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Circularly polarized states and propagating bound states in the continuum in a periodic array of cylinders

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Bound states in the continuum (BICs) in a periodic structure sandwiched between two homogeneous media have interesting properties and useful applications in photonics. The topological nature of BICs was previously revealed based on a topological charge related to the far-field polarization vector of the surrounding resonant states. Recently, it was established that when symmetry-protected BICs (with a nonzero topological charge) are destroyed by generic symmetry-breaking perturbations, pairs of circularly polarized resonant states (CPSs) emerge and the net topological charge is conserved. A periodic structure can also support propagating BICs with a nonzero wave vector. These BICs are not protected by symmetry in the sense of symmetry mismatch, but they need symmetry for their robust existence. Based on a highly accurate computational method for a periodic array of slightly noncircular cylinders, we show that a propagating BIC is typically destroyed by a structural perturbation that breaks only the in-plane inversion symmetry, and when this happens, a pair of CPSs of opposite handedness emerge so that the net topological charge is conserved. We also study the generation and annihilation of CPSs when a structural parameter is varied. It is shown that two CPSs with opposite topological charge and the same handedness, connected to two BICs or in a continuous branch from one BIC, may collapse and become a CPS with a zero charge. Our study clarifies the important connection between symmetry and topological charge conservation.

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I. INTRODUCTION

Bound states in the continuum (BICs) are trapped or guided modes with their frequencies in the radiation continua [1,2]. They exist in a variety of photonic structures including periodic structures sandwiched between two homogeneous media [3–13], waveguides with local defects [14,15], waveguides with lateral leakage channels [16–20], etc. In structures that are invariant or periodic in one or two spatial directions, a BIC is a special point with an infinite quality factor ($Q$ factor) in a band of resonant states [11,21–23], and it becomes a high-$Q$ resonance if the structure is perturbed generically [24,25]. High-$Q$ resonances lead to strong local field enhancement [26–28] and abrupt features in reflection and transmission spectra [29], and they are essential for sensing, lasing, switching, and nonlinear optics applications.

For theoretical interest and practical applications, it is important to understand how a BIC is affected by a perturbation of the structure. If the BIC is protected by a symmetry [3–8,14,15], i.e., there is a symmetry mismatch between the BIC and the compatible radiation modes, it naturally continues its existence if the perturbation preserves the symmetry [3,14,30]. Therefore, a symmetry-protected BIC is robust with respect to symmetry-preserving perturbations. If a perturbation breaks the symmetry, a symmetry-protected BIC typically, but not always, becomes a resonant state with a finite $Q$ factor [24,25,31]. In periodic structures sandwiched between two homogeneous media, there are also BICs with a nonzero Bloch wave vector (off-$\Gamma$ BICs), and they propagate in the periodic directions [9–12,29,32,33]. Such a propagating BIC is not protected by symmetry in the usual sense, but it can also be robust with respect to symmetry-preserving perturbations [34–36]. More precisely, in a periodic structure with an up-down mirror symmetry and an in-plane inversion symmetry, a generic low-frequency propagating BIC (with only one radiation channel) continues its existence if the structure is perturbed by a perturbation preserving these two symmetries [35,36].

The BICs in periodic structures exhibit interesting topological properties. Zhen et al. [34] realized that a BIC in a biperiodic structure is a polarization singularity in momentum space (the plane of two wave-vector components), and they defined a topological charge based on the winding number of the far-field polarization vector. Since the far field of a resonant state is typically elliptically polarized, Bulgakov and Makismov refined the definition using the major polarization vector [32]. The topological charge can be used to classify the BICs and illustrate their generation, interaction, and annihilation processes when structural parameters are tuned [32,34]. Importantly, the topological charge is a conserved quantity that cannot be changed by small structural perturbations. However, this does not imply that the BICs (with a nonzero topological charge) are robust with respect to arbitrary structural perturbations, because a resonant state can be circularly...
polarized and also has a nonzero topological charge. In a recent work, Liu et al. [37] showed that symmetry-protected at-Γ BICs in a photonic crystal slab, with topological charge ±1 and protected by the in-plane inversion symmetry, turn to pairs of circularly polarized resonant states (CPSs) when the structure is perturbed breaking the symmetry. Yoda and Notomi [38] considered an at-Γ symmetry-protected BIC with topological charge −2 in a photonic crystal slab, and they showed that CPSs or off-Γ BICs may emerge when the symmetry of the structure is lowered. For frequencies above the diffraction limit, the BICs and CPSs can also be connected when structure parameters are varied without breaking any symmetry [39].

Most propagating BICs are found in periodic structures with both up-down mirror symmetry and in-plane inversion symmetry. It is known that if one of these two symmetries is broken, a propagating BIC is usually, but not always, destroyed [31,33]. It has been shown that CPSs can exist in periodic structures when both up-down mirror symmetry and in-plane inversion symmetry are broken [40]. In this paper, we show that CPSs emerge when propagating BICs are destroyed by generic and arbitrarily small perturbations that break only the in-plane inversion symmetry.

Unlike the previous works for photonic crystal slabs [37–39], we focus on a structure with one-dimensional periodicity. We consider vectorial BICs in a periodic array of dielectric cylinders, introduce a small deformation of the cylinder boundary, and show that pairs of CPSs emerge when propagating BICs with topological charge ±1 are destroyed. In addition, we follow the CPSs as the deformation parameter is further increased, and we show that two CPSs with opposite topological charges may emerge and all plane waves can be connected in the structure is perturbed breaking the symmetry. Yoda and Notomi [38] showed that symmetry-protected BICs may emerge when the symmetry of the structure is lowered. For frequencies above the diffraction limit, the BICs and CPSs can also be connected when structure parameters are varied without breaking any symmetry [39].

