Anisotropy-induced photonic bound states in the continuum

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Bound states in the continuum (BICs) are radiationless localized states embedded in the parameter space that otherwise corresponds to radiative modes. Many decades after their original prediction and early observations in acoustic systems, such states have been demonstrated recently in photonic structures with engineered geometries. Here, we put forward a mechanism, based on waveguiding structures that contain anisotropic birefringent materials, that affords the existence of BICs with fundamentally new properties. In particular, anisotropy-induced BICs may exist in symmetric as well as in asymmetric geometries; they may form in tunable angular propagation directions; their polarization may be pure transverse electric, pure transverse magnetic or full vector with tunable polarization hybridity; and they may be the only possible bound states of properly designed structures, and thus appear as a discrete, isolated bound state embedded in a whole sea of radiative states.

Bound states in the continuum were originally predicted in 1929 by von Neumann and Wigner as discrete fully-bounded quantum states with energies above the continuum of the corresponding Hamiltonian. Signatures of acoustic BICs were observed experimentally several decades ago, but the implications of the almost century-old concept were properly appreciated only after the recent theoretical studies and landmark experiments conducted in classical photonic systems, which stimulated deeper understanding over their origin and inspired new schemes and applications. BICs discovered to date are almost-pure transverse-electric (TE) or transverse-magnetic (TM) waves, namely with a negligible fraction of energy being carried by the respective orthogonal polarization. The corresponding trapping mechanism can thus be intuitively viewed as a scalar or spinor potential. In contrast, photonic structures that contain anisotropic media can support bound states that, in general, involve the full-vector electric and magnetic-field components. This important feature opens up the possibility to search for full-vector BICs that cannot exist in scalar analogies. In this paper, we explore the concept and expose its potential.

By and large, coupling localized states with a coexisting radiative continuum results in energy being shed away and thus in unbound states that decay and fade away during propagation. Bound states can only exist when such transverse radiative leakage is suppressed by a suitable mechanism. Here we address the existence of such a mechanism in optical waveguiding structures fabricated in anisotropic media. We restrict ourselves to the simplest structures fabricated in birefringent uniaxial natural materials; the optical axes of the crystals are set to lie on the waveguide plane that forms an angle with the wave propagation direction. However, the concept is general and holds for a wealth of more complex structures, which include multilayer geometries, off-plane and unaligned optical axes, and structures that contain different anisotropic media, including biaxial media and other types of natural or artificial anisotropic materials.

In birefringent media, for an arbitrary direction of the light propagation relative to the optical axis, light fields are a superposition of ordinary and extraordinary waves, which are characterized, respectively, by the ordinary refractive index and the angle-dependent refractive index that varies between and the extraordinary refractive index where the subscripts ‘s’ and ‘t’ stand for the substrate and the core layer, respectively, are assumed to be larger than the refractive index of the cladding material, which here, for simplicity, we set to be air. The light cone is therefore defined as , where and are the angular frequency and the vacuum speed of light, respectively. is the vacuum wavenumber, is the vacuum wavelength and is the propagation constant. In this work, we consider that light is linearly polarized and we set the ordinary direction of polarization to coincide with the ordinary axis of the anisotropic medium. BICs can be thought of, in a generalized sense, as discrete fully-bounded quantum states that exist above the light cone — under such conditions, the wave is not required for a bound state to exist, or, more importantly,
because of a destructive interference of the radiative waves. Both mechanisms can be induced by anisotropy, as shown in Fig. 1b. The plot displays the frequency–momentum diagram of an illustrative structure made of a positive birefringent core and a negative birefringent core-layer film. The structure supports two families of standard guided modes in the areas shown as blue surfaces below the light cone, and leaky modes in the areas depicted as orange surfaces above the light cone. The corresponding dispersion relations as a function of the optical axis orientation are shown in Supplementary Fig. 1. The radiative channel is the extraordinary wave and the light cone is defined by the extraordinary refractive index. The decay length of the leaky modes, defined as the inverse of the imaginary part of the refractive index, is shown in Fig. 1c for a structure with $d/\lambda = 0.22$. The decay length exhibits discrete diverging peaks at specific off-axis optical axis orientations, which reveals the existence of fully-bound states embedded in the leaky branch.

