# Resonances and Bound States in the Continuum on Periodic Arrays of Slightly Noncircular Cylinders

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(Dated: November 22, 2017)

Optical bound states in the continuum (BICs), especially those on periodic structures, have interesting properties and potentially important applications. Existing theoretical and numerical studies for optical BICs are mostly for idealized structures with simple and perfect geometric features, such as circular holes, rectangular cylinders and spheres. Since small distortions are always present in actual fabricated structures, we perform a high accuracy numerical study for BICs and resonances on a simple periodic structure with small distortions, i.e., periodic arrays of slightly noncircular cylinders. Our numerical results confirm that symmetries are important not only for the so-called symmetry-protected BICs, but also for the majority of propagating BICs which do not have a symmetry mismatch with the outgoing radiation waves. Typically, the BICs continue to exist if the small distortions keep the relevant symmetries, and they become resonant modes with finite quality factors if the small distortions break a required symmetry.

## I. INTRODUCTION

In recent years, optical bound states in the continuum (BICs) have attracted much attention due to their intriguing properties and potentially significant applications [1]. A BIC on a periodic structure is a guided mode above the light line, and it can also be considered as a special resonant mode with an infinite quality factor. The so-called symmetry-protected BICs are well known [2–8]. They have a symmetry mismatch with the outgoing radiation waves, and are typically antisymmetric standing waves. There are also propagating BICs and symmetric standing waves that do not have the symmetry mismatch, but are still uncoupled with the outgoing waves [9–22]. Near each BIC, there is a family of resonant modes depending on the wavevector, and their quality factors approach infinity as the wavevector tends to the wavevector of the BIC. The strong resonant effect leads to enhanced local fields around the periodic structures, and it can be used to develop low-threshold lasers [23] and to enhance nonlinear and quantum optical effects [24]. The BICs also give rise to discontinuities in the transmission and reflection coefficients which can be explored in filtering, sensing, and switching applications [25, 26].

So far, existing theoretical studies on BICs are mostly for structures with simple and idealized geometric features. Two-dimensional (2D) structures usually consist of circular or rectangular cylinders or holes [2, 5, 6, 8–12, 14, 18, 19, 21]. Three-dimensional (3D) biperiodic structures are typically photonic crystal slabs with circular holes [3, 4, 7, 13, 17]. Rotationally symmetric structures consist of spheres or piecewise uniform circular rods [15, 16, 20, 22]. Since idealized structures cannot be realized in practice, it is essential to study non-perfect structures that are slightly distorted from the perfect ones. In particular, it is important to find out how small distortions affect the BICs. The existence and robustness of BICs are important theoretical questions. The symmetry-protected BICs are well understood [2, 6]. Their existence can be rigorously proved, and in general, they continue to exist when the structure is perturbed with the relevant symmetries kept intact. The majority of propagating BICs are found on structures with certain symmetries, and their frequencies and wavevectors satisfy conditions such that there is only one radiation channel for outgoing waves. It is known that these propagating BICs are robust against variations in the geometric or material parameters of the idealized structures [9, 12, 13, 27–29]. It has been suggested that these propagating BICs are in fact robust against arbitrary structural perturbations that preserve the relevant symmetries [28–30]. It should be pointed out that propagating BICs do exist when there are more than one radiation channels [9, 14], but they are less robust.

In this paper, we study BICs and resonances on periodic arrays of dielectric cylinders with slightly noncircular cross sections. A periodic array of circular cylinders is probably the simplest structure on which various BICs exist [5, 6, 8, 14, 19]. Based on a highly accurate numerical method, we show that the symmetry-protected BICs and the propagating BICs with one radiation channel are preserved when the distortion retains the relevant symmetries, and the BICs become resonances with finite quality factors when the distortion breaks the required symmetries. Our results are consistent with those reported in [28, 29] and provide a strong support for the analytic result developed in [30].

