Bound states in the continuum on periodic structures surrounded by strong resonances

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Bound states in the continuum (BICs) are trapped or guided modes with their frequencies in the frequency intervals of the radiation modes. On periodic structures, a BIC is surrounded by a family of resonant modes with their quality factors approaching infinity. Typically the quality factors are proportional to $1/|\boldsymbol{\beta}-\boldsymbol{\beta}_*|^2$, where $\boldsymbol{\beta}$ and $\boldsymbol{\beta}_*$ are the Bloch wavevectors of the resonant modes and the BIC, respectively. But for some special BICs, the quality factors are proportional to $1/|\boldsymbol{\beta}-\boldsymbol{\beta}_*|^4$. In this paper, a general condition is derived for such special BICs on two-dimensional periodic structures. As a numerical example, we use the general condition to calculate special BICs, which are antisymmetric standing waves, on a periodic array of circular cylinders, and show their dependence on parameters. The special BICs are important for practical applications, because they produce resonances with large quality factors for a very large range of $\boldsymbol{\beta}$.

I. INTRODUCTION

Bound states in the continuum (BICs), first studied by Von Neumann and Wigner for quantum systems [1], are trapped or guided modes with their frequencies in the frequency intervals of radiation modes that carry power to or from infinity [2]. For light waves, BICs have been analyzed and observed for many different structures, including waveguides with local distortions [3–7], waveguides with lateral leaky structures [8–11], and periodic structures sandwiched between or surrounded by homogeneous media [12–39]. The BICs on periodic structures are particularly interesting, because they are surrounded by families of resonant modes (depending on the wavevector) with quality factors (Q-factors) tending to infinity, and they give rise to collapsing Fano resonances corresponding to discontinuities in the transmission and reflection spectra [40, 41]. The high-Q resonances and the related strong local fields [42, 43] can be used to enhance light-matter interactions for applications in lasing [44], nonlinear optics [45], etc. Collapsing Fano resonances can be exploited in filtering, sensing, and switching applications [46, 47].

If the structures are symmetric, the BICs and the radiation modes may have incompatible symmetry so that they are automatically decoupled. These so-called symmetry-protected BICs are well known [12–18]. Their existence can be rigorously proved [5, 12, 16, 18], and they are robust against small structural perturbations that preserve the required symmetry. On periodic structures, there are also BICs that do not have a symmetry mismatch with the radiation modes [19–39]. These BICs are often considered as unprotected by symmetry, but for some important cases, they appear to depend crucially on the symmetry, and they continue to exist when geometric and material parameters are varied with the relevant symmetries kept intact [25, 36–39]. In fact, it has been shown that under the right conditions, these BICs are robust against any structural changes that preserve the relevant symmetries [37].

On periodic structures, a BIC is a guided mode, but it belongs to a family of resonant modes, and can be regarded as a special resonant mode with an infinite Q-factor. Let $\boldsymbol{\beta}_*$ be the Bloch wavevector of a BIC, then there is a related family of resonant modes depending on wavevector $\boldsymbol{\beta}$. The Q-factors of the resonant modes typically satisfy $Q \sim 1/|\boldsymbol{\beta}-\boldsymbol{\beta}_*|^2$. Clearly, a resonant mode with an arbitrarily large Q-factor can be obtained if $\boldsymbol{\beta}$ is chosen to be sufficiently close to $\boldsymbol{\beta}_*$, and an arbitrarily large local field can be induced by an incident wave with the wavevector $\boldsymbol{\beta}$. However, practical applications of the strong field enhancement can be limited by the difficulty of controlling $\boldsymbol{\beta}$ to high precision, in addition to other practical issues such as fabrication errors [48], material dissipation [43], variations in different periods, finite sizes [49–51], etc. In [45], we showed that for symmetric standing waves, which are BICs with $\boldsymbol{\beta}_* = \mathbf{0}$ and are unprotected by symmetry in the usual sense, the Q-factors of the associated resonant modes satisfy an inverse fourth power asymptotic relation, i.e., $Q \sim 1/|\boldsymbol{\beta}-\boldsymbol{\beta}_*|^4$. In that case, resonances with large Q-factors and strong local fields can be realized with a much more relaxed condition on $\boldsymbol{\beta}$. This property has been used to show that optical bistability can be induced by a very weak incident wave [45], and it should be useful in other applications that require a significant field enhancement. In general, resonant modes near antisymmetric standing waves (ASWs), which are symmetry-protected BICs with $\boldsymbol{\beta}_* = \mathbf{0}$, only satisfy the inverse quadratic asymptotic relation, but Bulgakov and Maksimov found a few examples for which the inverse fourth power relation is satisfied [49].

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In this paper, we derive a general condition for those special BICs with the Q-factors of the associated resonant modes satisfying the inverse fourth power relation. For simplicity, the theory is developed for two-dimensional (2D) periodic structures. We use a perturbation method assuming $|\boldsymbol{\beta} - \boldsymbol{\beta}_*|$ is small. The condition is given in integrals involving the BIC itself and related diffraction solutions for incident waves with the same frequency and same wavevector. With this general condition, it becomes feasible to systematically search the parameter values of the periodic structure supporting the special BICs. As numerical examples, we calculate special BICs on a periodic array of circular dielectric cylinders, and show their dependence on the parameters.

