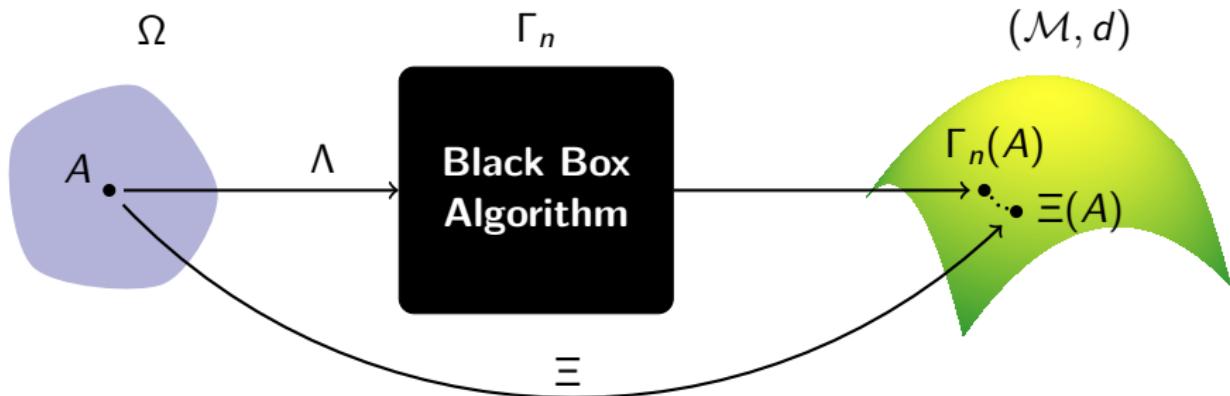


Recent results on the approximation of resonances

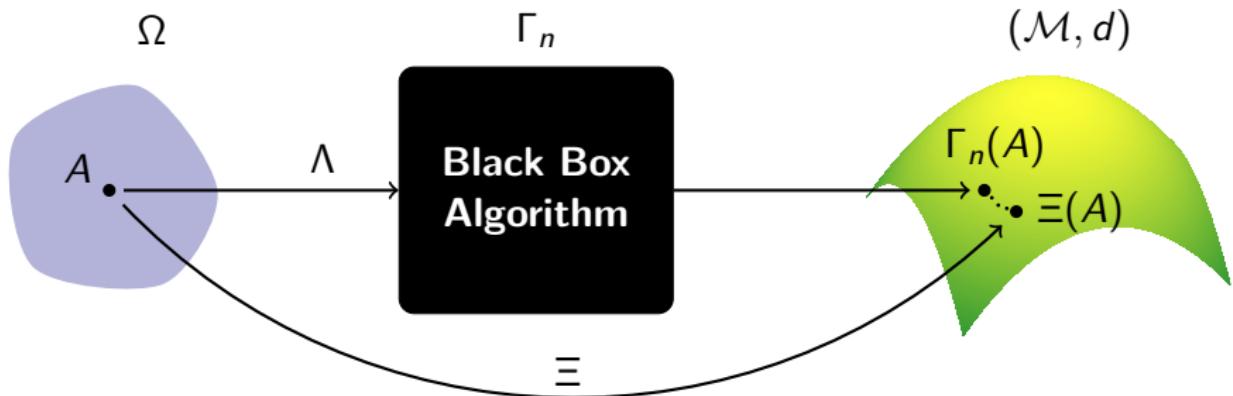
Jonathan Ben-Artzi (Cardiff University)

Spectral and Resonance Problems for
Imaging, Seismology and Materials Science
Université de Reims Champagne-Ardenne
20-24 novembre 2023

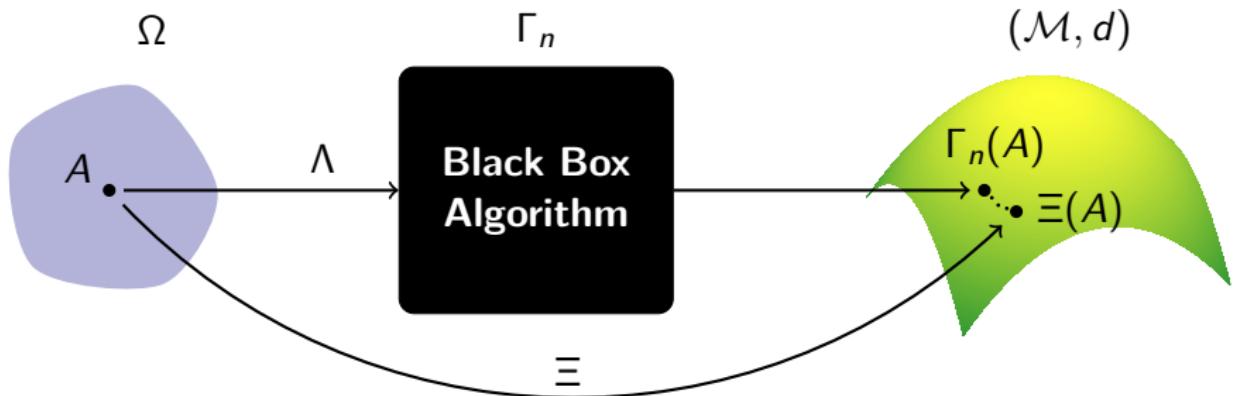
AN ABSTRACT QUESTION



- Ω a set,
- \mathcal{M} a metric space,
- $\Xi : \Omega \rightarrow \mathcal{M}$ a mapping,
- Λ a set of complex-valued functions on Ω
(input of the algorithm)



Does there exist an algorithm $\{\Gamma_n\}_{n=1}^{\infty}$ that can approximate Ξ for all A ?

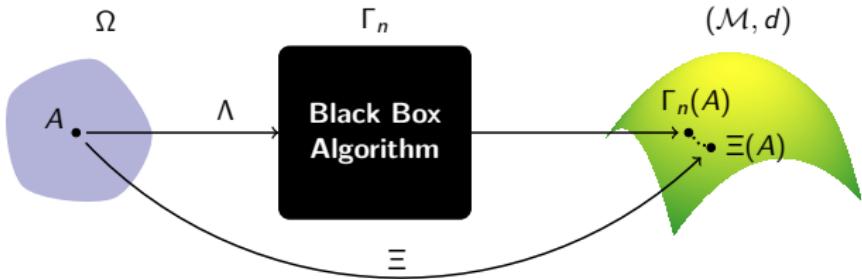


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The only two requirements of the algorithm:

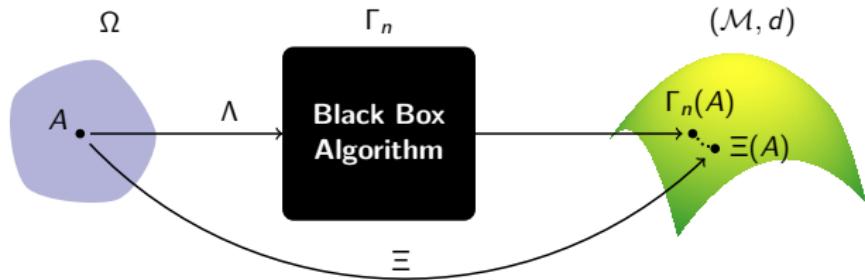
- At each iteration it can only access a finite subset $\Lambda_n \subset \Lambda$
- It operates consistently (the output depends only on Λ_n)

Example



Does there exist an algorithm for computing the spectrum of any $A \in \mathcal{B}^{\text{s.a.}}(\ell^2(\mathbb{N}))$?

