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A perturbation approach for near bound-state resonances of photonic crystal with defect

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This paper is concerned with scattering resonances of a 1D photonic crystal of finite extent. We propose a general perturbation approach to study the resonances that are close to the bound-state frequency of the infinite structure when some defect is embedded in the interior. It is shown that near bound-state resonances exist on the complex plane and the distance between the resonance and the associated bound-state frequency decays exponentially as a function of the number of periodic cells. A numerical approach based upon the perturbation theory is also proposed to calculate the near bound-state resonances accurately.

Key words: photonic crystal, scattering resonances, Helmholtz equation.

1 Introduction

The design of photonic crystals with high quality factors (low radiative leakage) has been extensively investigated in recent years, due to its potentially significant applications in areas of electron–photon interactions, nonlinear optics and quantum information processing [11, 17, 21]. The photonic crystals are periodic dielectric materials, and the ability to achieve low radiative leakage is usually achieved through the introduction of defects for the periodic structure. We refer the readers to [1,8,9,24] and references therein for both the experimental and numerical design of photonic structures of high quality factor that use such configurations.

In this paper, we consider the one-dimensional structure, which is essentially a layered dielectric medium as shown in Figure 1. The photonic crystal is homogeneous on the yz plane. It consists of periodic cells and some defect in the interior along the x direction. Let us denote the defect region $(0, D)$ by I_D and the length of each period cell by L. The defect medium may be inhomogeneous, whereas it is assumed that each period cell outside the defect region consists of two constant layers with length L_1 and L_2 respectively. Consider a TM polarized electromagnetic wave that propagates perpendicular to the layers (yz plane), and the magnetic field $\mathbf{H} = (0, 0, u)$. Then, the Maxwell equations that model the electromagnetic wave propagation are reduced to the following scalar wave equation for u:

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} - \frac{\partial}{\partial x}\left(\frac{1}{\varepsilon}\frac{\partial u}{\partial x}\right) = 0, \tag{1.1}$$

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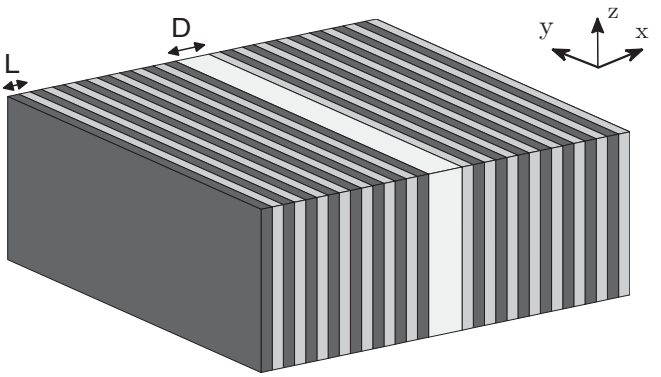

FIGURE 1. One-dimensional photonic crystal with a defect embedded in the interior. The medium is homogeneous in y and z directions. The defect region is denoted by $I_D := (0, D)$, and each period cell has a length of L.

where c is the wave speed. The relative permittivity ε is a positive function, and is given as follows inside the photonic structure:

$$\begin{aligned}
&\varepsilon(x) = \varepsilon_d(x), \quad x \in I_D \quad \text{(defect)};\\
&\varepsilon(x) = \varepsilon_p(x + nL), \quad x \in (-nL, -(n-1)L), \quad n = 1, 2, 3, \ldots N_l;\\
&\varepsilon(x) = \varepsilon_p(x - D - nL), \quad x \in (D + nL, D + (n+1)L), \quad n = 0, 2, 3, \ldots N_r - 1;
\end{aligned}$$

Here, N_l and N_r are the number of periods on each side, $\varepsilon_d(x) \in C^1(I_D)$, and ε_p is the relative permittivity inside each period defined by

$$\begin{aligned}
&\varepsilon_p(x) = \varepsilon_1 \quad x \in (0, L_1);\\
&\varepsilon_p(x) = \varepsilon_2 \quad x \in (L_1, L).
\end{aligned}$$

For brevity, let us denote $a = -N_l L$ and $b = D + N_r L$ as the boundaries of the photonic structure. The region (a, b) is also known as the photonic cavity. It is assumed that the photonic structure is placed in the vacuum so that the relative permittivity $\varepsilon = 1$ outside the region (a, b).

By assuming a time harmonic magnetic field $u(x, t) = \psi(x)e^{-i\omega t}$ for the wave equation, the scattering resonances are cast as solutions of the following eigenvalue problem:

$$\begin{cases}
-\dfrac{d}{dx}\left(\dfrac{1}{\varepsilon}\dfrac{d\psi}{dx}\right) = k^2\psi, \quad a < x < b,\\
\dfrac{1}{\varepsilon(a)}\dfrac{d\psi}{dx}(a) + ik\psi(a) = 0, \quad \dfrac{1}{\varepsilon(b)}\dfrac{d\psi}{dx}(b) - ik\psi(b) = 0,
\end{cases} \tag{1.2}$$

where $\omega = ck$. At each interface between two layers, the differential equation is interpreted in the sense that both the magnetic field ψ and the electric field $\frac{1}{i\omega\varepsilon}\frac{d\psi}{dx}$ are continuous across the interface. Outgoing radiation conditions are imposed on the boundaries by noting the fact that an outgoing wave takes the form $\psi = A^+e^{ikx}$ when $x > b$ ($\psi = A^-e^{-ikx}$ when $x < a$ respectively), and the continuity of the electromagnetic fields at $x = b$ ($x = a$ respectively). The eigenvalue problem (1.2) attains a sequence of complex resonances

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k_j with the imaginary part $\mathrm{Im}k_j < 0$ (see the Appendix), and the corresponding quasi-modes $\psi_j(x)$ are locally integrable.

In general, the electromagnetic energy leaks from photonic cavity (a, b) as time evolves, due to scattering or radiation loss to the surrounding medium. Such energy leakage is closely related to scattering resonances associated with the cavity as defined in (1.2). More precisely, the solution of the wave equation (1.1) can be approximated by the modes $e^{-ick_jt}\psi_j(x)$ in a manner that, for any $K > 0$,

$$\left\| u(\cdot, t) - \sum_{\mathrm{Im}k_j > -K} c_j e^{-ick_jt}\psi_j \right\|_{L^2(a,b)} = O(e^{-K(1+\delta)t}), \quad \text{for } t \geqslant \tau, \tag{1.3}$$

where $\delta(a, b, K)$, $\tau(a, b, K)$ are some positive constants and c_j are some complex coefficients. We refer the reader to [22] for more details of such an approximation. As indicated by (1.3), intuitively the imaginary part of resonances $\mathrm{Im}k_j$ determines the rate of the energy leakage. Thus, it is imperative to investigate the resonances so as to understand the radiation loss of the photonic cavity, and to develop efficient numerical methods to obtain those resonances accurately.

As the number of periodic cells becomes large, two types of complex resonances emerge for the photonic structure in the lower half plane:

(i) A set of discrete resonances in the neighbourhood of each eigenvalue (bound-state frequency) for the infinite layered structure. The eigenvalues, which are induced by the presence of the defect, are located in the band gaps of the continuous spectrum. Such resonances are referred to as near bound-state resonances, and as to be shown later in this paper, they converge exponentially fast to the associated eigenvalues.

(ii) A family of discrete resonances that lies underneath the continuous spectrum of the infinite structure. As N increases, such resonances become increasingly clustered and converge toward each closed interval of the continuous spectrum with a much slower rate [14, 15].

We would like to mention a closely related problem, in which the scattering resonances are defined as the complex eigenvalues of the Schrödinger operator with a potential barrier [23]. Two classes of resonances also arise in the lower complex plane when the potential is a low-energy well surrounded by a thick barrier, wherein a finite number of low-frequency resonances converge exponentially fast to the real eigenvalues and an infinite family of discrete scattering resonances approaches the continuous spectrum as the thickness of the barrier increases [3, 16, 23].

