Computing Resonances (in the spirit of the Solvability Complexity Index)

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Joint works with:

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Mathematical aspects of the physics with non-self-adjoint operators
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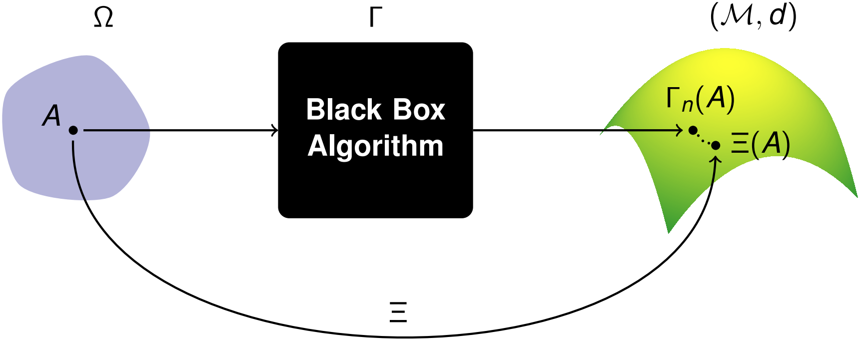
THE SOLVABILITY COMPLEXITY INDEX

Main idea of the Solvability Complexity Index (SCI)



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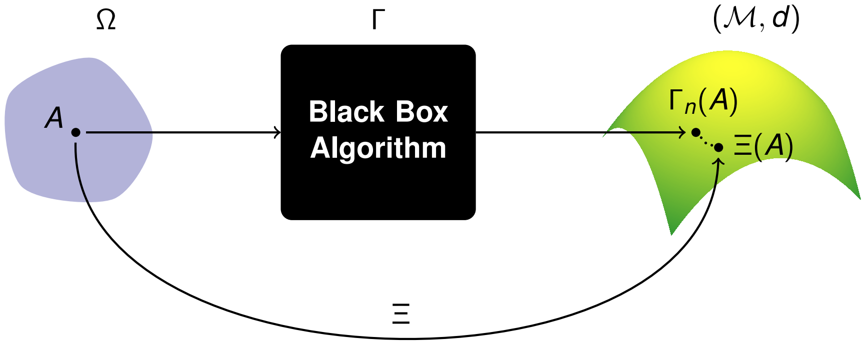

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Not always. Sometimes multiple limits might be necessary, requiring $\Gamma_{n_k, n_{k-1}, \ldots, n_1}$. The SCI theory characterizes this, as well as questions of error control.

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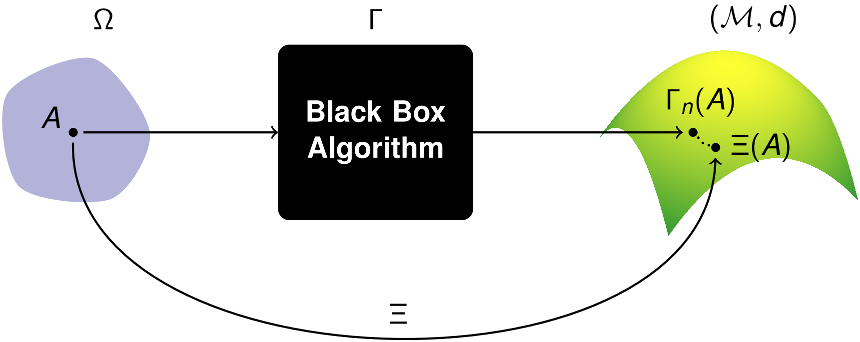

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Hansen (*JAMS* 2011), JBA–Colbrook–Hansen–Nevanlinna–Seidel (arXiv:1508.03280)

S. Smale, *Bull. AMS*, 1985

Let $\mathscr{P}_d$ be the space of polynomials of degree $\leq d$. A purely iterative algorithm is a rational map $T_p : \mathbb{C} \to \mathbb{C}$ depending on $p \in \mathscr{P}_d$ and its derivatives up to some fixed order k, and having the form $T_p(z) = F(z, p(z), \ldots, p^{(k)}(z))$ where F is a rational map.

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T_p is generally convergent if $\exists$ set $\mathcal{U} \subset \mathbb{C} \times \mathscr{P}_d$ of full measure s.t. $T_p^n(z) \xrightarrow{n\to\infty}$ root of p for any $(z, p) \in \mathcal{U}$.

