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Spectral and temporal evidence of robust photonic bound states in the continuum on terahertz metasurfaces

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Photonic bound states in the continuum (BICs) are protected eigenstates in optical systems with infinite lifetimes. This unique property, which translates in infinite $Q$-factor resonances, makes BICs extremely interesting not only from a fundamental perspective but also for various applications such as lasing and sensing. General means to achieve robust BICs are, however, elusive. Here we demonstrate analytically that BICs emerge in metasurfaces formed by arrays of detuned resonant dipolar dimers as a universal behavior occurring regardless of both dipole position within the unit cell and lattice constant in the nondiffracting regime. These resonances evolve continuously from a Fano resonance into a symmetry-protected BIC as the dipole detuning vanishes. We have experimentally verified this very robust response at terahertz frequencies through dimer rod arrays with different rod sizes by simultaneously measuring the reduction of linewidth and the increase of lifetime before the BIC is formed, as it is impossible to couple to it from the continuum. Similar configurations can be straightforwardly envisioned throughout the electromagnetic spectrum, enabling a simple geometry that is easy to fabricate with resonances of arbitrarily high $Q$ factors.

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1. INTRODUCTION

Bound states in the continuum (BICs) have attracted much interest lately in physics for their (theoretically) infinite $Q$ factor. These states are leaky modes that in a certain limit of some parameter space cannot couple to any radiation channel [1]. In the absence of material losses, BICs have infinite lifetimes and zero linewidths. An approach to trap light in such remarkable electromagnetic modes is to exploit metasurfaces [2–9], i.e., subwavelength arrays (in the nondiffractive region) where only the specular reflection/transmission channels are allowed by symmetry, wherein outgoing specular channels can be suppressed by tuning the parameters of the system in various manners, leading to symmetry-protected BICs. Achieving robust BICs and quasi-BICs will be of great interest for the realization of cavities with arbitrarily high $Q$-factor and for applications such as lasing and sensing [10–12]. Nonetheless, there are no fundamental works describing how to achieve robust BICs on a general basis, except for well-known symmetry-protected and accidental degeneracies appearing in photonic crystals [3] and asymmetric metasurfaces [7]. A variety of resonant phenomena, such as surface plasmon lattice resonances in the optical domain [13–19], Fano resonances [20–26], and electromagnetically induced transparency at optical and THz frequencies [27–36], have been reported in metasurfaces; however, robust symmetry-protected BICs remain unexplored. Metasurfaces are especially interesting for this purpose due to their enhanced collective response [21,26,37–40].

In this paper, we will show that a simple and easily experimentally accessible configuration based on metasurfaces of tunable dipoles supports robust BICs that emerge in the nondiffractive regime. The symmetry protection of these BICs is not broken or lost by displacements of the dipoles within the unit cell, which increase the tolerance of these systems to imperfections. In addition, we will unequivocally demonstrate experimentally that such BICs emerge at terahertz (THz) frequencies in gold-rod dimer metasurfaces formed by two rods per unit cell by observing the vanishing linewidth in the THz transmission spectra accompanied by the pronounced increase of the resonance lifetime, when rods are made identical. The negligible Ohmic losses of metals at THz frequencies and the dipolar-like = λ/2 resonances of metallic rods at these frequencies are responsible for the appearance of BICs in this system. Apart from full numerical calculations in agreement with the experimental results, a simple
model for arrays of detuned-resonant-dipole dimers is developed to yield physical insight. Hereby, we show analytically a very general condition for the emergence of symmetry-protected BICs in the parameter space of dipole detuning, from a dark Fano resonance (hybridized dipole lattice mode) that becomes an infinite-Q-factor BIC for zero detuning. These calculations fully explain the experimental results in this wider theoretical context of detuned-dipole arrays.