The goal of this paper is to develop a general perturbation theory to study the near bound-state resonances of the photonic structure. We show that for each non-degenerate bound-state frequency k_b belonging to the point spectrum σ_p, there exists some resonance k close to k_b. In addition, the distance $|k - k_b|$ decays exponentially as a function of the number of periodic cells. This implies that the negative imaginary part is exponentially small, and according to (1.3), the radiation loss for the associated photonic structure is small. A similar decay rate for near bound-state resonances has also been investigated in [15] for a symmetric structure with $\varepsilon(x) = \varepsilon(-x)$ and a constant defect layer. It should

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be pointed out that for the symmetric case, one has initial conditions that can be exploited and the eigenvalue problem (1.2) can be reduced to an initial value problem. In addition, the defect is assumed to be a constant layer such that an explicit expression for the wave fields at the edges of defect become possible [15]. No such equivalent conditions are available for a general asymmetric structure and inhomogeneous defects. Instead, a boundary value problem has to be investigated. As such, in order to analyse near bound-state resonances, we have to devise an entirely different approach. A key ingredient of the new approach is to reformulate the bound-state and scattering resonance problems over the defect region by introducing suitable boundary conditions, and obtain an equivalent *resonance condition* by examining the associated boundary value problem for the difference between the bound state and the quasi-mode. The study of resonances for the photonic crystal is then based upon the perturbation analysis of the nonlinear resonance condition. The idea of obtaining the resonance condition is suggested by our recent studies on the Schrödinger operator [16]. Very interestingly, the perturbation analysis also suggests a natural non-iterative numerical scheme to calculate the near bound-state resonances accurately. This is also discussed at the end of the paper. Finally, we would like to point out [18], in which the calculation is also presented for resonances of the structure considered in this paper.

The rest of the paper is organized as follow. Section 2 introduces the propagation matrix method, which converts solving the wave equation over the periodic structures to a matrix recurrence equation on the boundaries of dielectric layers. The spectrum for the structure with infinite periodic cells is briefly reviewed in Section 3, followed by the statement of the main theorem for near bound-state resonances. We derive the resonance condition in Section 4 in an innovative way through the solvability condition in elliptic theory, and give the proof of the main theorem in Section 5. A numerical perturbation approach is presented in Section 6 to calculate the near bound-state resonance accurately, and the paper is concluded with a general discussion.

2 Preliminaries

In this section, we introduce the propagation matrix briefly and collect some useful results to be used in later sections. The readers are referred to [15] for the details of the proof. Let us introduce the vector wave function

$$\Psi(x;k) = \begin{bmatrix} \psi(x;k) \\ \dfrac{1}{\varepsilon(x)}\dfrac{d\psi(x;k)}{dx} \end{bmatrix}, \tag{2.1}$$

where $\psi(x;k)$ is the solution of the ordinary differential equation (ODE):

$$\frac{d}{dx}\left(\frac{1}{\varepsilon}\frac{d\psi}{dx}\right) + k^2\psi = 0. \tag{2.2}$$

Then, the propagation of the wave field over each layer with constant permittivity ε can be expressed as

$$\Psi(x;k) = P(x - x_0;\varepsilon,k)\Psi(x_0;k) \quad \text{for } x > x_0,$$

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where the propagation matrix is

$$P(l;\varepsilon,k)=\begin{bmatrix}\cos(k\sqrt{\varepsilon}\,l) & \frac{\sqrt{\varepsilon}}{k}\sin(k\sqrt{\varepsilon}\,l)\\ -\frac{k}{\sqrt{\varepsilon}}\sin(k\sqrt{\varepsilon}\,l) & \cos(k\sqrt{\varepsilon}\,l)\end{bmatrix}. \tag{2.3}$$

Here, l denotes the propagation distance. It is well known that P is related to the fundamental matrix of the ODE defined in (2.2). In addition, $P(l;\varepsilon,k)$ is unimodular in the sense that $\det(P(l;\varepsilon,k))\equiv 1$. In this way, the propagation matrix $P_L(k)$ for each period cell of the photonic crystal is the product of the associated propagation matrix over each constant layer, and is given by

$$P_L(k)=P(L_2;\varepsilon_2,k)P(L_1;\varepsilon_1,k). \tag{2.4}$$

First, we have the following lemma for P_L', the derivative of P_L with respect to k.

Lemma ([15]) *Let Ψ_0 be a vector in $\mathbb{C}^2$, $k\in\mathbb{C}\backslash\{0\}$, then*

$$P_L'(k)\Psi_0=P_L(k)\int_0^L P^{-1}(x;k)O(k)P(x;k)\Psi_0 dx, \tag{2.5}$$

where

$$O(k)=\begin{bmatrix}0 & 0\\ -2k & 0\end{bmatrix}, \tag{2.6}$$

and $P(x;k)$ is the propagation matrix inside one period cell given by

$$P(x;k)=\begin{cases}P(x;\varepsilon_1,k), & x\in[0,L_1];\\ P(x-L_1;\varepsilon_2,k)P(L_1;\varepsilon_1,k), & x\in[L_1,L].\end{cases} \tag{2.7}$$

Let $k_0\in\mathbb{C}\backslash\{0\}$ be such that $P_L(k_0)$ has two distinct eigenvalues $\lambda_1(k_0)$ and $\lambda_2(k_0)$. Then the two eigenvalues $\lambda_1(k)$ and $\lambda_2(k)$ are analytic functions in the neighbourhood of k_0 [10, 12, 15]. The corresponding eigenvectors for the two distinct eigenvalues $\lambda_1(k)$ and $\lambda_2(k)$ can be expressed explicitly. Indeed, let us denote each entry of the matrix $P_L(k)$ by p_{ij}^L, and define V_1, V_2, U_1 and U_2 as follows:

$$V_1(k)=\begin{bmatrix}p_{21}^L(k)\\ \lambda_1(k)-p_{11}^L(k)\end{bmatrix},\qquad V_2(k)=\begin{bmatrix}p_{21}^L(k)\\ \lambda_2(k)-p_{11}^L(k)\end{bmatrix}; \tag{2.8}$$

and

$$U_1(k)=\begin{bmatrix}\lambda_1(k)-p_{22}^L(k)\\ p_{21}^L(k)\end{bmatrix},\qquad U_2(k)=\begin{bmatrix}\lambda_2(k)-p_{22}^L(k)\\ p_{21}^L(k)\end{bmatrix}. \tag{2.9}$$

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Then, it can be shown that the above vectors are the left and right eigenvectors of $P_L(k)$ respectively such that

$$V_1^T P_L = \lambda_1 V_1^T, \qquad V_2^T P_L = \lambda_2 V_2^T;$$
$$P_L U_1 = \lambda_1 U_1, \qquad P_L U_2 = \lambda_2 U_2.$$

For brevity, here and henceforth, we adopt the notation below to denote entries of the eigenvectors U_1 and U_2:

$$u_{11} = \lambda_1(k) - p_{22}^L(k), \quad u_{21} = p_{21}^L(k); \tag{2.10}$$
$$u_{12} = \lambda_2(k) - p_{22}^L(k), \quad u_{22} = p_{21}^L(k). \tag{2.11}$$

We also normalize the left eigenvectors by letting

$$\overline{V}_1(k) = \frac{1}{p_{21}^L(2\lambda_1 - (p_{11}^L + p_{22}^L))} V_1(k), \quad \text{and} \quad \overline{V}_2(k) = \frac{1}{p_{21}^L(2\lambda_2 - (p_{11}^L + p_{22}^L))} V_2(k). \tag{2.12}$$

Then, it follows that $\overline{V}_i^T(k) U_j(k) = \delta_{ij}$.

It is clear that the eigenvectors $V_1(k)$, $V_2(k)$, $U_1(k)$, and $U_2(k)$ are also analytic in the neighbourhood of k_0 since $\lambda_1(k)$, $\lambda_2(k)$ and $p_{ij}^L(k)$ are analytic. Furthermore, the sensitivity of the right eigenvectors on the parameter k may be characterized in the following Lemma. We refer to [15] for its proof (Lemma 2.2).

Lemma *Let $k \in \mathbb{C}\backslash\{0\}$ such that $\lambda_1(k)$ and $\lambda_2(k)$ are two distinct eigenvalues of $P_L(k)$. The corresponding left and right eigenvectors $\overline{V}_1(k)$, $\overline{V}_2(k)$, $U_1(k)$, $U_2(k)$ are defined by (2.12) and (2.9) respectively. Define the matrix $U(k) = [U_1(k), U_2(k)]$, then the derivative $U'(k)$ exists. Furthermore, there exists a 2×2 complex matrix $Q(k)$ such that $U'(k) = U(k)Q(k)$, where the off-diagonal entries of $Q(k)$ are*

$$q_{ij}(k) = \frac{1}{\lambda_j - \lambda_i} \overline{V}_i^T(k) P_L'(k) U_j(k) \qquad i \neq j, \quad i, j = 1, 2.$$

We end this section with an auxiliary lemma, which is useful for the proof of the main theorem in Section 5.

