

Computing Scattering Resonances

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joint work with
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Engineering and Physical Sciences
Research Council

Introduction

Introduction

General questions:

- ▶ Can one always compute the spectrum of an operator?
- ▶ (later) Can one always compute the scattering resonances of an obstacle?

\mathcal{H} Hilbert space, $\Omega =$ some class of operators on \mathcal{H} .

- ▶ Does there exist a sequence (Γ_N) of computer algorithms s.t.

$$\Gamma_N(T) \rightarrow \sigma(T) \quad \text{for all } T \in \Omega ?$$

Introduction

Definition: A *computational (spectral) problem* consists of

- ▶ Class of operators Ω ,
- ▶ Spectral function $T \mapsto \sigma(T)$,
- ▶ A set Λ of *input information*
(e.g. matrix elements: $T \mapsto \langle e_i, T e_j \rangle$).

Definition: An *Algorithm* is a map

$$\Gamma : \Omega \rightarrow [\text{closed subsets of } \mathbb{C}]$$

such that

- ▶ $\Gamma(T)$ depends only on finitely many $f \in \Lambda$,
- ▶ $\Gamma(T)$ can be computed using finitely many arithmetic operations on these $f(T)$.

Introduction

Example:

- ▶ $\mathcal{H} = \ell^2(\mathbb{N})$ with canonical basis,
- ▶ $\Omega = \mathcal{K}(\mathcal{H})$ (compact operators),
- ▶ $\Lambda = \{T \mapsto \langle e_i, Te_j \rangle\}_{i,j \in \mathbb{N}}$

Algorithm:¹ Let $N \in \mathbb{N}$ and choose lattice $L_N := \frac{1}{N}(\mathbb{Z} + i\mathbb{Z}) \cap B_N(0)$ and $\mathcal{H}_N := \text{span}\{e_1, \dots, e_N\}$.

$$\Gamma_N(T) := \left\{ z \in L_N \mid \| (z - P_N T|_{\mathcal{H}_N})^{-1} \| \geq N \right\}$$

Can show: $\Gamma_N(T) \rightarrow \sigma(T)$ in Hausdorff sense.

¹[Ben-Artzi-Colbrook-Hansen-Nevanlinna-Seidel(2015)]