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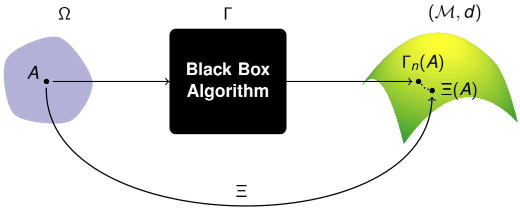
McMullen, *Ann. Math.* 1987: ***yes*** **for $d = 3$, *no* otherwise**

The Quintic

Doyle–McMullen, *Acta Math.* 1989: **the cases $d = 4, 5$ can be solved by *towers of algorithms***

A tower of algorithms is a finite sequence of generally convergent algorithms, linked together serially, so the output of one or more can be used to compute the input to the next. The final output of the tower is a single number, computed rationally from the original input and the outputs of the intermediate generally convergent algorithms.

Main Questions



1. Does there exist an algorithm for computing the resonances $\mathrm{Res}(H_q)$ of $H_q := -\Delta + q$ for any 'nice' $q : \mathbb{R}^d \to \mathbb{C}$?

2. Does there exist an algorithm for computing the resonances $\mathrm{Res}(U)$ of $-\Delta$ on $\mathbb{R}^d \setminus U$ for any 'nice' $U \subset \mathbb{R}^d$?

MAIN RESULTS

Quantum Scattering Resonances

Theorem (JBA–Marletta–Rösler, to appear in *JEMS*)

There exists an arithmetic algorithm that can approximate the resonances of $H_q = -\Delta + q$ *for any* $q \in \Omega = C_0^1(\mathbb{R}^d; \mathbb{C})$.

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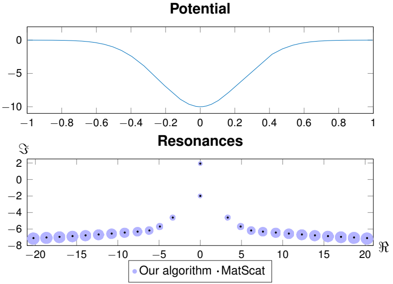
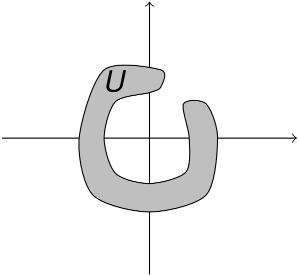
Comparison of our algorithm with MatScat (Bindel–Zworski) for a Gaussian well supported in $[-1, 1]$.



Classical Scattering Resonances

Theorem (JBA–Marletta–Rösler, *FoCM* 2022)

There exists an arithmetic algorithm that can approximate the Dirichlet resonances of U for any
$U \in \Omega = \{\emptyset \neq U \subset \mathbb{R}^d \mid U \text{ open, bounded and } \partial U \in C^2\}$.



PROOF:

QUANTUM SCATTERING RESONANCES

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But $v = (-\Delta - z^2)u = -qu = -\chi qu = \chi v$ for any $\chi \in C_0^\infty(\mathbb{R}^d; [0, 1])$ which is identically 1 on $\mathrm{supp}(q)$.

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4. Define a discretized version $K_n(z)$ which can be computed with finitely many arithmetic operations.

5. Identify the poles of $(\mathrm{Id}_{L^2} + K(z))^{-1}$ via the discretized operator $(I + K_n(z))^{-1}$.

An Abstract Approximation Result

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$$\begin{aligned} \|K(z) - P_n K(z) P_n\|_{L(\mathcal{H})} &\leq C a_n, \\ \|K(z) - K_n(z) P_n\|_{L(\mathcal{H})} &\leq C a_n, \\ \|P_n K(z)|_{\mathcal{H}_n} - K_n(z)\|_{L(\mathcal{H}_n)} &\leq C a_n. \end{aligned}$$

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Let $G_n = \frac{1}{a_n}(\mathbb{Z} + i\mathbb{Z})$ and define

$$\Gamma_n^B(K) = \left\{ z \in G_n \cap B \,\middle|\, \left\|(I + K_n(z))^{-1}\right\|_{L(\mathcal{H}_n)} \ge \frac{1}{2\sqrt{a_n}} \right\}$$

An Abstract Approximation Result (cont)

Proposition

We have $\Gamma_n^B(K) \to \{z \in B \mid -1 \in \sigma(K(z))\}$ *in the Hausdorff metric.*

Where we remind that

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Crucially: if we assume that $K_n(z)$ can be computed with finitely arithmetic operations, then $\Gamma_n^B(K)$ can be completely determined with finitely many operations.

