Polarization diversity close to the optical bound states in the continuum

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Abstract

Bound states in the continuum (BICs) realized in two-dimensional (2D) photonic crystal slabs (PhCSs) have attracted considerable attentions, owing to the advantages in the fabrications and on-chip applications. The polarization vortex centered at the BICs in the momentum space displayed by the linear polarization vectors of far-field radiation is a striking property of BICs. In this work, by constructing K-point BICs in photonic graphenes, we theoretically demonstrate that the far-field polarization states close to BICs can exhibit remarkable polarization diversity including circular polarizations, linear and elliptical polarizations with variant orientations and ellipticities. Thus, we propose that, along a loop enclosing BICs in the momentum space, the trajectories of the far-field polarization states on the shell of the Poincaré sphere could provide a general and straightforward means to characterize the topological natures of BICs. Our findings could open a gateway towards the applications of BICs in lasers with full polarizations and the generation and manipulation of vector beams of light.
Optical bound states in the continuum (BICs) [1] are embedded and infinite-lifetime eigenstates existing in continuous spectral range spanned by the propagating modes. BICs are mainly achieved by the symmetry incompatibility with the free-space radiations leading to the forbidden leaking or the destructive interferences among the different radiation channels in the far field [2]. The former is sensitively dependent on the geometric symmetry of the photonic structures and is called symmetry-protected BIC. It was observed in one-dimensional (1D) waveguide arrays [3] and two-dimensional (2D) photonic crystal slabs (PhCSs) at the Γ-point [4]. The latter could be efficiently constructed through tuning parameters of the photonic structures [1], such as 1D waveguiding structures containing anisotropic birefringent materials [5], coupled-waveguide arrays [6], dielectric gratings (1D PhCSs) [7, 8, 9], 2D PhCSs [10, 11, 12] and arrays of dielectric spheres [13]. Meanwhile, in compact systems, a single layered sphere coated with zero-epsilon meta-materials [14] and a single sub-wavelength high-index-dielectric cylindrical resonator [15, 16] have also been demonstrated to support BIC and quasi-BIC, respectively.

Recently, BICs in 2D PhCSs have gained increasing attentions due to their advantages in the designs, fabrications and on-chip applications. Different from guided modes in PhCSs, the optical BICs reside within the light cone of the surrounding medium and thus are compatible with free-space radiation, which facilitates the experimental observation of BICs. In the previous studies, Off-Γ BICs in both passive and active PhCS have been demonstrated by the disappearance of Fano features in the reflectivity spectrum [10] and the vanishing photocurrent [11], respectively. Double-degenerate BICs at Γ point supported by a square-lattice PhCS were also exploited in optically pumped BIC lasers [12]. Furthermore, when the far fields are linear polarizations, BICs have been verified to be momentum-space vortices centers exhibited by the far-field polarization vectors [17]. The topological property opens new applications for BICs in on-chip creation and manipulation of vector beams and polarization vortices [9, 18, 19]. However, it fails to characterize degenerate BICs because the far-field polarization directions of any degenerate states in the continuum are indeterminate and spontaneously present as a vortex center in the momentum space [19]. Thus, the previously observed polarization vortices were limited to the linear polarizations and non-degenerate BICs in the interior region of the first Brillouin zone (FBZ) whose topological charges were integers [9,17-19]. In addition, the reported theoretical models based on numerical methods [9-12, 20] have relatively little insight on the mechanism underlying the realization of BICs.
In this letter, focusing on the far-field polarization states close to BICs, we study $\mathbf{K}$-point BICs supported by the honeycomb-lattices PhCSs called photonic graphene. They are direct analogue to graphene, and could introduce two degrees of freedom, pseudospins [21, 22] and valleys [23, 24] to the photons, which are widely used in 2D topological photonics [25]. We theoretically demonstrate that the far fields of the PhCSs supporting BICs could exhibit remarkable polarization diversity. Circular polarizations, linear and elliptical polarizations with variant orientations and ellipticities can appear in the vicinity of the BICs. Therefore, instead of the linear polarization vortices centered at BICs, we propose to use the trajectories of the far-field polarization states on the Poincaré sphere to characterize the BICs with differently topological natures. Furthermore, considering the couplings between propagation modes inside the PhCSs and the free-space radiations, an analytical model is developed to describe BICs realized by the destructive interferences, which could provide great insight on the realization of BICs and the polarization diversity close to them. It is worth noting that our findings involving the polarization diversity are inconsistent with the reported consequence that when the slab was invariant under symmetry operator $C_z^2 T$, the far field of eigenmodes supporting by the slabs was linearly polarized [10, 17] (for details see the Supplementary Material Note 1).

