# Spectral problems and new resolvent based methods

## Computational foundations of spectral problems

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W. Arveson in 90s (leading operator theorist): "**Unfortunately, there is a dearth of literature on this basic problem, and there are no proven techniques.**"

Since then a lot of progress, but still much to be done!

# Set-up

In discrete setting, operator acting on $l^2(\mathbb{N})$:

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots \\ a_{21} & a_{22} & a_{23} & \dots \\ a_{31} & a_{32} & a_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad (Ax)_j = \sum_{k\in\mathbb{N}} a_{jk}x_k.$$

In continuous setting, deal with PDEs, integral operators etc.

| **Finite Case** | | **Infinite Case** |
|---|---|---|
| Eigenvalues | $\Rightarrow$ | Spectrum<br>$\mathrm{Sp}(A) = \{z \in \mathbb{C} : A - zI \text{ not bounded invertible}\}$ |
| Eigenvectors | $\Rightarrow$ | Spectral Measure (normal case) |
| Pseudospectrum<br>$\mathrm{Sp}_\epsilon(A) = \{z \in \mathbb{C} : \|(A - zI)^{-1}\|^{-1} \leq \epsilon\}$ | | |

Goal: compute spectral properties of the operator from matrix elements.

# Why study spectra numerically?

- Appears in a huge number of applications (e.g. quantum mechanics).
- Open problem for $> 50$ years whether we can compute spectra, even for just discrete Schrödinger operators in 1D.
- Main challenges:
  1. **Convergence:** Avoiding spectral pollution/gaining error bounds.
  2. **Lack of methods and algorithms in infinite dimensions:** Which assumptions do we need on the operators and how do we compute the spectral quantities?

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Common theme: use the resolvent $(A - zI)^{-1}$

# Magneto-graphene

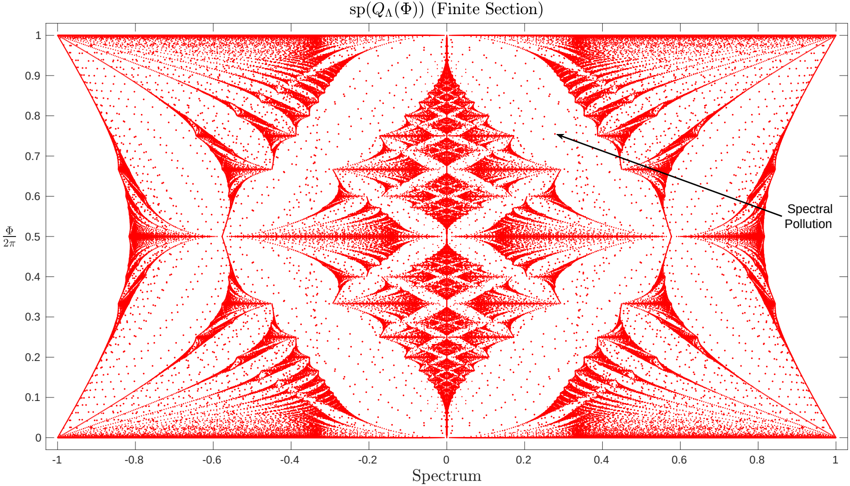



Figure: Finite section.

