

# Generation and Annihilation of Topologically Protected Bound States in the Continuum and Circularly Polarized States by Symmetry Breaking

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We demonstrate by breaking the  $C_6$  symmetry for higher-order at- $\Gamma$  bound states in the continuum (BICs) with topological charge  $-2$  in photonic crystals (i) deterministic generation of off- $\Gamma$  BICs from the at- $\Gamma$  BIC and (ii) a variety of pair-creation and annihilation processes of circularly polarized states with opposite topological charges and the same handedness. To explain these phenomena, we introduce the handedness-wise topological charge quantized to a half-integer. The handedness-wise charge gives a unified picture of various phenomena involving BICs and circularly polarized states.

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**Introduction.**—The concept of topology has been widely applied to photonic systems [1–3]. Various intriguing phenomena associated with nontrivial Bloch wave functions have been studied extensively. Recent studies suggest that far-field polarization vector fields radiated from photonic crystals (PhCs), also determined from Bloch wave functions, possess intriguing topological natures, including bound states in the continuum (BICs) [4–11], band degeneracies [8,12,13], and circularly polarized states (CPSs) [14–16].

BICs are resonances with infinite quality factors, although their frequencies fall inside continuous spectrum of radiation modes. At the  $\Gamma$  point, BICs result from the symmetry mismatch between PhC modes and radiative plane waves; this type of BIC is called an at- $\Gamma$  BIC or symmetry-protected BIC. Because of the symmetry protection, the occurrence of at- $\Gamma$  BICs does not depend on structural parameters. Interestingly, it was found that BICs can also exist at finite wave vectors apart from the symmetry point in a certain type of PhC, called off- $\Gamma$  BICs or topologically protected BICs [4,5]. Off- $\Gamma$  BICs have attracted much attention to applications such as on-chip beam steering [17,18] and generation of directive vector beams [19–21]. Moreover, off- $\Gamma$  BICs can propagate without radiation loss even though their frequency is above the light line [22–24]. In spite of these interesting properties, a systematic way to generate off- $\Gamma$  BICs is still lacking. Previously, off- $\Gamma$  BICs have been formed by accidental cancellation of outgoing waves, and thus they are sometimes called *accidental* BICs. In stark contrast to at- $\Gamma$  BICs, we must tune structural parameters carefully to generate off- $\Gamma$  BICs.

CPSs have other polarization singularities for far-field polarization vector fields in PhCs without  $C_2$  symmetry [14–16]. CPSs are resonances with *finite* quality factors,

and they couple to circularly polarized radiative plane waves. Both BICs and CPSs are polarization vortex centers in the reciprocal space and carry quantized topological charges  $\nu$ . The charge  $\nu$  is an integer for BICs and a half-integer for CPSs. So far, most previous studies dealt with topological processes involving BICs with  $\nu = \pm 1$  such as annihilation of two BICs with opposite charges.

In this study, we focus on at- $\Gamma$  BICs with a higher topological charge and demonstrate that a variety of interesting phenomena arise from breaking the crystal symmetry of PhCs having a higher-order charge. First, we demonstrate that this leads to a systematic way to generate off- $\Gamma$  BICs. We show that an at- $\Gamma$  BIC with  $\nu = -2$  in triangular-lattice PhCs can be split into two off- $\Gamma$  BICs by breaking  $C_6$  symmetry but preserving  $C_2$  symmetry. These off- $\Gamma$  BICs can be *deterministically* generated by an infinitesimal perturbation without fine-tuning parameters. Second, we demonstrate a wide variety of ways to generate and annihilate CPSs. We show that a perturbation breaking the  $C_2$  symmetry but preserving  $C_3$  symmetry generates six CPSs and that a variety of pair creations and annihilations of CPSs having *opposite charges* and the *same handedness* can be achieved through symmetry control starting from the at- $\Gamma$  BIC with  $\nu = -2$ . Importantly, we show that all these phenomena are governed by the conservation of topological charges. Although previous studies have already pointed out the importance of the charge conservation in far-field topological photonics [5] with an analogy to singular optics for beam propagation [25–27], it is still not clear how far this law can hold for PhCs. Actual examples where the charge conservation plays a key role are limited to the case where  $|\nu|$  of BIC is 1 [4–16], and the applicability of the conservation has not been fully explored. We introduce handedness-wise charges ( $\nu_{\pm}$ ) and clearly prove that they can fully explain

a variety of ways to generate and annihilate BICs and CPSs.

