surfaces.
A. $\mathbb{Z}_2$ topological characterization for exceptional surfaces

We begin with topological characterization of exceptional surfaces in $PT$-symmetric non-Hermitian systems. Before going into the details, we introduce a topological invariant for the zero-dimensional non-Hermitian systems with $PT$ symmetry according to Ref. [30]. The $PT$-symmetric Hamiltonians $H_{PT}$ are classified by a $\mathbb{Z}_2$ topological invariant given by

$$ s = \text{sgn} \det(H_{PT}) = (-1)^{n_{\text{R}}}, \quad (7) $$

where $n_{\text{R}}$ is the number of the real negative energy eigenvalues. The topological invariant $s$ is defined when $H_{PT}$ does not have zero-energy eigenvalues. If $s = +1(-1)$, the system has an even (odd) number of energy eigenvalues on the negative energy axis.[30] Therefore, when the system has zero-energy eigenvalues, it can be understood as a topological phase transition.

When a non-Hermitian $PT$-symmetric system has band degeneracy, the momentum space is divided by the exceptional surfaces, as illustrated in Figs. [4]c and (d). To characterize the exceptional surfaces, we regard each point $k$ in the momentum space as a zero-dimensional system with $PT$ symmetry. Because the Hamiltonian satisfies $(PT)H(k)(PT)^{-1} = H(k)$ for all $k$, we can define $s(k)$ on each point by using Eq. (7). By assumption, we can interpret the exceptional surface as a topological phase transition in the momentum space by changing $k$. Thus, exceptional surfaces can be characterized by the $\mathbb{Z}_2$ topological invariant leading to topological protection.[33] This argument is consistent with the change of $n_{\text{R}}(k)$ on the exceptional surface, as discussed in Sec. [13].

Next, we consider $CP$-symmetric non-Hermitian systems. Similarly, zero-dimensional $CP$-symmetric systems are classified by a $\mathbb{Z}_2$ topological invariant.[34] Thus, the $\mathbb{Z}_2$ topological invariant can characterize exceptional surfaces in the $CP$-symmetric systems. For the zero-dimensional $CP$-symmetric Hamiltonian $H_{CP}$, the $\mathbb{Z}_2$ topological invariant is

$$ s' = \text{sgn} \det(iH_{CP}) = (-1)^{n_{\text{I}}}, \quad (8) $$

where $n_{\text{I}}$ is the number of the energy eigenvalues on the positive imaginary axis. We define the topological invariant $s'$ when $H_{CP}$ does not have zero-energy eigenvalues. Eventually, we can also characterize the exceptional surfaces in a similar way to $PT$-symmetric systems if we define $s'(k)$ for each point $k$ in the momentum space.

In both of the $PT$- and the $CP$-symmetric systems, the exceptional surfaces can be characterized by the $\mathbb{Z}_2$ topological invariants. The same $\mathbb{Z}_2$ classifications stem from topological unification of time-reversal and particle-hole symmetries in the non-Hermitian gapped systems.[30,32] By the transformation $H \rightarrow iH$, the two symmetries can be actually treated as one symmetry called $K$ symmetry in non-Hermitian systems.[28,82,83] As a result, the topological unification can be found in the characterization of the exceptional surfaces.

B. Topological stability and drumhead bulk states

In order to see the topological stability, we consider a simple exceptional line in the two-dimensional system. The results in this subsection can be generalized to exceptional surfaces. Suppose that the exceptional line is described by

$$ H(k) = k_x\sigma_x + k_y\sigma_y + i\delta\sigma_z, \quad (9) $$

where $\delta$ is a real constant. This model can be regarded as a two-dimensional Dirac cone with non-Hermitian term $i\delta\sigma_z$, and realized in a honeycomb photonic crystal with gain and loss.[24,76] The Hamiltonian has $PT$-symmetry represented by $PT = \sigma_z K$. (If we perform the transformation $H \rightarrow iH$, the model becomes $CP$-symmetric.) The eigenvalues are

$$ E_{\pm}(k) = \pm \sqrt{k_x^2 + k_y^2 - \delta^2}. \quad (10) $$

Therefore, the exceptional line appears on $k_x^2 + k_y^2 = \delta^2$. Then, the topological invariant for the exceptional line is

$$ s(k) = \begin{cases} +1 & (k_x^2 + k_y^2 < \delta^2) \\ -1 & (k_x^2 + k_y^2 > \delta^2) \end{cases}. \quad (11) $$