# Can be turned into this!

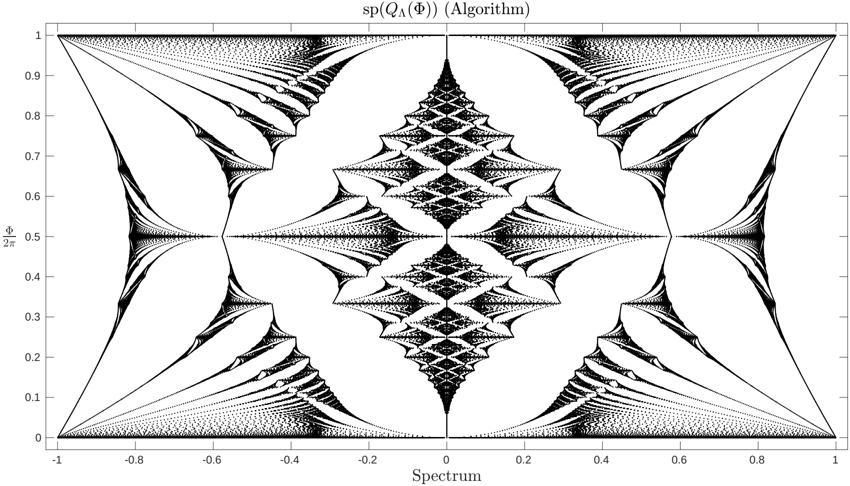



Figure: Guaranteed error bound of $10^{-5}$.

**Pseudospectra** (square + rectangular finite)

Efficient numerics and rich theory [Wright & Trefethen 2001 and 2002, Toh & Trefethen 1996, Trefethen & Embree 2005]

**Quadratic methods** (second order relative spectra)

For self-adjoint A [Levitin & Shargorodsky 2004, Shargorodsky 2000]:

$$\mathrm{Sp}_2(A, P_n) = \{z \in \mathbb{C}\colon P_n(A - zI)^2 P_n \text{ not invertible}\}$$

Some success with spectral pollution [Boulton & Levitin 2007] but doesn't always converge (can be arbitrarily bad) [Shargorodsky 2012].

**Spectral problem solved?**

Three limit algorithm proposed by Hansen in 2011. First computes pseudospectrum using two limits and a quadratic method. Then requires a third limit to compute spectrum. Sharp without further assumptions [Ben-Artzi, C., Hansen, Nevanlinna, Seidel. Preprint 2019] and hence cannot be used in practice!

**NEED ASSUMPTIONS**

**Directly deal with infinite dimensional operator**

In some cases apply classical algorithms (some in other talks!); IQR [C. & Hansen 2019], IQL [Olver & Webb. Preprint 2019], FEAST [Horning & Townsend. Preprint 2019],... Many use sparse spectral methods based on ultraspherical [Olver & Townsend 2013] or code such as Chebfun, ApproxFun,...

## From eigenvalues to spectra: Using the resolvent norm

Recall for bounded operator $T$:

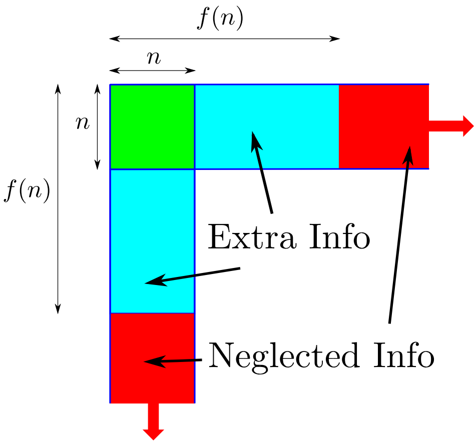
$$\|T\| = \sup\{\|Tx\| : \|x\| = 1\}$$

**Main message:** the resolvent norm allows computation of spectra with error control.

## Definition 1 (Dispersion: off-diagonal decay)

Dispersion of $A \in \mathcal{B}(l^2(\mathbb{N}))$ is bounded by the function $f : \mathbb{N} \to \mathbb{N}$ if

$$c_n = \max\{\|(I - P_{f(n)})AP_n\|, \|P_nA(I - P_{f(n)})\|\} \to 0 \quad \text{as } n \to \infty.$$



## Definition 2 (Controlled growth of the resolvent: well-conditioned)

Continuous increasing function $g : [0, \infty) \to [0, \infty)$ with $g(x) \leq x$.
Controlled growth of the resolvent by $g$ if

$$\|(A - zI)^{-1}\|^{-1} \geq g(\mathrm{dist}(z, \mathrm{Sp}(A))) \quad \forall z \in \mathbb{C}.$$