2. THz TIME-DOMAIN SPECTROSCOPY MEASUREMENTS

Using optical lithography, metal deposition, and lift-off, we have fabricated samples containing 2D periodic lattices of gold rods on top of a 1.5 mm thick amorphous quartz substrate. These samples were clamped against another 1.5 mm substrate with an index matching liquid in between to suppress unwanted reflections, making the total sample thickness 3 mm. Before the thermal evaporation of the 100 nm gold layer, a 3 nm Ti adhesion layer was deposited. All the samples consist of 2D periodic lattices of two gold rods per unit cell. The lattice has a square symmetry with a pitch of $a = b = 300 \mu m$. One of the rods has a fixed dimension of $200 \mu m \times 40 \mu m$, while the dimensions of the other rods are different for each sample that is investigated. The long dimensions of the rods are aligned with the $y$ axis, and the rods inside the unit cell are separated by a distance $d_x$ along the $x$ axis. Both rods support $\lambda/2$ resonances in the THz range given by their length. The resonance frequency is controlled by the long axis of the rods, so we classify each lattice by the length of the second rod $L_2$, which covers the range $L_2 = 125a/250 \mu m$ in steps of $25 \mu m$ while keeping $L_1 = 200 \mu m$ constant. The width of the rods is scaled such that surface area covered with gold is comparable between the rods and therefore between all samples.

Two different sets of samples have been measured, with separation between rods fixed at $d_x = 120$ and $150 \mu m$. THz transmittance spectra of these samples have been measured at normal incidence using a $4f^0$ far-field THz time-domain spectrometer (Menlo TeraK15). The transmittance of the lattices for different $L_2$ is shown in Fig. 1(a). Numerical simulations calculated through SCUFF [41,42] (an open-source software package for analysis of electromagnetic scattering problems using the method of moments) are shown in Fig. 1(b), corresponding to transmittance spectra at normal incidence for the same geometrical parameters, but considering gold rods as planar perfectly conducting rectangles embedded in a uniform medium with $n = 1.55$ (the average of those of air and the supporting quartz substrate [43]).

The more relevant feature in Fig. 1 is that for $L_2 \neq 200 \mu m$ all spectra present a strong Fano resonance with a narrow asymmetric line shape, with a high contrast approaching zero to total transmittance. The resonance moves toward lower frequencies as $L_2$ is increased and disappears for $L_2 = 200 \mu m$. In addition, as the rods become more similar in size, the resonance becomes narrower; it should be mentioned, though, that the resonance narrowing is not clearly visible in the measurements for $L_2 = 175, 225 \mu m$ due to the limited frequency resolution in the measurements. The Fano resonance can be understood in terms of the lattice resonances that the array supports: a bright, broad symmetric mode and a dark, narrow antisymmetric mode [33]. Incidentally, by lattice resonances we mean the resonances resulting from the lattice-induced modification of meta-atom resonances [44] rather than those emerging near Rayleigh anomalies [14]. The symmetry of these modes is preserved in the lattice, and they interfere either destructively or constructively, producing a characteristic dip/peak pair in the spectra. Moreover, the dark mode becomes inaccessible at $L_2 = 200 \mu m$ and the interference disappears; as we will show below, the width of the resonance thus tends to zero, leading to a BIC that cannot be detected in the far field.

It should be noted that when $d_x = 150 \mu m$, the BIC state is connected to the guided mode that the lattice supports. Indeed, for $L_2 = 200 \mu m$ both rods are identical, so the array becomes a single rod lattice with the lattice constant halved along the $x$ axis. We call this condition as the “half-period lattice.” The Brillouin zone is doubled when $d_x = a/4$; thus, if one artificially assumes that the actual lattice constant is still $a$ (instead of $a/2$), part of the lowest guided mode band (always below the light line of the true Brillouin zone) will be bent back into the propagating region (above the light line) of the artificially reduced Brillouin zone, indeed leading to an artificial BIC (stemming from a guided mode rather than from a leaky mode) at the $\Gamma$ point. Furthermore, the number of resonances that the lattice supports can be associated
with the number of particles per unit cell. For the identical half-period lattice, i.e., one particle per unit cell, there is only a bright (symmetric) mode. Therefore, for the half-period lattice it is difficult to relate the BIC with a real state.

Nonetheless, for a lattice with \(d_s = 120 \mu m\), where the half-period lattice is not recovered at \(L_2 = 200 \mu m\) for equal rods, the BIC is no longer directly connected to any guided mode, so the system has two well-defined lattice modes, and a true BIC emerges. This is further verified through numerical calculations at oblique incidence (see Supplement 1, Figure S1), which reveal a Fano resonance emerging for equal rods only in the case of the lattice with \(d_s = 2\alpha/5\); this is yet another evidence of the true BIC behavior.

