Propagating Bloch modes above the lightline on a periodic array of cylinders

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Abstract. Optical bound states in the radiation continuum (BICs) have interesting properties and potentially important applications. On periodic structures, the BICs are guided modes above the lightline, and they can be either standing waves or propagating Bloch modes. A one-dimensional (1D) array of circular dielectric cylinders is probably the simplest structure on which different types of BICs exist. Using a highly efficient numerical method, we perform an extensive numerical study for propagating BICs on 1D arrays of circular dielectric cylinders. In addition to the known Bloch BIC which is symmetric with respect to the axis of the array, we obtain a new BIC which is antisymmetric. The existence domains (in the plane of radius and dielectric constant of the cylinders) of both BICs are determined. The boundaries of these domains correspond to either standing waves which are not protected by symmetry or the opening of the second diffraction channel. Numerical results are also presented to illustrate the discontinuities of transmission and reflection coefficients at the BICs, and the resonant behavior near the BICs.

Keywords: periodic waveguides, bound state in the continuum, Bloch modes

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1. Introduction

A bound state in the continuum (BIC) is a localized or trapped mode with a frequency in the frequency interval where outgoing radiation modes exist. The concept of BIC first appeared in quantum mechanics [1–3]. Mathematically, a BIC corresponds to a discrete eigenvalue in a continuous spectrum, and leads to the non-uniqueness of a boundary value problem for given incident waves [4]. Recently, a number of theoretical and experimental studies on optical BICs have appeared in the literature [5–24]. Existing BICs for classical electromagnetic or sound waves involve a number of different configurations. The simplest BICs are trapped modes around a local distortion in a waveguide [5, 6, 25, 26]. They exist at frequencies for which the waveguide has outgoing propagating modes. BICs are also found on special z-invariant waveguides or waveguide arrays (z is the waveguide axis) with a transverse radiation channel [7–10]. In that case, the BICs are guided modes that propagate along the z axis, and they do not couple to the outgoing waves in the radiation channel. Many BICs are found on periodic structures surrounded by a homogeneous medium [4, 11–24, 27, 28]. These BICs exist above the lightline (or in the light-cone for biperiodic structures), and can be either standing waves or propagating Bloch modes.

BICs can be regarded as resonances with infinite Q-factors, and may have potentially significant applications. A BIC on a periodic structure cannot couple to an incident wave if they have exactly the same frequency and wavevector, but it becomes a resonance with a large Q-factor, when the wavevector is slightly changed. The resonant mode can couple with an incident wave producing a large local field in the structure. In addition, the transmission spectrum may exhibit a rapid variation from total transmission to total reflection [29, 30]. Such properties may find applications in filtering, sensing and switching, and can be used to enhance nonlinear effects.

In many cases, the BICs do not couple to the outgoing radiation waves since they have incompatible symmetries [4, 11–16, 28]. The existence of these so-called symmetry-protected BICs are well-known and can be rigorously proved [4, 26, 28]. BICs that are not symmetry-protected also exist. On a periodic structure with a reflection symmetry along the periodic direction, in addition to the antisymmetric standing waves which are symmetry-protected BICs, there could be propagating Bloch modes above the lightline (or in the lightcone), and they are not symmetry-protected [17–23, 27].

A one-dimensional (1D) periodic array of parallel and infinitely long cylinders is a particularly simple periodic structure. Bloch BICs are first found around a periodic array of rectangular non-penetrable cylinders [27]. Recently, Bulgakov and Sadreev [23] analyzed BICs on a periodic array of circular dielectric cylinders, and found propagating Bloch modes above the lightline for some values of the cylinder radius. However, the conditions for existence and nonexistence of Bloch BICs on such a periodic array are not fully clarified. In this paper, we perform a comprehensive study for Bloch BICs on 1D arrays of circular dielectric cylinders. We found two families of BICs with different symmetries, determined their domains of existence for different radius and dielectric constant of the cylinders, and analyzed the conditions for their disappearance.