Introduction

~~~ Recap of strategy:

- ▶ Start with infinite matrix,
- ▶ Truncate matrix to finite size,
- ▶ Compute spectral approximation for truncated matrix,
- ▶ Let truncation size go to  $\infty$ .

Does this always work?

# Introduction



## Counterexample

**Claim:** There exists no sequence of algorithms  $(\Gamma_N)$  s.t.

$$\Gamma_N(T) \rightarrow \sigma(T) \quad \text{for all } T \in \mathcal{B}(\mathcal{H})$$

**Proof:<sup>1</sup>** By Contradiction. Assume that  $\exists \Gamma_N$  and construct “diagonal sequence” operator.

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<sup>1</sup>[Ben-Artzi-Colbrook-Hansen-Nevanlinna-Seidel(2015)]

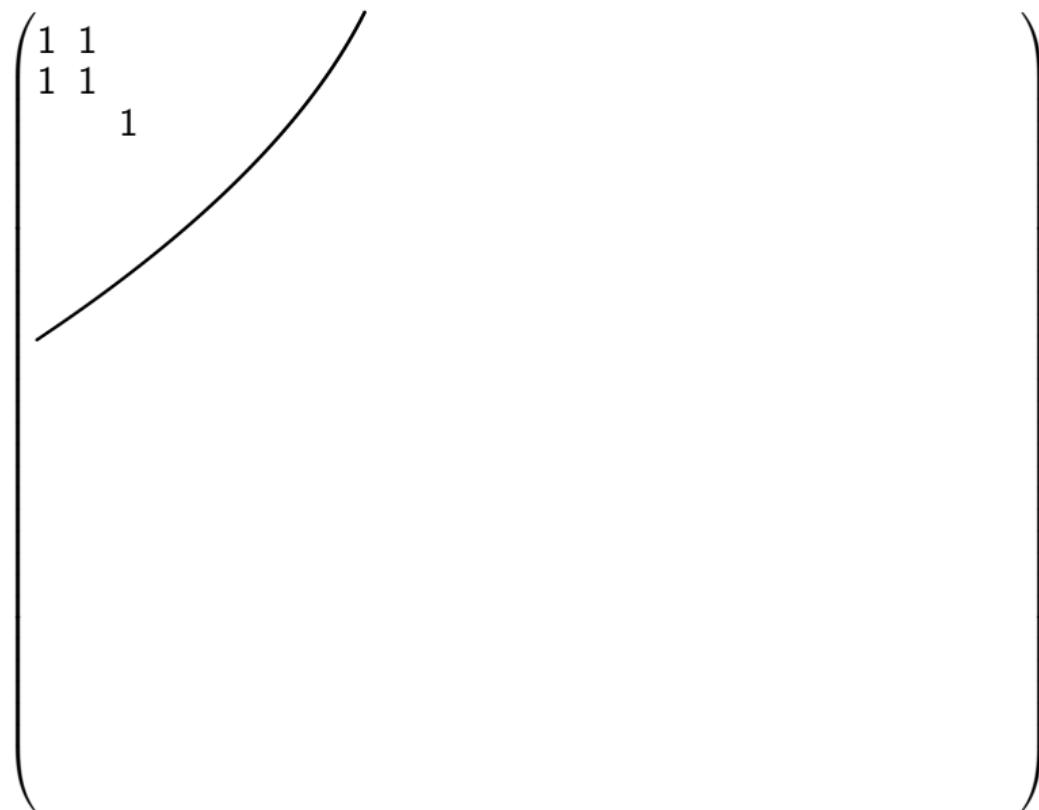
## Counterexample

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

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$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \\ & 1 \end{pmatrix}$$

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$$\left( \begin{array}{cc} 1 & 1 \\ 1 & 1 \\ 1 & \end{array} \right)$$
A 3x3 matrix is shown in parentheses. The top-left 2x2 submatrix is  $\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ . The bottom-right entry is missing, indicated by a blank space.