## II. FORMULATION AND METHOD

We consider a periodic array of parallel and infinitely long dielectric cylinders as shown in Fig. 1. The cylinders are placed periodically along the $y$ axis with period $L$, are parallel to the $z$ axis and surrounded by air. The dielectric constant of the cylinders is $\epsilon_1$. For the $E$ po-

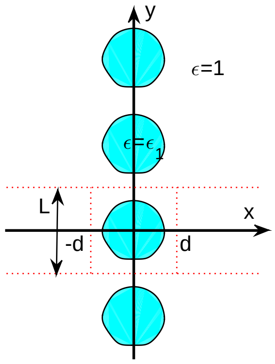


FIG. 1. A periodic array of dielectric cylinders with slightly noncircular cross sections.

larization, the $z$ component of the electric field, denoted by $u$, satisfies the following 2D Helmholtz equation

$$\partial_x^2 u + \partial_y^2 u + k_0^2 \epsilon(x,y) u = 0, \tag{1}$$

where $k_0 = \omega/c$ is the free space wavenumber, $\omega$ is the angular frequency and $c$ is the speed of light in vacuum. The time dependence is assumed to be $e^{-i\omega t}$. The function $\epsilon(x,y)$ is defined such that $\epsilon = \epsilon_1$ in the cylinders and $\epsilon = 1$ in the surrounding medium (air). A guided mode on the periodic array is a solution of Eq. (1) given in the Bloch form

$$u(x,y) = e^{i\beta y}\phi(x,y), \tag{2}$$

where $\beta$ is a real Bloch wavenumber satisfying $|\beta| \le \pi/L$, $\phi$ is periodic in $y$ with period $L$, and $\phi \to 0$ as $x \to \pm\infty$. A BIC is a guided mode with the additional condition $k_0 > |\beta|$. The case $\beta = 0$ gives a standing wave.

Assuming the cylinders are bounded by the vertical lines at $x = \pm d$ for some $d > 0$, we can expand the solution for $|x| > d$ in plane waves as

$$u(x,y) = \sum_{m=-\infty}^{\infty} c_m^{\pm} e^{i(\beta_m y \pm \alpha_m x)}, \quad \pm x > d, \tag{3}$$

where

$$\beta_m = \beta + 2\pi m/L, \quad \alpha_m = \sqrt{k_0^2 - \beta_m^2}. \tag{4}$$

If $\alpha_m$ is real, then the plane waves $e^{i(\beta_m y \pm \alpha_m x)}$ can propagate to infinity, and they correspond to radiation channels for outgoing waves. If we further assume that $k_0 < 2\pi/L - |\beta|$, then $\alpha_0$ is positive, and for all $m \ne 0$, $\alpha_m = i\sqrt{\beta_m - k_0^2}$ is pure imaginary. If $u$ is a BIC, it must decay to zero as $|x| \to \infty$, thus the coefficients $c_0^{\pm}$ must vanish.

In the $\beta$-$\omega$ plane, the BICs correspond to isolated points, but they belong to families of resonant modes that depend on $\beta$ continuously. A resonant mode is a nonzero solution of Eq. (1) for a complex frequency. It is also given in the Bloch form as in Eq. (2), but $\phi$ does not decay to zero as $|x| \to \infty$. Instead, a resonant mode satisfies outgoing radiation conditions as $x \to \pm\infty$. In addition, the expansion (3) is also valid for resonant modes, but in general $c_0^{\pm} \ne 0$. Since $\omega$ is complex, $\alpha_0$ has a nonzero imaginary part, the plane wave $\exp[i(\beta_0 y \pm \alpha_0 x)]$ blows up as $x \to \pm\infty$. The quality factor of a resonant mode is $Q = -0.5\mathrm{Re}(\omega)/\mathrm{Im}(\omega)$, where $\mathrm{Re}(\omega)$ and $\mathrm{Im}(\omega)$ denote the real and imaginary parts of $\omega$.

