Analysis of two-dimensional photonic crystals using a multidomain pseudospectral method

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An analysis method based on a multidomain pseudospectral method is proposed for calculating the band diagrams of two-dimensional photonic crystals and is shown to possess excellent numerical convergence behavior and accuracy. The proposed scheme utilizes the multidomain Chebyshev collocation method. By applying Chebychev-Lagrange interpolating polynomials to the approximation of spatial derivatives at collocation points, the Helmholtz equation is converted into a matrix eigenvalue equation which is then solved for the eigenfrequencies by the shift inverse power method. Suitable multidomain division of the computational domain is performed to deal with general curved interfaces of the permittivity profile, and field continuity conditions are carefully imposed across the dielectric interfaces. The proposed method shows uniformly excellent convergence characteristics for both the transverse-electric and transverse-magnetic waves in the analysis of different structures. The analysis of a mini band gap is also shown to demonstrate the extremely high accuracy of the proposed method.

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I. INTRODUCTION

Band structures are essential characteristics of photonic crystals (PCs), from which possible photonic band gaps (PBGs) can be identified [1–3]. For frequencies within the PBGs, wave propagation is forbidden and many photonic devices have been proposed and designed based on this phenomenon. In particular, two-dimensional (2D) PCs composed of either dielectric rods or air columns have been widely employed in many applications such as waveguiding, resonant cavity formation, and wavelength filtering. In this paper, we propose an analysis scheme with excellent numerical convergence behavior and accuracy for calculating the band structures of 2D PCs. The currently most used numerical methods for such calculations have been the plane-wave expansion (PWE) method [3–6] and the finite-difference time-domain (FDTD) method [7,8]. The finite-difference eigenvalue problem formulation has also been employed by Yang [9] and Shen et al. [10], and more recently by Yu and Chang [11] based on the Yee mesh as often employed in the FDTD method [12]. The Yee-mesh-based formulation was named the finite-difference frequency-domain (FDFD) method. Yu and Chang [11] used the FDFD method to analyze the band structures of 2D PCs with either square or triangular lattices and adopted a fourth-order accurate compact finite-difference scheme [13] to increase numerical efficiency and accuracy. Although the FDFD method offers results with accuracy comparable to those obtained using the MIT photonic-bands (MPB) package [14] based on the PWE method, the numerical convergent speed was found not to be uniformly fast among different bands in the two methods.

The numerical formulation proposed in this paper is based on the multidomain pseudospectral method using Chebyshev polynomials. The pseudospectral method has recently attracted raised attention as an alternative treatment for computational electromagnetics because of its high-order accuracy and fast convergence behavior over traditional techniques while retaining formulation simplicity. It has a long history of being applied to fluid dynamics [15] and has recently been extended to the analysis of electromagnetics both in the time [16–18] and in the frequency domain [19]. However, while the theory of the pseudospectral method has been well elaborated, the application in the frequency domain has not received much focus compared with that in the time domain in the electromagnetics community. In [19], the pseudospectral frequency-domain method was proposed and applied to solve the nonhomogeneous (nonzero-source) Helmholtz equation in a simple two-subdomain problem with rectangular structure shape. Our proposed scheme in this paper utilizes the multidomain Chebyshev collocation method supported by the curvilinear mapping technique [20] to facilitate and ameliorate the simulation of 2D PCs of arbitrary permittivity profile. The formulation is derived in the form of an eigenvalue problem so that we can readily obtain the eigenmodes by available mathematical tools. Here, we adopt the shift inverse power method (SIPM) for its particularly fast convergence characteristic over other conventional methods applying matrix inversion. Both the multidomain pseudospectral algorithm and the SIPM furnish our pseudospectral mode solver (PSMS) as a quite powerful and flexible method. To obtain high-accuracy full-vectorial modal solutions for dielectric structures, proper satisfaction of dielectric interface conditions is essential, whether it is based on the finite-difference method [21,22], the finite-element method [23], or others. Such proper treatment of interface conditions will be carefully considered in our formulation.