- $g$ is a measure of the conditioning of the problem of computing $\mathrm{Sp}(A)$ through the formula

$$\mathrm{Sp}_\epsilon(A) = \bigcup_{\|B\| \leq \epsilon} \mathrm{Sp}(A + B).$$

- Self-adjoint and normal operators ($A$ commutes with $A^*$) have well-conditioned spectral problems since

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$\boxed{\text{Know } f, g \Rightarrow \text{can compute } \mathrm{Sp} \text{ with error control!}}$[1]

[1] C., Roman, Hansen. PRL 2019

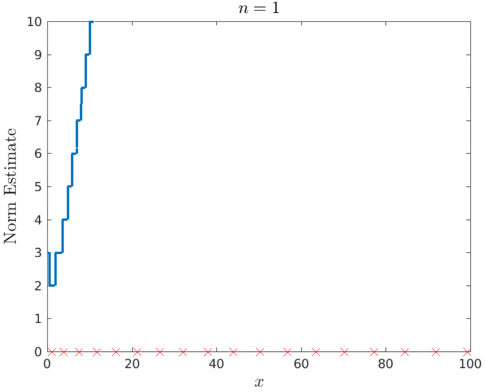
**Idea:** approximate locally via smallest singular value:

$$\gamma_n(z) = \min\{\sigma_1(P_{f(n)}(A - zI)P_n), \sigma_1(P_{f(n)}(A^* - \overline{z}I)P_n)\} + c_n \downarrow \|(A - zI)^{-1}\|^{-1}$$

$$\|(A - zI)^{-1}\|^{-1} \leq \mathrm{dist}(z, \mathrm{Sp}(A)) \leq g^{-1}(\|(A - zI)^{-1}\|^{-1}) \leq g^{-1}(\gamma_n(z)).$$

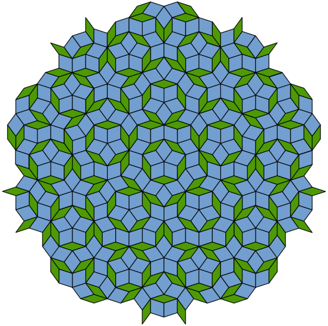
Local search routine computes $\Gamma_n(A)$ and $E(n, \cdot)$ with

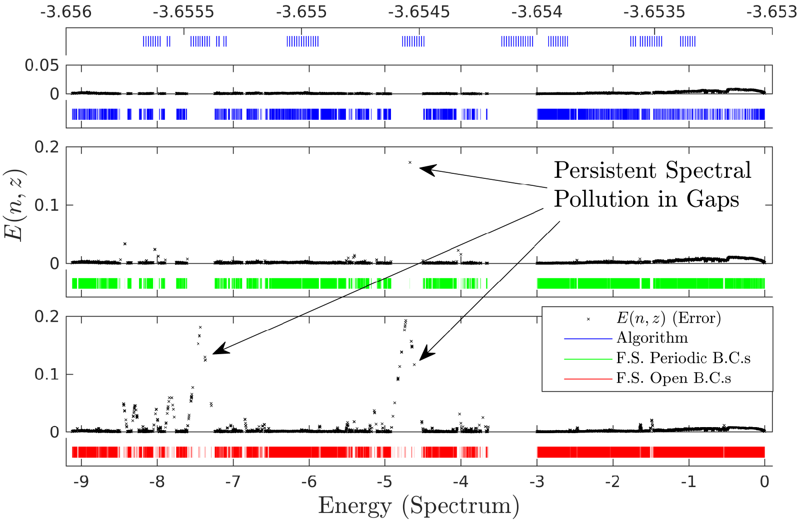
$$\Gamma_n(A) \to \mathrm{Sp}(A), \quad \mathrm{dist}(z, \mathrm{Sp}(A)) \leq E(n, z), \quad \sup_{z \in \Gamma_n(A)} E(n, z) \to 0$$



