The Computational Spectral Problem and a New Classification Theory

Novel Algorithms, Impossibility Results and Computer Assisted Proofs

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Motivation

- Motivating example: spectra of infinite-dimensional operators. Many applications but W. Arveson (leading operator theorist U.C. Berkeley) pointed out in nineties, "**Unfortunately, there is a dearth of literature on this basic problem, and ... there are no proven techniques.**" Situation even worse for the Schrödinger case.

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- Naive discretisations can fail spectacularly even when V real valued.
- Talk will present solution to this problem and how to compute spectra for much more general cases.

Computational Schrödinger Problem

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Studied by great scientists and mathematicians throughout 20th and 21st centuries. **Very** incomplete list - P.W. Anderson [2], J. Schwinger [3], A. Weyl [4], T. Digernes, V.S. Varadarajan and S.R.S. Varadhan [5], A. Böttcher [6, 7], P.A. Deift, L.C. Li and C. Tomei [8], C. Fefferman and L. Seco [9, 10, 11, 12, 13, 14, 15, 16, 17], P. Hertel, E. Lieb and W. Thirring [18], L. Demanet and W. Schlag [19], M. Zworski [20, 21]...

Computational Schrödinger Problem

M. Zworski's result: Let $V : \mathbb{R}^2 \to \mathbb{R}$ be in L^∞_{comp} and define

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Let $\{z_j(\epsilon)\}_{j=1}^\infty$ be eigenavlues of P_ϵ (has discrete spectrum) then uniformly on compact subsets of $\{z : \arg(z) \in (-\pi/4, 7\pi/4)\}$

$$z_j(\epsilon) \to z_j \text{ as } \epsilon \downarrow 0.$$

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Later - can compute $\mathrm{Sp}(P_\epsilon)$ via algorithm Γ_n^ϵ, get resonances in sector of $\mathbb{C}$ via two limits

$$\lim_{\epsilon \downarrow 0} \lim_{n \to \infty} \Gamma_n^\epsilon(A).$$

More on complex potentials and more general PDEs later...

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Theorem 1

For $\mathbb{P}_d$ there exists a generally convergent algorithm only for $d \leq 3$. Towers of algorithms exist additionally for $d = 4$ and $d = 5$ but not for $d \geq 6$.

Another example of limits

Problem: Given an infinite matrix (acting as a bounded operator on $l^2(\mathbb{N})$)

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

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Answer [25]: 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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Computational problem: decide whether there is an $x \in \mathbb{R}^N$ such that

$$(1) \quad \langle x, c\rangle_K \leq M \text{ subject to } Ax = y, \quad x \geq 0,$$

where

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Irrational input numbers means that A and y are only known approximately, however, to any precision one wants.
Not computable. But if replace $\langle x, c \rangle_K \leq M$ by $\langle x, c \rangle_K < M$ then problem is verifiable. If there had been cases with equality, the Flyspeck program may never have resolved Kepler's conjecture!

Motivation: Dirac-Schwinger conjecture

Proven by C. Fefferman and L. Seco in a series of papers


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The key result: show asymptotic behaviour of $E(Z)$ for large Z,

$$E(Z) = -c_0 Z^{7/3} + \frac{1}{8} Z^2 - c_1 Z^{5/3} + \mathcal{O}(Z^{5/3-1/2835}),$$

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for explicit constants c_0 and c_1.
To prove this, one verifies that $F''(\omega) \leq c < 0$ for some specific function F, for some c and for all $\omega \in (0, \omega_c)$ where ω_c is specifically defined. The intricate computer assisted proof hinges on several problems that are **not computable** but **are verifiable**.

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(iii) Δ_2^α is the set of problems that can be computed using one limit, the SCI $= 1$, but error control may not be possible.

(iv) Δ_{m+1}^α, for $m \in \mathbb{N}$, is the set of problems that can be computed by using m limits, the SCI $\leq m$.

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One side version of error control.
What about other spaces such as Hausdorff metric?

