A Multipole Dirichlet-to-Neumann Map Method for Photonic Crystals with Complex Unit Cells

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Abstract

The periodicity of photonic crystals can be utilized to develop efficient numerical methods for analyzing light waves propagating in these structures. The Dirichlet-to-Neumann (DtN) operator of a unit cell maps the wave field on the boundary of the unit cell to its normal derivative, and it can be used to reduce the computation to the edges of the unit cells. For two-dimensional photonic crystals with complex unit cells each containing a number of possibly different circular cylinders, we develop an efficient multipole method for constructing the DtN maps. The DtN maps are used to calculate the transmission and reflection spectra for finite photonic crystals with complex unit cells.

1 Introduction

Due to the existence of bandgaps, photonic crystals (PhCs) [1] can be used to manipulate and control light. Two-dimensional (2D) PhCs are relatively easy to fabricate and they still have many useful applications. A typical 2D PhC is composed of a lattice of parallel cylinders in a homogeneous background (either air-holes in a dielectric medium or dielectric or metallic rods in air). The simplest 2D PhCs consist of cylinders with circular cross sections, but cylinders with more complicated cross sections [2] may exhibit useful features, such as larger bandgaps. A unit cell of a typical 2D PhC contains only one cylinder, but more complicated lattice structures, such as the honeycomb lattice, may have more than one cylinders in a unit cell, and they often have interesting and useful properties. For example, a 2D resonator array [3] obtained by removing one cylinder in every three or four rows and columns, has flattened bands that can be used to reduce the group velocity of light. A similar structure is also considered in [4]. In this paper,

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we consider general 2D PhCs with unit cells containing a number of cylinders. These cylinders can be different and they are randomly placed in the unit cell. We call such a unit cell a complex unit cell.

For PhCs that are finite in one direction, numerical methods are needed to study their transmission and reflection properties. Existing methods for diffractive optics, such as the Fourier modal method [5, 6] and the finite element method [7] can be used, but special methods [8, 9, 10, 11] that take advantage of the properties of the PhC are often more efficient. The multipole method [12] was developed for analyzing scattering from a finite number of parallel cylinders, but it has been extended to PhCs with infinite number of cylinders using lattice sums techniques [8, 9]. In [11], Huang *et al.* developed a DtN operator marching method for PhCs of finite size. The method is based on the DtN operator that maps the wave field on the edges of the unit cell to its normal derivative. The method is efficient, since it avoids computing the wave field inside the unit cells. The DtN map is also useful for band structure calculations [13]. For a simple unit cell containing a circular cylinder, the DtN map can be easily constructed from a cylindrical wave expansion [11]. For a unit cell containing a cylinder with an arbitrary cross section, a boundary integral equation method can be used to find the DtN operator [14]. If a complex unit cell can be regarded as the union of simple cells (each containing at most one cylinder), the DtN map of the complex cell can be obtained by merging the DtN maps of the simple cells [15].

In this paper, we develop a multipole method for computing the DtN maps of complex unit cells. The method is more general than the merging technique developed in [15], since the cylinders in the complex unit cell can now be randomly placed. For all the cylinders in a complex unit cell, we solve scattering problems for a number of different incident waves using the multipole method. The solutions are then used to construct the DtN map. Since only a finite number of cylinders are involved in the scattering problems, sophisticated lattice sums techniques [8, 9] are not needed. The method is illustrated by computing the transmission and reflection spectra for a number of PhCs with complex unit cells.

2 A multipole approach to DtN maps of complex unit cells

For 2D structures and time harmonic waves in the E polarization, the z component of the electric field, denoted by u here, satisfies

$$\partial_x^2 u + \partial_y^2 u + k_0^2 n^2 u = 0, \tag{1}$$

where $n = n(x, y)$ is the refractive index function and k_0 is the free space wavenumber. For a 2D PhC, the refractive index is periodic in two linearly independent directions in