Example



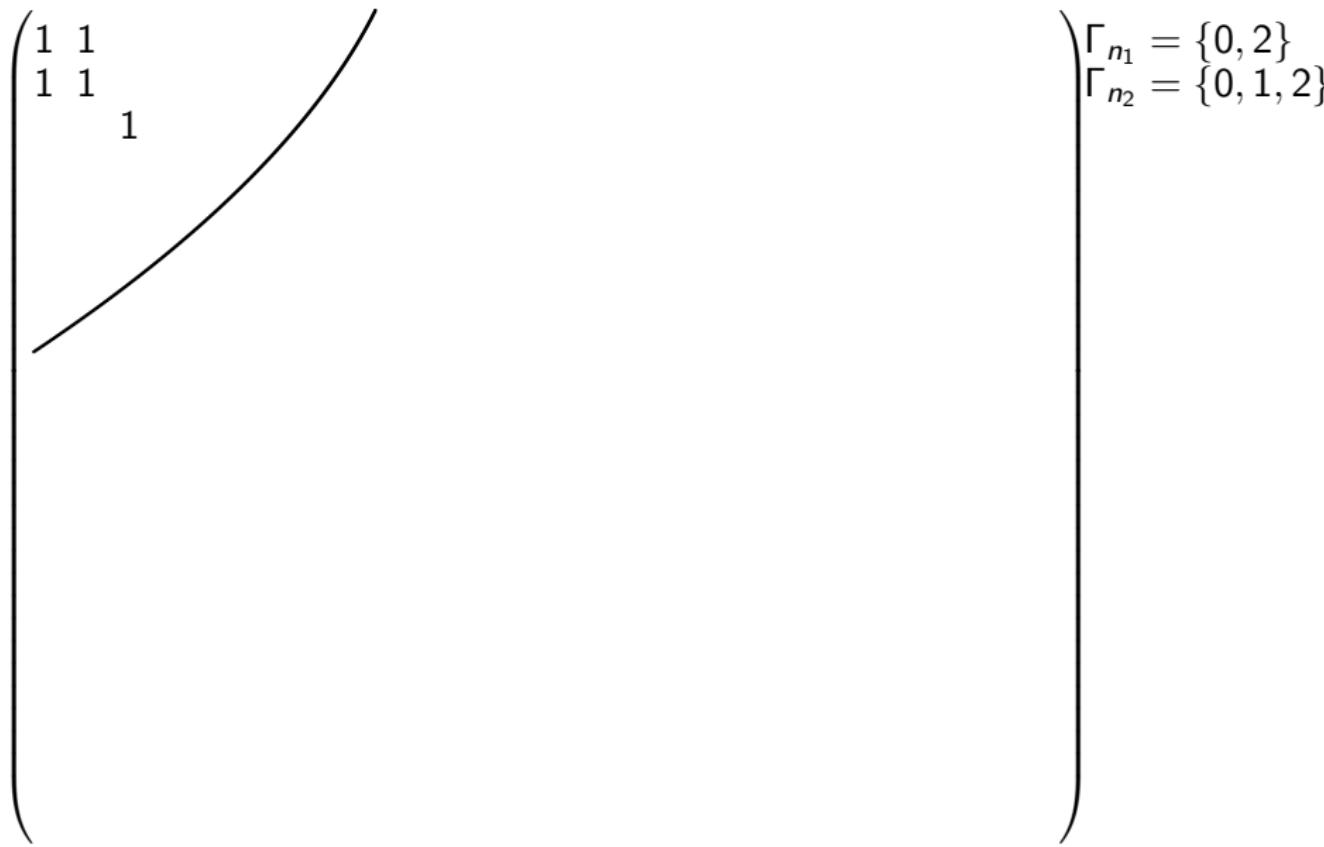
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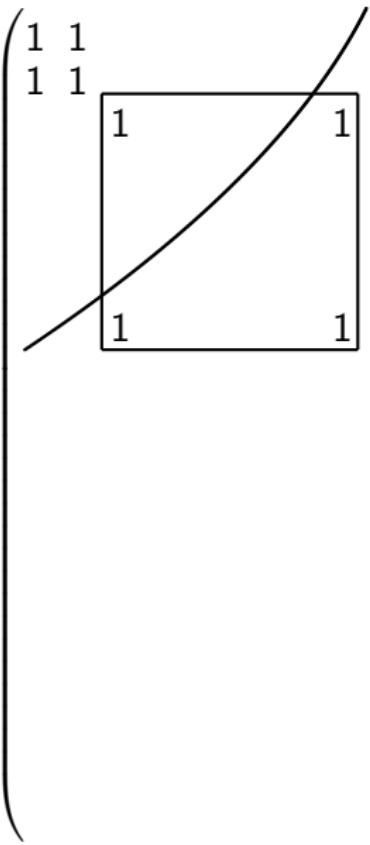
Here:

- $\Omega = \mathcal{B}^{\text{s.a.}}(\ell^2(\mathbb{N}))$,
- \mathcal{M} = compact subsets of \mathbb{C} with Hausdorff distance,
- $\Xi(A) = \sigma(A)$,
- $\Lambda = \{(Ae_i, e_j)\}_{i,j=1}^\infty$

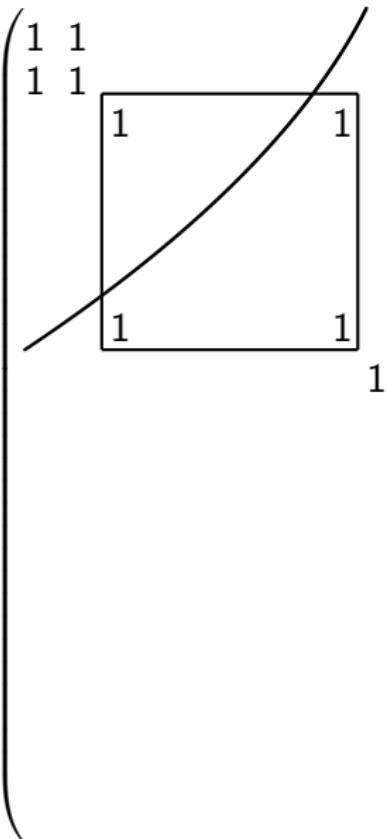
$$\left(\begin{array}{cc} 1 & 1 \\ 1 & 1 \end{array} \right) \Gamma_{n_1} = \{0, 2\}$$

$$\left(\begin{array}{cc} 1 & 1 \\ 1 & 1 \\ & 1 \end{array} \right) \quad \left. \begin{array}{l} \Gamma_{n_1} = \{0, 2\} \\ \Gamma_{n_2} = \{0, 1, 2\} \end{array} \right\}$$

