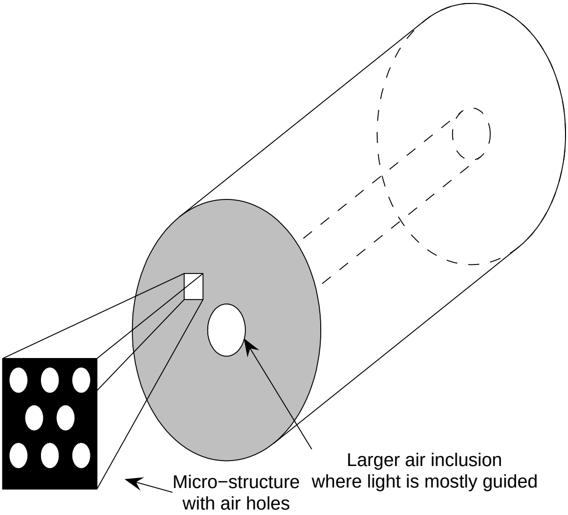
Convergence Analysis of Planewave Expansion for Band Gap Computations in Photonic Crystal Fibres

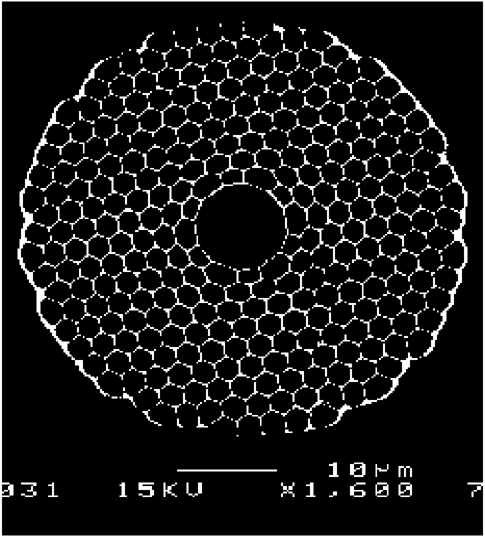
Richard Norton

Supervised by Dr Robert Scheichl, University of Bath

25 July 2007

Cross section of a PCF




10 μm
031 15KV X1,600 7

Problem Definition

Maxwell's Equations $\Rightarrow$ full 2D Problem:

$$\nabla^2 \mathbf{h} + \gamma \mathbf{h} + (\nabla \eta) \times (\nabla \times \mathbf{h}) = \beta^2 \mathbf{h}$$

where

- ∇ is 2D gradient op.
- γ and η are piecewise constant periodic functions in 2D.
- $\mathbf{h}$ is 2D vector field of transverse components of magnetic field.
- β is z-component of wave vector.

1D Problem Definition - TE and TM

We define the TE problem in terms of an operator L on a Hilbert Space $L^2(\mathbb{R})$.

$$\mathsf{L} = -\frac{d^2}{dx^2} + \gamma(x)$$

where $\gamma(x)$ is a piecewise constant periodic function with period cell $Q = [-\frac{1}{2}, \frac{1}{2}]$ and

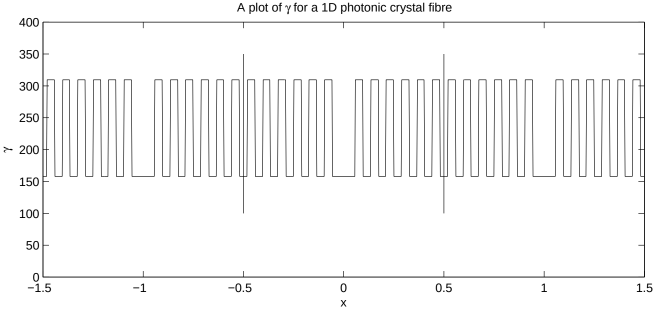
$$0 < \gamma(x) \leq \mathsf{F}$$

The problem:

Calculate $\sigma(\mathsf{L})$

TM Problem: $\mathsf{L} = -\frac{d^2}{dx^2} + \gamma(x) + \frac{d\eta}{dx}\frac{d}{dx}$