The rest of this paper is outlined as follows. The physical problem involving the Helmholtz equations is described in Sec. II along with the required Dirichlet and Neumann type boundary conditions across the dielectric interfaces. The formulation of the PSMS is presented in Sec. III. Numerical examples including 2D PCs with either a square or a trian-

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II. THE PHYSICAL EQUATIONS

Assume that the 2D PC considered is composed of lossless isotropic dielectric materials, and is uniform along the z direction and periodic in the transverse x-y plane. We will only consider the in-plane propagation that has zero propagation constant in the z direction so that the wave modes in the PC are either transverse electric (TE) or transverse magnetic (TM) to the z modes. To obtain the band structures, we need only solve the electromagnetic problem within a 2D unit cell. Assume that the PC possesses a piecewise uniform refractive index distribution n; Fig. 1 shows a boundary of arbitrary shape between two homogeneous regions within the unit cell with n=n_a and n=n_b, respectively, and the same permeability as in free space. For TM modes, only E_x, H_y, and H_z components exist. For TE modes, only E_z, H_x, and H_y components exist. The fields are governed by the Helmholtz equation

\[(\nabla^2 + k^2)\phi(x,y) = -k^2 \phi(x,y)\]  \hspace{1cm} (1)

where \(\nabla\) is the del operator, \(k = \omega / c\) is the free-space wave number, \(\omega\) is the angular frequency, \(c\) is the speed of light in vacuum, and \(\phi = H_z\) and \(E_z\) for the TE and TM modes, respectively. By the Chebyshev collocation method which will be introduced in Sec. III, Eq. (1) leads to an \(\omega/c\)-formulation matrix eigenvalue equation of the form

\[ [P] \{\phi\} = - (\omega/c)^2 \{\phi\} \]  \hspace{1cm} (2)

where \(\{\phi\}\) is a vector composed of \(\phi\) values at grid points and \([P]\) is the operator matrix. The eigenvalues can be solved by applying the SIPM.

We now discuss the boundary conditions for the TE and TM modes. Since the tangential fields \((H_x, E_z)\) should be made continuous across the dielectric interfaces, referring to regions \(a\) and \(b\) in Fig. 1, we have the Dirichlet type boundary conditions

\[ H_x^a = H_x^b \]  \hspace{1cm} (3a)

for the TE mode and

\[ E_z^a = E_z^b \]  \hspace{1cm} (3b)

for the TM mode. We have another continuity condition in terms of the transverse components

\[ n_x \times (E_x^a + E_x^b) = n_x \times (E_x^b + E_x^a) \]  \hspace{1cm} (4a)

for the TE mode and

\[ n_y \times (H_y^a + H_y^b) = n_y \times (H_y^b + H_y^a) \]  \hspace{1cm} (4b)

for the TM mode, where \(n_x = n_a x + n_b y\) is the normal unit vector to the dielectric interface. From Maxwell’s curl equations, we have

\[ j \omega n E_x = -\frac{\partial H_z}{\partial y}, \]  \hspace{1cm} (5a)

\[ j \omega n E_y = -\frac{\partial H_z}{\partial x}, \]  \hspace{1cm} (5b)

for the TE mode and

\[ j \omega \mu_0 H_x = -\frac{\partial E_z}{\partial y}, \]  \hspace{1cm} (5c)

\[ j \omega \mu_0 H_y = -\frac{\partial E_z}{\partial x}, \]  \hspace{1cm} (5d)

for the TM mode. By substituting Eqs. (5a)–(5d) into Eqs. (4a) and (4b), we derive the following Neumann type boundary conditions

\[ n_x \frac{\partial H_y^a}{\partial y} + n_y \frac{\partial H_y^a}{\partial x} = \left( \frac{n_a}{n_b} \right)^2 \left( n_x \frac{\partial H_y^b}{\partial y} + n_y \frac{\partial H_y^b}{\partial x} \right) \]  \hspace{1cm} (6a)

for the TE mode and

\[ n_x \frac{\partial E_z^a}{\partial y} + n_y \frac{\partial E_z^a}{\partial x} = \left( \frac{n_a}{n_b} \right)^2 \left( n_x \frac{\partial E_z^b}{\partial y} + n_y \frac{\partial E_z^b}{\partial x} \right) \]  \hspace{1cm} (6b)

for the TM mode.