The other four field components can be obtained from the following equations:

\[
\begin{align*}
\tilde{E}_y & = \frac{i}{\eta} (\alpha \tilde{H}_x + k P \cdot \nabla \tilde{H}_z), \\
\tilde{E}_z & = \frac{i}{\eta} (\alpha \tilde{H}_x - k P \cdot \nabla \tilde{E}_y).
\end{align*}
\]

If \(\alpha = 0\), the equations for \(E_x\) and \(\tilde{H}_x\) are decoupled, and we say the corresponding wave is scalar. The case \(\alpha \neq 0\) is referred to as vectorial.

Due to the periodicity in \(y\), any eigenmode of the structure is a Bloch mode with an electric field given by

\[
E(r) = F(r) e^{i\beta y},
\]

where \(\beta\) is a real Bloch wave number satisfying \(|\beta| \leq \pi/L\), and \(F\) is periodic in \(y\) with period \(L\). For \(|z| > D\), the field can be expanded in plane waves as

\[
E(r) = \sum_{m=-\infty}^{\infty} c_m e^{i(\beta_0 y + \gamma_m z)}, \quad |z| > D,
\]

where \(\beta_0 = \beta\), and

\[
\beta_m = \beta + \frac{2\pi m}{L}, \quad \gamma_m = \sqrt{k^2 - \alpha^2 - \beta_m^2}.
\]

A guided mode satisfies the condition \(E \to 0\) as \(z \to \pm \infty\) for a positive \(k\). A guided mode usually exists when \(k > \sqrt{\alpha^2 + \beta^2}\), so that all \(\gamma_m\) are pure imaginary, and all plane waves on the right-hand side of Eq. (7) are evanescent in \(z\). A BIC is also a guided mode, but it satisfies the condition \(k > \sqrt{\alpha^2 + \beta^2}\); thus \(\gamma_0\) and probably a few other \(\gamma_m\) are real positive. We study BICs with a real \(k\), a real \(\alpha\), and a real \(\beta\) such that

\[
\sqrt{\alpha^2 + \beta^2} < k < \sqrt{\alpha^2 + \left(\frac{2\pi}{L} - |\beta|\right)^2}.
\]

The above condition implies that \(\gamma_0\) is positive and all other \(\gamma_m\) are pure imaginary. Since the plane waves \(\exp[i(\beta_0 y + \gamma_m z)]\) can propagate to infinity, the coefficients \(c_m\) of the BIC must vanish.

A resonant state is also an eigenmode, but it satisfies an outgoing radiation condition as \(z \to \pm \infty\). Because of the radiation loss, the amplitude of a resonant state decays in time, thus the frequency \(\omega\) or \(k\) must be complex with a
negative imaginary part. This implies that the real and imaginary parts of \( \gamma_0 \) are positive and negative, respectively, and \( \exp[i(\theta_0 + \gamma_0 z)] \) is an amplifying outgoing plane wave as \( z \to +\infty \). We are concerned with resonant states with only one radiating plane wave for either \( z > D \) or \( z < -D \). Therefore, it is assumed that \( \text{Im}(\gamma_0) > 0 \) for all \( m \neq 0 \). Resonant states form bands where each band corresponds to \( k \) being a complex-valued function of \( \alpha \) and \( \beta \). The \( Q \) factor of a resonant mode is given by \( Q = -0.5 \text{Re}(k)/\text{Im}(k) \). A BIC is a special point (with a real \( k \)) in a band of resonant states.

We assume the periodic structure has an up-down mirror symmetry, i.e., \( \varepsilon(\mathbf{r}) = \varepsilon(\mathbf{v}, -z) \) for all \( \mathbf{r} \). It is then sufficient to study the field of any eigenmode in the upper half-space (\( z > 0 \)), because the field components are either even in \( z \) or odd in \( z \). For a BIC with a frequency and wave vector satisfying Eq. (9), it is possible to define a topological charge based on the far-field polarization vector of the surrounding resonant states [32,34]. Let \( C \) be a closed contour in the \( \alpha-\beta \) plane. Each point on \( C \) corresponds to a resonant state in a band that contains the BIC. The resonant state contains a far-field outgoing plane wave (for \( z \to +\infty \)) with a vector amplitude \( \mathbf{c}_{0z}^{+} \). Its projection on the \( x-y \) plane is

\[
\mathbf{E} = \begin{bmatrix} c_{0x}^{+} \\ c_{0y}^{+} \end{bmatrix} e^{i(\alpha x + \beta y + \gamma_0 z)}, \tag{10}
\]

where \( c_{0x}^{+} \) and \( c_{0y}^{+} \) are the \( x \) and \( y \) components of \( \mathbf{c}_{0z}^{+} \). For any fixed \( z > D \), the real projected electric field \( \text{Re}(\mathbf{E}e^{-i\omega t}) \) is typically elliptically polarized, and the major polarization vector (along the major axis of the polarization ellipse) forms an angle \( \theta \) with the \( x \) axis. If it is possible to define \( \theta \) continuously as \( (\alpha, \beta) \) traverses along \( C \) in a counterclockwise direction from a starting point back to the same point (the ending point), and \( \theta|_{\text{end}} - \theta|_{\text{start}} = 2\pi q \) for some \( q \), where \( \theta|_{\text{start}} \) and \( \theta|_{\text{end}} \) are the values of \( \theta \) at the starting point and the ending point, respectively, then \( q \) is the winding number (of the projected major polarization vector) on \( C \). Alternatively, \( q \) can be evaluated by the integral formula

