Convergence Analysis of Planewave Expansion Methods for 2D Schrödinger Operators with Discontinuous Periodic Potentials

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Introduction

Spectral method + discontinuous coefficients =

Not every applied mathematician's first choice

(not exponential convergence, large dense matrices)

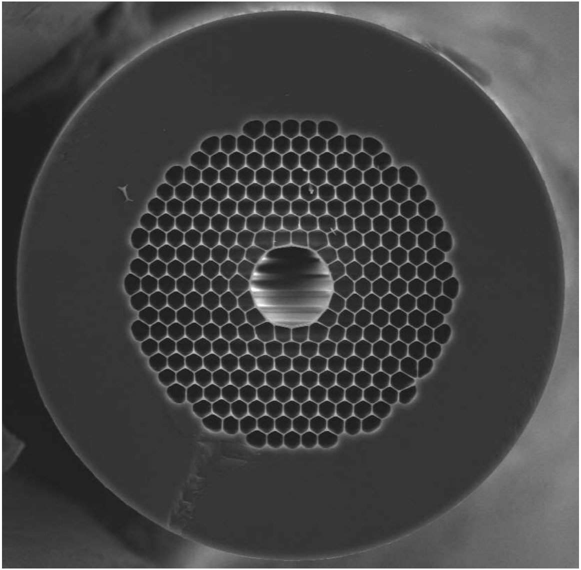
Why not use FEM?

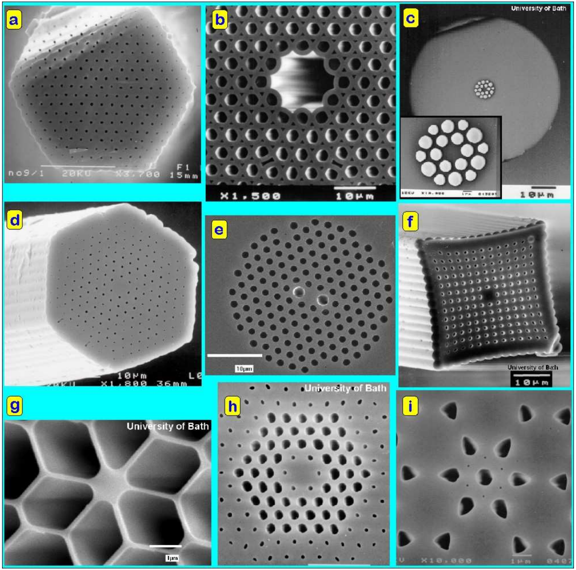
Will show that planewave expansion method has several desirable features that make it competitive with FEM

- converges at same rate as FEM on uniform grid
- can use FFT to make linear systems effectively sparse
- optimal preconditioner

Physicists have tried using smooth coefficients... will show if this is a good idea or not.

Will see that regularity plays and important role in everything.




a
b
X1,500
10μm
c
University of Bath
10μm
d
10μm
e
10μm
f
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10μm
g
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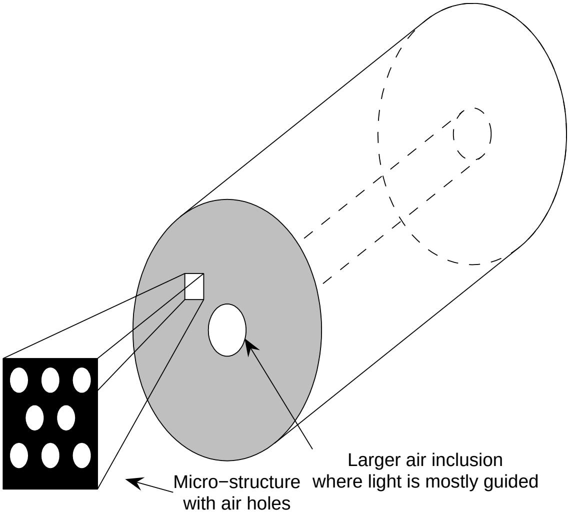
1μm
h
University of Bath
i

Cross section of a PCF



Problem Definition

Idea: given PCF structure and frequency, look for existence of light.

Maxwell's Equations and $\mathbf{H}(x, y, z) = (\mathbf{h}(x, y) + h_z(x, y)\hat{\mathbf{z}})\, \mathrm{e}^{i\beta z}$
$\Rightarrow$ (formally):

$$-\nabla^2 \mathbf{h} + V\mathbf{h} + (\nabla U) \times (\nabla \times \mathbf{h}) = -\beta^2 \mathbf{h} \qquad \text{on } \mathbb{R}^2,$$

where $\mathbf{h} = (h_x, h_y, 0)$, and $V = V(x, y)$ and $U = U(x, y)$ are given piecewise constant functions.