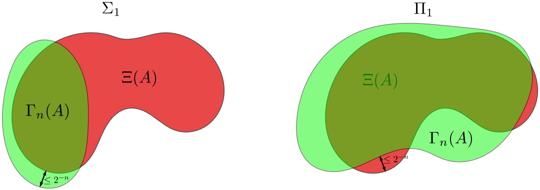

Figure: Meaning of Σ_1 and Π_1 convergence for problem function Ξ. The red area represents $\Xi(A)$ whereas the green areas represent the output of the algorithm $\Gamma_n(A)$. Σ_1 convergence means convergence as $n \to \infty$ but each output point in $\Gamma_n(A)$ is at most distance 2^{-n} from $\Xi(A)$. Similarly for Π_1, we have convergence as $n \to \infty$ but any point in $\Xi(A)$ is at most distance 2^{-n} from $\Gamma_n(A)$.

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- It is **crucial** in rigorous numerical analysis to understand the difference between Δ_1 (convergence with global error control), Σ_1 (convergence with error control of output) and Δ_2 (convergence with no error control).
- Problems in Σ_1 and Π_1 can be used in computer assisted proofs in pure maths and mathematical physics.

Recall

$$\mathrm{Sp}(A) := \{z \in \mathbb{C} : A - zI \text{ not invertible}\}.$$

$$\mathrm{Sp}_\epsilon(A) := \overline{\{z \in \mathbb{C} : \|(A - zI)^{-1}\|^{-1} < \epsilon\}}.$$

Notation: $\{\Xi, \Omega, \mathcal{M}\}$ denotes a computational problem.

$\Xi : \Omega \to (\mathcal{M}, d)$ thing we want to compute

Ω class of objects we work on e.g. class of operators or potentials

$(\mathcal{M}, d)$ metric space

Schrödinger Operators

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- Unsolved for a long time when considering H acting on $\mathrm{L}^2(\mathbb{R}^d)$. Also allow non self-adjointness (complex potentials).
- $(\mathcal{M}, d)$ the Attouch-Wets metric defined by

$$d_{\mathrm{AW}}(A, B) = \sum_{i=1}^{\infty} 2^{-i} \min\left\{1, \sup_{|x|<i} |d(x, A) - d(x, B)|\right\},$$

  for non-empty close A and B - generalises Hausdorff metric.

Schrödinger operators: Bounded potential

$$\phi : [0,\infty) \to [0,\infty) \text{ some increasing function and } M > 0$$
$$\Omega_{\phi,g} := \{H \in \Omega_\phi : \|(-\Delta + V - zI)^{-1}\|^{-1} \geq g(\mathrm{dist}(z, \mathrm{Sp}(H)))\},$$

- Controlled oscillation: $\mathrm{BV}_\phi(\mathbb{R}^d) = \{f : \mathrm{TV}(f_{[-a,a]^d}) \leq \phi(a)\}$
- Controlled resolvent growth near spectrum: $g : \mathbb{R}_+ \to \mathbb{R}_+$ continuous increasing function with $g(x) \leq x$, $\lim_{x\to\infty} g(x) = \infty$.

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

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Theorem 2 (Bounded potential [25])

$$\Delta_1^G \not\ni \{\Xi_{\mathrm{sp}}, \Omega_{\phi,g}\} \in \Sigma_1^A, \quad \Delta_1^G \not\ni \{\Xi_{\mathrm{sp},\epsilon}, \Omega_{\phi,g}\} \in \Sigma_1^A.$$

Schrödinger operators: Unbounded sectorial potential

$\theta_1, \theta_2 \geq 0$ such that $\theta_1 + \theta_2 < \pi$.

$\Omega_\infty = \{V \in \mathrm{C}(\mathbb{R}^d) : \forall x \arg(V(x)) \in [-\theta_2, \theta_1], |V(x)| \to \infty \text{ as } x \to \infty\}$.

$H = h^{**}$, $h = -\Delta + V$, $\mathcal{D}(h) = \mathrm{C}_c^\infty(\mathbb{R}^d)$.

