Dirichlet-to-Neumann transparent boundary conditions for photonic crystal wave-guides

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***Abstract*—In this work we present a method for the exact computation of guided modes in photonic crystal (PhC) wave-guides. In contrast to the super-cell method [1], [2], our proposed approach does not introduce any modelling error and is hence independent of the confinement of the modes. The approach is based on Dirichlet-to-Neumann (DtN) transparent boundary conditions that yield a non-linear eigenvalue problem. For the solution of this non-linear eigenvalue problem we propose a direct technique using Chebyshev interpolation. We show numerical results that demonstrate the convergence of our method.**

***Index Terms*—Photonic crystals, Boundary conditions, Eigenvalues and eigenfunctions, Finite element methods, Nonlinear equations.**

I. Introduction

We consider the problem of finding guided modes in 2D planar PhCs. For simplicity we restrict our presentation to the transverse magnetic (TM) mode, but the whole method can directly be transferred to the transverse electric (TE) mode.

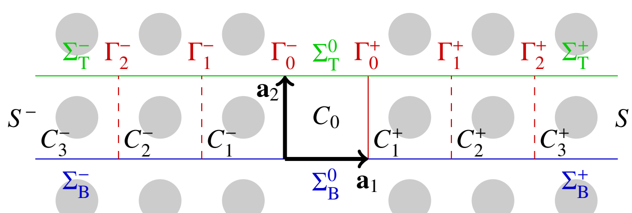

Figure 1: Sketch of the PhC wave-guide and the periodicity strip $S = S^+ \cup C_0 \cup S^-$, its unit cells $C_n^\pm$ with left/right boundaries $\Gamma_n^\pm$, its top/bottom boundaries $\Sigma_T = \Sigma_T^+ \cup \Sigma_T^0 \cup \Sigma_T^-$ and $\Sigma_B = \Sigma_B^+ \cup \Sigma_B^0 \cup \Sigma_B^-$, and its periodicity vectors $\mathbf{a}_1$ and $\mathbf{a}_2$.

Guided modes, which are modes that decay for $|\mathbf{x}_1| \to \infty$, are represented by Bloch modes e_k that satisfy

$$-\Delta e_k(\mathbf{x}) - \omega^2 \varepsilon(\mathbf{x}) e_k(\mathbf{x}) = 0 \tag{1a}$$

in the infinite strip $S = S^+ \cup C_0 \cup S^- \subset \mathbb{R}^2$, *c.f.* Fig. 1, with quasi-periodic boundary conditions

$$e_k|_{\Sigma_T} = e^{ik|\mathbf{a}_2|} e_k|_{\Sigma_B}, \qquad \partial_{\mathbf{n}} e_k|_{\Sigma_T} = -e^{ik|\mathbf{a}_2|} \partial_{\mathbf{n}} e_k|_{\Sigma_B}, \tag{1b}$$

where the parameter $k \in B$ is the so-called quasi-momentum in the one-dimensional Brillouin zone $B = [-\pi/|\mathbf{a}_2|, \pi/|\mathbf{a}_2|]$, and the operator $\partial_{\mathbf{n}}$ denotes the normal derivative $\partial_{\mathbf{n}} = \mathbf{n} \cdot \nabla$ with the unit normal vector $\mathbf{n}$ outward to the domain S. We assume a piecewise definition of the relative permittivity $\varepsilon : \mathbb{R}^2 \mapsto \mathbb{R}^+$, taking different values in the holes/rods (grey circles in Fig. 1) and in the bulk (white).

With the substitution $e_k(\mathbf{x}) = e^{ikx_2} u(\mathbf{x})$, the eigenvalue problem (1) is equivalent to: find couples $(\omega^2, k) \in \mathbb{R}^+ \times B$ such that there exists a guided mode u that satisfies

$$-(\nabla + ik\mathbf{a}_2) \cdot (\nabla + ik\mathbf{a}_2) u(\mathbf{x}) - \omega^2 \varepsilon(\mathbf{x}) u(\mathbf{x}) = 0, \qquad \mathbf{x} \in S. \tag{2}$$

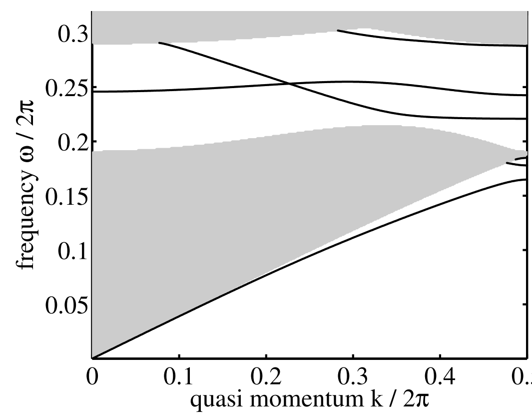

Figure 2: Band structure of hexagonal W1 PhC wave-guide.