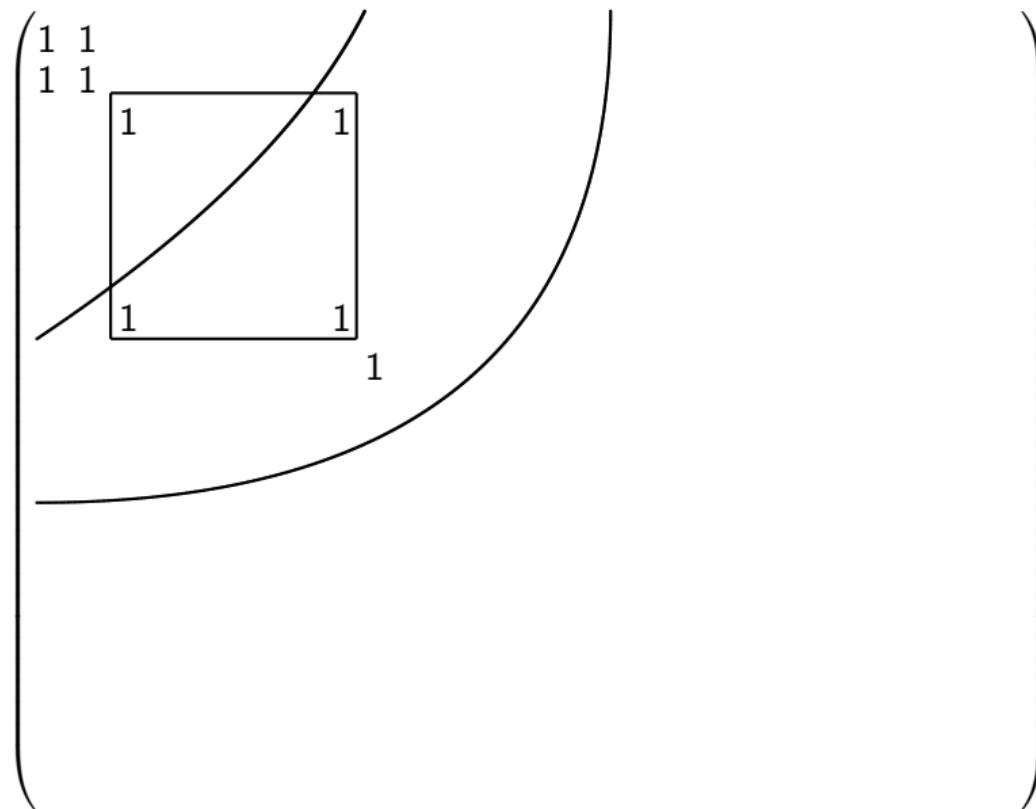
## Counterexample

$$\left( \begin{array}{cc} 1 & 1 \\ 1 & 1 \\ \hline 1 & \\ & 1 \\ \hline 1 & 1 \end{array} \right)$$

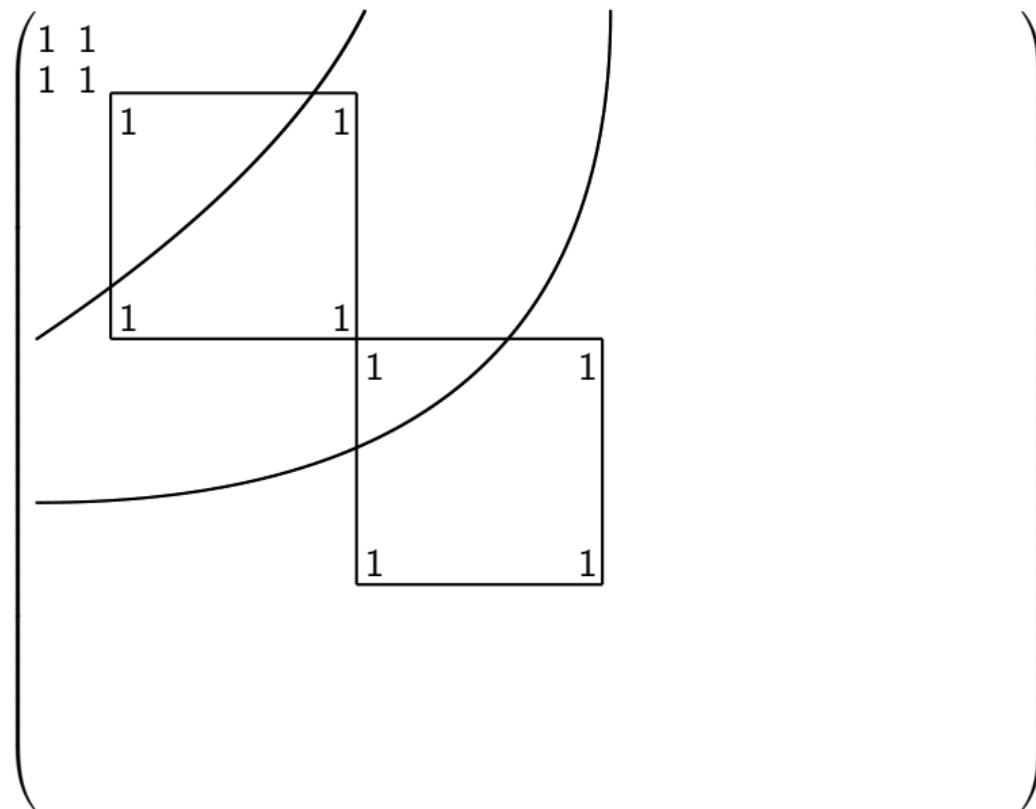
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$$\left( \begin{array}{cc} 1 & 1 \\ 1 & 1 \\ \hline 1 & 1 \\ 1 & 1 \\ \hline 1 & 1 \end{array} \right)$$

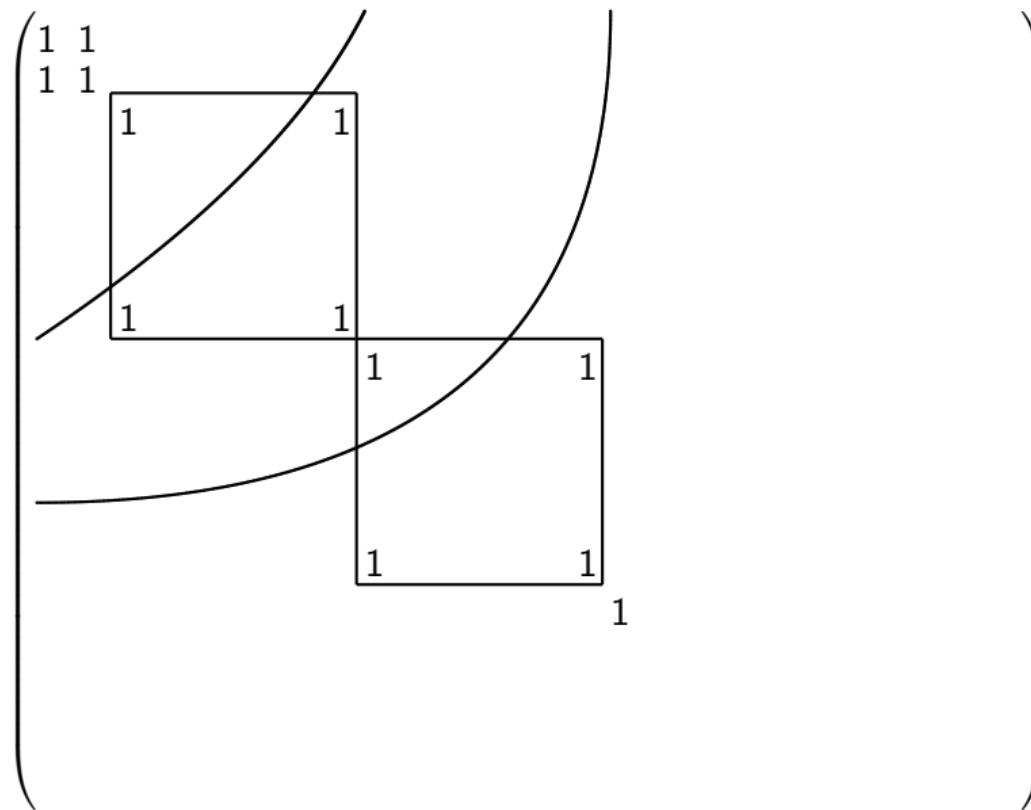
## Counterexample



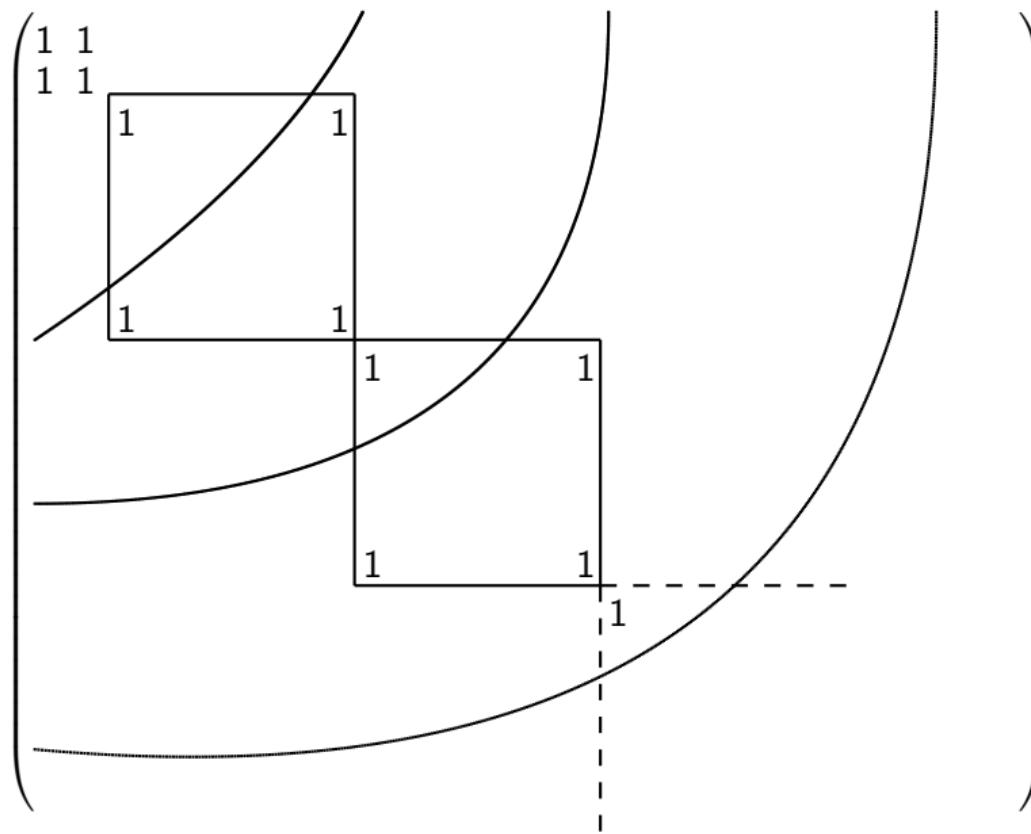
## Counterexample



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## Counterexample



## Counterexample

- ▶  $\rightsquigarrow$  bounded operator  $A$  with  $\sigma(A) = \{0, 2\}$ ;
  - ▶ but  $\Gamma_N(A) \approx \{0, 1, 2\}$  for infinitely many  $N$ .
- $\rightsquigarrow$  Different levels of computational complexity for the classes  $\mathcal{K}(\mathcal{H})$  vs.  $\mathcal{B}(\mathcal{H})$ .

## Motivation

- ▶  $\rightsquigarrow$  Allow more than 1 limit:<sup>3</sup>
- ▶ Approximate  $\sigma(A)$  by

$$\lim_{N_k \rightarrow \infty} \cdots \lim_{N_1 \rightarrow \infty} \Gamma_{N_1, \dots, N_k},$$

where  $\Gamma_{N_1, \dots, N_k}$  is algorithm.

