Resolving the resolvent
How to ‘diagonalise’ infinite matrices

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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.**”

Aim of talk: **Solve this problem!**

Set-up

Work in canonical Hilbert space $l^2(\mathbb{N})$ with

$$\langle x, y\rangle = \sum_{j\in\mathbb{N}} x_j \overline{y}_j, \quad \|x\|^2 = \sum_{j\in\mathbb{N}} |x_j|^2 .$$

Operator acting on $l^2(\mathbb{N})$:

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

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

Why?

- Appears in a huge number of applications.
- Hard numerical problem! Naïve discretisations/truncations can fail spectacularly even for "nice" self-adjoint, tridiagonal case (hence Arveson's quote).
- Talk will present first algorithm that computes spectra of a very general class of operators and how to compute spectra with (rigorous provable) error control.
- Everything in this talk in discrete setting, but can be extended to continuous setting (e.g. PDE/integral operators).

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

Magneto-graphene

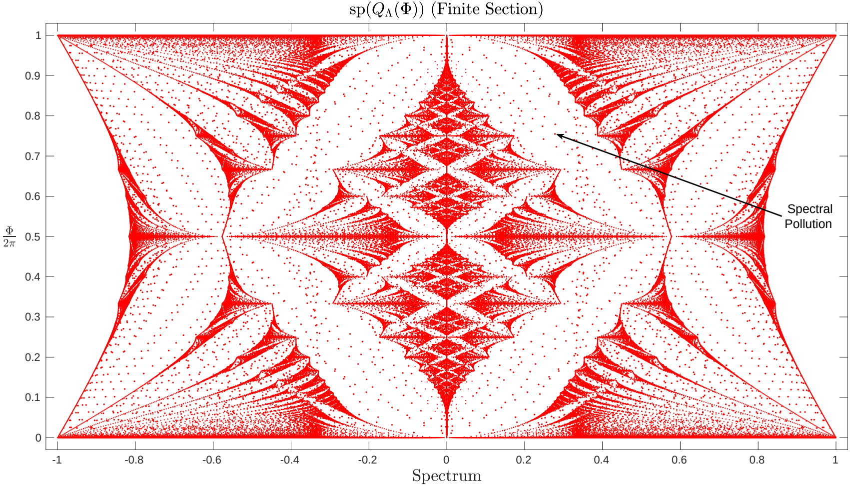


Figure: Finite section.

Can be turned into this!

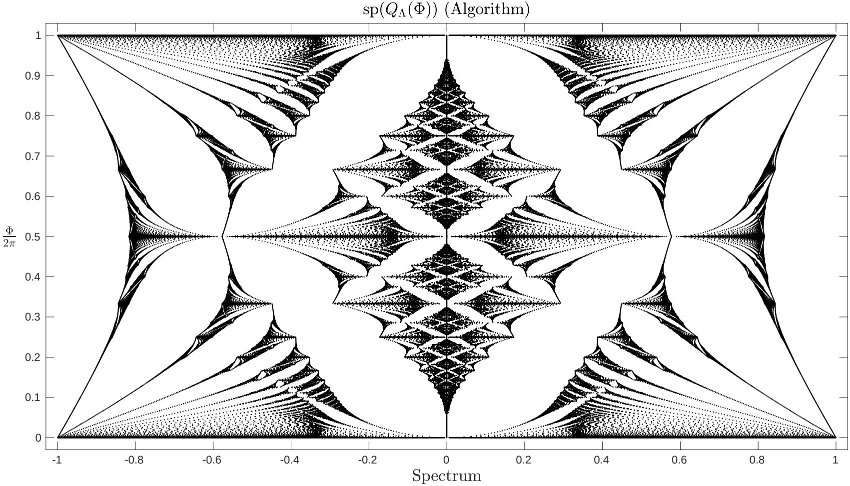
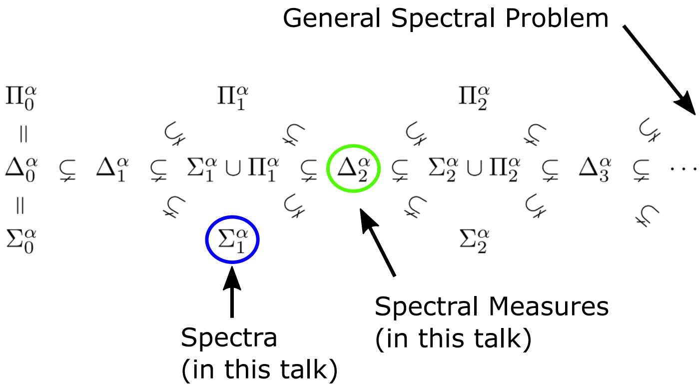


Figure: Guaranteed error bound of 10^{-5}.

The algorithms presented are optimal from a computational foundations point of view (SCI hierarchy)[1]:



Deep connections with logic and descriptive set theory.[2]

All algorithms are local and parallelisable, suitable for high performance computation.