Some V and U regimes allow further simplification:

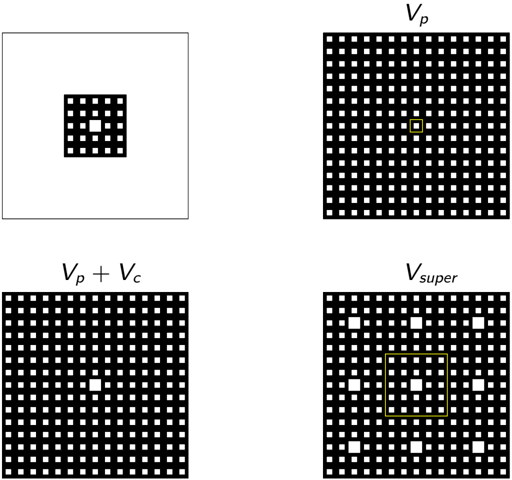
$$-\nabla^2 \mathbf{h} + V\mathbf{h} = -\beta^2 \mathbf{h} \qquad \text{on } \mathbb{R}^2.$$

Can decouple this into h_x and h_y.

Find $\sigma(L)$ where

$$L := -\nabla^2 + V(\mathbf{x}) + K$$

operates on $L^2(\mathbb{R}^2)$, with domain $D(L) = H^2(\mathbb{R}^2)$, $V \in L^\infty(\mathbb{R}^2)$, K is a constant.



$$\sigma(V_p) = \sigma_{ess}(V_p) = \sigma_{ess}(V_p + V_c),$$
$$\sigma(V_{super}) = \sigma_{ess}(V_{super}) \approx \sigma(V_p + V_c).$$

Floquet/Bloch Transform

V periodic with period cell $\Omega = (-\frac{1}{2}, \frac{1}{2})^2 \Rightarrow$ use Floquet/Bloch theory. It says... since the coefficients are periodic, every eigenfunction can be separated into modes that have the form

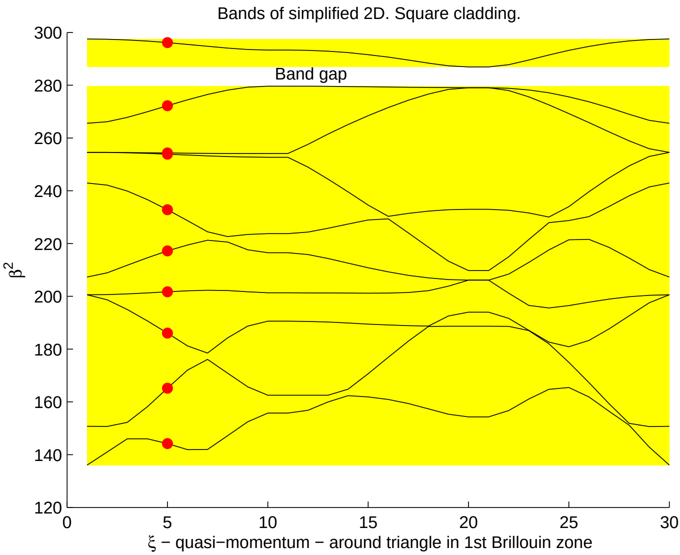
$$\mathbf{h}(\mathbf{x}) = e^{i2\pi\boldsymbol{\xi}\cdot\mathbf{x}}\,\mathbf{u}(\mathbf{x})$$

with $\mathbf{u}$ periodic where $\boldsymbol{\xi}$ is from the first Brillouin zone $B = [-\pi, \pi]^2$. We get a family of operators parameterized by $\boldsymbol{\xi} \in B$. For each fixed $\boldsymbol{\xi} \in B$,

$$L \text{ on } L^2(\mathbb{R}^2) \quad \text{becomes} \quad L_{\boldsymbol{\xi}} = -(\nabla + i\boldsymbol{\xi})^2 + V(\mathbf{x}) + K \text{ on } L^2_p.$$

