Bound States in the Continuum on Periodic Structures: Perturbation Theory and Robustness

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On periodic structures, a bound state in the continuum (BIC) is a standing or propagating Bloch wave with a frequency in the radiation continuum. Some BICs (e.g., antisymmetric standing waves) are symmetry-protected, since they have incompatible symmetry with outgoing waves in the radiation channels. The propagating BICs do not have this symmetry mismatch, but they still depend crucially on the symmetry of the structure. In this Letter, a perturbation theory is developed for propagating BICs on two-dimensional periodic structures. The study shows that these BICs are robust against structural perturbations that preserve the symmetry, indicating that these BICs are in fact implicitly protected by symmetry.

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A periodic structure sandwiched between two homogeneous media can be considered as a (periodic) waveguide. Guided modes on such a structure usually exist below the light line, so that plane waves with the same frequency and consistent wavevector can only decay exponentially in the surrounding homogeneous media. However, it is known that on periodic structures, guided modes can also exist above the light line [1–18], and they are special cases of bound states in the continuum (BICs), a notion originally introduced by Von Neumann and Wigner [19]. Due to their interesting properties and potentially important applications, optical BICs have recently attracted much attention [20]. Mathematically, the BICs correspond to discrete eigenvalues in continuous spectra, and are related to the nonuniqueness of diffraction problems [1]. BICs are also known to exist on waveguides with local distortions [21–26], and on waveguides with lateral leaky structures [27–30]. Related to a BIC on a periodic structure, diffraction problems for given incident waves exhibit interesting properties such as nonuniqueness, total transmission, total reflection, and discontinuities in transmission (reflection) coefficients [1, 31, 32]. These properties can be explored in filtering, sensing and switching applications. Near a BIC, there is a family of resonant modes with Q-factors approaching infinity. The resulting strong field enhancement and light confinement can be used to design high-quality laser [33], enhance nonlinear optical effects [34], quantum optical effects, and other emission processes.

On periodic structures, the so-called symmetry-protected BICs are well-known [1–7]. They cannot couple to the outgoing waves in the radiation channels due to a symmetry mismatch. The more interesting BICs are the propagating Bloch modes that do not have incompatible symmetry with the outgoing waves [8–18]. It has been observed that the propagating BICs are robust against structural changes that preserve the relevant symmetry [11, 12]. If the structure is slightly changed (keeping the relevant symmetry), the original BIC is simply shifted to a new one with a slightly different frequency and a slightly different wavevector. This phenomenon was investigated numerically for photonic crystal slabs and periodic arrays of spheres by a number of authors [35–37]. Zhen *et al.* [36] considered the polarization directions of the far-field radiation and suggested that the Bloch BICs on photonic crystal slabs are topologically protected. Bulgakov and Maksimov [37] reached the same conclusion for BICs on a periodic array of spheres by considering the phase singularities of a certain coupling coefficient. In this Letter, we present a perturbation theory for BICs on general periodic structures. Our result reveals the link between the relevant symmetry and the robustness of BICs directly and constructively. Namely, if the periodic structure is changed with a small perturbation that preserve the symmetry, the BIC is shifted to a nearby one which can be solved by the perturbation method. On the other hand, if the perturbation does not preserve the symmetry, the method breaks down which indicates that no BICs exist in the neighborhood.

We consider a two-dimensional (2D) periodic structure given by a real dielectric function $\epsilon(x,y)$ which is periodic in y with period L and has reflection symmetry in both x and y directions. The reflection symmetry implies that

$$\epsilon(x,y) = \epsilon(-x,y) = \epsilon(x,-y) \quad \textbf{(1)}$$

for all (x,y). In addition, we assume that the periodic structure is bounded in the x direction by $|x| < D$ and surrounded by vacuum, i.e., $\epsilon(x,y) = 1$ for $|x| > D$. For the E polarization, the z component of the electric field, denoted as u, satisfies the following Helmholtz equation

$$[\partial_x^2 + \partial_y^2 + k^2\epsilon(x,y)]u = 0, \quad \textbf{(2)}$$

where $k = \omega/c$ is the free-space wavenumber, ω is the angular frequency, and c is the speed of light in vacuum.