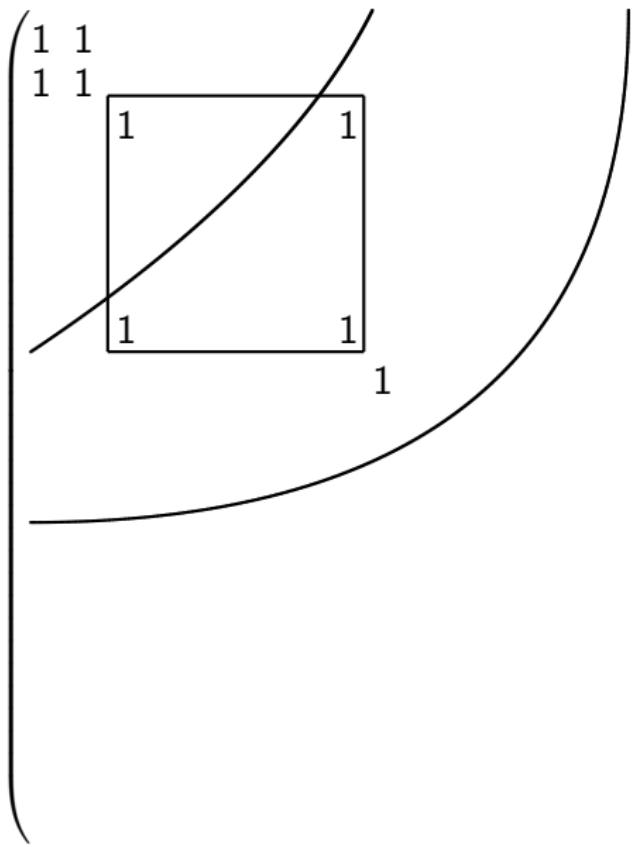
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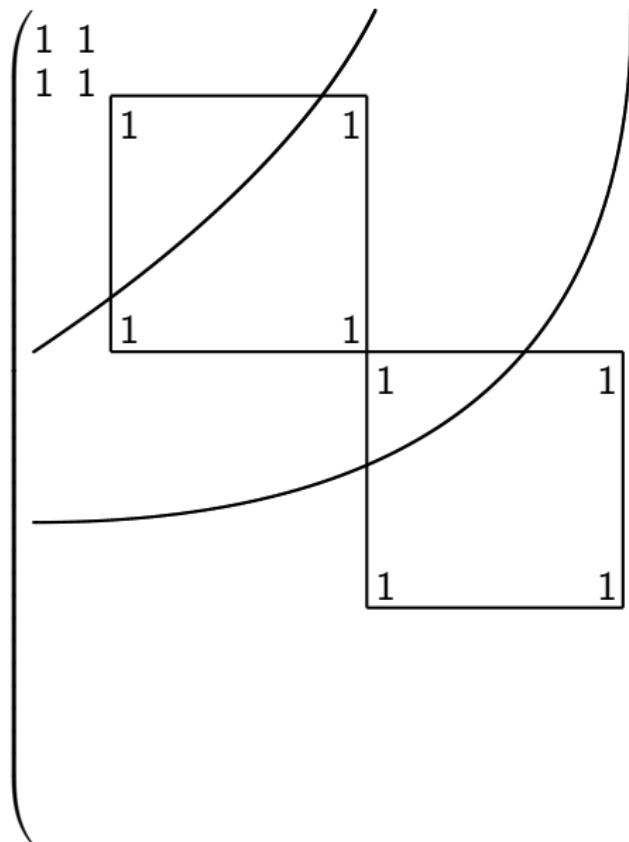
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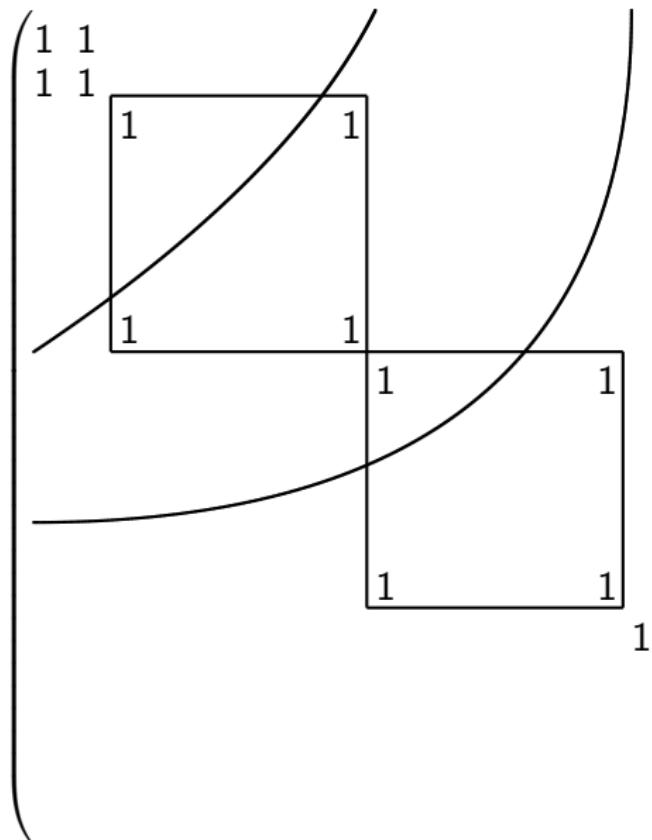
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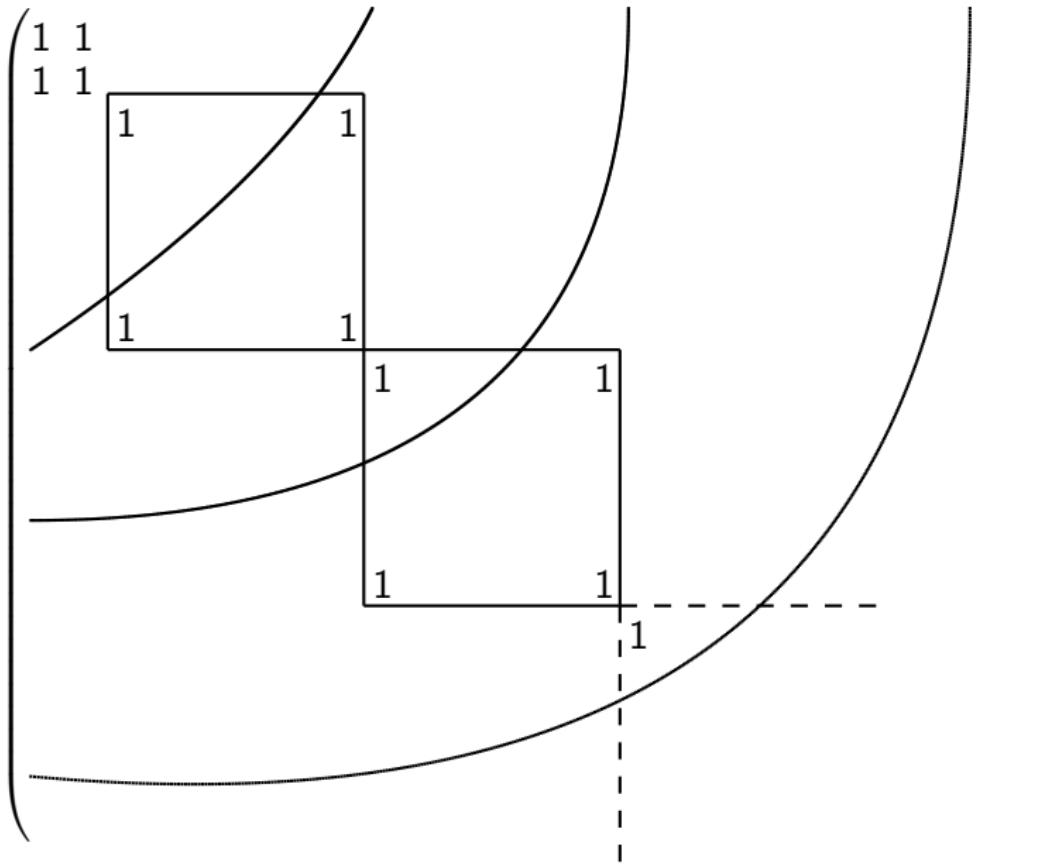
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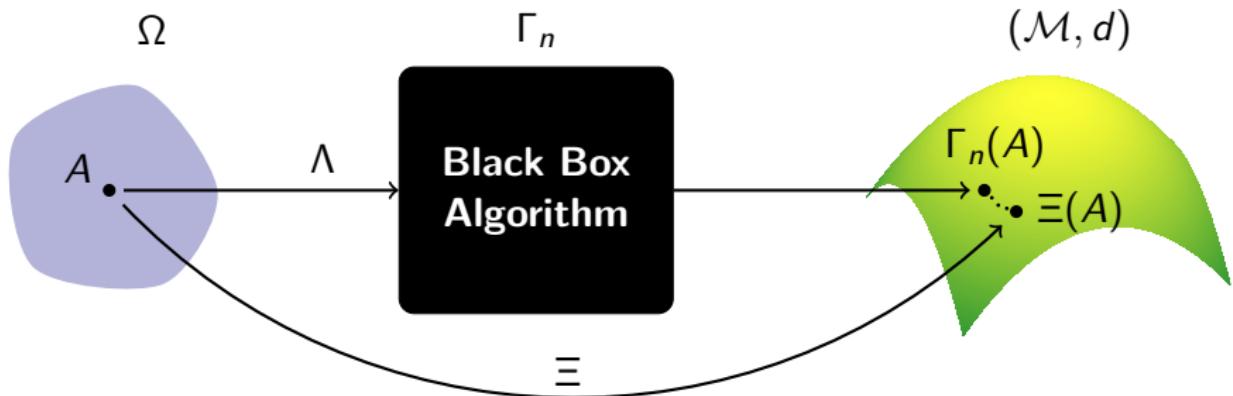


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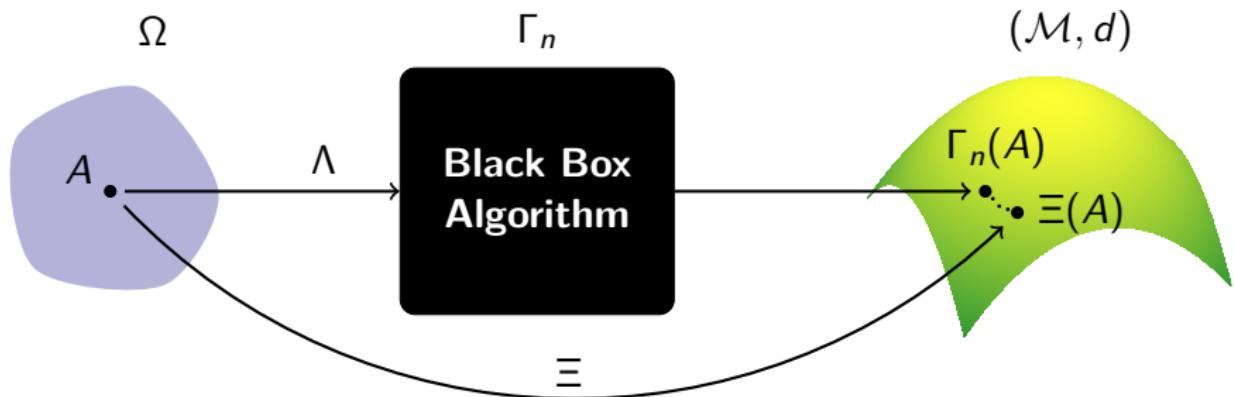
$$\sigma(A) = \{0, 2\}$$

Does there exist an algorithm for computing the spectrum of any $A \in \mathcal{B}^{\text{s.a.}}(\ell^2(\mathbb{N}))$?