The key result is

$$\sigma(L) = \bigcup_{\boldsymbol{\xi}\in B} \sigma(L_{\boldsymbol{\xi}}).$$


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

Planewave Expansion Method

To apply the planewave expansion method to

$$-(\nabla + i\xi)^2 u + Vu + Ku = \lambda u \qquad \text{on } \Omega$$

we look for approximate eigenfunctions of the form

$$u_G(\mathbf{x}) = \sum_{\mathbf{k}\in\mathbb{Z}^2_G} [u_G]_{\mathbf{k}}\, \mathrm{e}^{i2\pi\mathbf{k}\cdot\mathbf{x}}$$

where $\mathbb{Z}^2_G = \mathbb{Z}^2 \cap \overline{B(0,G)}$, and $[\cdot]_{\mathbf{k}}$ denotes Fourier coefficient with index $\mathbf{k}$, and $G \in \mathbb{N}$. Comparing coefficients...

$$(|2\pi\mathbf{k} + \boldsymbol{\xi}|^2 + K)[u_G]_{\mathbf{k}} + \sum_{|\mathbf{k}'|\leq G} [V]_{\mathbf{k}-\mathbf{k}'}[u_G]_{\mathbf{k}'} = \lambda_G[u_G]_{\mathbf{k}} \qquad \mathbf{k} \in \mathbb{Z}^2_G,$$

which is equivalent to a matrix eigenproblem

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

where $\mathbf{u}$ is a vector of Fourier coefficients $[u_G]_{\mathbf{k}}$ for $|\mathbf{k}| \leq G$ and $A = D + W$ is Hermitian, positive definite. V even $\Rightarrow$ A s.p.d.

Implementation

- Want smallest eigenvalues $\Rightarrow$ subspace iteration with A^{-1}. E.g. Arnoldi's method (ARPACK).
- Each subspace iteration requires a solve with A . Use PCG.
- Diagonal scaling is optimal preconditioner for solves with A. Theorem to support this - uses Gershgorin's circle theorem.
- Main cost: multiplications with A . Use FFT $\Rightarrow \mathcal{O}(N \log N)$ ops. ($N = \mathcal{O}(G^2)$).

Variational Problem

For fixed $\boldsymbol{\xi} \in B$, find $\lambda \in \mathbb{R}$ and $0 \neq u \in H_p^1$ such that

$$a(u, v) = \lambda \, (u, v)_{L^2(\Omega)} \qquad \forall v \in H_p^1(\Omega)$$

$$a(u, v) = \int_\Omega (\nabla + i\boldsymbol{\xi}) \, u \overline{(\nabla + i\boldsymbol{\xi}) \, v} + (V + K) u \overline{v} d\mathbf{x}$$

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

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

Spectral Galerkin Method

The planewave expansion method can be written as the following spectral Galerkin method. Define

$$S_G := \text{span}\{e^{i2\pi \mathbf{k}\cdot\mathbf{x}} : \mathbf{k} \in \mathbb{Z}^2, |\mathbf{k}| \leq G\} \subset H_p^1.$$

Find $\lambda_G \in \mathbb{R}$ and $0 \neq u_G \in S_G$ such that

$$a(u_G, v_G) = \lambda_G \left(u_G, v_G\right)_{L^2(\Omega)} \qquad \forall v_G \in S_G$$

which is equivalent to the same matrix eigenproblem

$$A\mathbf{u} = \lambda_G \mathbf{u}.$$

Periodic Sobolev Spaces

- Can define $\mathcal{D}'_p(\mathbb{R}^2)$ - space of periodic distributions.
- Every $u \in \mathcal{D}'_p(\mathbb{R}^2)$ has well-defined Fourier coefficients and Fourier Series.

For $s \in \mathbb{R}$ define

$$H_p^s := \{u \in \mathcal{D}'_p(\mathbb{R}^2) : \|u\|_{H_p^s} < \infty\}$$

where

$$\|u\|_{H_p^s}^2 := \sum_{\mathbf{k} \in \mathbb{Z}^2} |\mathbf{k}|_\star^{2s} |[u]_{\mathbf{k}}|^2, \quad \text{and} \quad |\mathbf{k}|_\star = \begin{cases} 1 & \mathbf{k} = 0 \\ |\mathbf{k}| & \mathbf{k} \neq 0 \end{cases}$$

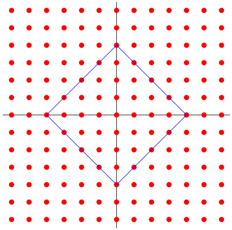
Regularity determined from decay of Fourier coefficients.
Also have expected Sobolev embeddings and inequalities.