**Definition:** *Solvability Complexity Index* (SCI) is smallest number of limits needed to solve the computational problem.

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<sup>3</sup>[Doyle-McMullen(1989)], [Hansen(2011)]

## Background

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Finding roots of polynomials:

- ▶ [Smale, *Bull. AMS* (1985)]: Newton's method not generally convergent in dimension  $d > 2$ .  
~~> **Does there exist a generally convergent purely iterative algorithm?**
- ▶ [McMullen, *Ann. Math.* (1987)]: **YES for  $d = 3$ , NO otherwise.**

## Background

- ▶ [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."

## Back to Spectra:

- ▶  $\rightsquigarrow$  Allow more than 1 limit:<sup>3</sup>
- ▶ Approximate  $\sigma(A)$  by

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## Background

Recent work:

[Hansen(2011)], [Ben-Artzi-Colbrook-Hansen-Nevanlinna-Seidel(2015)]:

- ▶ Definition of SCI;
- ▶ SCI classification of some (spectral and other) problems;
- ▶ wider theory of SCI hierarchy.

[Colbrook-Hansen(2020)], [Colbrook(2020)]:

- ▶ SCI classification for wider classes of spectral problems: computing spectra, spectral measures, spectral gaps, ...

## SCI for Resonances

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Abstract and numerical study of resonance problems have long history:

[Aguilar-Combes(1971)], [Balslev-Combes(1971)], [Simon(1973)]:

- ▶ Identify resonances as eigenvalues of an associated non-selfadjoint operator;
- ▶ ↵ method of complex scaling;

[Hislop-Martinez(1991)]:

- ▶ Explicit asymptotics for resonances of Helmholtz resonators

[Brown-Eastham(2000)]:

- ▶ 1-d numerical computation of resonances based on complex scaling.

[Bindel-Zworski(2007)]:

- ▶ MATLAB package for computing 1-d resonances by solving associated quadratic eigenvalue problem.

Textbooks: [Hislop-Sigal(1996)], [Dyatlov-Zworski(2019)]

And MANY others...

## SCI for Resonances

- ▶ Scattering resonances of a Schrödinger Operator  $H = -\Delta + V$  on  $L^2(\mathbb{R}^d)$  are poles of the scattering matrix;
- ▶ Can be alternatively defined as poles of analytic continuation of  $(I + V(-\Delta - z^2)^{-1}\chi)^{-1}$ , where  $\chi \equiv 1$  on  $\text{supp}(V)$  and  $\text{supp}(\chi)$  compact.

Computational problem [Res1]:

- ▶ Class of operators

$$\Omega_1 = \{-\Delta + V : \|V\|_{C^1} \leq C, \text{ supp}(V) \text{ compact}\}$$

- ▶ Resonance function  $H \mapsto \text{Res}(H)$