II. BICS AND RESONANT MODES

We consider 2D dielectric structures which are invariant in z, periodic in y with period L, and bounded in the x direction by $|x| < D$ for some constant D, where $\{x, y, z\}$ is a Cartesian coordinate system. The surrounding medium for $|x| > D$ is assumed to be vacuum. Therefore, the dielectric function ϵ satisfies $\epsilon(x, y+L) = \epsilon(x, y)$ for all (x, y), and $\epsilon(x, y) = 1$ for $|x| > D$. For the E polarization, the z-component of the electric field, denoted as u, satisfies the Helmholtz equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + k^2 \epsilon u = 0, \tag{1}$$

where $k = \omega/c$ is the free space wavenumber, ω is the angular frequency, c is the speed of light in vacuum, and the time dependence is assumed to be $e^{-i\omega t}$.

A Bloch mode on the periodic structure is a solution of Eq. (1) given as

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

where ϕ is periodic in y with period L and β is the real Bloch wavenumber. Due to the periodicity of ϕ, β can be restricted to the interval $[-\pi/L, \pi/L]$. If $\phi \to 0$ as $|x| \to \infty$, then u given in Eq. (2) is a guided mode. Typically, guided modes that depend on β and ω continuously can only be found below the light line, i.e., for $k < |\beta|$. A BIC is a special guided mode above the light line, i.e., β and k satisfy the condition $k > |\beta|$. For a given structure, BICs can only exist at isolated points in the $\beta\omega$ plane.

In the homogeneous media given by $|x| > D$, we can expand a Bloch mode in plane waves, that is

$$u(x, y) = \sum_{j=-\infty}^{\infty} c_j^{\pm} e^{i(\beta_j y \pm \alpha_j x)} \tag{3}$$

where the "+" and "−" signs are chosen for $x > D$ and $x < -D$ respectively, and

$$\beta_j = \beta + \frac{2\pi j}{L}, \quad \alpha_j = \sqrt{k^2 - \beta_j^2}. \tag{4}$$

If $k < |\beta_j|$, then $\alpha_j = i\sqrt{\beta_j^2 - k^2}$ is pure imaginary, and the corresponding plane wave is evanescent. For a BIC, one or more α_j are real, then the corresponding coefficients $c_j^{\pm}$ must vanish, since the BIC must decay to zero as $|x| \to \infty$.

Above the light line, if the frequency ω is allowed to be complex, there are Bloch mode solutions that depend on a real wavenumber β continuously. These solutions are the resonant modes, and they satisfy outgoing radiation conditions as $x \to \pm\infty$. Due to the time dependence $e^{-i\omega t}$, the imaginary part of the complex frequency of a resonant mode must be negative, so that its amplitude decays with time. The Q-factor is given by $Q = -0.5\mathrm{Re}(\omega)/\mathrm{Im}(\omega)$. The expansion (3) is still valid, but the complex square root for α_j must be defined to maintain continuity as $\mathrm{Im}(\omega) \to 0$. This can be achieved by using a square root with a branch cut along the negative imaginary axis (instead of the negative real axis), that is, if $\xi = |\xi| e^{i\theta}$ for $-\pi/2 < \theta \le 3\pi/2$, then $\sqrt{\xi} = \sqrt{|\xi|} e^{i\theta/2}$. Notice that α_0 and probably a few other α_j have negative real parts. Therefore, a resonant mode blows up as $|x| \to \infty$. As β is continuously varied following a family of resonant modes, $\mathrm{Im}(\omega)$ may become zero at some special values of β, and they correspond to the BICs. Therefore, although a BIC is a guided mode, it belongs to a family of resonant modes, and it can be regarded as a special resonant mode with an infinite Q-factor.

III. PERTURBATION ANALYSIS

Given a BIC on a periodic structure with frequency ω_* and Bloch wavenumber β_*, we are interested in the complex frequency ω and the Q-factor of the nearby resonant mode for wavenumber β close to β_*. For simplicity, we scale the BIC such that

$$\frac{1}{L^2} \int_{\Omega} |\phi_*|^2 d\boldsymbol{r} = 1, \tag{5}$$

where Ω is one period of the structure given by $-L/2 < y < L/2$ and $-\infty < x < \infty$. We also assume $k_* = \omega_*/c$ satisfies the following condition

$$|\beta_*| < k_* < \frac{2\pi}{L} - |\beta_*|. \tag{6}$$

This implies that α_{*0} (also denoted as α_* below) is positive and all α_{*j} for $j \ne 0$ are pure imaginary, where α_{*0} and α_{*j} are defined as in Eq. (4) with k and β replaced by k_* and β_*, respectively. To analyze this problem, we use a perturbation method assuming $\delta = \beta - \beta_*$ is small.

Let $u_* = \phi_* e^{i\beta_* y}$ and $u = \phi e^{i\beta y}$ be the BIC and the nearby resonant mode, respectively, we expand ω and ϕ as

$$\omega = \omega_* + \omega_1 \delta + \omega_2 \delta^2 + \omega_3 \delta^3 + \omega_4 \delta^4 + \ldots \tag{7}$$

$$\phi = \phi_* + \phi_1 \delta + \phi_2 \delta^2 + \phi_3 \delta^3 + \phi_4 \delta^4 + \ldots \tag{8}$$

In terms of the periodic function ϕ given in Eq. (2), the Helmholtz equation becomes

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+2i\beta\frac{\partial\phi}{\partial y}+\left(k^2\epsilon-\beta^2\right)\phi=0. \tag{9}$$

Inserting Eqs. (7)-(8) into Eq. (9), and comparing terms of equal powers of δ, we obtain

$$\mathcal{L}\phi_*=0, \tag{10}$$
$$\mathcal{L}\phi_1=-2i\partial_y\phi_*+2(\beta_*-k_*k_1\epsilon)\phi_*, \tag{11}$$
$$\begin{aligned}\mathcal{L}\phi_2=&-2i\partial_y\phi_1+2(\beta_*-k_*k_1\epsilon)\phi_1\\&+(1-k_1^2\epsilon-2k_*k_2\epsilon)\phi_*,\end{aligned} \tag{12}$$

where $k_j=\omega_j/c$ for $j\geq 1$, and

$$\mathcal{L}=\partial_x^2+\partial_y^2+2i\beta_*\partial_y+k_*^2\epsilon-\beta_*^2. \tag{13}$$

In addition, ϕ_j must satisfy proper outgoing radiation conditions as $|x|\to\infty$.

