Spectral resolvent based methods

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Motivation

- Spectra of infinite-dimensional operators, vast number of applications.
- W. Arveson in 90s: "**Unfortunately, there is a dearth of literature on this basic problem, and … there are no proven techniques.**"
- Naïve discretisations/truncations can fail spectacularly even for "nice" self-adjoint.
- Talk will present solution to this problem and how to compute spectra for much more general cases.
- Everything in this talk in discrete setting - but can be extended to continuous setting!
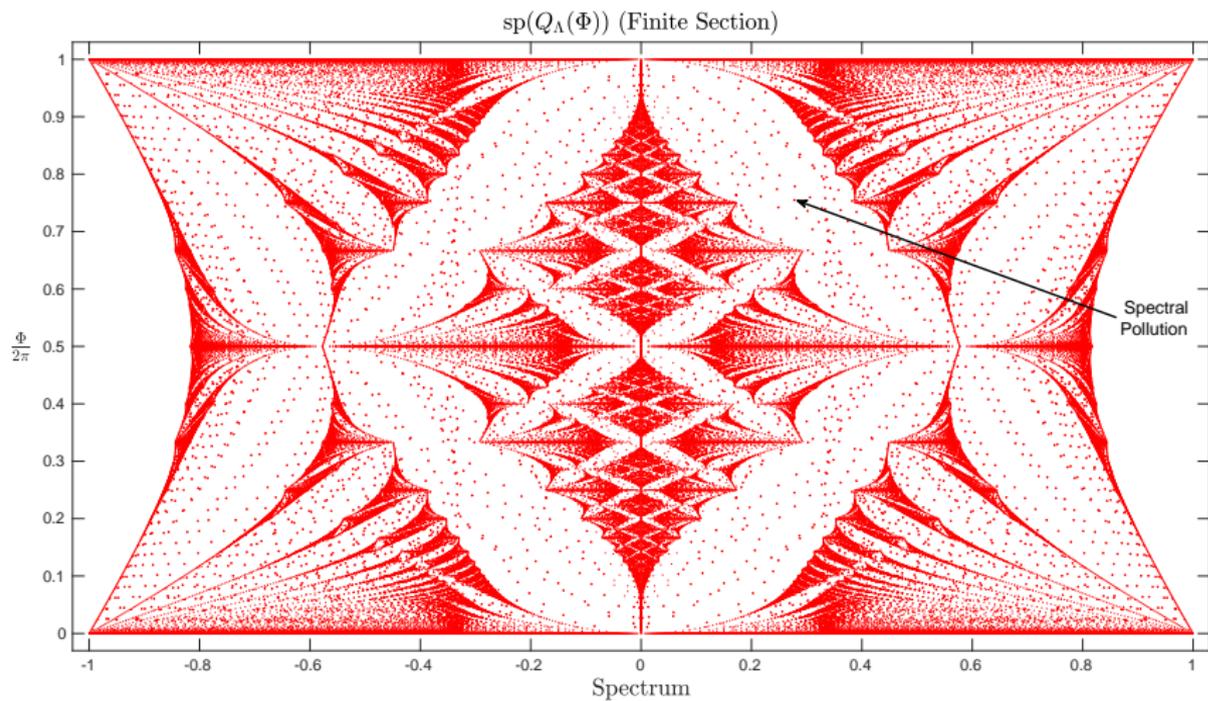
Magneto-graphene