The central insight put forward in this paper is that the interplay between the values of the ordinary and extraordinary refractive indices of the core layer and the substrate, the positive or negative nature of the crystals, the optical axes orientations, the cladding refractive index and the waveguide thickness for a given operating wavelength/frequency afford the existence of BICs with pure-TE, pure-TM and tunable full-vector polarization in a wealth of modal spectroscopies. Some of the different possibilities are illustrated in Fig. 2, which displays isofrequency sections of the frequency–momentum diagram obtained for six different suitable material configurations. In all the plots, the BICs that occur at discrete points embedded in the leaky branches are displayed as blue dots. Figure 2a illustrates the existence of BICs with properties similar to those previously reported in photonic crystals. Namely, a TM-polarized BIC that coexists with standard guided modes elsewhere in the parameter space. The BIC occurs as a bounded state that propagates at 90° relative to the crystal optical axis, surrounded by radiating modes in all angular (polar and azimuthal) directions. The BIC is not allowed anywhere, but discrete TM-polarized BICs do exist at exactly such orientations, as shown by Fig. 2c. Structures that support on-axis as well as off-axis BICs can be obtained by turning the core-layer birefringent, as illustrated in Fig. 2d (where $n_c = 1 < n_{os} < n_{id} < n_{ef}$). Finally, Fig. 2e (in which $n_c = 1 < n_{os} < n_{id} < n_{ef}$) and Fig. 2f (in which $n_c = 1 < n_{os} < n_{id} < n_{ef}$) correspond to structures built in a negative birefringent material as a substrate with a core layer having refractive indices that lay between the extraordinary and ordinary indices of the substrate. Under such conditions, standard guided modes are not allowed anywhere, but discrete BICs do exist, and therefore are the only fully-bound states supported by the structure. They occur as TE-polarized states or as full-vector states. Other modal spectroscopies (not shown in the plot), such as multiple TE-polarized or TM-polarized BICs only or full-vector BICs only (the latter case requires relaxing the condition $\theta_2 = \theta_3$), are also possible.

The physical origin and nature of the different BICs is dictated critically by the light-propagation direction relative to the crystal optical axis. The peaks that diverge to infinity reveal the existence of discrete BICs at specific orientations. The colour bar in c, used also in b, displays the radiative losses in logarithmic scale calculated using the imaginary part of the effective index of the leaky modes.