Equation (10) is simply the governing Helmholtz equation of the BIC. The first order term ϕ_1 satisfies the inhomogeneous Eq. (11) which is singular and has no solution, unless the right hand side is orthogonal to ϕ_*. Multiplying $\overline{\phi}_*$ (the complex conjugate of ϕ_*) to both sides of Eq. (11) and integrating on domain Ω, we obtain

$$k_1=\frac{\omega_1}{c}=\frac{\beta_*\int_\Omega|\phi_*|^2d\boldsymbol{r}-i\int_\Omega\overline{\phi}_*\partial_y\phi_*\,d\boldsymbol{r}}{k_*\int_\Omega\epsilon|\phi_*|^2\,d\boldsymbol{r}}. \tag{14}$$

It is easy to show that k_1 is real. Therefore, in general $\text{Im}(\omega)$ is proportional to $(\beta-\beta_*)^2$.

For k_1 given above, Eq. (11) has a solution. Similar to the plane wave expansion (3), ϕ_1 can be written down explicitly for $|x|>D$. Importantly, ϕ_1 contains only a single outgoing plane wave as $x\to\pm\infty$, that is

$$\phi_1\sim d_0^{\pm}e^{\pm i\alpha_*x},\quad x\to\pm\infty, \tag{15}$$

where $d_0^{\pm}$ are unknown coefficients and $\alpha_*=\sqrt{k_*^2-\beta_*^2}$. A formula for k_2 can be derived from the solvability condition of Eq. (12). In particular, the imaginary part of k_2 has the following simple formula

$$\text{Im}(k_2)=\frac{\text{Im}(\omega_2)}{c}=-\frac{L\alpha_*\left(|d_0^+|^2+|d_0^-|^2\right)}{2k_*\int_\Omega\epsilon|\phi_*|^2\,d\boldsymbol{r}}. \tag{16}$$

A special case of Eq. (16) was previously derived in [45]. Additional details on the derivation of Eqs. (14) and (16) are given in Appendix.

Notice that if ϕ_1 radiates power to $x=\pm\infty$, d_0^+ and d_0^- are nonzero, then $\text{Im}(\omega_2)\neq 0$. In that case, the imaginary part of the complex frequency satisfies

$$\text{Im}(\omega)\sim-\frac{cL\alpha_*\left(|d_0^+|^2+|d_0^-|^2\right)}{2k_*\int_\Omega\epsilon|\phi_*|^2\,d\boldsymbol{r}}(\beta-\beta_*)^2, \tag{17}$$

and the Q-factor satisfies

$$Q\sim\frac{k_*^2\int_\Omega\epsilon|\phi_*|^2\,d\boldsymbol{r}}{L\alpha_*\left(|d_0^+|^2+|d_0^-|^2\right)}(\beta-\beta_*)^{-2}. \tag{18}$$

On the other hand, if ϕ_1 does not radiate power to infinity, then $d_0^{\pm}=0$, $\text{Im}(\omega_2)=0$, and Eqs. (17) and (18) are no longer valid. In that case, $\text{Im}(\omega_3)$ must also be zero, since otherwise, $\text{Im}(\omega)$ changes signs when β passes through β_*. This is not possible, since $\text{Im}(\omega)$ of a resonant mode is always negative. Therefore, if ϕ_1 is non-radiative, we expect $\text{Im}(\omega)\sim(\beta-\beta_*)^4$ and $Q\sim(\beta-\beta_*)^{-4}$.

IV. STRONG RESONANCES

On periodic structures, the Q-factors of resonant modes around certain special BICs satisfy an inverse fourth power asymptotic relation $Q\sim(\beta-\beta_*)^{-4}$. This happens when the first order perturbation ϕ_1 does not radiate power to infinity, i.e., $d_0^{\pm}=0$. However, to check this condition, it is necessary to solve ϕ_1 from Eq. (11). This is not very convenient. Ideally, one would like to have a condition that involves the BIC ϕ_* only. This does not seem to be possible. In the following, we derive a condition that involves the BIC ϕ_* and related diffraction solutions for incident waves with the same ω_* and β_* as the BIC.

For Eq. (1) with k replaced by k_*, we consider two diffraction problems with incident waves $e^{i(\beta_*y+\alpha_*x)}$ and $e^{i(\beta_*y-\alpha_*x)}$ given in the left and right homogeneous media, respectively. The solutions of these two diffraction problems are denoted as u_l and u_r, respectively, and they satisfy

$$u_j=\varphi_j(x,y)e^{i\beta_*y},\quad j\in\{l,r\}, \tag{19}$$

where φ_l and φ_r are periodic in y with period L. It should be pointed out that the existence of a BIC implies that the corresponding diffraction problems have no uniqueness [12, 16], but the diffraction solutions are uniquely defined in the far field as $|x|\to\infty$. In fact, φ_l and φ_r have the following asymptotic formulae

$$\begin{aligned}\varphi_l&\sim\begin{cases}e^{i\alpha_*x}+R_le^{-i\alpha_*x}, & x\to-\infty\\ T_le^{i\alpha_*x}, & x\to+\infty,\end{cases}\\ \varphi_r&\sim\begin{cases}T_re^{-i\alpha_*x}, & x\to-\infty\\ e^{-i\alpha_*x}+R_re^{i\alpha_*x}, & x\to+\infty,\end{cases}\end{aligned} \tag{20}$$

where R_l, T_l, R_r and T_r are the reflection and transmission amplitudes associated with the left and right incident waves, respectively. It is well known that the scattering matrix $\boldsymbol{S}=\begin{bmatrix}R_l & T_r\\ T_l & R_r\end{bmatrix}$ is unitary. Notice that u_l and u_r are easier to solve than ϕ_1, since they satisfy a homogeneous Helmholtz equation with a zero right hand side.