- ▶ Input information:  $\Lambda = \{V(x) \mid x \in \mathbb{R}^d\}$   
+ values of Bessel potential

**Theorem (Ben-Artzi, Marletta, R. 2020):**

The resonance problem [Res1] can be solved in one limit, i.e.  $\text{SCI}(\Omega_1) = 1$ .

**Proof:**

Explicitly construct algorithm  $\Gamma_n$  that computes resonances:

- ▶ Use Bessel potential to write  $V(-\Delta - z^2)^{-1}\chi$  as integral operator  $\int_{\mathbb{R}^d} K(z; x, \cdot)$ ;
- ▶ replace the integral kernel by discretised version  $K_n$
- ▶ prove norm error estimates for  $K - K_n$ ;
- ▶ determine regions where  $\|(I + K_n)^{-1}\|$  is large
- ▶ Let  $n \rightarrow \infty$ .

Proof:

- ▶ Fix lattice  $L_n \subset \mathbb{C}$ .
- ▶ Algorithm:

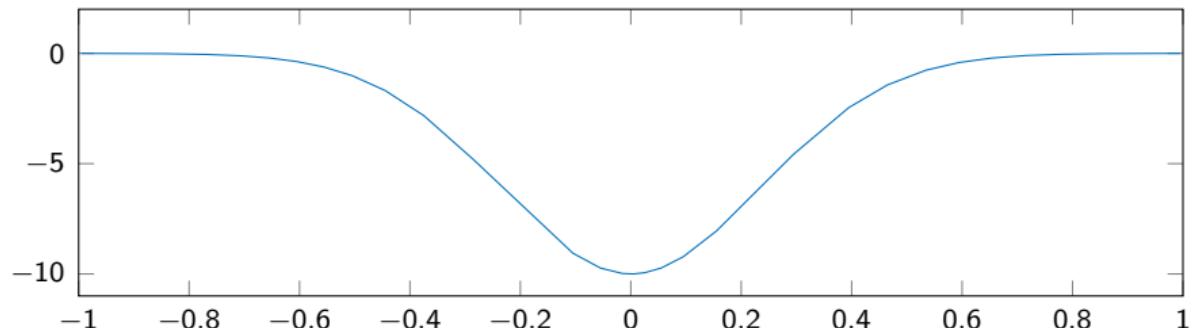
$$\Gamma_n(H) = \left\{ z \in L_n : \|(I + K_n(z))^{-1}\| > n^{\frac{1}{2d}} \right\}$$

- ▶ From bound on  $|\nabla V|$ : Error bound  $\|K(z) - K_n(z)\| < Cn^{-\frac{1}{d}}$ ;
- ▶ then for  $z_n \in \Gamma_n(H)$ ,  $z_n \rightarrow z \in \mathbb{C}$  one has  $\|(I + K_n(z_n))^{-1}\| \rightarrow \infty$  ;
- ▶ and hence  $\|(I + K(z_n))^{-1}\| \rightarrow \infty$  (Neumann series argument).
- ▶  $\Rightarrow z$  is pole of  $(I + K(z))^{-1}$