II. Non-linear eigenvalue problem using DtN operators

A. Definition of the DtN operators

In order to define the DtN operators, let us introduce Dirichlet problems in the infinite half-strips $S^\pm$: for any Dirichlet trace φ on $\Gamma_0^\pm$ find $u^\pm \equiv u^\pm(\mathbf{x}; \omega, k, \varphi)$ such that

$$-(\nabla + ik\mathbf{a}_2) \cdot (\nabla + ik\mathbf{a}_2) u^\pm - \omega^2 \varepsilon(\mathbf{x}) u^\pm = 0, \qquad \mathbf{x} \in S^\pm, \tag{3a}$$

$$u^\pm|_{\Gamma_0^\pm} = \varphi. \tag{3b}$$

Then we define the DtN operators $\Lambda^\pm(\omega, k)$ as linear mappings of the Dirichlet trace φ to the Neumann trace on $\Gamma_0^\pm$

$$\Lambda^\pm(\omega, k)\,\varphi = \mp \partial_1 u^\pm(\cdot\,; \omega, k, \varphi)|_{\Gamma_0^\pm}\,. \tag{4}$$

With this definition of the DtN operators the problem (2) is equivalent to: find couples $(\omega^2, k) \in \mathbb{R}^+ \times B$ such that there exists a non-trivial u that satisfies

$$-(\nabla + ik\mathbf{a}_2) \cdot (\nabla + ik\mathbf{a}_2) u(\mathbf{x}) - \omega^2 \varepsilon(\mathbf{x}) u(\mathbf{x}) = 0 \tag{5a}$$

in the defect cell C_0 with DtN transparent boundary conditions

$$-\partial_1 u(\mathbf{x}) = \Lambda^+(\omega,k)\, u(\mathbf{x}), \qquad \mathbf{x} \in \Gamma_0^+, \tag{5b}$$

$$\partial_1 u(\mathbf{x}) = \Lambda^-(\omega,k)\, u(\mathbf{x}), \qquad \mathbf{x} \in \Gamma_0^-. \tag{5c}$$

In contrast to (2) this eigenvalue problem is non-linear but posed on the bounded domain C_0.

B. Characterization of the DtN operators

Let us introduce the propagation operator $\mathcal{P}^\pm(\omega,k)$ that maps a Dirichlet trace φ on $\Gamma_0^\pm$ to the Dirichlet trace of the half strip solution $u^\pm$ of (3) on $\Gamma_1^\pm$, *i. e.* $\mathcal{P}^\pm(\omega,k)\,\varphi = u^\pm(\cdot\,;\omega,k,\varphi)\,|_{\Gamma_1^\pm}$. The propagation operator $\mathcal{P}^\pm(\omega,k)$ is the unique solution of the quadratic equation

$$\mathcal{T}_{10}^\pm(\mathcal{P}^\pm)^2 + (\mathcal{T}_{00}^\pm + \mathcal{T}_{11}^\pm)\mathcal{P}^\pm + \mathcal{T}_{01}^\pm = 0 \tag{6}$$

with spectral radius strictly less than 1, where the operators $\mathcal{T}_{ij}^\pm = \mathcal{T}_{ij}^\pm(\omega,k)$ are defined by $\mathcal{T}_{ij}^\pm(\omega,k)\,\varphi = \partial_{\mathbf{n}} u_i^\pm(\cdot\,;\omega,k,\varphi))|_{\Gamma_j^\pm}$ for any Dirichlet trace φ on $\Gamma_0^\pm$, where $u_i^\pm \equiv u_i^\pm(\mathbf{x};\omega,k,\varphi)$, solve the Dirichlet cell problems

$$-(\nabla + \mathrm{i}k\mathbf{a}_2)\cdot(\nabla + \mathrm{i}k\mathbf{a}_2)u_i^\pm - \omega^2\varepsilon(\mathbf{x})u_i^\pm = 0, \qquad \mathbf{x} \in C_1^\pm, \tag{7a}$$

$$u_i^\pm\,|_{\Gamma_j^\pm} = \delta_{ij}\,\varphi. \tag{7b}$$

Then the DtN operators $\Lambda^\pm(\omega,k)$ are given by

$$\Lambda^\pm(\omega,k) = \mathcal{T}_{00}^\pm(\omega,k) + \mathcal{T}_{10}^\pm(\omega,k)\,\mathcal{P}^\pm(\omega,k). \tag{8}$$

III. Discretization

For the discretization of this problem we use high-order finite elements on quadrilaterals with curved edges as provided by the C++ library Concepts [5].