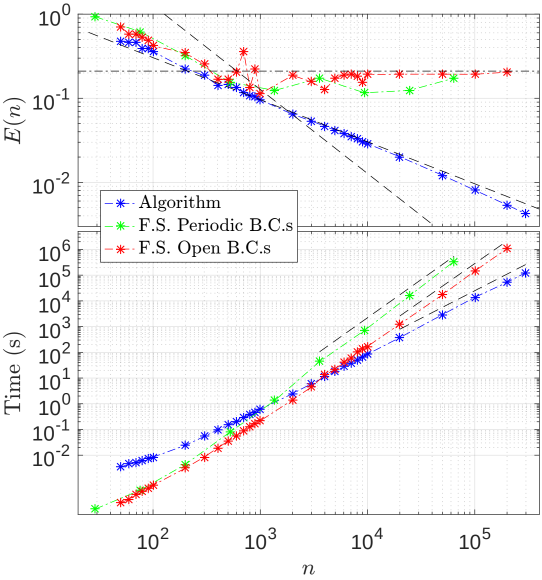
# Laplacian on Penrose Tile

Aperiodic, no known method for analytic study.





-3.656
-3.6555
-3.655
-3.6545
-3.654
-3.6535
-3.653
0.05
0
0.2
0.1
0
0.2
0.1
0
$E(n, z)$
Persistent Spectral Pollution in Gaps
$E(n, z)$ (Error)
Algorithm
F.S. Periodic B.C.s
F.S. Open B.C.s
-9
-8
-7
-6
-5
-4
-3
-2
-1
0
Energy (Spectrum)



$10^0$
$10^{-1}$
$10^{-2}$
$E(n)$
Algorithm
F.S. Periodic B.C.s
F.S. Open B.C.s
$10^6$
$10^5$
$10^4$
$10^3$
$10^2$
$10^1$
$10^0$
$10^{-1}$
$10^{-2}$
Time (s)
$10^2$
$10^3$
$10^4$
$10^5$
$n$

## Computing spectral measures: Using the resolvent operator

**Main message:** the resolvent operator allows computation of spectral measures - "diagonalisation."

- If $A$ normal, associated projection-valued measure $E^A$ s.t.

$$Ax = \int_{\mathrm{Sp}(A)} \lambda dE^A(\lambda)x, \quad \forall x \in \mathcal{D}(A),$$

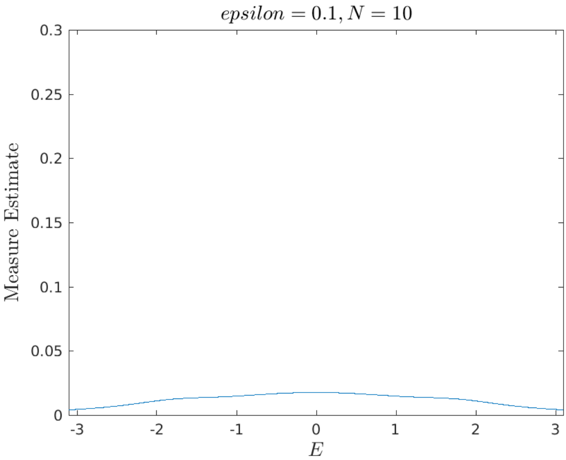
- View this as diagonalisation - allows computation of functional calculus, has interesting physics etc.
- Only previous work deals with $A$ tridiagonal Toeplitz + compact [Olver and Webb. Preprint 2019].

Suppose, for simplicity, $A$ self-adjoint...