Figure 1(a) shows our considered 2D PhCS composed of a honeycomb array (a lattice constant $a$) of cylindrical holes (identical radii $r$) etched in a free-standing dielectric slab (a thickness $h$ and a refractive index $n=2.02$ corresponding to Si$_3$N$_4$ [10]). Due to the z-mirror symmetry (invariance under the operation $\sigma_z$ changing $z$ to $-z$), the eigenmodes of the PhCS could be divided into TM-like (defined by $\sigma_z=-1$) and TE-like ($\sigma_z=1$) modes, respectively [26]. Figure 1(b) depicts the FBZ of a honeycomb lattice. At its corners, three equivalent $\mathbf{K}$ points, denoted by $\mathbf{K}_j$, $j=1, 2, 3$, provide six free-space radiation channels. They are the TM and TE polarized plane waves with the in-plane wave vector equal to $\mathbf{K}_j$. Distinct from $\Gamma$-point BICs, none of $\mathbf{K}$-point BICs is symmetry-protected because three $\mathbf{K}$ points are equivalent. At the fixed Bloch wave vector $\mathbf{K}_i$, owing to the $\gamma$-mirror symmetry, the TM and TE polarized plane waves are only symmetry compatibility with even (defined by $\sigma_z=1$ in the Letter) and odd ($\sigma_z=-1$) modes of the PhCS, respectively. Figures 1(c) and 1(d) respectively show the distributions of the reflectivity spectra when TM and TE polarized plane waves incident onto the PhCSs with the fixed radii $r=0.15a$ and different thickness $h$. From the disappearances of Fano features in the reflectivity, we obtain that the PhCSs with the thickness and the normalized frequency $(h, \omega a/2\pi c)$ equal
to (1.27a, 0.7062) and (0.9074a, 0.7998) support non-degenerate even and odd BICs, respectively. Meanwhile, their eigen fields exhibit different z-mirror symmetries. The non-degenerate odd and even BIC are TE- and TM-like modes, respectively.