A guided mode on this periodic structure is a special solution of Eq. (2) given in the Bloch form

$$u(x,y) = e^{i\beta y}\phi(x,y), \tag{3}$$

where β is the Bloch wavenumber, ϕ is periodic in y with period L, and $\phi(x,y) \to 0$ as $|x| \to \infty$. The Bloch wavenumber β can be restricted to the interval $[-\pi/L, \pi/L]$. In terms of ϕ, Eq. (2) becomes $\mathcal{L}\phi = 0$, where

$$\mathcal{L} = \partial_x^2 + \partial_y^2 + 2i\beta\partial_y + k^2\epsilon(x,y) - \beta^2. \tag{4}$$

A BIC is a special guided mode above the light line, i.e., $k > |\beta|$. In the surrounding free space, plane waves with the same frequency and compatible y-dependence have wavevectors $(\pm\alpha_j, \beta_j)$, where

$$\beta_j = \beta + 2\pi j/L, \quad \alpha_j = \sqrt{k^2 - \beta_j^2}, \tag{5}$$

and $\alpha = \alpha_0$ is positive. We further assume that $k < 2\pi/L - |\beta|$, then if $j \neq 0$, $\alpha_j = i\sqrt{\beta_j^2 - k^2}$ is pure imaginary. Therefore, for all $j \neq 0$, the plane waves with wavevectors $(\pm\alpha_j, \beta_j)$ are evanescent. The only opening diffraction channel corresponds to plane waves with wavevectors $(\pm\alpha, \beta)$. For $|x| > D$, the BIC can be expanded in plane waves as

$$u(x,y) = \sum_{j=-\infty}^{\infty} c_j^{\pm} e^{i(\beta_j y \pm \alpha_j x)}, \tag{6}$$

for $x > D$ and $x < -D$, respectively. Since $u \to 0$ as $|x| \to \infty$, we must have $c_0^{\pm} = 0$. In addition, it can be assumed that the BIC is either even in x or odd in x. Notice that if $u(x,y)$ is a BIC, then so is $u(-x,y)$, we can construct even or odd BICs from $u(x,y) + u(-x,y)$ or $u(x,y) - u(-x,y)$. It is clear that $c_j^+ = \pm c_j^-$ depending on whether u is even or odd in x.

It can be easily verified that if u is a BIC, then so it $\overline{u}(x,-y)$, where $\overline{u}$ denotes the complex conjugate of u, and they have the same frequency and same Bloch wavenumber β. We further assume that u is non-degenerate (i.e. single), then there must be a constant C, such that $u(x,y) = C\overline{u}(x,-y)$. Let Ω be one period of the structure given by $-\infty < x < \infty$ and $-L/2 < y < L/2$, then the integral of $|u|^2$ on Ω is finite, since u decays to zero exponentially as $|x|$ is increased. Substituting the above into this integral, we get $|C| = 1$. If $C = e^{i2\tau}$ for some real number τ, then $w = e^{-i\tau}u$ is also a BIC, and it satisfies $w(x,y) = \overline{w}(x,-y)$. Therefore, without loss of generality, we can assume $C = 1$, or

$$u(x,y) = \overline{u}(x,-y). \tag{7}$$

The above is a case of the $\mathcal{PT}$-symmetry. It is clear that ϕ given in (3) satisfies the same $\mathcal{PT}$-symmetry.

For the periodic structure, we also consider diffraction problems for incident plane waves with the same frequency and the same wavenumber (y-component of the wavevector, β). To obtain a solution $\tilde{v}_e$ that is even in x, we specify two incident waves $\exp[i(\beta y \pm \alpha x)]$ for $x < -D$ and $x > D$, respectively. The function $\tilde{v}_e$ can be assumed to be even in x, since otherwise, it can be replaced by $[\tilde{v}_e(x,y) + \tilde{v}_e(-x,y)]/2$ which solves the same diffraction problem. For large $|x|$, $\tilde{v}_e$ has the following asymptotic form