the xy plane. A unit cell corresponds to one period in each of these two directions. Let Ω be a unit cell and Γ be the boundary of Ω, we define the DtN map Λ as the operator that maps u on Γ to the normal derivative of u on Γ. That is, $\Lambda u = \partial u/\partial \nu$, where u is any solution of (1) and ν is a unit vector of Γ. If we choose K sampling points on Γ, the operator Λ can be approximated by a $K \times K$ matrix. More precisely, we find K special solutions of (1), say ϕ_k for $k = 1, 2, ..., K$, then approximate the general solution of (1) by $u = \sum_{k=1}^{K} c_k \phi_k$. If we evaluate ϕ_k at the K sampling points on Γ, we obtain a matrix Λ_1 that maps the coefficients $\{c_k\}$ to the values of u at these K points. We can also find the normal derivatives of ϕ_k at the K points on Γ. This gives rise to another matrix Λ_2 that maps $\{c_k\}$ to the normal derivatives of u at these K points. The DtN map is then approximated by the matrix $\Lambda = \Lambda_2 \Lambda_1^{-1}$.

For a simple unit cell containing one circular cylinder, we can use the cylindrical waves as the special solutions [11]. If the cylinder has a more general cross section, the special solutions can be obtained by solving a boundary integral equation. In this section, we calculate the special solutions by solving scattering problems for all the cylinders in the complex unit cell. A typical rectangular complex unit cell is shown in Fig. 1. We assume

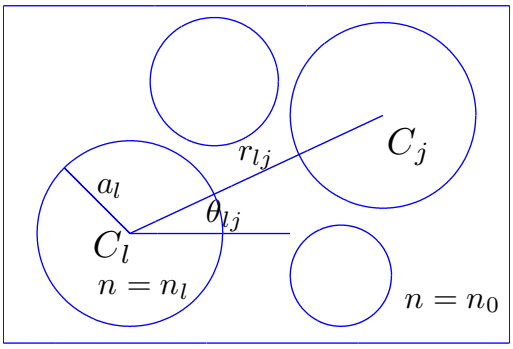

Figure 1: A complex unit cell containing a few circular cylinders.

that the cell includes N randomly placed cylinders. The l-th cylinder has its center at C_l, a radius a_l and a refractive index n_l. The refractive index of the background medium in the cell is n_0. The scattering problem is solved in the entire xy plane with only these N cylinders in the same background medium now extended to infinity. Let $\phi_k = \phi_k^{(i)} + \phi_k^{(s)}$, where $\phi_k^{(i)}$ is a plane incident wave with the incident angle $\rho_k = 2\pi k/K$, i.e.,

$$\phi_k^{(i)}(x, y) = \exp[ik_0 n_0 (x \cos \rho_k + y \sin \rho_k)], \tag{2}$$

and $\phi_k^{(s)}$ is the scattered wave. The scattering problem is solved by the multipole method

described in [12]. We write down the scattered wave outside the cylinders as

$$\phi_k^{(s)} = \sum_{l=1}^{N} \sum_{m=-\infty}^{\infty} b_{lm}^{(k)} \Phi_{lm} \quad \text{for} \quad \Phi_{lm}(x,y) = H_m^{(1)}(\zeta) e^{im\theta_l}, \tag{3}$$

where $H_m^{(1)}$ is the Hankel function, (r_l, θ_l) are the local polar coordinates of (x, y) with respect to the center C_l of the l-th cylinder, $\zeta = k_0 n_0 r_l$, and $\{b_{lm}^{(k)}\}$ are unknown coefficients. These coefficients can be solved from the following system:

$$\begin{bmatrix} I & -S_1T_{12} & -S_1T_{13} & \cdots \\ -S_2T_{21} & I & -S_2T_{23} & \cdots \\ -S_3T_{31} & -S_3T_{32} & I & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} b_1^{(k)} \\ b_2^{(k)} \\ b_3^{(k)} \\ \vdots \end{bmatrix} = \begin{bmatrix} S_1 g_1^{(k)} \\ S_2 g_2^{(k)} \\ S_3 g_3^{(k)} \\ \vdots \end{bmatrix}, \tag{4}$$