Lemma *Let $O(k)$ and $P(x;k)$ be the matrices given by (2.6) and (2.7) respectively, and $V_2(k)$ and $U_1(k)$ be the left and right eigenvectors of $P_L(k)$ defined in (2.8)–(2.9). If k is a real positive number, then*

$$\int_0^L V_2^T(k) P^{-1}(x;k) O(k) P(x;k) U_1(k)\, dx > 0.$$

Proof. First it is observed that $V_2 = RU_1$, where

$$R = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}.$$

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Therefore, the integral

$$\int_0^L V_2^T(k)P^{-1}(x;k)O(k)P(x;k)U_1(k)\,dx = \int_0^L U_1^T\ [\ R^T P^{-1}(x;k)O(k)P(x;k)\ ]\ U_1\,dx.$$

For each $x \in [0, L]$, let us denote the entry of the propagation matrix $P(x;k)$ by $p_{ij}(x;k)$. Using the fact that $\det(P(x;k)) \equiv 1$, then $P^{-1}(x;k)$ can be expressed explicitly as

$$P^{-1}(x;k_b) = \begin{bmatrix} p_{22}(x;k) & -p_{12}(x;k) \\ -p_{21}(x;k) & p_{11}(x;k) \end{bmatrix},$$

and a direct calculation yields

$$R^T P^{-1}(x;k)O(k)P(x;k) = 2k \begin{bmatrix} p_{11}^2(x;k) & p_{11}(x;k)p_{12}(x;k) \\ p_{11}(x;k)p_{12}(x;k) & p_{12}^2(x;k) \end{bmatrix}.$$

Let $A(x;k) = R^T P^{-1}(x;k)O(k)P(x;k)$. Then from the above formula, it is seen that $A(x;k)$ is a semi-positive definite matrix such that

$$U_1^T\ A(x;k)\ U_1 \geqslant 0 \qquad \forall x \in [0, L].$$

Furthermore

$$U_1^T\ A(x;k)\ U_1 = 0 \quad \text{if and only if} \quad U_1 \cdot \tilde{\zeta}(x;k) = 0,$$

wherein the vector $\zeta(x;k) = [p_{11}(x;k), p_{12}(x;k)]^T$.

The direction of the non-zero vector $\zeta(x;k)$ is not constant inside the interval $[0, L_1]$, while U_1 is independent of x. Hence, there exists at least one point $x_0 \in [0, L_1]$ such that $U_1 \cdot \tilde{\zeta}(x_0;k) \neq 0$, and $U_1^T\ A(x_0;k)\ U_1 > 0$. Consequently

$$\int_0^L U_1^T\ A(x;k)\ U_1\,dx > 0.$$

follows by the continuity of the matrix $A(x;k)$. □

3 Near bound-state resonances

In this section, we state the main theorem for the resonances of (1.2) that are close to the bound-state frequency of the infinite structure, or so-called near bound-state resonances. To this end, we first recall the spectrum of the photonic structure with infinite period cells on each side of the defect in Section 3.1.

3.1 Spectrum of the photonic structure with infinite periods

If $N_l = N_r = +\infty$, the associated eigenvalue problem becomes

$$-\frac{d}{dx}\left(\frac{1}{\varepsilon_\infty}\frac{d\psi}{dx}\right) = k^2\psi, \quad -\infty < x < \infty, \tag{3.1}$$

where ε_∞ is the relative permittivity for the infinite structure with the defect. Let us denote the associated operator in (3.1) by H_∞. Then H_∞ is an unbounded self-adjoint operator in $L^2(\mathbb{R})$, and its spectrum consists of a set of continuous spectrum and a point spectrum

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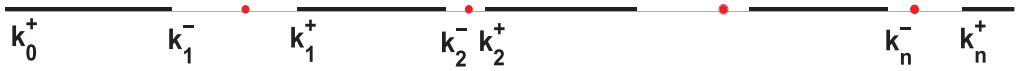

FIGURE 2. Spectrum of H_∞.

on the real line as shown in Figure 2. In the following, we discuss briefly the spectrum of H_∞ and its relation to eigenvalues of the propagation matrix $P_L(k)$. The readers are referred to [4, 15] for more details.

The continuous spectrum $\sigma_c = \cup_{n=1}^{\infty}[k_{n-1}^+, k_n^-]$, where $k_{n-1}^+ < k_n^- < k_n^+$, and each subset $[k_{n-1}^+, k_n^-]$ is separated by the band gap (k_n^-, k_n^+) (cf. Figure 2). The continuous spectrum σ_c coincides with the entire spectrum of the same periodic structure without the defect. This follows from the stability of essential spectrum by the Weyl's Theorem [5, 19]. The point spectrum $\sigma_p = \cup_{j=1} k_{b_j}$ is induced by the defect inside the photonic structure. It has been shown that as long as the defect is large enough, eigenvalues with finite multiplicity exist [5, 6]. The point spectrum consists of a set of discrete numbers with each eigenvalue k_{b_j} located in some band gap (k_n^-, k_n^+). The associated eigenmode is a localized function that decays exponentially away from the defect. For this reason, the eigenmode is usually called a bound state, and we call the associated eigenvalue k_{b_j} the bound-state frequency.

As illustrated by the following theorem, the spectrum of H_∞ is closely related to the eigenvalues of the propagation matrix $P_L(k)$ defined in (2.4).

Theorem 3.1 *Let $\lambda_1(k)$ and $\lambda_2(k)$ be the eigenvalues of $P_L(k)$.*

(i) *If $k \in \sigma_c$, then $\lambda_1(k)$ and $\lambda_2(k)$ are conjugate pairs with $|\lambda_1(k)| = |\lambda_2(k)| = 1$.*

(ii) *If $k \in \sigma_p$ and the associated eigenmode decays exponentially away from the defect, then*

  (a) $|\lambda_1(k)| > 1 > |\lambda_2(k)|$;

  (b) $\Psi(0;k) \parallel U_1(k)$ *and* $\Psi(D;k) \parallel U_2(k)$, *wherein* $\Psi(0;k)$ *and* $\Psi(D;k)$ *are the wavefields at the edges of the defect layer.*

We refer the readers to Section 3 of [4] and [15] for a detailed justification of the above theorem.

3.2 Estimate of near bound-state resonances

As demonstrated in the Appendix, all resonances of (1.2) lie in the lower half complex plane. Here, we are interested in those that are close to the bound-state frequency of the infinite structure. The main result regarding the near bound-state resonances is stated as follows:

Theorem 3.2 *Let $N = \min\{N_l, N_r\}$. Assume that $k_b \in \sigma_p$ is a bound-state frequency for the infinite structure with multiplicity one, then there exists an integer N_0 such that if $N \geqslant N_0$, there is a resonance k of (1.2) such that*

$$|k - k_b| \leqslant C(\varepsilon, k_b) e^{-\mu(\varepsilon, k_b)N}.$$

Here, $C(\varepsilon, k_b)$ and $\mu(\varepsilon, k_b)$ are positive constants independent of N.

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Table 1. *Near bound-state resonances (first column), and the difference between resonances and the bound-state frequency for different number of periodic cells (second column)*

N	k	$k-k_b$
2	$0.5852454436-0.0183888293i$	$-1.290\times10^{-2}-1.839\times10^{-2}i$
4	$0.5960350399-0.0030827089i$	$-2.108\times10^{-3}-3.083\times10^{-3}i$
8	$0.5980658187-0.0001120105i$	$-7.747\times10^{-5}-1.120\times10^{-4}i$
16	$0.5981431787-0.0000001626i$	$-1.126\times10^{-7}-1.626\times10^{-7}i$

To validate the conclusion of Theorem 3.2, let us consider a photonic structure with the size of the defect $D = 6$. The length of two layers in one period cell is $L_1 = 2$ and $L_2 = 1$ respectively. The relative permittivity of each layer inside one period is given by $\varepsilon_1 = 4$ and $\varepsilon_2 = 1$. We also assume that the defect is a constant layer with $\varepsilon_D = 2$.

The smallest bound-state frequency in the point spectrum can be calculated by the Newton's method and its value $k_b = 0.598143291317602$. Let $N_l = N_r = N$, then the resonance near k_b is given in Table 1 for the considered photonic structure with different number of periods. It is seen that the difference between k and k_b decays exponentially as a function of N.

4 Resonance condition

To prove Theorem 3.2, we first establish a nonlinear equation for the scattering resonances of (1.2) (*resonance condition*) in this section. As it can be seen in the following, this is accomplished by examining the associated boundary value problem for the difference between the bound state and the quasi-mode, and obtained through the solvability condition in elliptic theory. To this end, the bound-state problem (3.1) and the scattering resonance problem (1.2) are reformulated over the defect region by introducing suitable boundary conditions at the edges of the defect (Section 4.1). We point out that it is essential to choose the domain for the boundary value problem to be the defect region so as to obtain the desired estimates for the near bound-state resonances. In what follows, for brevity we denote the differential operator $-\frac{d}{dx}(\frac{1}{\varepsilon_d(x)}\frac{d}{dx})$ by $\mathscr{L}$.

