Computation of the band structure of two-dimensional Photonic Crystals with \textit{hp} Finite Elements

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Outline

Introduction

Problem Formulation

\textit{hp}-adaptive FEM with Concepts

Quasi-periodic basis functions

Numerical Results
Photonic Crystals (PCs) have got a periodic diffractive index → material with novel properties:

- forbidden frequencies (band gap = range of frequencies light can't propagate through crystal in no direction)
- optimal mirror,
- wave-guiding, bending and switching light,
- slow light pulses, negative refraction, ...

→ increasing number of applications in Photonics.

Properties are caused by periodicity ⇒ Investigation of PCs with perfect periodicity

Introduction
Methods for Simulation

Bandstructure = eigenvalues in dependence on quasi-momentum $k$.

Variety of methods

- Plane wave expansion (PWM, fourier expansion in $k$) and Finite Difference Time Domain. Algebraic convergence when smoothing out the dielectric contrast.
- Expansion by Kohn, Korrtinga and Rostocker (KKR) and augmented plane wave expansion. Both restricted to cylindrical structures.
- Separation of variables. Restricted to tensor product geometries.

Our approach based on $hp$-adaptive FEM

- is suitable for high-contrast material,
- is suitable for smooth and polygonal interfaces, and
- converges for both with exponential convergence.

Objective is the numerical investigation of the convergence of the eigenvalues.
Maxwell's equations for linear, loss-less, non-magnetic media
→ for 2D crystal decoupling of eigenvalue problem in TE- and TM-mode

\[
\begin{align*}
\text{(TM)} & \quad - \text{div} \, \text{grad} \, e(x) = \left(\frac{\omega_{\text{TM}}}{c}\right)^2 e(x) e(x) \\
\text{(TE)} & \quad - \text{div} \left( \frac{1}{\varepsilon(x)} \text{grad} \, h(x) \right) = \left(\frac{\omega_{\text{TE}}}{c}\right)^2 h(x)
\end{align*}
\]

\(h, e\) ... component of magnetic and electric field to plane of periodicity \\
\(\omega\) ... angular frequency, \(c\) ... vacuum speed of light, \(\varepsilon(x)\) ... (relative) dielectric constant

Eigenfunctions fulfill Neumann transmission conditions

\[
\begin{bmatrix}
\partial_n e(x) \\
\partial_n h(x)
\end{bmatrix} = \frac{1}{\varepsilon(x)} \begin{bmatrix}
\varepsilon(x) \\
\end{bmatrix}
= 0
\]

Problem formulation
Formulation on the elementary cell

Perfect 2D Photonic Crystal with pattern
\(\varepsilon(x + a_j) = \varepsilon(x), \ i = \{1, 2\}\)
\(\Omega\) ... elementary cell, \(a_1, a_2\) ... directions of periodicity

Reciprocal lattice associated,
\(B\) ... Brillouin zone, \(b_1, b_2\) ... periodicity directions

\[
a_i \cdot b_j = 2\pi \delta_{ij} , \ i, j = \{1, 2\}
\]

Transformation

\[
\tilde{u}(k, x) = (Tu)(k, x) = e^{i k \cdot x} (F u)(k, x)
\]

\[
u(x) = (T^{-1} \tilde{u})(x) = \int_B \tilde{u}(k, x) \, dk
\]

where \(F\) is the Floquet transform (Kuchment, 1993), which is an isomorphism between \(L^2(\mathbb{R}^2)\) and \(L^2(\Omega \times B)\)

Properties

\[
\tilde{u}(k, x + a_j) = e^{i k \cdot a_j} \tilde{u}(k, x) \quad \rightarrow \tilde{u}(k, x) \text{ in } \Omega \text{ defines } \tilde{u} \text{ whole } \mathbb{R}^2
\]

\[
\text{grad} \, u(x) = \text{grad}_x \tilde{u}(k, x) \quad \rightarrow \text{PDE's for } \tilde{u} \text{ and PDE for } u \text{ formally identical}
\]
Problem formulation

Formulation on the elementary cell

Transformation of eigenvalue problems for \( e(x) \) and \( h(x) \) in \( \mathbb{R}^2 \) into family of eigenvalue problems for \( \tilde{e}(k,x) \) and \( \tilde{h}(k,x) \) in \( \Omega \) (for each \( k \in B \))