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Theorem 3 (Unbounded potential [25])

$$\Sigma_1^G \cup \Pi_1^G \not\ni \{\Xi_{\mathrm{sp}}, \Omega_\infty\} \in \Delta_2^A, \quad \Sigma_1^G \cup \Pi_1^G \not\ni \{\Xi_{\mathrm{sp},\epsilon}, \Omega_\infty\} \in \Delta_2^A.$$

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Exactly same classification as compact operators acting on $l^2(\mathbb{N})$.
Strictly harder than previous problem despite compact resolvent.

Generalisations to PDEs

$$Tu(x) = \sum_{|k|\leq N} a_k(x)\partial^k u(x), \quad T^*u(x) = \sum_{|k|\leq N} \tilde{a}_k(x)\partial^k u(x).$$

Formally defined on $L^2(\mathbb{R}^d)$ and assume

1. $C_0^\infty(\mathbb{R}^d)$ a core of T and T^*.
2. Exists a positive constant A_k and integer B_k such that a.e.

$$|a_k(x)|, |\tilde{a}_k(x)| \leq A_k(1+|x|^{2B_k}).$$

3. Can access to functions $\{g_m\}$ such that

$$g_m(\mathrm{dist}(z, \mathrm{Sp}(T))) \leq \left\|(T-zI)^{-1}\right\|^{-1}, z \in B_m(0).$$

Generalisations to PDEs

$$\|f\|_{\mathcal{A}_r} = \|f\|_\infty + (3^d + 1)\mathrm{TV}_{[-r,r]^d}(f).$$

Assume $a_k, \tilde{a}_k \in \mathcal{A}_r$ for all $r > 0$.

Ω_1 : given positive c_n with $\|a_k\|_{\mathcal{A}_n}, \|\tilde{a}_k\|_{\mathcal{A}_n} \leq c_n$,

Ω_2 : given positive b_n with $\sup_{n\in\mathbb{N}} \frac{\max\{\|a_k\|_{\mathcal{A}_n}, \|\tilde{a}_k\|_{\mathcal{A}_n} : |k| \leq N\}}{b_n} < \infty$.

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Theorem 4 (PDEs [26])

With $\Xi = \mathrm{Sp}(\cdot)$ *or* $\mathrm{Sp}_\epsilon(\cdot)$

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Generalisations to PDEs

- Similar state of affairs (including distinction) for analytic coefficients replacing TV norm by decay rates of Taylor series.
- Can extend to super-polynomial growth at infinity too.
- Easy to extend to different domains (such as half line, polygons etc.) and different boundary conditions.

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What structure do we need to lower the SCI?

Recall the problem

Given an infinite matrix (acting as a bounded operator on $l^2(\mathbb{N})$)

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

Want to compute the spectrum $\mathrm{Sp}(A)$.
What about other properties like discrete spectra, fractal dimensions, spectral gaps,...?
What structure do we need to lower the SCI?
Simply taking square truncations $\mathrm{Sp}(P_n A P_n)$ (finite section) can fail spectacularly even in self-adjoint case (spectral pollution - false eigenvalues in gaps of essential spectrum).

First ever algorithm that computes spectrum without spectral pollution

Definition 5 (Dispersion - off-diagonal decay)

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

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

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Definition 6 (Controlled growth of the resolvent - well-conditioned)

$g : [0,\infty) \to [0,\infty)$ continuous, strictly increasing, vanishing only at $x = 0$ and tending to infinity as $x \to \infty$ with $g(x) \leq x$.
Controlled growth of the resolvent by g if

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

What does this mean?

- Dispersion - think banded matrices.

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

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

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Turns out if we know f and g we can compute the spectrum with Σ_1 error control! A completely different method to other previous approaches - local, fast and rigorous [27].

Point spectrum

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- Is there an algorithm that can compute the closure of the point spectrum (could also be empty)?
- Turns out for general bounded operators the problem is in Σ_2^A. Can we do better with more structure?

No. Even with nice Schrödinger operators on $l^2(\mathbb{Z})$:

$$A = \begin{pmatrix} \ddots & \ddots & & & \\ \ddots & q_{-1} & 1 & & \\ & 1 & q_0 & 1 & \\ & & 1 & q_1 & \ddots \\ & & & \ddots & \ddots \end{pmatrix}.$$

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Potential $\{q_n\}_{n\in\mathbb{Z}} \subset \mathbb{R}$ a bounded sequence.
There does **NOT** exist a one limit algorithm [28]. Proof uses a nice non-trivial construction of Anderson localisation via fractional moment method.