4.1 Boundary value problems in the defect region

Let k_b be a non-degenerate bound-state frequency, and ψ_b be the corresponding eigenfunction. By virtue of Theorem 3.1, we have two distinct eigenvalues of $P_L(k_b)$ with $|\lambda_1(k_b)| > 1 > |\lambda_2(k_b)|$. Let $U_1(k_b)$ and $U_2(k_b)$ be the corresponding eigenvectors of $P_L(k_b)$ given by (2.9). Then the wave fields at boundaries of the defect region are parallel to the eigenvectors in a manner that $\Psi(0;k_b) \parallel U_1(k_b)$ and $\Psi(D;k_b) \parallel U_2(k_b)$. This implies the boundary conditions

$$\frac{1}{\varepsilon_d(0)}\frac{d\psi_b}{dx}(0)-\beta_0\psi_b(0)=0, \quad \text{and} \quad \frac{1}{\varepsilon_d(D)}\frac{d\psi_b}{dx}(D)-\beta_D\psi_b(D)=0.$$

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Here, we adopt the notation given in (2.10), and define β_0 and β_D as

$$\beta_0 = \frac{u_{21}(k_b)}{u_{11}(k_b)}, \quad \text{and} \quad \beta_D = \frac{u_{22}(k_b)}{u_{12}(k_b)}. \tag{4.1}$$

Using the boundary conditions at $x = 0$ and $x = D$, the bound-state problem (3.1) can be reformulated in the defect region as

$$\begin{cases} \mathscr{L}\,\psi_b = k_b^2 \psi_b \quad \text{in } I_D, \\ \dfrac{1}{\varepsilon_d(0)}\dfrac{d\psi_b}{dx}(0) - \beta_0 \psi_b(0) = 0, \quad \dfrac{1}{\varepsilon_d(D)}\dfrac{d\psi_b}{dx}(D) - \beta_D \psi_b(D) = 0. \end{cases} \tag{4.2}$$

It is clear that (4.2) is self-adjoint since β_0 and β_D are real numbers.

For the resonance problem (1.2), by expanding $\Psi(D;k)$ in the neighbourhood of k_b as

$$\Psi(D;k) = c_1 U_1(k) + c_2 U_2(k),$$

for some coefficients c_1 and c_2, the wave vector $\Psi(b;k)$ at the right boundary of the photonic structure ($x = b$) becomes

$$\Psi(b;k) = c_1 \lambda_1^{N_r} U_1(k) + c_2 \lambda_2^{N_r} U_2(k).$$

On the other hand, note that

$$\psi = A^+ e^{ikx} \quad \text{for} \quad x > b.$$

Imposing the continuity conditions over $x = D$ and $x = b$ leads to the boundary condition

$$\frac{1}{\varepsilon_d(D)}\frac{d\psi}{dx}(D) - \alpha_D(k)\psi(D) = 0, \tag{4.3}$$

where the coefficient

$$\alpha_D(k) = \frac{\lambda_2^{N_r}(k)(u_{22}(k) - iku_{12}(k))u_{21}(k) + \lambda_1^{N_r}(k)(iku_{11}(k) - u_{21}(k))u_{22}(k)}{\lambda_2^{N_r}(k)(u_{22}(k) - iku_{12}(k))u_{11}(k) + \lambda_1^{N_r}(k)(iku_{11}(k) - u_{21}(k))u_{12}(k)}. \tag{4.4}$$

Again the notation in (2.10) is used above. Similarly, for $x = a$, by imposing the continuity conditions over $x = 0$ and $x = a$, it can be obtained that

$$\frac{1}{\varepsilon_d(0)}\frac{d\psi}{dx}(0) - \alpha_0(k)\psi(0) = 0, \tag{4.5}$$

where the coefficient

$$\alpha_0(k) = \frac{\lambda_1^{N_l}(k)(u_{22}(k) + iku_{12}(k))u_{21}(k) - \lambda_2^{N_l}(k)(u_{21}(k) + iku_{11}(k))u_{22}(k)}{\lambda_1^{N_l}(k)(u_{22}(k) + iku_{12}(k))u_{11}(k) - \lambda_2^{N_l}(k)(u_{21}(k) + iku_{11}(k))u_{12}(k)}. \tag{4.6}$$

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Now by using (4.3) and (4.5), the resonance problem (1.2) can be recast as the following boundary value problem:

$$\begin{cases} \mathscr{L}\,\psi = k^2\psi \quad \text{in } I_D, \\ \dfrac{1}{\varepsilon_d(0)}\dfrac{d\psi}{dx}(0) - \alpha_0(k)\psi(0) = 0, \quad \dfrac{1}{\varepsilon_d(D)}\dfrac{d\psi}{dx}(D) - \alpha_D(k)\psi(D) = 0. \end{cases} \tag{4.7}$$

4.2 Resonance condition

Let k_b be a non-degenerate bound-state frequency of (4.2), and ψ_b be the corresponding eigenfunction. Let (k, ψ) be a resonance pair of (4.7) such that k is a scattering resonance and ψ is the associated quasi-mode. We define the difference $\xi = \psi - \psi_b$. By a direct comparison of (4.2) and (4.7), it is observed that ξ is a solution of following boundary value problem:

$$\begin{cases} \mathscr{L}\,\xi - k_b^2\xi = (k^2 - k_b^2)\psi \quad \text{in } I_D, \\ \dfrac{1}{\varepsilon_d(0)}\dfrac{d\xi}{dx}(0) - \beta_0\xi(0) = \gamma_0(k)\psi(0), \quad \dfrac{1}{\varepsilon_d(D)}\dfrac{d\xi}{dx}(D) - \beta_D\xi_b(D) = \gamma_D(k)\psi(D). \end{cases} \tag{4.8}$$

It is clear that the coefficients $\gamma_0(k)$ and $\gamma_D(k)$ above are given respectively by

$$\gamma_0(k) = \alpha_0(k) - \beta_0 \quad \text{and} \quad \gamma_D(k) = \alpha_D(k) - \beta_D. \tag{4.9}$$

Note that the corresponding homogeneous (self-adjoint) problem coincides with the boundary value problem for the bound state as stated in (4.2). Since k_b is a non-degenerate bound-state frequency, it follows that the solution space $\mathscr{N}$ for the homogeneous problem is given by $\text{span}\{\psi_b\}$.

Let us denote the standard inner product $\displaystyle\int_0^D \xi(x)\overline{\eta(x)}dx$ on $L^2(I_D)$ by (ξ, η). Then, ξ solves the variational problem

$$a(\xi, \eta) = b(\eta) \qquad \forall \eta \in H^1(I_D),$$

where the bilinear form

$$a(\xi, \eta) = \left(\frac{1}{\varepsilon_d}\xi', \eta'\right) - k_b^2(\xi, \eta) + \beta_0\xi(0)\overline{\eta(0)} - \beta_D\xi(D)\overline{\eta(D)},$$

and the linear functional

$$b(\eta) = (k^2 - k_b^2)(\psi, \eta) - \gamma_0(k)\psi(0)\overline{\eta(0)} + \gamma_D(k)\psi(D)\overline{\eta(D)}.$$

Since k_b has multiplicity one, following the standard argument for second order elliptic equations, the solvability condition for the boundary value problem (4.8) reads:

$$(k^2 - k_b^2)(\psi, \psi_b) - \gamma_0(k)\psi(0)\overline{\psi_b(0)} + \gamma_D(k)\psi(D)\overline{\psi_b(D)} = 0. \tag{4.10}$$

The nonlinear equation (4.10) is referred to as the *resonance condition*. We give its derivation briefly and introduce notation to be used in the proof of the main theorem.