No, but....

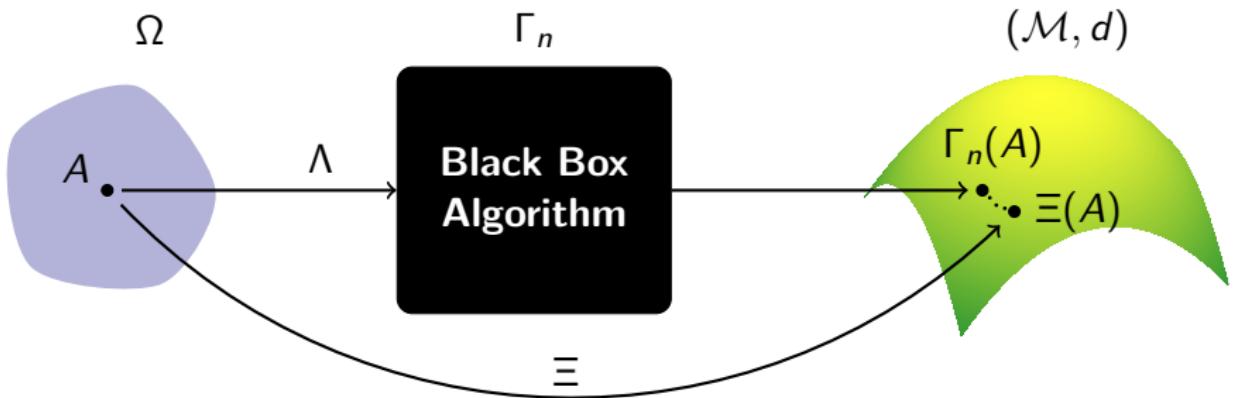


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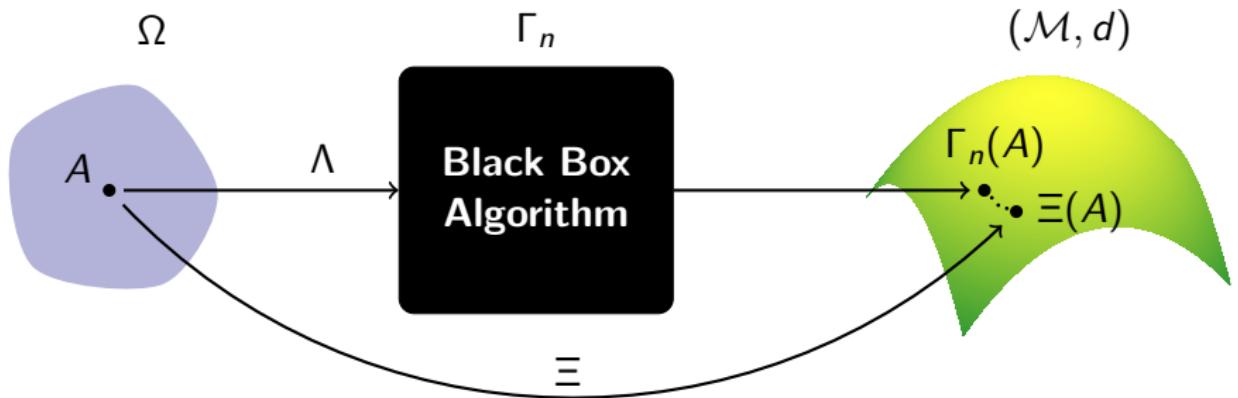
A: Not always.



Does there exist an algorithm $\{\Gamma_n\}_{n=1}^{\infty}$ that can approximate Ξ for all A ?

A: Not always. Sometimes multiple limits with multiple indices may be necessary $\Gamma_{n_k, n_{k-1}, \dots, n_1}$, a tower of algorithms:

$$\Xi(A) = \lim_{n_k \rightarrow \infty} \left(\lim_{n_{k-1} \rightarrow \infty} \cdots \left(\lim_{n_1 \rightarrow \infty} \Gamma_{n_k, n_{k-1}, \dots, n_1}(A) \right) \right)$$



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The **SCI** is the minimal number of limits necessary.

COMPUTING SPECTRA - ON THE SOLVABILITY COMPLEXITY INDEX HIERARCHY AND TOWERS OF ALGORITHMS

J. BEN-ARTZI, M. J. COLBROOK, A. C. HANSEN, O. NEVANLINNA, AND M. SEIDEL

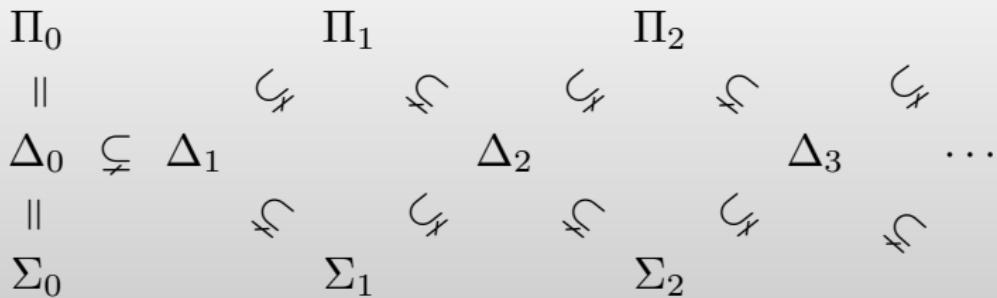
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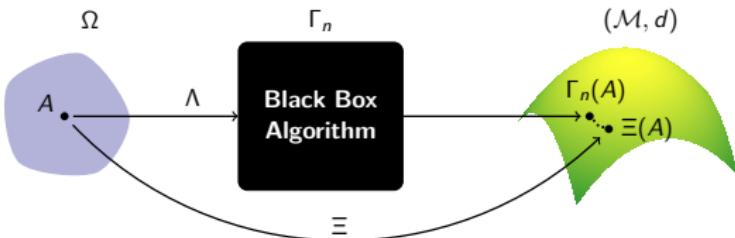
J. BEN-ARTZI, M. J. COLBROOK, A. C. HANSEN, O. NEVANLINNA, AND M. SEIDEL

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We define a hierarchical structure



Natural Questions



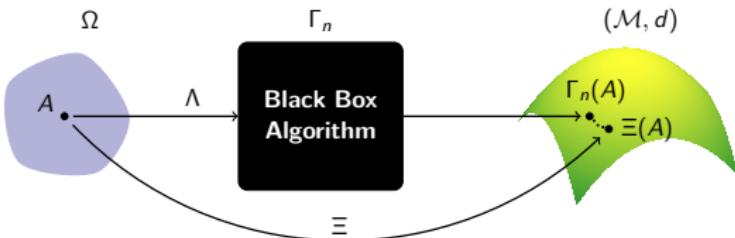
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JBA–Colbrook–Hansen–Nevanlinna–Seidel, *preprint*

Natural Questions



Does there exist an algorithm for computing the spectrum of any $A \in \mathcal{B}(\ell^2(\mathbb{N}))$? **SCI=3**

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JBA–Colbrook–Hansen–Nevanlinna–Seidel, *preprint*

RELATIONSHIP TO OTHER BRANCHES OF MATHEMATICS:

