How one can compute wrong eigenvalues and believe they are correct...

and how to remedy

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A Maxwell story: 1st act

A plain Galerkin discretization

Cavity modes with perfectly conducting conditions

Cavity Ω bounded domain. Permittivity ε and permeability μ.

Cavity electromagnetic mode

Triple $(\omega, \boldsymbol{E}, \boldsymbol{H})$ with

- Frequency $\omega \neq 0$
- Electromagnetic field $(\boldsymbol{E}, \boldsymbol{H}) \neq 0$, solution of:

Maxwell equations

$$\begin{cases} \mathbf{curl}\, \boldsymbol{E} - i\omega\, \mu \boldsymbol{H} = 0 & \text{in} \quad \Omega \\ \mathbf{curl}\, \boldsymbol{H} + i\omega\, \varepsilon \boldsymbol{E} = 0 & \text{in} \quad \Omega \end{cases}$$

Perfectly Conducting conditions

$$\begin{cases} \boldsymbol{E} \times \boldsymbol{n} = 0 & \text{on} \quad \partial\Omega \\ \boldsymbol{H} \cdot \boldsymbol{n} = 0 & \text{on} \quad \partial\Omega \end{cases}$$

To simplify, consider *homogeneous and isotropic* medium:
ε, μ constant > 0. By a change of unknown, assume without restriction

$$\varepsilon = \mu = 1.$$

Eliminate $\boldsymbol{H}$

$\boldsymbol{E}$ and $\boldsymbol{H}$ are searched in $H(\mathbf{curl}, \Omega)$, i.e. $\boldsymbol{E}$, $\boldsymbol{H}$, $\mathbf{curl}\,\boldsymbol{E}$, $\mathbf{curl}\,\boldsymbol{H} \in L^2(\Omega)$.

Multiply equation $\mathbf{curl}\,\boldsymbol{E} - i\omega\,\mu\boldsymbol{H} = 0$ by $\mathbf{curl}\,\boldsymbol{E}'$ and integrate over Ω

$$(1) \qquad \int_\Omega (\mathbf{curl}\,\boldsymbol{E} - i\omega\,\boldsymbol{H}) \cdot \mathbf{curl}\,\boldsymbol{E}' \, d\boldsymbol{x} = 0, \quad \forall \boldsymbol{E}' \in H(\mathbf{curl}, \Omega)$$

Multiply equation $\mathbf{curl}\,\boldsymbol{H} + i\omega\,\boldsymbol{E} = 0$ by $i\omega\boldsymbol{E}'$ and integrate over Ω

$$(2) \qquad \int_\Omega (i\omega\,\mathbf{curl}\,\boldsymbol{H} - \omega^2\,\boldsymbol{E}) \cdot \boldsymbol{E}' \, d\boldsymbol{x} = 0, \quad \forall \boldsymbol{E}' \in H(\mathbf{curl}, \Omega)$$

Integrate by parts if, moreover $\boldsymbol{E}' \times \boldsymbol{n} = 0$ on $\partial\Omega$, i.e. $\boldsymbol{E}' \in H_0(\mathbf{curl}, \Omega)$

$$\int_\Omega \mathbf{curl}\,\boldsymbol{H} \times \boldsymbol{E}' \, d\boldsymbol{x} = \int_\Omega \boldsymbol{H} \times \mathbf{curl}\,\boldsymbol{E}' \, d\boldsymbol{x}$$

Add (1) and (2)

$$\int_\Omega \mathbf{curl}\,\boldsymbol{E} \cdot \mathbf{curl}\,\boldsymbol{E}' - \omega^2\,\boldsymbol{E} \cdot \boldsymbol{E}' \, d\boldsymbol{x} = 0, \quad \forall \boldsymbol{E}' \in H_0(\mathbf{curl}, \Omega)$$

Variational electric formulation

Find $\lambda \neq 0$ such that there exists non-zero $\boldsymbol{E} \in H_0(\mathbf{curl}, \Omega)$:

$$\int_\Omega \mathbf{curl}\, \boldsymbol{E} \cdot \mathbf{curl}\, \boldsymbol{E}' \; d\boldsymbol{x} = \lambda \int_\Omega \boldsymbol{E} \cdot \boldsymbol{E}' \; d\boldsymbol{x}, \quad \forall \boldsymbol{E}' \in H_0(\mathbf{curl}, \Omega)$$

Seems suitable for Galerkin approximation: Replace $H_0(\mathbf{curl}, \Omega)$ with a sequence of finite element subspaces $\boldsymbol{W}_h$.