\( k \) is parameter \( \rightarrow e_k(x) := \tilde{e}(k,x), \ h_k(x) := \tilde{h}(k,x) \)

\( \begin{align*}
\text{(TM)} & \quad - \text{div} \ \text{grad} \ e_k(x) = \left( \frac{\omega_{TM}}{c} \right)^2 \varepsilon(x) e_k(x) \\
\text{(TE)} & \quad - \text{div} \left( \frac{1}{\varepsilon(x)} \text{grad} \ h_k(x) \right) = \left( \frac{\omega_{TE}}{c} \right)^2 h_k(x) \\
\end{align*} \)

in \( \Omega \)

with enclosed quasi-periodic boundary conditions on \( \partial \Omega \) and for \( j = 1, 2 \)

\( e_k(x + a_j) = e^{i k \cdot a_j} e_k(x) \quad h_k(x + a_j) = e^{i k \cdot a_j} h_k(x) \)

and the Neumann boundary conditions on \( \partial \Omega \) and for \( j = 1, 2 \)

\[ \partial_n e_k(x + a_j) = e^{i k \cdot a_j} \frac{1}{\varepsilon(x + a_j)} \partial_n e_k(x) \quad \frac{1}{\varepsilon(x + a_j)} \partial_n h_k(x) = e^{i k \cdot a_j} \frac{1}{\varepsilon(x)} \partial_n h_k(x) \]

Problem formulation

Band structure

Family of eigenvalue problems

\( \begin{align*}
\text{(TM)} & \quad - \text{div} \ \text{grad} \ e_k(x) = \left( \frac{\omega_{TM}}{c} \right)^2 \varepsilon(x) e_k(x) \\
\text{(TE)} & \quad - \text{div} \left( \frac{1}{\varepsilon(x)} \text{grad} \ h_k(x) \right) = \left( \frac{\omega_{TE}}{c} \right)^2 h_k(x) \\
\end{align*} \)

in \( \Omega \)

with enclosed quasi-periodic boundary conditions on \( \partial \Omega \) and for \( j = 1, 2 \)

\( e_k(x + a_j) = e^{i k \cdot a_j} e_k(x) \quad h_k(x + a_j) = e^{i k \cdot a_j} h_k(x) \)

and the Neumann boundary conditions on \( \partial \Omega \) and for \( j = 1, 2 \)

\[ \partial_n e_k(x + a_j) = e^{i k \cdot a_j} \frac{1}{\varepsilon(x + a_j)} \partial_n e_k(x) \quad \frac{1}{\varepsilon(x + a_j)} \partial_n h_k(x) = e^{i k \cdot a_j} \frac{1}{\varepsilon(x)} \partial_n h_k(x) \]

band structure = eigenvalues in dependence on quasi-momentum \( k \)
Function space with quasi-periodic boundary conditions

\[ H^1_k(\Omega) := \{ v \in H^1(\Omega) : v(x + a_j) = e^{i k \cdot a_j} v(x) \text{ on } \partial \Omega, j = 1, 2 \} , \]

Weak formulation

Seek \( e_k, h_k \in H^1_k(\Omega) \) such that \( \forall e'_k, h'_k \in H^1_k(\Omega) \)

\[ \begin{align*}
(TM) & \quad \int_{\Omega} \text{grad} e_k(x) \cdot \text{grad} e'_k(x) \, d\Omega = \left( \frac{\omega_{TM}}{c} \right)^2 \int_{\Omega} \varepsilon(x) e_k(x) e'_k(x) \, d\Omega \\
(TE) & \quad \int_{\Omega} \frac{1}{\varepsilon(x)} \text{grad} h_k(x) \cdot \text{grad} h'_k(x) \, d\Omega = \left( \frac{\omega_{TE}}{c} \right)^2 \int_{\Omega} h_k(x) h'_k(x) \, d\Omega
\end{align*} \]

Properties

- Bilinearforms hermitian and positiv semidefinite \( \rightarrow \) eigenvalues \( \omega_{TM}, \omega_{TE} \) are real.
- Zero eigenvalues for constant eigenfunctions \( \rightarrow \) only possible for \( k = 0 \).