2. Formulation and numerical method

In Fig. 1(a), we show a 1D periodic array of parallel and infinitely long circular dielectric cylinders surrounded by air. The Cartesian coordinate system $\{x, y, z\}$ is chosen so that the cylinders are parallel to the z axis, the array is periodic in y with period L, and the origin is located at the center of one cylinder. For the E-polarization, the z-component of the electric field, denoted by u, satisfies the following two-dimensional (2D) Helmholtz

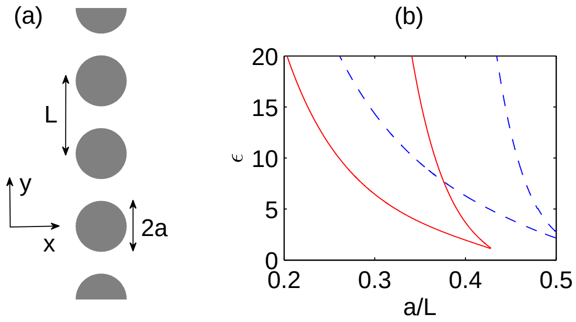

Figure 1. (a): A 1D array of circular cylinders (radius a and dielectric constant ϵ_1) periodic in y with period L. (b): Existence domains of the x-even and x-odd BICs bounded by the solid red curves and the dashed blue curves, respectively. For any point in an existence domain, there is a pair (ω, β) corresponding to a BIC.

equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + k_0^2 \epsilon \, u = 0, \tag{1}$$

where $k_0 = \omega/c$ is the freespace wavenumber, ω is the angular frequency, c is the speed of light in vacuum, and $\epsilon = \epsilon(x, y)$ is a real dielectric function satisfying $\epsilon = \epsilon_1$ in the cylinders and $\epsilon = 1$ outside the cylinders.

A guided Bloch mode of this periodic structure is a solution of Eq. (1) given by

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

where ϕ is periodic in y with period L, $\phi \to 0$ as $|x| \to \infty$, and β is the real Bloch wavenumber (or propagation constant). Due to the periodicity of ϕ and the reflection symmetry in y, β can be restricted to the interval $[0, \pi/L]$. Since the periodic array can be regarded as a waveguide, there are well-known guided Bloch modes below the lightline, i.e., $k_0 < \beta$. These modes exist continuously with respect to β and ω. On the other hand, a BIC is a Bloch mode above the lightline, i.e., $k_0 > \beta$. They only exist as isolated points in the frequency-wavenumber plane. Special BICs with $\beta = 0$ are the standing waves, and their existence is well established [4,15,28]. We are concerned with Bloch BICs with $\beta \neq 0$.

Since ϕ is periodic in y, it can be expanded in a Fourier series. Consequently, the Bloch mode given in Eq. (2) can be written as

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

for $x > a$ and $x < -a$, respectively, where

$$\beta_j = \beta + \frac{2j\pi}{L}, \quad \alpha_j = \sqrt{k_0^2 - \beta_j^2}, \tag{4}$$

and $c_j^{\pm}$ are unknown coefficients. Notice that α_j is either real or pure imaginary (with positive imaginary part). In particular, since we assume $k_0 > \beta$, α_0 is always positive. If

α_j is real, the coefficients $c_j^{\pm}$ must vanish, otherwise ϕ cannot decay to zero as $|x| \to \infty$. If we introduce a linear operator $\mathcal{T}$ satisfying

$$\mathcal{T} e^{\mathrm{i}\beta_j y} = \mathrm{i}\alpha_j \, e^{\mathrm{i}\beta_j y}, \quad j = 0, \pm 1, \pm 2, ... \tag{5}$$

then u satisfies the following boundary conditions

$$\frac{\partial u}{\partial x} = \pm \mathcal{T} u, \quad x = \pm \frac{L}{2}. \tag{6}$$

In addition, the Bloch mode satisfies the quasi-periodic conditions

$$u(x, L/2) \qquad = e^{\mathrm{i}\beta L} u(x, -L/2), \tag{7}$$

$$\frac{\partial u}{\partial y}(x, -L/2) = e^{\mathrm{i}\beta L} \frac{\partial u}{\partial y}(x, -L/2). \tag{8}$$