First of all, let us begin with describing two-dimensional (2D) PhC slabs with a finite thickness [28]. Above the light line and below the diffraction limit, a nondegenerate eigenmode with an in-plane wave vector  $\mathbf{k}_{\parallel} = (k_x, k_y)$  generally couples to a propagating plane wave with the same  $\mathbf{k}_{\parallel}$  and a polarization vector  $\mathbf{d}(\mathbf{k}_{\parallel})$  in the  $sp$  plane [4,5]. To discuss the topology in  $\mathbf{k}_{\parallel}$  space, we introduce a 2D polarization vector projected onto the  $xy$  plane,  $\mathbf{d}'(\mathbf{k}_{\parallel}) = d'_x(\mathbf{k}_{\parallel})\hat{x} + d'_y(\mathbf{k}_{\parallel})\hat{y}$  (see Sec. S1 in the Supplemental Material [29]). The topological charge of the polarization singularities for  $\mathbf{d}'(\mathbf{k}_{\parallel})$  is defined by [5–16,25–27]

$$\nu = \frac{1}{2\pi} \oint_C d\mathbf{k}_{\parallel} \cdot \nabla_{\mathbf{k}_{\parallel}} \phi(\mathbf{k}_{\parallel}), \quad (1)$$

where  $C$  is a closed loop in the  $\mathbf{k}_{\parallel}$  space,  $\phi(\mathbf{k}_{\parallel}) = \frac{1}{2} \arg[S_1(\mathbf{k}_{\parallel}) + iS_2(\mathbf{k}_{\parallel})]$  is the angle between its long axis of the polarization ellipse and the  $x$  axis, and  $S_i(\mathbf{k}_{\parallel})$  is the Stokes parameter of  $\mathbf{d}'(\mathbf{k}_{\parallel})$ .  $\nu$  describes how many times the polarization ellipse of the polarization vector winds along a loop  $C$ . The charge  $\nu$  is an integer if a loop  $C$  encloses a BIC where  $S_1 = S_2 = S_3 = 0$  [5–11]. The charge  $\nu$  is a half-integer if a loop  $C$  encloses a CPS where  $S_1 = S_2 = 0$  and  $S_3 = \pm 1$  [14–16]. The half-integer nature of  $\nu$  originates from the fact that the polarization ellipse is described by the real symmetric tensor [25,26]. Equation (1) takes the same form as quantized Berry phases in  $PT$ -symmetric systems because both the polarization ellipse and  $PT$ -symmetric system are described by real symmetric matrices (see Sec. S3 in the Supplemental Material [29]).

*Generation of off- $\Gamma$  BIC from at- $\Gamma$  BIC.*—The possible charge of an at- $\Gamma$  BIC is determined by the eigenvalues of the rotational symmetry of the system [5]. Here we particularly focus on an at- $\Gamma$  BIC with a symmetry-protected higher-order charge (see Ref. [43] and Sec. S4 in the Supplemental Material [29]). Although at- $\Gamma$  BICs with  $|\nu| \geq 2$  can be moved by splitting into off- $\Gamma$  BICs. The perturbations reduce the charge of the BIC and then the change of  $\nu$  generates new off- $\Gamma$  BICs. Since this splitting relies on the charge conservation and crystalline symmetry, the generation of off- $\Gamma$  BICs can be controlled by systematic deformation of the lattice symmetry in contrast to the generation of off- $\Gamma$  BICs by an accidental fine-tuning of structural parameters [5]. It is worth noting that, although the destruction of at- $\Gamma$  BICs by reducing symmetry has been reported [44,45], the splitting of an at- $\Gamma$  BIC into off- $\Gamma$  BICs has not been pointed out in previous works.