[1] Ben-Artzi, Colbrook, Hansen, Nevanlinna, Seidel. Preprint 2019

[2] Colbrook. Preprint 2019

From eigenvalues to spectra: Using the resolvent norm

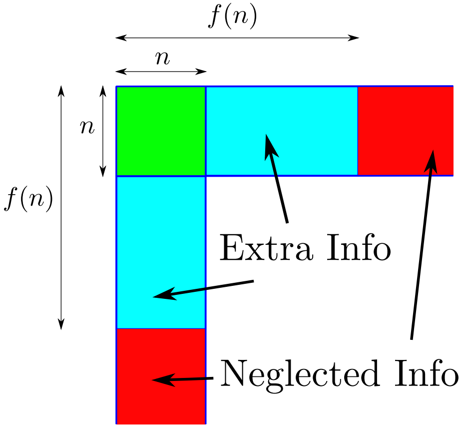
Recall for bounded operator T:

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

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

$$\left\|(A - zI)^{-1}\right\|^{-1} = \mathrm{dist}(z, \mathrm{Sp}(A)), \quad g(x) = x.$$

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Know $f, g \Rightarrow$ can compute Sp with error control![3]

[3] Colbrook, Roman, Hansen. PRL 2019

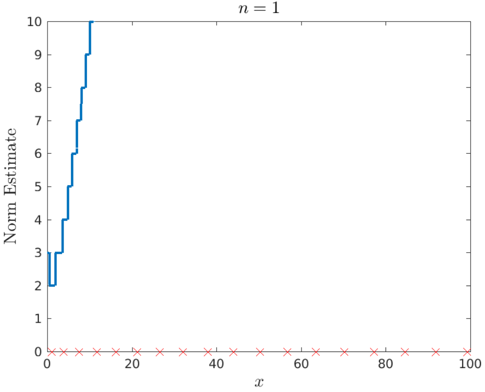
Idea: approximate locally via smallest singular value:

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

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

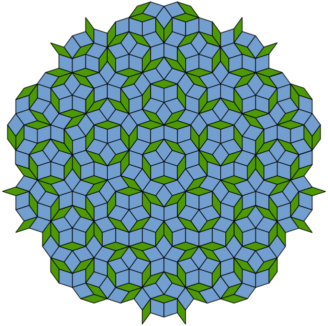
Local search routine computes $\Gamma_n(A)$ and $E(n, \cdot)$ with

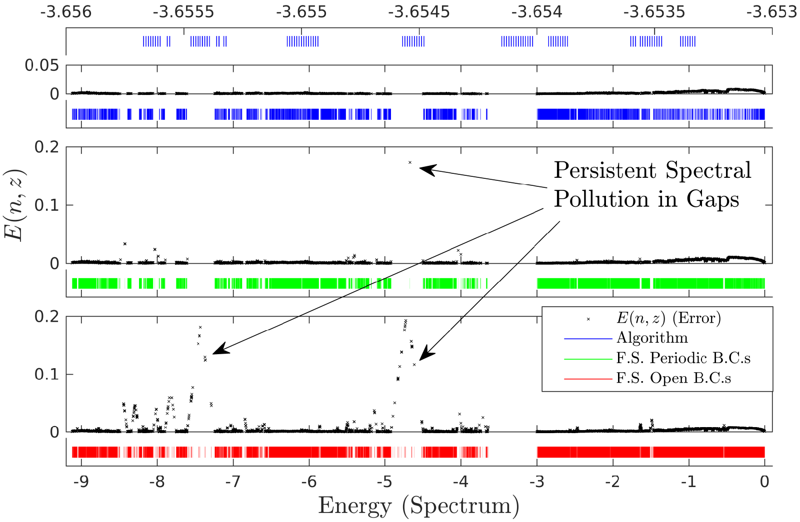
$$\Gamma_n(A) \to \mathrm{Sp}(A), \quad \mathrm{dist}(z, \mathrm{Sp}(A)) \leq E(n, z), \quad \sup_{z \in \Gamma_n(A)} E(n, z) \to 0$$

