Metasurface engineering through bound states in the continuum

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Metasurfaces have attracted a lot of attention in recent years due to novel ways they provide for the efficient wavefront control and engineering of the resonant transmission. We introduce a new concept for effective engineering of the sharp Fano resonances in metasurfaces associated with a new type of bound states in the continuum. We demonstrate that by breaking the symmetry transversely, in the direction perpendicular to a metasurface with a complex unit cell, we can control the number, frequency, and type of high-Q resonances originating from bound states in the continuum. As example, we demonstrate experimentally the metasurfaces with magnetic dipole and toroidal dipole responses governed by the physics of multipolar bound states.

Bound states in the continuum (BICs) are waves that remain localized in dynamic systems even though they coexist with a continuous spectrum of radiating waves. Although BICs were first introduced in quantum mechanics [1, 2], it is a general wave phenomenon that has been found in many physical systems, such as electromagnetic, acoustic, water and elastic waves. Specifically, these states have also been identified in a wide range of optical systems, including dielectric gratings [3], optical waveguides [4, 5], photonic crystals [6, 7], graphene quantum-dot structures [8], and hybrid plasmonic-photonic systems [9] (see a comprehensive review on BICs in Ref. 10 and references therein).

One interesting type of BICs relies on the symmetry properties of both discrete mode and coexisted radiative continuum. When a discrete mode is characterized by a particular symmetry class, radiative continuum belonging to a different symmetry classes completely decouples from such a discrete state [6, 11]. The coupling between the bound states and continuum band is forbidden as long as their symmetry properties are preserved, and they are classified as symmetry-protected BICs [6].

A particular signature of symmetry-protected BICs in the field of optical metasurfaces is the observation of exceptionally narrow resonances (sometimes called trapped modes) in the optical spectra of metasurfaces composed of in-plane asymmetric structural elements [12, 13]. The appearance of ultrahigh-Q resonances are attributed to the excitation of asymmetric modes whose electromagnetic field distributions are slightly deviated from the, otherwise inaccessible, symmetric modes. The corresponding quality factors of leaky resonances depend on the degree of the introduced structural asymmetry [14].

The concept of manipulating the transition between the symmetry-protected BICs and leaky resonances was first proposed for plasmonic metasurfaces composed of metallic split-ring resonators [15], and then it was developed for all-dielectric metasurfaces [16–24].

In general, BIC modes transform into leaky resonances when the symmetry of either eigenmodes of the structure or radiative continuum is broken. As a result, one needs to break the symmetry of either discrete mode or radiative continuum in order to access such symmetry protected multipolar BICs. To date, all the mechanisms reported so far for manipulating the transition between BICs and radiative continuum can be classified as in-plane symmetry breaking. No effort has been paid to manipulate the transition between BICs and leaky resonances utilizing the out-of-plane symmetry, which will...
provide more flexible approach to engineer and control the resonant properties of metasurfaces.

In this Letter, we introduce a new concept for effectively controlling the high-Q Fano resonances, which are originated from the BICs of optical metasurfaces, by utilizing out-of-plane symmetry breaking in the unit cell of an all-dielectric metasurface. We demonstrate that our idea is quite general, which has been validated in metasurfaces composed of lattices of particle clusters corresponding to different symmetries. By introducing this unique degree of freedom beyond the in-plane symmetry, one can efficiently control the symmetry of the discrete mode and thus manipulate its interaction with the continuum. Employing this concept, we realize accesses to various kinds of multipolar BIC associated leaky modes existed in the cluster-based all-dielectric metasurfaces. We further perform proof-of-principle microwave experiments by demonstrating leaky resonances associated with the toroidal dipole BICs in both far-field and near-field measurements.

Without loss of generality, we consider an all-dielectric metasurface whose unit cell consists of different types of particle clusters [Fig. 1(a)]. The simplest configuration of the unit cell is a disk dimer arranged in a square lattice, as shown in [Fig. 1(b)]. Therefore, we start from the demonstration of our concept by evaluating how the out-of-plane symmetry breaking will affect on the transition between various BIC modes and the corresponding leaky resonances in a dimer-based metasurface. Then it is generalized to a more complex trimer-based metasurface composed of equilateral triangular unit cells [Fig. 1(c)].

All notations and parameters related to the geometry of the metasurface under study are summarized in Fig. 1. The disks are made of a non-magnetic material with relative permittivity $\varepsilon_d$ and the metasurface is placed on a dielectric substrate with relative permittivity $\varepsilon_s$. We consider that the metasurface is illuminated by a normally incident ($\vec{k} = \{0, 0, -k_z\}$) linearly polarized plane wave with the electric field vector directed either along the $x$ axis ($\vec{E} = \{E_x, 0, 0\}$, $x$-polarized wave) or the $y$ axis ($\vec{E} = \{0, E_y, 0\}$, $y$-polarized wave).