To find the resonant modes and the BICs, we can fix $\beta$ and solve an eigenvalue problem where the eigenvalue is $\omega$ (or $k_0^2$). This eigenvalue problem is for Eq. (1) in a 2D domain that covers one period of the structure, i.e., for $-L/2 < y < L/2$. Numerical methods that discretize the 2D domain directly are not very efficient. For our problem, since the cylinders are slightly distorted from the perfect circular ones, high accuracy is needed to distinguish resonant modes with a small imaginary part of $\omega$ from true BICs. We choose to implement a numerical method that reformulates the eigenvalue problem on two line segments. These line segments are $x = \pm d$ for $|y| < L/2$. The eigenvalue problem is written as

$$\mathcal{A}\boldsymbol{u} = \boldsymbol{0}, \tag{5}$$

where $\boldsymbol{u}$ is a column vector of $u(d,y)$ and $u(-d,y)$ for $|y| < L/2$, $\mathcal{A}$ is an operator that depends on $\beta$ and $\omega$. If the line segments are discretized by $N$ points, then $u(d,y)$ and $u(-d,y)$ are approximated by vectors of length $N$, and $\mathcal{A}$ is approximated by a $(2N)\times(2N)$ matrix. Notice that this formulation gives a nonlinear eigenvalue problem. For any given real $\beta$, we can solve the complex $\omega$ from

$$\lambda_1(\mathcal{A}) = 0 \tag{6}$$

where $\lambda_1$ is the eigenvalue of $\mathcal{A}$ with the smallest magnitude. A method for computing operator $\mathcal{A}$ is described in Appendix.

## III. ANTISYMMETRIC STANDING WAVES

It is easy to find antisymmetric standing waves on a periodic array of circular dielectric cylinders [5, 8]. These standing waves are symmetry-protected BICs, where the relevant symmetry is the reflection symmetry along the $y$ direction. If the center of one circular cylinder is chosen to be the origin, then the dielectric function $\epsilon(x,y)$ is even in $y$, and the antisymmetric standing waves are odd functions of $y$. On an array of cylinders with radius $a = 0.3L$ and dielectric constant $\epsilon_1 = 4$, two antisymmetric standing waves can be found, and their frequencies are $\omega L/(2\pi c) = 0.67131588$ and $0.92718676$, respectively. It turns out that these two standing waves are even and odd in $x$, respectively.

For the same $a$ and $\epsilon_1$, we consider an array of slightly noncircular cylinders with a boundary given by

$$\begin{cases} x = a\cos(\theta+\theta_0) + \delta\cos(2\theta)\sin(\theta_0) \\ y = a\sin(\theta+\theta_0) - \delta\cos(2\theta)\cos(\theta_0) \end{cases} \tag{7}$$

for $0 \leq \theta < 2\pi$, where $\theta_0$ is a rotation angle and $\delta$ is a small parameter. The case for $\delta = 0.2a$ is shown in Fig. 2(a). It is well known that the antisymmetric standing waves are robust against small structural variations that preserve the reflection symmetry in $y$ [2, 5]. For $\theta_0 = \pm 90°$ and $\delta \neq 0$, the reflection symmetry in $x$ is broken, but the reflection symmetry in $y$ is preserved, thus the antisymmetric standing waves should continue to exist when $\delta$ is small. As a simple test, we consider the case for $\theta_0 = 90°$ and $\delta = 0.005a$. Two antisymmetric standing waves are found, and their frequencies are $\omega L/(2\pi c) = 0.67131674$ and $0.92718463$, respectively.

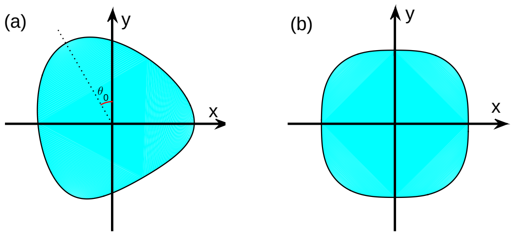


FIG. 2. Cross sections of two noncircular cylinders. (a) Cylinder given by Eq. (7) for rotation angle $\theta_0$ and $\delta = 0.2a$. (b) Cylinder given by Eq. (8) for $\delta = 0.05a$.