Due to the periodic geometry, we need to consider periodic boundary conditions (PBCs) at the boundaries of the unit cell for the field distribution in the PC. We will describe the PBCs for the respective cases in Sec. IV. In our numerical scheme, we combine the adjacent regions by imposing the Dirichlet and Neumann type boundary conditions on two sides of the interface to guarantee numerical stability.

III. THE MULTIDOMAIN PSEUDOSPECTRAL METHOD

The construction of the multidomain spectral collocation scheme for solving the Helmholtz equation is described in this section. The procedure to obtain a general form of the \([P]\) matrix in such a multidomain scheme will be discussed in detail.

A. The Chebyshev spectral method

For achieving better approximation characteristics in solving partial differential equations, we select the widely used
where the Chebyshev-Gauss-Lobatto grid \( x_i \) \( \cos \left( \frac{i \pi}{N} \right) \), \( i = 0, 1, 2, \ldots, N \). (8)

The Chebyshev collocation method provides a means to approximate the function \( f(x) \) by global Chebyshev-Lagrange interpolating polynomials of degree \( N \),

\[
 f(x) \approx \sum_{i=0}^{N} g(x_i) \xi(x),
\]

where the interpolating Chebyshev-Lagrange polynomials are given by

\[
 g_i(x) = \frac{(1-x^2)T_i'(x_i)(-1)^{i+1}}{c_i N^2(x-x_i)}
\]

with \( c_0 = c_N = 2 \) and \( c_i = 1 \) for \( 1 \leq i \leq N-1 \). Then, with the interpolation in Eq. (10), the spatial derivatives of \( f(x) \) at a collocation point \( x_i \) can be computed by a matrix operator with element entries \( D_{ij} = g_j'(x_i) \), i.e.,

\[
 \frac{df(x_i)}{dx} \approx \sum_{j=0}^{N} g_j'(x_i)f(x_j) = \sum_{j=0}^{N} D_{ij}f(x_j)
\]

where the explicit expression for \( D_{ij} \) is given in [15] as

\[
 D_{ij} = \begin{cases} 
 c_j \frac{(-1)^{i+j}}{x_i-x_j}, & i \neq j, \\
 -\frac{x_i}{2(1-x^2)}, & 1 \leq i = j \leq N-1, \\
 \frac{2N^2+1}{6}, & i = j = 0, \\
 -\frac{2N^2+1}{6}, & i = j = N. 
\end{cases}
\]

To extend the one-dimensional (1D) formula to a higher-dimensional problem, matrix products should be the most convenient treatment for computational simplicity. For the 2D PC analysis, we need to consider a 2D setting and define the approximation to \( f(x,y) \) as

\[
 f(x,y) = \sum_{i=0}^{M} \sum_{j=0}^{N} f(x_i,y_j)g_i(x)g_j(y)
\]

where the Chebyshev-Gauss-Lobatto grid \( y_j \) has been introduced. This approach has the benefit that the derivatives can be calculated through the 1D formula Eq. (11) and thus the differential formulas at the 2D collocation points arranged in a rectangular domain can be expressed as in the following matrix multiplication form:

\[
 \begin{bmatrix} 
 \frac{\partial f(x_0,y_0)}{\partial x} & \frac{\partial f(x_0,y_1)}{\partial x} & \cdots & \frac{\partial f(x_0,y_N)}{\partial x} \\
 \frac{\partial f(x_1,y_0)}{\partial x} & \frac{\partial f(x_1,y_1)}{\partial x} & \cdots & \frac{\partial f(x_1,y_N)}{\partial x} \\
 \vdots & \vdots & \ddots & \vdots \\
 \frac{\partial f(x_M,y_0)}{\partial x} & \frac{\partial f(x_M,y_1)}{\partial x} & \cdots & \frac{\partial f(x_M,y_N)}{\partial x} 
\end{bmatrix} = \frac{\partial f_{\text{rect}}}{\partial x}
\]