To find a BIC, we search a pair (ω, β), such that Eq. (1) has a nonzero Bloch mode solution that decays to 0 as $|x| \to \infty$. As described in [15], we can approximate the problem by

$$\boldsymbol{A}(\omega, \beta)\boldsymbol{u} = \boldsymbol{0}, \tag{9}$$

where $\boldsymbol{A}$ is a small matrix depending on ω and β, and $\boldsymbol{u}$ is a column vector approximating u on three edges of the square S given by $|x| < L/2$ and $|y| < L/2$. To obtain Eq. (9), we use cylindrical wave expansions in S and apply the boundary conditions (6), (7) and (8). If each edge of the square S is approximated by N points, then $\mathcal{T}$ can be approximated by an $N \times N$ matrix, and $\boldsymbol{A}$ is a $(3N) \times (3N)$ matrix. A BIC corresponds to a pair (ω, β) such that $\boldsymbol{A}$ is singular. We calculate (ω, β) by solving $\lambda_1(\boldsymbol{A}) = 0$, where λ_1 is the eigenvalue of $\boldsymbol{A}$ with the smallest magnitude. This nonlinear equation can be iteratively solved by a globally convergent Newton-Krylov method [31].

3. Results

We search Bloch BICs for frequencies satisfying $\omega L/(2\pi c) < 1$, and for $1 < \epsilon_1 < 20$ and $0 < a < 0.5L$, where a and ϵ_1 are the radius and dielectric constant of the cylinders, respectively. Two families of Bloch BICs are found, and they are even and odd in x respectively. The existence domains of these Bloch BICs are shown in Fig. 1(b). The domains bounded by the solid red curves and the dashed blue curves correspond to the x-even and x-odd BICs, respectively. The array also has symmetry-protected BICs which are y-odd standing waves [15], and they are not shown in Fig. 1(b). We point out that the x-even BICs are first found by Bulgakov and Sadreev [23] for the case of $\epsilon_1 = 12$. Notice that for a particular array with a given a and ϵ_1, it is possible to have 0, 1, or 2 Bloch BICs, depending on whether (a, ϵ_1) is outside both domains, inside one domain, or inside both domains. For any point in an existence domain, we have a pair (ω, β) for the corresponding BIC. In Figs. 2(a) and 2(b), we show the normalized frequency $\omega L/(2\pi c)$ and normalized wavenumber $\beta L/(2\pi)$ for the x-even BICs, respectively. The corresponding results for the x-odd BICs are shown in Figs. 2(c) and 2(d). We can see that β and ω of the BICs decrease as a or ϵ_1 is increased. To show the results more

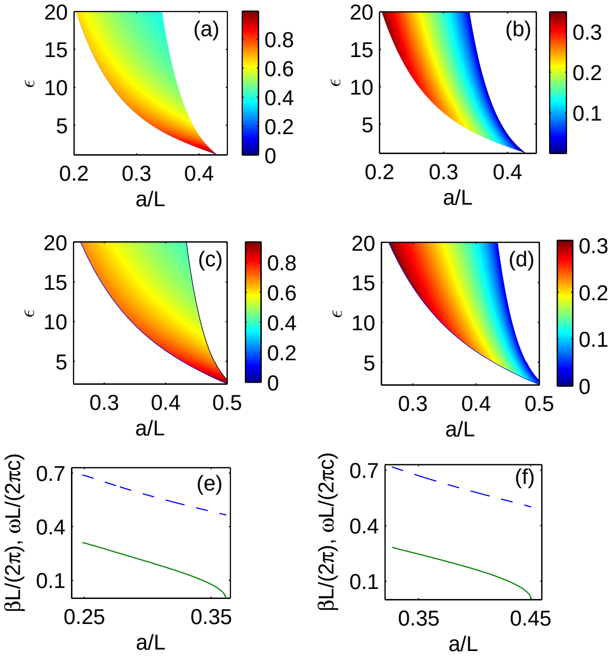

Figure 2. Frequency and wavenumber of the BICs as functions of a and ϵ_1: (a) frequency of the x-even BIC; (b) wavenumber of the x-even BIC; (c) frequency of the x-odd BIC; (d) wavenumber of the x-odd BIC; (e) and (f): frequency (dashed line) and wavenumber (solid line) at fixed $\epsilon_1 = 11.56$ for the x-even and x-odd BICs, respectively.