To verify the splitting of the at- $\Gamma$  BIC, we numerically investigate a triangular-lattice PhC slab of circular air holes with lattice constant  $a$ , hole radius  $r = 0.28a$ , slab

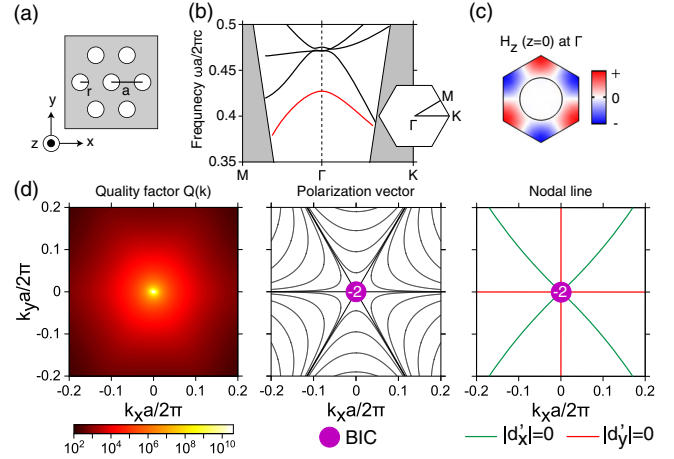


FIG. 1. (a) Schematics of a PhC slab with a triangular lattice of circular air holes. (b) Calculated TE-like band structure. The red line is the lowest TE-like band. The gray region indicates a region below the light line. The inset is the first Brillouin zone. (c) Mode profile in the unit cell for the lowest TE-like band. (d) Calculated quality factor (left), polarization vector (middle), and nodal lines of  $d'_x$  and  $d'_y$  (right). The projected polarization vector is represented by the line field tangent to the long axis of the polarization ellipse [8,10–16,25,26].

thickness  $h = 0.38a$ , and refractive index  $n_0 = 3.48$  [Fig. 1(a)] by the finite-element method. The lowest TE-like band at the  $\Gamma$  point belongs to the representation  $B_1$  of the  $C_{6v}$  point group [Figs. 1(b) and 1(c)] and thus becomes an at- $\Gamma$  BIC with  $\nu = -2 + 6n$  [5]. The calculated quality factor and polarization vector of the lowest TE-like band are plotted in Fig. 1(d). We find that the quality factor ( $Q$ ) diverges at the  $\Gamma$  point and that the polarization vector winds twice around it. We also plot nodal lines of  $d'_x$  and  $d'_y$  in Fig. 1(d) and find that both nodal lines are doubly degenerate at the  $\Gamma$  point. These results demonstrate that a BIC with charge  $-2$  exists at the  $\Gamma$  point [5,9,19].

Next, we introduce perturbations breaking the  $C_6$  symmetry but preserving the  $C_2$  symmetry. Here we slightly vary the angle  $\theta$  between two translational vectors defined in Fig. 2(a) [46]. When  $\theta$  is deviated from  $60^\circ$  (corresponding to uniaxial deformation in the triangular lattice), the symmetry of the eigenmode for the lowest TE-like band at the  $\Gamma$  point is reduced to the  $B_1$  representation of the  $C_{2v}$  point group. As mentioned before, we can expect that the perturbation split the original BIC with  $\nu = -2$  into two off- $\Gamma$  BICs with  $\nu = -1$  through the charge conservation. We numerically calculate  $Q$  for  $\theta = 58^\circ$  and  $\theta = 62^\circ$  [Figs. 2(b) and 2(c) left]. We can observe two high- $Q$  states at finite wave vectors on a mirror-invariant axis ( $k_x = 0$  or  $k_y = 0$ ). To prove that these states are exact BICs, not quasi-BICs [47,48], we also plot the polarization vector and nodal lines of  $d'_x$  and  $d'_y$  in Figs. 2(b) and 2(c). The polarization ellipse winds by  $-2\pi$  around the high- $Q$  states [Figs. 2(b) and 2(c) middle]. This plot shows that