For the metasurface under study we can recognize the BIC modes by performing an eigenvalue analysis using the RF module of commercial COMSOL Multiphysics® finite-element electromagnetic solver [25]. Such BIC modes can be distinguished by their real-valued eigenfrequencies. In accordance with our experimental possibilities, we consider the BICs mode in the microwave part of the spectrum (8 - 12 GHz). From the known set of modes we selected several BIC modes which appear in the chosen frequency band for the given parameters of the structure. We denoted the modes of interest by symbols D1-D4 [Fig. 2(a)].

These modes manifest themselves by distinct displacement current geometries, which can be regarded as specific combinations of magnetic dipole (MD) and electric dipole (ED) moments inherent to an individual disk [Fig. 2(b)]. In particular, for Mode D2 the magnetic field vector is anti-parallel located in the $x$-$y$ plane, whereas displacement current flows inside the particles in the $y$-$z$ plane and has a solenoid-like behavior enclosing the magnetic field. It resembles the typical out-of-plane toroidal dipole (TD) BIC mode which was theoretically studied recently [11]. Rather than enabling the coupling between TD BIC mode and the obliquely incident plane wave, we show that this TD BIC mode can be turned to a TD leaky resonance by breaking the out-of-plane symmetry, as shown in Fig. 2(c). Specifically, such a coupling to Mode D2 can be realized for the $y$-polarized incident wave as soon as a difference in the thicknesses of disks forming a dimer is introduced [we denote this difference as the asymmetry parameter $\theta$, see Fig. 2(b)]. Notice that the group of symmetry in the $x$-$y$ plane of the non-perturbed dimer with $\theta = 0$ is $C_2$, and of the perturbed dimer with $\theta \neq 0$ is $C_s$.

Indeed, while the symmetry of dimer is preserved, there is no peculiarities in the transmitted spectra of the metasurface under study at the frequencies of the BIC modes [the eigenfrequency of Mode D2 is denoted as $f_{BIC}$, see Fig. 2(c)]. As soon as the asymmetry is introduced, there is a leaky resonance (the resonant frequency of the leaky mode originated from Mode D2 is denoted as $f_{LM}$) in the transmission spectrum and such resonance acquires a peak-and-trough (Fano) profile which is typi-

![FIG. 2. (a) A set of the BIC-type eigenstates and (b) the corresponding electromagnetic near-field distribution for metasurfaces with the unit cell composed of a pair of disks (dimer). (c) Access to leaky resonance originated from the BIC Mode D2 of the dimer metasurface via out-of-plane symmetry breaking. (d) Dependence of the quality factors of leaky resonances originated from BIC modes D1-D4 on the out-of-plane asymmetry parameter $\theta$. Parameters of the metasurface are: $r_d = 4$ mm, $h_d = 3.5$ mm, $d = 20$ mm, $l = 0.5$ mm, $\varepsilon_d = 22$, $\varepsilon_s = 1$.](attachment:image.png)
FIG. 3. (a) A set of BIC-type eigenstates and (b) their electromagnetic near-field distributions for metasurfaces with the twin-trimer unit cell. (c) Schemes of access to Mode T1 in the trimer-based metasurface. (d) Evolution of the transmission spectra vs the asymmetry parameter $\theta$. (e) Electromagnetic near-field distribution of the leaky mode at the resonant frequency corresponding to the manifestation of Mode T1. $d = 31.1$ mm, all other parameters are the same as in Fig. 2.

It should be pointed out that breaking the out-of-plane symmetry of the cluster composed of disks has fundamentally different effects on the quality factor of the BIC modes compared with the case of breaking the in-plane symmetry. One can anticipate that introduced asymmetry in the thicknesses of disks forming the dimer has a stronger effect on its out-of-plane ED moment and in-plane MD moment, since the polarization currents are parallel to such plane. In contrast, breaking the in-plane symmetry by changing the radius of one disk has more pronounced effect on the in-plane ED moment and out-of-plane MD moment. For instance, among the selected BIC modes of dimer, Mode D2 is considered as a TD BIC composed of two anti-parallel in-plane MD moments. Therefore, symmetry breaking in the out-of-plane direction turns such a TD-BIC into a leaky resonance much more efficiently compared with other types of BIC modes. At the same time, the decrease of $Q$-factor for Mode D4 consisted in the in-plane MD moments is also faster than that for Modes D1 and D3, as shown in Fig. 2(d). As a result, the out-of-plane symmetry breaking can be regarded as a new degree of freedom and an efficient way to tailor the resonant properties of the symmetry protected BIC modes, especially for the out-of-plane TD BIC and in-plane magnetic BIC modes.