The Operator $K(z) = q(-\Delta - z^2)^{-1}\chi$

For $x \in \mathbb{R}^d$, $z \in \mathbb{C}$, the Green's function of the Helmholtz operator $-\Delta - z^2$ is

$$G(x,z) := \begin{cases} \frac{i}{4}\left(\frac{z}{2\pi|x|}\right)^{\frac{d-2}{2}} H_{\frac{d-2}{2}}(z|x|), & d \geq 2, \\ \frac{i}{2z} e^{iz|x|}, & d = 1, \end{cases}$$

where H_ν = Hankel function of the first kind.

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We shall approximate the kernel (slight abuse of notation)

$$K(x,y) := q(x)G(x-y,z)\chi(y)$$

Approximation of $K(x, y) = q(x)G(x - y, z)\chi(y)$

Split $\mathbb{R}^d$ into small cubes:

$$\mathbb{R}^d = \bigcup_{i \in \frac{1}{n}\mathbb{Z}^d} S_{n,i} := \bigcup_{i \in \frac{1}{n}\mathbb{Z}^d} \left(\left[0, \tfrac{1}{n}\right)^d + i \right),$$

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Define

$$K_n(x,y) := \sum_{i,j\in\frac{1}{n}\mathbb{Z}^d} K(i,j)\chi_{S_{n,i}}(x)\chi_{S_{n,j}}(y).$$

The Algorithm: the Poles of $(I + K_n(z))^{-1}$

Let $\emptyset \neq B \subset \mathbb{C}$ be compact and let $G_n := \frac{1}{a_n}(\mathbb{Z} + i\mathbb{Z})$

$$\Gamma_n^B : \Omega \to \mathrm{cl}(\mathbb{C})$$
$$\Gamma_n^B(q) = \left\{ z \in G_n \cap B \,\middle|\, \left\| (I + K_n(\cdot,\cdot))^{-1} \right\|_{L(\mathcal{H}_n)} \geq \frac{1}{2\sqrt{a_n}} \right\}$$

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Theorem

For any $q \in \Omega$ we have $\Gamma_n^B(q) \to \mathrm{Res}(q) \cap B$ in the Hausdorff distance as $n \to +\infty$.

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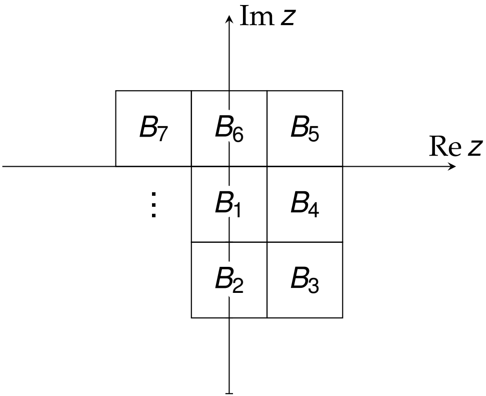

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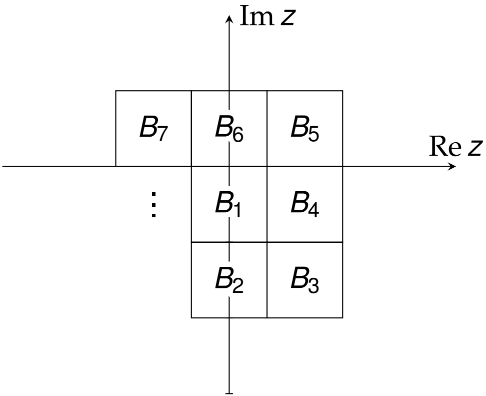


And finally define:

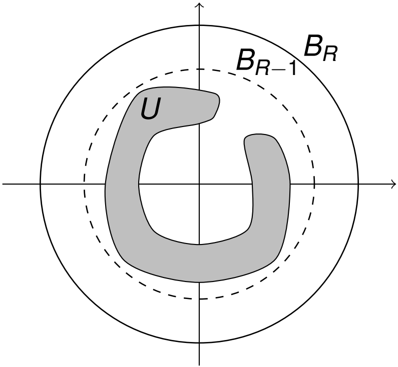
$$\Gamma_n(q) := \bigcup_{j=1}^{n} \Gamma_n^{B_j}(q)$$

PROOF:

CLASSICAL SCATTERING RESONANCES

Proof: Classical Scattering Resonances

1. Assume that the support B_R of U is known.



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2. Write the Dirichlet-to-Neumann (DtN) maps for $-\Delta - k^2$, $k \in \mathbb{C}^+$:

$$\begin{array}{rcl} M_{\mathrm{in}}(k) & \text{in} & B_R \setminus \overline{U} \\ M_{\mathrm{out}}(k) & \text{in} & \mathbb{R}^d \setminus \overline{B}_R \end{array}$$

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5. Approximate $\mathcal{C}$ & find values of k for which $\left|\det_{\lceil p \rceil}(\mathrm{Id}_{L^2} + \mathcal{C}(k))\right| < \epsilon$.