clearly, we fix $\epsilon_1 = 11.56$ and plot ω and β as functions of radius a in Figs. 2(e) and 2(f). For $\epsilon_1 = 11.56$ and $a = 0.35L$, we have one x-even BIC with $\beta L/(2\pi) = 0.0776$ and $\omega L/(2\pi c) = 0.4854$, and one x-odd BIC with $\beta L/(2\pi) = 0.2483$ and $\omega L/(2\pi c) = 0.6702$. The wave field patterns of these two modes are shown in Figs. 3(a) and 3(b), respectively.

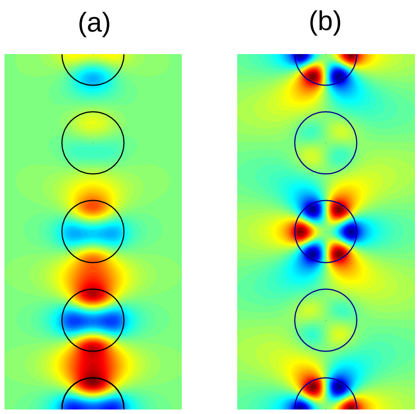

Figure 3. (a) and (b): Wave field patterns (i.e. real part of u) of the x-even and x-odd BICs, respectively, for $\epsilon_1 = 11.56$ and $a = 0.35L$.

From Figs. 2(b), 2(d), 2(e) and 2(f), we observe that the right boundaries of both existence domains correspond to $\beta = 0$, i.e., the BICs there are standing waves. For $\epsilon_1 = 10$, the two standing waves exist at $a = 0.36665158L$ and $a = 0.45746377L$, respectively. Their wave field patterns are shown in Figs. 4(a) and 4(b). Standing waves

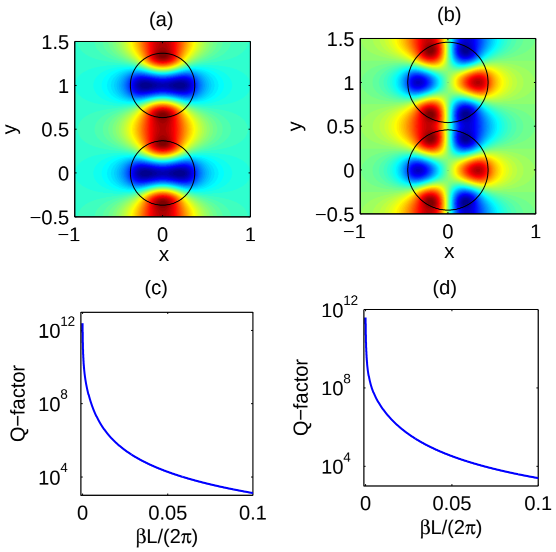

Figure 4. (a): Wave field pattern (i.e. real part of u) of the x-even BIC with $\beta = 0$ for $\epsilon_1 = 10$ and $a = 0.36665158L$, and $\omega L/(2\pi c) = 0.49114236$. (b): Wave field pattern (i.e. real part of u) of the x-odd BIC with $\beta = 0$ for $\epsilon_1 = 10$, $a = 0.45746377L$, and $\omega L/(2\pi c) = 0.52756851$. (c) and (d): Q-factors of the resonant modes near the x-even and x-odd BICs with $\beta = 0$, respectively.

on periodic arrays of circular dielectric cylinders have been extensively investigated [15, 23]. With reference to the reflection symmetry in the y direction, antisymmetric standing waves (odd functions of y) are symmetry-protected BICs, and their existence can be rigorously proved [4, 15, 28]. However, the two standing waves shown in Fig. 4 are different. We can see that they are even functions of y, thus are not protected by symmetry. Note that an x-odd standing wave (for $\epsilon_1 = 12$) was previously found by Bulgakov and Sadreev [23].

