Efficient method for computing leaky modes in two-dimensional photonic crystal waveguides

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***Abstract*—An accurate and efficient numerical method is developed for computing leaky modes of two-dimensional photonic crystal (PhC) waveguides corresponding to line defects surrounded by finite PhCs. The method reformulates the eigenvalue problem on a single edge of the defect cell and uses exact boundary conditions at the edges of the surrounding PhC. Unlike previous works for leaky modes, perfectly matched layers or other absorbing boundary conditions are avoided.**

I. Introduction

Due to a periodic modulation of the refractive index, photonic crystals (PhCs) [1] exhibit frequency intervals, i.e. bandgaps, in which propagating electromagnetic waves do not exist. For frequencies in a bandgap, a line defect in a PhC can be used to guide light. Such PhC waveguides based on the bandgap effect can transmit light through sharp bends [2] and they are expected to play important roles in future photonic integrated circuits. In most theoretical studies, it is often assumed that the core of a PhC waveguide is surrounded by infinite bulk PhCs. In that case, the PhC waveguide support true guided modes with real propagation constants. In practice, the line defect is often surrounded by a finite PhC, then the PhC waveguide may have only leaky modes with complex propagation constants.

Many numerical methods have been developed to analyze band structures of PhCs [3]–[10]. If we replace the unit cell by one period of the waveguide, all these methods can be used to analyze PhC waveguides. To find the dispersion relation of a guide mode in a PhC waveguide, these methods follow the standard approach that calculates the frequency assuming that the Bloch wave vector component (i.e. the propagation constant of the PhC waveguide) is real and given [1]. However, for leaky modes, the complex propagation constant cannot be specified. Therefore, it is necessary to use the alternative approach that calculates the propagation constant for a given real frequency [11]–[17]. In the transverse direction, a leaky mode is very different from a guided mode. It behaves like an outgoing wave, but its magnitude actually increases as the distance from the waveguide core is increased (except in the finite PhC cladding). Most existing numerical methods for PhC waveguides require a truncation of the transverse variable so that one period of the waveguide is reduced to a finite computation domain. The perfectly matched layer (PML) is a widely used technique for truncating variables in modeling outgoing waves, and it has been used to analyze leaky PhC waveguides [16]. However, parameters in the PML profile must be chosen carefully, since the imaginary part of the complex propagation constant of a leaky mode is typically very small and improper PMLs can lead to large relative errors.

In this paper, we develop a new method for computing leaky modes in two-dimensional (2D) PhC waveguides. As in [17], we use exact boundary conditions to terminate the semi-infinite homogeneous media outside the finite PhC claddings. This allows us to avoid the PMLs, but it also turns the original linear eigenvalue problem to a nonlinear one. To solve the nonlinear eigenvalue problem effectively, we develop a fast method to establish a condition for the eigenvalue on one single edge. This is achieved by taking advantage of the geometric features of a typical PhC waveguide and calculating the Dirichlet-to-Neumann (DtN) maps of the unit cells. The DtN map of a unit cell is an operator (to be approximated by a small matrix) that maps the wave field to its normal derivative on the boundary of the cell. In earlier works, the DtN maps have been used to analyze band structures [13], [14], non-leaky PhC waveguides [15], microcavities [18], and various boundary value problems for PhC structures and devices [19]–[21]. Compared with the method in [15], our new method has the additional capability of computing leaky modes, and it is also more efficient because the problem established on one single edge is small and easy to solve.

II. Eigenvalue problems

We consider ideal 2D structures which are invariant in the z direction and assume that light waves are propagating in the xy plane, where $\{x, y, z\}$ forms a Cartesian coordinate system. Under these conditions, we can separately consider the E and H polarizations. For simplicity, we present our method only for the E polarization, since the treatment for the H polarization is similar. For the E polarization, the frequency domain Maxwell's equations are reduced to the following Helmholtz equation:

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

where U is the z component of the electric field, $n = n(x, y)$ is the refractive index, $k_0 = \omega/c$ is the free space wavenumber, ω is the angular frequency, the time dependence is assumed to be $e^{-i\omega t}$ and c is the speed of light in vacuum.