Problem formulation

Regularity in 1D

TE mode at \( k = 0 \), for \( \varepsilon = 9 \) in \([0, 1]\)

\[ -\left( \frac{1}{\varepsilon(x)} h'(x) \right)' = \omega^2 h(x) \quad \text{in } [1, 1] \]

with first non-zero eigenvalue

\( \omega = \arccos(1/4) \)

\[ p = 1 \quad p = 2 \quad p = 3 \]

\[ h = 1 \quad h = 1/2 \quad h = 1/4 \]

\( p \)-FEM with exponential convergence
Problem formulation

Dielectric pattern typically piecewise constant
Let us assume piecewise analytic pattern in two subdomains. \( \Omega_1, \Omega_2 \)

\[ \varepsilon(x)|_{\Omega_i} \in \mathcal{A}(\Omega_i) \]

Interface \( \Gamma := \partial \Omega_1 \cap \partial \Omega_2 \) p.w. analytic.
Set of corners on the interface \( \mathcal{C} \).

**Smooth case :** \( \mathcal{C} = \emptyset \)

- eigenfunctions analytic up to the interface
- \( p \)-FEM on a fixed mesh has exponential convergence

**Polygonal case :** \( \mathcal{C} \neq \emptyset \)

- eigenfunctions analytic up to the interface except the corners
- singularity at interface corners, depends on \( \varepsilon(x) \) in surrounding
- \( hp \)-FEM with geometric meshes and linearly from the corners increasing polynomial degrees has exponential convergence

Problem formulation

\( hp \)-adaptive refinement

**hp-adaptive FEM**
- Combination of cell refinement and polynomial order enrichment

**Geometric mesh**
- Layers of constant polynomial order around interface corner
- Polynomial order is raised away from interface corner
- Cells are refined close to interface corner

Exponential convergence also with sharp corners expected

\[ |\lambda - \lambda_N| \leq C \exp(-\beta N^{1/3}). \] (1)
C++ class library Concepts

- Used and improved by Frauenfelder, Matache, Schmidlin, Schmidt, Kauf and several students.
- Concept Oriented Design using mathematical principles [1].
- Currently two parts: $hp$-FEM (nodal and edge elements), BEM (wavelet and multipole methods).
- $hp$-FEM-part (in 2D and 3D) is released under GPL, http://www.concepts.math.ethz.ch


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Elements with large error should be refined.

Non-conforming meshes

Remedy

Our approach: Use only tensor elements and process hanging nodes.
Local shape functions on the reference element \( \hat{K} = [0,1]^2 \)

\[
\phi_{k,l}(\hat{\mathbf{x}}) = N_k(\hat{x}_1) N_l(\hat{x}_2)
\]

of the hierarchical 1D basis

\[
N_k(\xi) = \begin{cases} 
1 - \xi & k = 0 \\
\xi & k = 1 \\
\xi(1 - \xi)P_{k-2}^{1,1}(2\xi - 1) & k > 1 
\end{cases}
\]

with the Jacobi polynomials \( P_{k-2}^{1,1}(\xi) \) = scaled integrated Legendre polynomials

Mapping to physical element with Blending techniques

Basis function is mapped shape function

\[
\Phi_i(x)|_K = \sum_{k,l} [T_K]_{kl,i} \phi_{kl}(F_K^{-1} x),
\]

T-matrix = topological connection between local and global dof

- for conforming meshes only values +1, −1 and zeros
- ensures continuity of \( H^1 \) basis functions

Quasi-periodic basis functions

Periodic basis functions

- topological identification between nodes and edges on opposite sides of \( \Omega \)

\[
\begin{array}{ccc}
\pi & \gamma_1 & \pi \\
\gamma_2 & \gamma_2 & \Rightarrow \end{array}
\]

Quasi-periodic basis functions

- Cutting of each periodic basis function \( b^0_i(x) \) into parts \( b^1_i(x), \ldots, b^4_i(x) \)

- this is done by introducing four spaces, where in each element \( K \) some entries in the T-matrix are suppressed

