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Topological Nature of Optical Bound States in the Continuum

Bo Zhen,1,∗ Chia Wei Hsu,1,2 Ling Lu,1 A. Douglas Stone,3 and Marin Soljačić1
1Department of Physics, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, Massachusetts 02139, USA
2Department of Physics, Harvard University, 17 Oxford Street, Cambridge, Massachusetts 02138, USA
3Department of Applied Physics, Yale University, Post Office Box 208284, New Haven, Connecticut 06520, USA

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Optical bound states in the continuum (BICs) have recently been realized in photonic crystal slabs, where the disappearance of out-of-plane radiation turns leaky resonances into guided modes with infinite lifetimes. We show that such BICs are vortex centers in the polarization directions of far-field radiation. They carry conserved and quantized topological charges, defined by the winding number of the polarization vectors, which ensure their robust existence and govern their generation, evolution, and annihilation. Our findings connect robust BICs in photonics to a wide range of topological physical phenomena.

Bound states in the continuum (BICs) are unusual solutions of wave equations describing light or matter: they are discrete and spatially bounded, but exist at the same energy as a continuum of states which propagate to infinity. Until recently, BICs were constructed through fine-tuning parameters in the wave equation [1–8] or exploiting the separability of the wave equation due to symmetry [9–13]. More recently, BICs in periodic extended structures (different from the original proposal of BICs [14]) that are both robust and not symmetry protected (“accidental”) have been predicted [15–20] and experimentally realized [20]; the simplest such system is a periodic dielectric slab [20], which also has symmetry-protected BICs. Here we show that both types of BICs in such systems are vortex centers in the polarization direction of far-field radiation. The robustness of these BICs is due to the existence of conserved and quantized topological charges, defined by the number of times the polarization vectors wind around the vortex centers. Such charges can only be generated or annihilated by making large changes in the system parameters, and then only according to strict rules, which we derive and test numerically. Our results imply that laser emission based on such states will generate vector beams [21].

These BICs exist in photonics crystal slabs, which are dielectric slabs with a periodic modulation of refractive index at the wavelength scale [22] surrounded by air or a low-index medium. Photonic crystal slabs are used in many applications including surface-emitting lasers [23], photovoltaics [24], LEDs [25], and biosensing [26–28]. The periodic modulation alters the dispersion relation of light in the slabs and gives rise to photonic bands, analogous to electronic band structures in solids. In general, light can escape from the surface of the slab and propagate to the far field, but for a portion of the photonic band (that is “below the light line”) light is perfectly confined to the slab by the generalized form of total internal reflection [22]. In contrast, modes above the light line appear generically as resonances with finite lifetimes due to their coupling to the continuum of extended modes [29]. It has been known for some time that bound states with infinite lifetimes also exist above the light line at isolated high-symmetry wave vectors. This type of BIC arises from the symmetry mismatch between their mode profiles inside the photonic crystal and those of the external propagating modes (radiation continuum) [13,29–31]. Recently, a new type of BIC, unprotected by symmetry, has been found (both theoretically and experimentally) to exist at arbitrary wave vectors in bands above the light line in photonic crystal slabs [20]. These BICs occur accidentally when the relevant couplings to the continuum (see below) all vanish simultaneously. However, their existence does not require fine-tuning of system parameters; small changes in parameters simply shift the position of these special points along the band diagram. An intuitive understanding of why such BICs exist and are robust was previously lacking. Recently, an explanation based on accidental triangular symmetry of the radiating fields was proposed [32] but does not explain the robustness of these BICs and their occurrences in TE-like bands.

We now show that both types of BICs in photonic crystal slabs are vortex centers in the polarization direction of the far-field radiation. Using the Bloch theorem for photonic crystals [22], we write the electric field of a resonance as $\mathbf{E}_k(\rho, z) = e^{ik \cdot \rho} \mathbf{u}_k(\rho, z)$, where $\mathbf{k} = k_x \hat{x} + k_y \hat{y}$ is the two-dimensional wave vector, $\rho = x\hat{x} + y\hat{y}$ is the in-plane coordinate, $\mathbf{u}_k$ is a periodic function in $\rho$, and $z$ is the normal direction to the slab. While the fields inside the slab are periodically modulated, outside the slab each state consists of propagating plane waves and/or evanescent waves that decay exponentially away from the surface. For states above the light line (resonances), and wavelengths below the diffraction limit, the only nonzero propagating-wave amplitudes are the zero-order (constant in-plane) Fourier coefficients of $\mathbf{u}_k$, given by $c_k(\mathbf{k}) = c_{k_x}(\mathbf{k}) \hat{x} + c_{k_y}(\mathbf{k}) \hat{y}$ [Fig. 1(a)]. Here, $c_{k_x}(\mathbf{k}) = \mathbf{\hat{k}} \cdot (\mathbf{u}_k)$,
Along the nodal line of the BIC, as illustrated in Fig. 1(b), for the simplest case. A resonance turns into a BIC if and only if \( c_x = c_y = 0 \). (b) Schematic illustration for the nodal lines of \( c_x \) (green) and of \( c_y \) (red) in a region of \( k \) space near a BIC. The direction of vector \( e \) (shown in arrows) becomes undefined at the nodal line crossing, where a BIC is found. (c) Two possible configurations of the polarization field near a BIC. Along a closed loop in \( k \) space containing a BIC (loop goes in counterclockwise direction, \( 1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \)), the polarization vector either rotates by angle \( 2\pi \) (denoted by topological charge \( q = +1 \)) or rotates by angle \(-2\pi \) (denoted by topological charge \( q = -1 \)). Different regions of the \( k \) space are colored in four gray-scale colors according to the signs of \( c_x \) and \( c_y \). In this way, a BIC happens where all four gray-scale colors meet, and charge \( q = +1 \) corresponds to the color changing from white to black along the counterclockwise loop \( C \), and charge \( q = -1 \) corresponds to the color changing from black to white.