\[
q = \frac{1}{2\pi} \oint_C d\alpha \cdot \nabla_\alpha \theta(\alpha), \tag{11}
\]

where \( \alpha = (\alpha, \beta) \) and \( \nabla_\alpha = (\partial_\alpha, \partial_\beta) \). A BIC is a polarization singularity, since it does not have a far field (\( \mathbf{c}_{0z}^{+} = 0 \)). The topological charge of a BIC is defined as the winding number \( q \) if \( C \) is sufficiently close to the BIC and encloses the BIC in the \( \alpha-\beta \) plane [32,34].

It is important to note that the major polarization vector or the angle \( \theta \) is undefined if the projected far-field plane wave is circularly polarized. This implies that a circularly polarized state (CPS), i.e., a resonant state with a circularly polarized projected far field, is also a polarization singularity. If \( C \) contains the wave vector of a CPS, the winding number on \( C \) is undefined. The definition of topological charge requires the underlying assumption that no CPSs exist in a small neighborhood (in the \( \alpha-\beta \) plane) of the BIC. Since the definition is based on the projected field given in Eq. (10), the far field of a CPS is not really circularly polarized, only the projection of the far field onto the \( xy \) plane is circular. It is possible to avoid the projected field and use the true polarization vector to define the topological charge [38]. The resulting CPSs are different, but the topological charge for any BIC remains the same.

Finally, we recall that the polarization state of the plane wave given by Eq. (10) can be characterized by the Stokes parameters [41]

\[
S_0 = |c_{0x}^{+}|^2 + |c_{0y}^{+}|^2, \quad S_1 = |c_{0x}^{+}|^2 - |c_{0y}^{+}|^2, \tag{12}
\]

\[
S_2 = 2|c_{0x}^{+}|^2 \cos(\varphi_x - \varphi_c), \tag{13}
\]

\[
S_3 = 2|c_{0x}^{+}|^2 \sin(\varphi_y - \varphi_c), \tag{14}
\]

where \( \varphi_x = \arg(c_{0x}^{+}) \) and \( \varphi_y = \arg(c_{0y}^{+}) \) are the phases of \( c_{0x}^{+} \) and \( c_{0y}^{+} \), respectively. Since a BIC has no radiation, it corresponds to the point \((S_0, S_1, S_2, S_3) = 0 \). A CPS satisfies the condition \((S_1, S_2, S_3)/S_0) = (0, 0, +1) \), where the ellipticity \( S_3/S_0 = +1 \) for the left CPS and \( -1 \) for right CPS. A linearly polarized state is any point with \( S_3 = 0 \). The principal value of angle \( \theta \) is given by \( \theta = \arg(S_1 + iS_2)/2 \).

**III. CIRCULAR CYLINDERS**

A periodic array of circular dielectric cylinders surrounded by air, as shown in Fig. 1, is a simple structure supporting many different BICs [7,12,29,30,32]. In general, a BIC may be a standing wave \((\alpha = \beta = 0)\), may propagate along the \( y \) axis \((\alpha = 0 \text{ and } \beta \neq 0)\), along the \( x \) axis \((\alpha \neq 0 \text{ and } \beta = 0)\), or in both \( x \) and \( y \) directions \((\alpha \neq 0 \text{ and } \beta \neq 0)\). Those BICs with \( \alpha = 0 \) are scalar ones with either the \( H \) or \( E \) polarization. The BICs with \( \alpha \neq 0 \) are vectorial ones with nonzero \( E_x \) and \( H_z \). In Table I, we list four BICs for periodic arrays with a fixed dielectric constant \( \varepsilon_r = 15 \). The topological charges of the BICs are listed in the last column. More BICs in this periodic array can be found in Ref. [32].

**TABLE I. A few BICs in periodic arrays of circular cylinders with radius \( a \) and dielectric constant \( \varepsilon_r = 15 \).**

| BIC   | \( a/L \) | \( aL \) | \( \beta L \) | \( \kappa L \) | \( q \) |
|-------|----------|---------|---------|---------|-----|
| BIC1  | 0.45042  | 0       | 0       | 3.512894| -1  |
| BIC2  | 0.45042  | 0.584168| 0       | 3.523918| +1  |
| BIC3  | 0.45     | 0       | 0.479401| 3.471973| +1  |
| BIC4  | 0.3      | 1.190401| 0.96714 | 3.196556| +1  |
Normally, the resonant states and the BICs are computed by solving an eigenvalue problem for Maxwell’s equations. To take advantage of the special geometry of the circular cylinders, we use a semianalytic method based on cylindrical wave expansions. Since the structure is invariant in $x$ and periodic in $y$, it is sufficient to solve the eigenmodes in one period of the structure, i.e., a 2D domain $\Omega_\infty$ given by $|y| < L/2$ and $|z| < \infty$. Inside $\Omega_\infty$, there is a square $\Omega$ given by $|y| < L/2$ and $|z| < L/2$. We assume one cylinder is located at the center of $\Omega$. For given $\alpha$ and $\omega$, the electromagnetic field in $\Omega$ can be expanded in vectorial cylindrical waves with unknown coefficients [42]. If $\beta$ is also specified, we can expand the electromagnetic field in plane waves (also with unknown coefficients) for $|z| > L/2$. Relating the field at $y = \pm L/2$ by the quasiperiodic condition, assuming even or odd symmetry in $y$, and imposing continuity conditions at $z = L/2$, we can obtain an operator $\mathcal{A}$, such that