Equation (11) for ϕ_1 can be written as $\mathcal{L}\phi_1=2G$, where

$$G=-i\partial_y\phi_*+(\beta_*-k_*k_1\epsilon)\phi_*. \tag{21}$$

Since $G \to 0$ exponentially as $x \to \pm\infty$, the following integrals

$$F_j = \int_\Omega \overline{\varphi}_j G d\boldsymbol{r}, \quad j \in \{l, r\} \tag{22}$$

are well defined. On the other hand, φ_j and ϕ_1 (in general) do not decay to zero as $|x| \to \infty$, it is not immediately clear whether $\overline{\varphi}_j \mathcal{L} \phi_1$ is integrable on the unbounded domain Ω. However, for any $h \geq D$, we can define a rectangular domain Ω_h given by $|y| < L/2$ and $|x| < h$, and evaluate the integral on Ω_h, then take the limit as $h \to \infty$. Clearly, the limit must exist and

$$\lim_{h\to\infty} \int_{\Omega_h} \overline{\varphi}_j \mathcal{L} \phi_1 d\boldsymbol{r} = 2F_j, \quad j \in \{l, r\}.$$

In Appendix, we show that

$$\lim_{h\to\infty} \int_{\Omega_h} \overline{\varphi}_l \mathcal{L} \phi_1 d\boldsymbol{r} = 2iL\alpha_* \left(d_0^+ \overline{T}_l + d_0^- \overline{R}_l \right), \tag{23}$$

$$\lim_{h\to\infty} \int_{\Omega_h} \overline{\varphi}_r \mathcal{L} \phi_1 d\boldsymbol{r} = 2iL\alpha_* \left(d_0^+ \overline{R}_r + d_0^- \overline{T}_r \right). \tag{24}$$

Therefore,

$$F_l = iL\alpha_* \left(d_0^+ \overline{T}_l + d_0^- \overline{R}_l \right),$$
$$F_r = iL\alpha_* \left(d_0^+ \overline{R}_r + d_0^- \overline{T}_r \right).$$

Using the unitarity of the scattering matrix $\boldsymbol{S}$, it is easy to show that

$$|d_0^+|^2 + |d_0^-|^2 = \frac{|F_l|^2 + |F_r|^2}{(L\alpha_*)^2}. \tag{25}$$

If $(F_l, F_r) \neq (0, 0)$, Eq. (17) can be written as

$$\mathrm{Im}(\omega) \sim -\frac{c\left(|F_l|^2 + |F_r|^2\right)}{2L\alpha_* k_* \int_\Omega \epsilon |\phi_*|^2 \, d\boldsymbol{r}} (\beta - \beta_*)^2. \tag{26}$$

Clearly, the condition $d_0^+ = d_0^- = 0$ is equivalent to

$$F_l = F_r = 0. \tag{27}$$

BICs are most easily found on structures with suitable symmetries. If the structure has a reflection symmetry in the y direction, it is often possible to find ASWs which are symmetry-protected BICs with $\beta_* = 0$. Assuming the origin is chosen so that $\epsilon(x, y) = \epsilon(x, -y)$, then the ASWs are odd functions of y. From Eq. (14), it is easy to see that $k_1 = 0$, thus $G = -i\partial_y \phi_*$ and

$$F_j = -i \int_\Omega \overline{\varphi}_j \frac{\partial \phi_*}{\partial y} d\boldsymbol{r}, \quad j \in \{l, r\}. \tag{28}$$

Notice that symmetric standing waves (which are even functions of y) may also exist on periodic structures with a reflection symmetry in y. In [45], it is shown that $d_0^\pm = 0$ is always true for the symmetric standing waves. This is so, because $k_1 = 0$ and $G = -i\partial_y \phi_*$ are still valid, thus G is odd in y. Meanwhile, φ_l and φ_r are even in y. Therefore, $F_l = F_r = 0$.

Propagating BICs (with $\beta_* \neq 0$) are often found on structures with an additional reflection symmetry in the x direction. With a properly chosen origin, the dielectric function satisfies

$$\epsilon(x, y) = \epsilon(x, -y) = \epsilon(-x, y) \tag{29}$$

for all (x, y). In that case, we can reduce the condition $F_l = F_r = 0$ to a single real condition. In [37], it is shown that if the BIC $u_* = \phi_* e^{i\beta_* y}$ is a single mode, then it is either even in x or odd in x, and it can be scaled to satisfy the $\mathcal{PT}$-symmetric condition

$$u_*(x, y) = \overline{u}_*(x, -y). \tag{30}$$

In particular, the ASWs should be scaled as pure imaginary functions.