where $b_l^{(k)}$ is the infinite column vector of $b_{lm}^{(k)}$ for all m, $g_l^{(k)}$ is a given infinite column vector, I is the identity matrix, T_{lj} is a given infinite matrix and S_l is a given infinite diagonal matrix. The m-th entry of $g_l^{(k)}$ is

$$(g_l^{(k)})_m = i^m \exp[ik_0 n_0 d_l \cos(\rho_k - \varphi_l) - im\rho_k],$$

where (d_l, φ_l) are the polar coordinates of C_l with respect to the origin. The (m, q) entry of T_{lj} is

$$(T_{lj})_{mq} = H_{m-q}^{(1)}(k_0 n_0 r_{lj})\, e^{i(q-m)\theta_{lj}},$$

where (r_{lj}, θ_{lj}) are the local polar coordinates of C_j with respect to C_l. The (m, m) entry of S_l is

$$(S_l)_{mm} = \frac{n_l J_m(\xi) J_m'(\eta) - n_0 J_m(\eta) J_m'(\xi)}{-n_l H_m^{(1)}(\xi) J_m'(\eta) + n_0 J_m(\eta) H_m^{(1)\prime}(\xi)},$$

where $\xi = k_0 n_0 a_l$ and $\eta = k_0 n_l a_l$. More details can be found in [12].

To construct the DtN map, we need the normal derivatives of ϕ_k at the K sampling points on Γ. They are related to the gradients of $\phi_k^{(i)}$ and Φ_{lm} given by

$$\begin{aligned} \nabla \phi_k^{(i)}(x,y) &= ik_0 n_0 \exp[ik_0 n_0 (x\cos\rho_k + y \sin\rho_k)] \begin{bmatrix} \cos\rho_k \\ \sin\rho_k \end{bmatrix}, \\ \nabla \Phi_{lm}(x,y) &= k_0 n_0 e^{im\theta_l} H_m^{(1)\prime}(\zeta) \begin{bmatrix} \cos\theta_l \\ \sin\theta_l \end{bmatrix} + \frac{im}{r_l} e^{im\theta_l} H_m^{(1)}(\zeta) \begin{bmatrix} -\sin\theta_l \\ \cos\theta_l \end{bmatrix}. \end{aligned}$$

In practice, the integer m is truncated from $-m_*$ to m_*. Therefore, Eq. (4) is a system of $N_{tol} = (2m_* + 1)N$ unknowns. Notice that the different incident waves correspond to different right hand sides of (4). If K is on the same order as N_{tol}, the required number of operations for solving all K scattered waves is only $O(N_{tol}^3)$.

3 The DtN operator marching scheme

The DtN map of a unit cell can be used to formulate eigenvalue problems for band structure problems [13], it can also be used to calculate transmission and reflection spectra for PhCs that are finite in one direction [11]. In the following, we consider a 2D structure that is periodic in the x direction with period L and finite in the y direction for $0 < y < D$. For $y > D$ and $y < 0$, we have homogeneous media with refractive indices n_{top} and n_{bot}, respectively. For a given plane incident wave in $y > D$, the problem is to calculate the transmitted wave in $y < 0$ and the reflected wave in $y > D$. Assuming a time dependence of $e^{-i\omega t}$, the incident wave is given as

$$u^{(i)}(x, y) = e^{i[\alpha_0 x - \beta_0 (y-D)]}, \quad y > D, \tag{5}$$

where α_0 and β_0 satisfy $\alpha_0^2 + \beta_0^2 = k_0^2 n_{top}^2$ and $\beta_0 > 0$. It is well known that the reflected wave $u^{(r)}$ and the transmitted wave $u^{(t)}$ can be written down as

$$u^{(r)}(x, y) = \sum_{j=-\infty}^{\infty} R_j e^{i[\alpha_j x + \beta_j (y-D)]}, \quad y > D, \tag{6}$$

$$u^{(t)}(x, y) = \sum_{j=-\infty}^{\infty} T_j e^{i(\alpha_j x - \gamma_j y)}, \quad y < 0, \tag{7}$$

where

$$\alpha_j = \alpha_0 + \frac{2\pi j}{L}, \quad \beta_j = \sqrt{k_0^2 n_{top}^2 - \alpha_j^2}, \quad \gamma_j = \sqrt{k_0^2 n_{bot}^2 - \alpha_j^2},$$

R_j and T_j are the reflection and transmission coefficients to be determined.