For a PhC waveguide whose axis is in the y direction, the refractive index is periodic in y with a period a, i.e.,

$$n(x, y + a) = n(x, y). \tag{2}$$

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In that case, Eq. (1) has Bloch mode solutions given as

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

where β is the Bloch wavenumber (i.e. the propagation constant) and Φ is periodic in y with the same period a. Such a solution only exists when ω and β satisfy some dispersion relations. The Bloch mode (3) is a guided mode if β is real and $\Phi \to 0$ as $|x| \to \infty$. To calculate dispersion relations of guided modes, a popular approach solves ω assuming β is real [1]. In that case, we can solve Eq. (1) directly in one period of the waveguide

$$S = \{(x,y) | -\infty < x < \infty, 0 < y < a\}, \tag{4}$$

subject to the following quasi-periodic conditions:

$$U(x,a) = \mu\, U(x,0), \quad \frac{\partial U}{\partial y}(x,a) = \mu\, \frac{\partial U}{\partial y}(x,0), \tag{5}$$

where $\mu = \exp(i\beta a)$. This is an eigenvalue problem where k_0^2 (or ω^2) is the eigenvalue. The domain S is still unbounded in both positive and negative directions of x. In practical numerical implementations, x has to be truncated. This is relatively simple, since the field of a guided mode decays exponentially to zero as $|x| \to \infty$. The truncated domain is discretized in the finite element [4], [5] and finite difference [9] methods. Alternatively, as in the plane wave expansion method [3], [6], the wave field on the truncated domain is approximated by a finite sum of given functions.

However, the above approach is not applicable to leaky modes for which β is complex. If the waveguide core is surrounded by finite PhCs so that the refractive index is a constant n_0 for $|x|$ sufficiently large, and if the refractive index of the core is not larger than n_0, then the structure may have no guided modes. In that case, a general wave field in such a structure consists of only radiation modes. The leaky modes are relevant because they provide the leading asymptotic behavior for the radiation fields. The imaginary part of β is associated with the attenuation of the leaky mode as it propagates forward along the waveguide axis. In the transverse directions, a leaky mode satisfies outgoing radiation conditions. But since β is complex, it actually blows up as $|x| \to \infty$. As a complex β cannot be specified, it is necessary to use the alternative approach that solves β assuming ω is given. If we insert the Bloch mode solution (3) into the governing Helmholtz equation (1), we obtain

$$\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} + k_0^2 n^2 \Phi + 2i\beta \frac{\partial \Phi}{\partial y} - \beta^2 \Phi = 0. \tag{6}$$

Therefore, we can solve Eq. (6) as a quadratic eigenvalue problem for eigenvalue β, on domain S subject to the following periodic conditions:

$$\Phi(x,a) = \Phi(x,0), \quad \frac{\partial \Phi}{\partial y}(x,a) = \frac{\partial \Phi}{\partial y}(x,0). \tag{7}$$

The above quadratic eigenvalue problem can be easily reduced to a linear eigenvalue problem. For $\Psi = \partial_y \Phi + i\beta\Phi$, we have

$$\begin{bmatrix} \partial_y & -1 \\ \partial_x^2 + k_0^2 n^2 & \partial_y \end{bmatrix} \begin{bmatrix} \Phi \\ \Psi \end{bmatrix} = -i\beta \begin{bmatrix} \Phi \\ \Psi \end{bmatrix}. \tag{8}$$

This approach is especially useful for dispersive media, since Eq. (8) is a linear eigenvalue problem even when the refractive index n varies with ω.

The eigenvalue problems above are formulated on one period of the waveguide, i.e. on domain S. After a truncation of S and a discretization, both formulations give matrix eigenvalue problems involving relatively large matrices. In connection with the second approach that solves β for a given ω, it is possible to reformulate the eigenvalue problem on the boundary of S, i.e., on the two lines at $y = 0$ and $y = a$. These boundary formulations can be obtained by scattering matrices [11], [12] or the Dirichlet-to-Neumann (DtN) map [15]. For domain S, the DtN map is the 2×2 operator matrix M satisfying

$$M \begin{bmatrix} U(x,0) \\ U(x,a) \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} U(x,0) \\ U(x,a) \end{bmatrix} = \frac{\partial}{\partial y} \begin{bmatrix} U(x,0) \\ U(x,a) \end{bmatrix}, \tag{9}$$