Try in 2D first: Find non-zero λ_h and non-zero $\boldsymbol{E}_h \in \boldsymbol{W}_h$:

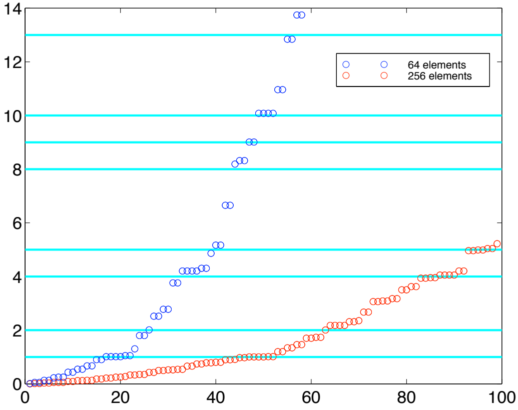
$$\int_\Omega \operatorname{rot} \boldsymbol{E}_h \operatorname{rot} \boldsymbol{E}'_h \; d\boldsymbol{x} = \lambda_h \int_\Omega \boldsymbol{E}_h \cdot \boldsymbol{E}'_h \; d\boldsymbol{x}, \quad \forall \boldsymbol{E}'_h \in \boldsymbol{W}_h$$

Example of the square

$\Omega = (0, \pi)^2$. Exact eigenvalues known explicitly

$$\lambda_1 = \lambda_2 = 1, \quad \lambda_3 = 2, \quad \lambda_4 = \lambda_5 = 4, \quad \lambda_6 = \lambda_7 = 5, \quad \lambda_8 = 8, \ldots$$

Galerkin approximation: h-version of FEM



$\Omega = (0, \pi)^2$

Plot $k \longrightarrow \lambda_{h,k}$

$\mathbb{Q}_1$ (bilinear) square elements

8 nodes per side

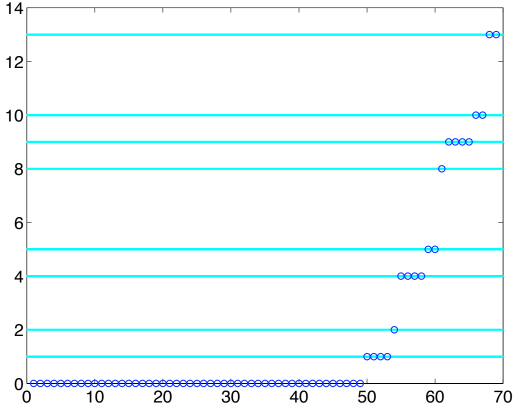
16 nodes per side

Exact values:

Horizontal lines

Raté! (Doesn't work)

Galerkin approximation: p-version of FEM



$$\Omega = (0, \pi)^2$$

Plot $k \to \lambda_{h,k}$

One single element $\mathbb{Q}_8$

Exact values:
Horizontal lines

Encore raté! (Correct values, but wrong multiplicity)

and the culprit is...

...the infinite-dimensional kernel:

For all potential $\varphi \in H_0^1(\Omega)$

$$\boldsymbol{E} = \mathbf{grad}\,\varphi,$$

belongs to $H_0(\mathrm{rot}, \Omega)$ and belongs to the kernel of our operator.

How to get rid of it?

A Maxwell story: 2nd act

Regularization

Introducing the divergence

Take the divergence of the equation $\mathbf{curl}\, \boldsymbol{H} + i\omega\, \boldsymbol{E} = 0$. Since $\omega \neq 0$:

$$\operatorname{div} \boldsymbol{E} = 0 \quad \text{in} \quad \Omega$$

Recall the formula

$$\mathbf{curl}\,\mathbf{curl} - \mathbf{grad}\operatorname{div} = -\Delta$$

and add the term $\int_\Omega \operatorname{div} \boldsymbol{E}\, \operatorname{div} \boldsymbol{E}'$ to our bilinear form

$$\int_\Omega \mathbf{curl}\, \boldsymbol{E} \cdot \mathbf{curl}\, \boldsymbol{E}'\, d\boldsymbol{x} + \int_\Omega \operatorname{div} \boldsymbol{E}\, \operatorname{div} \boldsymbol{E}'\, d\boldsymbol{x} = \lambda \int_\Omega \boldsymbol{E} \cdot \boldsymbol{E}'\, d\boldsymbol{x}.$$