$$\mathcal{A}(k, \alpha, \beta) u|_{z=L/2} = 0, \quad (15)$$

where $u$ is a column vector for $E_x$ and $H_z$, and $u|_{z=L/2}$ denotes $u$ at $z = L/2$ for $|y| < L/2$. Notice that $\mathcal{A}$ is an operator that acts on a vector of two single-variable functions. Since $\mathcal{A}$ depends on $k$, Eq. (15) is a nonlinear eigenvalue problem. In practice, $y \in (-L/2, L/2)$ is sampled by $N$ points, $u|_{z=L/2}$ becomes a vector of length $2N$, and $\mathcal{A}$ is approximated by a $(2N) \times (2N)$ matrix. The method can be extended to the case in which the boundaries of the cylinders are slightly and smoothly deformed. Details are given in the Appendix.

For computing resonant states, $\alpha$ and $\beta$ are given, and we look for a complex $k$ such that Eq. (15) has a nontrivial solution. One possible approach is to solve $k$ from

$$\lambda_1(\mathcal{A}) = 0, \quad (16)$$

where $\lambda_1$ is the eigenvalue of $\mathcal{A}$ with the smallest magnitude. A BIC is a special resonant state with $\text{Im}(\lambda(k)) = 0$. For propagating BICs, it is more efficient to treat $\alpha$ and/or $\beta$ also as unknowns. We can solve Eq. (16) for a real $k$, a real $\alpha$, and/or a real $\beta$.

**IV. SLIGHTLY NONCIRCULAR CYLINDERS**

In this section, we consider a periodic array of slightly noncircular cylinders, we study the emergence of CPSs when propagating BICs are destroyed, and also the annihilation and generation of CPSs. We assume that the boundary of the cylinder centered at the origin is given by

$$y = -a \sin(\tau) + \delta \cos(\tau), \quad z = a \cos(\tau) \quad (17)$$

for $0 \leq \tau < 2\pi$ and $g = 2$ or 4, where $\delta > 0$ is a small deformation parameter. The dielectric constant of the cylinders is fixed at $\varepsilon_c = 15$. The deformed cylinders for $\delta = 0.1a$ are shown in Figs. 2(a) and 2(b) for $g = 2$ and 4, respectively. The small boundary deformation is a perturbation that breaks the reflection symmetry in $y$ (the in-plane inversion symmetry), but it preserves the reflection symmetry in $z$ (the up-down mirror symmetry).

To calculate vectorial resonant states, we extend the method described in the previous section. Importantly, a general electromagnetic field in $\Omega$ (the square domain containing one cylinder centered at the origin) can still be expanded in cylindrical waves, although the expansions are more complicated due to the deformation of the cylinder boundary. As shown in the Appendix, the eigenvalue problem for resonant states is reduced to Eq. (15), where $\mathcal{A}$ is a $(2N) \times (2N)$ matrix depending on $k$, $\alpha$, and $\beta$, and $N$ is the number of sampling points for an interval of length $L$. It is highly desirable to compute a CPS without calculating all nearby resonant states. To find a left or right CPS, we solve a real $\alpha$, a real $\beta$, and a complex $k$, from Eq. (16) and

$$S_1 = 0, \quad S_3/S_0 = \pm 1, \quad (18)$$

where $S_0$, $S_1$, and $S_3$ are the Stokes parameters.

First, we show that when the deformation parameter $\delta$ is increased from zero, all four BICs listed in Table I are destroyed and pairs of CPSs emerge. If the topological charge of the BIC is 1 (or $-1$), a pair of CPSs with topological charge 1/2 (or $-1/2$) and different handedness emerge. The net topological charge is conserved. In Fig. 3, we show the emergence of CPSs from BIC$_1$ for a periodic array with $a = 0.45L$ and $g = 4$. The purple arrows indicate the direction of increasing $\delta$. The curve shows the wave vector $(\alpha, \beta)$ for a pair of left and right CPSs, and it is shown in color to indicate the value of $\delta$. These two CPSs exhibit a symmetry with respect to the $\beta$ axis. For each left CPS with wave vector $(\alpha, \beta)$, there is also a right CPS with wave vector $(-\alpha, \beta)$. The complex frequencies of these two CPSs are exactly the same. In Figs. 4(a) and 4(b), we show CPSs that emerged from BIC$_4$ for periodic arrays

![Fig. 2](image2.png) **FIG. 2.** Cross sections $\Omega_1$ of two deformed cylinders with a boundary given by Eq. (17) for $\delta = 0.1a$ and the cases (a) $g = 2$ and (b) $g = 4$. $\Omega_2$ is the exterior domain outside the cylinder and inside the square $\Omega = (-L/2, L/2) \times (-L/2, L/2)$.

![Fig. 3](image3.png) **FIG. 3.** A pair of CPSs with topological charge 1/2 that emerged from BIC$_1$ for a periodic array of slightly noncircular cylinders with $g = 4$. 