Some further fun questions

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   Answer [29]: Σ_3^A - two limits more than computing spectrum, which the finite section method was designed for!
2. Given self-adjoint A, what's the classification of computing the Hausdorff dimension of $\mathrm{Sp}(A)$?
   Answer [29]: Σ_4^A (but Σ_3^A for Schrödinger case). Non trivial and uses ideas from descriptive set theory (Baire/Borel hierarchies).

Have classifications of:

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

For a whole bunch of classes:

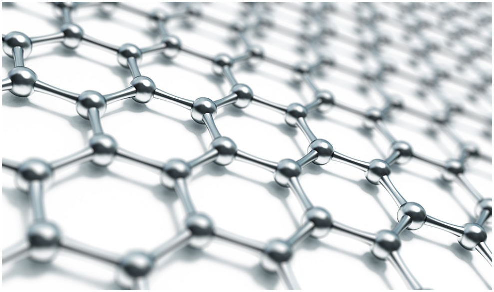
- Self-adjoint, normal, diagonal.
- Know the function g and/or know the function f.
- Even compact case not trivial.

Each problem tends to have an algorithm/proof of lower bound of a different flavour. A very rich classification theory.

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

Graphene

- Graphene is a two-dimensional material with carbon atoms situated at the vertices of a honeycomb lattice with interesting spectral properties (and has won some people Nobel prizes).
- Magnetic properties of graphene important due to experimental observation of quantum Hall effect and Hofstadter's butterfly.



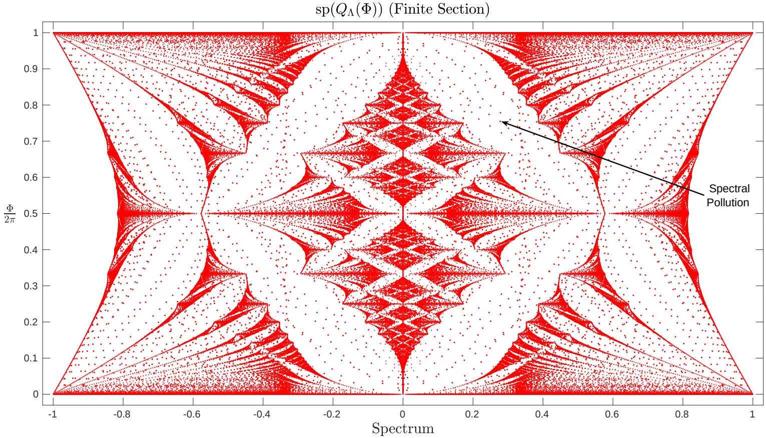


Figure: Finite section.

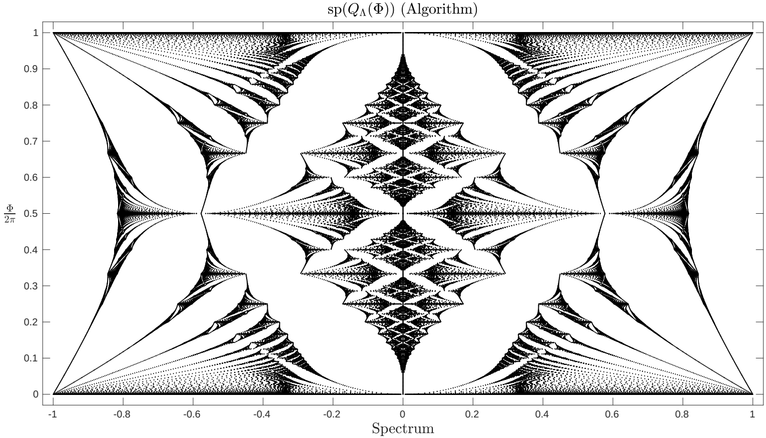


Figure: Guaranteed error bound of 10^{-5}.