where M_{jk} ($1 \le j,k \le 2$) are operators acting on functions of x. If the two lines at $y = 0$ and $y = a$ are truncated and discretized by N points each, then M_{jk} is approximated by an $N \times N$ matrix. Using the quasi-periodic conditions (5), we obtain a linear eigenvalue problem for $\mu = \exp(i\beta a)$:

$$\begin{bmatrix} M_{11} & -1 \\ M_{21} & 0 \end{bmatrix} \begin{bmatrix} U_0 \\ V_0 \end{bmatrix} = \mu \begin{bmatrix} -M_{12} & 0 \\ -M_{22} & 1 \end{bmatrix} \begin{bmatrix} U_0 \\ V_0 \end{bmatrix}, \tag{10}$$

where $U_0 = U(x,0)$ and $V_0 = \partial_y U(x,0)$.

The eigenvalue problems above are formulated on domain S (one period of the waveguide) or the two lines at $y = 0$ and $y = a$. In both cases, the variable x is still unbounded. For a guided mode, the field decays exponentially away from the waveguide core, and we can use some simple boundary conditions for truncating x. In the supercell approach of the plane wave expansion method, one usually uses a periodic condition in x. For the finite element and finite difference methods, we can simply assume $U = 0$ on the truncated boundaries of x. For a leaky mode, the field exhibits outgoing radiation behavior and diverges as $|x| \to \infty$, therefore the periodic and simple zero boundary conditions are incorrect. In fact, these boundary conditions will only produce solutions with a real β if the medium is lossless. To overcome this difficulty, the perfectly matched layer (PML) technique can be used. A PML corresponds to a complex coordinate stretching where x is replaced by $\hat{x} = \int_0^x s(\tau)d\tau$ for some complex function $s(x)$. In [16], leaky modes are solved from the eigenvalue problem (8) using a PML for truncating x. However, a PML introduces a small undesired imaginary part to β, even if the waveguide is non-leaky and β should be real. As the true imaginary part of β of a leaky mode is often very small, it is not obvious that the obtained small imaginary part of β is correct when PMLs are used. Furthermore, if PMLs are used with the eigenvalue problem (8), the truncated domain is still quite large compared with the unit cell of the bulk PhC. A discretization leads to a matrix eigenvalue problem which is expensive to solve, since the matrices are large, complex and non-Hermitian. While the size of the matrices can be significantly reduced if we use the DtN formulation (10), it is desirable to completely avoid the PMLs. We present such a method in the following sections.

III. Exact boundary conditions

For simplicity, we consider 2D PhCs composed of circular cylinders on a square lattice (of lattice constant a) surrounded by a homogeneous medium of refractive index n_0. The cylinders can be dielectric rods or air columns, where the surrounding medium can be air or a dielectric medium, respectively. The cylinders are infinitely long and parallel to the z axis. A PhC waveguide is formed by removing one row of cylinders which is assumed to be along the y axis. In the x direction, the bulk PhC is finite, and we assume that there are m rows of cylinders for both $x < 0$ and $x > 0$. In Fig. 1, we show one period of the PhC waveguide (i.e. the domain S) for the special case of $m = 3$. Besides the homogeneous medium that extends to plus and minus infinity, the domain S contains $2m + 1$ square unit cells ($2m$ regular and one defect unit cells). We assume that the vertical edges of these unit cells are located at x_j for $0 \le j \le 2m + 1$, where $x_j = x_{j-1} + a$ and $x_{2m+1} = -x_0 = (m + 0.5)a$.

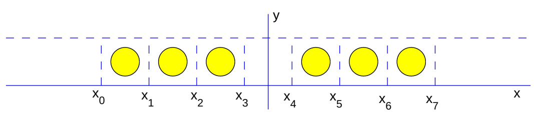

Fig. 1. One period of a leaky PhC waveguide with 3 rows of dielectric rods in each side of a missing row.

To avoid truncating x by PMLs or other absorbing layers, we can use exact boundary conditions at $x = x_0$ and $x = x_{2m+1}$ [17]. The price we pay is that the boundary conditions depend on both β and ω, and thus the eigenvalue problems become nonlinear. In fact, these boundary conditions are identical to those used in the theory of diffraction gratings [22]. However, some care is needed when these conditions are extended to cover leaky modes with complex β.