For $\theta_0 = 0$ and $\delta \neq 0$, the periodic array no longer has the reflection symmetry in $y$. Our numerical results confirm that the antisymmetric standing waves disappear and become resonant modes. For $\delta = 0.005a$ and $\beta = 0$, we found two resonant modes with complex frequencies $\omega L/(2\pi c) = 0.67131418 - i0.00000004$, and $0.92718448 - i0.00000020$, respectively. Since the resonant modes depend continuously on the real Bloch wavenumber $\beta$, we also calculate the resonant modes for $\beta$ near zero. In Fig. 3, we show the quality factors of the resonant modes as functions of $\beta$, for both circular and noncircular cylinders. The antisymmetric standing waves are located at $\beta = 0$ where the curves for $\delta = 0$ approach infinity. It is clear that if $\delta \neq 0$ the quality factor is finite for all $\beta$ around zero. Therefore, the antisymmetric standing waves are destroyed by the small distortions that break the reflection symmetry in $y$, and the distorted array has only resonant modes for $\beta$ around zero.

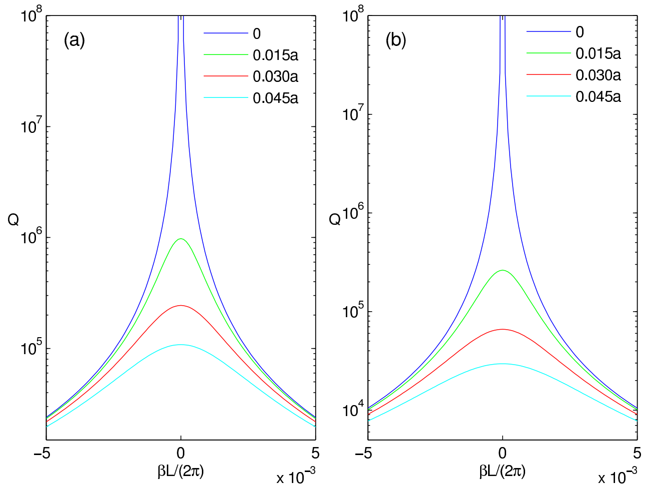


FIG. 3. Quality factors of the resonant modes (as functions of wavenumber $\beta$) on periodic arrays of distorted cylinders given by Eq. (7): (a) near the $x$-even standing wave; (b) near the $x$-odd standing wave.

Since the small distortion turns the antisymmetric standing waves to resonant modes with large quality factors, the transmission spectrum exhibits sharp resonant features. In Fig. 4, we compare the transmission spectra of normal incident plane waves for periodic arrays of circular and distorted cylinders. The distorted cylinders correspond to $\delta = 0.15a$ and $\theta_0 = 0$. For the circular cylinders, the transmission spectrum does not have any particular feature around the frequencies of the two antisymmetric standing waves, since these standing waves cannot couple to the normal incident waves. On the other hand, the transmission spectrum of the distorted array exhibits two sharp Fano resonance features, each having an asymmetric line shape with a total transmission and a total reflection in a very narrow frequency range around the real part of the complex frequency of the resonant modes. These resonant features can be explained by the theoretical models developed in [31, 32].

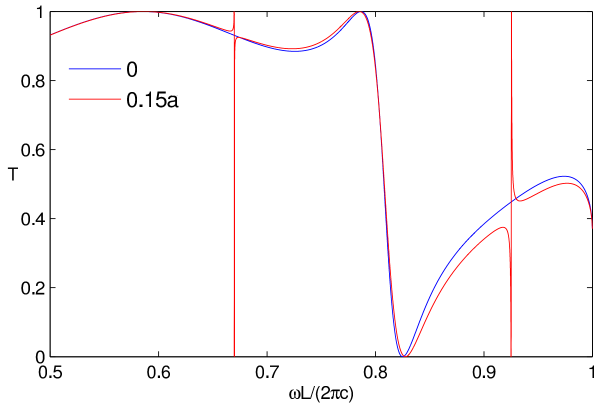


FIG. 4. Transmission spectra of normal incident waves for periodic arrays of circular cylinders ($a = 0.3L$ and $\epsilon_1 = 4$) and distorted cylinders given by Eq. (7) for $\delta = 0.15a$ and $\theta_0 = 0°$.