We further present an example utilizing the out-of-plane symmetry breaking induced transition between the symmetry protected BIC modes and the corresponding leaky resonances in an all-dielectric metasurface based on trimers [Fig. 1(c)]. The existence of the TD mode in the metasurface whose lattice is formed by trimers arranged in square unit cells was examined in [26]. Here we introduce some modifications to the structure of unit cell studied earlier to provide further degree of freedom for resonance manipulation in both near- and far-fields. Firstly, we consider that the unit cell has the form of an equilateral triangle. Secondly, two triangle unit cells are paired together in such a way that a rhomboid cluster appears, i.e., generally, the metasurface under study is constructed from the twin-trimer super-cells.
FIG. 4. Experimental results. (a) Transmission coefficient of the trimer-based metasurface. The inset presents a fragment of the metasurface prototype and several sets of particles. In the simulation actual material losses (tan δ = 1 × 10⁻³) in ceramic particles are taken into account, while the substrate is modeled as a loss-less dielectric. The asymmetry factor is θ = −1.0 mm. All other material and geometrical parameters of the metasurface are the same as in Fig. 3 (b) Simulated and (c) measured near-field distribution of the real part of the normal component of the electric field (Eₜ) at the resonant frequency f_{LM}. The measurement plane is 1 mm away from the metasurface. The field is normalized to the maximum value of Eₜ.

After the eigenvalue analysis of this metasurface, a set of BIC modes existed in the frequency band of interest are selected. We denote these modes by symbols T1-T3 [Fig. 3(a)]. All these modes present fruitful electromagnetic near-field distributions manifested as electric and magnetic hot-spots in the near-field [Fig. 3(b)]. Specifically, these BIC modes are composed of various MD moments in each disk, which are arranged in the x-y plane. When all disks are identical, the symmetry of the twin-trimer super-cell is C₂ᵥ and it belongs to the rhomboid system (see Fig. 3(c), upper part). As can be seen from this figure, neither the x-polarized nor the y-polarized normally incident plane wave can access to these BIC modes. As the in-plane MD moment is more sensitive to the out-of-plane asymmetry for the all-dielectric metasurface under consideration, these BIC modes can be effectively turned into leaky resonance by increasing the thickness of certain disks. For example, perturbation of the unit cell by two disks with different thicknesses reduces the symmetry to C₂ of the monoclinic system (Fig. 3(c), middle part). This perturbation allows one to excite the MD leaky resonance originated from BIC Mode T1. It should be pointed out that the metasurface has a polarization-dependent response, where the transmissions of the metasurface are different under the excitation by the x-polarized and y-polarized plane waves [Fig. 3(c)].

At the same time, the out-of-plane symmetry breaking can also be used to tailor the frequency and Q-factor of the leaky Fano resonance. By changing the asymmetry factor θ from 1 to −1 mm, one can observe the shift of the resonant frequency of the leaky mode f_{LM} compared with the eigenfrequency f_{T1} of Mode T1, as shown by Figs. 3(d). It can be observed that the Q-factor of this resonance can also be manipulated accordingly by using different degrees of out-of-plane symmetry breaking. More importantly, the electromagnetic near-field can also be manipulated by using the asymmetry parameter θ. The electromagnetic field distributions at the resonant frequency under the excitation of the y-polarized plane wave are shown in Figs. 3(e) for two typical asymmetry parameters θ = 1 and θ = −1, respectively. As can be seen from this figure, they are distinct by their electromagnetic near-field distributions though they are originated from the same BIC Mode T1, validating the concept of out-of-plane symmetry breaking for the manipulation of the vector near field. It should be pointed out that our concept is quite general and it can be easily generalized to resonant metasurfaces operating at the optical spectrum. (see two examples in Supplemental Material [27]). The ability to control the electromagnetic near-field by utilizing out-of-plane symmetry breaking provides possibility to precisely tailor both the emission of the ED and MD types of dipole emitters [28].

To experimentally verify the out-of-plane symmetry breaking effect as an effective mean to trigger the transition between BIC modes and high-Q Fano resonance, an all-dielectric metasurface is fabricated and studied in the microwave range. All details regarding to the samples preparation and the measurement setup can be found in Refs. [23] and [26] (see also Supplemental Material [27]). The manifestation of the corresponding leaky resonance is detected in the far-field measurement of the transmission coefficient of the metasurface [Fig. 4(a)]. In order to provide a reference for experiment, we present the simulated electric near-field distribution [Real(Eₜ)] of the metasurface at the frequency f_{LM}. As can be seen from Fig. 4(b), the electric field is mostly concentrated in the center of trimers, being out of phase in the pair of trimers forming the super-cell. The electromagnetic near field distribution are then experimentally measured for the all-dielectric metasurface at the same resonant frequency f_{LM}. Indeed, the simulated [Fig. 4(b)] and experimental [Fig. 4(c)] results show excellent agreement with each other, validating the excitation of MD leaky resonance originated from BIC Mode T1.

In summary, we have introduced a new mechanism for a highly efficient engineering and control of resonant metasurfaces via symmetry-breaking in the out-of-plane direction, which essentially trigger the transition between symmetry protected BIC modes and leaky resonances. We show that both the resonance frequency and Q-factor
of leaky resonance can be manipulated by the asymmetry factor $\theta$. At the same time, the electromagnetic near field can also be tailored simultaneously to address the electric and magnetic hot-spots locally. As an example, we have presented a microwave experiment to validate the concept of out-of-plane symmetry breaking for metasurface engineering.

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