To obtain the boundary condition at x_{2m+1}, we consider the Bloch mode given in (3). Using Fourier series of Φ for its y variable, we obtain

$$U(x,y) = \sum_{l=-\infty}^{\infty} c_l \, e^{i(\alpha_l x + \beta_l y)} \quad \text{for} \quad x > x_{2m+1}, \qquad (11)$$

where $\beta_l = \beta + 2\pi l/a$, α_l satisfies $\alpha_l^2 + \beta_l^2 = k_0^2 n_0^2$, n_0 is the real refractive index of the medium surrounding the cylinders, and c_l is an unknown coefficient. When β is real, we can choose α_l as

$$\alpha_l = \sqrt{k_0^2 n_0^2 - \beta_l^2}. \qquad (12)$$

If $k_0 n_0 < |\beta_l|$, we should have $\alpha_l = i\sqrt{\beta_l^2 - k_0^2 n_0^2}$, then the terms in (11) are either outgoing plane waves propagating towards $x = +\infty$ or evanescent waves that decay as $x \to +\infty$. Notice that the standard complex square root function is defined as $\sqrt{z} = \sqrt{|z|} e^{i\theta/2}$ if $z = |z| e^{i\theta}$ for $-\pi < \theta \le \pi$, and it has a branch cut along the negative real line. For a real β, this definition still gives the correct α_l for $k_0 n_0 < |\beta_l|$ due to its special choice for phase angle $\theta = \pi$. However, for a leaky mode, β has a small positive imaginary part. For some l, the complex number $k_0^2 n_0^2 - \beta_l^2$ has a negative real part and a small and negative imaginary part, then the standard square root function would produce an α_l with a negative imaginary part. This leads to incorrect exponential grow of the evanescent waves. To overcome this difficulty, we define the square root function by rotating the branch cut to the negative imaginary axis:

$$\sqrt{z} = \sqrt{|z|} e^{i\theta/2}, \text{ if } z = |z| e^{i\theta} \text{ for } -\frac{\pi}{2} < \theta \le \frac{3\pi}{2}. \qquad (13)$$

With this definition, when β has a small imaginary part, α_l given in (12) is always close to the positive real axis or the positive imaginary axis. This ensures the continuous dependence of α_l on the imaginary part of β. Notice that α_l may have a small negative imaginary part and a positive real part for some l. This corresponds to an outgoing wave (towards $x = +\infty$) with a growing amplitude.

Let us define a linear operator $\mathcal{L}$ by

$$\mathcal{L} \, e^{i\beta_l y} = i\alpha_l \, e^{i\beta_l y}, \quad l = 0, \pm 1, \pm 2, \ldots \qquad (14)$$

For a general quasi-periodic function g satisfying $g(y) = e^{i\beta y} h(y)$, where h is periodic in y with period a, we can expand h in its Fourier series and re-write g as

$$g(y) = \sum_{l=-\infty}^{\infty} \hat{h}_l e^{i\beta_l y},$$

where

$$\hat{h}_l = \frac{1}{a}\int_0^a h(y) e^{-i2\pi l y/a} dy = \frac{1}{a}\int_0^a g(y) e^{-i\beta_l y} dy.$$

From the linearity of $\mathcal{L}$, we evaluate $\mathcal{L} g$ by

$$(\mathcal{L} g)(y) = \sum_{l=-\infty}^{\infty} i\alpha_l \hat{h}_l e^{i\beta_l y}.$$

From (11), we can easily evaluate $\partial_x U$. This leads to the exact boundary condition at x_{2m+1} involving the operator $\mathcal{L}$:

$$\frac{\partial U}{\partial x} = \mathcal{L} U \quad \text{at} \quad x = x_{2m+1}. \qquad (15)$$

The exact boundary condition at x_0 is similar. We have

$$\frac{\partial U}{\partial x} = -\mathcal{L} U \quad \text{at} \quad x = x_0. \qquad (16)$$

If we use K sampling points on each vertical edge for $0 < y < a$, the operator $\mathcal{L}$ can be approximated by a $K \times K$ matrix.

Since the operator $\mathcal{L}$ depends on ω and β, the eigenvalue problems with the exact boundary conditions are nonlinear. In the next section, we develop an efficient method by reducing the nonlinear eigenvalue problem to a condition on one single edge.