![Fig. 4](image4.png)
CPS with a zero charge. BIC1 and BIC2 in Table I are found from BICs of opposite topological charge may collapse to a invariant in x vectors (respectively. As slightly noncircular cylinders with (a) are deformed cylinders with \( \delta > \delta_{GP} \), with \( \delta_{GP} \) being a self-generation point. However, annihilation and generation are relative terms depending on how the structure is tuned. For example, \( \delta_{GP} \) can also be regarded as a self-annihilation point if the structure is tuned by a decreasing \( \delta \). It is clear that the continuous branch of CPSs that emerged from BIC3, as shown in Fig. 6(a), exhibits a multivalued dependence on \( \delta \). In Figs. 6(b), 6(c) and 6(d), we show, respectively, the \( Q \) factor and the wave-vector components \( \alpha \) and \( \beta \) as multivalued functions of \( \delta \). Despite the generation and annihilation of CPSs as \( \delta \) is varied, the net topological charge is conserved and remains at 1/2.

V. CONCLUSION

Many applications of BICs are realized in periodic structures sandwiched between two homogeneous media. It is known that the existence and robustness of BICs, including the propagating BICs in periodic structures, depend crucially on symmetry \([11,34]\). More precisely, it has been proved that some propagating BICs are robust with respect to structural perturbations that preserve the in-plane inversion symmetry and the up-down reflection symmetry, even though these BICs do not have a symmetry mismatch with compatible radiating waves \([35,36]\). If the perturbation breaks one of these two symmetries, the propagating BICs are typically destroyed and become resonant states with a finite \( Q \) factor \([33]\). The

FIG. 4. Pairs of CPSs that emerged from BIC4 for periodic arrays of slightly noncircular cylinders with (a) \( g = 2 \) and (b) \( g = 4 \).

FIG. 5. Emergence of CPSs from BIC1 and BIC2, and annihilation of CPSs of opposite charges for periodic arrays of slightly noncircular cylinders with (a) \( g = 2 \) and (b) \( g = 4 \).

FIG. 6. (a) A continuous right CPS emerged from BIC3 for a periodic array with \( g = 2 \), with \( \delta \) increased from 0 to \( \delta_{AP} \), decreased to \( \delta_{GP} \), and increased again. The topological charge of the CPS has changed from 1/2 to \(-1/2\) and back to 1/2 accordingly. (b) The \( Q \) factor, (c) \( \alpha \), and (d) \( \beta \) of the right CPS as multivalued functions of \( \delta \). The blue and red curves correspond to topological charge 1/2 and \(-1/2\), respectively.

The topological charge of the CPS has changed from 1/2 to \(-1/2\), and back to 1/2 accordingly. In the process of an increasing \( \delta \), the critical value \( \delta_{AP} \) is the annihilation point where two CPSs of opposite topological charge and the same handedness collapse to a CPS with a zero charge, but these two CPSs are not connected to different BICs. In fact, the CPS with topological charge \(-1/2\) and another CPS with topological charge 1/2 emerge from a CPS of zero topological charge at \( \delta_{GP} \). We call \( \delta_{AP} \) a self-annihilation point and \( \delta_{GP} \) a self-generation point. However, annihilation and generation are relative terms depending on how the structure is tuned. For example, \( \delta_{GP} \) can also be regarded as a self-annihilation point if the structure is tuned by a decreasing \( \delta \). It is clear that the continuous branch of CPSs that emerged from BIC3, as shown in Fig. 6(a), exhibits a multivalued dependence on \( \delta \). In Figs. 6(b), 6(c) and 6(d), we show, respectively, the \( Q \) factor and the wave-vector components \( \alpha \) and \( \beta \) as multivalued functions of \( \delta \). Despite the generation and annihilation of CPSs as \( \delta \) is varied, the net topological charge is conserved and remains at 1/2.
topological charge of a BIC, defined using the polarization vector of the resonant states surrounding the BIC in momentum space, is an interesting concept and is useful for understanding the evolution of BICs as structural parameters are varied [32,34]. The definition of topological charge does not require in-plane inversion symmetry. When structural parameters are varied, the topological charge is always conserved, but this does not imply that the BICs are robust with respect to arbitrary structural perturbations, because a CPS is also a polarization singularity in momentum space and it can have a nonzero topological charge. Therefore, the conservation of topological charge is only valid when both BICs and CPSs are included. For propagating BICs, the connection between symmetry-breaking perturbations and the emergence of CPSs has not been clearly established in the existing literature. Using a periodic array of slightly noncircular cylinders as an example, we show that pairs of CPSs emerge when propagating BICs are destroyed by arbitrarily small perturbations that break only the in-plane inversion symmetry. We also study the generation and annihilation of CPSs when structural parameters are varied. It is shown that pairs of CPSs of opposite topological charge can collapse at special CPSs with a zero topological charge, but the net topological charge is still conserved.

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APPENDIX: CONSTRUCTION OF MATRIX $\mathcal{A}$

To obtain a matrix $\mathcal{A}$ satisfying Eq. (16) for the case of a periodic array of slightly noncircular cylinders, we need to find cylindrical wave solutions that are valid inside and outside a single cylinder, determine a matrix $\mathcal{C}$ mapping $\mathbf{u}$ to the normal derivative of $\mathbf{u}$ on $\partial \Omega$ (the boundary of $\Omega$), and finally construct the matrix $\mathcal{A}$. As shown in Fig. 2, $\Omega_1$ is a subdomain of $\Omega$ corresponding to the cross section of the cylinder, $\Omega_2=\Omega_1$, $e(\mathbf{r})=e_1$ or $e_2$ for $\mathbf{r} \in \Omega_1$ or $\Omega_2$, respectively. The boundary of $\Omega_1$ is $\Gamma$.