Theoretical Computer Science

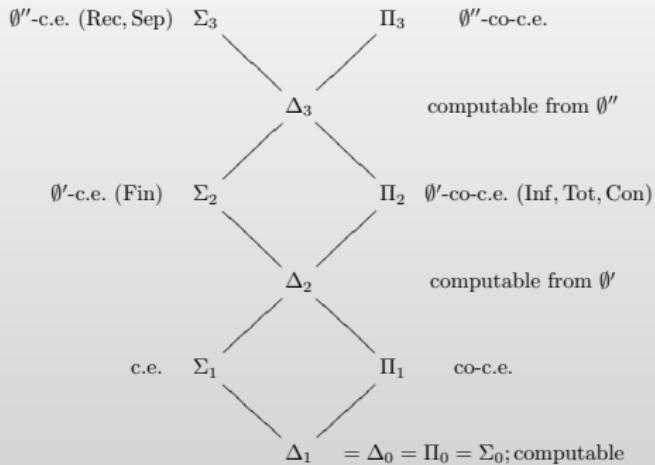
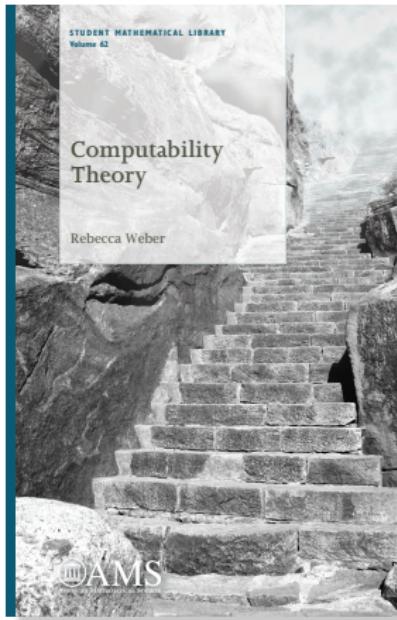


Figure 7.1. A picture of the arithmetical hierarchy.
Each set is contained in those directly above it and those above it to which it is connected by lines.

RELATIONSHIP TO OTHER BRANCHES OF MATHEMATICS:

Finding Roots of Polynomials

Let \mathcal{P}_d be the space of polynomials of degree $\leq d$. A **purely iterative algorithm** is a rational map $T_p : \mathbb{C} \rightarrow \mathbb{C}$ depending on $p \in \mathcal{P}_d$ and its derivatives up to some fixed order k , and having the form

$T_p(z) = F(z, p(z), \dots, p^{(k)}(z))$ where F is a rational map.

e.g. *Newton's algorithm*

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T_p is **generally convergent** if \exists set $\mathcal{U} \subset \mathbb{C} \times \mathcal{P}_d$ of full measure s.t.

$T_p^n(z) \xrightarrow{n \rightarrow \infty}$ root of p for any $(z, p) \in \mathcal{U}$.

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purely iterative algorithm?

S. Smale, Bull. AMS, 1985

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

Solving the quintic by iteration

by

PETER DOYLE⁽¹⁾

and

CURT McMULLEN⁽²⁾

*Princeton University
Princeton, NJ, U.S.A.*

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Show that the cases $d = 4, 5$ can be solved by towers of algorithms

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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.

RECENT RESULTS

Some Recent Results

All joint with M. Marletta and F. Rösler

Spectrum of periodic operators (*Num. Math.*, 2022)

Obstacle scattering resonances (*Found. Comp. Math.*, 2022)

Quantum scattering resonances (*J. Eur. Math. Soc.*, 2023)

The inverse Sturm-Liouville problem (*Pure Appl. Anal.*, to appear)

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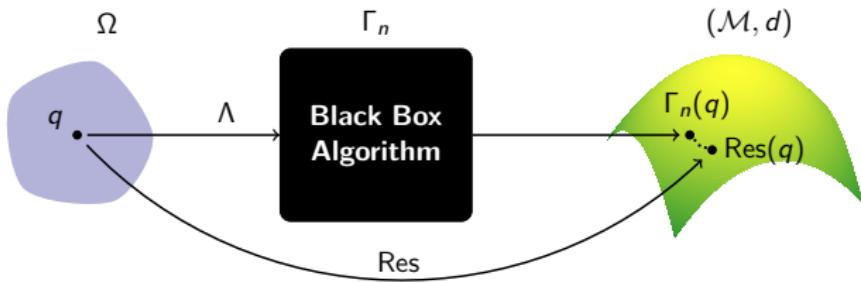
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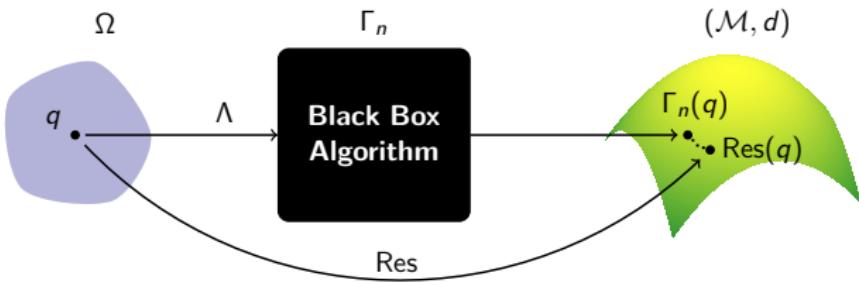
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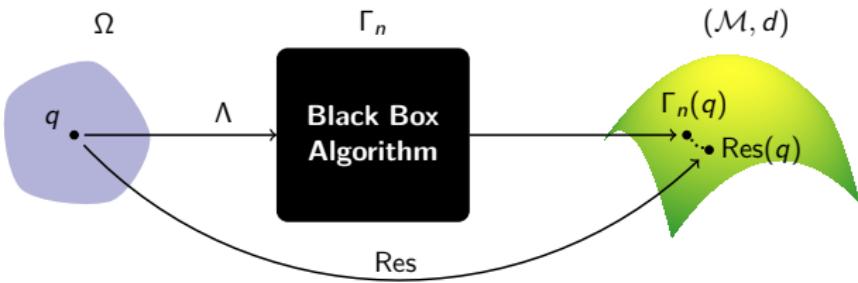
Does there exist an algorithm for computing the resonances $\text{Res}(q)$ of $H_q := -\Delta + q$ for **any** ‘nice’ $q : \mathbb{R}^d \rightarrow \mathbb{C}$?



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Theorem (JBA–Marletta–Rösler, *J. Eur. Math. Soc.* 2023)

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

Moreover, if one knows a priori that $\exists M > 0$ such that $\text{diam}(\text{supp}(q)) + \|q\|_\infty \leq M$ then the computation can be performed with error control.

Proof

1. Looking for resonances of $H_q = -\Delta + q$, where $q \in C_0^1(\mathbb{R}^d; \mathbb{C})$.

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$$\begin{aligned} (-\Delta + q)u &= z^2 u \\ \underbrace{(-\Delta - z^2)u}_{v} + qu &= 0 \\ v + q(-\Delta - z^2)^{-1}v &= 0 \end{aligned}$$

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 $\text{supp}(q)$.

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5. Poles of $(I + K_n(z))^{-1} \longrightarrow$ Poles of $(\text{Id}_{L^2} + K(z))^{-1}$.

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

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

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

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

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

let

$\mathcal{H}_n = L^2$ functions that are constant on each $S_{n,i}$

P_n = orthogonal projection onto \mathcal{H}_n

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

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

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

let

$\mathcal{H}_n = L^2$ functions that are constant on each $S_{n,i}$

P_n = orthogonal projection onto \mathcal{H}_n

Define

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

An Abstract Approximation Result

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

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

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Proposition

We have $\Gamma_n^B(K) \xrightarrow{n \rightarrow +\infty} \{z \in B \mid -1 \in \sigma(K(z))\}$ in the Hausdorff metric.

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Observe: $\Gamma_n^B(K)$ can be completely determined with finitely many operations if $K_n(z)$ can be computed with finitely arithmetic operations.

Applying the Abstract Result

The abstract result leads to (after proving it is applicable):

Theorem

For any $q \in \Omega$, we have $\Gamma_n^B(q) \xrightarrow{n \rightarrow +\infty} \text{Res}(q) \cap B$ in the Hausdorff metric.