The DtN operator marching method developed in [11] relies on two operators $Q(y)$ and $Y(y)$ (which act on functions of x) satisfying

$$Q(y)u(x, y) = \partial_y u(x, y), \quad Y(y)u(x, y) = u(x, 0). \tag{8}$$

At $y = 0$, these two operators are known from the transparent boundary condition and the definition of Y. The main process is to march Q and Y from $y = 0$ to $y = D$. Once $Q(D)$ and $Y(D)$ are known, we can compute the reflected and the transmitted waves, again using the boundary condition and the definition of Y. For a 2D PhC, the y direction has a number of layers separated by $0 = y_0 < y_1 < ... < y_m = D$, where Ω_j given by $y_j < y < y_{j+1}$ and $0 < x < L$ corresponds to a unit cell. From the DtN map Λ of the unit cell Ω_j and the quasi-periodic conditions for u and $\partial_x u$ on the two vertical edges of Ω_j, we can find the reduced DtN map M satisfying

$$M \begin{bmatrix} u_j \\ u_{j+1} \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} u_j \\ u_{j+1} \end{bmatrix} = \frac{\partial}{\partial y} \begin{bmatrix} u_j \\ u_{j+1} \end{bmatrix}, \tag{9}$$

where $u_j = u(x, y_j)$, etc. Using the operator M, we can march Q and Y from y_j to y_{j+1} as follows:

$$Z = [Q(y_j) - M_{11}]^{-1} M_{12}, \quad Q(y_{j+1}) = M_{22} + M_{21} Z, \quad Y(y_{j+1}) = Y(y_j) Z. \tag{10}$$

More details can be found in [11].

In the discrete case, the operators Q and Y are approximated by $K_x \times K_x$ matrices, where K_x is the number of sampling points used on the horizontal edges of the unit cells. The value of K_x is typically quite small. For PhCs, the unit cells are often identical. In that case, it is only necessary to compute the DtN map Λ and the reduced DtN map M once.

4 Numerical examples

In this section, we illustrate our method by a number of examples. The first example has been analyzed by Kusha *at al.* in [9]. It consists of an array of dielectric cylinders in vacuum. As shown in Fig. 2, the array contains two different types of cylinders. The

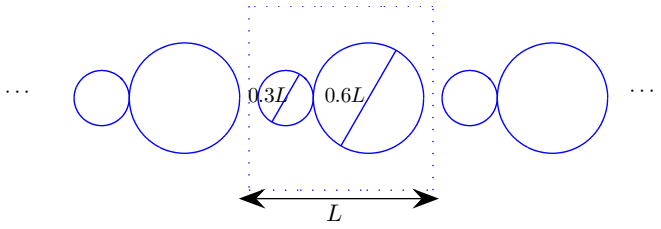

Figure 2: An array of two different dielectric cylinders.

diameters of the large and small cylinders are $0.6L$ and $0.3L$, respectively, where L is the period in the x direction (along the axis of the array). All cylinders have the same dielectric constant $\epsilon = n^2 = 2$. We use a square unit cell which contains a large and a small cylinders touching each other. The vertical edges of the unit cell lie exactly at the middle of the gaps between the cylinders, that is, the shortest distance between a vertical edge the unit cell to a nearby cylinder is $0.05L$. We calculate the DtN map Λ of this complex unit cell using 9 sampling points on each edge of the cell. The special solutions $\{\phi_k\}$ are obtained by solving the two-cylinder scattering problems using the multipole method. The index m in the multipole method is truncated to $|m| \leq 6$. For normal incident waves, we obtain the reflection spectrum shown in Fig. 3. The horizontal axis is the normalized frequency $\omega L/(2\pi c)$, where c is the speed of light in vacuum. The vertical axis is $|R_0|^2$, where R_0 is the reflection coefficient defined in (6). Our results are in good agreement with those in [9].