Special Classes of Periodic Functions

Starting point for regularity... $V \in H_p^s$ for what $s \in \mathbb{R}$?

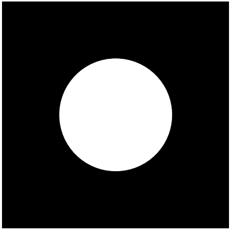
$$\mathcal{X}_p := \{f \in H_p^s \text{ for any } s < 1/2\} \cap L^\infty(\mathbb{R}^2)$$
$$\mathcal{Y}_p := \{f \in \mathcal{D}_p'(\mathbb{R}^2) : F_n(f) \lesssim n^{-1} \text{ for all } n \in \mathbb{N}\} \cap L^\infty(\mathbb{R}^2).$$

where $F_n(f) := \left(\sum_{|k_1|+|k_2|=n} |[f]_{\mathbf{k}}|^2 \right)^{1/2}$

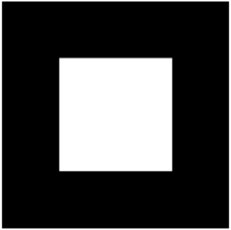


Easy to show $\mathcal{Y}_p \subset \mathcal{X}_p$. Also true that $\mathcal{Y}_p \neq \mathcal{X}_p$. What kind of functions are in $\mathcal{X}_p$ or $\mathcal{Y}_p$?

Examples of V in $\mathcal{Y}_p$



$$|[V]_{\mathbf{k}}| \lesssim |\mathbf{k}|_\star^{-3/2} \Rightarrow V \in \mathcal{Y}_p$$



$$|[V]_{\mathbf{k}}| \lesssim |k_1|_\star^{-1}|k_2|_\star^{-1} \Rightarrow V \in \mathcal{Y}_p$$

Regularity of Eigenfunctions

Suppose $V \in \mathcal{X}_p$ and $u \in H_p^1$ is an eigenvector of our variational problem. Then u is a weak solution to

$$\mathcal{L}u = f \qquad \text{on } \Omega, \text{ periodic b.c.s,}$$

where $\mathcal{L} := -(\nabla + i\xi)^2 + K$ and $f := \lambda u - Vu$.

Steps for Regularity:

1. Easy step:

$$u \in H_p^1 \text{ and } V \in L^\infty \quad \Rightarrow \quad f \in L_p^2$$
$$\Rightarrow \quad u \in H_p^2$$

2. Technical step:

$$u \in H_p^2 \text{ and } V \in H_p^{1/2-\epsilon} \quad \overset{\text{(Saranen \& Vainikko)}}{\Longrightarrow} \quad Vu \in H_p^{1/2-\epsilon}$$
$$\Longrightarrow \quad f \in H_p^{1/2-\epsilon}$$
$$\overset{\text{(Lions \& Magenes)}}{\Longrightarrow} \quad u \in H_p^{5/2-\epsilon}.$$

Approximation Error

We use this regularity to get

$$\inf_{\chi \in S_G} \|u - \chi\|_{H^1_p} \leq G^{-3/2+\epsilon} \|u\|_{H_p^{5/2-\epsilon}}$$

Error Analysis - the Solution Operator

- Define solution operator $T : L_p^2 \to H_p^1$ by

$$a(Tf, v) = (f, v) \qquad \forall v \in H_p^1(\Omega)$$

- Define $T_G : L_p^2 \to S_G$ for approx. var. problem.
- $T : H_p^1 \to H_p^1$ and $T_G : H_p^1 \to H_p^1$ 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.

(Now we know that $\sigma(L_\xi) = \sigma_d(L_\xi)$, i.e. no essential spectrum so ok to only talk about eigenvalues).

Using Babuska & Osborn theory we get...

Theorem

$V \in \mathcal{X}_p$, (λ, u) eigenpair of our variational problem, λ simple, $\|u\|_{H^1_p} = 1$. Then, for sufficiently large G, $\exists$ an eigenpair (λ_G, u_G) of the approx. var. problem, with $\|u_G\|_{H^1_p} = 1$, such that

$$\|u - u_G\|_{H^1_p} \lesssim \|(T - T_G)u\|_{H^1_p}$$

$$|\lambda - \lambda_G| \lesssim |a((T - T_G)u, u)| + \|(T - T_G)u\|^2_{H^1_p}$$

Cea's Lemma and Galerkin Orthogonality $\Rightarrow$

$$\|(T - T_G)u\|_{H^1_p} \lesssim \inf_{\chi \in S_G} \|u - \chi\|_{H^1(\Omega)} \leq G^{-3/2+\epsilon} \|u\|_{H_p^{5/2-\epsilon}}$$

$$|a((T - T_G)u, u)| \lesssim \left(\inf_{\chi \in S_G} \|u - \chi\|_{H^1(\Omega)} \right)^2 \leq G^{-3+2\epsilon} \|u\|^2_{H_p^{5/2-\epsilon}}$$

Theorem holds for multiple eigenvalues.