Proof: Classical Scattering Resonances

1. Assume that the support B_R of U is known.

2. Write the Dirichlet-to-Neumann (DtN) maps for $-\Delta - k^2$, $k \in \mathbb{C}^+$:

$$\begin{array}{rcl} M_{\text{in}}(k) & \text{in} & B_R \setminus \overline{U} \\ M_{\text{out}}(k) & \text{in} & \mathbb{R}^d \setminus \overline{B}_R \end{array}$$

These can be extended meromorphically to $k \in \mathbb{C}$.

3. $k \in \mathbb{C}^-$ is a resonance if and only if $\ker(M_{\text{in}}(k) + M_{\text{out}}(k)) \neq \{0\}$.

4. Find a compact operator $\mathcal{C}(k)$ in a p-Schatten class ($\forall p > 2$) such that $\ker(\mathrm{Id}_{L^2} + \mathcal{C}(k)) \neq \{0\} \quad \Leftrightarrow \quad \ker(M_{\text{in}}(k) + M_{\text{out}}(k)) \neq \{0\}$

5. Approximate $\mathcal{C}$ & find values of k for which $\left|\det_{\lceil p \rceil}(\mathrm{Id}_{L^2} + \mathcal{C}(k))\right| < \epsilon$.

6. Get rid of R dependence.

DtN Maps ($d = 2$)

In the orthonormal basis $e_n(\theta) := \frac{e^{in\theta}}{\sqrt{2\pi R}}$ on ∂B_R:

$$M_{\mathrm{out}}(k) = \mathrm{diag}\left(-k\frac{H'_{|n|}(kR)}{H_{|n|}(kR)}\right) = \mathrm{diag}\left(\frac{|n|}{R} - k\underbrace{\frac{H_{|n|-1}(kR)}{H_{|n|}(kR)}}_{\sim\frac{kR}{2|n|}}\right)$$

$H_\nu =$ Hankel functions of the first kind.

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$$M_{\mathrm{in}}(k) = M_{\mathrm{in},0}(k) + \mathcal{K}(k)$$

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J_ν = Bessel functions of the first kind.

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$$M_{\text{in}}(k) + M_{\text{out}}(k) = \frac{2}{R}N + \mathcal{H}(k) + \mathcal{J}(k) + \mathcal{K}(k)$$

DtN Maps ($d = 2$), cont.

$$\begin{aligned} M_{\mathrm{in}}(k)+M_{\mathrm{out}}(k) &= \frac{2}{R}N + \mathcal{H}(k) + \mathcal{J}(k) + \mathcal{K}(k) \\ &= \frac{2}{R}N^{\frac{1}{2}}\left(\mathrm{Id}_{L^2} + \frac{R}{2}N^{-\frac{1}{2}}\big(\mathcal{H}(k) + \mathcal{J}(k) + \mathcal{K}(k)\big)N^{-\frac{1}{2}}\right)N^{\frac{1}{2}} \end{aligned}$$

DtN Maps ($d = 2$), cont.

$$\begin{aligned} M_{\text{in}}(k)+M_{\text{out}}(k) &= \frac{2}{R}N + \mathcal{H}(k) + \mathcal{J}(k) + \mathcal{K}(k) \\ &= \frac{2}{R}N^{\frac{1}{2}}\left(\mathrm{Id}_{L^2} + \frac{R}{2}N^{-\frac{1}{2}}\left(\mathcal{H}(k)+\mathcal{J}(k)+\mathcal{K}(k)\right)N^{-\frac{1}{2}}\right)N^{\frac{1}{2}} \end{aligned}$$

Hence

$$\ker(M_{\text{in}}(k) + M_{\text{out}}(k)) = \{0\}$$

$$\Updownarrow$$

$$\ker\left(\mathrm{Id}_{L^2} + \frac{R}{2}\underbrace{N^{-\frac{1}{2}}\left(\mathcal{H}(k)+\mathcal{J}(k)+\mathcal{K}(k)\right)N^{-\frac{1}{2}}}_{\mathcal{C}(k)}\right) = \{0\}$$

Approximation of $\mathcal{C}(k)$

$$\mathcal{C}(k) = N^{-\frac{1}{2}}\big(\mathcal{H}(k) + \mathcal{J}(k) + \mathcal{K}(k)\big)N^{-\frac{1}{2}}$$