Simplified 2D Problem: $\mathsf{L} = -\nabla^2 + \gamma(x, y)$


A plot of γ for a 1D photonic crystal fibre
400
350
300
250
200
150
100
50
0
γ
−1.5
−1
−0.5
0
0.5
1
1.5
x

Floquet Transform

Apply Floquet Transform to get a family of problems on

$$L^2_p(Q) = \{f|_Q \in L^2(Q) : f \text{ periodic}\}$$

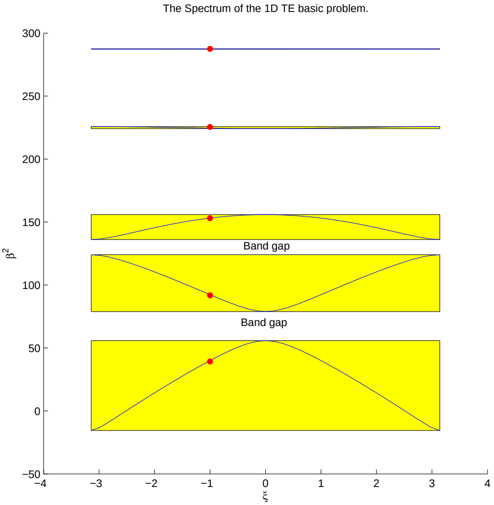
parameterized by $\xi \in B = [-\pi, \pi]$. The new operator is

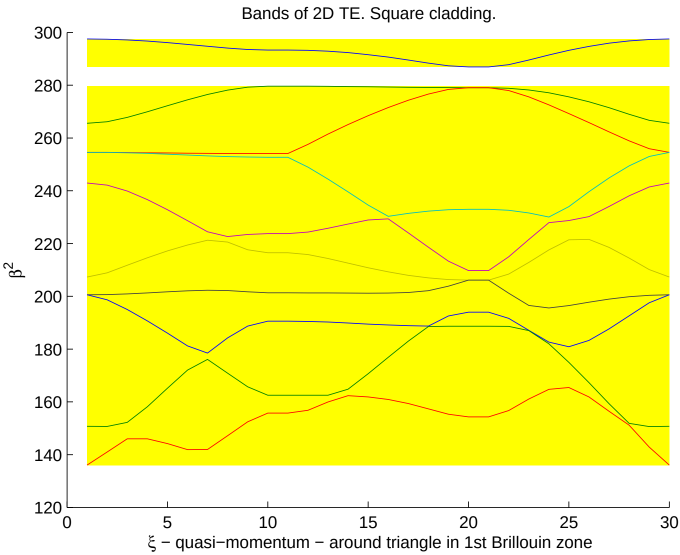
$$\mathsf{L}_\Phi(\xi) = -\left(\frac{d}{dx} + i\xi\right)^2 + \gamma(x)$$

$\sigma(\mathsf{L}_\Phi)$ is discrete.

Theorem (Reed & Simon)

$$\sigma(\mathsf{L}) = \bigcup_{\xi \in B} \sigma(\mathsf{L}_\Phi(\xi))$$


The Spectrum of the 1D TE basic problem.
300
250
200
150
100
50
0
−50
β2
Band gap
Band gap
−4
−3
−2
−1
0
1
2
3
4
ξ


Bands of 2D TE. Square cladding.
300
280
260
240
220
200
180
160
140
120
β2
0
5
10
15
20
25
30
ξ − quasi−momentum − around triangle in 1st Brillouin zone

Variational Problem

Find $\lambda \in \mathbb{C}$ and $0 \neq u \in H_p^1(Q)$ such that

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

$$a(u, v) = \int_Q \left(\frac{d}{dx} + i\xi\right) u \overline{\left(\frac{d}{dx} + i\xi\right) v} + \gamma u \overline{v} dx$$

$$H_p^1(Q) = \{f|_Q \in H^1(Q) : f \text{ periodic}\}$$

- $a(\cdot, \cdot)$ is bounded, coercive and hermitian.