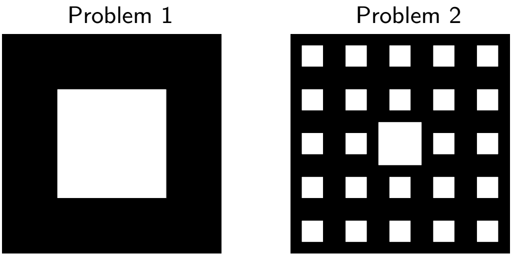
Error Analysis

$$\|u - u_G\|_{H^1_p} \lesssim G^{-3/2+\epsilon}$$

$$|\lambda - \lambda_G| \lesssim G^{-3+2\epsilon}$$

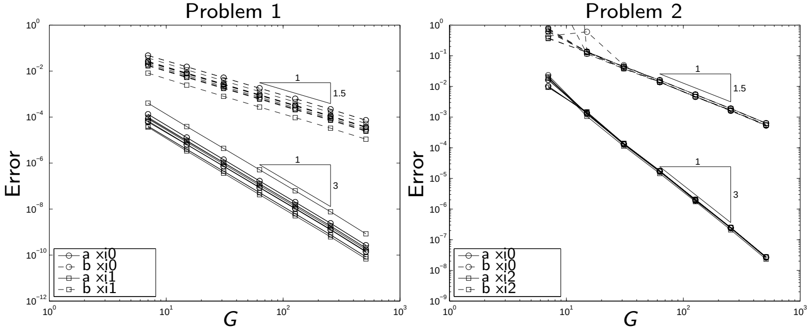
Not exponential since $u \notin C^\infty$

An Example



The period cell for $V(\mathbf{x})$ in Problems 1 and 2. $V = -162.0$ in the black regions and $V = -10.4$ in the white regions.

Observed Convergence



Eigenvalue error (a) and eigenfunction error in the H^1_p norm (b) plotted against G for selected eigenpairs in Problem 1 (1st-5th eigenpairs) and in Problem 2 (23rd-27th eigenpairs), where $\boldsymbol{\xi} = (0, 0)$ (xi0), (π, π) (xi1), and $(\frac{\pi}{5}, \frac{\pi}{5})$ (xi2). Reference solution computed with $G = 2^{10} - 1$.

Optimal Preconditioner

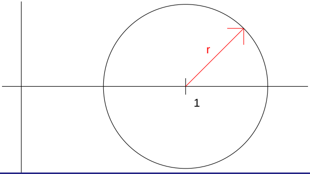
Define our preconditioner to be

$$P := \mathrm{diag}(A).$$

Want to prove

$$\kappa(P^{-1}A) \leq C.$$

Idea: Only ones on diagonal of $P^{-1}A$. Gershgorin's Circle Theorem then says that all the eigenvalues of $P^{-1}A$ will be in a disc centered at 1. Disc will have small radius if sum of off diagonal entries along every row is small. Off diagonal entries are (scaled) $[V]_{\mathbf{k}-\mathbf{k}'}$ and from regularity of V we know these decay.



Definition of A

Let $\mathbb{Z}^2_G := \mathbb{Z}^2 \cap \overline{B(0, G)}$ and $N = |\mathbb{Z}^2_G|$.

Define an ordering of the elements of $\mathbb{Z}^2_G$, $i : \mathbb{Z}^2_G \to \mathbb{N}$ (ascending magnitude).