To look into the far-field polarization distributions in the momentum space centered at the non-degenerate BICs, we study the eigenmodes of the PhCSs with the Bloch wave vector in the vicinity of $K_1$ point by using COMSOL simulations. Since $K_1$ point is a high-symmetry point in the FBZ, the TM-like non-degenerate even BICs is located at the top of the band with a quadratic dispersion [Fig. 2(a)]. Figure 2(b) displays the far-field polarization states of eigenmodes with different in-plan wave vector $k$. Where, the ellipses with different ellipticities and orientation angles are defined by the polarization states of the plane wave component with the given in-plan wave vector $k$ in the far field. Compatible with the even symmetry ($\sigma_z$=1) of the BICs, the far fields of the eigenmodes with Bloch wave vector along the $x$ direction are TM polarizations (shown as a short line in the $x$ direction). Very close to $K_1$ point ($|k - K_1| < 0.02K$), the far fields are nearly linear and radially oriented polarizations relative to $K_1$ point [Fig. 2(b)], which approximately exhibits a polarization vortex (topological charge equal to 1) centered at the BIC with an infinite quality factor (Q value) [Fig. 2(c)]. However, for the TE-like non-degenerate odd BICs located at the bottom of the band [Fig. 2(d)], the polarization vortex is not obvious. It is due to the fact that the far-field polarization states in the vicinity of the $K_1$ point exhibit the diversity, which cannot be simply described by the orientation angles [Fig. 2(e)]. Remarkably, when the Bloch wave number $k_x$ changes from -0.03K to 0.03K with the fixed $k_y$ equal to -1.02K, the far-field polarization states change from right-handedly circular to elliptical to TE (shown as a short line in the $y$ direction) to left-handedly elliptical and then to left-handedly circular polarizations without rotating their directions. While, on the other side of $K_1$ point, the far fields of eigenmodes with the fixed $k_x$ equal to -0.98K stay at nearly TE polarizations. It is worth noting that in Fig. 2(e) along the boundary between the right- and left-handed ellipses, denoted by a dash line, the far fields of eigenmodes are the linear polarizations whose predominant component of electric field is TM polarization. The point of intersection between the dash line and the line with Bloch wave number $k_y=0$ in the momentum space is just $K_1$ point (for details see the Fig. S1 in Supplementary Material Note 2). Owing to the $y$-mirror symmetry of the PhCS, the polarization direction of the far field at $K_1$ point is undefined [17]. Thus, the non-degenerate eigenmode at $K_1$ point becomes a BIC with an infinite Q value [Fig. 2(f)].
Moreover, the PhCS shown in Fig. 1(a) with the radii of cylindrical holes \( r = 0.143a \) and the thickness \( h = 1.036a \) supports a TE-like double-degenerate BICs at the \( \mathbf{K} \) point. Close to the BICs, two bands linearly cross each other and form the Dirac cone dispersion [Fig. 3(a)]. Figure 3(b) displays the far-field polarization states of eigenmodes in the lower band of the Dirac cone. It is obvious that not all of the far fields are linearly polarized. Due to the \( y \)-mirror symmetry of the PhCS and the undefined polarization states of double-degenerate modes at \( \mathbf{K}_1 \) point, the far fields of eigenmodes with Bloch wave number \( k_y = 0 \) are TM and TE polarizations on the left and right sides of \( \mathbf{K}_1 \) point, respectively. While, the infinite Q value of the eigenmode at \( \mathbf{K}_1 \) point demonstrates the mode is a BIC [Fig.3(c)]. Figure 3(d) and 3(e) present the similar results of eigenmodes in the upper band.

Considering the existence of the polarization diversity of eigenmodes in the vicinity of BICs, we record the varying polarization states along a closed loop around the BICs in the momentum and depict them on the shell of the Poincaré sphere to describe the different topological natures of BICs. The dash line in the Fig. 3(d) denotes our selected loop. For the PhCSs supporting the non-degenerate even BIC [Fig. 2(a)-(c)], and odd BIC [Fig. 2(d)-(f)], and the double-degenerate BICs [Fig. 3], Figs. 4(a)-4(d) show the trajectories of their far-field polarization states along the loop, respectively. Since the far fields are not linear polarizations, all of the trajectories are not located at the equator of the Poincaré sphere. Especially, the trajectory corresponding to the PhCS with non-degenerate odd BICs could traverses close to the south and north poles of the Poincaré sphere [Fig. 4(b)]. Owing to the \( y \)-mirror symmetry of PhCSs, all trajectories in Fig. 4 are invariant under the 180° rotation around \( S_1 \) axis. The common feature of the non-degenerate BICs are the ‘\( \infty \)’-sharped trajectories on the Poincaré sphere, which pass the crossing at \( (S_1, S_2, S_3) = (1,0,0) \) [TM polarization in Fig. 4(a)] and \( (S_1, S_2, S_3) = (-1,0,0) \) [TE polarization in Fig. 4(b)] two times, respectively. However, the two trajectories corresponding to the double-degenerate BICs are closed curves without any crossing point, which pass two points with \( (S_1, S_2, S_3) = (-1,0,0) \) and \( (1,0,0) \), and circle the Poincaré sphere one time [Fig. 4(c) and 4(d)]. Similar to the topological chargers of the polarization vortices centered at BICs and exhibited by the linear polarization directions of far fields, the above features of the four trajectories [Fig. 4] are determined by the spatial symmetry of the BICs, and do not alter when the square loop shrinks or expands in the vicinity of \( \mathbf{K}_1 \) point. Therefore, the trajectory of the far-field polarization states on the shell of the Poincaré sphere provides a general and straightforward means to character the topological natures of BICs. Where, the single-pass ‘\( \infty \)’-sharped trajectories and closed trajectories without any crossing point
corresponding to non- and double-degenerate $K$-point BICs are topologically equivalent to linear polarization vortices centered at BICs with the topological chargers equal to 1 and $1/2$ [27,28], respectively.