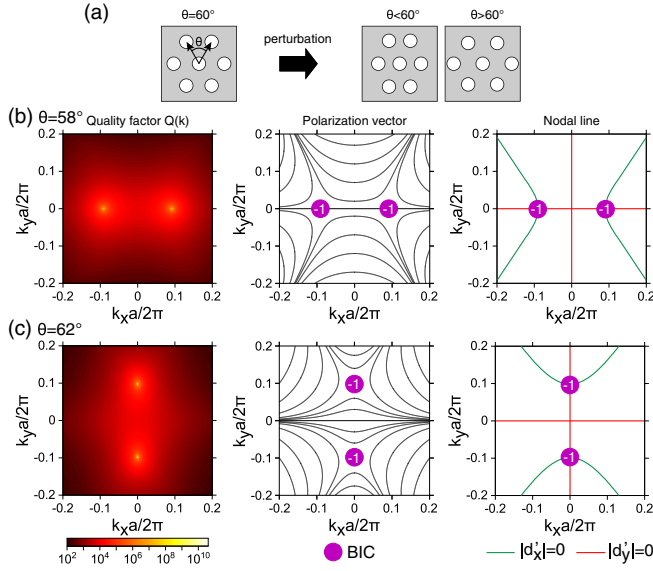


FIG. 2. (a) Definition of the angle  $\theta$  and schematics of perturbed PhCs. (b),(c) Calculated quality factor (left), polarization vector (middle), and nodal lines of  $d'_x$  and  $d'_y$  (right) for (b)  $\theta = 58^\circ$  and (c)  $\theta = 62^\circ$ .

the perturbation splits the degeneracy of the nodal lines at the  $\Gamma$  point. In addition, the nodal lines intersect each other at the high- $Q$  states [Figs. 2(b) and 2(c) right], where the polarization vector vanishes [4,5,30]. These results unambiguously verify that the at- $\Gamma$  BIC with  $\nu = -2$  is split into the two exact off- $\Gamma$  BICs with  $\nu = -1$  by the uniaxial deformation. This finding shows that there is always a systematic way to generate off- $\Gamma$  BICs from higher-order at- $\Gamma$  BICs.

Conventional off- $\Gamma$  BICs can exist only at a certain range of the structural parameters. In Sec. S5 in the Supplemental Material [29], we demonstrate that off- $\Gamma$  BICs do not exist when  $h < 0.97a$  for the PhC with  $r = 0.28a$ ,  $n_0 = 3.48$ , and  $\theta = 60^\circ$ . This contrasts with the present deterministic off- $\Gamma$  BICs that always exist at any thickness because the existence of at- $\Gamma$  BICs is guaranteed by the symmetry. Furthermore, we have confirmed that it is possible to widely change the wave vector of off- $\Gamma$  BICs by simply varying  $\theta$ , as shown in Sec. S6 in the Supplemental Material [29]. The result shows that one can widely change the emission angle of polarization vortex beams generated from BICs between  $0^\circ$  and  $90^\circ$ , which will be promising for vortex-beam steering devices.

*Generation and annihilation of CPSs.*—Recently, generation of two CPSs from splitting a BIC with charge  $\pm 1$  in PhCs by breaking spatial symmetries was reported [14–16]. Here we demonstrate that starting from a higher-order at- $\Gamma$  BIC with charge  $-2$ , we are able to observe far richer phenomena, including various pair creations and annihilations.