Then

$$A = D + W$$

where D and W have entries

$$D_{i(\mathbf{k}),i(\mathbf{k})} = |\boldsymbol{\xi} + 2\pi\mathbf{k}|^2 + K \quad \forall \mathbf{k} \in \mathbb{Z}^2_G,$$

$$W_{i(\mathbf{k}),i(\mathbf{k}')} = [V]_{\mathbf{k}-\mathbf{k}'} \quad \forall \mathbf{k}, \mathbf{k}' \in \mathbb{Z}^2_G.$$

A Sketch of the Proof

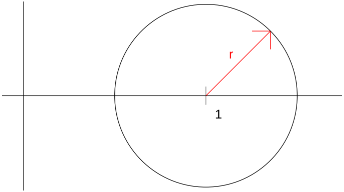
For any $C > 1$, if $V \in \mathcal{Y}_p$ ($\exists\, \gamma$ s.t. $F_n(V) \leq \gamma n^{-1}$) and $K \geq \frac{C+1}{C-1} 2^{11/4} \gamma \sqrt{G} + |[V]_0|$, then

summing the off diagonal entries in row $i(\mathbf{k})$ of $P^{-1}A$,

$$r_{\mathbf{k}} = \sum_{\mathbf{k} \neq \mathbf{k}' \in \mathbb{Z}_G^2} |(P^{-1}A)_{i(\mathbf{k}), i(\mathbf{k}')}| \leq \frac{1}{|\boldsymbol{\xi} + 2\pi \mathbf{k}|^2 + K - |[V]_0|} \sum_{\mathbf{k} \neq \mathbf{k}' \in \mathbb{Z}_G^2} |[V]_{\mathbf{k}-\mathbf{k}'}| \leq \cdots \leq \frac{C-1}{C+1}.$$

Gershgorin's Circle Theorem then says

$\sigma(P^{-1}A) \subset [1 - \frac{C-1}{C+1}, 1 + \frac{C-1}{C+1}] = [\frac{2}{C+1}, \frac{2C}{C+1}]$ and so $\kappa(P^{-1}A) \leq C$.



Compare the performance of preconditioner P with $K = \|V\|_{L^\infty} + \pi^2 + \frac{1}{2} \approx 172.4$ and $K = 5000$.

		IRA restarts			PCG iterations		
G	N	I	P	$P_{K=5000}$	I	P	$P_{K=5000}$
15	709	7	7	22	50	38	8
31	3001	7	7	41	99	38	8
63	12453	7	7	65	204	39	8
127	50617	7	7	96	410	39	8

Large $K \Rightarrow$ more IRA restarts, since relative spacing of eigenvalues is decreased.

We actually used the following preconditioner...

$$P = \begin{bmatrix} A_{11} & 0 \\ 0 & \mathrm{diag}(A_{22}) \end{bmatrix}.$$

Smoothing

Define normalized Gaussian

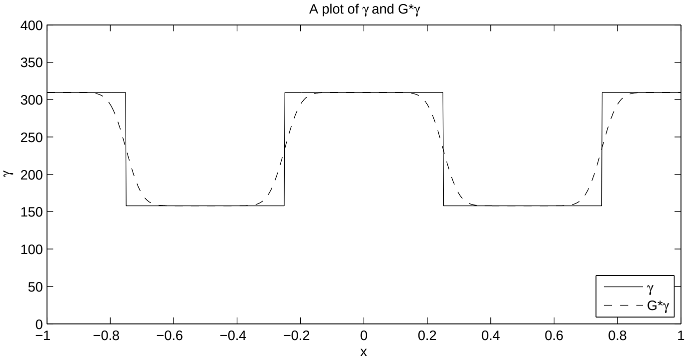
$$\mathcal{G}(\mathbf{x}) = \frac{1}{2\pi\Delta^2} \exp\left(-\frac{|\mathbf{x}|^2}{2\Delta^2}\right)$$

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

$$\widetilde{L} = -\nabla^2 + \widetilde{V}(\mathbf{x}) + K$$

where

$$\widetilde{V}(\mathbf{x}) = (\mathcal{G} * V)(\mathbf{x}) = \int_{\mathbb{R}^2} \mathcal{G}(\mathbf{x}-\mathbf{y})V(\mathbf{y})d\mathbf{y}.$$


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 $\widetilde{V}$

- $\widetilde{V}(\mathbf{x}) \to V(\mathbf{x})$ pointwise a.e. as $\Delta \to 0$.
- $$[\widetilde{V}]_{\mathbf{k}} = e^{-2\pi^2|\mathbf{k}|^2\Delta^2}[V]_{\mathbf{k}}$$
- If $V \in \mathcal{Y}_p$ and $\Delta \in (0,1)$ then
$$\|\widetilde{V} - V\|_{H_p^{-1}} \lesssim \Delta^{\frac{3}{2}}$$
- If $V \in \mathcal{Y}_p$ and $\Delta \in (0,1)$ then
$$\|\widetilde{V}\|_{H_p^s} \lesssim \begin{cases} (\Delta^{-1})^{s-1/2} & s > \frac{1}{2} \\ (1 + \log(\Delta^{-1}))^{1/2} & s = \frac{1}{2} \\ 1 & s < \frac{1}{2}. \end{cases}$$