Time-domain measurements [also with quasi-plane wave excitation as in Fig. 1(a)], shown in Fig. 2, yield further evidence of the transition to a BIC in the parameter space. Transmitted THz transients are plotted for lattices with a spacing of \(d_s = 120 \mu m\) and asymmetric dimer rods \(L_2 = 125, 150, 175 \mu m\). The transient for the BIC condition \((L_2 = 200 \mu m)\) is subtracted from these measurements to remove the contribution of the broad bright mode. On long time scales, only this narrow, dark (anti-symmetric) resonance remains, which is in turn fitted to a single frequency-damped harmonic oscillator with lifetimes of 5.9, 10, and 20 ps, respectively, and oscillation frequencies of 0.4, 0.39, and 0.375 THz, respectively.

![Fig. 2. Measured transient response after background subtraction for square lattices (\(\alpha = 300 \mu m\)) as in Fig. 1, consisting of two gold rods per unit cell, deposited on a quartz substrate, with rod separation \(d_s = 2\alpha/5\) (solid curves). One of the rods has fixed dimensions of \(L_2 = 200 \mu m\) for equal rods, the BIC is no longer directly connected to any guided mode, so the system has two well-defined lattice modes, and a true BIC emerges. This is further verified through numerical calculations at oblique incidence (see Supplement 1, Figure S1), which reveal a Fano resonance emerging for equal rods only in the case of the lattice with \(d_s = 2\alpha/5\); this is yet another evidence of the true BIC behavior.](image)

### 3. THEORETICAL MODEL: COUPLED DETUNED-DIPOLE PLANAR ARRAY

To shed light onto this rich phenomenology, we developed a simple coupled dipole-dimer model of an infinite array embedded in a homogeneous environment, shown in detail in Supplement 1. Dipoles are fully characterized by their polarizabilities along the \(y\) axis, namely, \(\alpha^{(1)}_y\) and \(\alpha^{(2)}_y\), where (1) and (2) account for each dimer dipole in the unit cell. The array is excited by an external plane wave, with \(\psi_0\) being its electric field polarization along the \(y\) axis. Upon imposing Bloch’s theorem and recalling that only normal incidence is considered, the local field at the position of the dipoles \(\psi^{(i)}_{loc}\), with \(i = 1, 2\), can be found through a self-consistent field equation

\[
\begin{bmatrix}
\psi^{(1)}_{loc} \\
\psi^{(2)}_{loc}
\end{bmatrix} = \left[\mathbb{I} - k^2 G_{b} \mathbb{\alpha}^{\dagger}\right]^{-1} \begin{bmatrix}
\psi^{(1)}_0 \\
\psi^{(2)}_0
\end{bmatrix},
\]

where \(\psi^{(i)}_0\) is the incident field on dipole \(i = 1, 2\), \(\mathbb{I}\) is the identity matrix, \(\mathbb{\alpha}\) is the polarizability tensor, and \(G_{b}\) is the lattice “depolarization” dyadic (or return Green function)

\[
\mathbb{\alpha} = \begin{bmatrix}
\alpha^{(1)}_y & 0 \\
0 & \alpha^{(2)}_y
\end{bmatrix},
\quad
G_{b} = \begin{bmatrix}
G_{yy}^{(1)} & G_{yy}^{(1-2)} \\
G_{yy}^{(2-1)} & G_{yy}^{(2)}
\end{bmatrix}.
\]

\(G_{yy}\) describes the self-interaction of each dipole array; \(G_{yy}^{(i-j)}\) is the interaction of the dipole array labeled as \(i\) over \(j\). Due to symmetry, at normal incidence \(G_{yy}^{(1-2)} = G_{yy}^{(2-1)}\).

Surface lattice resonances are the solutions of Eq. (1) in the absence of the external plane wave. To solve it, we diagonalize the system and find the condition at which the eigenvalues \(\Lambda\) are equal to zero. At real frequencies, the zeros of the real part of \(\Lambda\) give the resonance frequencies, whereas the imaginary parts define the resonance widths. Recall that the imaginary components of \(G_{b}\) and \(\mathbb{\alpha}\) (for lossless particles) are well defined and satisfy the following condition:

\[
3 \left[ \frac{1}{\alpha_y} - G_{by} \right] + G_{yy}^{(1-2)} = 0,
\]

where we define the magnitudes

\[
\frac{2}{\alpha_y} = \frac{1}{k^2} \left( \frac{1}{\alpha^{(1)}_y} + \frac{1}{\alpha^{(2)}_y} \right), \quad \Delta \alpha_y = \frac{1}{k^2} \left( \frac{1}{\alpha^{(1)}_y} - \frac{1}{\alpha^{(2)}_y} \right).
\]