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

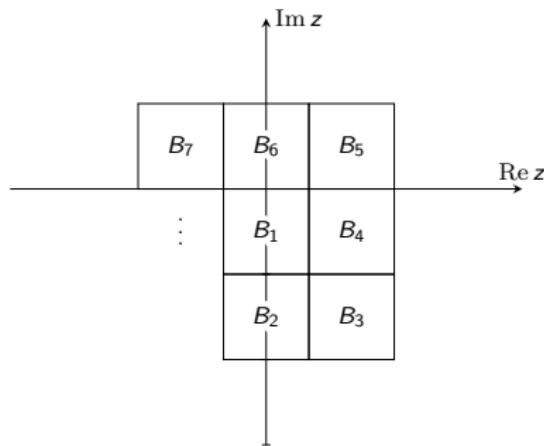
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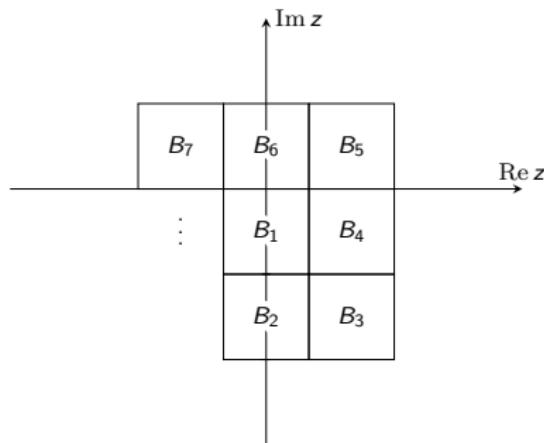
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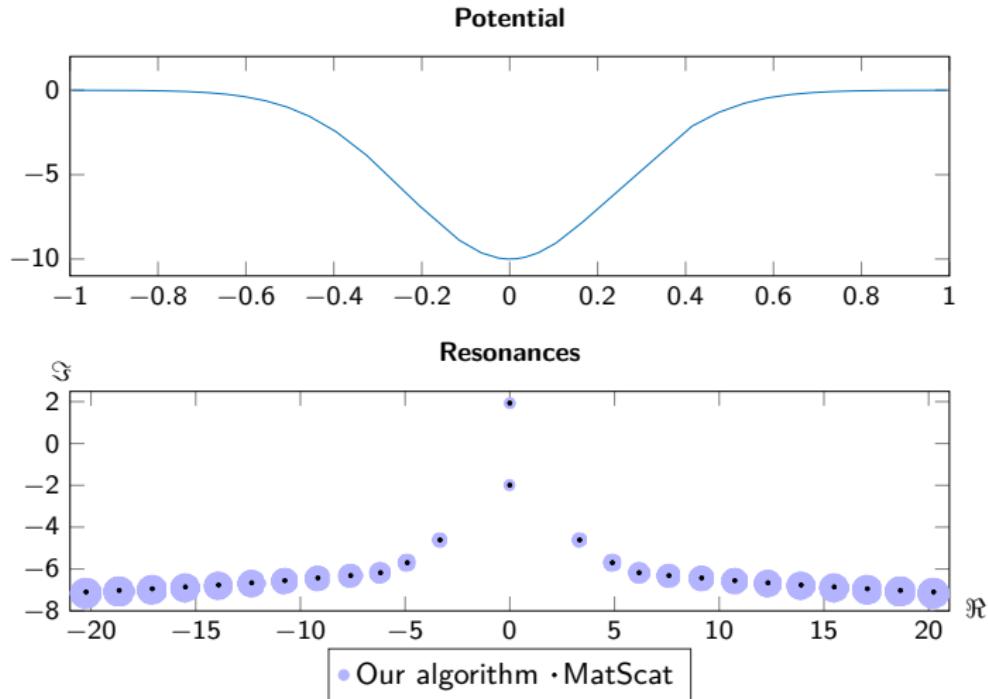
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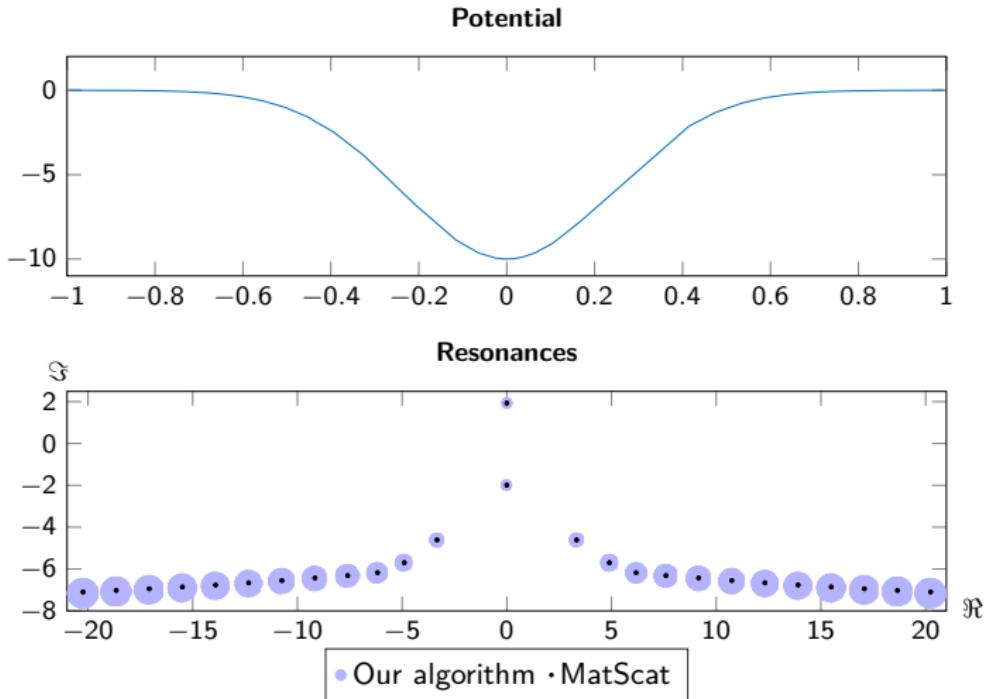
And finally define:

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

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



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Bindel–Zworski (2007): In 1D, assumes $\text{diam}(\text{supp}(q)) \leq M$ and relies on MATLAB's `eig`.

Our algorithm works in **any dimension** and is **self-contained** (does not rely on existing software).

Some Recent Results

All joint with M. Marletta and F. Rösler

Spectrum of periodic operators (*Num. Math.*, 2022)

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The inverse Sturm-Liouville problem (*Pure Appl. Anal.*, to appear)

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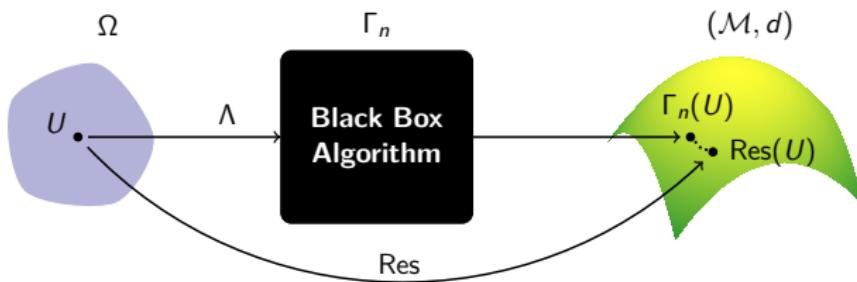
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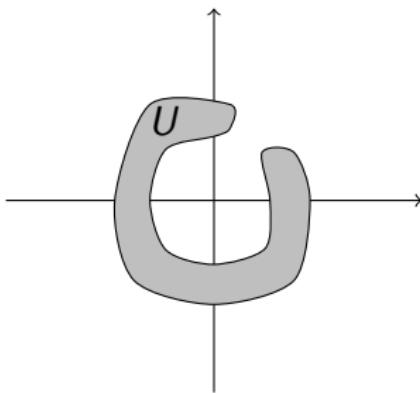
Does there exist an algorithm for computing the resonances $\text{Res}(U)$ of $-\Delta$ on $\mathbb{R}^d \setminus U$ for any 'nice' $U \subset \mathbb{R}^d$?

