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

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ABSTRACT

The computation of guided modes in photonic crystal wave-guides is a key issue in the process of designing devices in photonic communications. Existing methods, such as the super-cell method, provide an efficient computation of well-confined modes. However, if the modes are not well-confined, the modelling error of the super-cell method becomes prohibitive and advanced methods applying transparent boundary conditions for periodic media are needed. In this work we demonstrate the numerical realization of a recently proposed Dirichlet-to-Neumann approach and compare the results with those of the super-cell method. For the resulting non-linear eigenvalue problem we propose an iterative solution based on Newton's method and a direct solution using Chebyshev interpolation of the non-linear operator. Based on the Dirichlet-to-Neumann approach, we present a formula for the group velocity of guided modes that can serve as an objective function in the optimization of photonic crystal wave-guides.

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1. Introduction

Photonic crystals (PhCs) are nanostructures with a periodic refractive index [1]. The periodicity, which is in the order of the wavelength of light, is induced by periodically spaced holes in an otherwise homogeneous medium. A typical approximation, the so called 2*D planar PhC*, of this three dimensional structure is obtained by assuming invariance along the direction of the holes. PhCs have been studied extensively due to their ability to tailor the propagation of light; see for example [2–12] and the references therein.

Of particular interest are 2*D planar PhC wave-guides* which are obtained by introducing a line defect in a 2D planar PhC. Light is guided efficiently along the line defect of a 2D planar PhC wave-guide, while decaying exponentially in the PhC. For homogeneous line defects the existence of these so called *guided modes* was shown in [13], while the mathematical justification of this observation in full generality is still under investigation. An important feature of 2D planar PhC wave-guides is the possibility to tailor the dispersion of guided modes, and hence, obtaining, for example, slow light modes [14,15], i.e. guided modes with a small group velocity. Slow light modes lead to a simultaneous enhancement of the light intensity and are thus relevant for the construction of devices in non-linear optics [16].

For 2D planar PhC wave-guides with infinite extent, that we will deal with in this work, a plane wave expansion [17] as used in [11] for the homogeneous exterior domain of finite PhC wave-guides is not appropriate since it cannot account for the periodicity of the infinite medium. For the computation of guided modes the super-cell approach [18,19] has proven to be an efficient yet reliable method if the modes are well-confined, i.e. decay exponentially inside the PhCs with large decay

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rate. However, if the guided mode is not well-confined, the computational complexity of the super-cell method increases significantly. To overcome this problem, transparent boundary conditions for periodic media serve as an alternative that allow for an *exact* computation of guided modes without introducing a modelling error.

Transparent boundary conditions for periodic media using a Dirichlet-to-Neumann (DtN) approach were introduced in [20], see also [21–23]. Very recently, this approach was rigorously extended to the computation of guided modes in PhC wave-guides [24]. In this paper we want to elaborate on the numerical implementation of the approach in [24] for the exact computation of guided modes in PhC wave-guides, extend it by some important features, such as the computation of the group velocity of guided modes, and compare it to the results of the super-cell method.

This paper is organized as follows: In Section 2 we describe the model problem, introduce function spaces and summarize results of the spectral theory of the model problem. Furthermore, we provide in this section a short summary of the super-cell method. In Section 3 we introduce a non-linear eigenvalue problem for the computation of guided modes in PhC wave-guides using DtN operators and explain the computation of these DtN operators via local cell problems and a so called *Ricatti equation*. We finish this section with a proof of the differentiability of these DtN operators. In Section 4 we derive a formula for the group velocity of guided modes, that can for example be used to efficiently search for slow light modes. The discretization of the problem using the *finite element method* (FEM) is explained in Section 5. With the help of this discretization we will also show in Section 5 how to solve the discrete form of the Ricatti equation. We continue with solution techniques for the non-linear eigenvalue problem in Section 6 before we present numerical results in Section 7. Finally, we give some concluding remarks in Section 8.