\(\Delta \alpha_y\) thus represents the detuning between the two rods in the unit cell (introduced in the experiments by changing the size
of one rod). For a small detuning $\Delta a_j \ll 2G_{yy}^{(1-2)}$, the imaginary components of the eigenvalues can be approximated by

$$3[\Lambda^+] = 3 \left[ \frac{(\Delta a_j)^2}{8G_{yy}^{(1-2)}} \right],$$

and

$$3[\Lambda^-] = 3 \left[ 2 \left( \frac{1}{a_j} - G_{byy} \right) - \frac{(\Delta a_j)^2}{8G_{yy}^{(1-2)}} \right].$$

Finally, the corresponding eigenvectors are given by

$$\Lambda^\pm = 0 \rightarrow \nu^\pm = \begin{bmatrix} \psi^{(1)}_{\text{loc}} \\ \psi^{(2)}_{\text{loc}} \end{bmatrix} = \begin{bmatrix} 1 \\ \mp 1 \end{bmatrix}.$$

The lattice resonances are associated with two modes in which the rods are out of phase (antisymmetric/symmetric). From Eq. (3), it follows that $3[\Lambda^+]$ goes to zero as the detuning is suppressed, i.e., as the two rods are made equal. Hence, as expected, the out-of-phase mode $\Lambda^+$ is very narrow and becomes a BIC at zero detuning. On the other hand, $3[\Lambda^-]$ is always larger than zero, so the in-phase mode $\Lambda^-$ is broad. Therefore, for $L_1 \neq L_2$ ($a_j^{(1)} \neq a_j^{(2)}$) we have a broad mode that interferes with a very narrow mode, leading to a Fano resonance. For $L_1 = L_2$, the narrow mode converges into a BIC state, precluding any external coupling to it and the formation of the dip in transmission.

Interestingly, if there is also an additional displacement along the $y$ axis, given by $d_y$, Eq. (3) still holds. Moreover, this identity is also valid for rectangular (non-square) lattices where $a \neq b$. This is evidenced in the detailed formulation in Supplement 1, (Eq. S19), where the expressions of the imaginary parts of all three terms in Eq. (3) are shown to cancel out in the absence of diffraction orders despite the fact that both $G_{yy}^{(1-2)}$ and $G_{byy}$ depend on lattice parameters. Hence, Eq. (3) is universal and holds for: (i) any set of lattice constant parameters $a$ and $b$ and (ii) any relative displacement between dipoles inside the unit cell, not only along the $x$ axis, but extensive to the full $x-y$ plane. Therefore, a major conclusion is that the BIC state is symmetry protected and robust against changes in the specific lattice parameters: $a$, $b$, $d_x$, and $d_y$. In this regard, bear in mind that this statement is purely theoretical (no experimental evidence is provided). Indeed, it is thus restricted to the domain of applicability of our coupled detuned-dipole formulation, namely, dimer meta-atoms accounted for by parallel detuned dipoles, with couplings among them fully reproduced by dipole–dipole interactions, and within the spectral regime where no diffraction orders are allowed other than the specular ones.

Let us now analyze the Fano–BIC transition using our coupled dipole-dimer model. We plot in Figs. 3(a) and 3(c) the spectra of the transmission coefficient ($T = 1 - R$) intensity and phase, for a square lattice (lattice constant $a = b = 300 \mu$m) with two dipoles per unit cell, separated by a distance of $d_x = 120 \mu$m for varying $L_2$; cuts for fixed lengths are shown in Figs. 3(b) and 3(d).

The polarizability of the rods is calculated through SCUFF [41,42], considering the rods as perfect electric conductors [see Supplement 1, Fig. S2(b)].