Obstacle Scattering Resonances

Theorem (JBA–Marletta–Rösler, *Found. Comp. Math.* 2022)

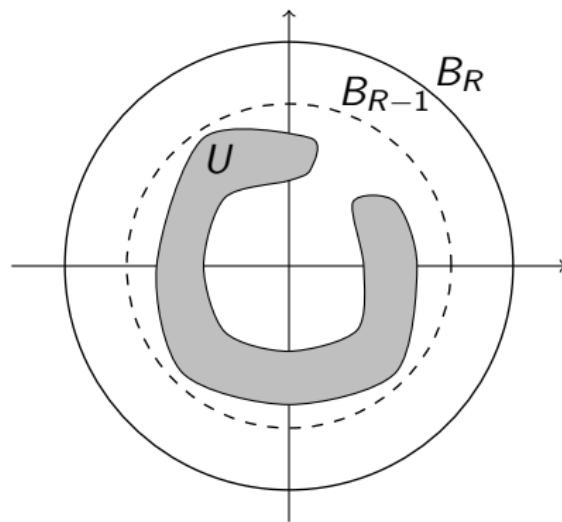
There exists an arithmetic algorithm that can approximate the Dirichlet resonances of U for any

$$U \in \Omega = \{\emptyset \neq U \subset \mathbb{R}^d \mid U \text{ open, bounded and } \partial U \in C^2\}.$$



Proof: Classical Scattering Resonances

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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 :

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

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

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Hence

$$\ker(M_{\text{int}}(k) + M_{\text{ext}}(k)) = \{0\}$$

\Updownarrow

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1. Truncate the matrix:

Lemma

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

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

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

$$\mathcal{K}(k) = \partial_\nu (H_D - k^2)^{-1} T_\rho S(k) : L^2(\partial B_R) \rightarrow L^2(\partial B_R)$$

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 $S(k) : H^1(\partial B_R) \rightarrow H^{\frac{3}{2}}(B_R)$ 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 $L^2(\partial B_R) \rightarrow H^{\frac{1}{2}}(B_R)$.

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- ∂_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 $S(k) : H^1(\partial B_R) \rightarrow H^{\frac{3}{2}}(B_R)$ 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 $L^2(\partial B_R) \rightarrow H^{\frac{1}{2}}(B_R)$.

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

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

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Goal: approximate

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

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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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$\times \quad \times \quad \checkmark$

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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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 .

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

\times \times \checkmark

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

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

where C is independent of h and α .

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Proof is about 4 pages long, 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

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

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Finally, a Young's inequality leads to:

Proposition

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

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

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

Recall that we had to approximate

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

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We know from before that

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

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The Proposition on the last slide leads to

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

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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

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

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

We finally have:

Proposition

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

$$\left| \det_{[\rho]} (\text{Id}_{L^2} + \mathcal{C}(k)) - \det_{[\rho]} (\text{Id}_{L^2} + \mathcal{C}_n(k)) \right| \leq C n^{-\frac{1}{2} + \frac{1}{|\rho|}}$$

The Algorithm

Goal: find values of k for which $\det_{[\rho]} (\text{Id}_{L^2} + \mathcal{C}_n(k))$ 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

$$\Gamma_n^Q : \Omega \rightarrow \text{cl}(\mathbb{C})$$

$$\Gamma_n^Q(U) := \left\{ k \in G_n \cap Q \mid \left| \det_{[\rho]} (\text{Id}_{L^2} + \mathcal{C}_n(k)) \right| \leq \frac{1}{\log(n)} \right\}.$$

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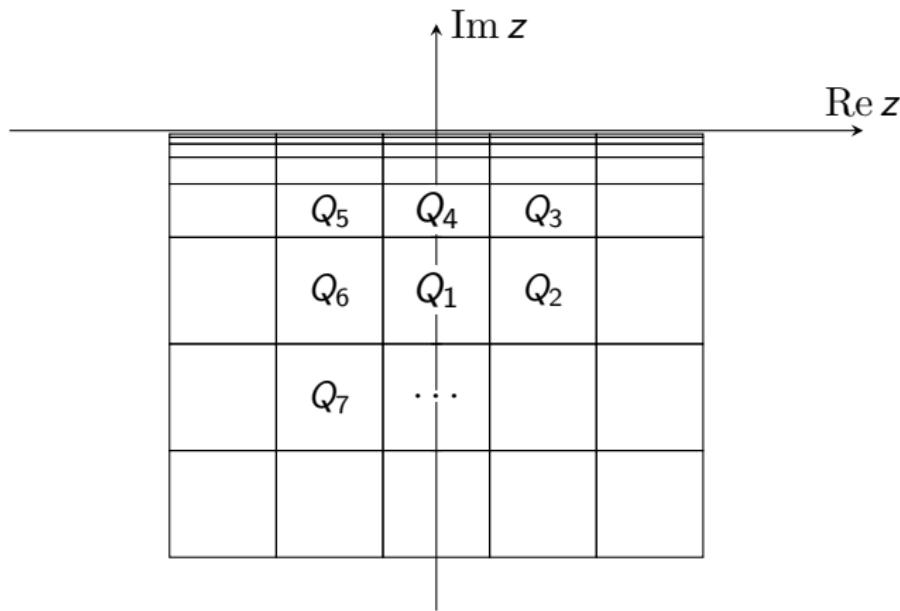
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Theorem

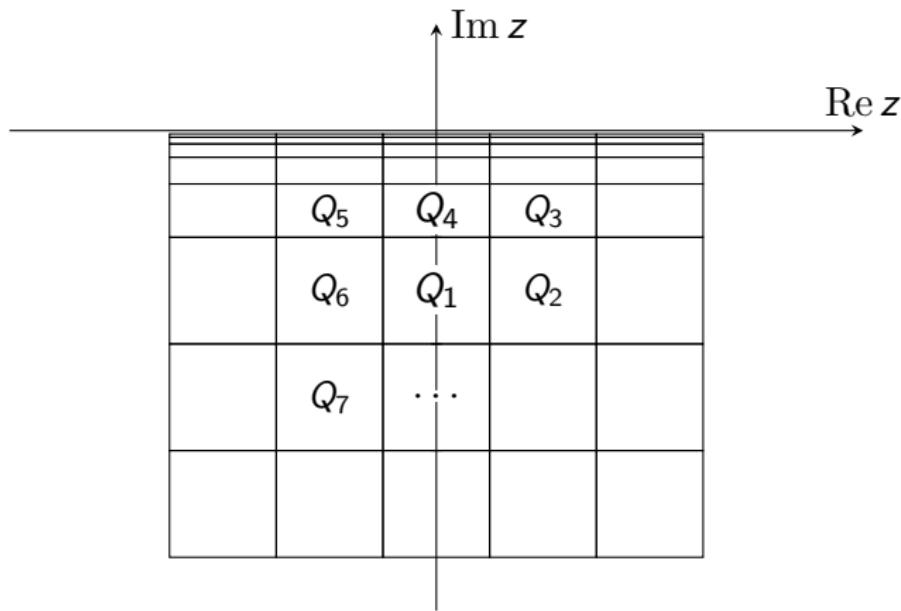
For any $U \in \Omega$ we have $\Gamma_n^Q(U) \xrightarrow{n \rightarrow +\infty} \text{Res}(U) \cap Q$ in the Hausdorff metric.