\[
 \begin{bmatrix} 
 \frac{\partial f(x_0,y_0)}{\partial y} & \frac{\partial f(x_0,y_1)}{\partial y} & \cdots & \frac{\partial f(x_0,y_N)}{\partial y} \\
 \frac{\partial f(x_1,y_0)}{\partial y} & \frac{\partial f(x_1,y_1)}{\partial y} & \cdots & \frac{\partial f(x_1,y_N)}{\partial y} \\
 \vdots & \vdots & \ddots & \vdots \\
 \frac{\partial f(x_M,y_0)}{\partial y} & \frac{\partial f(x_M,y_1)}{\partial y} & \cdots & \frac{\partial f(x_M,y_N)}{\partial y} 
\end{bmatrix} = \frac{\partial f_{\text{rect}}}{\partial y}
\]

where \( f_{\text{rect}} \) is an \((M+1) \times (N+1)\) matrix with entries \( f(x_i,y_j) \), \( i=0,1,2,\ldots,M \) and \( j=0,1,2,\ldots,N \), corresponding to collocation points in rectangular arrangement, \( D_{(M+1)\times(N+1)} \) is an \((M+1) \times (M+1)\) matrix with entries \( D_{ij} \) as defined by Eq. (12) but with \( N \) replaced by \( M \), and the superscript \( T \) denotes the transpose. However, the employment of matrix products is still restricted by the nature of rectangular grids, which is unsound to deal with curved boundaries. In the next section, a curvilinear representation will be introduced to overcome this barrier.

B. The curvilinear representation

In order to extend our numerical scheme defined above on rectangular grids to the analysis of structures with curved boundaries, a multidomain formulation and modified differential matrices will be established. We first split the whole computational domain into a series of nonoverlapping curvilinear quadrilaterals according to the profile and material distributions. Then by applying the transfinite blending function presented in [20], each curvilinear quadrilateral in Cartesian \((x,y)\) coordinates can be mapped onto a unit square one \([-1,1] \times [-1,1]\) in curvilinear \((\xi,\eta)\) coordinates, as shown in Fig. 2, under the transformation

\[
 \xi = \xi(x,y), \quad \eta = \eta(x,y).
\]

It yields the great advantage that we can thus calculate the spatial derivatives \( \partial f/\partial x \) and \( \partial f/\partial y \) in a subdomain with curved boundaries by the formulation defined on this unit element. By the fundamental differential principle, the modified differential matrices are expressed as
\[
\frac{\partial \xi(x,y)}{\partial x} \frac{\partial}{\partial \xi} = D_{\xi}\xi
\]

\[
= \begin{bmatrix}
\xi_{00} & \xi_{01}D_{01} & \cdots & \xi_{0M}D_{0M} \\
\xi_{10}D_{10} & \xi_{11}D_{11} & \cdots & \xi_{1M}D_{1M} \\
\vdots & \vdots & \ddots & \vdots \\
\xi_{M0}D_{M0} & \xi_{M1}D_{M1} & \cdots & \xi_{MM}D_{MM}
\end{bmatrix}_{(M+1)\times(M+1)}
\]

\[
\frac{\partial \eta(x,y)}{\partial x} \frac{\partial}{\partial \eta} = D_{\eta}\eta
\]

\[
= \begin{bmatrix}
\eta_{00} & \eta_{01}D_{01} & \cdots & \eta_{0N}D_{0N} \\
\eta_{10}D_{10} & \eta_{11}D_{11} & \cdots & \eta_{1N}D_{1N} \\
\vdots & \vdots & \ddots & \vdots \\
\eta_{N0}D_{N0} & \eta_{N1}D_{N1} & \cdots & \eta_{NN}D_{NN}
\end{bmatrix}_{(N+1)\times(N+1)}
\]