- Quantum mechanics, quasicrystals

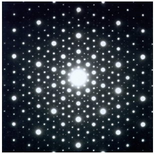
 

Figure: Left: Dan Shechtman, Nobel Prize in Chemistry 2011. Right: Electron diffraction pattern of quasicrystal.

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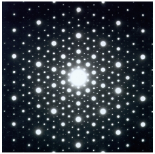

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- Intensely investigated since the 1950s, still very active today.

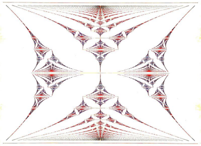
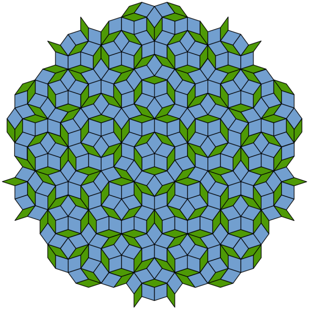


Figure: Left: Artur Avila, Fields Medal 2014. Right: Hofstadter butterfly.

Laplacian on Penrose Tile



Naïve Approximations

1. Finite section with open boundary conditions: compute eigenvalues of **truncated matrix** $P_n H_0 P_n$ for large n. Similar "Galerkin" methods - suffer from spectral pollution.

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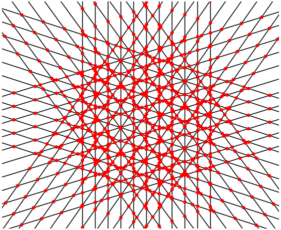

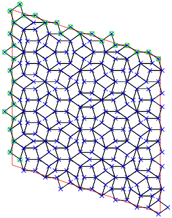

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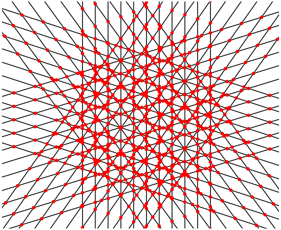
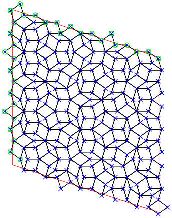
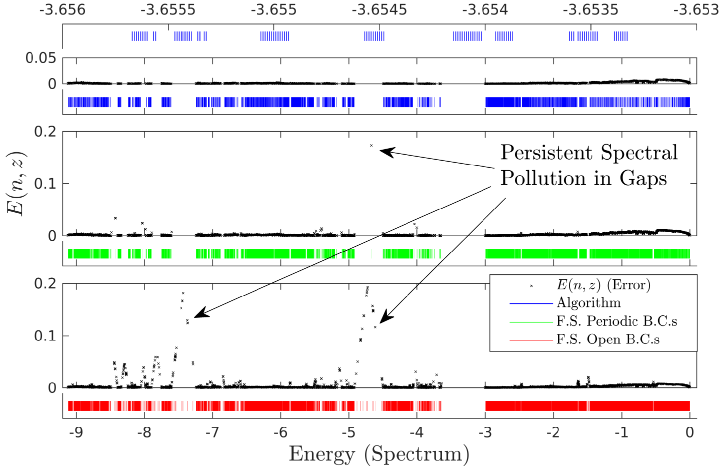




These represent state of art in (vast physics/maths) literature. Can we beat this?

Laplacian on Penrose Tile



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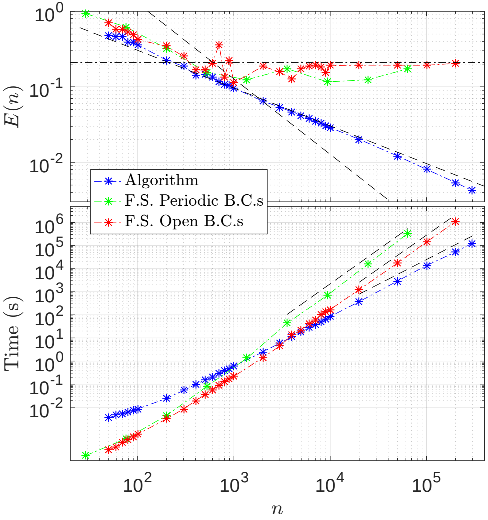


