CONVERGENCE ANALYSIS OF PLANEWAVE EXPANSION FOR BAND GAP COMPUTATIONS IN PHOTONIC CRYSTAL FIBRES

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Abstract

In this paper we consider the numerical computation of band gaps in photonic crystal fibres. We approximate the solution to a variational eigenvalue problem using the planewave expansion method (spectral Galerkin method). As well as presenting implementation and error analysis results we consider solving a modified problem where the piecewise constant coefficient function is replaced with a smooth function. The error analysis for the smooth problem is also presented and we answer the question: Is smoothing worth it?

Introduction

Photonic Crystal Fibres (PCFs) [1] are optical fibres that have a core surrounded by cladding. The structure of a PCF is described by its refractive index n. n is constant along the length of the fibre (z-axis) and we write $n = n(x, y)$. The function $n(x, y)$ is a piecewise constant function representing the refractive index of two materials. Light will be described by its frequency ω and its propagation constant in the z-direction β.

For certain designs of cladding and fixed ω, light propagation in the cladding may be forbidden for some values of β. These values of β are called 'band gaps'. Our task is to approximate the band gaps of a particular PCF and ω by approximating the solution to Maxwell's equations.

We will restrict ourselves to the case where $n = n(x)$. Physically, this is the case of a radially symmetric PCF or a planar PCF. Using time harmonic, source free Maxwell's equations for a non-magnetic material the problem decouples into two eigenvalue problems

$$\frac{d^2 h_x}{dx^2} + \gamma(x) h_x = \beta^2 h_x \qquad \text{(TE)}$$

$$\frac{d^2 h_y}{dx^2} + \gamma(x) h_y - \frac{d\eta(x)}{dx}\frac{dh_y}{dx} = \beta^2 h_y. \qquad \text{(TM)}$$

where

$$\gamma(x) = \frac{4\pi^2}{\lambda_0^2} n^2(x\Lambda)$$
$$\eta(x) = \log\left(n^2(x\Lambda)\right),$$

h_x is the x-component of the magnetic field, h_y is the y-component of the magnetic field, Λ is the period of the microstucture in the cladding and λ_0 is the wavelength of light relative to Λ. The remaining components of the magnetic and electric fields are uniquely determined given β, h_x and h_y.

We will work with the TE mode problem multiplied by -1 and shifted by K (making the operator positive definite). Similar numerical results are observed with the TM mode problem, however, we have not obtained any theoretical results for the TM mode problem. We apply the supercell method [2], [3] followed by the Floquet transform. Let $Q = [-\frac{1}{2}, \frac{1}{2}]$. The variational form of the problem is:

For a fixed $\xi \in [-\pi, \pi]$, find an eigenpair (λ, u) where $\lambda \in \mathbb{C}$ and $0 \neq u \in H^1_p(Q) = \{u \in H^1(Q) : u(\frac{1}{2}) = u(-\frac{1}{2})\}$ with $\|u\|_{H^1} = 1$ such that

$$a(u, v) = \lambda b(u, v) \qquad \forall v \in H^1_p(Q) \qquad (1)$$

where

$$a(u, v) = \int_Q \left(\tfrac{d}{dx} + i\xi\right) u \overline{\left(\tfrac{d}{dx} + i\xi\right) v} + (K - \gamma)\, u\overline{v}$$
$$b(u, v) = \int_Q u\overline{v}.$$

It is sufficient to solve (1) for $\xi = 0$ and π [4]. We want to find a few of the smallest eigenvalues of (1).

In this work we try two methods to solve (1). Method 1 applies the planewave expansion method. In Method 2 we modify the problem so that $\gamma(x)$ is smooth and then apply the planewave expansion method. We try this because the planewave expansion method is expected to perform better when the eigenfunctions are smooth. We present the error analysis for both of these methods together a corollary that considers the case where we must approximate the fourier coefficients of $\gamma(x)$ in Method 1.

For details and proofs of the implementation and error analysis please refer to our paper in preparation [5].

In the following, $C \lesssim D$ (for two quantities C, D) means that C/D is bounded above independent of the discretisation parameters N, M and Δ (defined below).

Methods and Convergence Analysis

Method 1 - discontinuous refractive index

We approximate (1) by using the planewave expansion (spectral Galerkin) method. We replace $H_p^1(Q)$ in (1) with a finite dimensional space $S_N = \operatorname{span}\{\mathrm{e}^{i2\pi nx} : |n| \leq N\}$ to get the following problem:

For a fixed $\xi \in [-\pi, \pi]$, find an eigenpair (λ_N, u_N) where $\lambda \in \mathbb{C}$ and $0 \neq u \in S_N$ with $\|u_N\|_{H^1} = 1$ such that

$$a(u_N, v_N) = \lambda b(u_N, v_N) \qquad \forall v_N \in S_N. \qquad (2)$$

This problem is equivalent to the following $(2N+1) \times (2N+1)$ matrix eigenvalue problem

$$A\mathbf{u} = \lambda_N \mathbf{u}$$

where $\mathbf{u}$ is a vector of Fourier coefficients of u_N. According to the definition of $a(\cdot, \cdot)$ we can write A as

$$A = D - V + KI$$

where D is a diagonal matrix (derivative contributions from $a(\cdot, \cdot)$), V is a Toeplitz matrix with entries that are the fourier coefficients of $\gamma(x)$ and I is the identity matrix. The smallest few eigenvalues of A are found using a subspace iteration method where linear systems are solved using the preconditioned conjugate gradient method (PCG). Matrix-vector products can be computed in $\mathcal{O}(N \log N)$ operations using two fast fourier transforms (FFTs).

Theorem. *Let $C > 1$ and $D_A = \operatorname{diag}(A)$. Then there exists a K such that $\kappa(D_A^{-1} A) \leq C$.*

The error analysis results are expressed in the following theorem.