Thanks to the topological protection, the exceptional line is stable as long as the Hamiltonian preserves the $PT$ symmetry.

Indeed, the exceptional line disappears by perturbations breaking the $PT$ symmetry of the Hamiltonian. If we add $\delta'\sigma_z$ term with a real constant $\delta'$ to Eq. (9), the exceptional line vanishes because the eigenvalues become $E_{\pm} = \pm \sqrt{k_x^2 + k_y^2 + \delta'^2 - \delta^2 + 2i\delta\delta'}$. On the other hand, if $i\kappa_x\sigma_x + i\kappa_y\sigma_y$ term is added, the exceptional line can become exceptional points.[29,61] When $\kappa_x$ and $\kappa_y$ are real, the exceptional points emerge at $(k_x, k_y) = \pm(-\kappa_y \sqrt{\frac{\kappa^2 + \kappa_x^2}{\kappa_x^2 + \kappa_y^2}}, \kappa_x \sqrt{\frac{\kappa^2 + \kappa_x^2}{\kappa_x^2 + \kappa_y^2}})$. From the topological property, the quasiparticle band gap becomes zero on a region bordered by exceptional lines. The quasiparticle band gap is given by $\Delta_q(k) = ReE_+ - ReE_-$ in the non-Hermitian system.[84] In this model, we can write the band gap as

$$ \Delta_q(k) = \begin{cases} 0 & (k_x^2 + k_y^2 \leq \delta^2) \\ 2\sqrt{k_x^2 + k_y^2 - \delta^2} & (k_x^2 + k_y^2 > \delta^2) \end{cases}. \quad (12) $$

Because $\Delta_q(k) = 0$ inside the exceptional line, the drumhead-like gapless quasiparticles appear in the bulk. Although the drumhead bulk states are analogous to drumhead surface states of nodal-line semimetals[21,22], these zero-gap bulk states can be found since the eigenvalues are purely imaginary inside the exceptional lines.

In general, we can see that a quasiparticle band gap can vanish in some regions with exceptional surfaces as
follows. From the energy eigenvalue of the effective model in Eq. (5), we obtain

$$\Delta_{q}(k) = (1 + \text{sgn}(b_0 \cdot b_0 - b_1 \cdot b_1)) \sqrt{b_0 \cdot b_0 - b_1 \cdot b_1}.$$  

(13)

Therefore, the zero-gap states can appear when \(\text{sgn}(b_0 \cdot b_0 - b_1 \cdot b_1)\) changes. Since the change of \(\text{sgn}(b_0 \cdot b_0 - b_1 \cdot b_1)\) corresponds to that of \(s(k)\), the zero-gap quasiparticle states are also protected by symmetry and topology. Correspondingly, if we create exceptional points from an exceptional line by breaking the symmetry externally in the two-dimensional system, the drumhead bulk states change into bulk Fermi arc states.