For given $k$ and $\alpha$ and an integer $p$, we construct a vectorial cylindrical wave solution that depends on two arbitrary coefficients $c_p$ and $r_p$. The $x$ components of this solution are assumed to be

$$E_x^{(p)} = \begin{cases} \sum a_{pq} J_{\rho_j(p)}(\rho) e^{i \rho \theta}, & \mathbf{r} \in \Omega_1, \\ c_p J_{\rho_j(p)}(\rho) e^{i \rho \theta} \left[ \sum b_{pq} Y_{\rho_j(p)}(\rho) e^{i \rho \theta} \right], & \mathbf{r} \in \Omega_2, \end{cases}$$

$$H_x^{(p)} = \begin{cases} \sum a_{pq} J_{\rho_j(p)}(\rho) e^{i \rho \theta}, & \mathbf{r} \in \Omega_1, \\ r_p J_{\rho_j(p)}(\rho) e^{i \rho \theta} \left[ \sum t_{pq} Y_{\rho_j(p)}(\rho) e^{i \rho \theta} \right], & \mathbf{r} \in \Omega_2, \end{cases}$$

where $\rho$ and $\theta$ are the polar coordinates of $\mathbf{r}$, $\rho_j=(k^2 \varepsilon_j - \alpha^2)^{1/2}$, $\alpha$ is the radius of the circle to which $\Gamma$ is close, $J_{\rho_j}$ and $Y_{\rho_j}$ are the first and second kinds of Bessel functions of order $p$, the sums are for $q$ from $-\infty$ to $+\infty$, and $a_{pq}$, $b_{pq}$, $s_{pq}$, and $t_{pq}$ (for all $q$) are unknown coefficients.

Let $v=(v_x, v_y)$ be the outward unit vector normal to $\Gamma$, and let $\tau=(-v_x, v_y)$ be a unit vector tangential to $\Gamma$. Then the tangential field components of this cylindrical wave solution are

$$H_t^{(p)} = i \frac{\partial E_z^{(p)}}{\partial v} + \frac{\gamma_0}{k} \frac{\partial H_x^{(p)}}{\partial \tau},$$

$$E_t^{(p)} = i \frac{\partial H_z^{(p)}}{\partial v} - \frac{\gamma_0}{k} \frac{\partial E_x^{(p)}}{\partial \tau}. \quad (A1)$$

We discretize $\Gamma$ using $M$ points (assuming $M$ is odd) and truncate the sums by $|q| \leq (M-1)/2$. The continuity conditions of $E_x, H_x, E_z,$ and $H_t$ at those $M$ points on $\Gamma$ give rise to the following linear system:

$$\begin{bmatrix} A_{11} & A_{12} & 0 & 0 \\ 0 & 0 & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix} \begin{bmatrix} a_{p} \\ b_{p} \\ s_{p} \\ t_{p} \end{bmatrix} = \begin{bmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \end{bmatrix} + \frac{r_p}{h_2} \begin{bmatrix} 0 \\ h_3 \\ h_3 \\ h_4 \end{bmatrix},$$

where $A_{jk}$ for $1 \leq j, k \leq 4$ are $M \times M$ matrices; $g_j$ and $h_j$ for $1 \leq j \leq 4$ are column vectors of length $M$; $a_p, b_p, s_p, t_p$ are also column vectors of length $M$; $a_p$ is the vector for all $a_{pq}$; etc. Solving the above linear system, we obtain column vectors $f_{jk}^{(p)}$ for $1 \leq j, k \leq 2$, such that

$$b_p = c_p f_{11}^{(p)} + r_p f_{12}^{(p)}, \quad t_p = c_p f_{21}^{(p)} + r_p f_{22}^{(p)}. \quad (A3)$$

Therefore, the cylindrical wave solution can be written as $\mathbf{u}_p = c_p \mathbf{u}_p^{(1)} + r_p \mathbf{u}_p^{(2)}$, where $\mathbf{u}_p^{(1)}$ and $\mathbf{u}_p^{(2)}$ are completely determined.

The general field in $\Omega$ can be expanded in the above cylindrical waves as

$$\mathbf{u} = \sum_{p=-\infty}^{\infty} \mathbf{u}_p = \sum_{p=-\infty}^{\infty} \left( c_p \mathbf{u}_p^{(1)} + r_p \mathbf{u}_p^{(2)} \right). \quad (A4)$$