In the $\omega\beta$ plane, the BICs are isolated points above the lightline. Let (ω_*, β_*) be the frequency and wavevector of a BIC, if β is slightly different from β_*, a nonzero Bloch mode solution of Eq. (1) exists for a complex ω. It is a resonant mode and its quality factor can be defined as $Q = -0.5\text{Re}(\omega)/\text{Im}(\omega)$. As $\beta \to \beta_*$, $\text{Re}(\omega) \to \omega_*$, $\text{Im}(\omega) \to 0$ and the Q-factor tends to infinity. Therefore, a BIC can also be regarded as a resonant mode with infinite Q-factor (and infinite lifetime). As simple examples, we consider the two standing waves on the right boundaries of the existence domains for $\epsilon_1 = 10$. In Figs. 4(c) and 4(d), we show the Q-factors of the resonant modes for different values of β. Clearly, the Q-factor blows up as $\beta \to 0$.

A close inspection reveals that the left boundaries of the existence domains are precisely the condition for opening the second diffraction channel. For $|x| > a$, the

Bloch mode has a plane wave expansion given in Eq. (3). A diffraction channel is simply a propagating diffraction order corresponding to a plane wave with a real wave vector. Since the Bloch BIC is confined around the array, the expansion coefficients of all propagating diffraction orders must be zero. For a Bloch mode above the lightline (i.e., $k_0 > \beta$), α_0 is real and positive, the zeroth diffraction order is always propagating, and it is the first diffraction channel. The left boundaries of the existence domains correspond to $\alpha_{-1} = 0$ or $k_0 = 2\pi/L - \beta$, assuming $0 \le \beta \le \pi/L$. BICs with more than one diffraction channels are more difficult to find, but they do exist [23, 27].

For a BIC with frequency ω_* and Bloch wavenumber β_*, the boundary value problem of Eq. (1) associated with an incident wave with $\omega = \omega_*$ and wave vector $\boldsymbol{k} = (k_x, k_y)$ where $k_y = \beta_*$, has no uniqueness [4], but the transmission and reflection coefficients (for normalized power) are well defined, since the incident wave and the BIC are uncoupled. For a periodic array of circular cylinders with radius a and dielectric constant ϵ_1, we may consider the reflection coefficient R (or transmission coefficient T) as a function of ω and k_y of the incident plane wave. It turns out that R, as a joint function of the two variables, is discontinuous at (ω_*, β_*). As shown in [29,30], if k_y is close to but not equal to β_*, the reflection (or transmission) spectrum exhibits resonant behavior near ω_* with a rapid change from 0 (total transmission) to 1 (total reflection). The frequencies for total transmission and total reflection can be arbitrarily close, if k_y is arbitrarily close to β_*. Similarly, if ω is close to but not equal to ω_*, R (or T) as a function of k_y exhibits arbitrarily close total reflection and total transmission near β_*. These properties are illustrated in Fig. 5 for the two BICs on the array with $\epsilon_1 = 11.56$ and $a = 0.35L$. In principle, this property can be used to separate two incident waves with the same k_y and arbitrarily close frequencies, and to separate two incident waves with the same frequency but arbitrarily close incident angles.

Similarly, if we fixed the incident wave with $\omega = \omega_*$ and $k_y = \beta_*$, where ω_* and β_* are the frequency and wavenumber of a BIC for an array with radius a_* and dielectric constant ϵ_*, and consider the reflection coefficient R and transmission coefficient T as functions of a and ϵ_1, then R and T are discontinuous at (a_*, ϵ_*). In an arbitrarily small neighborhood of (a_*, ϵ_*) (in the $a\epsilon_1$ plane), there are total reflection and total transmission points. When R (or T) is regarded as a function of radius a for fixed ϵ_1 near ϵ_*, or as a function of ϵ_1 for a fixed a near a_*, rapid changes from total transmission to total reflection can be observed. This is illustrated in Fig. 6 in connection with the x-even BIC for the array with $\epsilon_* = 11.56$ and $a_* = 0.35L$. In principle, these properties can be used to detect an infinitesimal change in radius a or dielectric constant ϵ_1 of the cylinders in the array, and may find applications in sensing and switching.