Before showing the actual examples, we point out that  $\nu$  defined by Eq. (1) cannot fully describe the processes involved with CPSs because it does not contain the Stokes parameter  $S_3$ . To overcome this difficulty, we express  $\mathbf{d}'(\mathbf{k}_{\parallel})$  in terms of the circular basis [26,27,49],

$$\mathbf{d}'(\mathbf{k}_{\parallel}) = d'_+(\mathbf{k}_{\parallel})\mathbf{e}_+ + d'_-(\mathbf{k}_{\parallel})\mathbf{e}_-, \quad (2)$$

where  $\mathbf{e}_{\pm} = (\hat{x} \pm i\hat{y})/\sqrt{2}$  and  $d'_{\pm}(\mathbf{k}_{\parallel}) = [d'_x(\mathbf{k}_{\parallel}) \mp id'_y(\mathbf{k}_{\parallel})]/\sqrt{2}$ . In this basis, zeros of  $d'_{\pm}(\mathbf{k}_{\parallel})$  correspond to CPSs. When both  $d'_+(\mathbf{k}_{\parallel})$  and  $d'_-(\mathbf{k}_{\parallel})$  are simultaneously zero, an eigenmode turns into a BIC. By writing  $d'_{\pm}(\mathbf{k}_{\parallel})$  as  $d'_{\pm}(\mathbf{k}_{\parallel}) = |d'_{\pm}|e^{i\alpha_{\pm}}$ , we introduce an integer [26,27],

$$\nu_{\pm} = \frac{1}{2\pi} \oint_C d\mathbf{k}_{\parallel} \cdot \nabla_{\mathbf{k}_{\parallel}} \alpha_{\pm}(\mathbf{k}_{\parallel}). \quad (3)$$

$\nu_{\pm}$  is a finite integer when a loop  $C$  encloses the zeros of  $d'_{\pm}(\mathbf{k}_{\parallel})$ .  $\nu$  and  $\nu_{\pm}$  are related by

$$\nu = \frac{1}{2}(\nu_- - \nu_+) \quad (4)$$

because  $\phi(\mathbf{k}_{\parallel})$  is given by  $\phi(\mathbf{k}_{\parallel}) = \frac{1}{2} \arg(d'_+ d'_-)$ . It follows from Eq. (4) that  $\nu_{\pm}$  is a handedness-wise charge, meaning the winding number weighted by its handedness  $S_3$ . Assuming the conservation for  $\nu$  and  $\nu_{\pm}$ , a BIC with  $\nu = \pm 1$  can be regarded as the superposition of two CPSs with  $(\nu_+, \nu_-) = \pm(-1, +1)$ , which indeed correctly explains the observation that a perturbation breaking  $C_2$  symmetry splits the BIC into two CPSs with the *same topological charge*  $\nu$  and *opposite handedness*  $S_3$  [14–16]. Furthermore, a CPS with  $\nu_{\pm} = +1$  can be removed through collision with another CPS with  $\nu_{\pm} = -1$ , i.e., *opposite topological charge*  $\nu$  and *same handedness*  $S_3$ . The introduction of  $\nu_{\pm}$  consistently explains the splitting of a BIC into two CPSs and predicts the rule for pair annihilation of two CPSs.

Here we examine actual examples. We break the  $C_2$  symmetry by deforming circular air holes into triangular air holes with a side length of  $d = 0.75a$ , a slab thickness of  $h = 0.38a$ , and  $\theta = 60^\circ$  [Fig. 3(a)]. This deformation reduces the crystalline symmetry from  $C_{6v}$  to  $C_{3v}$ , which allows CPSs. The perturbation does not break the at- $\Gamma$  BIC because  $C_3$  symmetry still protects an at- $\Gamma$  BIC with  $\nu = 1 + 3n$  [5]. We plot the calculated polarization vector for the lowest TE-like band [Fig 3(e)]. The polarization ellipse now winds only once in the opposite direction around the  $\Gamma$  point, indicating  $\nu$  of the at- $\Gamma$  BIC changes from  $-2$  to  $+1$ . Since the present PhC is no longer invariant under  $C_2$  symmetry, the change of  $\nu$  may generate six CPSs with  $\nu = -1/2$  through the charge conservation. This prediction is indeed confirmed in Fig. 3(e). We find that the polarization ellipse winds by  $-\pi$  around six CPSs. The