Spectral Galerkin Method

$$S_N := \text{span}\{e^{i2\pi nx} : |n| \leq N\} \subset H^1_p(Q)$$

The approx. variational problem is equivalent to the matrix eigenproblem

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

where $\mathbf{u}$ is a vector of Fourier coefficients of u_N and

$$(\mathrm{A})_{mn} = a(e^{i2\pi nx}, e^{i2\pi mx}) \quad m, n = -N, \ldots, N.$$

$$A = D + V$$

where

$$D \ldots \text{diagonal}$$
$$V \ldots \text{toeplitz}$$

$$V = \begin{bmatrix} \gamma_0 & \gamma_{-1} & \gamma_{-2} & \cdots & & & \gamma_{-2N} \\ \gamma_1 & \gamma_0 & \gamma_{-1} & & & & \\ \gamma_2 & \gamma_1 & \gamma_0 & \ddots & & & \vdots \\ \vdots & & \ddots & \ddots & & & \\ & & & & & \ddots & \gamma_{-2} \\ & & & & \ddots & \ddots & \gamma_{-1} \\ \gamma_{2N} & & \cdots & & \gamma_2 & \gamma_1 & \gamma_0 \end{bmatrix}$$

- A is a full p.d. matrix. (γ even $\Rightarrow$ A symmetric).

Implementation

- Want smallest eigenvalues $\Rightarrow$ subspace iteration.
- Diagonal scaling preconditioner for solves with A $\Rightarrow$ Thm. $\kappa(P\,\mathrm{A}) < 1$.
- Main cost: multiplications with A. Use FFT $\Rightarrow \mathcal{O}(N \log N)$ ops.

Error Analysis

- Define solution operator $\mathrm{T} : L^2_p(Q) \to H^1_p(Q)$ by

$$a(\mathrm{T}f, v) = (f, v) \qquad \forall v \in H^1_p(Q)$$

- Define T_N for approx. var. problem.
- On $H^1_p(Q)$ T,T_N are bounded, compact, self-adjoint and positive definite w.r.t. $a(\cdot,\cdot)$.
- (λ, u) eigenpair of $a(\cdot,\cdot) \iff (\frac{1}{\lambda}, u)$ eigenpair of T.

Theorem (Survey Article by Babuska & Osborn, 91)

(μ, u) eigenpair of T, $\|u\|_a = 1$. Then, for sufficiently large N, $\exists$ an eigenpair of T_N (μ_N, u_N), $\|u_N\|_a = 1$ such that.

$$\|u - u_N\|_a \lesssim \|(\mathsf{T} - \mathsf{T}_N)u\|_a$$

$$|\mu - \mu_N| \lesssim |a((\mathsf{T} - \mathsf{T}_N)u, u)| + \|(\mathsf{T} - \mathsf{T}_N)u\|_a^2$$

Cea's Lemma and Galerkin Orthogonality $\Rightarrow$

$$\|(\mathsf{T} - \mathsf{T}_N)u\|_a \lesssim \inf_{\chi \in S_N} \|u - \chi\|_{H^1(Q)}$$

$$|a((\mathsf{T} - \mathsf{T}_N)u, u)| \lesssim \left(\inf_{\chi \in S_N} \|u - \chi\|_{H^1(Q)} \right)^2$$

$$u'' \text{ discontinuous } \Rightarrow \inf_{\chi \in S_N} \|u - \chi\|_{H^1(Q)} \lesssim \frac{1}{N^{3/2}}$$

Theorem

$$\|u - u_N\|_a \lesssim \frac{1}{N^{3/2}}$$

$$|\lambda - \lambda_N| \lesssim \frac{1}{N^3}$$

Not exponential!!

Smooth Problem Definition

Define normalized Gaussian

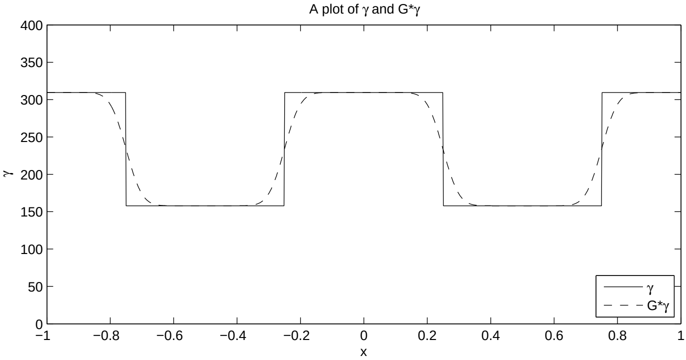
$$G(x) = \frac{1}{\sqrt{2\pi}\Delta} \exp\left(-\frac{x^2}{2\Delta^2}\right)$$

for small $\Delta > 0$. Perturb L to

$$\widetilde{L} = -\frac{d^2}{dx^2} + \widetilde{\gamma}(x)$$

where

$$\widetilde{\gamma}(x) = (G * \gamma)(x) = \int_{\mathbb{R}} G(x-y)\gamma(y)dy.$$