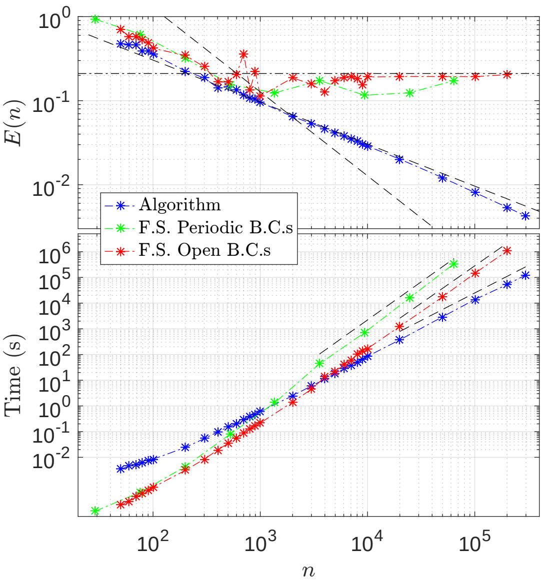


Laplacian on Penrose Tile

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

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

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

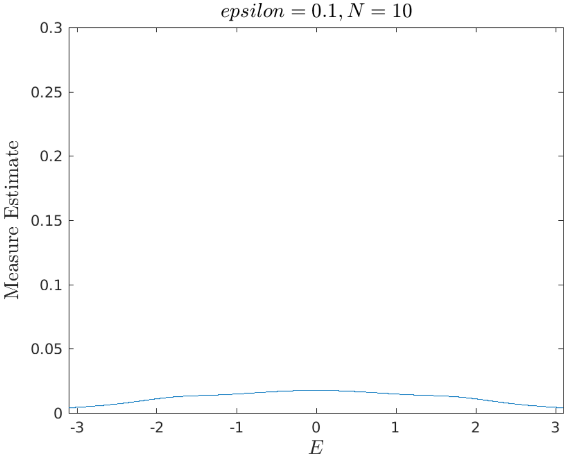
- View this as diagonalisation - allows computation of functional calculus, has interesting physics etc.
- Only previous work deals with A tridiagonal Toeplitz $+$ compact. Analogous in finite dimensions to being able to compute the location of eigenvalues but not eigenvectors!

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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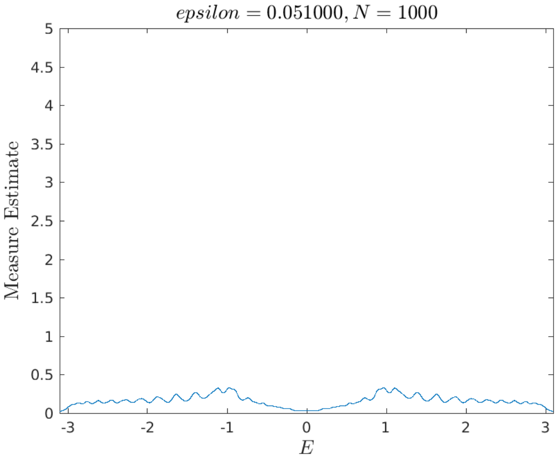
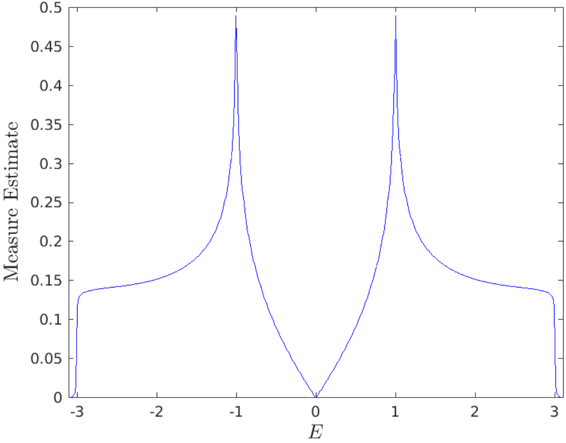


Know $f \Rightarrow$ can compute measure in one limit[4]!

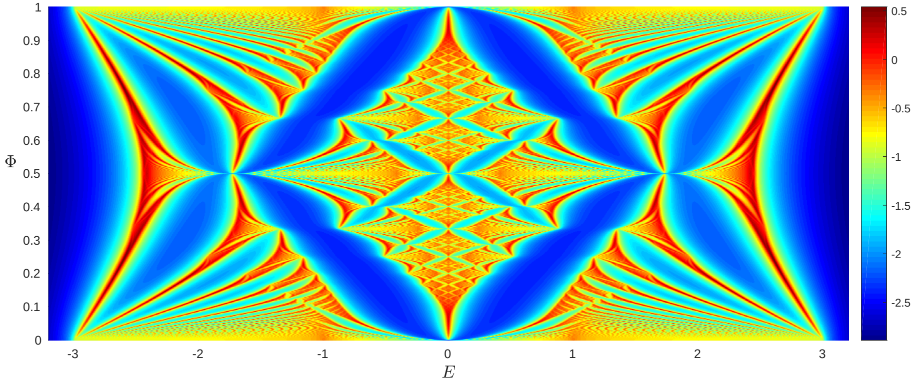
This is through a rectangular least squares type problem.



[4] Colbrook. Preprint 2019

Back to graphene

Beautiful fractal structure!



Can do things like study transport properties etc.

Conclusion

- Can now compute spectra of a large class of operators with error control (first algorithm that does this).
- New algorithm is fast, local and parallelisable, competitive with the current methods in the literature.
- Produced an algorithm that computes spectral measures.
- Algorithms part of a larger class of resolvent based techniques and hierarchical classification.
- Other problems can also be tackled such as fractal dimensions, discrete spectra,...

Coming soon: high performance numerical package with resolvent based algorithms for discrete and continuous problems.