It is also shown in [37] that there is a complex number C with unit magnitude, such that $u_e = C(u_l + u_r)$ and $u_o = C(u_l - u_r)$ are even and odd in x, respectively, and are also $\mathcal{PT}$-symmetric. As in Eq. (19), we associate two periodic functions φ_e and φ_o with u_e and u_o, respectively. It is easy to see that ϕ_*, φ_e, φ_o and G given in Eq. (21) are all $\mathcal{PT}$-symmetric. Furthermore, let F_e and F_o be defined as in Eq. (22) for $j \in \{e, o\}$, then $F_e = C(F_l + F_r)$ and $F_o = C(F_l - F_r)$. This leads to

$$|F_e|^2 + |F_o|^2 = 2(|F_l|^2 + |F_r|^2). \tag{31}$$

If $(F_e, F_o) \neq (0, 0)$, Eq. (26) can be written as

$$\mathrm{Im}(\omega) \sim -\frac{c\left(|F_e|^2 + |F_o|^2\right)}{4L\alpha_* k_* \int_\Omega \epsilon |\phi_*|^2 \, d\boldsymbol{r}} (\beta - \beta_*)^2. \tag{32}$$

Clearly, the condition $F_l = F_r = 0$ is equivalent to

$$F_e = F_o = 0. \tag{33}$$

If a function satisfies the $\mathcal{PT}$-symmetric condition (30), its real part is even in y and its imaginary part is odd in y. Therefore, F_e and F_o are always real. If the BIC is even in x, then F_o is always zero, and it is only necessary to check one real condition $F_e = 0$. Similarly, if the BIC is odd in x, the only condition is $F_o = 0$. For ASWs on periodic structures with the double reflection symmetry (29), $G = -i\partial_y \phi_*$ is real and even in y, and the corresponding diffraction solutions u_e and u_o are also real even functions of y.

V. NUMERICAL EXAMPLES

In this section, some numerical examples are presented to validate and illustrate the theoretical results developed in the previous sections. As shown in Fig. 1(a), we consider a single periodic array of dielectric circular cylinders surrounded by air. The radius and dielectric constant of the cylinders are a and ϵ_1, respectively. BICs on such

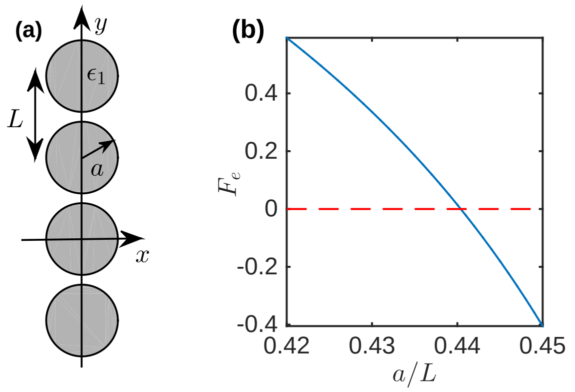

FIG. 1: (a): A periodic array of circular cylinders surrounded by air. (b) F_e (with unit L) of the first ASW as a function of radius a for $\epsilon_1 = 8.2$.

a periodic array have been extensively investigated before [15, 18, 26, 33]. Many BICs exist continuously with respect to ϵ_1 and a. For numerical results, we first consider an array with $\epsilon_1 = 8.2$. For $a = 0.4L$ and the E polarization, the array supports five ASWs and one propagating BIC. The frequencies and Bloch wavenumbers of these BICs are listed in the first and second columns of Table I, respectively.

$\omega_* L/(2\pi c)$	$\beta_* L/(2\pi)$	a_2: Eq. (35)	a_2: approximation
0.4104	0	0.0325	0.0325
0.5458	0	0.1330	0.1331
0.7087	0	0.1429	0.1428
0.8080	0	0.0824	0.0825
0.8749	0	0.0766	0.0769
0.6872	0.2038	0.1033	0.1040

TABLE I: Frequencies and Bloch wavenumbers of six BICs on a periodic array of circular cylinders with radius $a = 0.4L$ and dielectric constant $\epsilon_1 = 8.2$, and their exact and approximate coefficients a_2.

First, we check the formula for $\text{Im}(\omega)$ for ordinary BICs where ϕ_1 radiates power to infinity. The periodic array has reflection symmetries in both x and y directions, thus, Eq. (32) is applicable. In terms of the normalized frequency and normalized wavenumber, Eq. (32) can be written as

$$\frac{\text{Im}(\omega)L}{2\pi c} \sim -a_2 \left[\frac{(\beta-\beta_*)L}{2\pi}\right]^2, \tag{34}$$

where a_2 is a dimensionless coefficient given by

$$a_2 = \frac{\pi\left(|F_e|^2 + |F_o|^2\right)}{2L^2 k_* \alpha_* \int \epsilon |\phi_*|^2 d\boldsymbol{r}}. \tag{35}$$

Recall that F_e and F_o are real, and one of them is always zero. For each BIC listed in Table I, we calculate a_2 by Eq. (35), and also find an approximation of a_2 by a quadratic polynomial fitting the numerical values of $\text{Im}(\omega)$ for $\beta = \beta_*$ and $\beta_* \pm 0.02\pi/L$. As shown in the third and fourth columns of Table I, the exact and approximate values of a_2 agree very well. This confirms that Eqs. (34) and (35) are correct.