Regularity for smooth problem

Suppose $V \in \mathcal{Y}_p$, $\Delta \in (0,1)$ and $\widetilde{u}$ is an eigenfunction of the smooth problem. Then $\widetilde{u} \in C^\infty(\mathbb{R}^2)$ and

$$\|\widetilde{u}\|_{H_p^s} \lesssim \zeta(\Delta^{-1})\,\|u\|_{H_p^1}$$

where

$$\zeta(\Delta^{-1}) := \begin{cases} (\Delta^{-1})^{s-5/2}, & \text{for } s > \frac{5}{2}, \\ (1+\log(\Delta^{-1}))^{1/2}, & \text{for } s = \frac{5}{2}, \\ 1, & \text{for } s < \frac{5}{2}. \end{cases}$$

Approximation Error

$$\inf_{\chi \in S_G} \|\widetilde{u} - \chi\|_{H_p^1} \lesssim \begin{cases} (\Delta^{-1})^s G^{-s-3/2}\|\widetilde{u}\|_{H_p^1} & s > 0 \\ C_{G,\Delta^{-1}} G^{-3/2}\|\widetilde{u}\|_{H_p^1} \end{cases}$$

$C_{G,\Delta^{-1}} = \min\{G^\epsilon, (1+\log(\Delta^{-1}))^{1/2}\}$.

Error of Smoothing

Define $\widetilde{T}$ for the smooth variational problem and apply Babuska & Osborn.

$$\|u - \widetilde{u}\|_{H^1_p} \lesssim \|(T - \widetilde{T})u\|_{H^1_p}$$

$$|\lambda - \widetilde{\lambda}| \lesssim |a((T - \widetilde{T})u, u)| + \|(T - \widetilde{T})u\|_{H^1_p} \|(T - \widetilde{T}^*)u\|_{H^1_p}$$

where $\widetilde{T}^*$ is the adjoint of $\widetilde{T}$ w.r.t. $a(\cdot, \cdot)$.

Bounding the RHS

We bound $\|(T - \widetilde{T})u\|_{H^1_p}$ using Strang's 1st Lemma.

$$
\begin{aligned}
\|Tu - \widetilde{T}u\|_{H^1_p} &\lesssim \inf_{v \in H^1_p} \left\{ \|Tu - v\|_{H^1_p} + \sup_{w \in H^1_p} \frac{|a(v,w) - \tilde{a}(v,w)|}{\|w\|_{H^1_p}} \right\} \\
&\leq \sup_{w \in H^1_p} \frac{\int_\Omega |(\widetilde{V} - V) Tu\overline{w}| dx}{\|w\|_{H^1_p}} \quad \text{choosing } v = Tu \\
&\leq \sup_{w \in H^1_p} \frac{\|\widetilde{V} - V\|_{H^{-1}_p} \|Tu\overline{w}\|_{H^1_p}}{\|w\|_{H^1_p}} \\
&\lesssim \Delta^{3/2} \|Tu\|_{H^2_p} \\
&\lesssim \Delta^{3/2} \|u\|_{H^1_p}
\end{aligned}
$$

Error with Smoothing

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 is... for any $s > 0$

$$\|u - \widetilde{u}_G\|_{H^1_p} \lesssim \Delta^{3/2} + \begin{cases} (\Delta^{-1})^s G^{-s-3/2} \\ C_{G,\Delta^{-1}} G^{-3/2} \end{cases}$$

$$|\lambda - \widetilde{\lambda}_G| \lesssim \Delta^{3/2} + \begin{cases} (\Delta^{-1})^{2s} G^{-2s-3} \\ C^2_{G,\Delta^{-1}} G^{-3} \end{cases}$$