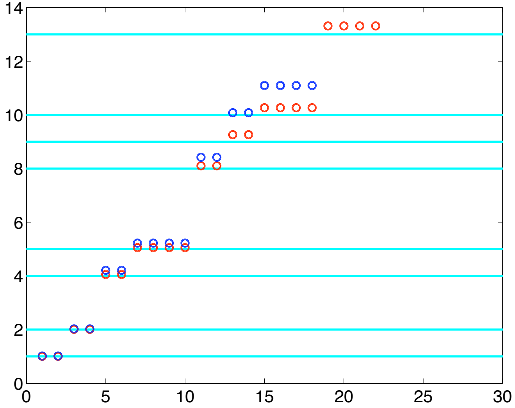
The variational space is now $\boldsymbol{X}_N(\Omega) := H_0(\mathbf{curl}, \Omega) \cap H(\operatorname{div}, \Omega)$.

Introduce new variational problems, for $s > 0$:

Find $\lambda \neq 0$, $\boldsymbol{E} \in \boldsymbol{X}_N(\Omega)$, $\boldsymbol{E} \neq 0$

$$\int_\Omega \left(\mathbf{curl}\, \boldsymbol{E} \cdot \mathbf{curl}\, \boldsymbol{E}' + s \operatorname{div} \boldsymbol{E}\, \operatorname{div} \boldsymbol{E}' \right) d\boldsymbol{x} = \lambda \int_\Omega \boldsymbol{E} \cdot \boldsymbol{E}'\, d\boldsymbol{x}, \quad \forall \boldsymbol{E}' \in \boldsymbol{X}_N(\Omega)$$

FEM approximation on the square, with regularization



$\Omega = (0,\pi)^2$.

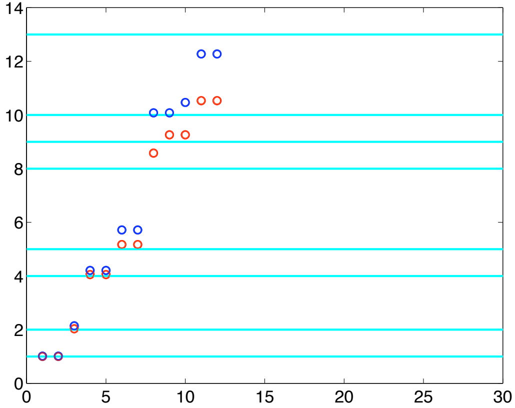
Regularizing parameter
$s = 1$

Plot $k \to \lambda_{h,k}$.
$\mathbb{Q}_1$ (bilinear) square elements
8 nodes per side
16 nodes per side

Exact values:
Horizontal lines

There is some hope...

FEM approximation on the square, with regularization



$\Omega = (0, \pi)^2$.

Regularizing parameter
$s = 10$

Plot $k \to \lambda_{h,k}$.
$\mathbb{Q}_1$ (bilinear) square elements

8 nodes per side

16 nodes per side

Exact values:
Horizontal lines

This is converging to the correct values with the correct multiplicity...

A Maxwell story: 3rd act

Regularization... and corners

The L-shape domain

Solve the regularized variational problems, for $s > 0$:
Find $\lambda \neq 0$, $\boldsymbol{E} \in \boldsymbol{X}_N(\Omega)$, $\boldsymbol{E} \neq 0$

$$\int_\Omega \big(\operatorname{rot} \boldsymbol{E} \cdot \operatorname{rot} \boldsymbol{E}' + s \operatorname{div} \boldsymbol{E} \operatorname{div} \boldsymbol{E}' \big)\, d\boldsymbol{x} = \lambda \int_\Omega \boldsymbol{E} \cdot \boldsymbol{E}'\, d\boldsymbol{x}, \quad \forall \boldsymbol{E}' \in \boldsymbol{X}_N(\Omega)$$