## IV. PROPAGATING BICS

It is known that propagating BICs with a nonzero wavenumber $\beta$ exist on periodic arrays of circular dielectric cylinders [14, 19]. If the radius of the cylinders is $a = 0.35L$ and the dielectric constant is $\epsilon_1 = 11.56$, then the periodic array supports two propagating BICs, and they are even and odd in $x$, respectively. The $x$-even BIC has a frequency $\omega L/(2\pi c) = 0.4854$ and a wavenumber $\beta L/(2\pi) = 0.0776$. The $x$-odd BIC appears when $\omega L/(2\pi c) = 0.6702$ and $\beta L/(2\pi) = 0.2483$. Notice that the periodic array of circular cylinders has reflection symmetries in both $x$ and $y$ directions. It has been suggested that the propagating BICs are robust against small structural changes that keep all relevant symmetries, and they become resonant modes with finite quality factors when the changes break a required symmetry [13, 28, 29]. However, existing numerical results supporting this conclusion are mostly for idealized structures with simple and perfect geometric features such as circular holes, circular rods, rectangular cylinders and spheres. In the following, we present numerical results for distorted structures involving slightly noncircular cylinders.

First, we consider a periodic array of distorted cylinders with a boundary given by Eq. (7) for $a = 0.35L$ and $\delta \neq 0$, and study three cases corresponding to $\theta_0 = 0°$, $45°$ and $90°$. The dielectric constant of the cylinders is kept at $\epsilon_1 = 11.56$. For all three cases, the reflection symmetries in one or both directions are broken. Our numerical results reveal that the BICs are indeed turned to resonant modes. In Fig. 5, we show the quality factors of the resonant modes as functions of wavenumber $\beta$ for a few different $\delta$. The curves for $\delta = 0$ diverge at wavenumbers corresponding to the BICs. It is also clear that the quality factors are finite on the curves for $\delta \neq 0$. Therefore, the two propagating BICs have been destroyed by the small distortions.

Next, we consider a periodic array of distorted cylinders that retains the reflection symmetries in both $x$ and $y$ directions. The array consists of noncircular cylinders with a boundary given by

$$\begin{cases} x = a\cos(\theta) - \delta\cos(4\theta)\cos(\theta) \\ y = a\sin(\theta) - \delta\cos(4\theta)\sin(\theta) \end{cases} \tag{8}$$

for $0 \le \theta < 2\pi$ and $a = 0.35L$. The case for $\delta = 0.05a$ is shown in Fig. 2(b). The dielectric constant of the cylinders is also $\epsilon_1 = 11.56$. For a few small values of $\delta$, we calculate the complex frequencies of the resonant modes for $\beta$ near the wavenumbers of the two propagating BICs. The quality factors of the resonant modes are shown in Fig. 6. The top and bottom panels correspond to the $x$-even and $x$-odd modes, respectively. It is clear that for each $\delta$, there are two BICs (one $x$-even and one $x$-odd), since all curves diverge for some real $\beta$. For $\delta = 0.005a$, we found an $x$-even BIC with $\beta L/(2\pi) = 0.0886$ and $\omega L/(2\pi c) = 0.48753358$, and an $x$-odd BIC with $\beta L/(2\pi) = 0.2628$ and $\omega L/(2\pi c) = 0.67101142$. Their electric field patterns are shown in Fig. 7. These numerical results indicate that the propagating BICs are robust against small distortions that keep the reflection symmetries in both $x$ and $y$ directions.