In discrete sense the operators $\mathcal{T}_{ij}^\pm$ are matrices $\mathbf{T}_{ij}^\pm$ whose number of columns/rows is equal to the number of degrees of freedom on the boundaries $\Gamma^\pm$. Consequently, also the propagation operators $\mathcal{P}^\pm$ are — in discrete sense — equivalent to matrices $\mathbf{P}^\pm$ of the same size as $\mathbf{T}_{ij}^\pm$ satisfying the quadratic, matrix-valued equation of the form (6) and having only eigenvalues of magnitude strictly less than 1. Finally, interpreting Eq. (8) in discrete sense, the DtN operators $\Lambda^\pm$ can be understood as matrices $\mathbf{D}^\pm$.

These DtN matrices $\mathbf{D}^\pm$ are added as dense blocks to the stiffness, mass and advection matrices that correspond to the left hand side of (5a). This yields the non-linear, matrix-valued eigenvalue problem

$$\mathbf{N}(\omega,k)\,\mathbf{u} = 0. \tag{9}$$

IV. Linearization of the non-linear eigenvalue problem

The non-linear, matrix-valued eigenvalue problem (9) can be linearized using the Chebyshev interpolation [6]. This linearization can be realized according to both, the ω-formulation and the k-formulation. If we choose the k-formulation for example, we have to fix — additionally to the value of the frequency ω — an interval of k that lies entirely inside the bandgap. In this interval we place d Chebyshev nodes to obtain a polynomial eigenvalue problem of degree d which can be linearized yielding a linear eigenvalue problem whose size is d-times larger than the original, non-linear eigenvalue problem. However, thanks to the special properties of the Chebyshev interpolation, we only have to invert a matrix of the same size as the original problem, if we apply a shift and invert strategy to the linear eigenvalue problem.

V. Numerical results

Let us now present numerical results of our proposed DtN method applied to a W1 PhC wave-guide with hexagonal lattice and holes of relative radius $r/|\mathbf{a}_2| = 0.31$ filled with air ($\varepsilon = 1$) in a homogeneous and isotropic dielectric material of relative permittivity $\varepsilon = 11.4$. We study the TE mode for which we plotted the band structure in Fig. 2. The computation was performed using a polynomial degree of $p = 7$ and taking $d = 10$ Chebyshev nodes.

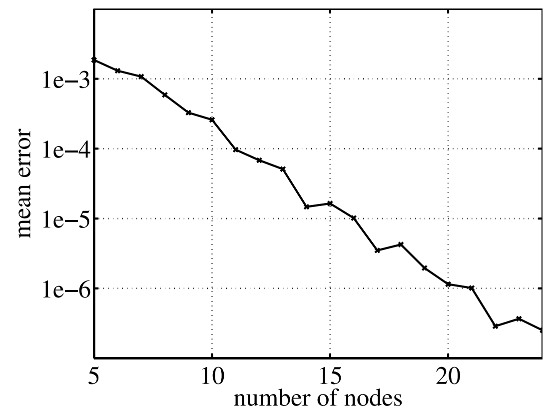

Figure 3: Convergence of the error of the Chebyshev linearization with respect to the number of Chebyshev nodes.

The error of the Chebyshev linearization is presented in Fig. 3, where the mean error $\frac{1}{200}\sum_{i=1}^{200}|k_{\mathrm{Cheb},i} - k_{\mathrm{ref},i}|$ of the eigenvalues $k_{\mathrm{Cheb},i}$ using the Chebyshev interpolation of the k-formulation in the reduced Brillouin zone $B = [0,\pi]$ over a sample of 200 frequencies in the band gap $[0.22\cdot 2\pi, 0.28\cdot 2\pi]$ is shown. The reference solutions $k_{\mathrm{ref},i}$ are computed using the Newton method [4] applied to the non-linear eigenvalue problem (9) of same polynomial degree $p = 7$.

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