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Let us choose a suitable function $\rho(x,k) \in H^2(I_D)$ such that

$$\frac{1}{\varepsilon_d(0)}\frac{d\rho}{dx}(0,k) - \beta_0\rho(0,k) = \gamma_0(k)\psi(0), \quad \frac{1}{\varepsilon_d(D)}\frac{d\rho}{dx}(D,k) - \beta_D\rho(D,k) = \gamma_D(k)\psi(D), \quad (4.11)$$

and

$$||\rho(\cdot,k)||_{H^2(I_D)} \leqslant C\left(|\psi(0)| + |\psi(D)|\right) \leqslant C||\psi||_{H^1(D)}.$$

By setting $\zeta = \xi - \rho$, (4.8) is reduced into the following boundary value problem:

$$\begin{cases} \mathscr{L}\,\zeta = (k^2 - k_b^2)\psi + \phi \quad \text{in } I_D, \\ \dfrac{1}{\varepsilon_d(0)}\dfrac{d\zeta}{dx}(0) - \beta_0\zeta(0) = 0, \quad \dfrac{1}{\varepsilon_d(D)}\dfrac{d\zeta}{dx}(D) - \beta_D\zeta(D) = 0, \end{cases} \quad (4.12)$$

wherein $\phi = -\mathscr{L}\rho$ and $||\phi||_{L^2(I_D)} \leqslant C||\psi||_{H^1(D)}$. Let

$$r(x;k) = (k^2 - k_b^2)\psi + \phi. \quad (4.13)$$

From the Lax–Milgram theorem, it is known that the variational problem $a(\zeta,\eta)+v(\zeta,\eta) = (r,\eta)$ has a unique solution in $H^1(I_D)$ for some sufficiently large constant v. Hence the induced operator $K_v^{-1} : r \to \zeta$ is bounded from $L^2(I_D)$ to $H^1(I_D)$, and compact from $L^2(I_D)$ to $L^2(I_D)$. Therefore, ζ is a weak solution of (4.12) if and only if

$$\zeta - vK_v^{-1}\zeta = K_v^{-1}r. \quad (4.14)$$

The solution of the corresponding homogeneous (self-adjoint) problem (4.2) satisfies

$$\psi_b - vK_v^{-1}\psi_b = 0. \quad (4.15)$$

Employing the Fredholm alternative and integrations-by-parts, we arrive at (4.10).

Remark *For clarity, here we may set $\rho(x,k)$ to be the solution of the elliptic equation $-\frac{d}{dx}(\frac{1}{\varepsilon_d}\frac{d\rho}{dx}) + v_0\rho = 0$ with the boundary condition (4.11), where v_0 is a sufficiently large constant. Define the vector $\boldsymbol{\gamma}(k) = [\gamma_0(k), \gamma_D(k)]^T$. From previous discussion, it is clear that the operator $\mathscr{M}_{\boldsymbol{\gamma}(k)} : \psi \to \rho(\cdot,k)$ is bounded from $H^1(I_D)$ to $H^2(I_D)$, and the composition operator $-\mathscr{L} \circ \mathscr{M}_{\boldsymbol{\gamma}(k)} : \psi \to \phi(\cdot,k)$ is bounded from $H^1(I_D)$ to $L^2(I_D)$.*

If we decompose $L^2(I_D)$ by letting $L^2(I_D) = \mathscr{N} \bigoplus \mathscr{N}^\perp$, then (4.15) admits only trivial solution in $\mathscr{N}^\perp$. Accordingly, (4.14) has a unique solution in $\mathscr{N}^\perp$, which can be expressed as

$$\hat{\zeta} = (I - vK_v^{-1})^{-1}K_v^{-1}r =: \mathscr{K}_b r. \quad (4.16)$$

The subscript b indicates that the operator depends only on bound-state frequency k_b. Let

$$\hat{\xi} = \hat{\zeta} + \rho, \quad \text{and} \quad \hat{\psi}_b = \psi - \hat{\xi}, \quad (4.17)$$

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and substitute these into (4.10), then the solvability condition (resonance condition) is recast as

$$(k^2-k_b^2)(\psi,\psi-\hat{\xi}(\cdot\,;k))-\gamma_0(k)\psi(0)\left(\overline{\psi(0)}-\overline{\hat{\xi}(0;k)}\right)+\gamma_D(k)\psi(D)\left(\overline{\psi(D)}-\overline{\hat{\xi}(D;k)}\right)=0. \tag{4.18}$$

Hence, if (k,ψ) is a resonance pair for (4.7), it satisfies the resonance condition (4.18). On the other hand, it is straightforward that those k satisfying (4.18) are scattering resonances of (4.7). Therefore, (4.18) is an equivalent condition for the resonances.

5 Proof of the main result

The spectrum for the infinite structure is symmetric with respect to the origin, thus we only need to consider positive k_b in the proof. Here and henceforth, we use the notation C to denote some generic positive constant independent of N_l and N_r.

Let us decompose the coefficients $\alpha_0(k)$ and $\alpha_D(k)$ given in (4.6) and (4.4) as

$$\alpha_0(k)=\alpha_{0,p}(k)+\alpha_{0,s}(k),\quad \text{and}\quad \alpha_D(k)=\alpha_{D,p}(k)+\alpha_{D,s}(k), \tag{5.1}$$

where

$$\alpha_{0,p}(k)=\frac{u_{21}(k)}{u_{11}(k)},\quad \alpha_{D,p}(k)=\frac{u_{22}(k)}{u_{12}(k)}, \tag{5.2}$$

$$\alpha_{0,s}(k)=\frac{-\left(\frac{\lambda_2}{\lambda_1}\right)^{N_l}(u_{21}+iku_{11})\det[U_1,U_2]}{(u_{22}+iku_{12})u_{11}^2-\left(\frac{\lambda_2}{\lambda_1}\right)^{N_l}(u_{21}+iku_{11})u_{11}u_{12}}, \tag{5.3}$$

and

$$\alpha_{D,s}(k)=\frac{-\left((\frac{\lambda_2}{\lambda_1}\right)^{N_r}(u_{22}-iku_{12})\det[U_1,U_2]}{\left(\frac{\lambda_2}{\lambda_1}\right)^{N_r}(u_{22}-iku_{12})u_{11}u_{12}+(iku_{11}-u_{21})u_{12}^2}. \tag{5.4}$$

Note that $\alpha_{0,p}$ and $\alpha_{D,p}(k)$ are independent of the number of periods N_l and N_r. Furthermore, $\alpha_{0,p}(k_b)$ and $\alpha_{0,D}(k_b)$ coincide with the impedance coefficients β_0 and β_D (cf.(4.1)) for the infinite structure.

Theorem 5.1 *Let $\gamma_0(k)$ be defined by (4.9) for $k\in\mathbb{C}$. If $k_b>0$ belongs to the point spectrum σ_p of the infinite structure with the defect, then $\gamma_0'(k_b)$ can be decomposed as $\gamma_0'(k_b)=-\gamma_{0,p}'+\gamma_{0,s}'$, where*

$$\gamma_{0,p}'>0,\quad \textit{and}\quad |\gamma_{0,s}'|<CN_le^{-\mu N_l}$$

for some positive constant C and μ, provided that N_l is sufficiently large.

Proof In light of (4.9) and (5.1), it follows that

$$\gamma_0'(k_b)=\alpha_0'(k_b)=\alpha_{0,p}'(k_b)+\alpha_{0,s}'(k_b). \tag{5.5}$$

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By a direct calculation, the following estimate holds for some positive constant C independent of N_l:

$$|\alpha'_{0,s}(k_b)| < CN_l \left| \frac{\lambda_2(k_b)}{\lambda_1(k_b)} \right|^{N_l}.$$

Since $k_b \in \sigma_p$, from Theorem 3.1 we see that two eigenvalues of $P_L(k_b)$ are distinct: $|\lambda_1(k_b)| > 1 > |\lambda_2(k_b)|$. Thus

$$|\alpha'_{0,s}(k_b)| < CN_l e^{-\mu N_l}, \tag{5.6}$$

wherein $\mu = \log \frac{|\lambda_1(k_b)|}{|\lambda_2(k_b)|} > 0$. Next we show that $\alpha'_{0,p}(k_b) < 0$. Then from (5.5) and (5.6), the proof is complete by setting $\gamma'_{0,p} = -\alpha'_{0,p}(k_b)$ and $\gamma_{0,s} = \alpha'_{0,s}(k_b)$.

First, we note that the derivative

$$\alpha'_{0,p}(k_b) = \frac{\det[U_1(k_b), U_1'(k_b)]}{u_{11}^2(k_b)}.$$

From Lemma 2, there exist complex numbers q_{11} and q_{21} such that

$$U_1'(k_b) = q_{11}U_1(k_b) + q_{21}U_2(k_b), \quad \text{where } q_{21} = \frac{1}{\lambda_1(k_b) - \lambda_2(k_b)} \overline{V}_2^T(k_b) P_L'(k_b) U_1(k_b).$$

Substitute the above formula into $\det[U_1(k_b), U_1'(k_b)]$, and using the fact that $\det[U_1, U_2] = p_{21}^L(\lambda_1 - \lambda_2)$, we obtain

$$\det[U_1(k_b), U_1'(k_b)] = p_{21}^L \overline{V}_2^T(k_b) P_L'(k_b) U_1(k_b).$$

This can be further simplified as

$$\det[U_1'(k_b), U_1(k_b)] = \frac{1}{\lambda_2(k_b) - \lambda_1(k_b)} V_2^T(k_b) P_L'(k_b) U_1(k_b), \tag{5.7}$$

by using the formula (2.12) for the normalized left eigenvector $\overline{V}_2(k_b)$ and the trace formula $p_{11}^L + p_{22}^L = \lambda_1 + \lambda_2$.