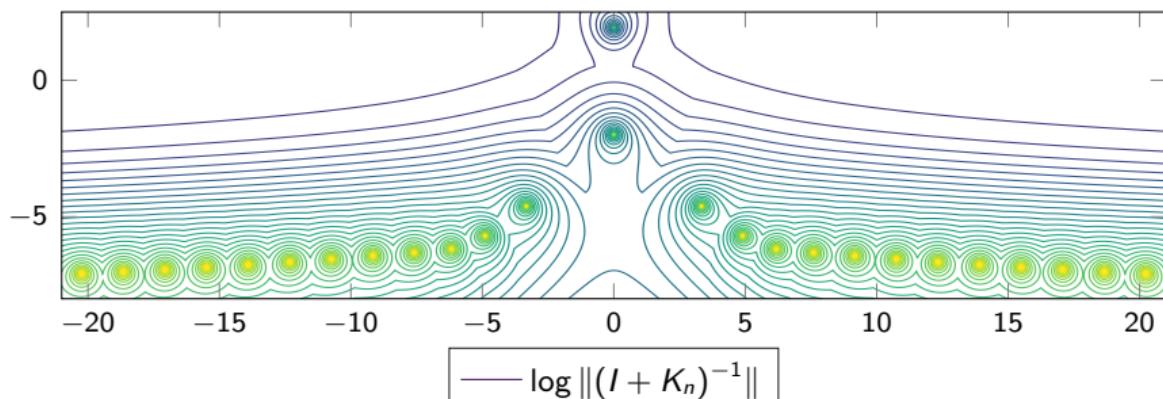
## Numerical Results

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Potential:

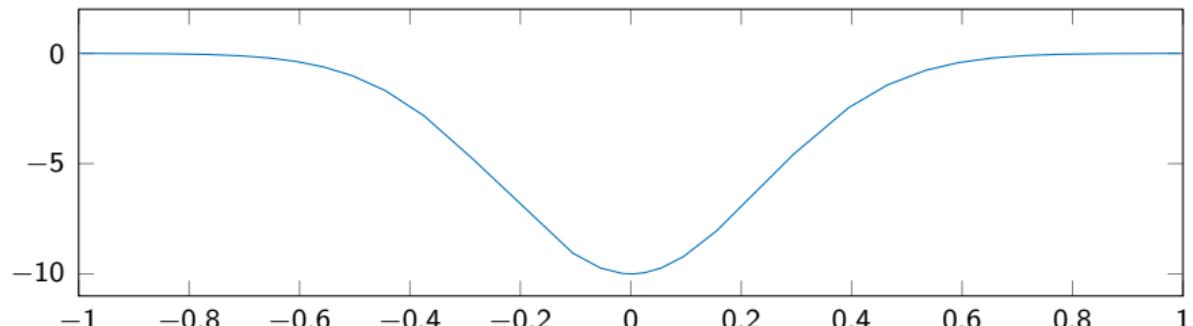


Resonances:

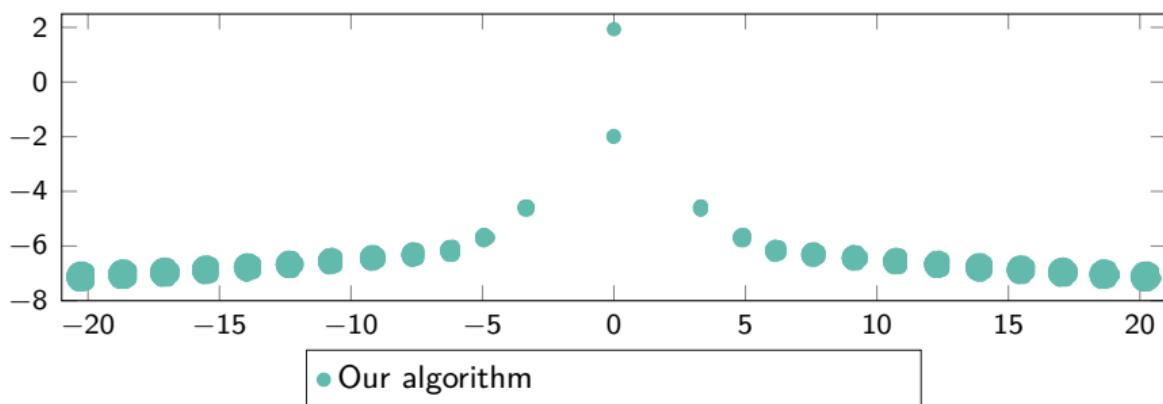


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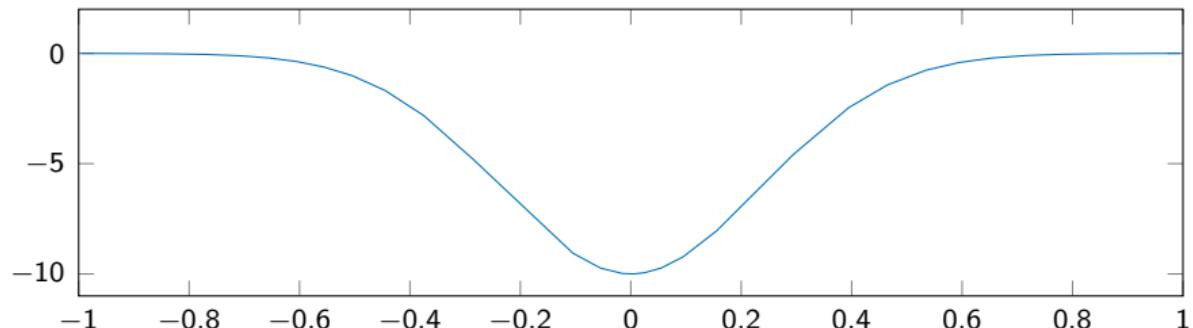


Resonances:

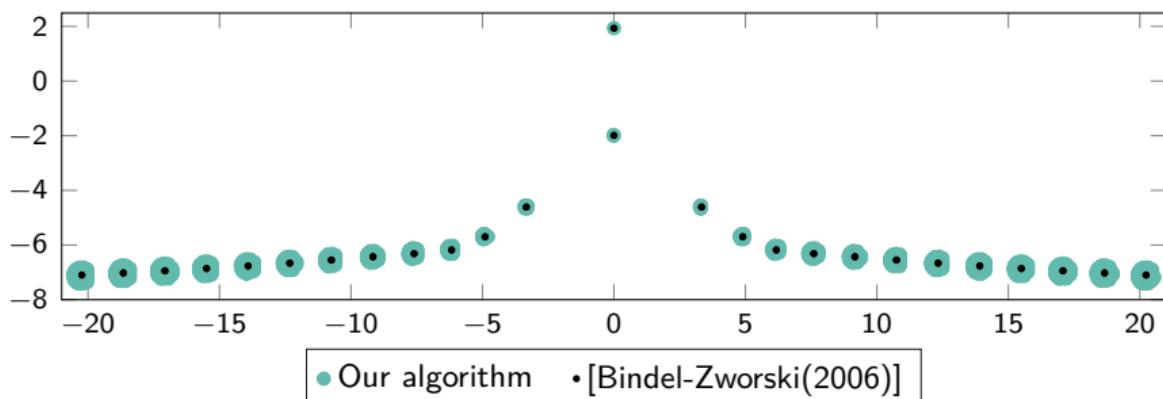


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Potential:

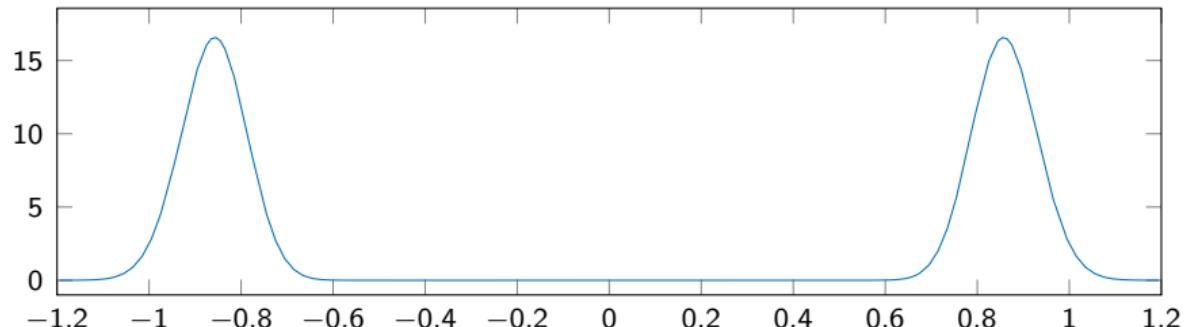


Resonances:

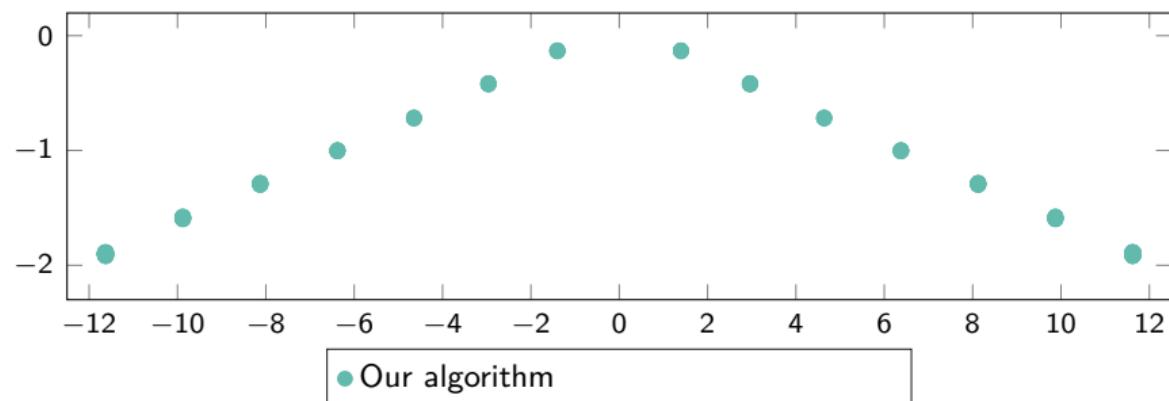


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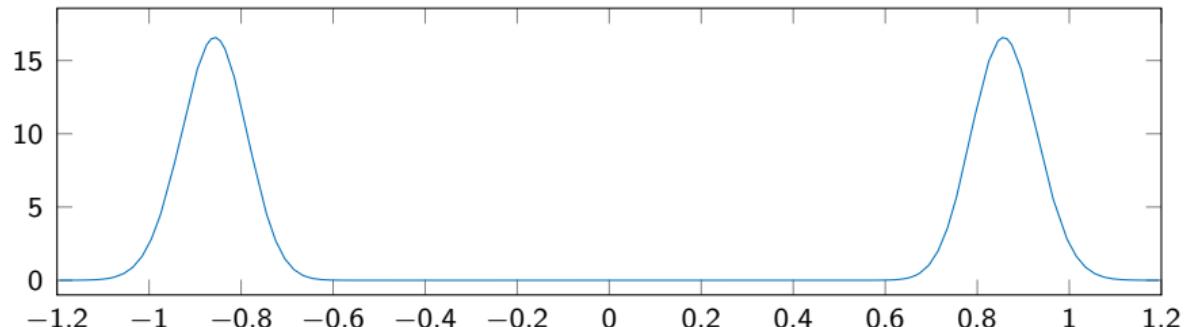


Resonances

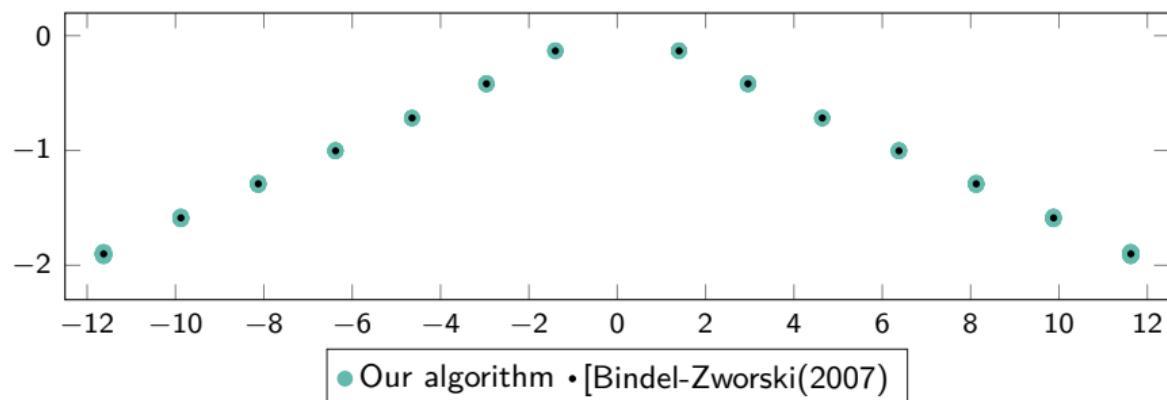


## Numerical Results

Potential



Resonances



# SCI for Obstacle Scattering

- ▶ Consider Dirichlet Laplacian  $-\Delta_D$  on  $L^2(\mathbb{R}^2 \setminus \overline{U})$  for some obstacle  $U$
- ▶ Boundary conditions on  $U$  induce trapping of waves and hence resonances.

Computational problem [Res2]:

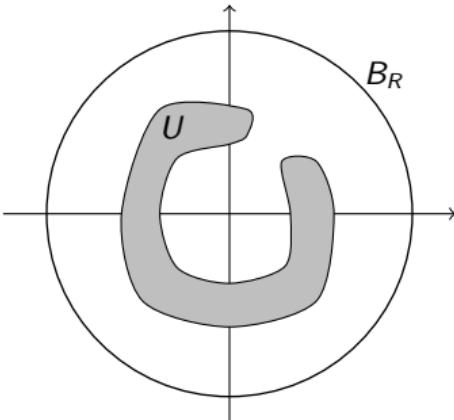
- ▶ Class of operators

$$\Omega_2 = \{-\Delta_D \text{ on } L^2(\mathbb{R}^2 \setminus \overline{U}) : U \text{ open, bounded and } \partial U \in C^2\}$$