Theorem. *Let (λ, u) be an eigenpair of* (1) *and (λ_N, u_N) be an eigenpair of* (2) *with $\|u - u_N\|_{H^1} < \|u + u_N\|_{H^1}$. Then*

$$\|u - u_N\|_{H^1} \lesssim N^{-3/2}$$
$$|\lambda - \lambda_N| \lesssim N^{-3}$$

In the method above we use the exact Fourier coefficients of $\gamma(x)$. In practice we may need to approximate the Fourier coefficients of $\gamma(x)$. A method for approximating the Fourier coefficients is to sample $\gamma(x)$ on a uniform grid and then compute the discrete Fourier transform of the samples (using FFT). The error analysis is expressed in the following corollary.

Corollary. *Let M be the number of samples taken of $\gamma(x)$, (λ, u) be an eigenpair of* (1) *and (λ_N, u_N) be an eigenpair of* (2) *(computed using approximate Fourier coefficients of $\gamma(x)$) with $\|u - u_N\|_{H^1} < \|u + u_N\|_{H^1}$. Then*

$$\|u - u_N\|_{H^1} \lesssim N^{-3/2} + M^{-1}$$
$$|\lambda - \lambda_N| \lesssim N^{-3} + M^{-1}$$

In practice we choose $M = \mathcal{O}(N)$ and this reduces the rate of convergence for the method to $\mathcal{O}(N)$ for both eigenfunction and eigenvalue error. We do not choose $M = \mathcal{O}(N^r)$ for $r > 1$ since the computational cost of the method is $\mathcal{O}(N \log N) + \mathcal{O}(M \log M)$.

Method 2 - smoothed refractive index

It has been proposed [6] that smoothing $\gamma(x)$ before applying the planewave expansion method may improve Method 1. Our error analysis shows that the rate of convergence is no better than Method 1.

The method for smoothing is to replace $\gamma(x)$ with $\widetilde{\gamma}(x) = G * \gamma(x)$ where $G(x)$ is the Gaussian $G(x) = \frac{1}{\sqrt{2\pi}\Delta} \exp(-\frac{x^2}{2\Delta^2})$, where we specify Δ, and then apply the planewave method as in Method 1. Large Δ results in more smoothing. The error analysis splits into two parts: the error introduced by smoothing and the error introduced by using the planewave expansion method. Using the triangle inequality we add the two errors together to obtain the following theorem

Theorem. *Let $p \in \mathbb{N} \cup \{0\}$ and let (λ, u) be an eigenpair of* (1) *and $(\widetilde{\lambda}_N, \widetilde{u}_N)$ be an eigenpair of* (2) *with $\gamma(x)$ replaced by $\widetilde{\gamma}(x)$ such that $\|u - \widetilde{u}_N\|_{H^1} < \|u + \widetilde{u}_N\|_{H^1}$. Then*

$$\|u - \widetilde{u}_N\|_{H^1} \lesssim \Delta^{3/2} + \Delta^{-p} N^{-p-3/2}$$
$$|\lambda - \widetilde{\lambda}_N| \lesssim \Delta^{3/2} + \Delta^{-2p} N^{-2p-3}$$

Trying to balance the two error terms, we choose $\Delta = N^r$ for some $r \in \mathbb{R}$ and find that choosing $\Delta = N^{-1}$ is the best choice of r for the eigenfunction error but this only recovers the same rate of convergence as in Method 1. If we balance the the eigenvalue error terms then we find that $r = -\frac{3+2p}{3/2+2p}$ and if we choose $r = -2$ then we recover the rate of convergence seen in Method 1. Other choices of r result in slower rates of convergence. We conclude that no amount of smoothing will improve the rate of convergence for the planewave expansion method.

Numerical Results

We now present an example to support the results from the theorems of the previous section. We choose $\gamma(x)$ as in Figure 1 with $1.0 \leq n \leq 1.4$ and $\lambda_0 = 0.5$. We then apply Method 1 for varying N. The errors of the 1st and 5th eigenpairs have been plotted in Figure 2. The reference solution was computed with $N = 2^{16} - 1$.

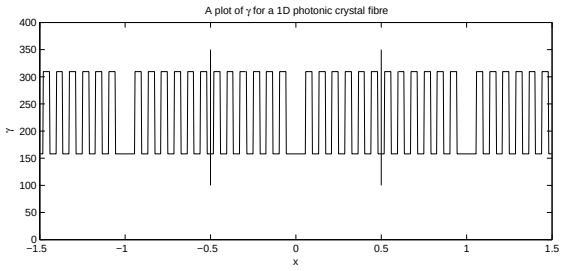

Figure 1: Plot of γ.

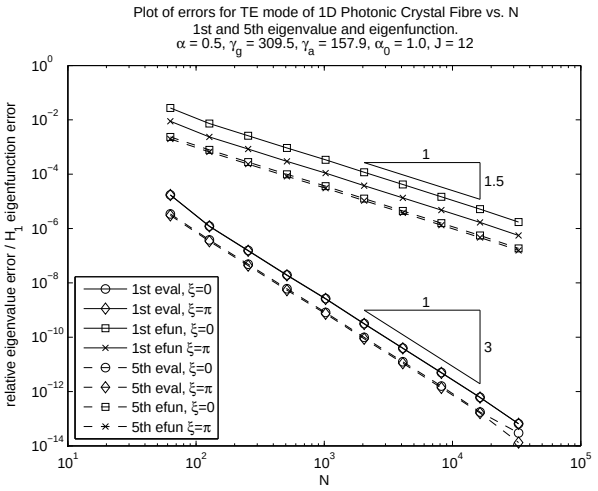

Figure 2: Plot of the errors for Method 1.

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