**Figure 1 | Modal spectroscopy.** a, Schematic of the waveguiding structure. A typical relationship among the refractive indices is shown in the inset. In all cases $n_i = 1$. b, Light cone (grey surface) for a structure composed of a negative birefringent core ($n_{op} = 1.75$, $n_{id} = 1.5$) on a positive birefringent substrate ($n_{os} = 1.25$, $n_{ef} = 2$). Standard guided modes exist in the blue areas and leaky modes exist in the orange areas. Polarization-separable (PS) and full-vector interferometric (INT) BICs exist in the loci indicated by blue lines within the yellow area. c, Decay length of the leaky states that exist at $d/\lambda = 0.22$ versus the propagation direction relative to the optical axis. The peaks that diverge to infinity reveal the existence of discrete BICs at specific orientations. The colour bar in c, used also in b, displays the radiative losses in logarithmic scale calculated using the imaginary part of the effective index of the leaky modes.
Figure 2 | Type of anisotropy-induced BICs. Isofrequency sections of the light-cone diagram for waveguiding structures with different constitutive parameters. The regions below and above the light cone are shown in blue and yellow/orange, respectively. Standard mode branches are shown as blue lines within the blue region. Radiating semileaky branches exist in the orange region and are shown as red lines. BICs are the discrete points highlighted with blue dots on the red semileaky branch. a, TM-polarized BICs coexist with guided modes for an isotropic film ($n = 2$ and thickness $d = 0.8\lambda$) and a positive birefringent substrate ($n_{ef} = 1.5$, $n_{os} = 1.75$). b, BICs disappear for substrates with a smaller birefringence ($n_{ef} = 1.5$, $n_{os} = 1.48$) and core layers with higher refractive index, even if the core layer is anisotropic ($n_{os} = 2$, $n_{ef} = 1.75$, $d = 0.8\lambda$). c, Guided modes and TM-polarized BICs coexist for an isotropic core layer with a refractive index ($n = 1.75$) between those of the positive birefringent substrate ($n_{ef} = 1.5$, $n_{os} = 2$). d, TE-polarized and multiple full-vector BICs appear for a core layer that is birefringent ($n_{os} = 1.75$, $n_{ef} = 1.5$, $d = 0.22\lambda$) on a birefringent substrate ($n_{ef} = 1.25$, $n_{os} = 2$). e,f, Structures in which BICs are the only non-radiating state: a TE-polarized BIC in an isotropic core layer ($n = 1.75$, $d = 0.5\lambda$) on a negative birefringent substrate ($n_{ef} = 2$, $n_{os} = 1.5$) (e) or TE-polarized and multiple full-vector BICs in a structure with a positive birefringent core layer ($n_{ef} = 1.5$, $n_{os} = 1.75$, $d = 0.68\lambda$) on a negative birefringent substrate ($n_{ef} = 2$, $n_{os} = 1.25$) (f).
to the usual BICs\(^{9,10,30}\) that exist as a single point in that representation. Also, in contrast to previously reported TE-like or TM-like BICs, the full-vector nature of the interferometric BICs allows tuning their TE/TM polarization content to a large degree by varying the structural or operational control parameters, such as the core-layer thickness or the wavelength. This is shown in Fig. 3a for the relevant BIC displayed in Fig. 2d. The plot also shows that, in contrast to standard BICs that exist in photonic crystals, which occur only along symmetry axes, the angular loci at which the full-vector interferometric anisotropy-induced BICs occur can be tuned readily. The TE/TM polarization content of the BIC also varies along the curve, which shows that various external parameters can be used to tune the practical properties of the full-vector BICs. Figure 3b illustrates how the BIC propagation direction can be controlled actively by changing any of the refractive indices of the structure, a possibility of particular practical interest. To highlight the point, Fig. 3b explores a variation of the extraordinary refractive index over a large range (\(\Delta n = 0.2\)), which causes a change of the BIC existence angular loci of more than \(\Delta \theta \approx 40^\circ\). However, \(\Delta n = 0.2\) is compatible with the change of the extraordinary refractive index of a liquid crystal under temperature tuning\(^{31}\). Additionally, Supplementary Fig. 4 shows the variation of the angular propagation direction of BICs generated in a suitable (yet non-optimized) proton-exchange LiNbO\(_3\) waveguide structure under the action of the Pockels effect. The plot illustrates that an applied external field of the order of 1 V \(\mu\)m\(^{-1}\) may result in a variation of the BIC existence angular loci of more than ten degrees. Such large angular loci steering, as well as the accompanying sharp transitions from bound modes to

Figure 3 | Polarization hybridity and angular locus of BICs. a, Degree of polarization hybridity of the BICs (left axis) and angular loci (right axis) at which the full-vector interferometric BICs occur as a function of the normalized thickness of the core layer. b, Angular loci at which the full-vector interferometric BICs occur as a function of the extraordinary refractive index of the film. Both a and b correspond to the BIC shown in Fig. 2d. The degree of polarization hybridity is measured as the fraction of the total BIC power density carried by the field components that correspond to the TE polarization. Black arrows point to the original case in Fig. 2d.

Figure 4 | Theoretical and experimental modal spectroscopy spectra for an antiguiding waveguide on a calcite substrate. a, TE-reflected intensity with TE incident polarization. Taking advantage of the specular symmetry of the structure, we compare transfer-matrix theoretical calculations (left-hand side, \(\theta = 0^\circ\)–90\(^\circ\)) with experimental observations (right-hand side, \(\theta = 90^\circ\)–0\(^\circ\)). The green dashed line shows the angular dependence of the extraordinary refractive index for calcite. b, TM-reflected intensity with TE incident polarization. c,d, Theoretical magnifications near the region of existence of polarization-separable BICs within the dashed boxes in b.
radiating states, may find applications in integrated photonic devices for sensing, spatial-light modulation or filtering.