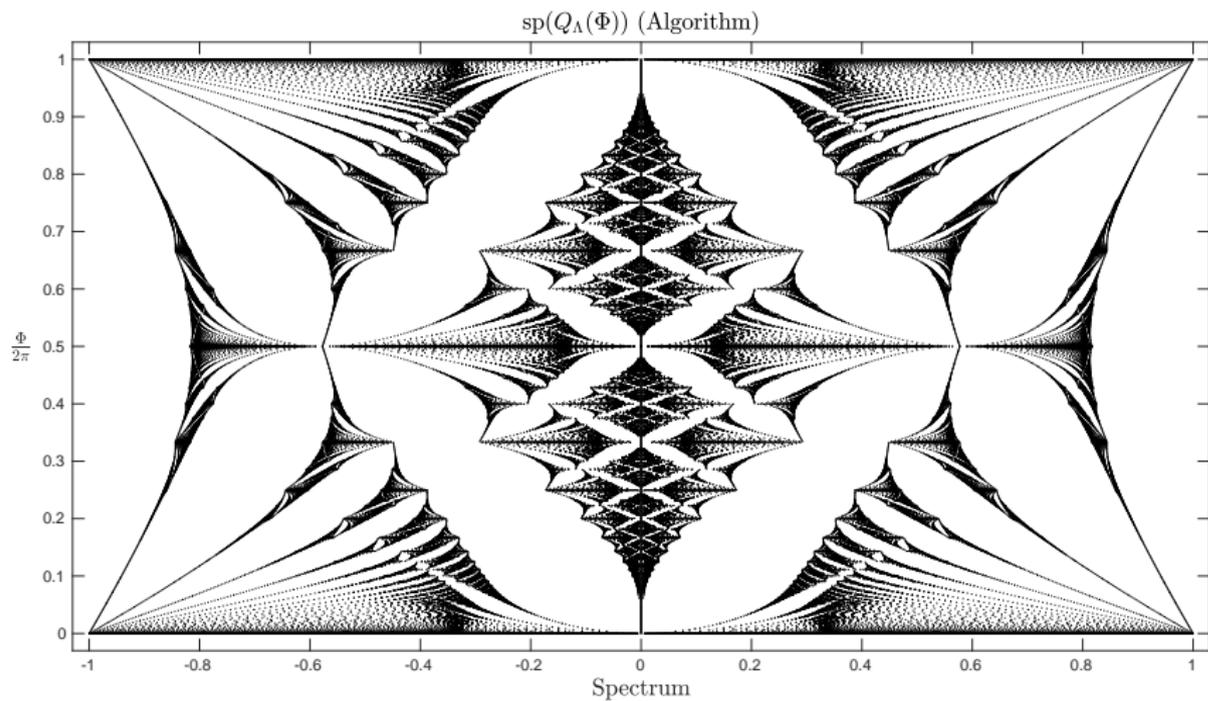Figure: Finite section.

Can be turned into this!

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

Motivation: a curious case of limits

Problem: Given class of general bounded operators

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \ldots \\ a_{21} & a_{22} & a_{23} & \ldots \\ a_{31} & a_{32} & a_{33} & \ldots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

can we compute $\mathrm{Sp}(A)$ in Hausdorff metric from matrix values?

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Answer [1]: No! Best one can do is compute using three successive limits:

$$\lim_{n_3 \to \infty} \lim_{n_2 \to \infty} \lim_{n_1 \to \infty} \Gamma_{n_3, n_2, n_1}(A) = \mathrm{Sp}(A)$$

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$\mathrm{SCI} =$ number of limits needed to solve problem.

How do we capture 'verifiable' problems that can be used in computer assisted proofs and rigorous numerics?
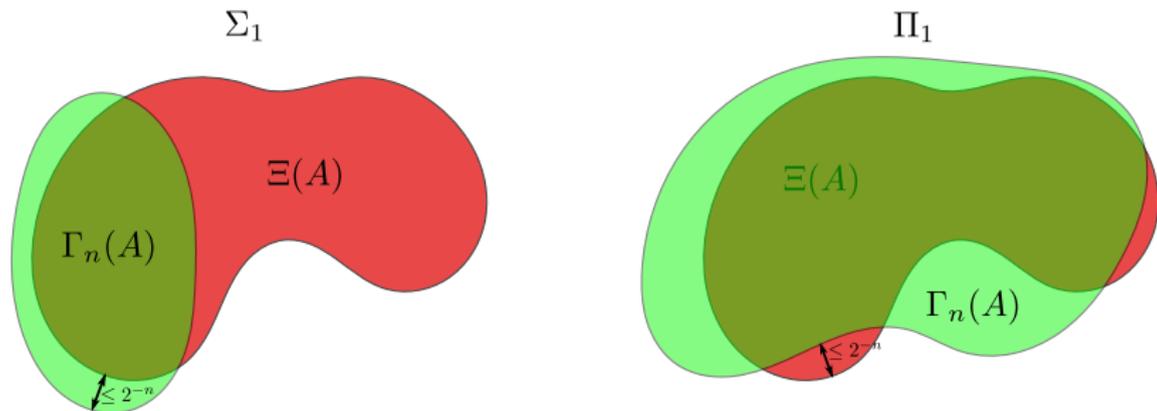

Figure: Meaning of Σ_1 and Π_1 convergence for problem function Ξ. The red area represents $\Xi(A)$ whereas the green areas represent the output of the algorithm $\Gamma_n(A)$.