As the second example, we consider air-holes in a dielectric medium. The original structure was first analyzed by Sakota [16]. It consists of 16 layers of air-holes in a medium with a dielectric constant $n_0^2 = 2.1$. The air-holes are arranged in a square lattice with a lattice constant h. The radii of the air-holes are $a = 19h/68 \approx 0.2794h$. The structure has a total thickness of $D = 16h$. The homogeneous medium outside of structure is air.

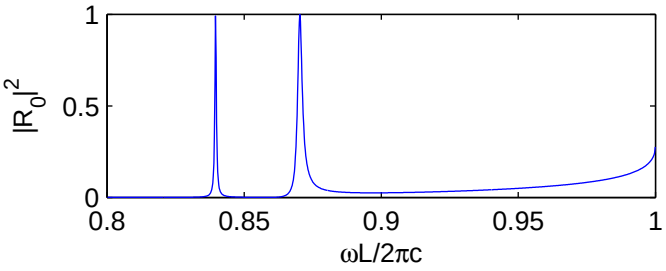

Figure 3: Reflection spectrum of the array of two different dielectric cylinders.

The transmission spectrum of this structure was first calculated by Sakoda [16] using a plane wave expansion of 2700 terms. Accurate solutions were obtained by the DtN operator marching method [11] using only 9 sampling points on each edge of the simple $h \times h$ unit cell. In that case, the operators Q and Y are approximated by 9×9 matrices.

In the following, we consider a modified structure where the cylinders are rearranged in groups of four. More precisely, the modified structure has $(2h) \times (2h)$ complex unit cells each containing four cylinders. It comprises 2 layers in the y direction (the total thickness is $D = 4h$) and is periodic in x with a period of $L = 2h$. As shown in Fig. 4, we consider two cases. In the first case, the four cylinders are moved close together

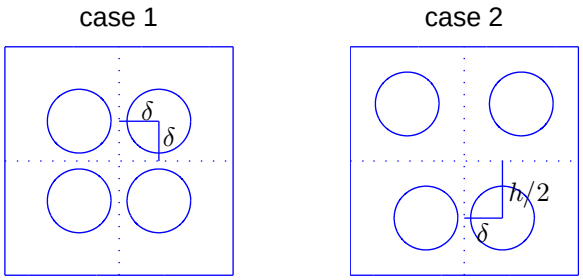

Figure 4: Complex unit cells of a finite photonic crystal structure (air-holes in a dielectric medium). Case 1: all four air-holes are moved closer to the center; case 2: two lower air-holes are moved closer horizontally.

approaching the center of the complex cell. If we consider the complex unit cell as given by $0 < x, y < 2h$, the x and y coordinates of the centers of the four cylinders are $h \pm \delta$. The original configuration corresponds to $\delta = h/2$. If $\delta = a$, the four cylinders touch each other. In the second case, the two lower cylinders in the complex cell are moved close together while the upper two cylinder are kept unchanged. The x coordinates of the centers of the two lower cylinders are $h \pm \delta$.

In our calculations, we use 9 sampling points on each edge of the complex unit cell. Therefore, the DtN map Λ is constructed from 36 special solutions corresponding to 36 different plane incident waves. The multipole method is used to compute these special

solutions with the integer m in (3) truncated to $|m| \leq 6$. To validate our method, we first consider the original configuration corresponding to $\delta = h/2$. The results are in good agreement with those in [11] and [16]. For the first case of the modified structure, we obtain the transmission spectra shown in Fig. 5 for $\delta = 1.5a$, $\delta = 1.1a$ and $\delta = 1.01a$.