**Idea:** Use the formula

$$\frac{(A - zI)^{-1} - (A - \overline{z}I)^{-1}}{2\pi i} = \int_{\mathrm{Sp}(A)} P(\mathrm{Re}(z) - \lambda, \mathrm{Im}(z))dE^A(\lambda),$$

$P(x, \epsilon) = \epsilon\pi^{-1}/(x^2 + \epsilon^2)$: convolution with Poisson kernel. Smoothed version of measure.



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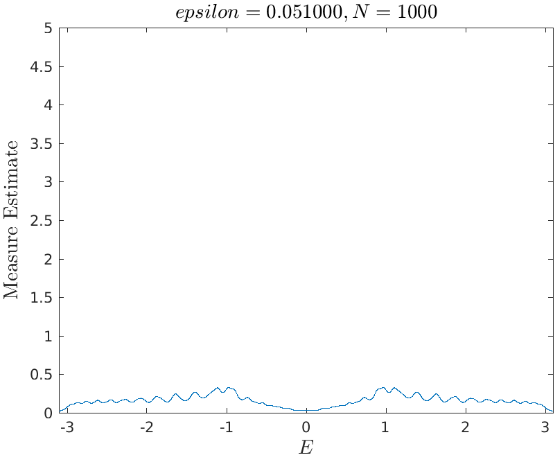
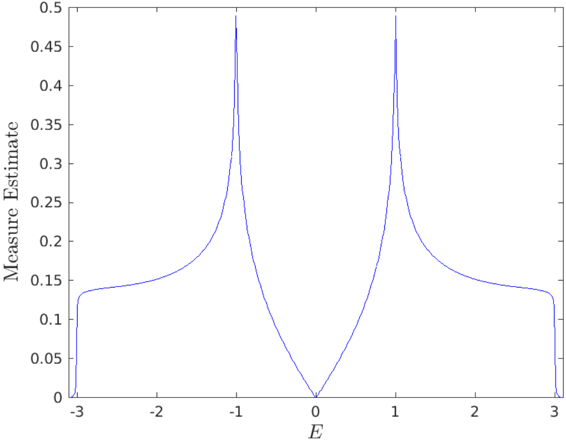


Know $f \Rightarrow$ can compute measure in one limit[2]!

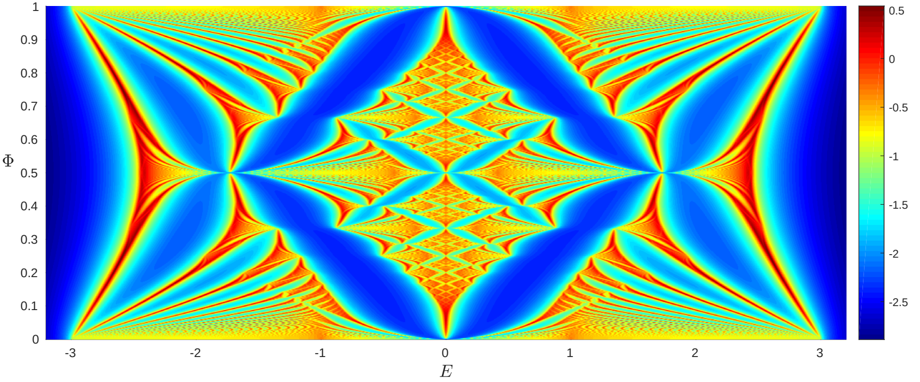
This is through a rectangular least squares type problem.




[2] C. Preprint 2019

# Back to graphene

Beautiful fractal structure!



# Easy to marry these algorithms with spectral methods

Current work with Andrew Horning and Alex Townsend: extending to continuous operators.