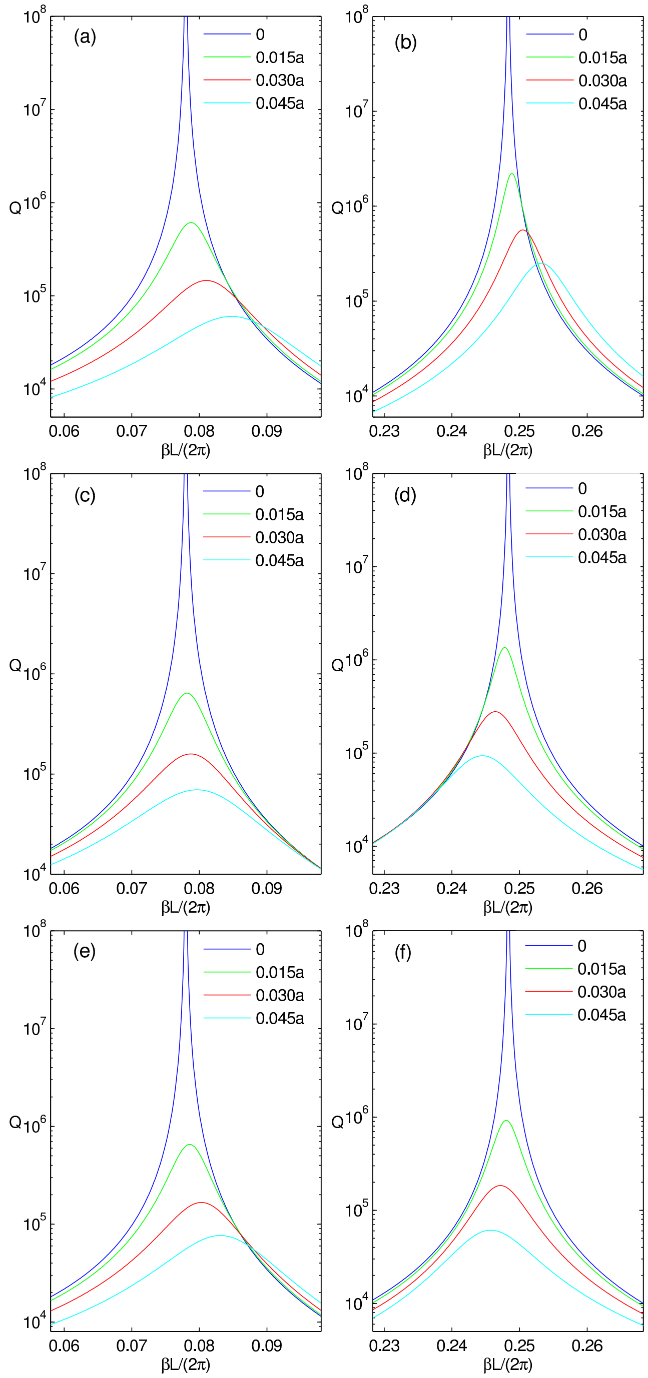


FIG. 5. Quality factors of the resonant modes (as functions of wavenumber $\beta$) on periodic arrays of distorted cylinders given by Eq. (7): (a,b) $\theta_0 = 0°$; (c,d) $\theta_0 = 45°$; (e,f) $\theta_0 = 90°$; (a,c,e) near the $x$-even propagating BIC; (b,d,f) near the $x$-odd propagating BIC.

## V. CONCLUSION

On periodic structures, BICs are guided modes that belong to the families of resonant modes, and they can be regarded as special resonant modes with infinite quality factors. Existing theoretical and numerical works on BICs are mostly for structures with simple and perfect geometric features, such as circular holes, rectangular rods and spheres. Since perfect structures can not be fabricated in practice, it is essential to study slightly dis-