A plot of γ and G*γ
400
350
300
250
200
150
100
50
0
γ
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1
x
γ
G*γ

Properties of $\widetilde{\gamma}$

- $\widetilde{\gamma}(x) \to \gamma(x)$ pointwise a.e. as $\Delta \to 0$.
- $$\widetilde{\gamma}_n = e^{-2\pi^2 n^2 \Delta^2} \gamma_n$$
- $$\|\widetilde{\gamma} - \gamma\|_{H^{-1}(Q)} \lesssim \Delta^{\frac{3}{2}}$$
- For $p \geq 0$,
$$\inf_{\chi \in S_N} \|u - \chi\|_{H^1(Q)} \lesssim \frac{1}{\Delta^p N^{p+\frac{3}{2}}}$$

The error splits into

$$\text{error} \leq \begin{pmatrix} \text{error of} \\ \text{smoothing} \end{pmatrix} + \begin{pmatrix} \text{error of} \\ \text{Galerkin method} \end{pmatrix}$$

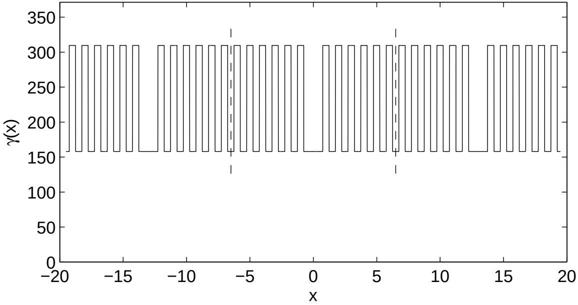
The result becomes...

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

Conclusion

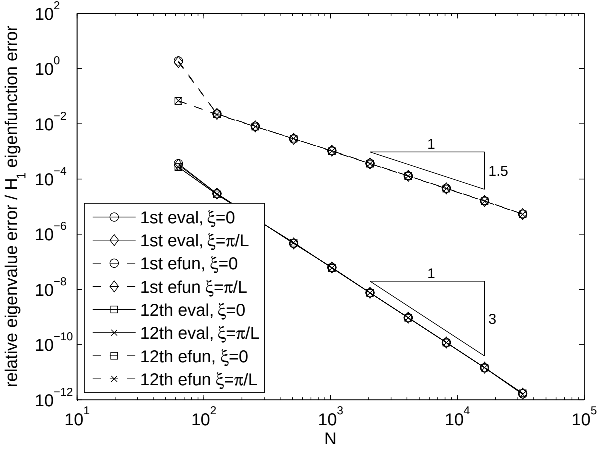
Balance the errors $\Rightarrow$ No amount of smoothing will improve the rate of convergence.

Example



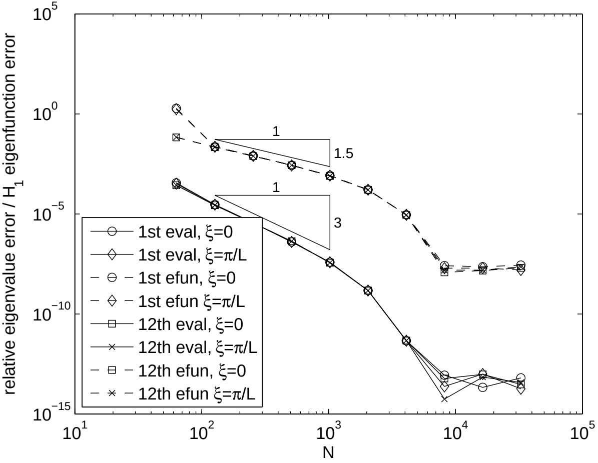
Standard Galerkin Method

Theory ⇒ eigenfunctions $\mathcal{O}(N^{-3/2})$, eigenvalues $\mathcal{O}(N^{-3})$.