We are interested in the special BICs surrounded by strong resonances with $Q \sim 1/(\beta-\beta_*)^4$. It is known that the symmetric standing waves (even in y) are examples of such special BICs [45], and they exist when a and ϵ_1 lie on a curve in the $a\epsilon_1$ plane [33]. Bulgakov and Maksimov [49] found a number of ASWs which also have this special property. Using the perturbation theory developed in previous sections, we can find these special BICs systematically by searching the parameters a and ϵ_1, such that $F_e = 0$ for an x-even BIC or $F_o = 0$ for an x-odd BIC. The first ASW listed in Table I, with $\omega_* L/(2\pi c) = 0.4101$ for $a = 0.4L$ and $\epsilon_1 = 8.2$, is even in x. We calculate F_e for this BIC as a function of a with a fixed $\epsilon_1 = 8.2$. The result is shown in Fig. 1(b). Since F_e is real and changes signs, it must have a zero. It turns out that $F_e = 0$ for $a = 0.4404L$. The frequency of the corresponding ASW is $\omega_* L/(2\pi c) = 0.3950$. Its wave field pattern is shown in Fig. 2(a).

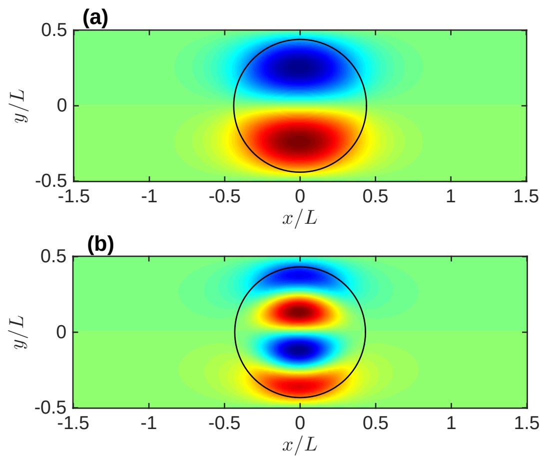

FIG. 2: Wave field patterns of two special x-even ASWs on periodic arrays of circular cylinders with $\epsilon_1 = 8.2$. (a) The first ASW for $a = 0.4404L$. (b) The fifth ASW for $a = 0.4323L$.

For other values of $\epsilon_1 > 1$, F_e of the first ASW can still reach zero for a properly chosen a. Those values of a and ϵ_1 such that $F_e = 0$ for the first ASW give rise to a curve in the $a\epsilon_1$ plane, shown as the red solid line in Fig. 3(a). The corresponding frequency ω_* is shown with a as the solid red curve in Fig. 3(b). It appears that as ϵ_1 is increased, the related a increases and approaches a constant as infinity. It should be pointed that the first ASW exists for all $\epsilon_1 > 1$ and $0 < a \le 0.5L$ [18]. The curve represents those parameter values such that the ASW becomes a special BIC surrounded by strong resonances.

For the other BICs listed in Table I, we also attempt to find parameters a and ϵ_1 such that $F_e = F_o = 0$. It seems that only the fifth ASW, with $\omega_* L/(2\pi c) = 0.8749$

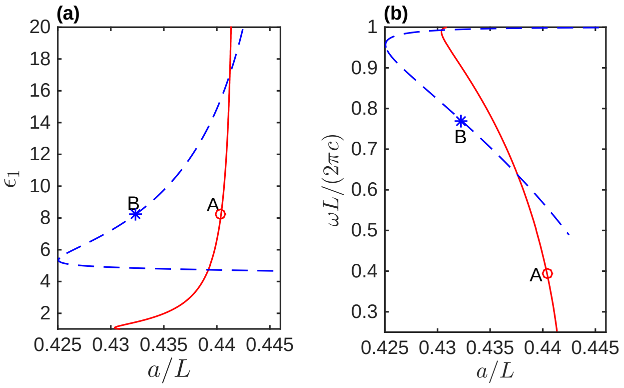

FIG. 3: (a): Parameters of the periodic array for two special ASWs: the first ASW (red solid curve) and the fifth ASW (blue dashed curve). (b) The corresponding frequencies of the two special ASWs. Points A and B correspond to Figs. 2(a) and 2(b), respectively.

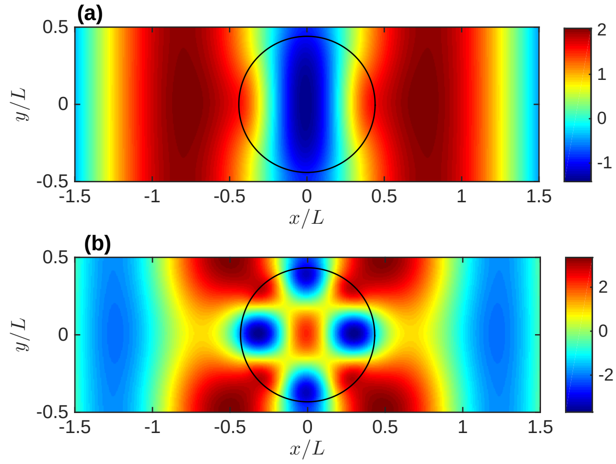

FIG. 4: (a) and (b): Diffraction solutions φ_e corresponding to the special ASWs shown in Figs. 2(a) and 2(b), respectively.