- ▶ Resonance function  $H \mapsto \text{Res}(H)$
- ▶ Input information:  $\Lambda = \{\mathbf{1}_U(x) \mid x \in \mathbb{R}^2\}$   
+ values of Hankel functions

**Theorem (Ben-Artzi, Marletta, R. 2020):**

The resonance problem [Res2] can be solved in one limit, i.e.  $\text{SCI}(\Omega_2) = 1$ .



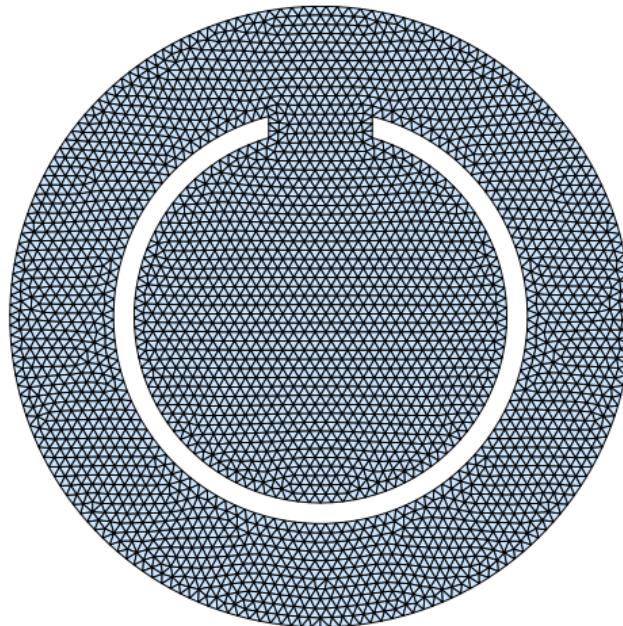
**Proof:** Explicitly construct algorithm  $\Gamma_n$  that computes resonances.

- ▶ Consider sum of inner and outer Dirichlet-to-Neumann maps associated with  $-\Delta - z^2$  on  $B_R \setminus \overline{U}$ ;
- ▶  $z$  is resonance iff  $\ker(M_{\text{inner}}(z) + M_{\text{outer}}(z)) \neq \{0\}$ ;
- ▶ transform  $M_{\text{inner}}(z) + M_{\text{outer}}(z)$  into an operator of the form  $I + A(z)$ , with  $A$  Schatten class;
- ▶ approximate  $A$  via finite element procedure on  $B_R \setminus \overline{U}$ ;
- ▶ compute approximated perturbation determinant  $\det(I + A(z))$ ;
- ▶ identify regions where  $\det(I + A(z)) \approx 0$ ;

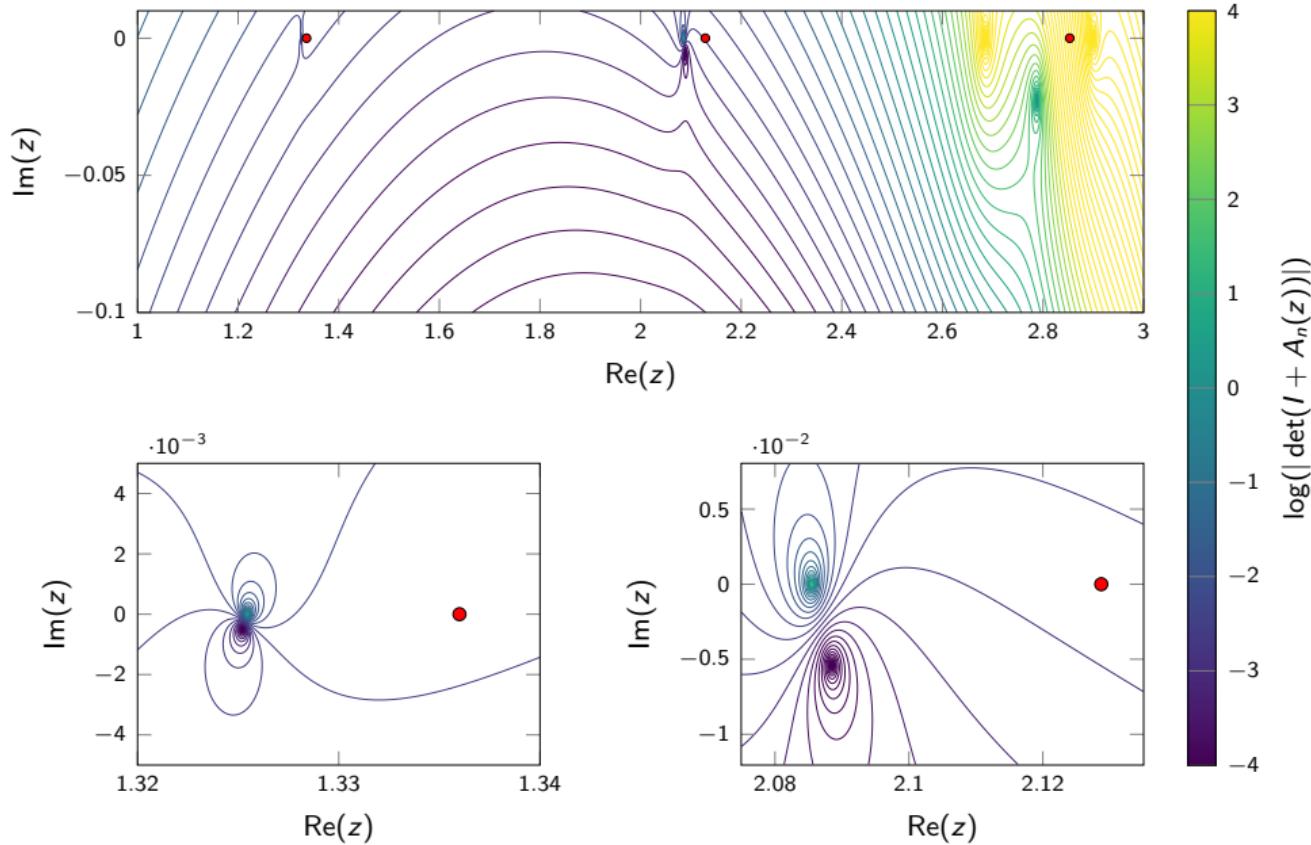
## Numerical Results

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Domain (triangulation via Distmesh [[Persson-Strang\(2004\)](#)]):



## Numerical Results



## Numerical Results

Thank You!