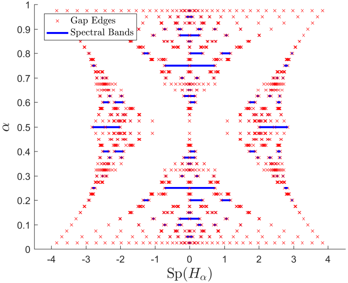
Discrete Spectrum for Normal Operators

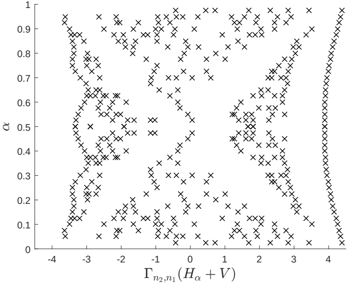
$$(H_\alpha x)_n = x_{n-1} + x_{n+1} + 2\cos(2\pi n\alpha + \nu)x_n, \quad \text{acts on } l^2(\mathbb{Z}).$$

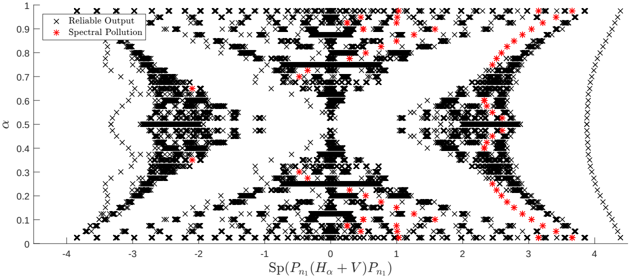
No discrete spectrum. To generate a discrete spectrum, add

$$V(n) = V_n/(|n| + 1),$$

where V_n are independent and uniformly distributed in $[-2, 2]$.
Perturbation compact so preserves essential spectrum.


Gap Edges
Spectral Bands
α
Sp(H_α)


α
$\Gamma_{n_2,n_1}(H_\alpha + V)$


Reliable Output
Spectral Pollution
α
Sp($P_{n_1}(H_\alpha + V)P_{n_1}$)

Pseudospectra of NSA Schrödinger operators - no discretisation!

Computed pseudospectra converge and guaranteed to be in true pseudospectra.

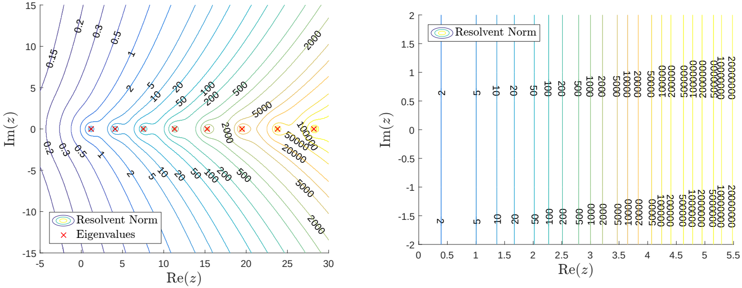


Figure: Left: $V(x) = ix^3$. Note the clear presence of eigenvalues. Right: $V(x) = ix$ (has empty spectrum).

Open Problems

- How to compute 'g' in general - applications in rigorous numerics for resonances in arbitrary dimension etc.

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- Current work is looking at **rigorous** computability results for **stable** neural networks (looking increasingly likely that this **can** be done).

Thank you for listening

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Matthew Colbrook.
Can we always compute point spectra?

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Solvability Complexity Index (SCI) [30, Hansen, JAMS]

Ω is some set, called the *primary* set,

Λ is a set of complex valued functions on Ω, called the *evaluation* set,

$\mathcal{M}$ is a metric space, where the thing we compute lives

Ξ is a mapping $\Omega \to \mathcal{M}$, called the *problem* function.