Each component of the polarization vector flips sign as its nodal line is crossed so as to create a net circulation of \( \pm 2\pi \) in the polarization field. At the nodal intersection the polarization direction becomes undefined, since at the BIC there is zero emission into the far field. Conversely, one could say that BICs cannot radiate because there is no way to assign a far-field polarization that is consistent with neighboring \( k \) points. Thus, robust BICs are only possible when there is vorticity in the polarization field.

Vortices are characterized by their topological charges. Here, the topological charge \( (q) \) carried by a BIC is defined as

\[
q = \frac{1}{2\pi} \oint_C d\mathbf{k} \cdot \nabla_k \phi(\mathbf{k}), \quad q \in \mathbb{Z},
\]

which describes how many times the polarization vector winds around the BIC. Here, \( \phi(\mathbf{k}) = \arg[c_x(\mathbf{k}) + ic_y(\mathbf{k})] \) is the angle of the polarization vector, and \( C \) is a closed simple path in \( k \) space that goes around the BIC in the counterclockwise direction. The fields \( \mathbf{u}_k \) are chosen to be smooth functions of \( k \), so \( \phi(\mathbf{k}) \) is differentiable in \( k \) along the path. The polarization vector has to come back to itself after the closed loop, so the overall angle change must be an integer multiple of \( 2\pi \), and \( q \) must be an integer. Figure 1(c) shows examples of how the polarization vector winds around a BIC with charge \( q = +1 \) and also around a BIC with charge \( q = -1 \) along a loop \( C \) marked by \( 1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 1 \). Similar
definitions of winding numbers can be found in describing
topological defects [34] of continuous two-dimensional
spins, dislocations in crystals, and quantized vortices in
helium II [35]. This formalism describing polarization
vortices is also closely related to Berry phases in describ-
ading adiabatic changes of polarization of light [36,37] and
Dirac cones in graphenes [38].

Lasing emission through BICs are naturally vector
beams [21] (see Supplemental Material [33]), where the
polarization of the outgoing beam has a spatial twist around
the center. The order number of the vector beam is given by
the topological charge of the BIC.

In the example of Fig. 2, we show the topological
charges of BICs for a structure that has been experimentally
realized in Ref. [20]. In this example, there are five BICs on
the lowest-frequency TM-like band as shown in Fig. 2(a).
Details about numerical simulation are provided in the
Supplemental Material [33]. The mode profiles of the $E_{z}$
component for two BICs are shown in Fig. S1 showing
localization in the $z$ direction. We numerically calculate
polarization vectors $c(k)$ [39], which reveal five vortices
with topological charges of $\pm 1$ at these five $k$ points
[Fig. 2(b)]. The BICs and their topological charges can also be identified from the nodal-line crossings and the
gray-scale colors of $c_{x}$ and $c_{y}$ [Fig. 2(c)].

The winding number of the polarization vector along a
closed path is given by the sum of the topological charges
carried by all BICs enclosed within this path [34]. When
system parameters vary continuously, the winding number
defined on this path remains invariant, unless there are
BICs crossing the boundary. Therefore, topological charge
is a conserved quantity. This conservation rule leads to
restrictions on the behaviors of BICs (see Supplemental
Material [33]). For example, as long as the Hermitian
system retains $C_{2v} T$ and $\sigma_{z}$ symmetries (Fig. S2), a BIC can
only be destroyed through annihilation with another BIC of
the exact opposite charge, or through bringing it outside of
the continuum (below the light line).