**IV. LATTICE MODELS**

**A. Exceptional surfaces in a PT-symmetric diamond lattice**

To obtain exceptional surfaces, we use a tight-binding model on a diamond lattice with PT symmetry. We write the three translation vectors as \(t_1 = \frac{a}{\sqrt{2}} (0, 1, 1)\), \(t_2 = \frac{a}{\sqrt{2}} (1, 0, 1)\), and \(t_3 = \frac{a}{\sqrt{2}} (1, 1, 0)\), where \(a\) is the lattice constant. The tight-binding model is

$$H = \sum_{<ij>} t_{ij} c_i^\dagger c_j + i \sum \lambda_i c_i^\dagger c_i,$$

(14)

where \(t_{ij}\) and \(\lambda_i\) are real constants. The first term is nearest-neighbor hoppings between the sublattices A and B. We assume that the hopping in the direction of \(\tau = \frac{a}{\sqrt{2}} (1, 1, 1)\) is different from the other three nearest-neighbor hoppings. We denote the nearest-neighbor hopping in the direction of \(\tau\) by \(t_\tau\), and the other hoppings by \(t\). The second term represents gain and loss leading to non-Hermiticity. \(\lambda_i\) takes values \(+\lambda(-\lambda)\) for the A(B) sublattices. The model without the second term has been studied as a nodal-line semiconductor\(^{84,85}\). The Hamiltonian in the momentum space is

$$H(k) = \left( t_\tau + t \sum_i \cos(k \cdot t_i) \right) \sigma_x + t \sum_i \sin(k \cdot t_i) \sigma_y + i \lambda \sigma_z.$$  

(15)

Here, \(\sigma_{x,y,z}\) are Pauli matrices acting on the sublattices. In this model, the PT operator is given by \(PT = \sigma_x K\).

We set \(t_\tau = 1.4t\) and \(\lambda = 0.1t\) to investigate an exceptional surface. The torus-like exceptional surface appears around the point \(L = \frac{a}{\sqrt{2}} (1, 1, 1)\), as shown in Fig. 2(a). Then, the topological invariant \(s(k)\) changes in the momentum space. Figure 2(b) shows change in \(s(k)\) by the exceptional surface. The red regions with \(s = +1\) give purely imaginary energy eigenvalues [Figs. 2(c) and (d)]. These results agree with the discussions in Secs. III and IV.

**B. Exceptional lines in a two-dimensional even-parity superconductor**

We study even-parity non-Hermitian superconductors with exceptional surfaces. We consider a Bogoliubov-de Gennes Hamiltonian given by \(H = \frac{1}{2} \sum_k \Psi_k^\dagger \mathcal{H}(k) \Psi_k \) with \(\Psi_k = (c^\dagger_{k\uparrow}, c^\dagger_{k\downarrow}, c_{-k\uparrow}, c_{-k\downarrow})\) and

$$\mathcal{H}(k) = \begin{pmatrix} \xi_k & 0 & 0 & \Delta(k) \\ 0 & \xi_k & -\Delta^*(k) & 0 \\ 0 & -\Delta(k) & -\xi_k & 0 \\ \Delta^*(k) & 0 & 0 & -\xi_k \end{pmatrix},$$  

(16)

where \(\xi_k\) is a kinetic energy, and \(\Delta(k)\) and \(\Delta^*(k)\) are gap functions. When \(\Delta(k) \neq \Delta^*(k)\), the superconductor becomes non-Hermitian. The energy eigenvalues are given by \(E_k = \pm \sqrt{\xi_k^2 + \Delta(k) \Delta^*(k)}\). In the even-parity superconductors, \(\Delta(k) = \Delta(-k)\) and \(\Delta^*(k) = \Delta^*(-k)\). Such non-Hermitian superconductors can be realized if the pairing potential is complex\(^{86}\).

Because of \(SU(2)\) symmetry, the superconducting Hamiltonian in Eq. (16) can be rewritten as two \(2 \times 2\) matrices. Here, we assume that \(\Delta(k) = -\Delta^*(k)\) to realize non-Hermiticity. Then, we obtain

$$\mathcal{H}_\pm(k) = \pm \text{Im}[\Delta(k)] \tau_x \pm \text{Re}[\Delta(k)] \tau_y + \xi_k \tau_z,$$

(17)

where \(\tau_{x,y,z}\) are Pauli matrices. The energy eigenvalues are \(E_k = \pm \sqrt{\xi_k^2 - |\Delta(k)|^2}\), which define exceptional surfaces as \(\xi_k^2 = |\Delta(k)|^2\). \(\mathcal{H}_\pm\) have particle-hole symmetry \(C = \tau_z K\) and inversion symmetry \(P = 1\). Therefore, we...