Figure 3 shows that the coupled dipole-dimer model reproduces all the features exhibited in Fig. 1, fully extending the characterization of the BIC into the $L_1$-parameter space. Remarkably, the contour map in Fig. 3(a) reveals the classical narrowing of the leaky resonance (Q factor tending to infinity) towards a BIC state, with the distinct feature that the resonant state [surface lattice dipole resonance with an abrupt $\pi$-phase jump shown in the contour map in Fig. 3(c)] manifests itself as a narrow Fano resonance instead. Transmittance spectra (intensity and phases) are shown in Figs. 3(b) and 3(d) for given $L_1$, illustrating this Fano-like behavior that disappears at $L_2 = L_1$ as a signature of the BIC.

Furthermore, we show in Fig. 4 the amplitudes ($\psi^{(1)}_{\text{loc}}, \psi^{(2)}_{\text{loc}}$) and phases ($\phi^{(1)}_{\text{loc}}, \phi^{(2)}_{\text{loc}}, \Delta \phi$) of the local fields over the dipoles for the dipole dimer corresponding to $L_2 = 150$ μm. At low frequencies, both dipoles are driven in phase. At $\nu = 0.38$ THz, coinciding with the zero of $\psi^{(2)}_{\text{loc}}$, $\Delta \phi$ presents a discontinuity and becomes maximum (rods out of phase, with a high dispersion in both). The field amplitudes are enhanced and, indeed, exhibit a resonant line shape, corresponding to the dark lattice resonance, where the Fano asymmetric line shape emerges in the far field. Then at $\nu = 0.48$ THz, upper-frequency end of the Fano resonance, $\Delta \phi$ presents another discontinuity exactly at the zero of $\psi^{(2)}_{\text{loc}}$. For higher frequencies the phase difference vanishes and the dipoles are in phase again. Thus, at given frequencies at the lower/upper band of the Fano resonance, the fields at the long/short rods are strictly zero, manifesting the strong interaction that exists between the different rods near resonance. In addition, the local field is enhanced by more than a factor of three in both rods. At $L_2 = L_1$, the anti-phase behavior is not allowed, so that the field at both rods is identical [cf. Figs. 4(a) and 4(b)], with no evidence whatsoever of a Fano resonance, and thus it becomes a BIC [as shown in Figs. 3(a) and 3(b)].

To reveal even more neatly the BIC behavior, we show a near-field map of the out-of-plane electric field component at the BIC frequency (0.357 THz) in Fig. 5. The field pattern is numerically calculated through FDTD simulations (Lumerical), for a
broadband (center frequency around the BIC, $\nu = 0.357$ THz) dipole source (located at the center of the image) inside both asymmetric and symmetric dimer rod arrays ($d = 120$ $\mu$m) lying on a quartz substrate, over a large area of $2.5 \times 2.5$ mm$^2$, with rod dimer dimensions (as highlighted in the schematic insets) of: $L_1 = 200$ $\mu$m and $L_2 = 125$ $\mu$m, [Fig. 5(a)]; $L_1 = L_2 = 200$ $\mu$m [Fig. 5(b)]. In Fig. 5(a) the excitation with a point dipole is radiated to the far field, showing negligible coupling or propagation to the neighboring rods. By contrast, the near field for equal rod dimers is effectively trapped in the BIC mode as shown in Fig. 5(b): many dimers in the lattice are resonantly excited, with the expected opposite phase for each rod within the (dimer) unit cell that protects the BIC and precludes out-of-plane radiation losses.

4. CONCLUSIONS

We have shown experimentally through the THz transmission spectra and transients that metasurfaces consisting of sub-wave-length gold-rod dimers support BICs when the rods are identical and that such BICs emerge from strong Fano resonances, which become narrower (higher $Q$ factor) as the dimensions of the rods approach each other. Such experimental results have been fully explained in the theoretical context of detuned-dipole arrays as a universal condition for the emergence of symmetry-protected BICs and vanishing dipole detuning. Remarkably, such BIC condition is shown to be independent of both the relative position between dipoles/rods inside the unit cells and the lattice constants (provided that no diffractive orders come into play). Hence, these properties make an array of detuned dipoles a general scenario to engineer robust and versatile metasurfaces supporting bound states in the continuum throughout the electromagnetic spectrum, with appealing implications in sensing, lasing, and related phenomenology. Finally, bear in mind that the formalism and phenomenology of our coupled detuned-dipole model could be extrapolated to other fields of wave physics with arrays of dipolar scatterers, such as acoustic, elastic, seismic, and even atom waves.


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See Supplement 1 for supporting content.

'These two authors contributed equally to this work.

REFERENCES