For example, basis choice of $L^2(\mathbb{R})$ :

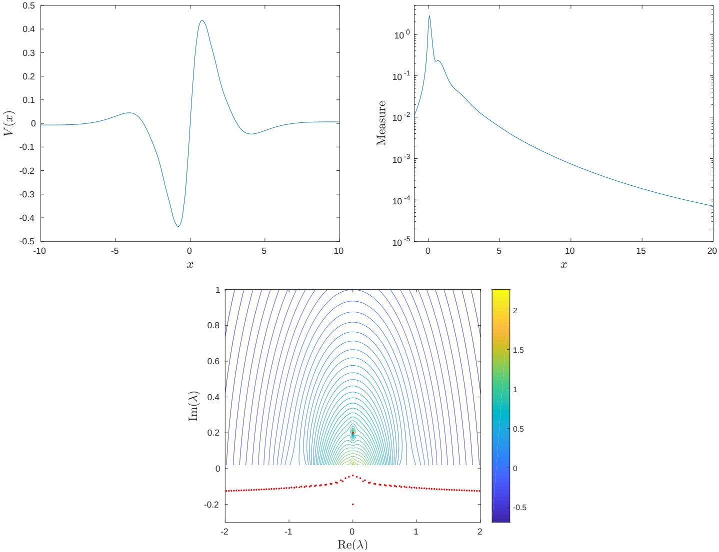
$$\rho_n(x) = \frac{1}{\sqrt{\pi}} \frac{(1+ix)^n}{(1-ix)^{n+1}}.$$

In 1D leads to banded representation of ODEs on real line, connections with Fourier series etc. Look at Schrödinger operator

$$A = -\frac{d^2}{dx^2} + V(x),$$

with $V$ bounded and real.

# Easy to marry these algorithms with spectral methods



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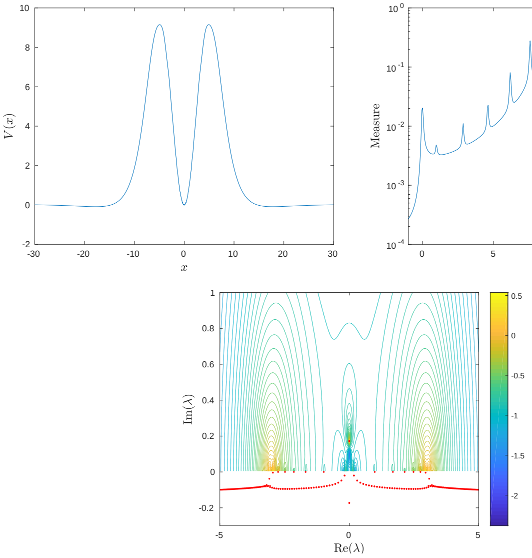

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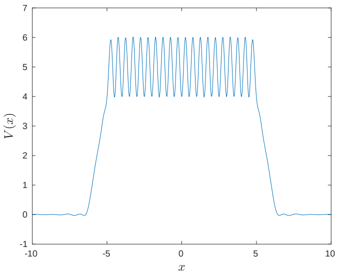


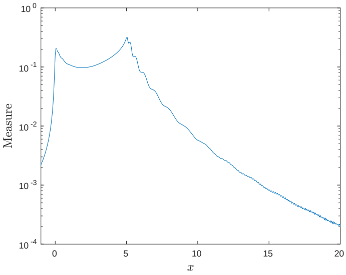


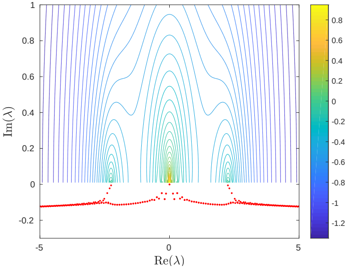

# Conclusion

**Challenges overcome:**

- Can now compute spectra of a large class of operators with error control. The new algorithm is fast, local and parallelisable.
- The resolvent can be use to compute spectral measures.

**Connected work:** Many other problems can also be tackled with the resolvent; spectral type, fractal dimensions, ...

**Future challenges:**

- Making these methods even faster - iterative methods for PDEs?
- Computing embedded eigenvalues.

**Coming soon: numerical package with resolvent based algorithms for discrete and continuous problems (with Andrew Horning).**