Focusing on the energy conservation, we utilize the general scattering-matrix model [29] to investigate the realization of BICs by the destructive interferences and the polarization diversity close to them. For eigenmode of the PhCS with frequency $\omega$ and in-plane Bloch wave vector $k$, the transversal field $\mathbf{E} = \mathbf{H}x E_x t = |\mathbf{E}| e^{-i\omega x - i\mathbf{k} \cdot \mathbf{x}}$, inside the slab satisfies

$$
-i\frac{\partial}{\partial z} |\psi\rangle = \mathbf{H}_k |\psi\rangle, \quad \mathbf{H}_k = \begin{bmatrix}
\varepsilon & 0 & 0 \\
0 & \varepsilon & 0 \\
0 & 0 & \mu
\end{bmatrix}
+ \frac{e^{-ikx}}{\omega}
\begin{bmatrix}
\partial_x \mu^{-1} \partial_x & \partial_y \mu^{-1} \partial_y \\
\partial_y \mu^{-1} \partial_x & -\partial_x \mu^{-1} \partial_y \\
-\partial_x \mu^{-1} \partial_x & \partial_y \mu^{-1} \partial_y
\end{bmatrix}
e^{ikx}. \quad (1)
$$

Where, $|\psi\rangle$ can be approximately expressed as a superposition of the eigen vectors $|\psi_m^{(\pm)}\rangle$ ($m = 1, 2, ..., N$) of the operator $\mathbf{H}_k$ [Eq. (1)] with the real eigen value $\pm \beta_m$, which indeed are waveguide modes of the corresponding 2D PhC (that is, the thickness $h$ of slab is infinity) propagating along $\pm z$ direction. That is, $|\psi\rangle = \sum_{m=1}^{N} \left[ \rho_m^{(+)} e^{i\beta_m(z-h/2)} |\psi_m^{(+)}\rangle + \rho_m^{(-)} e^{i\beta_m(h/2-z)} |\psi_m^{(-)}\rangle \right]$. $N$ is the amount of the propagating modes with the real propagation constants. At the interface between the PhCS and free space ($z = h/2$), these propagating modes partly reflect back into the slab, simultaneously, partly transmit into the free space and become the plane waves, which can be described by an interface-reflection matrix $r$ ($N \times N$ version) and an interface-transmission matrix $t$ ($6 \times N$ version in the vicinity of $K$ point). Meanwhile, taking in account the $z$-mirror symmetry of the PhCS, the column vector $\rho^{(+)} = [\rho_1^{(+)}, \rho_2^{(+)}, ..., \rho_N^{(+)}]^T$ composed by the mode coefficients satisfies

$$
(fr) \rho^{(+)} = \eta \rho^{(+)}, \quad (2)
$$

in which, $f = \text{diag}[e^{i\beta_h}, e^{i\beta_h}, ..., e^{i\beta_h}]$. The eigenvalue $\eta$ is equal to 1 and -1 for TE-like and TM-like modes of the PhCS, respectively. Equation (2) means the existence of BICs (corresponding to a real eigen-frequency) requires that the reflection matrix $r$ must be non-diagonal because there are symmetry-compatible radiation channels. Therefore, the inter-conversions among the waveguide modes in the slab (that is, each waveguide mode experiences not only reflection but also converts into other
modes at the two interfaces) play an important role in the realization of BICs by the destructive interferences.

At the \( \mathbf{K} \) point, due to the \( C_{3\nu} \) symmetries of the PhCS [Fig. 1(a)], the matrix \( \mathbf{r} \) and \( \mathbf{t} \) are block-diagonal since only waveguide modes with the compatible symmetries can be interconverted and transmit into the radiation channel with the compatible symmetries at the interfaces. For the sake of simplicity, in our designed non (double)-degenerate \( \mathbf{K} \)-point BICs in Fig. 2 (3), only two (four) waveguide modes and one (two) radiation channel are symmetry-matched and take part in the destructive interferences. The previously reported anisotropy-induced BICs [5] and off-\( \Gamma \) BICs [10] belonged to the simplest kind of the destructive interferences involving only two waveguide modes and one radiation channel. Where, one thickness (\( h \))-independent necessary condition for the existence of BIC in the \( z \)-mirror-symmetrical slabs (for detailed derivation see the Supplementary Material Note 3) can be given by the matrix \( \mathbf{r} \) (reduced to \( 2 \times 2 \) version) and \( \mathbf{t} \) (reduced to \( 1 \times 2 \) version). That is,

\[
\left| r_{11} - r_{22} t_{11} / t_{12} \right| = \left| r_{22} - r_{12} t_{11} / t_{12} \right| = 1.
\] (3)