IV. Condition on a single edge

The boundary conditions (15) and (16) allow us to formulate the problem on the finite domain

$$S_t = \{(x,y) | x_0 < x < x_{2m+1}, 0 < y < a\}. \qquad (17)$$

The Helmholtz equation (1), the quasi-periodic conditions (5) and the exact boundary conditions (15) and (16) give rise to a nonlinear eigenvalue problem on S_t. In general, it is expensive to solve this nonlinear eigenvalue problem on S_t directly. Tausch and Butler [17] suggested to calculate the operator $\mathcal{P}$ such that

$$\mathcal{P}\begin{bmatrix} U(x_0,y) \\ U(x_{2m+1},y) \end{bmatrix} = \frac{\partial}{\partial x}\begin{bmatrix} U(x_0,y) \\ U(x_{2m+1},y) \end{bmatrix}$$

for all U satisfying the Helhomtz equation (1) and the quasi-periodic condition (5), and use $\mathcal{P}$ to obtain a nonlinear condition on the two vertical edges at x_0 and x_{2m+1}. While the final nonlinear condition on the two edges is small, the operator $\mathcal{P}$ is expensive to calculate. In particular, $\mathcal{P}$ depends on β and ω. Therefore, in an iterative scheme for solving β, it is necessary to calculate a new $\mathcal{P}$ for each iteration.

We present a special method for PhC waveguides. As in Section 3, the domain S_t is composed of $2m+1$ unit cells. Our approach is to calculate the DtN maps of these unit cells and use them to establish a condition for β on one single edge. Unlike the operator $\mathcal{P}$ above, the DtN maps of the unit cells do not depend on β and they only need to be calculated once. Although we can use these DtN maps of the unit cells to find $\mathcal{P}$ and establish a condition on the two vertical edges at x_0 and x_{2m+1} as in [17], it is easier and more convenient to establish a condition on one horizontal edge in the waveguide core.

The unit cells in S_t are

$$\Omega_j = \{(x,y) \mid x_{j-1} < x < x_j,\, 0 < y < a\},$$

for $1 \le j \le 2m+1$. Notice that Ω_{m+1} is the defect unit cell of a homogeneous medium and all other unit cells are the regular unit cells of the bulk PhC. For a regular unit cell Ω_j, $j \ne m+1$, we find the DtN operator Λ that maps U on the boundary of Ω_j to its normal derivative. More precisely, we have

$$\Lambda \begin{bmatrix} u_{j-1} \\ v_{j0} \\ v_{ja} \\ u_j \end{bmatrix} = \begin{bmatrix} \partial_x u_{j-1} \\ \partial_y v_{j0} \\ \partial_y v_{ja} \\ \partial_x u_j \end{bmatrix}, \tag{18}$$

where $u_{j-1} = U(x_{j-1},y)$, $u_j = U(x_j,y)$ for $0 < y < a$ and $v_{j0} = U(x,0)$, $v_{ja} = U(x,a)$ for $x_{j-1} < x < x_j$, etc. The components in the right hand side of (18) are the x or y derivatives of U evaluated on the four edges of Ω_j. When each edge of Ω_j is discretized by K points, Λ is approximated by a $(4K)\times(4K)$ matrix. A simple method for constructing Λ is given in [13], [19]. It is based on approximating the general solution of the Helmholtz equation in Ω_j by a sum of $4K$ cylindrical waves. Similarly, we can find the DtN map $\tilde{\Lambda}$ of the defect cell Ω_{m+1}.

For a given β, using the DtN map Λ and the quasi-periodic conditions (5), we can eliminate the horizontal edges and find the reduced DtN map $\mathcal{M}$ satisfying

$$\mathcal{M}\begin{bmatrix} u_{j-1} \\ u_j \end{bmatrix} = \begin{bmatrix} \mathcal{M}_{11} & \mathcal{M}_{12} \\ \mathcal{M}_{21} & \mathcal{M}_{22} \end{bmatrix}\begin{bmatrix} u_{j-1} \\ u_j \end{bmatrix} = \begin{bmatrix} \partial_x u_{j-1} \\ \partial_x u_j \end{bmatrix}. \tag{19}$$