**FIG. 2.** (a) The exceptional surface around the \(L\) point in the diamond lattice with \(t_\tau = 1.4t\) and \(\lambda = 0.1t\). \(q\) is a wavevector measured from the point \(L\). (b) The topological invariant \(s(q)\) in the \(q_x = 0\) plane. The red and the white regions represent the areas with \(s(q) = +1\) and \(-1\), respectively. (c) and (d) The real and the imaginary parts of the energy bands along the dotted arrow in (b).
can use the topological invariant $s'$ to characterize exceptional surfaces for each of $\mathcal{H}_\pm$ although the bands of $\mathcal{H}$ are doubly degenerate.

In this model, we put $\xi_k = 2t'(\cos k_x + \cos k_y)$ and $\Delta(k) = \Delta x^2 - y^2 \cos(k_x - k_y) + i\Delta_{xy} \sin k_x \sin k_y$, as an example of the two-dimensional even-parity superconductors. The hopping $t'$ and the gap functions $\Delta x^2 - y^2$ and $\Delta_{xy}$ are real. We set the lattice constant to unity. Figure 3 shows exceptional lines in this model with $\Delta x^2 - y^2 = 0.2t'$ and $\Delta_{xy} = 0.1t'$. From Fig. 3(a), we find exceptional lines as changes of $s'(k)$, which are depicted by the boundaries between the red and the white regions in the momentum space. As seen in Fig. 3(b)-(d), the non-Hermitian superconductor has topological nodes even if $\Delta(k) \neq 0$.

\[ \text{FIG. 3. (a) The topological invariant } s'(k) \text{ for } \mathcal{H}_+ \text{ in the momentum space. The red (white) regions indicate } s'(k) = +1 (-1). \text{ The boundaries between the two regions correspond to the exceptional lines. (b) The solid (dotted) lines are the real (imaginary) part of the energy bands on the } k_y = 0 \text{ line. (c) and (d) The real and the imaginary parts of the energy bands.} \]

V. CONCLUSION AND DISCUSSION

In this paper, we have studied exceptional surfaces in non-Hermitian systems with $PT$ or $CP$ symmetry. We have shown that the exceptional surfaces are topologically stable when $PT$ or $CP$ symmetry is present. The results can be universally applied to $d$-dimensional non-Hermitian systems when $d \geq 1$. The exceptional surfaces yield novel zero-gap quasiparticle states. On the other hand, if the symmetry is broken by perturbations, the exceptional surfaces disappear. Our theory is also confirmed by our calculation based on the effective and the lattice models.

From our study, we can see how to realize topological exceptional surfaces. As a two-dimensional Dirac cone becomes an exceptional line by $PT$-symmetric non-Hermitian perturbations, a two-dimensional exceptional surface can be obtained from a nodal line in three-dimensional systems. Because a photonic crystal with a nodal line is suggested theoretically, photonic systems have potential for experimental realization of the exceptional surface. Meanwhile, topological phase transitions typically need band touching in the bulk. If the band touching happens by tuning parameters, an exceptional surface can appear in the $PT$- or $CP$-symmetric systems. Therefore, when the system has an exceptional surface, the phase may be regarded as a non-Hermitian intermediate phase between trivial and topological gapped phases. Moreover, because four-dimensional quantum Hall effects have been proposed by using synthetic dimension, non-Hermitian topological exceptional surfaces in higher-dimensional systems are feasible.

We became aware of a related work, which studies exceptional surfaces in view of Bernard and LeClair classes.

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Because the \( \mathbb{Z}_2 \) topological invariant characterizes the zero-dimensional systems, the characterization is applicable to general \((d-1)\)-dimensional Fermi surfaces as well as exceptional surfaces in \( PT \)-symmetric non-Hermitian systems.

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