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1. Truncate the matrix:

Lemma

Let $k \in \mathbb{C}^-$, $p > 2$, and for $n \in \mathbb{N}$ let $P_n : L^2(\partial B_R) \to \mathrm{span}\{e_{-n}, \dots e_n\}$ be the orthogonal projection. Then there exists a constant $C > 0$ depending only on the set U such that

$$\|\mathcal{C}(k) - P_n\mathcal{C}(k)P_n\|_{C_p} \leq Cn^{-\frac{1}{2}+\frac{1}{p}}.$$

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2. Approximate $\mathcal{K}(k)$.

The Operator $\mathcal{K}(k)$

$$\mathcal{K}(k) = \partial_\nu (H_{\mathrm{D}} - k^2)^{-1} T_\rho S(k) : L^2(\partial B_R) \to L^2(\partial B_R)$$

where:

- ∂_ν is the normal derivative on ∂B_R,
- H_{D} denotes the Laplacian on $L^2(B_R \setminus \overline{U})$ with homogeneous Dirichlet boundary condition on $\partial(B_R \setminus \overline{U})$,
- $T_\rho = 2\nabla\rho \cdot \nabla + \Delta\rho$ where ρ is a cutoff function that is 0 in B_{R-1} and 1 near ∂B_R,
- and $S(k) : H^1(\partial B_R) \to H^{\frac{3}{2}}(B_R)$ is defined by $S(k)\phi = w$, where w solves

$$\begin{cases} (-\Delta - k^2)w = 0 & \text{in } B_R, \\ w = \phi & \text{on } \partial B_R, \end{cases}$$

i.e. $S(k)\phi$ is the harmonic extension of ϕ into B_R, which extends to a bounded operator $L^2(\partial B_R) \to H^{\frac{1}{2}}(B_R)$.

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Writing $\mathcal{K}(k)$ in the basis $e_n(\theta)$

Recall: $\mathcal{K}(k) = \partial_\nu (H_\mathrm{D} - k^2)^{-1} T_\rho S(k)$ and $e_n(\theta) = (2\pi R)^{-\frac{1}{2}} e^{in\theta}$

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Goal: approximate

$$\begin{aligned}\mathcal{K}_{\alpha\beta} &:= \int_{\partial B_R} \overline{e_\beta} \mathcal{K}(k) e_\alpha \, d\sigma \\ &= \int_{\partial B_R} \overline{e_\beta} \partial_\nu \underbrace{(H_{\mathrm{D}} - k^2)^{-1} \underbrace{T_\rho S(k) e_\alpha}_{f_\alpha}}_{v_\alpha} \, d\sigma.\end{aligned}$$

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Define $E_n(r,\theta) = \rho(r) e_n(\theta)$ and use Green's first identity...

$$
\begin{aligned}
\mathcal{K}_{\alpha\beta} &= \int_{\partial B_R} \overline{e_\beta}\partial_\nu v_\alpha \, d\sigma \\
&= \int_{B_R\setminus\overline{U}} \overline{E_\beta}\Delta v_\alpha \, dx + \int_{B_R\setminus\overline{U}} \nabla\overline{E_\beta}\cdot\nabla v_\alpha \, dx \\
&= \int_{B_R\setminus\overline{U}} \overline{E_\beta}(-f_\alpha - k^2 v_\alpha) \, dx + \int_{B_R\setminus\overline{U}} \nabla\overline{E_\beta}\cdot\nabla v_\alpha \, dx \\
&= \int_{B_R\setminus\overline{U}} \nabla\overline{E_\beta}\cdot\nabla v_\alpha \, dx - k^2 \int_{B_R\setminus\overline{U}} \overline{E_\beta} v_\alpha \, dx - \int_{B_R\setminus\overline{U}} \overline{E_\beta} f_\alpha \, dx
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&= \int_{B_R \setminus \overline{U}} \nabla \overline{E_\beta} \cdot \nabla v_\alpha \, dx - k^2 \int_{B_R \setminus \overline{U}} \overline{E_\beta} v_\alpha \, dx - \int_{B_R \setminus \overline{U}} \overline{E_\beta} f_\alpha \, dx \\
& \qquad\qquad ✗ \qquad\qquad\qquad\qquad ✗ \qquad\qquad\qquad\qquad ✓
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$$

The last term can be approximated by standard methods; a mesh of size h leads to error of order h^2. First two terms are problematic.