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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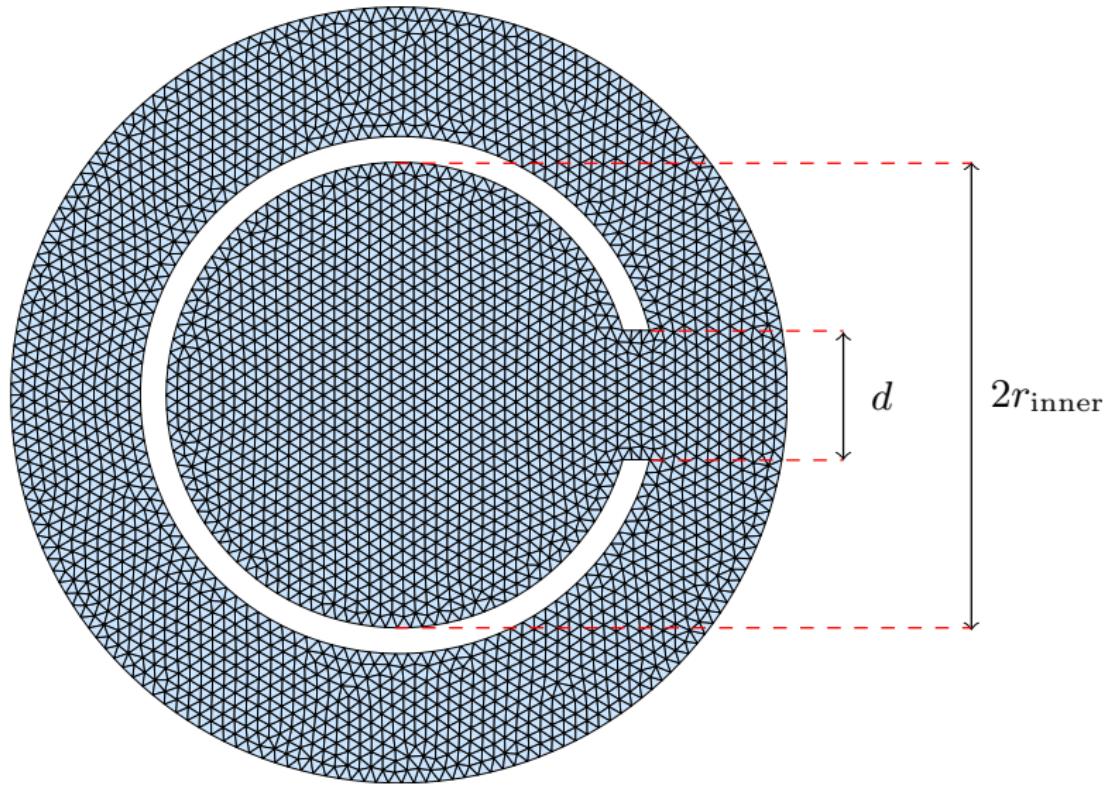


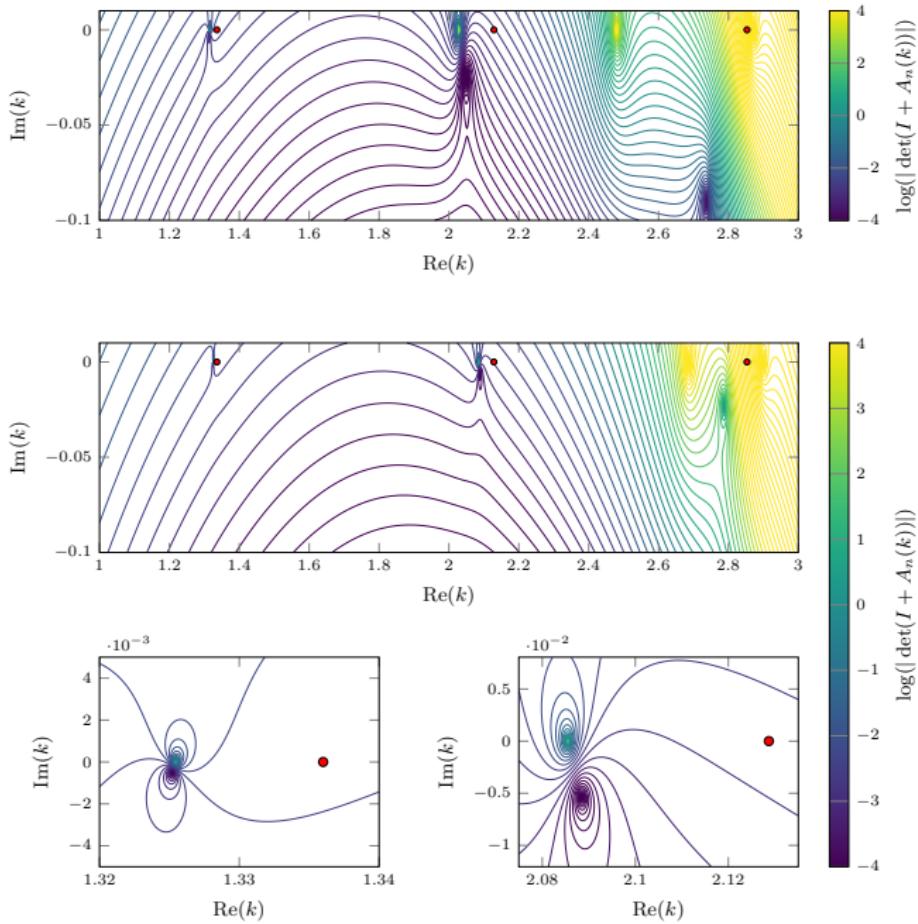
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And finally define:

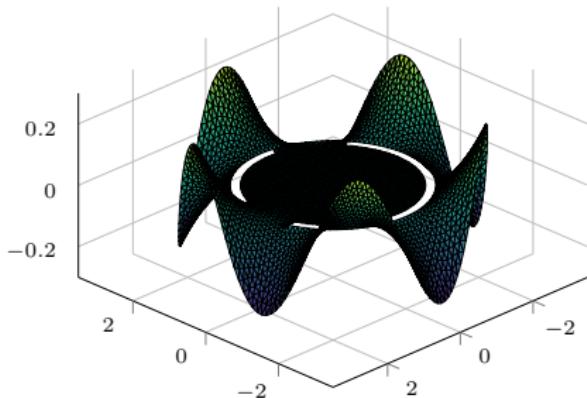
$$\Gamma_n(U) := \bigcup_{j=1}^n \Gamma_n^{Q_j}(U)$$





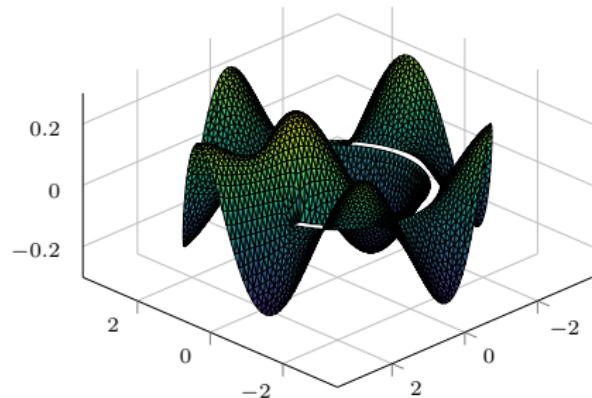
$$k = 1.0$$

(far from the resonances)



$$k = 2.049 - 0.026i$$

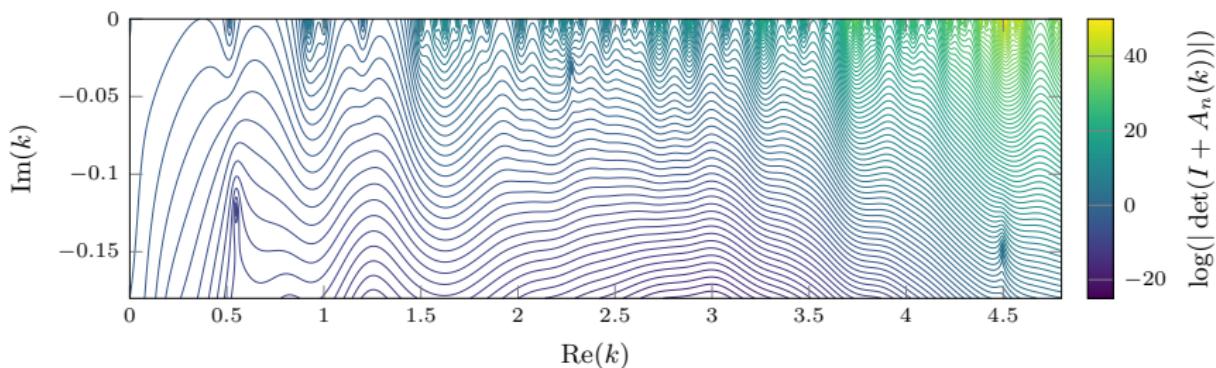
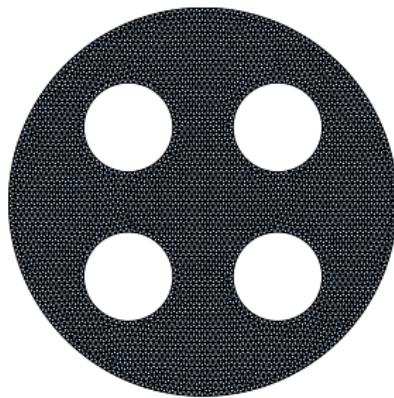
(close to the second resonance)



Solution of

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





Results agree with Evans–Porter (*Applied Ocean Research* 1997)

Thank you for your attention!