E.g. $\Omega = \mathcal{B}(\mathcal{H})$, problem function Ξ maps $A \mapsto \mathrm{Sp}(A)$, $(\mathcal{M}, d)$ set of all compact subsets of $\mathbb{C}$ with Hausdorff metric and evaluation functions in Λ consist of $f_{i,j} : A \mapsto \langle Ae_j, e_i \rangle$, $i, j \in \mathbb{N}$, which provide the entries of the matrix representation of A w.r.t. an orthonormal basis $\{e_i\}_{i \in \mathbb{N}}$.

Definition 7 (General Algorithm)

Given a computational problem $\{\Xi, \Omega, \mathcal{M}, \Lambda\}$, a *general algorithm* is a mapping $\Gamma : \Omega \to \mathcal{M}$ such that for each $A \in \Omega$:

(i) there exists a finite subset of evaluations $\Lambda_\Gamma(A) \subset \Lambda$,

(ii) the action of Γ on A only depends on $\{A_f\}_{f \in \Lambda_\Gamma(A)}$ where $A_f := f(A)$,

(iii) for every $B \in \Omega$ such that $B_f = A_f$ for every $f \in \Lambda_\Gamma(A)$, it holds that $\Lambda_\Gamma(B) = \Lambda_\Gamma(A)$.

No restrictions on the operations allowed (can consult any fixed oracle etc.). But can consider different types of towers. E.g. type-2 Turing machines, allow radicals, BSS model, ...

Definition 8 (Tower of algorithms)

Given $\{\Xi, \Omega, \mathcal{M}, \Lambda\}$, a *tower of algorithms of height k for* $\{\Xi, \Omega, \mathcal{M}, \Lambda\}$ is a collection of sequences of functions

$$\Gamma_{n_k} : \Omega \to \mathcal{M}, \quad \Gamma_{n_k, n_{k-1}} : \Omega \to \mathcal{M}, \ldots, \Gamma_{n_k, \ldots, n_1} : \Omega \to \mathcal{M},$$

where $n_k, \ldots, n_1 \in \mathbb{N}$ and the functions $\Gamma_{n_k, \ldots, n_1}$ are general algorithms. Moreover, for every $A \in \Omega$,

$$\lim_{n_k \to \infty} \ldots \lim_{n_1 \to \infty} \Gamma_{n_k, \ldots, n_1}(A) = \Xi(A)$$

with convergence in metric space $\mathcal{M}$.

Definition 9 (Solvability Complexity Index)

$\{\Xi, \Omega, \mathcal{M}, \Lambda\}$ is said to have $\mathrm{SCI}(\Xi, \Omega, \mathcal{M}, \Lambda)_\alpha = k$ with respect to a tower of algorithms of type α if k is the smallest integer for which there exists a tower of algorithms of type α of height k.

If no such tower exists then $\mathrm{SCI}(\Xi, \Omega, \mathcal{M}, \Lambda)_\alpha = \infty$.

If there exists a tower $\{\Gamma_n\}_{n\in\mathbb{N}}$ of type α and height one such that $\Xi = \Gamma_{n_1}$ for some finite n_1, then we define $\mathrm{SCI}(\Xi, \Omega, \mathcal{M}, \Lambda)_\alpha = 0$.

Definition 10 (The Solvability Complexity Index Hierarchy)

Consider a collection $\mathcal{C}$ of computational problems and let $\mathcal{T}$ be the collection of all towers of algorithms of type α for the computational problems in $\mathcal{C}$. Define

$$\Delta_0^\alpha := \{\{\Xi, \Omega\} \in \mathcal{C} \mid \mathrm{SCI}(\Xi, \Omega)_\alpha = 0\}$$
$$\Delta_{m+1}^\alpha := \{\{\Xi, \Omega\} \in \mathcal{C} \mid \mathrm{SCI}(\Xi, \Omega)_\alpha \leq m\}, \qquad m \in \mathbb{N},$$

as well as

$$\Delta_1^\alpha := \{\{\Xi, \Omega\} \in \mathcal{C} \mid \exists\ \{\Gamma_n\}_{n\in\mathbb{N}} \in \mathcal{T} \text{ s.t. } \forall A\ d(\Gamma_n(A), \Xi(A)) \leq 2^{-n}\}.$$