If $\partial \Omega$ is sampled by $4N$ points, we can truncate the index $p$ in the sum above to $-2N \leq p \leq 2N - 1$, and evaluate $\mathbf{u}$ and the normal derivative of $\mathbf{u}$ at the $4N$ points on $\partial \Omega$. This leads to $(8N) \times (8N)$ matrices $\mathcal{D}_1$ and $\mathcal{D}_2$ such that

$$\left. \mathbf{u} \right|_{\partial \Omega} = \mathcal{D}_1 \left[ \left. \mathbf{c} \right|_r \right], \quad \left. \frac{\partial \mathbf{u}}{\partial v} \right|_{\partial \Omega} = \mathcal{D}_2 \left[ \left. \mathbf{c} \right|_r \right]. \quad (A5)$$

where $\mathbf{u}|_{\partial \Omega}$ and $\partial_r \mathbf{u}|_{\partial \Omega}$ are column vectors of length $8N$, and $\mathbf{c}$ and $\mathbf{r}$ are column vectors of length $4N$ with entries $c_p$ and $r_p$, respectively. For simplicity, $\partial_r$ is simply taken to be $\partial_r$ or $\partial_\theta$ on the horizontal and vertical sides of $\Omega$. Therefore, we have matrix $\mathcal{C} = \mathcal{D}_2 \mathcal{D}_1^{-1}$, such that

$$\frac{\partial \mathbf{u}}{\partial v} \bigg|_{\partial \Omega} = \mathcal{C} \left. \mathbf{u} \right|_{\partial \Omega}. \quad (A6)$$

If $\beta$ is given, $\mathbf{u}$ and $\partial_\theta \mathbf{u}$ satisfies the following quasiperiodic condition:

$$\mathbf{u} \big|_{y=L/2} = e^{i \beta \theta} \mathbf{u} \big|_{y=-L/2}, \quad (A7)$$

$$\frac{\partial \mathbf{u}}{\partial y} \bigg|_{y=L/2} = e^{i \beta \theta} \frac{\partial \mathbf{u}}{\partial y} \bigg|_{y=-L/2}. \quad (A8)$$
Since the structure has up-down mirror symmetry, we have either $u(y, z) = u(y, -z)$ or $u(y, z) = -u(y, -z)$. Substituting these conditions into Eq. (A6), we obtain a matrix $\mathcal{R}_0$ such that

$$\frac{\partial u}{\partial z} \bigg|_{z=L/2} = \mathcal{R}_0 u \bigg|_{z=L/2}. \quad (A9)$$

For $z > L/2$, the field can be expanded in plane waves as in Eq. (7). Using the plane-wave expansion for $u$ and $\partial u/\partial z$ at $z = L/2$, and eliminating the unknown coefficients, we obtain a matrix $\mathcal{R}_1$, such that

$$\frac{\partial u}{\partial z} \bigg|_{z=L/2} = \mathcal{R}_1 u \bigg|_{z=L/2}. \quad (A10)$$

This leads to Eq. (15) for $\mathcal{A} = \mathcal{R}_1 - \mathcal{R}_0$. 