The conservation of topological charges allows us to
predict and understand the behaviors of BICs when the
parameters of the system are varied over a wide range. First,
consider the lowest-frequency TM-like mode (TM$_{1}$ band)
of a 1D-periodic structure in air shown in Fig. 3(a). This
grating consists of a periodic array of dielectric bars
with periodicity of $a$, width $w = 0.45a$, and refractive
index $n = 1.45$. Its calculated band structure is shown in
Fig. 3(b). When the thickness of the grating is $h = 1.50a$,
there are two BICs on the $k_{c}$ axis, as indicated by the
radiative quality factor of the resonances [Fig. 3(c)]. The
polarization vector $c(k)$, also shown in Fig. 3(c), character-
izes both BICs as carrying charges $q = \pm 1$. When the
grating thickness is decreased to $h/a = 1.43$ (all other
parameters fixed), the two BICs move towards the center of
the Brillouin zone, meet at the $\Gamma$ point, and deflect onto the
$k_{c}$ axis [Fig. 3(d)]. This is inevitable due to the conservation
of the topological charges: annihilation cannot happen
between two BICs of the same charge.

Annihilation of BICs is only possible when charges of
opposite signs are present. This can be seen in the lowest-
frequency TE-like band of the same structure [Figs. 3(e)
and 3(f)]. When $h/a = 1.04$, there are two off-$\Gamma$ BICs
with charge $-1$ and a BIC with charge $+1$ at the $\Gamma$
point [Fig. 3(e)]. As $h/a$ decreases, the two $-1$ charges move
to the center and eventually annihilate with the $+1$ charge,
leaving only one BIC with charge $q = -1$ [Fig. 3(f)].

Generation of BICs is also restricted by charge conser-
vation, and can be understood as the reverse process of
charge annihilation. We provide an example by considering
the lowest-frequency TE-like mode in a photonic crystal slab
of $n = 3.6$ with a square lattice of cylindrical air holes of
diameter $d = 0.5a$ (Fig. S3(a) in the Supplemental Material
[33]). As the slab thickness increases, BICs are generated
at the $\Gamma$ point. Each time, four pairs of BICs with exact
opposite charges are generated, consistent with charge
conservation and $C_{4\sigma}$ symmetry of the structure. With
further increases of the slab thickness, the eight BICs move

![FIG. 2 (color online). Characterization of BICs using topological charges. (a) Calculated radiative quality factor $Q(k)$ of the TM$_{1}$ band on a square-lattice photonic crystal slab (as in Ref. [20]), plotted in the first Brillouin zone. Five BICs can be seen. (b) Directions of the polarization vector field reveal vortices with topological charges of $\pm 1$ at each of the five $k$ points. The area shaded in blue indicates modes below the light line and thus bounded by total internal reflection. (c) Nodal lines and gray-scale colors of the polarization vector fields (same coloring scheme as in Fig. 1(c)).]
outward along high-symmetry lines and eventually go outside of the continuum (fall below the light line).

Although the examples discussed so far only show topological charges of $\pm 1$, other values of charges can be found in higher-frequency bands of the PhC or in structures with higher rotational symmetry. For example, Fig. S4 shows a stable BIC of charge $-2$ at the $\Gamma$ point arising from the double degeneracy of nodal lines caused by the $C_{6v}$ symmetry of the system.

The symmetries of the system also restrict the possible values of topological charges, since the nodal curves must respect the point symmetry. BICs at $k$ points related by in-plane point-group symmetries of the system (mirror reflections and rotations) have the same topological charges (see Supplemental Material [33]). Using a similar method, all possible charges at the $\Gamma$ point on a nondegenerate band of any system with $C_n$ symmetry are given in Table S1. This is consistent with all examples in this Letter. This table can be used to predict the charges in other systems of interest and to design high order vector beams.

In conclusion, we have demonstrated that BICs in photonic crystal slabs are associated with vortices in the polarization field and explained their robustness in terms of conserved topological charges. We derive the symmetries that constrain these charges and explain their generation, evolution, and annihilation. We conjecture that most robust BICs [9,12,13,16–20] will correspond to topological defects in appropriate parameter spaces. Our finding connects electromagnetic BICs to a wide range of physical phenomena including Berry phases around Dirac points [37,38], topological defects [34], and general vortex physics [35]. Optical BICs in photonic crystals have a wealth of applications. Lasing action can naturally occur at BIC states where the quality factor diverges. The angular (wave vector) tunability of the BICs makes them great candidates for on-chip beam steering [40]. Furthermore, photonic crystal lasers through BICs are naturally vector beams [41,42,43], which are important for particle accelerations, optical trapping, and stimulated emission depletion microscopy.

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BICs in the original proposal [1] are spatially bounded in all three dimensions and therefore integrable in the whole three-dimensional space. On the other hand, BICs in periodic extended structures are Bloch eigenstates: they are extended in the direction(s) where the system is periodic, but spatially confined in all other directions. Therefore, BICs in periodic extended structures are integrable within one unit cell instead of the whole space. These states, which are the focus of this Letter, are essentially resonances with zero linewidths and infinitely long lifetimes.

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[33] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.113.257401 for (A) Numerical methods and setups; (B) Symmetry requirements for stable BICs; (C) BICs and vector beams; (D) Conservation of topological charges; (E) Example of charge -2; (F) BICs related to point group symmetries have the same topological charges; (G) Allowed charges at the center of the Brillouin zone. They are mostly providing detailed information, proofs, and examples for the claims made in the main text.