First algorithm that computes Sp 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

$$\max\{\|(I - P_{f(m)})AP_m\|, \|P_m A(I - P_{f(m)})\|\} \to 0 \quad \text{as } m \to \infty.$$

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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

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

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Know $f, g \Rightarrow$ can compute Sp with Σ_1 error control [2]!
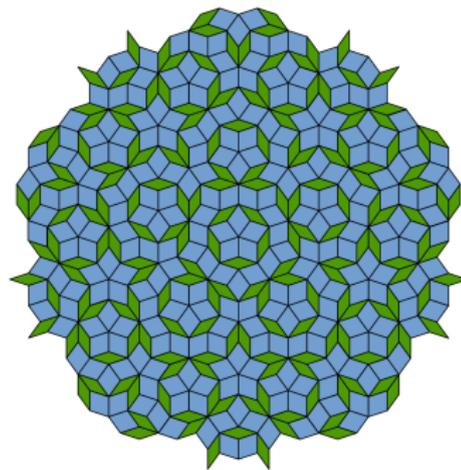
Idea: can we approximate the quantity $\|(A - zI)^{-1}\|^{-1}$ locally? Then gain an upper bound:

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

Compute $E(n, z)$ with $\text{dist}(z, \text{Sp}) \leq E(n, z)$, $\quad E(n, z) \downarrow \text{dist}(z, \text{Sp})$.

Laplacian on Penrose Tile

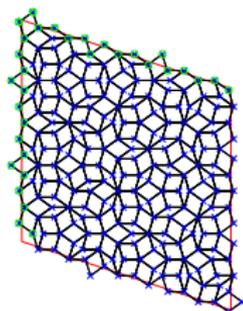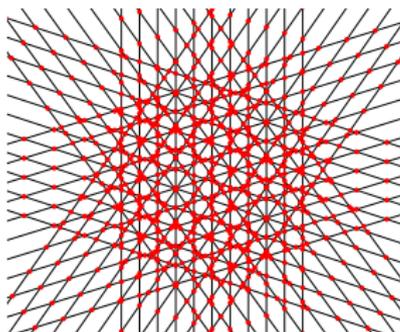Aperiodic, no known method for analytic study.

Naïve Approximations

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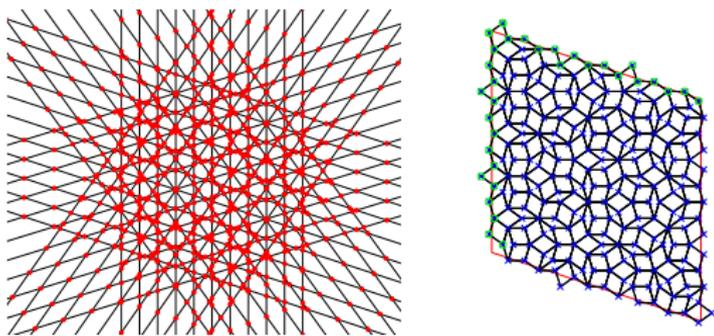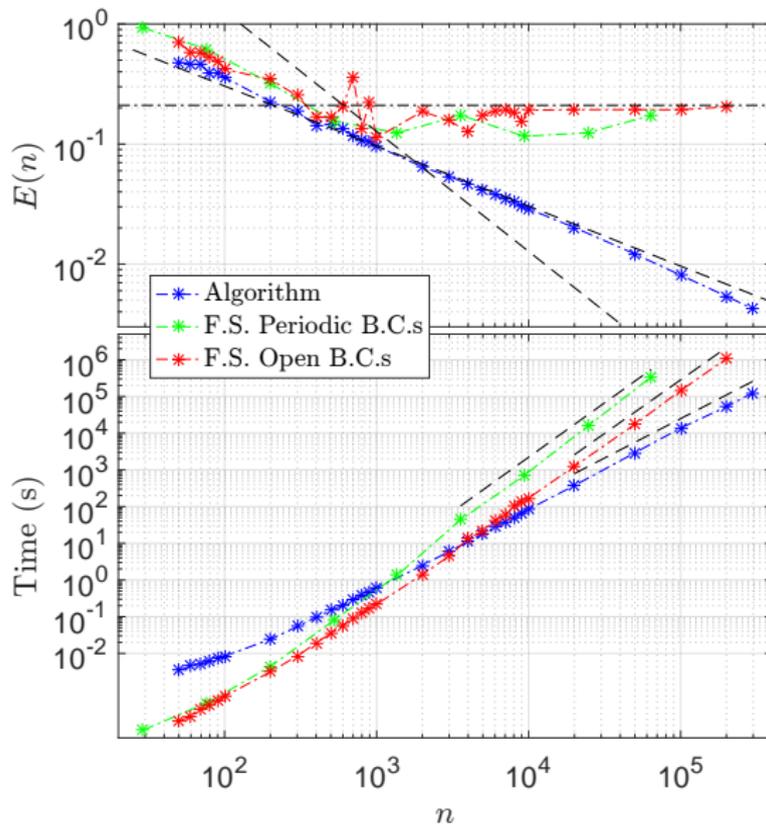