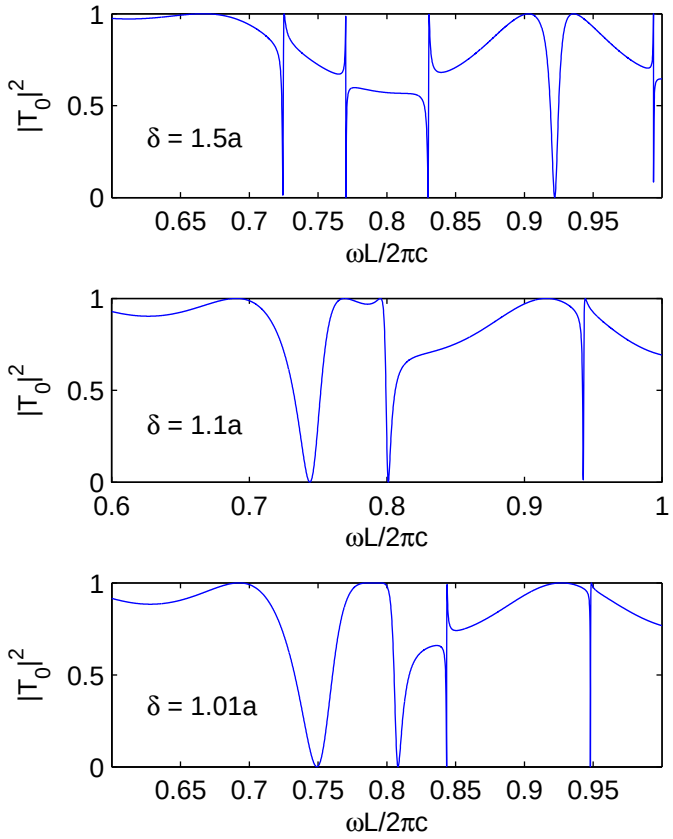

Figure 5: Transmission spectra of a finite photonic crystal (air-holes in a dielectric medium). Case 1: four air-holes are moved closer to the center.

In terms of the original lattice constant h, these values are $\delta \approx 0.4191h$, $\delta \approx 0.3074h$ and $\delta \approx 0.2822h$, respectively. For the second case where only the lower cylinders are moved, we obtain the transmission spectra shown in Fig. 6 for $\delta = 1.5a$ and $\delta = a$. For $\delta = a$, the two lower cylinders touch each other.

5 Conclusion

The Dirichlet-to-Neumann (DtN) operator of the unit cells of a photonic crystal can be used to develop efficient numerical algorithms. It allows us to take advantage of the periodicity of the PhC and to avoid computing the wave field in the interiors of the

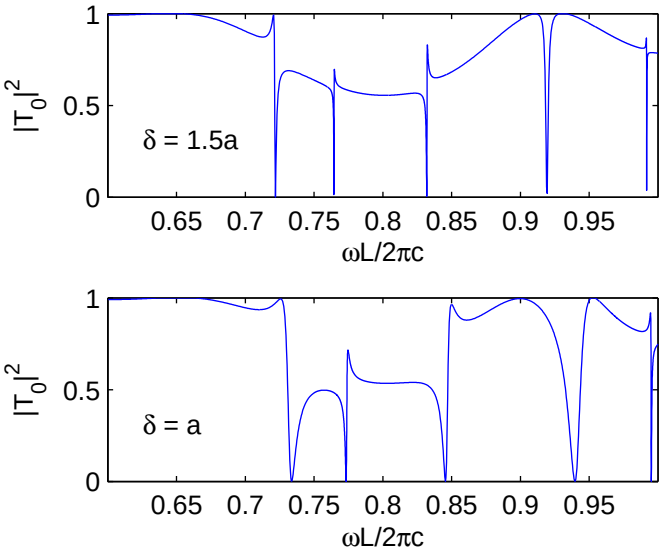

Figure 6: Transmission spectra of a finite photonic crystal (air-holes in a dielectric medium). Case 2: two lower air-holes are moved closer together.

unit cells. The DtN map of a simple unit cell containing one circular cylinder can be easily constructed from cylinderical waves [11]. In this paper, we developed a multipole method for constructing the DtN maps for complex unit cells containing more than one cylinders. The multipole method is used to solve scattering problems associated with the finite number of cylinders in one complex unit cell. Previous multipole methods [8, 9] for photonic crystals require sophisticated lattice sums techniques due to the involvement of infinitely many cylinders. The multipole DtN technique is illustrated by a number of calculations for structures with complex unit cells.

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