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&= \underbrace{\int_{B_R\setminus\overline{U}} \nabla\overline{E_\beta}\cdot\nabla v_\alpha \, dx}_{\text{✗}} - k^2 \underbrace{\int_{B_R\setminus\overline{U}} \overline{E_\beta} v_\alpha \, dx}_{\text{✗}} - \underbrace{\int_{B_R\setminus\overline{U}} \overline{E_\beta} f_\alpha \, dx}_{\text{✓}}
\end{aligned}$$

The last term can be approximated by standard methods; a mesh of size h leads to error of order h^2. First two terms are problematic.

We need to approximate v_α.

$$\mathcal{K}_{\alpha\beta} = \int_{B_R \setminus \overline{U}} \nabla \overline{E_\beta} \cdot \nabla v_\alpha \, dx - k^2 \int_{B_R \setminus \overline{U}} \overline{E_\beta} v_\alpha \, dx - \int_{B_R \setminus \overline{U}} \overline{E_\beta} f_\alpha \, dx$$

✗ ✗ ✓

Proposition

For small $h > 0$ there exists a piecewise linear function v_α^h which is computable in finitely many algebraic steps, which satisfies the error estimate

$$\|v_\alpha - v_\alpha^h\|_{H^1(B_R \setminus \overline{U})} \leq C h^{\frac{1}{3}} \|f_\alpha\|_{H^1(B_R \setminus \overline{U})},$$

where C is independent of h and α.

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Proof is about 4 pages, so we skip. Ingredients: triangulation of $B_R \setminus \overline{U}$, tools from numerical analysis (e.g. Céa's Lemma) and functional analysis (e.g. Sobolev embeddings).

$$\mathcal{K}_{\alpha\beta} = \int_{B_R \setminus \overline{U}} \nabla \overline{E_\beta} \cdot \nabla v_\alpha \, dx - k^2 \int_{B_R \setminus \overline{U}} \overline{E_\beta} v_\alpha \, dx - \int_{B_R \setminus \overline{U}} \overline{E_\beta} f_\alpha \, dx$$

✓ ✓ ✓

Thus we have a quantitative way to approximate these integrals:

$$(\mathcal{K}_h)_{\alpha\beta} = \int_{B_R \setminus \overline{U}} (\Pi^h \nabla \overline{E_\beta}) \cdot \nabla v_\alpha^h \, dx - k^2 \int_{B_R \setminus \overline{U}} (\Pi^h \overline{E_\beta}) v_\alpha^h \, dx - \int_{B_R \setminus \overline{U}} (\Pi^h \overline{E_\beta}) f_\alpha^h \, dx$$

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This ultimately leads to

$$\begin{aligned}|\mathcal{K}_{\alpha\beta} - (\mathcal{K}_h)_{\alpha\beta}| &\le C(k)\beta^2\left(h^{\frac{1}{3}}\|f_\alpha\|_{L^2(B_R\setminus\overline{U})} + h^2\|f_\alpha\|_{H^2(B_R\setminus\overline{U})}\right)\\ &\le C(k)\beta^2\left(h^{\frac{1}{3}}|\alpha| + h^2|\alpha|^3\right)\end{aligned}$$

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Finally, a Young's inequality leads to:

Proposition

For any $n \in \mathbb{N}$, one has the operator norm estimate:

$$\| P_n \mathcal{K} P_n - \mathcal{K}_h \|_{L(\mathcal{H})} \le C(k)(h^{\frac{1}{3}} n^3 + h^2 n^5),$$

Approximation of $\mathcal{C}(k)$ Revisited

Recall that we had to approximate

$$\mathcal{C}(k) = N^{-\frac{1}{2}}\big(\mathcal{H}(k) + \mathcal{J}(k) + \mathcal{K}(k)\big)N^{-\frac{1}{2}}.$$

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We know from before that

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The Proposition on the last slide leads to

$$\Big\|\mathcal{C}(k) - \underbrace{P_n N^{-\frac{1}{2}}(\mathcal{H} + \mathcal{J} + \mathcal{K}_{h(n)})N^{-\frac{1}{2}} P_n}_{\mathcal{C}_n(k)}\Big\|_{C_p} \leq Cn^{-\frac{1}{2}+\frac{1}{p}}$$

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$\mathcal{C}_n(k)$ is something that we can compute with finitely many arithmetic operations!