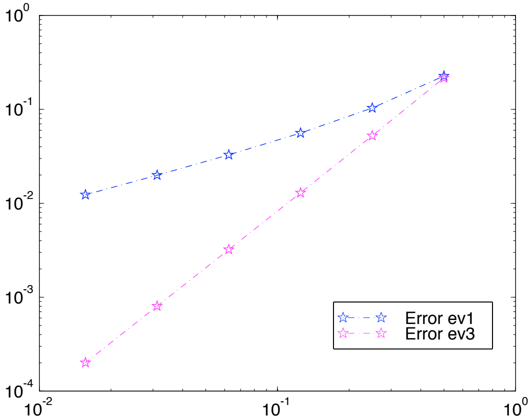
in the L-shape domain (a square minus a square)

$$\Omega_{\mathrm{L}} = (-1,1)^2 \setminus (-1,0)^2$$

No analytic solution known.

Compute error by comparing with a finer approximation (denoted by $\lambda_{0,k}$).

FEM approximation on the L, with regularization



$\Omega = \Omega_{\mathrm{L}}$.

Regularizing parameter
$s = 1$

Plot relative errors

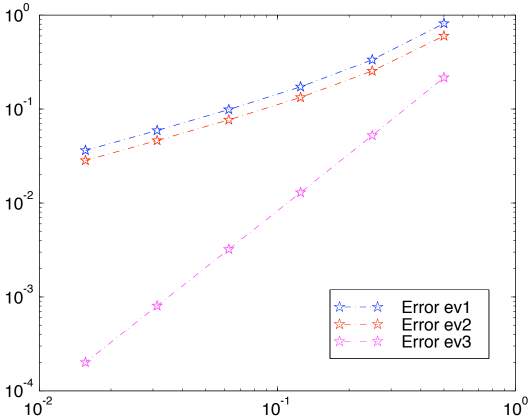
$$h \to \frac{\lambda_{h,k} - \lambda_{0,k}}{\lambda_{0,k}}$$

$k = 1, 2$ and $k = 3$

$\mathbb{Q}_1$ nodal squares
(h goes from $\frac{1}{2}$ to $\frac{1}{64}$)

This is converging...

FEM approximation on the L, with regularization



$\Omega = \Omega_{\mathrm{L}}$.

Regularizing parameter
$s = 10$

Plot relative errors

$$h \to \frac{\lambda_{h,k} - \lambda_{0,k}}{\lambda_{0,k}}$$

$k = 1$, $k = 2$ and $k = 3$

$\mathbb{Q}_1$ nodal squares
(h goes from $\frac{1}{2}$ to $\frac{1}{64}$)

Convergence rate: 0.706 for λ_1 and λ_2, 2.000 for λ_3.

Are computed eigenvalues correct?

What did we find as numbers?

	$s = 1$	$s = 10$
λ_1	3.53420	3.53450
λ_2	3.53420	5.68315
λ_3	9.86960	9.86960

What should we expect?
The eigenvalues of the regularized formulation with parameter s globally depend on s:

$$\mathfrak{S}_{\text{regularized}}(s) = \mathfrak{S}_{\text{Maxwell}} \cup s\,\mathfrak{S}_{\text{Dirichlet }\Delta}$$

The second eigenvalue is doubtful...

And, worse...

New information:
In 2D, electric Maxwell eigenvectors are the curls of Neumann Laplace eigenvectors

$$\boldsymbol{E} = \mathbf{curl}\,\psi, \quad \text{with} \quad -\Delta\psi = \lambda\psi \text{ (in } \Omega) \quad \text{and} \quad \partial_n\psi = 0 \text{ (on } \partial\Omega)$$

	$s = 1$	$s = 10$	Neumann Δ
λ_1	3.53420	3.53450	1.47562
λ_2	3.53420	5.68315	3.53403
λ_3	9.86960	9.86960	9.86960

We missed the first one! (and caught the second one)

Why?