By virtue of Lemma 2,

$$P_L'(k_b)U_1 = P_L(k_b) \int_0^L P^{-1}(x; k_b) O(k_b) P(x; k_b) U_1 \, dx,$$

with the matrices $O(k)$ and $P(x,k)$ given by (2.6) and (2.7) respectively. It is obtained that

$$\begin{aligned} \det[U_1'(k_b), U_1(k_b)] &= \frac{1}{\lambda_2(k_b) - \lambda_1(k_b)} V_2^T(k_b) P_L(k_b) \int_0^L P^{-1}(x; k_b) O(k_b) P(x; k_b) U_1 \, dx \\ &= \frac{\lambda_2(k_b)}{\lambda_2(k_b) - \lambda_1(k_b)} \int_0^L V_2^T P^{-1}(x; k_b) O(k_b) P(x; k_b) U_1 \, dx, \end{aligned} \tag{5.8}$$

since $V_2^T P_L = \lambda_2 V_2^T$. From $\lambda_1(k_b)\lambda_2(k_b) = 1$ and $|\lambda_1(k_b)| > 1 > |\lambda_2(k_b)|$, we deduce that

$$\frac{\lambda_2(k_b)}{\lambda_2(k_b) - \lambda_1(k_b)} < 0.$$

Applying Lemma 2 for (5.8), it is concluded that $\det[U_1(k_b), U_1'(k_b)] < 0$, and $\alpha'_{0,p}(k_b) < 0$ follows. □

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Following a similar proof as in Theorem 5.1, the following theorem also holds.

Theorem 5.2 *Let $\gamma_D(k)$ be defined by (4.9) for $k \in \mathbb{C}$. Assume that $k_b \in \sigma_p$ and k_b is positive. If N_r is sufficiently large, then $\gamma'_D(k_b) = \gamma'_{D,p} + \gamma'_{D,s}$ where*

$$\gamma'_{D,p} > 0, \quad \text{and} \quad |\gamma'_{D,s}| < CN_r e^{-\mu N_r}$$

for some positive constant C and μ.

Next, we analyse the roots for the resonance condition (4.18). Let us rewrite it as

$$\begin{aligned} f(k) = (k^2 - k_b^2)||\psi||^2_{L^2(I_D)} - (k^2 - k_b^2)(\psi, \hat{\xi}(\cdot\,;k)) - \gamma_0(k)|\psi(0)|^2 + \gamma_D(k)|\psi(D)|^2 \\ +\gamma_0(k)\psi(0)\overline{\hat{\xi}(0;k)} - \gamma_D(k)\psi(D)\overline{\hat{\xi}(D;k)} = 0. \end{aligned} \tag{5.9}$$

The function $f(k)$ is analytic in the neighbourhood of k_b on the complex plane. For clarity, let us denote this neighbourhood as Ω. In addition, the eigenvalues of $P_L(k_b)$ satisfy $|\lambda_1(k_b)| > 1 > |\lambda_2(k_b)|$. Thus the eigenvalues $\lambda_1(k)$ and $\lambda_2(k)$ of $P_L(k)$ are distinct in the neighbourhood of k_b. Without loss of generality, we may assume that

$$|\lambda_1(k)| > 1 > |\lambda_2(k)| \quad \text{for} \quad k \in \Omega.$$

Let Γ be the boundary of the disk with radius δ centred at k_b such that its interior is contained in Ω. Let $\kappa = k - k_b$. By Taylor's theorem [2], we have

$$f(k) = f(k_b) + f_1(k_b)\kappa + f_2(k)\kappa^2, \tag{5.10}$$

where

$$f_1(k_b) = f'(k_b), \quad f_2(k) = \frac{1}{2\pi i}\int_\Gamma \frac{f(s)}{(s-k_b)^2(s-k)}ds. \tag{5.11}$$

To obtain $f(k_b)$ and $f_1(k_b)$ explicitly, we expand $\gamma_0(k)$ and $\gamma_D(k)$ at the bound-state frequency k_b:

$$\gamma_0(k) = \gamma_0(k_b) + \gamma'_0(k_b)\kappa + \gamma_{0,h}(k); \quad \gamma_D(k) = \gamma_D(k_b) + \gamma'_D(k_b)\kappa + \gamma_{D,h}(k), \tag{5.12}$$

where $\gamma_{0,h}(k)$ and $\gamma_{D,h}(k)$ represent the high order terms. Let $\rho(x,k)$ and $\phi(x,k)$ be the functions as defined in Section 4.2. Similarly, we may expand ρ and ϕ as

$$\begin{aligned} \rho(\cdot,k) &= \rho_0 + \kappa\rho_1 + \rho_h(k), \\ \phi(\cdot,k) &= \phi_0 + \kappa\phi_1 + \phi_h(k). \end{aligned}$$

It follows from a direct comparison that

$$\begin{aligned} &\rho_0 = \mathscr{M}_{\gamma(k_b)}(\psi), \quad \rho_1 = \mathscr{M}_{\gamma'(k_b)}(\psi), \quad \rho_h = \mathscr{M}_{\gamma_h(k)}(\psi), \\ &\phi_0 = -\mathscr{L}\rho_0, \quad \phi_1 = -\mathscr{L}\rho_1, \quad \phi_h = -\mathscr{L}\rho_h. \end{aligned}$$

Here the vectors

$$\boldsymbol{\gamma}(k_b) = [\gamma_0(k_b), \gamma_D(k_b)]^T, \quad \boldsymbol{\gamma}'_1(k_b) = [\gamma'_0(k_b), \gamma'_D(k_b)]^T, \quad \text{and } \boldsymbol{\gamma}_h(k_b) = [\gamma_{0,h}(k), \gamma_{D,h}(k_b)]^T.$$

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The operators $\mathscr{M}_{\gamma(k_b)}$, $\mathscr{M}_{\gamma'(k_b)}$, and $\mathscr{M}_{\gamma_h(k_b)}$ are bounded from $H^1(I_D)$ to $H^2(I_D)$ (cf. Section 4.2). From (4.13), (4.16), (4.17), and using the above expansions, we see that $\hat{\xi}$ can be written as

$$\hat{\xi}(\cdot,k) = \hat{\xi}_0 + \kappa\hat{\xi}_1 + \hat{\xi}_h(k), \tag{5.13}$$

wherein $\hat{\xi}_0 = \mathscr{K}_b\phi_0 + \rho_0$, $\hat{\xi}_1 = \mathscr{K}_b[2k_b\psi + \phi_1] + \rho_1$ and $\hat{\xi}_h = \mathscr{K}_b[\kappa^2\psi + \phi_h(k)] + \rho_h$. Substituting the expansions (5.12)–(5.13) into (5.9), it is obtained that

$$\begin{aligned} f(k_b) &= -\gamma_0(k_b)|\psi(0)|^2 + \gamma_D(k_b)|\psi(D)|^2 + \gamma_0(k_b)\psi(0)\overline{\hat{\xi}_0(0)} - \gamma_D(k_b)\psi(D)\overline{\hat{\xi}_0(D)};\\ f_1(k_b) &= 2k_b||\psi||^2_{L^2(I_D)} - 2k_b(\psi,\hat{\xi}_0) - \gamma_0'(k_b)|\psi(0)|^2 + \gamma_D'(k_b)|\psi(D)|^2 + \gamma_0'(k_b)\psi(0)\overline{\hat{\xi}_0(0)}\\ &\quad -\gamma_D'(k_b)\psi(D)\overline{\hat{\xi}_0(D)} + \gamma_0(k_b)\psi(0)\overline{\hat{\xi}_1(0)} - \gamma_D(k_b)\psi(D)\overline{\hat{\xi}_1(D)}. \end{aligned}$$

Theorem 5.3 *Let $N = \min\{N_l, N_r\}$. There exist an integer N_0 that if $N \geqslant N_0$, then*

$$|f(k_b)| < C_0e^{-\mu N}, \quad \textit{and} \quad f_1(k_b) \geqslant c_0$$

for some positive constants C_0, c_0, and μ independent of N.