[1] J. von Neumann and E. Wigner, Über merkwürdige diskrete Eigenwerte, Phys. Z. 30, 465 (1929).
[2] C. W. Hsu, B. Zhen, A. D. Stone, J. D. Joannopoulos, and M. Soljačić, Bound states in the continuum, Nat. Rev. Mater. 1, 16048 (2016).
[3] A.-S. Bonnet-Bendhia and F. Starling, Guided waves by electromagnetic gratings and nonuniqueness examples for the diffraction problem, Math. Methods Appl. Sci. 17, 305 (1994).
[4] P. Paddon and J. F. Young, Two-dimensional vector-coupled-mode theory for textured planar waveguides, Phys. Rev. B 61, 2090 (2000).
[5] T. Ochiai and K. Sakoda, Dispersion relation and optical transmittance of a hexagonal photonic crystal slab, Phys. Rev. B 63, 125107 (2001).
[6] S. G. Tikhodeev, A. L. Yablonskii, E. A. Muljarov, N. A. Gippius, and T. Ishihara, Quasi-guided modes and optical properties of photonic crystal slabs, Phys. Rev. B 66, 045102 (2002).
[7] S. P. Shipman and S. Venakides, Resonance and bound states in photonic crystal slabs, SIAM J. Appl. Math. 64, 322 (2003).
[8] J. Lee, B. Zhen, S. L. Chua, W. Qiu, J. D. Joannopoulos, M. Soljačić, and O. Shapira, Observation and Differentiation of Unique High-Q Optical Resonances Near Zero Wave Vector in Macroscopic Photonic Crystal Slabs, Phys. Rev. Lett. 109, 067401 (2012).
[9] R. Porter and D. Evans, Embedded Rayleigh-Bloch surface waves along periodic rectangular arrays, Wave Motion 43, 29 (2005).
[10] D. C. Marinica, A. G. Borisov, and S. V. Shabanov, Bound States in the Continuum in Photonicics, Phys. Rev. Lett. 100, 183902 (2008).
[11] C. W. Hsu, B. Zhen, J. Lee, S.-L. Chua, S. G. Johnson, J. D. Joannopoulos, and M. Soljačić, Observation of trapped light within the radiation continuum, Nature (London) 499, 188 (2013).
[12] E. N. Bulgakov and A. F. Sadreev, Bloch bound states in the radiation continuum in a periodic array of dielectric rods, Phys. Rev. A 90, 053801 (2014).
[13] R. Gansch, S. Kalchmair, P. Genevet, T. Zederbauer, H. Detz, A. M. Andrews, W. Schrenk, F. Capasso, M. Lončar, and G. Strasser, Measurement of bound states in the continuum by a detector embedded in a photonic crystal, Light: Sci. Appl. 5, e16147 (2016).
[14] D. V. Evans, M. Levitin and D. Vassiliev, Existence theorems for trapped modes, J. Fluid Mech. 261, 21 (1994).
[15] E. N. Bulgakov and A. F. Sadreev, Bound states in the continuum in photonic waveguides induced by defects, Phys. Rev. B 78, 075105 (2008).
[16] C.-L. Zou, J.-M. Cui, F.-W. Sun, X. Xiong, X.-B. Zou, Z.-F. Han, and G.-C. Guo, Guiding light through optical bound states in the continuum for ultrahigh-Q microresonators, Laser Photon. Rev. 9, 114 (2015).
[17] E. A. Bezuš, D. A. Bykov, and L. L. Doskolovich, Bound states in the continuum and high-Q resonances supported by a dielectric ridge on a slab waveguide, Photon. Res. 6, 1084 (2018).
[18] T. G. Nguyen, G. Ren, S. Schoenhardt, M. Knoerzer, A. Boes, and A. Mitchell, Ridge resonance in silicon photonics harnessing bound states in the continuum, Laser Photon. Rev. 13, 1900035 (2019).
[19] Z. Yu, X. Xi, J. Ma, H. K. Tsang, C.-L. Zou, and X. Sun, Photonic integrated circuits with bound states in the continuum, Optica 6, 1342 (2019).
[20] D. A. Bykov, E. A. Bezuš, and L. L. Doskolovich, Bound states in the continuum and strong phase resonances in integrated Gires-Tournois interferometer, Nanophotonics 9, 83 (2020).
[21] L. Yuan and Y. Y. Lu, Strong resonances on periodic arrays of cylinders and optical bistability with weak incident waves, Phys. Rev. A 95, 023834 (2017).
[22] L. Yuan and Y. Y. Lu, Bound states in the continuum on periodic structures surrounded by strong resonances, Phys. Rev. A 97, 043828 (2018).
[23] J. Jin, X. Yin, L. Ni, M. Soljačić, B. Zhen, and C. Peng, Topologically enabled ultrahigh-Q guided resonances robust to out-of-plane scattering, Nature (London) 574, 501 (2019).
[24] K. Koshelev, S. Lepeshov, M. Liu, A. Bogdanov, and Y. Kivshar, Asymmetric Metasurfaces with high-Q Resonances Governed by Bound States in the Continuum, Phys. Rev. Lett. 121, 193903 (2018).
[25] L. Yuan and Y. Y. Lu, Perturbation theories for symmetry-protected bound states in the continuum on two-dimensional periodic structures, Phys. Rev. A 101, 043827 (2020).
[26] V. Moccia and S. Romano, Giant field enhancement in photonic lattices, Phys. Rev. B 92, 155117 (2015).
[27] J. W. Yoon, S. H. Song, and R. Magnusson, Critical field enhancement of asymptotic optical bound states in the continuum, Sci. Rep. 5, 18301 (2015).
[28] Z. Hu, L. Yuan, and Y. Y. Lu, Resonant field enhancement near bound states in the continuum on periodic structures, Phys. Rev. A 101, 043825 (2020).
[29] L. Yuan and Y. Y. Lu, Propagating Bloch modes above the lightline on a periodic array of cylinders, J. Phys. B 50, 05LT01 (2017).
[30] S. Shipman and D. Volkov, Guided modes in periodic slabs: existence and nonexistence, SIAM J. Appl. Math. 67, 687 (2007).
[31] L. Yuan and Y. Y. Lu, Parametric dependence of bound states in the continuum on periodic structures, Phys. Rev. A 102, 033513 (2020).
[32] E. N. Bulgakov and D. N. Maksimov, Bound states in the continuum and polarization singularities in periodic arrays of dielectric rods, Phys. Rev. A 96, 063833 (2017).

[33] Z. Hu and Y. Y. Lu, Resonances and bound states in the continuum on periodic arrays of slightly noncircular cylinders, J. Phys. B 51, 035402 (2018).

[34] B. Zhen, C. W. Hsu, L. Lu, A. D. Stone, and M. Soljačić, Topological Nature of Optical Bound States in the Continuum, Phys. Rev. Lett. 113, 257401 (2014).

[35] L. Yuan and Y. Y. Lu, Bound states in the continuum on periodic structures: Perturbation theory and robustness, Opt. Lett. 42, 4490 (2017).

[36] L. Yuan and Y. Y. Lu, Conditional robustness of propagating bound states in the continuum in structures with two-dimensional periodicity, Phys. Rev. A 103, 043507 (2021).

[37] W. Liu, B. Wang, Y. Zhang, J. Wang, M. Zhao, F. Guan, X. Liu, L. Shi, and J. Zi, Circularly Polarized States Spawning from Bound States in the Continuum, Phys. Rev. Lett. 123, 116104 (2019).

[38] T. Yoda and M. Notomi, Generation and Annihilation of Topologically Protected Bound States in the Continuum and Circularly Polarized States by Symmetry Breaking, Phys. Rev. Lett. 125, 053902 (2020).

[39] W. Ye, Y. Gao, and J. Liu, Singular Points of Polarizations in the Momentum Space of Photonic Crystal Slabs, Phys. Rev. Lett. 124, 153904 (2020).

[40] X. Yin, J. Jin, M. Soljačić, C. Peng, and B. Zhen, Observation of topologically enabled unidirectional guided resonances, Nature (London) 580, 467 (2020).

[41] W. H. McMaster, Polarization and the Stokes parameters, Am. J. Phys. 22, 351 (1954).

[42] Y. Wu and Y. Y. Lu, Dirichlet-to-Neumann map method for analyzing periodic arrays of cylinders with oblique incident waves, J. Opt. Soc. Am. B 26, 1442 (2009).