$$\tilde{v}_e(x,y) \sim e^{i(\beta y \pm \alpha x)} + S_e e^{i(\beta y \mp \alpha x)}, \quad x \to \mp\infty,$$

where $S_e = e^{2i\theta_e}$ is a complex number satisfying $|S_e| = 1$. Let $v_e = e^{-i\theta_e}\tilde{v}_e$, then we can assume that v_e satisfies the $\mathcal{PT}$-symmetry, since otherwise, it can be replaced by $[v_e(x,y) + \overline{v}_e(x,-y)]/2$ which solves the same diffraction problem with the same asymptotic behavior as infinity. Similarly, we can construct a diffraction solution $v_o(x,y)$ which is odd in x and is $\mathcal{PT}$-symmetric. Finally, we define φ_e and φ_o as in Eq. (3). That is,

$$v_e(x,y) = e^{i\beta y}\varphi_e(x,y), \; v_o(x,y) = e^{i\beta y}\varphi_o(x,y), \tag{8}$$

where φ_e and φ_o are periodic in y with period L, are $\mathcal{PT}$-symmetric, and are even and odd in x, respectively.

Assuming that the periodic structure given by $\epsilon(x,y)$ has a non-degenerate BIC $u = e^{i\beta y}\phi$ for free-space wavenumber k (frequency ω) and Bloch wavenumber β, we now consider a perturbed structure given by

$$\tilde{\epsilon}(x,y) = \epsilon(x,y) + \delta F(x,y), \tag{9}$$

where δ is a small real number and F is a real $O(1)$ function satisfying $F(x,y) = 0$ for $|x| > D$. We look for a BIC $\tilde{u} = e^{i\tilde{\beta}y}\tilde{\phi}$ with Bloch wavenumber $\tilde{\beta}$ and free-space wavenumber $\tilde{k}$. In the perturbation method, $\tilde{\phi}$, $\tilde{k}$ and $\tilde{\beta}$ are expanded in power series of δ:

$$\tilde{\phi} = \phi + \delta\phi_1 + \delta^2\phi_2 + \cdots \tag{10}$$

$$\tilde{\beta} = \beta + \delta\beta_1 + \delta^2\beta_2 + \cdots \tag{11}$$

$$\tilde{k} = k + \delta k_1 + \delta^2 k_2 + \cdots \tag{12}$$

Inserting the above expansions into the equation for $\tilde{\phi}$, i.e., $\tilde{\mathcal{L}}\tilde{\phi} = 0$, where $\tilde{\mathcal{L}}$ is defined as $\mathcal{L}$ given in (**??**), with ϵ, β and k replaced by $\tilde{\epsilon}$, $\tilde{\beta}$ and $\tilde{k}$, respectively, we obtain a sequence of equations for ϕ_1, ϕ_2, etc. They can be written as

$$\mathcal{L}\phi_j = B_1\beta_j + B_2 k_j - C_j, \tag{13}$$

for any integer $j \geq 1$, where B_1 and B_2 are independent of j, and C_j does not involve β_j and k_j. More precisely,

$$B_1 = 2\beta\phi - 2i\partial_y\phi, \tag{14}$$

$$B_2 = -2k\epsilon\phi, \tag{15}$$

$$C_1 = k^2 F\phi, \tag{16}$$

$$\begin{aligned} C_2 &= (k_1^2\epsilon - \beta_1^2 + 2kk_1F)\phi \\ &+ (2kk_1\epsilon - 2\beta\beta_1 + k^2F)\phi_1 + 2i\beta_1\partial_y\phi_1, \end{aligned} \tag{17}$$

and the general formula for C_j is

$$\begin{aligned} C_j = &\left[\sum_{l=1}^{j-1}(k_l k_{j-l}\epsilon - \beta_l\beta_{j-l}) + F\sum_{l=0}^{j-1} k_l k_{j-1-l}\right]\phi \\ &+ \sum_{n=1}^{j-1}\left[\sum_{l=0}^{n}(k_l k_{n-l}\epsilon - \beta_l\beta_{n-l}) + F\sum_{l=0}^{n-1} k_l k_{n-1-l}\right]\phi_{j-n} \\ &+ 2i\sum_{n=1}^{j-1}\beta_n\partial_y\phi_{j-n}, \end{aligned} \tag{18}$$

where $\beta_0 = \beta$ and $k_0 = k$.