\[
\frac{\partial \xi(x,y)}{\partial y} \frac{\partial}{\partial \xi} = D_{\xi}\xi
\]

\[
= \begin{bmatrix}
\xi_{00} & \xi_{01}D_{01} & \cdots & \xi_{0M}D_{0M} \\
\xi_{10}D_{10} & \xi_{11}D_{11} & \cdots & \xi_{1M}D_{1M} \\
\vdots & \vdots & \ddots & \vdots \\
\xi_{M0}D_{M0} & \xi_{M1}D_{M1} & \cdots & \xi_{MM}D_{MM}
\end{bmatrix}_{(M+1)\times(M+1)}
\]

\[
\frac{\partial \eta(x,y)}{\partial y} \frac{\partial}{\partial \eta} = D_{\eta}\eta
\]

\[
= \begin{bmatrix}
\eta_{00} & \eta_{01}D_{01} & \cdots & \eta_{0N}D_{0N} \\
\eta_{10}D_{10} & \eta_{11}D_{11} & \cdots & \eta_{1N}D_{1N} \\
\vdots & \vdots & \ddots & \vdots \\
\eta_{N0}D_{N0} & \eta_{N1}D_{N1} & \cdots & \eta_{NN}D_{NN}
\end{bmatrix}_{(N+1)\times(N+1)}
\]

The operator matrix \([P]\) in Eq. (2) can be expressed in terms of other operators in Eq. (18) with slight modification.

The operator matrix \([P]\) in Eq. (2) can be expressed in terms of other operators in Eq. (18) with slight modification.
In Eq. (19), \( k = (M+1)(N+1) \),

\[
\tilde{D}_{\alpha\alpha} = \frac{\tilde{D}_{\alpha\alpha}}{\tilde{D}_{\alpha\alpha}} + \tilde{D}_{\alpha\beta} + \tilde{D}_{\beta\alpha} + \tilde{D}_{\beta\beta},
\]

\[
\begin{bmatrix}
\tilde{D}_{\alpha\alpha} & 0 & \ldots & 0 \\
0 & \tilde{D}_{\alpha\alpha} & \ldots & \vdots \\
\vdots & \ddots & \ddots & \vdots \\
0 & \ldots & 0 & \tilde{D}_{\alpha\alpha}
\end{bmatrix}
\]

where \( \tilde{D}_{\alpha\alpha} \) is a diagonal matrix of order \( M+1 \) with all diagonal elements being the constant \( a \).

In the generalization to the multidomain situation, we assume that the computational domain is divided into \( s \) subdomains. Under the \( \beta \) formulation, the matrix eigenvalue equation without imposing boundary conditions across the subdomain boundaries can be written as

\[
[P] = n^{-1} \begin{bmatrix}
\tilde{D}_{\alpha\alpha} & \tilde{D}_{\alpha\beta} \\
\tilde{D}_{\beta\alpha} & \tilde{D}_{\beta\beta}
\end{bmatrix} [\phi] = \omega \begin{bmatrix}
\phi_1 \\
\phi_2 \\
\vdots \\
\phi_s
\end{bmatrix}
\]

where the subscript of \( [P] \), \( i = 1, 2, \ldots, s \) represents the numbering of each subdomain. Then we can connect the adjacent subdomains by imposing the boundary conditions and possible PBCs on those matrix elements in Eq. (16) that correspond to the boundary nodes of the subdomain. In our numerical scheme, we have intentionally applied different types of boundary conditions (Dirichlet or Neumann type) to the adjacent subdomains to guarantee numerical stability. In the Appendix, we show how Eq. (20) will be modified when the boundary conditions are imposed. Finally, the field distributions (eigenvectors) and the eigenfrequencies (eigenvalues) can be obtained by using the SIPM.