Singular and regular eigenvectors

For $k = 1, 2, 3, 4$

$$\boldsymbol{E}_k = \textbf{curl}\, \psi_k^{\text{neu}}, \quad \text{with} \quad -\Delta \psi_k^{\text{neu}} = \lambda_k^{\text{neu}} \psi_k^{\text{neu}} \quad \text{and} \quad \partial_n \psi_k^{\text{neu}} = 0$$

1. ψ_1^{neu}, the first non-constant eigenvector, is odd with respect to the diagonal $x = y$ of Ω_{L}. It does not belong to $H^2(\Omega_{\text{L}})$

   $$\psi_1^{\text{neu}} = u + c\, r^{2/3} \cos \tfrac{2\theta}{3}, \quad u \in H^2(\Omega_{\text{L}}), \quad c \neq 0.$$

   Thererfore $\boldsymbol{E}_1 \notin H^1(\Omega_{\text{L}})^2$.
2. ψ_2^{neu}, is even with respect to the diagonal $x = y$. It belongs to $H^2(\Omega_{\text{L}})$
3. One can take

   $$\psi_3^{\text{neu}}(x, y) = \cos(\pi x) \quad \text{and} \quad \psi_4^{\text{neu}}(x, y) = \cos(\pi y)$$

   and $\lambda_3^{\text{neu}} = \lambda_4^{\text{neu}} = \pi^2 \simeq 9.86960$.

A density issue

- Recall that $\boldsymbol{W}_h$ are the discrete spaces.
- Let $\boldsymbol{H}^m_N(\Omega) = H^m(\Omega)^2 \cap \boldsymbol{X}_N(\Omega), \quad m = 1, 2, \ldots$

1. Any $\boldsymbol{u}_h \in \boldsymbol{W}_h$ is piecewise polynomial and continuous across inter-element boundaries. Therefore

$$\boldsymbol{W}_h \subset \boldsymbol{H}^1_N(\Omega)$$

2. On the other hand, there holds

Theorem **COSTABEL-DAUGE**

(i) For any $\boldsymbol{u} \in \boldsymbol{H}^2_N(\Omega)$, $\displaystyle\int_\Omega |\operatorname{rot} \boldsymbol{u}|^2 + |\operatorname{div} \boldsymbol{u}|^2 \, d\boldsymbol{x} = \int_\Omega |\mathbf{grad}\, \boldsymbol{u}|^2 \, d\boldsymbol{x}$.

(ii) $\boldsymbol{H}^2_N(\Omega)$ is dense in $\boldsymbol{H}^1_N(\Omega)$.

(iii) $\boldsymbol{H}^1_N(\Omega)$ is closed in $\boldsymbol{X}_N(\Omega)$ for the norm of $\boldsymbol{X}_N(\Omega)$.

3. If Ω has non-convex corners, the embedding $\boldsymbol{H}^1_N(\Omega) \subset \boldsymbol{X}_N(\Omega)$ is strict.

Convergence does not imply consistency

Conclusion

If Ω has non-convex corners, there exists $\delta > 0$ such that any nodal conforming finite element subspace $\boldsymbol{W}_h$ of $\boldsymbol{X}_N(\Omega)$ satisfies

$$\mathrm{dist}(\boldsymbol{X}_N(\Omega), \boldsymbol{W}_h) \geq \mathrm{dist}(\boldsymbol{X}_N(\Omega), \boldsymbol{H}^1_N(\Omega)) > \delta.$$

But the first Maxwell eigenvector $\boldsymbol{E}_1$ does not belong to $\boldsymbol{H}^1_N(\Omega)$.

Therefore $\boldsymbol{E}_1$ cannot be approached by nodal Finite Element spaces $\boldsymbol{W}_h$.

A Maxwell story: Epilogue

Weighted Regularization... and other methods

Consistent methods

1. **Weighted regularization**: introduce a positive exponent γ and the weighted integral

$$s \int_\Omega r^{2\gamma} \operatorname{div} \boldsymbol{E} \operatorname{div} \boldsymbol{E}' \, d\boldsymbol{x}$$

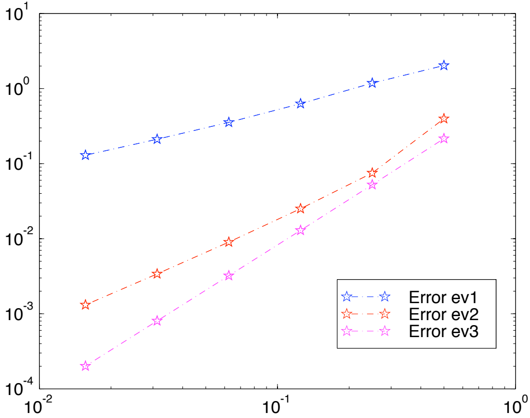
COSTABEL-DAUGE

2. **Singular Function Methods**: Add non-H^1 singularities to the FEM spaces $\boldsymbol{W}_h$. LOHRENGEL et al., CIARLET JR et al.