These represent state of art in (vast physics/maths) literature. Can we beat this?

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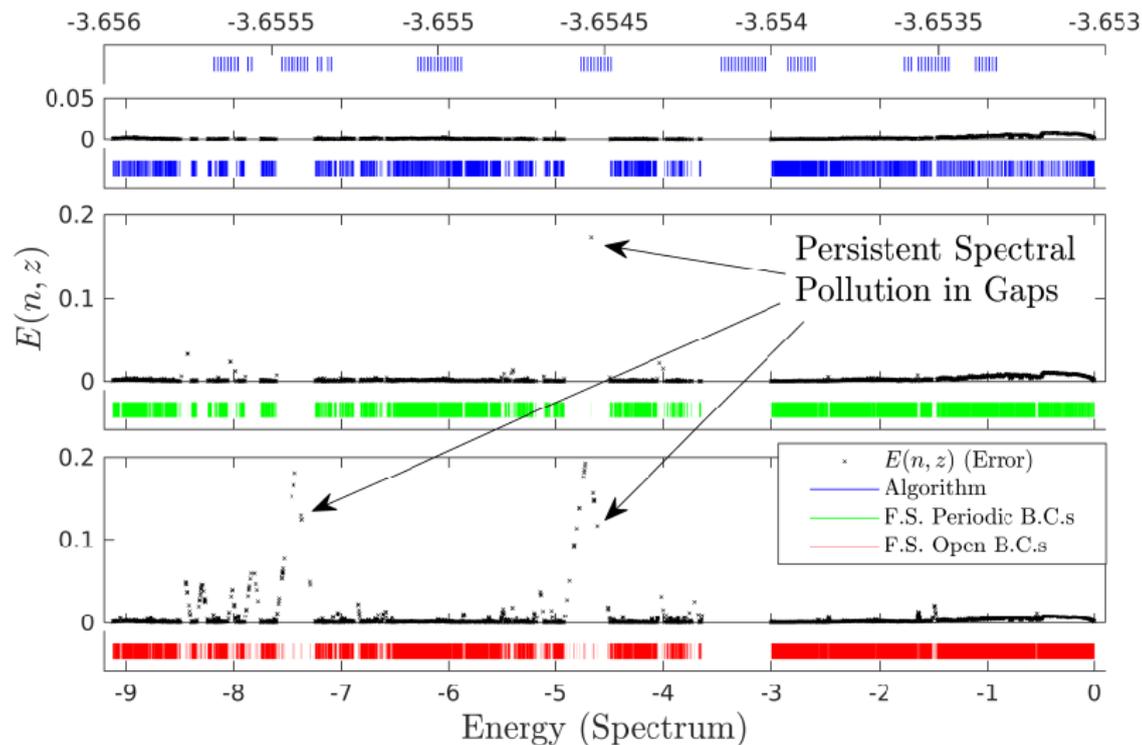
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What about spectral measures?

- If T normal (commutes with adjoint) then has associated projection-valued measure (resolution of the identity) E^T s.t.

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

- View this as diagonalisation - allows computation of functional calculus, has interesting physics etc.
- Previous work: can compute $\mathrm{Sp}(T)$ but not the measure, unless T of special form (tridiagonal Toeplitz + compact). Analogous in finite dimensions to being able to compute the location of eigenvalues but not eigenvectors!

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Know $f \Rightarrow$ can compute measure in one limit [3]!