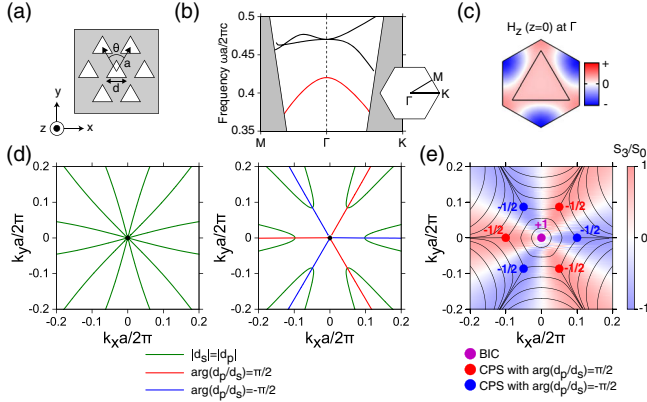


FIG. 3. (a) A triangular-lattice PhC with triangular air holes. (b) Calculated TE-like band structure. (c) Mode profile in the unit cell for the lowest TE-like band. (d) Lines for  $|d_s|=|d_p|$  (green) and  $\delta = \pm\pi/2$  (red and blue) for PhCs with circular (left) and triangular (right) holes. (e) Calculated polarization vector and normalized Stokes parameter  $S_3/S_0 = 2|d_s||d_p| \sin \delta / (|d_s|^2 + |d_p|^2)$ . The attached numbers denote topological charges  $\nu$ .

half-winding indicates  $\nu = -1/2$ . Among the six CPSs, three CPSs are left-handed with  $\delta = \pi/2$  [ $\delta \equiv \arg(d_p/d_s)$ ] and the others are right-handed with  $\delta = -\pi/2$ , which is explained by the conservation of  $\nu_{\pm}$ .

For better understanding, we plot lines for  $|d_s|=|d_p|$  (Lines A) and  $\delta = \pm\pi/2$  (Lines B). For the circular-hole PhC [Fig. 3(d) left], Lines A emerge between the lines for  $d_s = 0$  and  $d_p = 0$  [30]. Lines B do not exist due to the  $C_2$  symmetry. For the triangular-hole PhC [Fig. 3(d) right], the degeneracy of Lines A at the  $\Gamma$  point is lifted, and Lines B emerge. The six intersections between Lines A and B

correspond to CPSs, which guarantees the topological protection of CPSs in a similar way to that of BICs [5].

Finally, we vary the angle  $\theta$  from  $60^\circ$  to introduce the uniaxial deformation. It is expected from the conservation of  $\nu_{\pm}$  that perturbations breaking the  $C_3$  symmetry splits the at- $\Gamma$  BIC into two CPSs with the same charge  $+1/2$  and opposite handedness [Figs. 4(a) and 4(d)]. For  $\theta > 60^\circ$  ( $\theta < 60^\circ$ ), the CPS with  $\delta = -\pi/2$  splits in the direction of  $k_x > 0$  ( $k_x < 0$ ). As the perturbation is increased, two CPSs with opposite charges and the same handedness approach [Figs. 4(b) and 4(e)] and eventually collide with each other, resulting in pair annihilation of CPSs [Figs. 4(c) and 4(f)]. Finally, the two pairs of CPSs with charge  $-1/2$  and opposite handedness survive. Note that these two pair of CPSs can be regarded as generated from the off- $\Gamma$  BICs in Figs. 2(b) and 4(c) as a result of breaking  $C_2$  symmetry. Let us point out that all through these processes [Figs. 4(a)–(f)], the topological charges  $\nu_{\pm}$  are consistently conserved and prove that conventional topological charges  $\nu$  are not sufficient for explaining the results.