The perturbation theory is developed to investigate the existence of BICs on the perturbed structure. If there is a BIC on the perturbed structure $\tilde{\epsilon}$ and it is near the original one, we expect to carry out the perturbation process successfully, that is, β_j, k_j and ϕ_j can be solved, β_j and k_j are real, and ϕ_j decays to zero exponentially as $|x| \to \infty$. On the other hand, if the perturbation process breaks down, that is, β_j and/or k_j become complex, or

ϕ_j does not decay to zero at infinity, then we believe there is no BIC near the original one.

In the jth step, β_j and k_j are solved from the linear system

$$\mathbf{A}\begin{bmatrix}\beta_j\\ k_j\end{bmatrix} = \begin{bmatrix}a_{11} & a_{12}\\ a_{21} & a_{22}\end{bmatrix}\begin{bmatrix}\beta_j\\ k_j\end{bmatrix} = \begin{bmatrix}b_{1j}\\ b_{2j}\end{bmatrix}, \quad (19)$$

where $\mathbf{A}$ is a 2×2 matrix,

$$a_{11} = \int_\Omega \overline{\phi} B_1 d\mathbf{r},\ a_{12} = \int_\Omega \overline{\phi} B_2 d\mathbf{r},\ b_{1j} = \int_\Omega \overline{\phi} C_j d\mathbf{r},$$

B_1, B_2 and C_j are given in Eqs. (14), (15) and (18), respectively, and $\mathbf{r} = (x, y)$. The second row depends on whether ϕ is even or odd in x. If ϕ is even in x, then

$$a_{21} = \int_\Omega \overline{\varphi}_e B_1 d\mathbf{r},\ a_{22} = \int_\Omega \overline{\varphi}_e B_2 d\mathbf{r},\ b_{2j} = \int_\Omega \overline{\varphi}_e C_j d\mathbf{r}.$$

If ϕ is odd in x, then we replace φ_e by φ_o. The first equation in (19) is obtained by multiplying Eq. (13) by $\overline{\phi}$ and integrating both sides on Ω. It can be verified that $\int_\Omega \overline{\phi}\mathcal{L}\phi_j d\mathbf{r} = 0$, and a_{11} and a_{12} are both real. The second equation in (19), for the case when ϕ is even in x, is a result of requiring

$$\int_\Omega \overline{\varphi}_e (B_1\beta_j + B_2 k_j - C_j) d\mathbf{r} = 0. \quad (20)$$

Since φ_e is $\mathcal{PT}$-symmetric, it can be shown that a_{21} and a_{22} are also real. If matrix $\mathbf{A}$ is invertible, β_j and k_j can be determined, then ϕ_j can be solved from Eq. (13). The right hand side of Eq. (13) represents a given source distribution.

In the following, we show that if $\mathbf{A}$ is invertible and if F has the same symmetry as ϵ, that is,

$$F(x, y) = F(x, -y) = F(-x, y) \quad (21)$$

for all (x, y), then the above perturbation process can be carried out successfully. For $j = 1$, since both ϕ and φ_e (or φ_o) are $\mathcal{PT}$-symmetric, it is easy to see that b_{11} and b_{21} are real. Therefore, β_1 and k_1 can be uniquely solved and they are real. The governing equation for ϕ_1 has a nonzero source term in the right hand side, thus in general, ϕ_1 should satisfy outgoing radiation conditions as $x \to \pm\infty$. When ϕ is even in x, the right hand side of Eq. (13) (for $j = 1$) is even in x, thus, we can assume ϕ_1 is even in x, since otherwise, it can be replaced by $[\phi_1(x, y) + \phi_1(-x, y)]/2$. Since ϕ is known to decay exponentially as $|x| \to \infty$, it is easy to construct particular solutions for Eq. (13), $j = 1$, for $|x| > D$, and these particular solutions decay exponentially as $|x| \to \infty$. The general solution for ϕ_1 is a sum of the particular solution and a solution of the homogeneous equation. Because of the symmetry in x and the outgoing radiation condition, we have