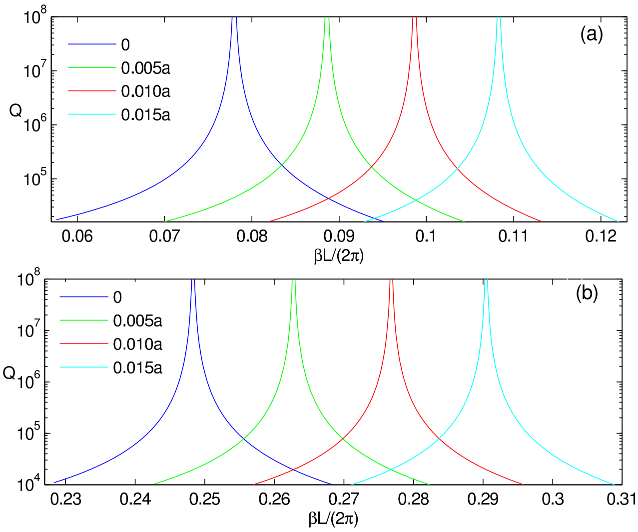


FIG. 6. Quality factors of the resonant modes (as functions of wavenumber $\beta$) on periodic arrays of distorted cylinders given by Eq. (8): (a) near the $x$-even propagating BIC; (b) near the $x$-odd propagating BIC.

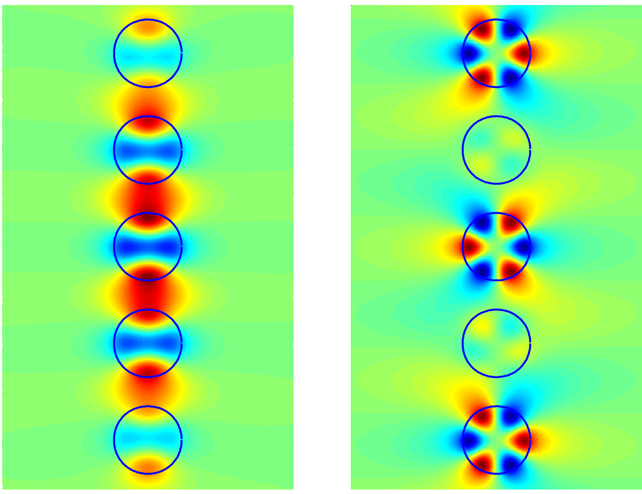

FIG. 7. Electric field patterns of the $x$-even (left) and $x$-odd (right) propagating BICs on a periodic array of distorted cylinders given by Eq. (8) for $\delta = 0.005a$.

torted structures. In particular, it is important to find out whether a BIC is preserved or destroyed by a small distortion. This is related to the robustness of BICs.

For the symmetry-protected BICs, the existence and robustness are well understood. The propagating BICs are not symmetry-protected in the usual sense, since they do not have a symmetry mismatch with the outgoing radiation waves. Most propagating BICs are found on symmetric structures for frequencices that are not too large, so that there is only one outgoing radiation channel. It has been realized that these BICs crucially depend on symmetries [12, 13]. Using topological concepts, the existence and robustness of propagating BICs on a photonic crystal slab and an array of spheres have been analyzed [28, 29]. These studies provide a clear descrition for the generation, evolution and annihilation of the BICs as some parameters such as the radius of the holes, the refractive index and the thickness of the slab, are varied. Notice that although the parameters can change, the structure keep the symmetries, and the perfect geometric features. In this work, we analyzed periodic arrays of slightly noncircular cylinders. Our numerical results indicate that if the cylinders are slightly distorted so that the reflection symmetry with respect to either the $x$ axis or the $y$ axis is broken, then the propagating BICs disappear, that is, they turn to resonant modes. On the other hand, if the distortion does not break the reflection symmetries, then the propagating BICs continue to exist at slightly different frequencies and slightly different wavenumbers. This is consistent with existing results for different periodic structures [28, 29], and gives a strong support to the theoretical result of [30]. Finally, it should be pointed out that BICs can turn to resonant modes for many different reasons, including, for example, when the periodic structure is truncated to a finite one [35], and when the homogeneous media in the two sides of the structure are no longer the same [36].

## ACKNOWLEDGMENT

The work is partially supported by the Fundamental Research Funds for the Central Universities of China (Project No. 2015B19614) and the Research Grants Council of Hong Kong Special Administrative Region, China (Project No. CityU 11301914).