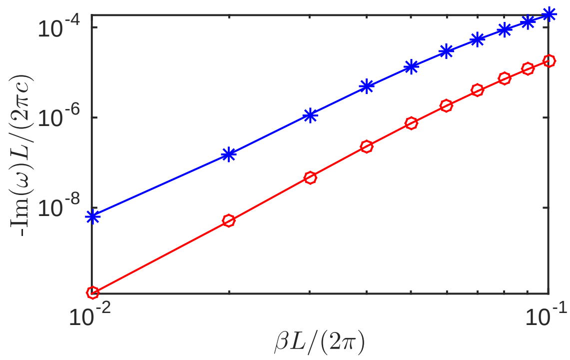

FIG. 5: Imaginary parts of the complex frequencies vs. β for resonant modes near ASWs shown in Fig. 2(a) ($\circ$) and Fig. 2(b) ($*$), respectively.

for $a = 0.4L$ and $\epsilon_1 = 8.2$, can be tuned to a special BIC. For $\epsilon_1 = 8.2$, the fifth ASW, which is also even in x, gives $F_e = 0$ for $a = 0.4323L$. Its frequency is $\omega_* L/(2\pi c) = 0.7701$, and its field pattern is shown in Fig. 2(b). For other values of ϵ_1, we also found the corresponding values of a such that $F_e = 0$ for the fifth ASW. The results are given as a curve in the $a\epsilon_1$ plane, i.e., the blue dashed line in Fig. 3(a). The corresponding frequency ω_* is shown as the blue dashed line in Fig. 3(b). Notice that ϵ_1 has a lower bound around 4.67, and it is achieved as $a \to 0.5L$. In addition, a as a function of ϵ_1, has a minimum around $\epsilon_1 = 5.35$, and it seems to approach a constant as ϵ_1 tends to infinity.

In order to evaluate F_e for an x-even BIC, we need to calculate the x-even diffraction solution $u_e = C(u_l + u_r)$, where C is chosen so that u_e is $\mathcal{PT}$-symmetric and $C = e^{-i\tau}$ for a real constant τ. As shown in [37], this leads to

$$\varphi_e \sim 2\cos(\alpha_* x \pm \tau), \quad x \to \pm\infty. \tag{36}$$

In Fig. 4, we show the diffraction solutions corresponding to the two special ASWs shown in Fig. 2.

In Sec. III, we argued that if $\text{Im}(\omega_2) = 0$, then $\text{Im}(\omega_3)$ should also be zero, and $\text{Im}(\omega)$ should be proportional to $(\beta - \beta_*)^4$ in general. For the two ASWs shown in Fig. 2, we check this result by computing the complex frequencies of some nearby resonant modes directly. In Fig. 5, we show $\text{Im}(\omega)$ as functions of β in a logarithmic scale for some resonant modes near these two ASWs. The numerical results confirm the fourth order relation between $\text{Im}(\omega)$ and β.

VI. CONCLUSION

BICs on periodic structures are surrounded by resonant modes with Q-factors approaching infinity. High-Q resonances and the resulting strong local field enhancement have important applications in lasing, nonlinear optics, etc. On 2D periodic structures, the Q-factors of the resonant modes near a BIC usually satisfy $Q \sim 1/(\beta - \beta_*)^2$, where β and β_* are the Bloch wavenumbers of the resonant mode and the BIC, respectively. In this paper, we derived a general condition for special BICs so that their nearby resonant modes have $Q \sim 1/(\beta - \beta_*)^4$. These special BICs produce high-Q resonances for a very large range of β, and they are useful because precise control of β may be difficult in practice. The conditions for the special BICs are given in integrals involving the BIC and related diffraction solutions, and they imply that the first order perturbation ϕ_1 does not radiate power to infinity. It was previously shown that the symmetric standing waves are special BICs with $Q \sim 1/(\beta - \beta_*)^4$ [45]. Other BICs can also become special ones, if the parameters of the periodic structure are properly tuned. The general conditions derived in this paper can be used to find new special BICs. Numerical examples are given for two families of ASWs on a periodic array of circular cylinders.

In practical applications, the BICs always dissolve into resonant modes with finite Q-factors, because the structures are always finite and fabrication errors will break the required symmetries and periodicity. We expect the special BICs have advantages over the ordinary BICs in practical structures with fabrication errors and in finite structures, but a rigorous analysis is still under development. In addition, the results of this paper are restricted to 2D structures. Clearly, it is worthwhile to derive similar conditions for special BICs on bi-periodic three-dimensional (3D) structures and rotationally symmetric 3D structures.

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APPENDIX

For operator $\mathcal{L}$ given in Eq. (13), it is easy to verify that

$$\overline{\phi}_*\mathcal{L}\phi_1 - \phi_1\overline{\mathcal{L}\phi_*} = \nabla\cdot\left(\overline{\phi}_*\nabla\phi_1 - \phi_1\nabla\overline{\phi}_*\right) + 2i\beta_*\partial_y(\phi_1\overline{\phi}_*),$$

where ∇ is the 2D gradient operator. The integral on Ω of the right hand side can be reduced to an integral on $\partial\Omega$ (the boundary of Ω) by the divergence theorem. It is zero, since ϕ_* and ϕ_1 are periodic in y and $\phi_* \to 0$ exponentially as $|x| \to \infty$. Meanwhile, ϕ_* satisfies Eq. (10), thus $\int_\Omega \overline{\phi}_*\mathcal{L}\phi_1 d\boldsymbol{r} = 0$. From Eq. (11) for ϕ_1, it is clear that

$$\int_\Omega \overline{\phi}_*\left[-2i\partial_y\phi_* + 2(\beta_* - k_*k_1\epsilon)\phi_*\right]d\boldsymbol{r} = 0.$$

This leads to Eq. (14). Meanwhile, $\int \overline{\phi}_*\partial_y\phi_* d\boldsymbol{r}$ is pure imaginary, since

$$\int_\Omega \overline{\phi}_*\partial_y\phi_* d\boldsymbol{r} = \int_\Omega \partial_y|\phi_*|^2 d\boldsymbol{r} - \int_\Omega \phi_*\partial_y\overline{\phi}_* d\boldsymbol{r} = -\int_\Omega \phi_*\partial_y\overline{\phi}_* d\boldsymbol{r}.$$

Therefore, k_1 is real.