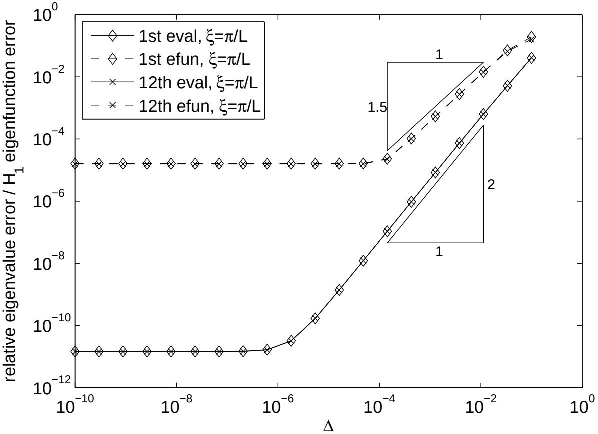


Standard Galerkin on Smooth Problem

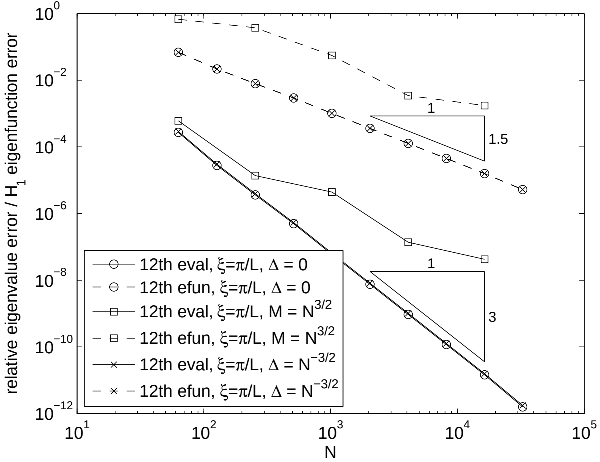
Theory ⇒ eigenfunctions $\mathcal{O}(\Delta^{-p} N^{-p-3/2})$, eigenvalues $\mathcal{O}(\Delta^{-2p} N^{-2p-3})$.



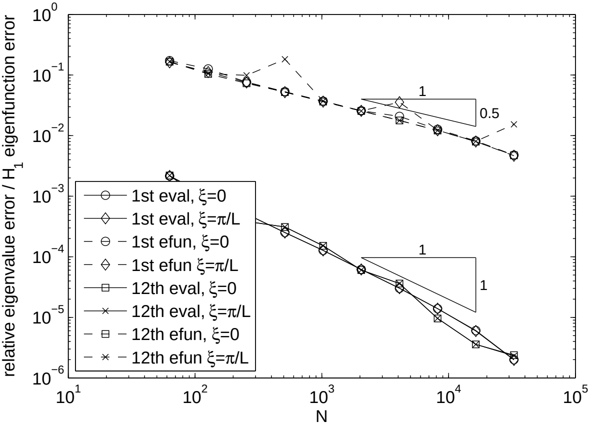
Smoothing error. Large N, varying Δ.
Theory $\Rightarrow$ eigenfunctions and eigenvalues $\mathcal{O}(\Delta^{-3/2})$.



Balancing Errors. Sampling error $\mathcal{O}(M^{-1})$.



TM Problem. Regularity: u' discontinuous.



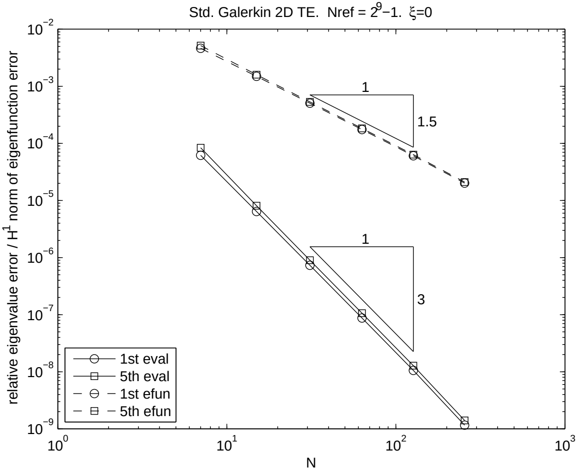
Simplified 2D problem / 2D version of TE

$$L = -\nabla^2 + \gamma(x, y)$$

Do we see the same convergence rates in 2D?