In conclusion, we have demonstrated deterministic generation of off- $\Gamma$  BICs and a variety of ways to generate and annihilate CPSs by using a single at- $\Gamma$  BIC with charge  $-2$  and perturbations that lower the symmetry of PhCs. All processes are successfully explained by the charge conservation for handedness-wise topological charges  $\nu_{\pm}$ . This clearly demonstrates the wide applicability of the charge conservation of  $\nu_{\pm}$  for far-field topological photonics by PhCs and guarantees the stability of their polarization singularities in parameter spaces. As another possibility, the accidental merging of two CPSs with opposite handedness and opposite charges causes accidental BICs without any in-plane symmetry [16]. The merging of two CPSs with

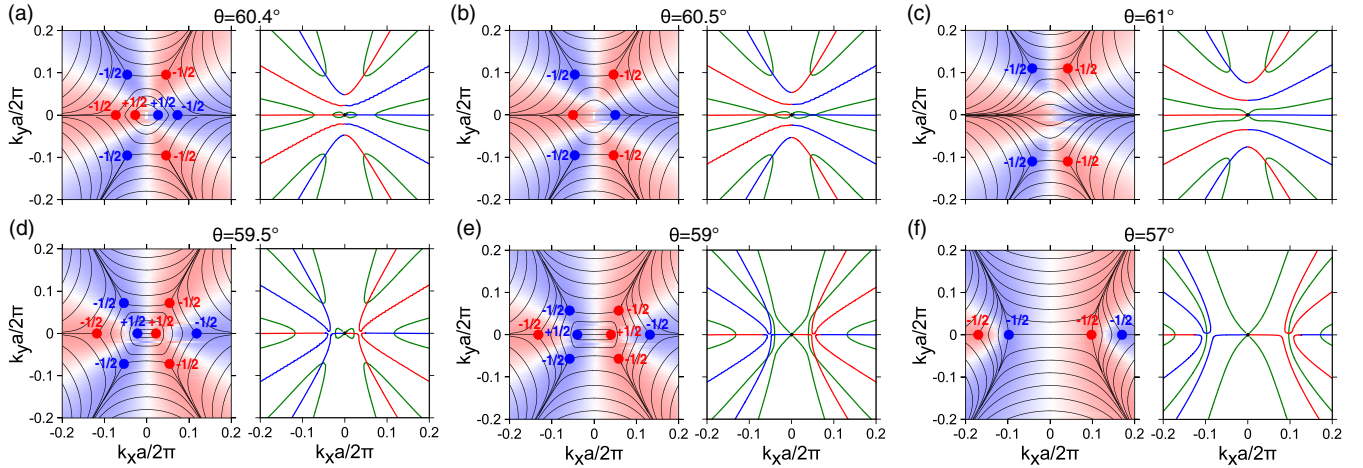


FIG. 4. Evolution of CPSs. In (a)–(f), left panels show calculated polarization vector and normalized Stokes parameter  $S_3/S_0$ , and right panels show lines for  $|d_s|=|d_p|$  (green) and  $\delta = \pm\pi/2$  (red and blue). For (a)  $\theta = 60.4^\circ$  and (d)  $\theta = 59.5^\circ$ , the at- $\Gamma$  BIC ( $\nu = +1$ ) split into two CPSs ( $\nu = +1/2$ ). For (b)  $\theta = 60.5^\circ$  and (e)  $\theta = 59^\circ$ , two CPSs with opposite charges and the same handedness approach each other. For (c)  $\theta = 61^\circ$  and (f)  $\theta = 57^\circ$ , two CPSs with opposite charges and the same handedness collide, and then they annihilate by the collision. In (a)–(f), one of five lines for  $\delta = \pm\pi/2$  is pinned at the  $\Gamma$  point due to  $\sigma T$  symmetry (see Sec. S2 in the Supplemental Material [29]).

the same handedness and same charge may generate a higher-order CPS with  $|\nu| \geq 1$ . Practically, our findings suggest a novel method for creating various polarization singularities of far-field radiations such as circularly polarized light emission [50–52]. This novel way for generating off- $\Gamma$  BICs will be especially promising for on-chip vortex-beam steering [17,18] and dynamic tuning of a quality factor [44].

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*Correction:* A byline footnote has been added for the second author.