## APPENDIX

The eigenvalue problem for BICs and resonant modes has been written as Eq. (5) for an operator $\mathcal{A}$. To find $\mathcal{A}$, we need two operators $\mathcal{T}$ and $\Lambda$, where $\mathcal{T}$ is used to write down exact boundary conditions at $x = \pm d$ and $\Lambda$ (the so-called Dirichlet-to-Neumann or DtN map) is used to link $u$ and its normal derivative on the boundary of the rectangular domain $S$ given by $|x| < d$ and $|y| < L/2$. All operators are approximated by small matrices in practice.

Based on $\beta_m$ and $\alpha_m$ given in Eq. (4), if we define a linear operator $\mathcal{T}$ such that $\mathcal{T} e^{i\beta_m y} = i\alpha_m e^{i\beta_m y}$ for all integers $m$, then $u$, given in Eq. (3), must satisfy the following boundary conditions

$$\pm \frac{\partial u}{\partial x} = \mathcal{T} u, \quad x = \pm d. \tag{9}$$

For a slightly noncircular cylinder with cross section $\Omega$, if the radius $a$ of the original circular cylinder is not too large (i.e., not close to $0.5L$), we may choose $d = L/2$, then $S$ is a square of side length $L$. For any $u$ satisfying

Eq. (1) in $S$, we have

$$u(x,y) = \sum_{m=-\infty}^{\infty} c_m \phi_m(x,y), \tag{10}$$

where $c_m$ is an unknown coefficient, and $\phi_m$ is a special solution satisfying

$$\phi_m(x,y) = \sum_{q=-\infty}^{\infty} a_{mq} \frac{J_q(k_0 n_1 r)}{J_q(k_0 n_1 a)} e^{iq\theta}$$

for $(x,y) \in \Omega$, and

$$\phi_m(x,y) = \frac{J_m(k_0 n_0 r)}{J_m(k_0 n_0 a)} e^{im\theta} + \sum_{q=-\infty}^{\infty} b_{mq} \frac{Y_q(k_0 n_0 r)}{Y_q(k_0 n_0 a)} e^{iq\theta}$$

for $(x,y)$ outside $\Omega$. In the above, $r$ and $\theta$ are the radial and angle variables of the polar coordinate system, $n_1 = \sqrt{\epsilon_1}$ and $n_0 = 1$ are the refractive indices of the cylinder and the surrounding medium (air), respectively, $J_q$ and $Y_q$ are Bessel functions of order $q$, $a_{mq}$ and $b_{mq}$ are unknown coefficients. To find these coefficients, we can truncate the sums in $q$, choose a finite number of points on the boundary of $\Omega$, set up a linear system for these coefficients by matching $u$ and its normal derivative at these points. After obtaining the special solutions $\phi_m$, we can construct the DtN map $\Lambda$ as in [33, 34]. Notice that $\Lambda$ satisfies

$$\Lambda \begin{bmatrix} u(-d,y) \\ u(x,L/2) \\ u(d,y) \\ u(x,-L/2) \end{bmatrix} = \begin{bmatrix} \partial_x u(-d,y) \\ \partial_y u(x,L/2) \\ \partial_x u(d,y) \\ \partial_y u(x,-L/2) \end{bmatrix}, \tag{11}$$

where $u$ and its normal derivative are evaluated on the boundary of $S$.

For $u$ given in the Bloch form, we have the quasi-periodic conditions $u(x,L/2) = e^{i\beta L} u(x,-L/2)$ and $\partial_y u(x,L/2) = e^{i\beta L} \partial_y u(x,-L/2)$. These conditions can be combined with Eq. (11) to find an operator $\mathcal{M}$ satisfying

$$\mathcal{M} \begin{bmatrix} u(-d,y) \\ u(d,y) \end{bmatrix} = \begin{bmatrix} \partial_x u(-d,y) \\ \partial_x u(d,y) \end{bmatrix}. \tag{12}$$

Finally, Eqs. (9) and (12) are used to eliminate $\partial_x u$ and obtain the operator $\mathcal{A}$.


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