Proof From (4.1), (4.9), and (5.1)–(5.2), it is apparent that

$$\gamma_0(k_b) = \alpha_{0,s}(k_b), \quad \text{and} \quad \gamma_D(k_b) = \alpha_{D,s}(k_b).$$

Note that at the bound-state frequency k_b, the eigenvalues for $P_L(k_b)$ satisfy $|\lambda_1(k_b)| > 1 > |\lambda_2(k_b)|$. We deduce from the expansion of $\alpha_{0,s}$ and $\alpha_{D,s}$ in (5.3)–(5.4) that, for sufficiently large N,

$$|\gamma_0(k_b)| < Ce^{-\mu N}, \quad \text{and} \quad |\gamma_D(k_b)| < Ce^{-\mu N}, \tag{5.14}$$

where $\mu = \log\frac{|\lambda_1(k_b)|}{|\lambda_2(k_b)|} > 0$. In addition, the standard energy estimate for $\hat{\xi}_0$ and $\hat{\xi}_1$ defined in (5.13) yields

$$||\hat{\xi}_0||_{H^1(I_D)} \leqslant C\left(||\phi_0||_{L^2(I_D)} + ||\rho_0||_{H^1(I_D)}\right) \leqslant C||\psi||_{H^1(I_D)}, \tag{5.15}$$

$$||\hat{\xi}_1||_{H^1(I_D)} \leqslant C(||\psi||_{L^2(I_D)} + ||\phi_1||_{L^2(I_D)} + ||\rho_1||_{H^1(I_D)}) \leqslant C||\psi||_{H^1(I_D)}. \tag{5.16}$$

From (5.14)–(5.15), and the trace theorem, it is deduced that

$$|f(k_b)| < Ce^{-\mu N}||\psi||^2_{H^1(I_D)}. \tag{5.17}$$

Employing Theorems 5.1 and 5.2, $\gamma_0'(k_b)$ and $\gamma_D'(k_b)$ can be decomposed as

$$\gamma_0'(k_b) = -\gamma_{0,p}' + \gamma_{0,s}', \quad \text{and} \quad \gamma_D'(k_b) = \gamma_{D,p}' + \gamma_{D,s}',$$

where $\gamma_{0,p}'$ and $\gamma_{D,p}'$ are positive constants independent of N, and

$$|\gamma_{0,s}'| < CNe^{-\mu N}, \quad |\gamma_{D,s}'| < CNe^{-\mu N} \quad \text{for sufficiently large } N. \tag{5.18}$$

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Consequently

$$f_1(k_b) > 2k_b||\psi||^2_{L^2(I_D)} - \left\{2k_b|(\psi, \hat{\xi}_0)| + |\gamma'_{0,s}(k_b)||\psi(0)|^2 + |\gamma'_{D,s}(k_b)||\psi(D)|^2\right\}$$
$$-\left\{|\gamma'_0(k_b)||\psi(0)|\left|\hat{\xi}_0(0)\right| + |\gamma'_D(k_b)||\psi(D)|\left|\hat{\xi}_0(D)\right| + |\gamma_0(k_b)||\psi(0)|\left|\hat{\xi}_1(0)\right|\right.$$
$$\left.+|\gamma_D(k_b)||\psi(D)|\left|\hat{\xi}_1(D)\right|\right\}.$$

In light of (5.14)–(5.16), and (5.18), we see that there exist an integer N_0 such that if $N \geqslant N_0$,

$$f_1(k_b) > k_b||\psi||^2_{L^2(I_D)} \geqslant c_0, \tag{5.19}$$

and c_0 is some constant independent of N.

□

Proof of Theorem 3.2. Since $f_1(k_b) > 0$ in the Taylor expansion (5.10) (cf. Theorem 5.3), we may rewrite the resonance condition (5.9) as

$$\kappa = -\frac{f(k_b)}{f_1(k_b)} + \kappa^2 \Lambda(\kappa),$$

where $\Lambda(\kappa) = -\frac{f_2(k_b+\kappa)}{f_1(k_b)}$, and $f_1(k_b)$, $f_2(k)$ are given by (5.11). We recall that Γ is the boundary of the disk with radius δ centred at k_b such that its interior is contained in Ω, the neighbourhood of k_b.

Define the iteration sequence

$$\kappa_0 = -\frac{f(k_b)}{f_1(k_b)}, \quad \text{and} \quad \kappa_{n+1} = \kappa_0 + \kappa_n^2 \Lambda(\kappa_n), \quad n \geqslant 1. \tag{5.20}$$

In the following, we show that κ_{n+1} remains in the neighbourhood of the origin, and $\kappa^2\Lambda(\kappa)$ is a contraction map. As such, the nonlinear equation attains a solution κ, and the iterations sequence $\{\kappa_n\}_{n=0}^{\infty}$ converges to κ. Moreover, for all n, it is shown that $|\kappa_n| \leqslant Ce^{-\mu N}$ for some constant $C > 0$ independent of N.

First, a combination of (5.17) and (5.19) in Theorem 5.3 leads to

$$|\kappa_0| \leqslant \frac{C}{2}e^{-\mu N}.$$

Without loss of generality, it is assumed that $Ce^{-\mu N} \leqslant \frac{\delta}{2}$. Suppose that

$$|\kappa_n| \leqslant Ce^{-\mu N},$$

then

$$|\kappa_{n+1}| \leqslant \frac{C}{2}e^{-\mu N}\left(1 + 2|\kappa_n||\Lambda(\kappa_n)|\right).$$

Therefore

$$|\kappa_{n+1}| \leqslant Ce^{-\mu N},$$

if $|\kappa_n||\Lambda(\kappa_n)| \leqslant \frac{1}{2}$. In what follows, we establish such an estimate.

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For any $k \in \Gamma$, using (4.9) and (5.1), it is observed that $\gamma_0(k) = \alpha_{0,p}(k) - \beta_0(k) + \alpha_{0,s}(k)$. It is apparent that $|\alpha_{0,p} - \beta_0|$ is bounded in $\bar{\Omega}$, and the bound is independent of N. On the other hand, by noting that $|\lambda_1(k)| > 1 > |\lambda_2(k)|$ in Ω, we have $|\alpha_{0,s}| \leqslant 1$ for sufficiently large N. Thus, there exists a constant C_0 such that

$$\sup_{k\in\Omega} |\gamma_0(k)| \leqslant C_0.$$

Similarly, $\sup_{k\in\Omega} |\gamma_D(k)| \leqslant C_D$ for positive constant C_D. By the definition of $\hat{\xi}$ in (4.17), we deduce that

$$\sup_{k\in\Omega} ||\hat{\xi}(\cdot\,;k)||_{H^1(I_D)} \leqslant C||\psi||_{H^1(I_D)}.$$

By combining all the above estimates for $f(k)$ in (5.9), it is obtained that $\sup_{k\in\Omega} |f(k)| \leqslant C$. A direct estimate for $f_2(k)$ now yields

$$|f_2(k_b + \kappa_n)| \leqslant \frac{1}{2\pi} \int_\Gamma \frac{|f(s)|}{|s - k_b|^2 |s - (k_b + \kappa_n)|} ds \leqslant \frac{C}{\delta^2},$$

and

$$|\kappa_n||\Lambda(\kappa_n)| \leqslant Ce^{-\mu N} \frac{|f_2(k_b + \kappa_n)|}{|f_1(k_b)|} \leqslant \frac{1}{2},$$

follows provided N is large. We thus have shown that $|\kappa_{n+1}| \leqslant Ce^{-\mu N}$ and, in particular, $|\kappa_{n+1}| \leqslant \frac{\delta}{2}$.