3. **Edge elements**, which are **curl**-conforming but not div conforming, and part of a discrete commuting diagram. NÉDÉLEC, KIKUCHI, and many others.

More about (1) and (3) in my next talk.

Computing with Weighted Regularization Method



$\Omega = \Omega_{\mathrm{L}}$.

Regularizing parameters $\gamma = 1$ and $s = 10$

Plot relative errors

$$h \to \frac{\lambda_{h,k} - \lambda_{0,k}}{\lambda_{0,k}}$$

$\mathbb{Q}_1$ nodal squares (h goes from $\frac{1}{2}$ to $\frac{1}{64}$)

Compared with "exact eigenvalues" ($\lambda_{0,k} =$ Laplace-Neumann $\lambda_k^{\mathrm{neu}})_{k=1,2,3}$

Convergence rate 0.707 for λ_1, 1.37 for λ_2, and 2.00 for λ_3.

Another example of...

... dangerous eigenvalue computations

The Schrödinger operator with magnetic potential

$\mathcal{A}$ magnetic potential $\frac{1}{2}(-y, x)$.
Schrödinger operator $-(\varepsilon\nabla - i\mathcal{A})^2$ with **small** ε, and Neumann BC.
Variational space $H^1(\Omega)$ (classical).

Square $\Omega = (-1, 1)^2$. $\varepsilon = 1/50$. Eigenvalues $\lambda_k(\varepsilon)$.
Discretize by FEM and compute the first two eigenpairs.

$\lambda_{h,1}(\varepsilon) = 0.020032$ $\lambda_{h,2}(\varepsilon) = 0.020092$

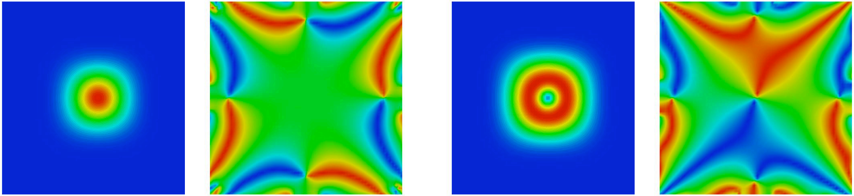
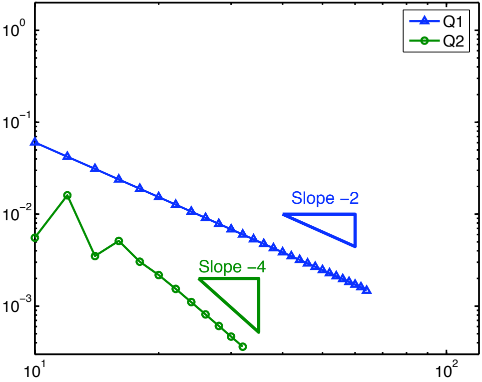


Figure: Modulus and phase of modes 1 and 2, $\mathbb{Q}_1$-approximation on 63×63 mesh

Convergence



$$\Omega = (-1, 1)^2.$$

Apparent limiting value $\lambda_{0,1}(\varepsilon) = \varepsilon = 0.02.$

Plot relative errors

$$\frac{1}{h} \rightarrow \frac{\lambda_{h,1}(\varepsilon) - \lambda_{0,1}(\varepsilon)}{\lambda_{0,1}(\varepsilon)}$$

in loglog scale.

Is it correct?

If we are not very curious, and know little about this problem, we shall be satisfied with the result. We recognize Landau modes in the eigenvectors...

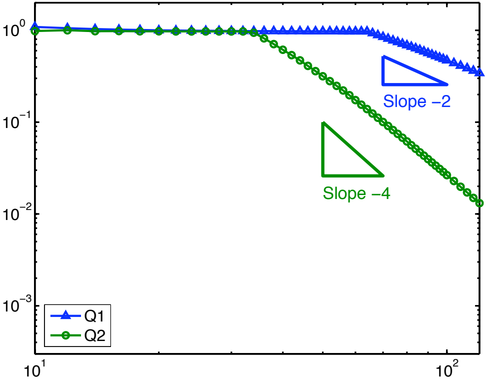
$$(x, y) \to (X + iY)^{k-1} \exp(-\frac{1}{4}(X^2 + Y^2)), \quad X = \frac{x}{\sqrt{\varepsilon}}, \; Y = \frac{y}{\sqrt{\varepsilon}}.$$