Figure 4 shows the experimental signature of the anisotropy-induced BICs, obtained by modal spectroscopy in a prism-coupling geometry (Methods and Supplementary Fig. 5). We used calcite as the substrate material and a spinned-coated polymer for the core-layer film to form an antiguiding configuration that features the salient phenomenon described in Fig. 2e; in which BICs are the only existing non-radiating bound states. The plots compare the theoretical and the experimental reflectance when TE-polarized light is used as illumination. Figure 4a shows that above the light cone the incoming light is fully reflected, except when it couples to a radiative leaky mode or to a TE-polarized BIC, which then results in a dip in the image. The hybrid polarization of the leaky modes means that light coupled to the modes is partially converted into TM polarization, which in this structure is predominantly an ordinary wave. Therefore, the TE–TM polarization conversion reflectance shown in Fig. 4b (the corresponding transmittance is given in Supplementary Fig. 6) is an indirect indication of the leakage losses of the different states. At light propagation orthogonal to the crystal optical axis (θ = 90°), the two branches in Fig. 4b (magnifications are shown in Fig. 4c,d) exhibit no visible polarization-conversion reflectance, consistent with the existence there of the two fully-bound states displayed in Fig. 2e. In contrast to previous experiments carried out in photonic crystals, our sample is highly asymmetric and the BICs are excited by prism coupling from the cladding and not from the substrate; thus, Fano resonances do not occur.

In closing, we stress that the occurrence of BICs in fully vectorial settings opens the door to the exploration of such bound states beyond traditional scalar or spinor analogies. Anisotropy affords new radiation-suppression mechanisms based on the concept of semileaky modes by which BICs can occur readily in both symmetric and highly asymmetric structures. All the modal spectroscopy combinations, that is, modes only, modes and BICs, and BICs only, may be realized. In the BICs-only case, the BICs are not higher-order modes, but rather the only possible bound state. Anisotropy-induced BICs can be polarization separable or intrinsically polarization hybrid. Full-vector BICs exhibit tunable angular propagation direction and tunable polarization hybridity, as well as highly directional, ultrasharp transitions from radiationless to radiative states, properties that may find applications in photonic filters, spatial-light modulators and sensors based on angular selectivity. We anticipate similar phenomena in off-plane geometries, multilayer and multimaterial structures, biaxial crystals and generalized anisotropic media, such as chiral and hyperbolic materials, as well as in engineered natural and artificial materials crafted in geometries, including high-contrast ultrathin structures and metasurfaces, with form anisotropy.

Methods

Methods and any associated references are available in the online version of the paper.

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Author contributions

All authors contributed equally to the work.

Additional information

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Competing financial interests

The authors declare no competing financial interests.
Methods

Theoretical and numerical methods. A detailed description of the derivation of the eigenvalue equations for interferometric BICs and the related transfer matrix and beam propagation methods are provided as Supplementary Information.

Experimental methods. Modal spectroscopy in a prism-coupling geometry was performed to demonstrate the BIC existence. The experimental layout is shown in Supplementary Fig. 6. The spin-coated polymeric film used as a core film was measured using profilometry and ellipsometry techniques, which gave thickness \( d = 1.6 \, \mu m \) and \( n_i = 1.553 + 0.0005i \). We placed a 5 mm equilateral SF11 prism \( (n = 1.779) \) on top of the sample, using a liquid to match the prism refractive index and minimize any air gap between the sample and the prism. We focused an 8-mm-diameter laser beam \( (\lambda_0 = 632.8 \, nm) \) with an \( f = 25 \, mm \) lens on the top surface of the sample through the tilted prism facet. The light reflected by the sample, coming out from the opposite prism facet, illuminated a CCD (charge-coupled device) camera with its sensing surface \( (6 \, mm \, \times \, 8 \, mm \, \text{high}) \) perpendicular to the reflection direction, in such a way that the vertical axis of the CCD image provided in one shot the dependence with the angle of incidence \( (\phi) \). The incident and reflected light polarizations were selected by means of two independent polarizers. The propagation direction (angle \( \theta \) with respect to the sample’s optical axis) was defined by the plane of incidence and controlled by rotating the sample with a goniometer. The measurement was performed by changing the propagation angle in steps of \( 2^\circ \) and building Fig. 4 by stitching together the central part of the images obtained.

Data availability. The data that support the plots within this paper and other findings of this study are available from the corresponding author on reasonable request.