This is a simple elimination step and an explicit formula is given in [19]. In the discrete case, $\mathcal{M}$ is approximated by a $(2K)\times(2K)$ matrix. Next, we consider a sequence of operators $\mathcal{Q}_j$, for $0 \le j \le 2m+1$, satisfying

$$\partial_x u_j = \mathcal{Q}_j u_j. \tag{20}$$

At x_0, we have the exact boundary condition (16), therefore $\mathcal{Q}_0 = -\mathcal{L}$. Now for $j = 1, 2, ..., m$, if $\mathcal{Q}_{j-1}$ is known, we can find $\mathcal{Q}_j$ based on the reduced DtN map $\mathcal{M}$. Using (20) at the right hand side of (19), we obtain

$$\mathcal{Q}_j = \mathcal{M}_{22} + \mathcal{M}_{21}\left(\mathcal{Q}_{j-1} - \mathcal{M}_{11}\right)^{-1}\mathcal{M}_{12}. \tag{21}$$

This leads to $\mathcal{Q}_m$ at x_m. Similarly, we can calculate $\mathcal{Q}_{m+1}$ at $x = x_{m+1}$ starting from $\mathcal{Q}_{2m+1} = \mathcal{L}$ at $x = x_{2m+1}$.

The DtN map of the defect cell Ω_{m+1} satisfies

$$\tilde{\Lambda}\begin{bmatrix} u_m \\ w_0 \\ w_1 \\ u_{m+1} \end{bmatrix} = \begin{bmatrix} \partial_x u_m \\ \partial_y w_0 \\ \partial_y w_1 \\ \partial_x u_{m+1} \end{bmatrix}, \tag{22}$$

where $w_0 = v_{m+1,0} = U(x,0)$ and $w_1 = v_{m+1,a} = U(x,a)$ for $x_m < x < x_{m+1}$. Writing $\tilde{\Lambda}$ in 4×4 blocks ($\tilde{\Lambda}_{kl}$ for $1 \le k,l \le 4$) where each block is a $K\times K$ matrix, using the quasi-periodic condition (5) and the operators $\mathcal{Q}_m$ and $\mathcal{Q}_{m+1}$, we can eliminate w_1, u_m and u_{m+1}, and obtain

$$\mathcal{A}\, w_0 = 0 \tag{23}$$

where

$$\begin{aligned} \mathcal{A} &= \tilde{\Lambda}_{32} - \mu\tilde{\Lambda}_{22} + \mu\tilde{\Lambda}_{33} - \mu^2\tilde{\Lambda}_{23} \\ &- \left[\tilde{\Lambda}_{31} - \mu\tilde{\Lambda}_{21}, \quad \tilde{\Lambda}_{34} - \mu\tilde{\Lambda}_{24}\right]\mathcal{X}, \end{aligned}$$

and $\mathcal{X}$ satisfies

$$\begin{bmatrix} \tilde{\Lambda}_{11} - \mathcal{Q}_m & \tilde{\Lambda}_{14} \\ \tilde{\Lambda}_{41} & \tilde{\Lambda}_{44} - \mathcal{Q}_{m+1} \end{bmatrix}\mathcal{X} = \begin{bmatrix} \tilde{\Lambda}_{12} + \mu\tilde{\Lambda}_{13} \\ \tilde{\Lambda}_{42} + \mu\tilde{\Lambda}_{43} \end{bmatrix}.$$

Notice that the operators $\mathcal{A}$, $\mathcal{Q}_j$ and $\mathcal{M}$ all depend on β, but Λ and $\tilde{\Lambda}$ are independent of β. To actually find β, we apply a nonlinear equation solver such as the Müller's method to

$$\lambda_1(\mathcal{A}) = 0, \tag{24}$$

where λ_1 is the smallest eigenvalue of $\mathcal{A}$ in absolute value. Our method is efficient, since $\mathcal{A}$ can be approximated by a very small matrix.

