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An Efficient Calculation of Photonic Crystal Band Structures Using Taylor Expansions

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Abstract. In this paper we present an efficient algorithm for the calculation of photonic crystal band structures and band structures of photonic crystal waveguides. Our method relies on the fact that the dispersion curves of the band structure are smooth functions of the quasi-momentum in the one-dimensional Brillouin zone. We show the derivation and computation of the group velocity, the group velocity dispersion, and any higher derivative of the dispersion curves. These derivatives are then employed in a Taylor expansion of the dispersion curves. We control the error of the Taylor expansion with the help of a residual estimate and introduce an adaptive scheme for the selection of nodes in the one-dimensional Brillouin zone at which we solve the underlying eigenvalue problem and compute the derivatives of the dispersion curves. The proposed algorithm is not only advantageous as it decreases the computational effort to compute the band structure but also because it allows for the identification of crossings and anti-crossings of dispersion curves, respectively. This identification is not possible with the standard approach of solving the underlying eigenvalue problem at a discrete set of values of the quasi-momentum without taking the mode parity into account.

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1 Introduction

Photonic crystals (PhCs) are nanostructures with a periodic refractive index, where the periodicity is in the order of the wavelength of light [19]. In general one has to distinguish between 1D, 2D, and 3D PhCs, where the number of the dimension stands for the

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number of axes of periodicity. In this work we shall focus on 2D PhCs whose periodicity is usually induced by periodically spaced holes in a dielectric material, or by periodically spaced rods of a dielectric material. A typical approximation, the so called *2D planar PhC*, of this three dimensional structure is obtained by assuming invariance along the direction of the holes and rods. Due to their ability to tailor the propagation of light, 2D PhCs and their band structures, *i.e.* eigenfrequencies in dependence of the quasi-momentum, have been studied extensively, see for example [2–4, 6, 10, 13, 15–18, 24, 26–28] and the references therein. Of particular interest in PhC band structure calculations is the identification of frequency intervals, so called *band gaps* or *complete band gaps*, for which no light can propagate in the PhC. These band gaps are relevant for *PhC waveguides*. PhC waveguides are PhCs with a line defect, that is usually induced by omitting one (W1 PhC waveguide), two (W2 PhC waveguide), or more rows of holes/rods [19]. Inside the band gaps there can exist modes, so called *guided modes*, that propagate along the line defect while decaying exponentially in perpendicular direction.

In the design process of devices in photonics the calculation of band structures of PhC waveguides is a key issue. The frequently used supercell method [35, 38] is a simple procedure for the approximative computation of guided modes in PhC waveguides. While giving good results for well-confined modes (guided modes with a large decay rate in perpendicular direction to the line defect), the supercell methods lacks accuracy for modes that are close to the boundaries of the band gaps, the so called *band edges*, since the decay rate for these modes is significantly smaller [38]. Very recently, an approach for an exact computation of guided modes in PhC waveguides was proposed that uses Dirichlet-to-Neumann (DtN) transparent boundary conditions at the interfaces of periodic medium and line defect [11]. A numerical realization and comparison to the supercell method was shown in [22]. This DtN method does not introduce any modelling error and hence, it is also suited for guided modes close to the band edges.

A full band structure calculation, that resolves all phenomena like *crossings* and *anticrossings* [30, 31] of dispersion curves in full detail, is very time-consuming with either method and there is a need for efficient yet reliable methods that provide good approximations to both, well-confined modes and modes close to the band edge. We propose in this work a method that is based on the fact that the dispersion curves in band structures are smooth functions and hence, a Taylor expansion of these functions is possible. We show how to compute the first derivative of the dispersion curves, which corresponds to the so called *group velocity* [5,20], the second derivative, known as *group velocity dispersion*, and any higher derivative of the dispersion curves. The computation of the derivatives relies directly on the differentiability of the underlying operator of the eigenvalue problem with respect to the quasi-momentum. In particular, we do not employ the perturbation theory as done in earlier works [9,14,37], where the vector $\mathbf{k}\cdot\mathbf{p}$ approach of electronic band structure theory is transferred to PhC band structure calculations. Our computational procedure has two main advantages: (*i*) it is "exact" in the way that no additional modelling error is introduced in comparison to the perturbation approach in [9, 14, 37] where an infinite sum for the computation of the group velocity dispersion has to be