Example 1

$$J = \begin{pmatrix} b_1 & a_1 & 0 & \cdots \\ a_1 & b_2 & a_2 & \cdots \\ 0 & a_2 & b_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

Jacobi polynomials defined for $\alpha, \beta > -1$ which have

$$a_k = 2\sqrt{\frac{k(k+\alpha)(k+\beta)(k+\alpha+\beta)}{(2k+\alpha+\beta-1)(2k+\alpha+\beta)^2(2k+\alpha+\beta)}},$$

$$b_k = \frac{\beta^2 - \alpha^2}{(2k+\alpha+\beta)(2k-2+\alpha+\beta)}.$$

Measure on $[-1, 1]$:

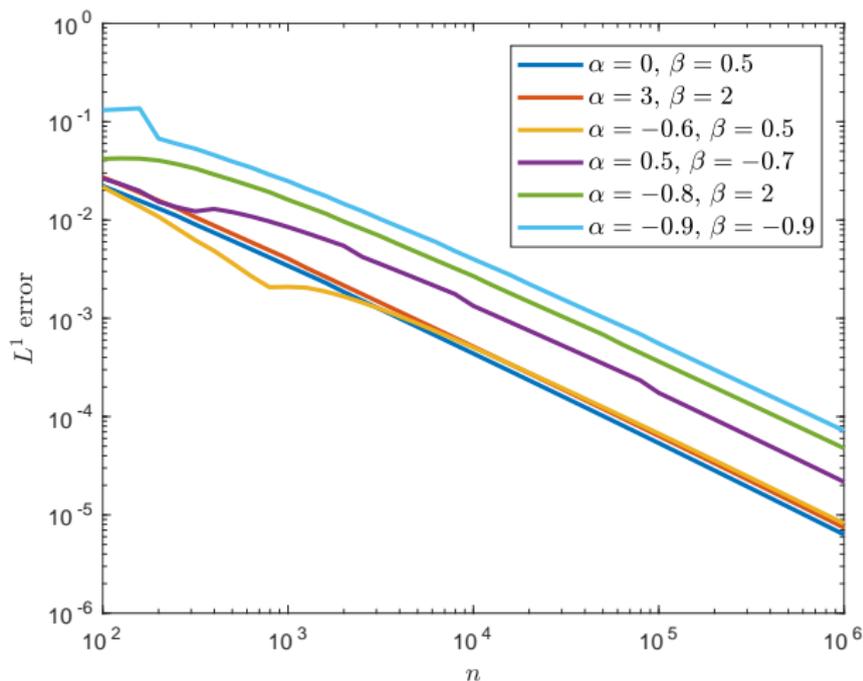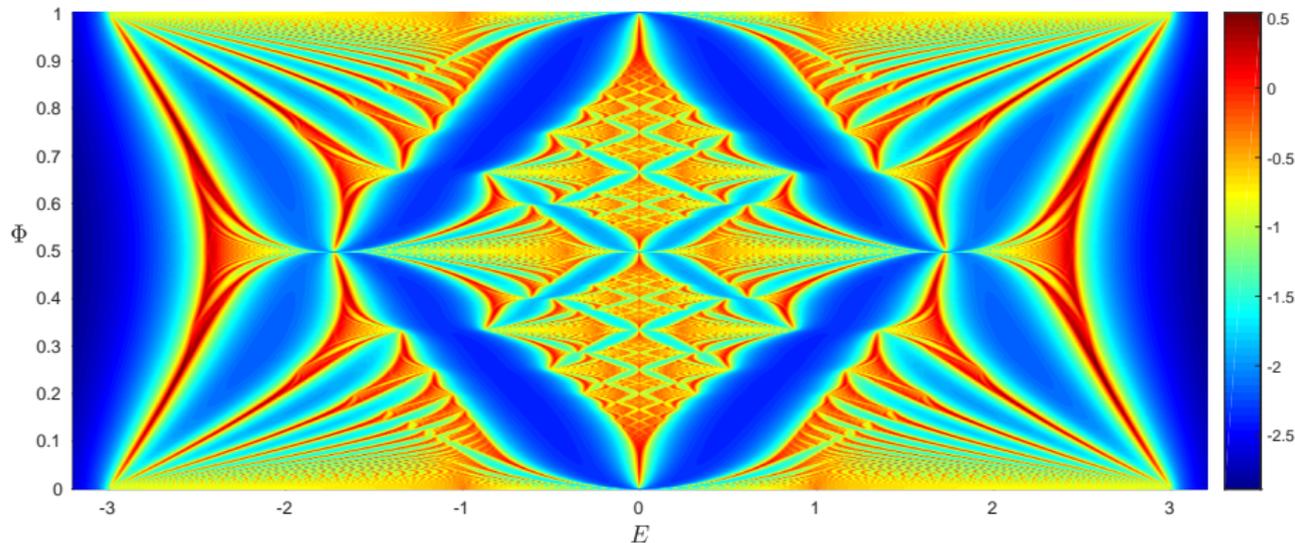$$d\mu_J = \frac{(1-x)^\alpha(1+x)^\beta}{N(\alpha, \beta)}dx = f_{\alpha,\beta}(x)dx.$$

Example 1

Figure: Convergence in L^1 for various parameters α, β as we increase the matrix size n. Fast $\mathcal{O}(n)$ solver!