Balance Errors / Optimal Choice of Smoothing

Balance errors by taking $\Delta = G^r$ for some $r \leq 0$. At best we get

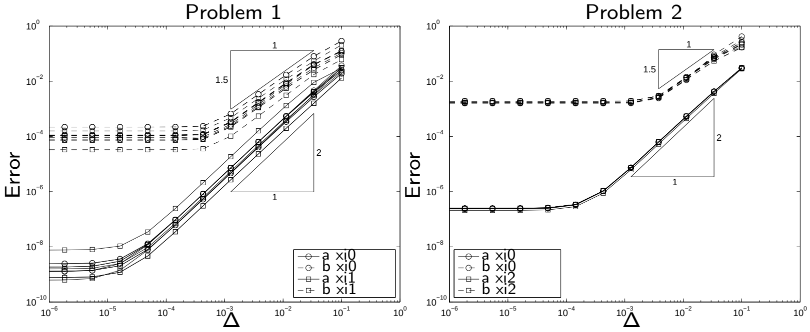
$$\|u - \widetilde{u}_G\|_{H^1_p} \lesssim G^{-3/2} \qquad \text{taking } r \leq -1$$

$$|\lambda - \widetilde{\lambda}_G| \lesssim G^{-3} \log G \qquad \text{taking } r \leq -2$$

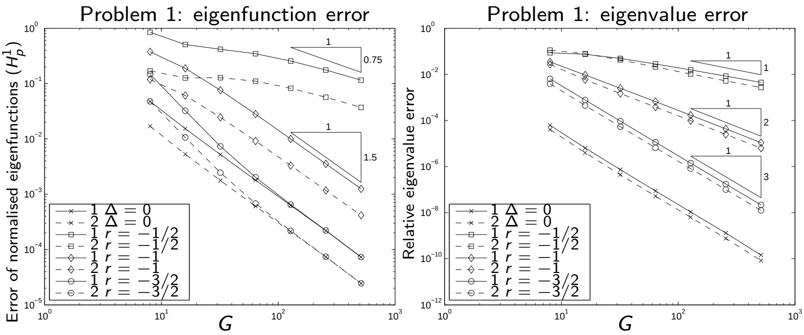
Conclusion

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

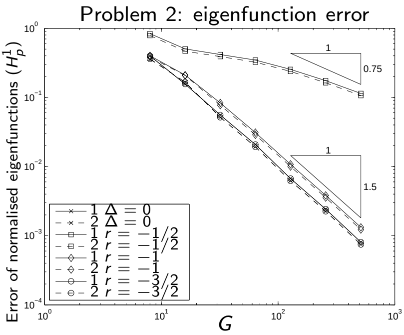
An Example



Eigenvalue error (a) and eigenfunction error in the H^1_p norm (b) plotted against Δ for selected eigenpairs in Problem 1 (1st-5th eigenpairs) and in Problem 2 (23rd-27th eigenpairs), where $\boldsymbol{\xi} = 0$ (xi0), (π, π) (xi1), and $(\frac{\pi}{5}, \frac{\pi}{5})$ (xi2). $G = 2^8 - 1$ used.



Errors for the 1st eigenpair in Problem 1 plotted against G with $\Delta = G^r$ for different $r \in \mathbb{R}$. (Solid lines correspond to $\boldsymbol{\xi} = (0,0)$, whereas dashed lines are $\boldsymbol{\xi} = (\pi,\pi)$.) Reference solution computed with $G = 2^{10} - 1$.



Errors for the 1st eigenpair in Problem 2 plotted against G with $\Delta = G^r$ for different $r \in \mathbb{R}$. (Solid lines correspond to $\boldsymbol{\xi} = (0, 0)$, whereas dashed lines are $\boldsymbol{\xi} = (\frac{\pi}{5}, \frac{\pi}{5})$.) Reference solution computed with $G = 2^{10} - 1$.

Summary / Conclusions

- Put the planewave expansion method in Galerkin method framework.
- Sharp regularity and convergence results for the standard planewave expansion method, no smoothing.
- Optimal preconditioner.
- Improved regularity and convergence rate (w.r.t. G) with smoothing, but additional smoothing error.
- Quantified smoothing error. Sharp for eigenfunctions, not for eigenvalues.
- Optimal choice of smoothing. Conclude that smoothing does not help (but it does not hurt either).
- Numerical experiments agree with theory.
- Planewave expansion method competitive with FEM on uniform grid.

Further / Future Work

- Caveat: have assumed we have explicit formula for $[V]_{\mathbf{k}}$. In practice need approximation, e.g. sample V on uniform grid, compute approximate $[V]_{\mathbf{k}}$ using FFT. Include this error. Maybe smoothing is beneficial here.
- Extend analysis to full problem - Maxwell.
- Analysis of supercell method error.

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