V. Numerical examples

For numerical examples, we consider PhC waveguides formed by removing one row from a square lattice of dielectric rods in free space. As in [16], we assume that the radius and the refractive index of the rods are $0.2a$ and $\sqrt{11.9}$, respectively, and analyze the waveguide at the fixed normalized frequency $\omega a/(2\pi c) = 0.35$. In the direction perpendicular to the waveguide axis, the PhC is finite, and there are m rows in each side of the waveguide core (i.e., the missing row at the center). One period of the waveguide is shown in Fig. 1 for $m = 3$. The structure has been previously analyzed by Zhang and Jia [16] based on the scattering matrix for one period of the waveguide. The scheme is similar to the eigenvalue problem (10) formulated on the two lines at $y = 0$ and $y = a$, since the scattering matrix is associated with field expansions on these two lines. The scattering matrix requires extra effort to calculate, but it gives rise to much smaller matrices compared with the eigenvalue problem (8) formulated on domain S (one period of the waveguide) directly. In [16], Zhang and Jia used

PMLs to terminate the transverse direction, Fourier series in the x direction for discretization, divided S into many small y-invariant segments, calculated the scattering matrix for each segment and then obtained the scattering matrix for the whole domain S. Both the staircase approximation in y and the PMLs can limit the accuracy of their solutions.

Based on our method that formulates the eigenvalue problem on one edge of the defect cell (i.e. at $y = 0$ for $|x| < a/2$), we have obtained accurate solutions with minimal computation effort. The normalized propagation constant up to 7 digits are given as follows:

$$\begin{aligned} \beta a/(2\pi) &\approx 0.2128996 + 0.0012394i, \quad m = 2, \\ \beta a/(2\pi) &\approx 0.2126575 + 0.0000956i, \quad m = 3, \\ \beta a/(2\pi) &\approx 0.2126399 + 0.0000006i, \quad m = 4. \end{aligned}$$

The corresponding eigenmodes are shown in Fig. 2. Our results agree with those in [16] up to the first three digits in the real part of β and first four digits in the imaginary parts of β. To further validate our results, we have varied K (the number of sampling points on each edge) from $K = 5$ to $K = 30$. A clear convergence is observed to the 7 digits shown above. Since the wave field in each unit cell is approximated by $4K$ cylindrical waves (implicit in the construction of the DtN maps) and cylindrical wave expansions are known to have exponential convergences, a typical value of K can be quite small. In fact, we can obtain 5 significant digits for K less than 10.

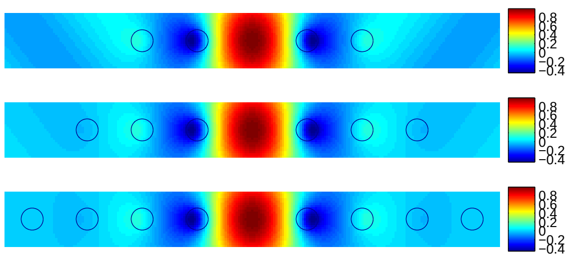

Fig. 2. Electric field patterns (real part of U) of the leaky photonic crystal waveguide modes.

Although we need to solve a nonlinear eigenvalue problem, only a few iterations are needed when Müller's method is applied to solve (24). Before the iteration for β is started, we need to calculate the DtN maps Λ and $\hat{\Lambda}$ for the regular and defect unit cells, respectively. These two operators are represented by $(4K)\times(4K)$ matrices and they can be obtained using $O((4K)^3)$ operations [13], [19]. Since Λ and $\tilde{\Lambda}$ do not depend on β, they are only calculated once. For each iteration where an approximate β is given, we need to find the boundary operator $\mathcal{L}$, calculate the reduced DtN map $\mathcal{M}$, find $\mathcal{Q}_m$ and $\mathcal{Q}_{m+1}$ by marching $\mathcal{Q}_j$ cell by cell, and finally calculate the matrix $\mathcal{A}$. The whole process requires only $O(mK^3)$ operations. Once the eigenvalue β is obtained, we first calculate the wave field on the edges of the unit cells and then use the cylindrical wave expansions in each unit cell to reconstruct the field at any desired location.

VI. Conclusion

In this paper, we developed an efficient numerical method for computing leaky modes in 2D PhC waveguides. These modes have a complex propagation constant β at a real frequency. The small imaginary part of β is an important parameter that indicates the attenuation of the field propagating along the waveguide. Finding the imaginary part of β accurately is not easy using existing numerical methods involving perfectly matched layers and staircase approximations for dielectric interfaces. Instead of solving an eigenvalue problem on a 2D domain covering one period of the waveguide, we reduce the problem to one single edge of the defect cell. The reduction process makes use of the the DtN maps of the unit cells. Our method also avoids PMLs by imposing exact boundary conditions that terminate the homogeneous semi-infinite media outside the PhC claddings. The accuracy and efficiency of our method are illustrated in numerical examples.

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