- With the phase factors \( \phi_k^0 := 1, \phi_k^1 := e^{i \mathbf{k} \cdot a_1}, \phi_k^2 := e^{i \mathbf{k} \cdot a_2}, \phi_k^3 := e^{i \mathbf{k} \cdot (a_1 + a_2)} \)

\[
b^k_i(x) := \sum_n \phi_k^n b^n_i(x).
\]
Quasi-periodic basis functions

- Cutting of each periodic basis function $b_i^0(x)$ into parts $b_i^1(x), \ldots, b_i^4(x)$
- With the phase factors $\phi_k^1 := 1, \phi_k^2 := e^{i k \cdot a_1}, \phi_k^3 := e^{i k \cdot a_2}, \phi_k^4 := e^{i k \cdot (a_1 + a_2)}$

\[ b_k^i(x) := \sum_n \phi_k^i b_n^i(x). \quad (2) \]

Matrix eigenvalue problems

\[ A^k \vec{x}^k = \lambda^k M^k \vec{x}^k \]

with the system matrices

\[ A^k = \left( a(b^k_j, b^k_j) \right)_{i,j=1}^N, \quad M^k = \left( b(b^k_j, b^k_j) \right)_{i,j=1}^N. \]

Building system matrices

With (2) and the definition of the sixteen matrices

\[ A^{mn} := \left( a(b^m_j, b^n_j) \right)_{i,j=1}^N \Rightarrow A^k = \sum_{m,n=1}^4 \phi_k^m \phi_k^n A^{mn}. \]

\Rightarrow Non-recurring assembling of matrices for different quasi-momenta $k$

Numerical Results

Comparison of different pattern

- Contrast $\varepsilon = 20$
- Diameter of cylinder or length of square 0.9 $a$
- Convergence of $p$-FEM at $k = (\pi/2, 0)/a$
Numerical Results

Comparison of bandstructure

- Dielectric veins of thickness $0.1\ a$ with $\varepsilon = 20$ and air holes ($\varepsilon = 1$)
- Mesh with 9 cells and $p = 15$ ($\#dof=963$)
- Our algorithm computes the right bandstructure, with some more digits

\[
|\lambda - \lambda_N| \leq C \exp(-\beta N^{1/3}).
\]  

(3)

<table>
<thead>
<tr>
<th>TM spectrum</th>
<th>TE spectrum</th>
</tr>
</thead>
<tbody>
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<td>Band No.</td>
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</tr>
<tr>
<td></td>
<td>3.43</td>
</tr>
<tr>
<td></td>
<td>3.4379333(62)</td>
</tr>
</tbody>
</table>

Numerical Results
Comparison of refinement strategies

- Dielectric veins of thickness 0.2\(a\) with \(\varepsilon = 8.9\) and air holes (\(\varepsilon = 1\))
- Coarse Mesh with 9 cells
- \(p\)-FEM with algebraic convergence, as expected
- \(hp\)-FEM with exponential convergence, as expected

**Numerical Results**
Computation of eigenfunctions

The FEM deliver in addition the eigenfunctions \(e_k(x)\) and \(h_k(x)\).

**Example**

- Elementary cell consists of dielectric veins (\(\varepsilon = 20\)) of thickness \(a/90\) and a perturbation in the middle
- \(|h_k(x)|^2\) for first TE eigenfunction at \(k = (\pi, \pi)/a\) (double eigenvalue, second is rotated \(x \leftrightarrow y\))
- \(|e_k(x)|^2\) for first TM eigenfunction at \(k = (\pi, \pi)/a\)
Conclusions

Problem Formulation
- Formulation of Maxwell’s eigenvalue problem for perfect 2D photonic crystals with quasi-periodic boundary conditions.

*hp*-adaptive FEM
- Handling of non-conforming meshes and polynomial degree distribution.
- Quasi-periodic basis functions as linear combination of cutted periodic ones.

Numerical Results
- Exponential convergence of eigenvalues for *hp*-adaptive FEM when interface corners are present.
- There is a pre-asymptotic range, where *p*-FEM performs better than *hp*-FEM.

Outlook
Expectation, that *hp*-adaptive FEM will converge exponentially as well
- for geometries of finite size with polygonal interfaces,
- for 3D Photonic crystals → edge elements or weighted regularisation.