Similarly, we have $\int_\Omega \overline{\phi}_*\mathcal{L}\phi_2 d\boldsymbol{r} = 0$. Multiplying both sides of Eq. (12) and integrating on Ω, we obtain

$$k_2 = \frac{\int_\Omega (1 - k_1^2\epsilon)|\phi_*|^2 d\boldsymbol{r} + \int_\Omega R\, d\boldsymbol{r}}{2k_*\int_\Omega \epsilon|\phi_*|^2 d\boldsymbol{r}},$$

where $R = \overline{\phi}_*[-2i\partial_y\phi_1 + 2(\beta_* - k_*k_1\epsilon)\phi_1]$. Therefore,

$$\mathrm{Im}(k_2) = \frac{\mathrm{Im}\left[\int_\Omega R\, d\boldsymbol{r}\right]}{2k_*\int_\Omega \epsilon|\phi_*|^2 d\boldsymbol{r}}.$$

From the complex conjugate of Eq. (11), we obtain

$$\int_{\Omega_h} \phi_1\overline{\mathcal{L}\phi_1} d\boldsymbol{r} = \int_{\Omega_h} R\, d\boldsymbol{r},$$

where Ω_h is the rectangular domain defined in Sec. IV. The right hand side above requires an integration by parts that switches the integral from $\phi_1\partial_y\overline{\phi}_*$ to $-\overline{\phi}_*\partial_y\phi_1$. Meanwhile, it is easy to verify that

$$\int_{\Omega_h} \phi_1\overline{\mathcal{L}\phi_1} d\boldsymbol{r} = \int_{\partial\Omega_h} \phi_1\frac{\partial\overline{\phi}_1}{\partial\nu}ds + \int_{\Omega_h}\left[(k_*^2\epsilon - \beta_*^2)|\phi_1|^2 - |\nabla\phi_1|^2 - 2i\beta_*\phi_1\frac{\partial\overline{\phi}_1}{\partial y}\right]d\boldsymbol{r},$$

where $\partial\Omega_h$ is the boundary of Ω_h and ν is its unit outward normal vector. The second term in the right hand side above is real. Therefore,

$$\mathrm{Im}\left[\int_{\Omega_h} R\, d\boldsymbol{r}\right] = \mathrm{Im}\left[\int_{\partial\Omega_h} \phi_1\frac{\partial\overline{\phi}_1}{\partial\nu}ds\right].$$

Since ϕ_1 is periodic in y, the line integrals at $y = \pm L/2$ are canceled. Therefore

$$\int_{\partial\Omega_h} \phi_1\frac{\partial\overline{\phi}_1}{\partial\nu}ds = \int_{-L/2}^{L/2}\left[\phi_1\frac{\partial\overline{\phi}_1}{\partial x}\right]_{x=-h}^{x=h} dy,$$

where $P(x,y)|_{x=-h}^{x=h}$ denotes $P(h,y) - P(-h,y)$.

For $|x| > D$, the equation for ϕ_1 is quite simple. It is not difficult to see that

$$\phi_1 = d_0^{\pm}e^{\pm i\alpha_* x} + \sum_{j\neq 0} d_j^{\pm}(x)e^{i2\pi jy/L}e^{\pm\gamma_{*j}x}$$

for $x > D$ and $x < -D$ respectively, where $\gamma_{*j} = -i\alpha_{*j}$ is positive, $d_0^{\pm}$ are unknown coefficients, and $d_j^{\pm}(x)$ $(j \neq 0)$ are unknown linear polynomials of x. The above gives

$$\lim_{h\to+\infty}\int_{-L/2}^{L/2}\left[\phi_1\frac{\partial\overline{\phi}_1}{\partial x}\right]_{x=-h}^{x=h} dy = -iL\alpha_*(|d_0^+|^2 + |d_0^-|^2),$$

and $\mathrm{Im}\left[\int_\Omega R\, d\boldsymbol{r}\right] = -L\alpha_*(|d_0^+|^2 + |d_0^-|^2)$, and finally Eq. (16).

To show Eq. (23), we notice that

$$\overline{\varphi}_l\mathcal{L}\phi_1 - \phi_1\overline{\mathcal{L}}\overline{\varphi}_l = \nabla\cdot\left[\overline{\varphi}_l\nabla\phi_1 - \phi_1\nabla\overline{\varphi}_l\right] + 2i\beta_*\partial_y(\phi_1\overline{\varphi}_l).$$

Since φ_l satisfies the Helmholtz equation and both ϕ_1 and φ_l are periodic in y, we have

$$\int_{\Omega_h} \overline{\varphi}_l\mathcal{L}\phi_1 d\boldsymbol{r} = \int_{\partial\Omega_h}\left[\overline{\varphi}_l\frac{\partial\phi_1}{\partial\nu} - \phi_1\frac{\partial\overline{\varphi}_l}{\partial\nu}\right]ds.$$

In the right hand side above, the integrals on the two edges at $y = \pm L/2$ are canceled. Therefore

$$\int_{\Omega_h} \overline{\varphi}_l \mathcal{L}\phi_1 d\boldsymbol{r} = \int_{-L/2}^{L/2} \left[\overline{\varphi}_l \frac{\partial \phi_1}{\partial x} - \phi_1 \frac{\partial \overline{\varphi}_l}{\partial x} \right]_{x=-h}^{x=h} dy.$$

Based on the asymptotic formula (20), it is easy to show that as $h \to +\infty$, the right hand side above tend to $2iL\alpha_*(d_0^+\overline{T}_l + d_0^-\overline{R}_l)$. This leads to Eq. (23). The proof for Eq. (24) is similar.

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