$$\phi_1(x, y) \sim d_1 e^{\pm i\alpha x}, \quad x \to \pm\infty, \quad (22)$$

for an unknown coefficient d_1. To show that d_1 is actually zero, we choose $h > D$, multiply Eq. (13) for $j = 1$, by $\overline{\varphi}_e$, and integrate on the rectangular domain Ω_h given by $|x| < h$ and $|y| < L/2$. From Eq. (20), it is clear that

$$\lim_{h\to\infty} \int_{\Omega_h} \overline{\varphi}_e \mathcal{L}\phi_1 d\mathbf{r} = 0.$$

Using integration by parts and the asymptotic formulas for φ_e and ϕ_1, it can be shown that the left hand side above is $4id_1\alpha L e^{-i\theta_e}$. Therefore, we must have $d_1 = 0$. Finally, since the right hand side of Eq. (13) is $\mathcal{PT}$-symmetric, we can assume ϕ_1 is also $\mathcal{PT}$-symmetric, since otherwise, we can replace ϕ_1 by $[\phi_1(x, y) + \overline{\phi}_1(x, -y)]/2$.

The same reasoning can be used in all perturbation steps for $j \geq 2$. If F satisfies Eq. (21) and $\mathbf{A}$ is invertible, in the jth step, we can show that β_j and k_j are real, $\phi_j \to 0$ exponentially as $x \to \pm\infty$, ϕ_j is even or odd in x (same as ϕ), and ϕ_j is $\mathcal{PT}$-symmetric.

If F does not satisfy Eq. (21), then the perturbation process is likely to fail. In the first step, if ϕ is even in x, in order to have a real b_{21}, we need $\int F\phi\overline{\varphi}_e d\mathbf{r}$ to be real. This implies

$$\int_\Omega [F(x, y) - F(x, -y)]\phi\overline{\varphi}_e d\mathbf{r} = 0. \quad (23)$$

Meanwhile, Eq. (20) should remain valid when φ_e is replaced by φ_o. This gives rise to the condition $\int F\phi\overline{\varphi}_o d\mathbf{r} = 0$, which can be written as

$$\int_\Omega [F(x, y) - F(-x, y)]\phi\overline{\varphi}_o d\mathbf{r} = 0. \quad (24)$$

If ϕ is odd in x, we swap φ_e and φ_o in Eqs. (23) and (24). If F does not satisfy Eq. (23) or (24), then the perturbation process fails in the first step. If F satisfies these two conditions, it may be possible to find ϕ_1 that decays to zero as $|x| \to \infty$, but the perturbation method can still fail in the second step. In order to obtain real β_2 and k_2, F must satisfy additional conditions that involve ϕ_1. It is clear that in order to to carry out the perturbation process to all steps, F must satisfy an infinite sequence of conditions. Therefore, if F does not satisfy Eq. (21), the perturbation process is likely to fail. When this happens, we believe there is no BIC near the original one of the unperturbed structure.

The perturbation process also requires a non-singular matrix $\mathbf{A}$. This condition is independent of the perturbation profile F, since $\mathbf{A}$ involves only the BIC ϕ and the diffraction solutions φ_e or φ_o. If $\mathbf{A}$ is singular, we expect that at least for some symmetry-preserving perturbations, the BIC will fail to exist. In general, when the structure is continuously varied while the required symmetry is preserved, a BIC may cease to exist. As shown in Ref. [18], this could happen when the frequency and wavenumber of the BIC have reached the condition for the opening of the second diffraction channel, or when the the BIC becomes a symmetric standing wave which is even in y. For a symmetric standing wave, we have $a_{11} = a_{21} = 0$, thus $\det\mathbf{A} = 0$. If the BIC approaches the opening of second diffraction channel ($k = 2\pi/L - |\beta|$), usually it becomes more and more extended, and the entries of $\mathbf{A}$ tend to infinity.