- If we are more curious, we keep decreasing h, and suddenly the convergence to 0.02 disappears, $\lambda_{h,k}(\varepsilon)$ starts to decrease below 0.02, very slowly.
- If we know more (Bonnaillie-Dauge), we expect the asymptotic behavior

$$\lambda_k(\varepsilon) = \varepsilon \times \Lambda_1(\tfrac{\pi}{2}), \quad k = 1, 2, 3, 4$$

where $\Lambda_1(\frac{\pi}{2}) \sim 0.507$ is the first eigenvalue of the Schrödinger operator with $\varepsilon = 1$ in an infinite sector of opening π.

True convergence: h-version



$$\Omega = (-1,1)^2.$$

Actual limiting value $\lambda_{0,1}(\varepsilon) = \varepsilon \times 0.5072662 = 0.01145324.$

Plot relative errors

$$\frac{1}{h} \longrightarrow \frac{\lambda_{h,1}(\varepsilon) - \lambda_{0,1}(\varepsilon)}{\lambda_{0,1}(\varepsilon)}$$

in loglog scale.

It is desperate to perform precise computations using low degree elements.

Use *p*-version of FEM instead.

True convergence: p-version

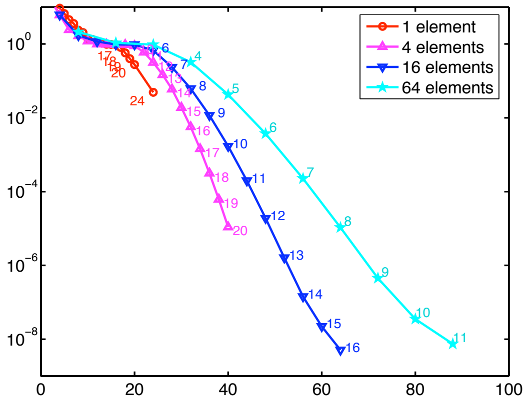


Figure: Relative errors for first eigenvalue, vs. number of Dof per side

Semi-logarithmic scale from 10^{-9} *to* 10 *for errors. Integers mark polynomial degree.*

Why it is difficult to compute

$\lambda_{h,1}(\varepsilon) = 0.0101454$ $\lambda_{h,2}(\varepsilon) = 0.0101726$

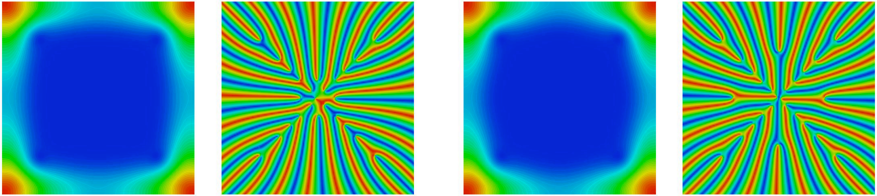


Figure: Modulus and phase of modes 1 and 2, $\mathbb{Q}_{10}$-approximation on 8×8 mesh

The eigenmodes have two-scale boundary layer structure,
in $\sqrt{\varepsilon}$ (corner layers) and ε (oscillations), which causes...

... intertwining eigenvalues

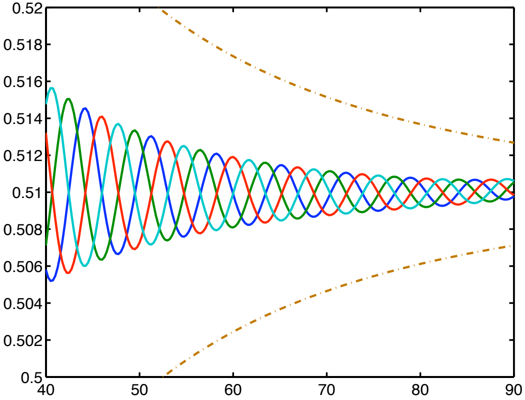


Figure: $\frac{1}{\varepsilon} \to \frac{\lambda_k(\varepsilon)}{\varepsilon}$, for $k = 1, \ldots, 4$

To conclude

Common features of non reliable eigenvalue approximations:

- Essential spectrum
- Corners
- Both
- and... ignorance, leading to hazard computations