Example 2: Back to Graphene

Beautiful fractal structure!

Can do things like study transport properties etc.

Have classifications computing:

- Lebesgue measure and fractal dimensions of spectra (different types).
- Discrete spectra, essential spectra, eigenvectors (if they exist) + multiplicity, spectral type...
- Spectral radii, essential numerical ranges, geometric features of spectrum such as capacity...
- Decision problems such as whether compact set intersects spectrum...

For a whole bunch of classes:

- Self-adjoint, normal.
- Know the function g and/or know the function f.
- Even compact case not trivial!
- Continuous operators such as PDEs with coefficients of locally bounded total variation (this can be done with Σ_1 error control).

ALL constructed algorithms can cope with inexact input using only arithmetic over $\mathbb{Q}$, are stable and recursive.

Open Problems and Future Work

- How to compute "g" in general - applications in rigorous numerics for resonances in arbitrary dimension etc.
- Non-linear eigenvalue problems, extensions to Banach spaces...
- Current work is looking at this framework applied to **rigorous** computability results for **stable** neural networks (this **can** be done).
- Computing embedded point spectra (in general needs two limits but for certain classes can be done in one).
- How can we use interval arithmetic in this framework?
- Next step: efficient and easy to use code!

Want to hear about problems like these that interest people like yourselves for future work!

Thank you for listening!
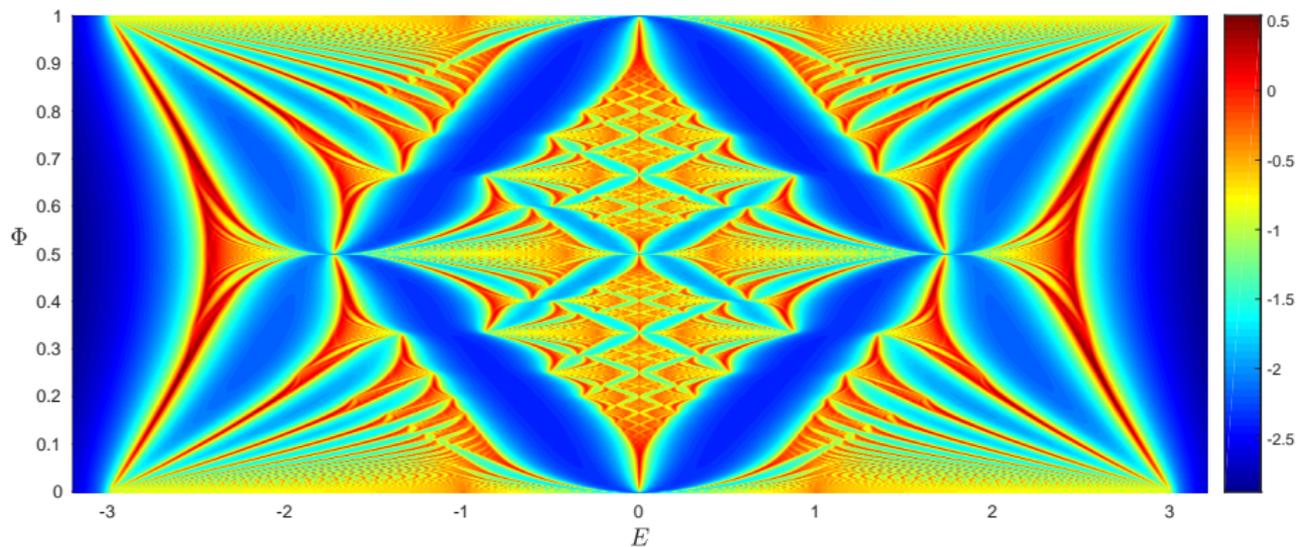
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Preprint, 2019.

Idea: Use the formula

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

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

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