By solving Eq. (2), we can obtain the thicknesses of PhCSs supporting BICs with desired symmetries and the far-field polarization states consistent with the results shown in Fig. 2 and 3 [for details see the Supplementary Material Notes 4-6]. Therefore, our analytical model could efficiently describe the realization of BICs formed by the destructive interferences and the far-field polarization diversity.

In conclusion, by constructing \( \mathbf{K} \)-point BICs in honeycomb-lattices PhCSs, we have theoretically demonstrated that the far-field radiation close to BICs could exhibit the polarization diversity (e.g. circular polarization, elliptical and linear polarizations with variant orientations, polarization vortices with the different topological charges). Where, the spatial symmetry and the interferences among the different radiation channels play important roles. The trajectories of the far-field polarization states on the shell of the Poincaré sphere provide a general means to characterize the topological natures of BICs displayed by the diverse polarizations of far-field radiation. The polarization diversity close to BICs may bring about opportunities to generate and manipulate vector beams with diverse polarization states and different vortices in the momentum space.

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[30] See Supplemental Material at http://link.aps.org/supplemental/ for the details of the polarization states of eigenmodes in the continuum of the slab and Fig. 2(e) in the main text and the derivation of Eq. (3) and K-point BICs realized by the destructive interferences.

Figures 1-4:
FIG. 1 Schematic illustration of the two-dimensional photonic crystal slab with a honeycomb array of cylindrical holes etched in a free-standing dielectric slab (a). The first Brillouin zone (b) in the reciprocal space of the honeycomb lattice with positions of $K_1 = -K_e$, $K = 4\pi/(3a)$. (c) and (d) Reflectivity spectra of TM and TE polarized plane waves with the wave vector matching with the $K_1$ incident on the PhCS with different thicknesses, respectively. The two circles are used to denote the positions where the two non-degenerate BICs appear.
FIG. 2 Band structures and far-field polarization states of eigenmodes supported by the PhCS ($r=0.15a$) in the momentum space close to the non-degenerate $\mathbf{K}$-point BIC. (a), (b) and (c) Band structure, far-field polarization states with different in-plan wave vectors $[k_x, k_y]$ and the dependence of the quality factors (Q) & eigen-frequencies over the Bloch wave vector along the $x$ direction of the PhCS with the thickness $1.27a$, respectively. In (b), the ellipse (circle) denoted by +(-) means the polarization state of the far field is a right (left)-handed ellipse (circle). (d)-(f) Corresponding results of the PhCS with the thickness $0.9074a$. 
FIG. 3 Band structure (a) and far-field polarization states of TE-like eigenmodes supported by the PhCS with the thickness $1.036a$ $(r=143\,nm)$ in the momentum space close to the double-degenerate $\mathbf{K}$-point BIC. (b) Far-field polarization states of eigenmodes in the lower band. (c) Dependence of the quality factors (Q) and eigen-frequencies over the Bloch wave vector along the $x$ direction. (d) and (e) Corresponding results of eigenmodes in the upper band. The dash line in (d) defines the square loop which will be used in Fig. 4. The wave vectors $[k_x, k_y]$ corresponding to the four corners of it are $[-1.03, -0.03]K$, $[-0.97, -0.03]K$, $[-1.03, 0.03]K$, $[-0.97, 0.03]K$, respectively.
FIG. 4 Trajectories of the far-field polarization states on the shell of the Poincaré sphere when the in-plan wave vector of eigemodes move along the square loop enclosing the $K_1$-point BICs. (a) and (b) Trajectories of the PhCSs supporting non-degenerate $K$-point BICs shown in Figs. 2(a-c) and 2(d-f), respectively. (c) and (d) Trajectories of the PhCSs supporting double-degenerate $K$-point BICs shown in Figs. 3(b) and 3(d), respectively.