2. Model problem

2.1. The geometry of photonic crystal wave-guides

A general approach to describe the medium of a 2D PhC wave-guide in the above mentioned configuration is a piecewise definition of its permittivity ε, where the permittivity in the holes is equal to the vacuum permittivity and in the bulk it takes some constant value. Let us first consider two (infinite) PhCs in 2D which are characterized by their periodic permittivities $\varepsilon^{\pm}_{\mathrm{PhC}} : \mathbb{R}^2 \to \mathbb{R}^+ \setminus \{0\}$ that satisfy $\varepsilon^{\pm}_{\mathrm{PhC}}(\mathbf{x} + \mathbf{a}^{\pm}_i) = \varepsilon^{\pm}_{\mathrm{PhC}}(\mathbf{x})$ with the periodicity vectors $\mathbf{a}^{\pm}_i \in \mathbb{R}^2$, $i = 1, 2$, where we assume that $\mathbf{a}^+_1 = \mathbf{a}^-_1$ and w.l.o.g. $\mathbf{a}_1 := \mathbf{a}^{\pm}_1 = a_1\,(1, 0)^{\mathrm{T}}$, $a_1 > 0$. The periodicity vectors $\mathbf{a}^{\pm}_2$, however, do not need to be identical or parallel, and neither do they have to be orthogonal to $\mathbf{a}_1$. Here and in the sequel, the superscript "+" indicates quantities related to the PhC on top of the guide and the superscript "−" indicates quantities related to the PhC below the guide.

Note that for a PhC with square lattice the periodicity vectors are equal to the unit vectors in $\mathbb{R}^2$ scaled with the length of the square. For an infinite PhC with hexagonal lattice, however, the periodicity vectors can either be chosen as two orthogonal vectors of different length or as two vectors of the same length that are not mutually orthogonal, e.g. $\mathbf{a}_1 = (1, 0)^{\mathrm{T}}$ and $\mathbf{a}_2 = (0.5, \sqrt{0.75})^{\mathrm{T}}$, [25].

Moreover, we consider a line defect of height a^0_2 characterized by the permittivity $\varepsilon_{\mathrm{defect}} : \mathbb{R}\times]-\frac{a^0_2}{2}, \frac{a^0_2}{2}[\to \mathbb{R}^+ \setminus \{0\}$ which is periodic in $\mathbf{a}_1$-direction, i.e. $\varepsilon_{\mathrm{defect}}(\mathbf{x} + \mathbf{a}_1) = \varepsilon_{\mathrm{defect}}(\mathbf{x})$. Usually, the line defect of a PhC wave-guide has constant permittivity, i.e. there are no holes in the guide. In fact, in the numerical examples in Section 7 the permittivity $\varepsilon_{\mathrm{defect}}$ in the guide is chosen to be constant.

Then we can define the permittivity ε of the PhC wave-guide by

$$\varepsilon(\mathbf{x}) = \begin{cases} \varepsilon^-_{\mathrm{PhC}}(\mathbf{x}), & \text{if } \mathbf{x} \in \Omega^- := \mathbb{R} \times \left]-\infty, -\dfrac{a^0_2}{2}\right[, \\ \varepsilon_{\mathrm{defect}}(\mathbf{x}), & \text{if } \mathbf{x} \in \Omega^0 := \mathbb{R} \times \left]-\dfrac{a^0_2}{2}, \dfrac{a^0_2}{2}\right[, \\ \varepsilon^+_{\mathrm{PhC}}(\mathbf{x}), & \text{if } \mathbf{x} \in \Omega^+ := \mathbb{R} \times \left]\dfrac{a^0_2}{2}, \infty\right[. \end{cases} \tag{1}$$

2.2. Model problem of finding guided modes

In PhC wave-guides there exist guided modes, sometimes also called trapped modes, which are eigensolutions of the time-harmonic Maxwell's equations and which propagate along the line-defect (i.e. along the x_1-axis) while decaying in the directions orthogonal to the line defect (i.e. along the x_2-axis).

It is a well known fact that in 2D the time-harmonic Maxwell's equations decouple into a transverse magnetic (TM) and a transverse electric (TE) mode that satisfy a 2D linear Helmholtz equation [1,19]. For simplicity let us consider the TM-mode, for which

$$-\Delta E(\mathbf{x}) - \omega^2 \varepsilon(\mathbf{x}) E(\mathbf{x}) = 0, \quad \mathbf{x} \in \mathbb{R}^2,$$

defines the electric field E in x_3-direction.

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