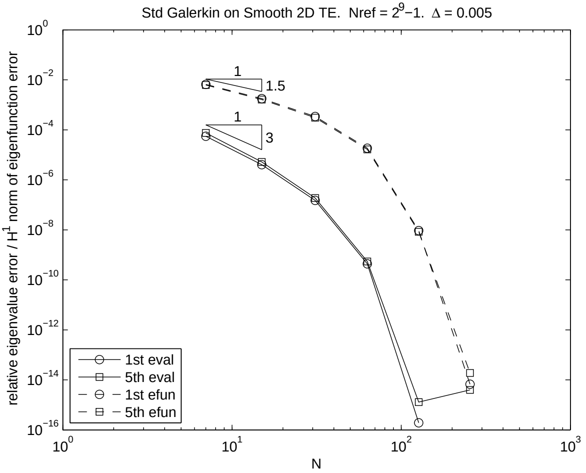
Standard Galerkin Method

Same as TE 1D. Eigenfunctions $\mathcal{O}(N^{-3/2})$, eigenvalues $\mathcal{O}(N^{-3})$.

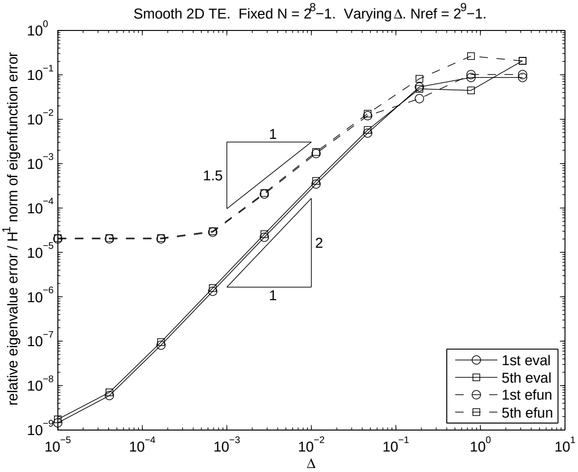


Standard Galerkin on Smooth Problem

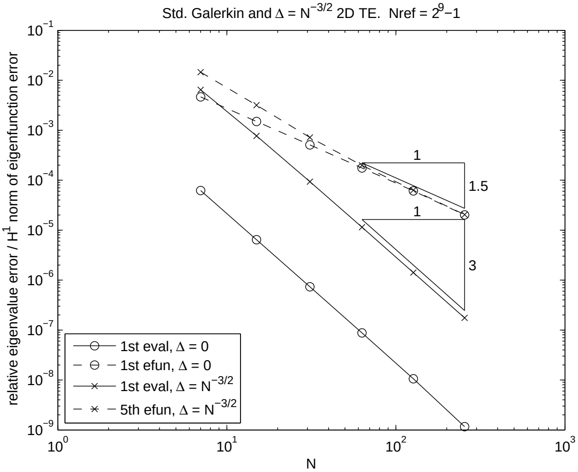
Again, same as TE 1D. Eigenfunctions and eigenvalues exponential convergence.



Smoothing error. Large N, varying Δ. Observe same rates as 1D TE.



Balancing Errors. Choosing $\Delta = N^{-3/2}$.



Conclusion

- 1D TE. No improvement from smoothing.
- 1D TE. Approximating γ_n. Large error.
- 1D TM. Less regularity $\Rightarrow$ convergence slower.
- 1D TM. Smoothing might be useful.
- 2D version of TE. Observe same convergence as 1D.

Work in Progress

- 2D version of TE. Theory. Already have some results.
- 2D Full. Numerical computations.

References

- Babuska, I. & Osborn J., *Eigenvalue Problems*, 1991.
- Hackbusch, W., *Elliptic Differential Equations*, 1992.
- Hardy, G.H. & Rogosinski, W.W., *Fourier Series*, 1956.
- Reed, M. & Simon, B., *Methods of Modern Mathematical Physics IV Analysis of Operators*, 1978.