Transformation of guided modes into bound states in the continuum

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Abstract. We study a silicon-based structure composed of parallel rods arranged in a periodic array. The structure supports guided modes which due to the deformation of structure in general become leaky modes. At the same time the modes split at the Brillouin zone surface by a pair with certain symmetry. Here we report on guided modes transformation into symmetry-protected BIC under deforming the structure, because of inherent field distribution governed by the Bragg-related mode hybridization.

INTRODUCTION

In photonics resonances are widely used for increasing light-matter interaction in vast applications and sophisticated optical devices such as biological and chemical sensors, microcavity lasers, modulators to name a few [1–?]. The conventional merit of resonator efficiency is its quality (Q) factor, which determines the time of photon restraint before it leaks into free space off. For resonator modes decoupled from the radiating waves of free space Q factor tends to infinity and that resonator is perfect. Almost a century ago, in quantum mechanics a special type of electron states, bound states in the continuum (BIC), were considered [2]. These states have discrete energy embedded in the continuum of free space states, nevertheless BIC are stay localized by a certain spatial distribution of potential. Essentially the adaption of the BIC concept to optics paves the way to realization of the perfect resonators.

Unlike electrons, photonic BIC are mostly interesting because the photon energy is always positive and lies in the continuum of propagating waves. Therefore, the problem of trapping a photon near a certain dielectric structure for arbitrary time is of great practical importance. Recently, many applications of BIC in photonics were demonstrated [3, 4, 5].

We notice that perfect BIC cannot exist in finite structures, however they managed to be identified in systems that are infinitely extended in at least one direction. In extend periodic structures we distinguish resonant modes above the light line and guided mode below. Mathematically, in a homogeneous waveguide the wave number $k$ can be combined with the frequency $\omega$ into an effective energy and then the modes above the light line $\omega/c > k$ correspond

![FIGURE 1. Schematic representation of the structure composed of silicon rods. (a) Periodic array of silicon rods along zx direction with radius $r$ and dielectric index $\varepsilon = 12$. (b) Deformed structure wherein rods in each dimer are shifted at arbitrary distances in opposite directions along the $x$ and $y$ axes. Gray arrows specify the direction of dotted circles displacement in place of rods marked black solid circles. These shifted rods form the primitive cell depicted by black dashed lines.](image-url)
to positive energy thus they are extend into a free space, and the modes under the light line $\omega/c < k$ correspond to negative energy. In this approach, the guided modes (below the light line) are considered as ordinary non-radiant localized states with negative effective energy. Although periodicity makes this treatment to be nonstrict it is still really illustrative. Using this approach BIC can only be modes over the light line, among other leaky modes. The periodicity leads to opening diffraction channels up, thus a portion of guided modes occur above the light line where they become leaky modes. Occasionally a structure deformation increases the period resulting to additional diffraction channels to appear in photonic band structure.

Here we show that different types of structure deformation lead to transforming guided modes into leaky ones, however Bragg interaction of two guided modes might allow one of them become BIC.

RESULTS

We consider a structure made of silicon rods with circular profile ($\varepsilon = 12$), lattice constant $a = 330$ $\mu$m, radius of rods $r = 100$ $\mu$m (Fig. 1). The system under study is homogeneous along the $z$ axis and infinitely extended along the $x$ axis. Similar finite structure is known to support BIC related high-Q supercavity modes [6].

We numerically simulated photonic band structure by using the eigenfrequency solver of COMSOL Multiphysics software. Figure 2 demonstrates modes sustained by the structure. It is important to clarify that we calculate only eigen modes of the system. Free space modes lie above the light line which is shown by black solid line. The modes of light cone occur beyond the Brillouin zone because uncertainty of the wave vector up to summation with any reciprocal lattice vector. A pair of guided modes corresponding to the opposite direction of propagation split up at the boundary of the Brillouin zone, which we refer as mode 1 (at the low frequencies) and mode 2 (at the high frequencies).

Now we deform the metasurface. So that let us consider the structure as an array of dimers consisting of two rods (Fig. 1). Parameter $h$ is a shift of the dimerized rods in the direction to each other along the $x$ axis; parameter $b$ defines an offset along the normal (the $y$ axis) such that the one rod moves upside and the other to the opposite direction. Thus one rod shifts at a vector $(h, b)^T$ and the other one has the opposite displacement $-(h, b)^T$. We consider two types of deformation and we call the horizontal deformation as the $x$-deformation, while vertical deformation by $b$ parameter as the $y$-deformation. Both structural transformations change the primitive cell and result to open up additional light cone centered at $\pi/a$. So the both guided modes become resonant leaky modes above the light line.

Figure 3 exhibits that the modes under study are localized in different regions of structure. The magnetic field of mode 1 predominantly concentrates in site of the rod centers and localization areas protrude beyond the rod in the form of ellipses elongated in the vertical direction and the mode 1 is even relative the vertical plane passing through
FIGURE 3. Eigen modes profiles. The intensity of blue and red colors shows, respectively, positive and negative values of the magnetic field component $H_z$ amplitude. These modes are even or odd relative to two vertical planes: brown dashed line is symmetry element, which is located in the middle of the rod and green dashed line is symmetry element which is located between adjacent rods.

Owing to primitive cell doubling we observe appearance of additional diffraction channels whereupon modes cease to be guided. They appear above light line and propagate into free space with their Q factor reduction. We found Q-factor dependence on structure deformation whereby mode 1 stay BIC with the x-deformation while mode 2 became leaky, the opposite occurs when we deform structure with the y-deformation. Modes 1 and 2 become BIC due to even symmetry protection. We consider symmetry-protected BIC at the $\Gamma$ point, although they might also exist on Brillouin zone boundary [8]. In addition we obtain that the leaky modes 1 and 2 (not protected by the symmetry) have quadratic dependence on the deformation.

CONCLUSION

We have shown that the deformation of structure leads to transformation guided modes into leaky resonances, however the field distribution at the Brillouin zone surface match the symmetry and some guided modes become symmetry-protected BIC. BIC resulting from guided modes inherit their field distribution in the material and outside the material which allows us to find different various possible applications in low-threshold lasers, high-sensitivity sensors and switchable modulators. Although we considered a structure with periodicity in one direction, similar physics is inherent in structures with more complex symmetry of systems consisting of resonant particles bounded in two directions.

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