4. Conclusion

In summary, we analyzed Bloch BICs, i.e., Bloch modes above the lightline, for a periodic array of circular dielectric cylinders. Extending the work of Bulgakov and Sadreev [23], we found two families of Bloch BICs that depend on the radius a and dielectric constant

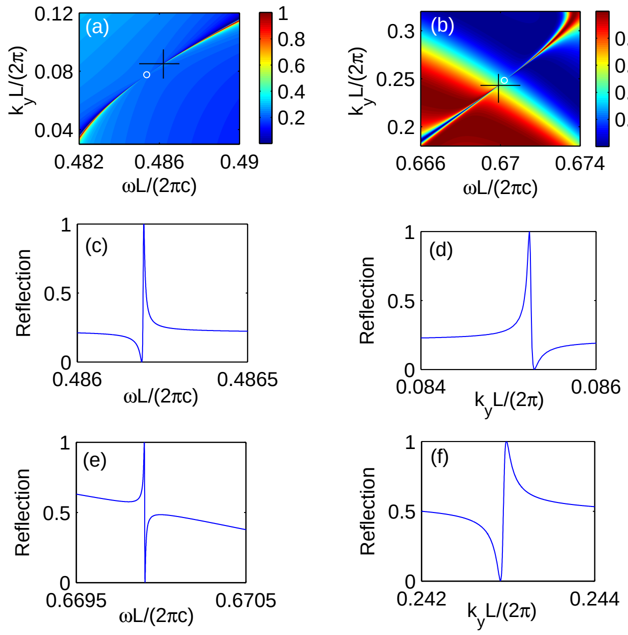

Figure 5. Reflection coefficient R as a function of ω and k_y for an array with $\epsilon_1 = 11.56$ and $a = 0.35L$. The BICs are indicated by the while circles. Plots are shown along the lines in the black crosses. (a) Near the x-even BIC; (b) near the x-odd BIC; (c) $k_yL/(2\pi) = 0.0852$; (d) $\omega L/(2\pi c) = 0.4862$; (e) $k_yL/(2\pi) = 0.243$; (f) $\omega L/(2\pi c) = 0.6699$.

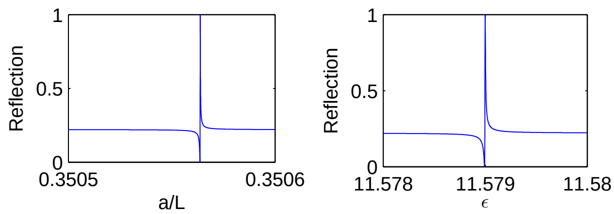

Figure 6. Reflection coefficient R as a function of a or ϵ_1 for an incident wave with frequency $\omega L/(2\pi c) = 0.4854$ and wavenumber $k_yL/(2\pi) = 0.0776$. (a) For $\epsilon_1 = 11.52$; (b) for $a = 0.3497L$.

ϵ_1 continuously. In the $a\epsilon_1$ plane, the domain of existence of each BIC family is bounded by two curves, one corresponding to standing waves and the other corresponding to the opening of the second diffraction channel. We also investigated some interesting properties of Bloch BICs, including nearby resonant modes with arbitrarily high Q-factors, discontinuities in reflection and transmission coefficients, and arbitrarily close total reflections and total transmissions. The y-even standing waves on the right boundaries of the existence domains are particularly interesting, since their nearby resonances have unusually large Q-factors. We are currently developing a theory for these resonances, and considering their applications for nonlinearity enhancement.

Our study is limited to the special case of circular cylinders, since we believe it is worthwhile to thoroughly analyze BICs in the simplest setting, in order to have a better understanding of the intriguing wave phenomena. For BICs on periodic structures, the importance of some key symmetries has been revealed [19, 20], but even for the very simple periodic array of circular dielectric cylinders considered in this paper, existing physical or mathematical theories cannot predict the existence or nonexistence of Bloch BICs (unprotected by symmetry) for a given pair (a, ϵ_1). As shown in Fig. 1(b), for a given pair (a, ϵ_1), it is possible to have 0, 1 or 2 Bloch BICs, but there is currently no theory to predict this. Therefore, direct numerical calculations are still needed to get a complete picture about BICs on such a simple periodic structure. Of course, general physical or mathematical theories on the existence and robustness of BICs are very important. Further studies are needed for BICs on more general periodic arrays and for their potential applications.

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