Approximation of $\mathcal{C}(k)$ Revisited

$$\mathcal{C}(k) = N^{-\frac{1}{2}}\big(\mathcal{H}(k) + \mathcal{J}(k) + \mathcal{K}(k)\big)N^{-\frac{1}{2}}$$

$$\mathcal{C}_n(k) = P_n N^{-\frac{1}{2}}(\mathcal{H}(k) + \mathcal{J}(k) + \mathcal{K}_{h(n)}(k))N^{-\frac{1}{2}}P_n$$

We finally have:

Proposition

There exists $C > 0$ which is independent of k for k in a compact subset of $\mathbb{C}^-$ such that:

$$\left|\det_{\lceil p \rceil}(\mathrm{Id}_{L^2} + \mathcal{C}(k)) - \det_{\lceil p \rceil}(\mathrm{Id}_{L^2} + \mathcal{C}_n(k))\right| \leq Cn^{-\frac{1}{2}+\frac{1}{\lceil p \rceil}}$$

The Algorithm

Goal: find values of k for which $\det_{\lceil p \rceil}(\mathrm{Id}_{L^2} + \mathcal{C}_n(k))$ is small.

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Let $\emptyset \neq Q \subset \mathbb{C}^-$ be compact and let $G_n = \frac{1}{n}(\mathbb{Z} + i\mathbb{Z})$. Define

$$\Gamma_n^Q : \Omega \to \mathrm{cl}(\mathbb{C})$$
$$\Gamma_n^Q(U) := \left\{ k \in G_n \cap Q \,\middle|\, \left|\det_{\lceil p \rceil}(\mathrm{Id}_{L^2} + \mathcal{C}_n(k))\right| \leq \frac{1}{\log(n)} \right\}.$$

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$$\Gamma_n^Q(U) := \left\{ k \in G_n \cap Q \,\middle|\, \left|\det_{\lceil p \rceil}(\mathrm{Id}_{L^2} + \mathcal{C}_n(k))\right| \leq \frac{1}{\log(n)} \right\}.$$

Theorem

For any $U \in \Omega$ we have $\Gamma_n^Q(U) \to \mathrm{Res}(U) \cap Q$ in the Hausdorff distance as $n \to +\infty$.

We need to extend this to the whole of $\mathbb{C}^-$. We do this by tiling $\mathbb{C}^-$ with compact sets:

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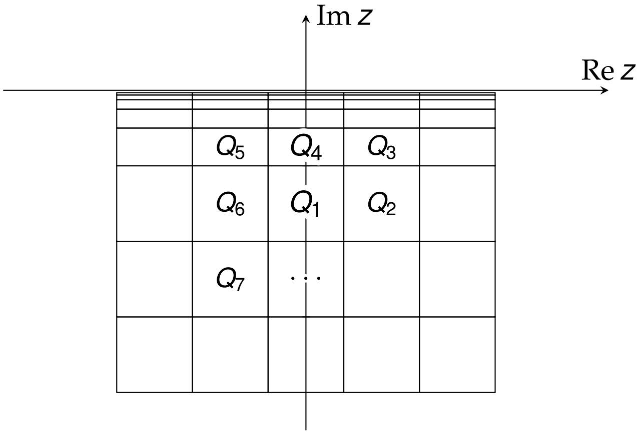