To validate the perturbation result, we consider a periodic array of dielectric rods on which various BICs exist [7, 13, 18]. In particular, if the radius of the rods is $0.35L$, there is a family of x-even BICs for $3.711 < \epsilon_1 \leq 15.701$, where ϵ_1 is the dielectric constant of the rods. The free-space wavenumber k and Bloch wavenumber β of the BICs are shown as functions of ϵ_1 in Figs. 1(b) and 1(c). Notice that for $\epsilon_1 = 15.701$, the BIC becomes a symmetric standing wave (even in y). The perturbation theory is applicable, if we let $F(x, y) = 1$ for (x, y) in the rods and $F(x, y) = 0$ otherwise, and in that case, β_1 and k_1 in the first order perturbation are simply the derivatives of β and k with respect to ϵ_1. In Fig. 2, we show the perturbation results k_1 and β_1 for different values of ϵ_1, and compare them with finite difference approximations for $dk/d\epsilon_1$ and $d\beta/d\epsilon_1$. The excellent agreement in Fig. 2 indicates that our perturbation theory is correct. As ϵ_1 tends to 15.701, β_1 or $d\beta/d\epsilon_1$ becomes negative infinity. In fact, $\mathbf{A}$ is singular for $\epsilon_1 = 15.701$. As $\epsilon_1 \to 3.711$,

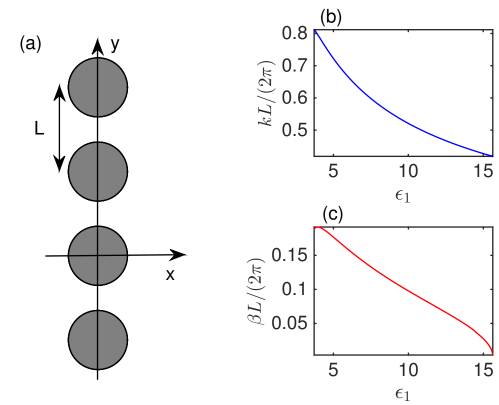

Fig. 1. (a) A periodic array of circular dielectric rods with radius $0.35L$ and dielectric constant ϵ_1. (b) Free-space wavenumber k as a function of ϵ_1 for a family of x-even BICs on the periodic array. (c) Bloch wavenumber β as a function of ϵ_1 for the same BIC family.

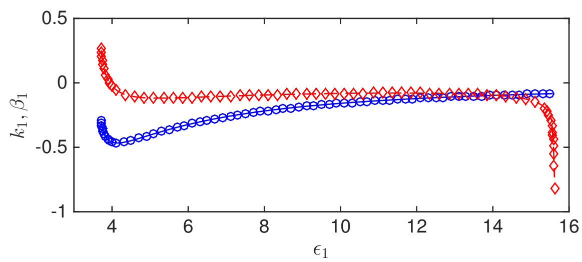

Fig. 2. First order perturbation results k_1 (shown as "$\circ$") and β_1 (shown as "$\diamond$") of a BIC family for different values of ϵ_1, and finite difference approximations of $dk/d\epsilon_1$ (solid blue line) and $d\beta/d\epsilon_1$ (red dashed line), all in unit $1/L$.

the BIC ceases to exist because k and β approach the condition $k = 2\pi/L - \beta$, that corresponds to the opening of the second diffraction channel. In this limit, the entries of $\mathbf{A}$ tend to infinity, but β_1 and k_1 approach constants.

In summary, a perturbation theory is developed for BICs on general 2D periodic structures with reflection symmetry in both x and y directions, and it shows that the propagating BICs are robust with respect to structural perturbations that preserve the reflection symmetry. The importance of symmetry for propagating BICs on periodic structures was first realized by Hsu *et al.* [11, 12], and the existence and robustness of these BICs have been investigated numerically for particular periodic structures involving a few parameters [36, 37]. Our perturbation theory is analytic, and it is applicable to general 2D periodic structures and general perturbations. Our perturbation results could also be useful for sensitivity analysis and optimal design of periodic structures. In this work, we have concentrated on the 2D case for simplicity. Clearly, it is worthwhile to extend the perturbation theory to three-dimensional (3D) rotationally symmetric structures with one periodic direction, or 3D structures with two periodic directions.

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