To show that $\kappa^2\Lambda(\kappa)$ is a contraction map in the neighbourhood of origin, note that $(\kappa^2\Lambda(\kappa))' = 2\kappa\Lambda(\kappa) + \kappa^2\Lambda'(\kappa)$. Following the parallel lines as above, it can be shown that $|(\kappa^2\Lambda(\kappa))'| < 1$ if $|\kappa| \leqslant \frac{\delta}{2}$. We omit the proof the clarity of exposition. □

6 A perturbation approach to calculate near bound-state resonances

The iteration scheme (5.20) suggests a natural numerical method to obtain the near bound-state resonance. In practice, the calculation of the bound-state frequency k_b and corresponding eigenfunction ψ_b can be implemented efficiently by the supercell method [20]. Since $|k - k_b| \sim O(e^{-\mu N})$ for sufficiently large N, if one knows the bound-state frequency k_b and corresponding eigenfunction ψ_b, then without resorting to the iteration process, a simplified perturbation approach may be employed to calculate the resonance k via a linear approximation of the resonance condition (5.9). That is, by neglecting the high order terms in (5.10) and exponentially small terms for $f(k_b)$ and $f_1(k_b)$, an approximation of κ is computed by

$$\kappa_{\text{approx}} = \frac{-\gamma_0(k_b)|\psi_b(0)|^2 + \gamma_D(k_b)|\psi_b(D)|^2}{2k_b||\psi_b||^2_{L^2(I_D)} + \gamma'_{0,p}(k_b)|\psi_b(0)|^2 + \gamma'_{D,p}(k_b)|\psi_b(D)|^2}. \tag{6.1}$$

The approximate resonance

$$k_{\text{approx}} = k_b + \kappa_{\text{approx}}. \tag{6.2}$$

Next, we present an example to show the accuracy of the approximation. Let us consider the same photonic structure as in Section 3.2, i.e., the parameters are specified by $D = 6$,

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Table 2. *Resonance k_{Newton} and the associated linear approximation k_{approx} for different number of periodic cells*

N	k_{Newton}	k_{approx}
2	$0.585245443593 - 0.018388829293i$	$0.598143178712 - 0.000000162563i$
4	$0.596035039932 - 0.003082708901i$	$0.596167795232 - 0.003053231994i$
8	$0.598065818707 - 0.000112010544i$	$0.598065956311 - 0.000111825473i$
16	$0.598143178712 - 0.000000162563i$	$0.598143178610 - 0.000000162560i$

$L_1 = 2$, $L_2 = 1$, and $N_l = N_r = N$. The permittivity of each layer is given by $\varepsilon_D = 2$, $\varepsilon_1 = 4$, and $\varepsilon_2 = 1$, respectively. In order to make a comparison, we set up a direct resonance condition by letting the wave propagate from the left endpoint of the photonic structure ($x = a$) to the right ($x = b$), and imposing the continuity conditions at the interfaces of layers. The resonance are then obtained by solving this nonlinear equation directly via Newton's method (denoted as k_{Newton}). In Table 2, we compare k_{Newton} and the calculation obtained by the approximation formula (6.2). It is seen that the resonance is approximated accurately by the proposed perturbation formula. In particular, the errors decay with increasing number of periodic cells.

7 Discussions

A general perturbation approach has been proposed to study the near bound-state resonances for one-dimensional photonic crystal with some defect. It is shown that near bound-state resonances exit and the distance between the resonance and the associated bound-state frequency decays exponentially as a function of the number of periodic cells. Some challenging research in this direction is to extend such perturbation theory for the study of resonances in higher dimensions. As indicated in the derivation of the resonance condition in Section 4, the key is to reformulate eigenvalue problems in the defect region by introducing suitable Dirichlet-to-Neumann maps on its boundary, and obtain an equivalent resonance condition by examining the associated equation for the difference between the bound state and quasi-mode. This is our ongoing work and will be reported elsewhere.

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References

[1] Akahane, Y., Asano, T., Song, B. & Noda, S. (2003) High-Q photonic nanocavity in a two-dimensional photonic crystal. *Nature* **425** (no. 6961), 944–947.

https://doi.org/10.1017/S0956792515000340 Published online by Cambridge University Press

[2] Ahlfors, L. (1953) *Complex Analysis,* 2nd ed., McGraw-Hill, New York.
[3] Dobson, D., Santosa, F., Shipman, S. & Weinstein, M. (2013) Resonances of a potential well with a thick barrier. *SIAM J. Appl. Math.* **73**, 1489–1512.
[4] Figotin, A. & Gorentsvieig, V. (1998) Localized electromagnetic waves in a layered periodic dielectric medium with a defect. *Phy. Rev. B* **58**, 180–188.
[5] Figotin, A. & Klein, A. (1997) Localized classical waves created by defects. *J. Stat. Phys.* **86**, 165–177.
[6] Figotin, A. & Klein, A. (1998) Midgap defect modes in dielectric and acoustic media. *SIAM J. Appl. Math.* **58**, 1748–1773.
[7] Figotin, A. & Kuchment, P. (1996) Band-gap structure of spectra of periodic dielectric and acoustic media. I. scalar model. *SIAM J. Appl. Math.* **56**, 68–88.
[8] Heider, P., Berebichez, D., Kohn, R. V. & Weinstein, M. I. (2008) Optimization of scattering resonances. *Struct. Multidiscip. Optim.* **36**, 443–456.
[9] Kao, C. Y. & Santosa, F. (2008) Maximization of the quality factor of an optical resonator. *Wave Motion* **45**, 412–427.
[10] Kato, T. (1995) *Perturbation Theory for Linear Operators*, Springer-Verlag, Berlin .
[11] Khitrova, G., Gibbs, H. M., Jahnke, F., Kira, M. and Koch, S. W. (1999) Nonlinear optics of normal-mode-coupling semiconductor microcavities. *Rev. Mod. Phys.* **71**, 1591–1639.
[12] Knopp, K. (1996) *Theory of Function, Parts I and Parts II*, Dover Publications, New York.
[13] Krantz, S. (2001) *Function Theory of Several Complex Variables*, 2nd ed., American Mathematical Society.
[14] Iantchenko, A. (2006) Resonance spectrum for one-dimensional layered media. *Appl. Anal.* **85**(11), 1383–1410.
[15] Lin, J. & Santosa, F. (2013) Resonances of a finite one-dimensional photonic crystal with a defect. *SIAM J. Appl. Math.* **73**, 1002–1019.
[16] Lin, J. & Santosa, F. (2015) Scattering resonances for a two-dimensional potential well with thick barrier. *SIAM J. Math. Anal.* **47**, 1458–1488.
[17] Michler, P. *et al.* (2000) A quantum dot single-photon turnstile device. *Science* **290**, 2282–2285.
[18] Ramdani, K. & Shipman, S. (2008) Transmission through a thick periodic slab. *Math. Models Methods Appl. Sci.* **18**, 543–572.
[19] Reed, M. & Simon, B. (1978) *Methods of Modern Mathematical Physics*, Vol. 4, Analysis of operators. Academic Press, New York.
[20] Soussi, S. (2005) Convergence of the supercell method for defect modes calculations in photonic crystals. *SIAM J. Numer. Anal.* **43**, 1175–1201.
[21] Spillane, S. M., Kippenberg, T. J. & Vahala, K. J. (2002) Ultralow-threshold Raman laser using a spherical dielectric microcavity. *Nature* **415**, 621–623.
[22] Tang, S. & Zworski, M. (2000) Resonance expansions of scattered waves. *Commun. Pure. Appl. Math.* **53**, 1305–1334.
[23] Zworski, M. (1999) Resonances in physics and geometry, Notices of the AMS, **46**, 319–328.
[24] Vahala, K. J. (2004) *Optical Microcavities*, World Science Publishing, Singapore.

Appendix A

Lemma *Let $k \in \mathbb{C}\backslash\{0\}$ be a resonance of (1.2), then k has negative imaginary part.*

Proof Multiply the differential equation in (1.2) by $\bar{\psi}$ and integrate by parts, it follows that

$$\int_a^b \frac{1}{\varepsilon}\left|\frac{d\psi}{dx}\right|^2 - k^2|\psi|^2\,dx - ik(|\psi(a)|^2 + |\psi(b)|^2) = 0. \tag{A 1}$$

Let $k = \mathrm{Re}k + i\ \mathrm{Im}k$. First, let us consider the case when the real part $\mathrm{Re}k \neq 0$. By a simple calculation, it can be shown that the imaginary part of the left-hand side

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of (A 1) is

$$-\mathrm{Re}k\left(2\,\mathrm{Im}k\int_0^a|\psi|^2\,dx+|\psi(a)|^2+|\psi(b)|^2\right).$$

If $\mathrm{Im}k\geqslant 0$, then $\psi(a)=\psi(b)=0$, and $\frac{d\psi(a)}{dx}=\frac{d\psi(a)}{dx}=0$ by the boundary condition. It follows that $\psi\equiv 0$ in (a,b), which contradicts $\psi\not\equiv 0$.

Now if the $\mathrm{Re}k=0$, (A 1) becomes

$$\int_a^b\frac{1}{\varepsilon}\left|\frac{d\psi}{dx}\right|^2+(\mathrm{Im}k)^2|\psi|^2\,dx+\mathrm{Im}k(|\psi(a)|^2+|\psi(b)|^2)=0.$$

If $\mathrm{Im}k>0$, again we see that $\psi\equiv 0$ in (a,b). Consequently, $\mathrm{Im}k$ has to be negative. □

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