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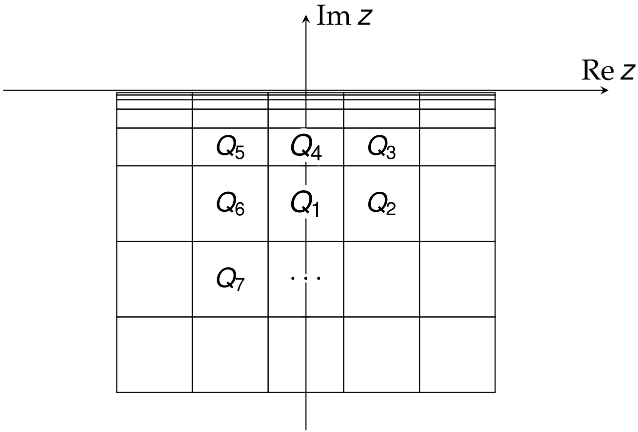
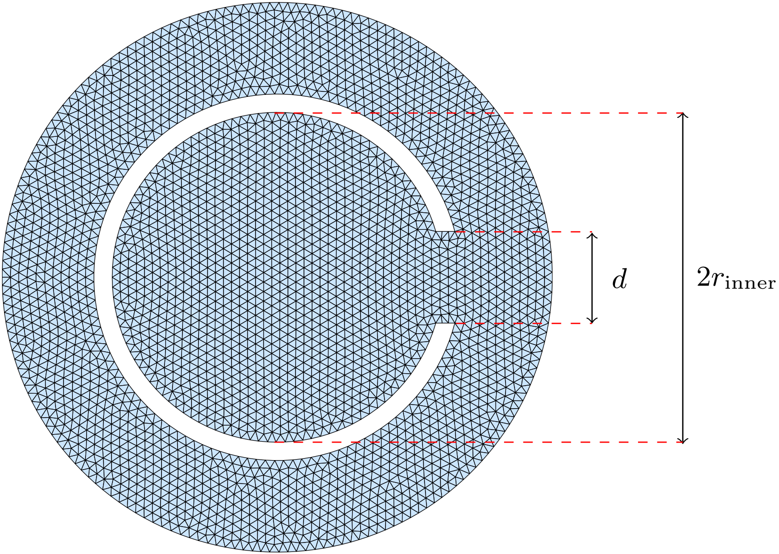
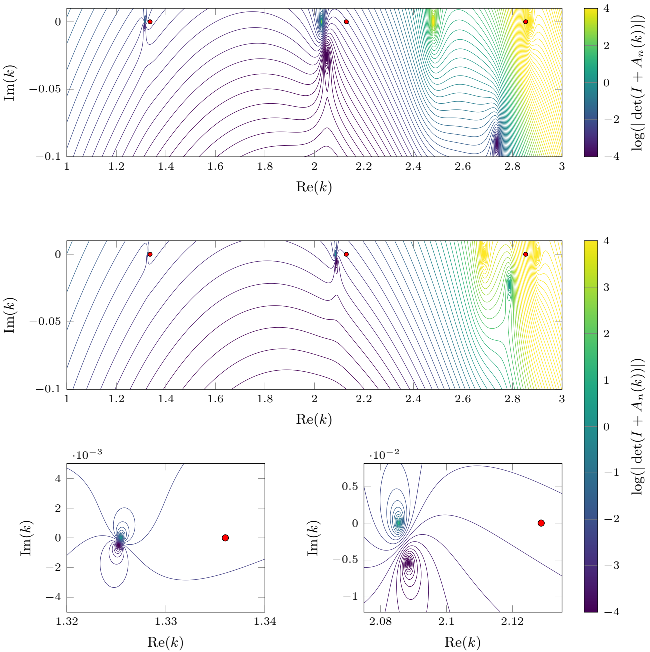
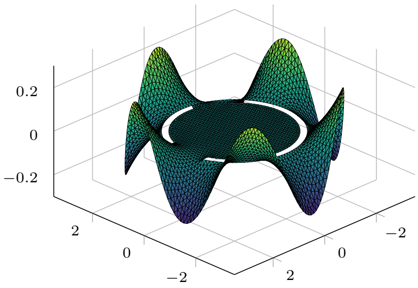


And finally define:

$$\Gamma_n(U) := \bigcup_{j=1}^{n} \Gamma_n^{Q_j}(U)$$


d
$2r_{\text{inner}}$

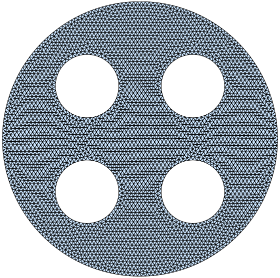

Im(k)
Re(k)
log(| det(I + A_n(k))|)
·10^{−3}
·10^{−2}

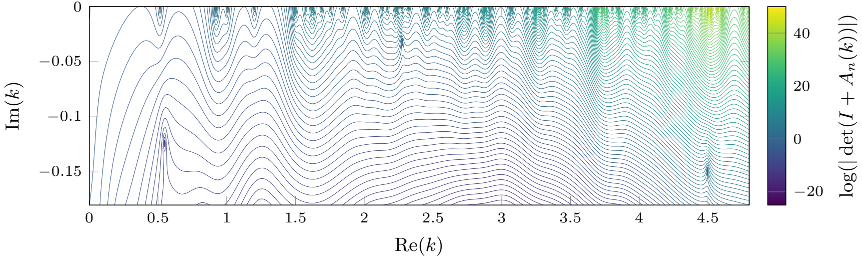


Solution of

$$\begin{cases} (-\Delta - k^2)u = 0 & \text{in } B_R \setminus \overline{U}, \\ u = e_5 & \text{on } \partial B_R, \\ u = 0 & \text{on } \partial U. \end{cases}$$

Left: $k = 1.0$ (far from resonance)
Right: $k = 2.049 - 0.026i$ (near second resonance)




0
−0.05
−0.1
−0.15
Im(k)
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
Re(k)
40
20
0
−20
log(| det($I + A_n(k)$)|)

Thank you for your attention!