FIG. 3. (Color online) (a) Cross section of a 2D square-lattice PC and its unit cell specified by the dashed lines. (b) Mesh and domain division profile for the unit cell.
IV. NUMERICAL EXAMPLES

We present in this section five numerical examples to demonstrate the inherent accuracy and excellent numerical convergence behavior of the PSMS in the analysis of 2D PCs. Comparison will be made with the FDFD method and the PWE method in the first four examples. The first two, the square-lattice and the triangular-lattice PCs, are those discussed in [11]. The third one is a PC having a large air hole in the unit cell. The fourth one relates to a PC composed of large dielectric pixels designed to possess large absolute band gaps [24]. The last example discusses the analysis of a mini band gap.

TABLE I. Normalized frequencies of TE first and second bands at the $M$ point for the square-lattice PC obtained with different polynomial degrees.

<table>
<thead>
<tr>
<th>$N$</th>
<th>Grid points</th>
<th>TE first mode</th>
<th>TE second mode</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>325</td>
<td>0.548961563774</td>
<td>0.603564998825</td>
</tr>
<tr>
<td>5</td>
<td>468</td>
<td>0.548847662048</td>
<td>0.602451830831</td>
</tr>
<tr>
<td>6</td>
<td>637</td>
<td>0.548861905144</td>
<td>0.601878879371</td>
</tr>
<tr>
<td>8</td>
<td>1053</td>
<td>0.548843381514</td>
<td>0.601903085785</td>
</tr>
<tr>
<td>12</td>
<td>2197</td>
<td>0.548843155002</td>
<td>0.60189903235</td>
</tr>
<tr>
<td>14</td>
<td>2925</td>
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<td>0.601898894833</td>
</tr>
<tr>
<td>18</td>
<td>4693</td>
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<td>0.601898894955</td>
</tr>
<tr>
<td>20</td>
<td>5733</td>
<td>0.548843160880</td>
<td>0.601898894965</td>
</tr>
</tbody>
</table>

A. PC with square lattice

We first investigate the square-arranged 2D PC, with its cross section in the $x$-$y$ plane as shown in Fig. 3(a), formed by parallel alumina rods with refractive index $n=8.91/2$ and radius $r=0.2a$ in the air, where $a$ is the lattice distance. The unit cell is specified by the dashed lines. The unit cell is divided into 13 subdomains, as shown in Fig. 3(b), with the four corner subdomains and the central subdomain being in a square shape and the other eight subdomains not in any rectangular shape. The mesh pattern of each subdomain shown is for $M=N=8$. When applying the boundary conditions Eqs. (3) and (6) at the boundaries of the unit cell, the following PBCs need to be carefully taken into account:

$$\psi(x, y + a) = e^{-jk_ya} \psi(x, y) \quad \text{(PBC1)},$$
$$\psi(x + a, y) = e^{-jk_xa} \psi(x, y) \quad \text{(PBC2)},$$

where $k_x$ and $k_y$ are the wave numbers in the $x$ and $y$ directions, respectively, and the boundaries at which the PBC1 or the PBC2 applies are indicated in Fig. 3(b). The calculated band diagrams of the TE and TM modes are plotted in Figs. 4(a) and 4(b), respectively. Each point along the boundary of the first Brillouin zone shown as the inset in Fig. 4(a) provides $k_x$ and $k_y$ in Eq. (21). The crosses are the results obtained using our PSMS based on Chebyshev polynomials of degree 12 ($M=N=12$). (In fact, using just $M=N=4$, the obtained results would be indistinguishable when plotted, as can be seen in the later discussion.) The circles are the results of the compact FDFD algorithm with the index average scheme and using 40 grid points in each lattice distance [11]...
where $J$ denotes the TE or TM mode, with $B_{ui}^{1\text{TE}} = n_x D_{xui} + n_y D_{yui}$, $B_{vi}^{1\text{TE}} = -(n_x/n_y)^2(n_x D_{xvi}^2 + n_y D_{yvi}^2)$, $B_{ui}^{1\text{TM}} = n_x D_{xui}$, and $B_{vi}^{2\text{TM}} = -(n_x D_{xvi}^2 + n_y D_{yvi}^2)$, where $i = 0, 1, \cdots, h$.

Note that, after imposing the two boundary conditions at one grid point, the dimension of the matrix eigenvalue equation is reduced by 2.