The Computational Spectral Problem and a New Classification Theory

Novel Algorithms, Impossibility Results and Computer Assisted Proofs

Matthew Colbrook
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Motivation

- Motivating example: spectra of infinite-dimensional operators, vast number of applications. W. Arveson (leading operator theorist U.C. Berkeley) in 90s: "**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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  Can we compute the spectrum from point samples of the potential $V(x)$ (or similar appropriate data)? Very important open problem both in continuous and discrete cases.
- 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.

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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].

A curious case of limits

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

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Answer [22]: 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

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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!

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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?

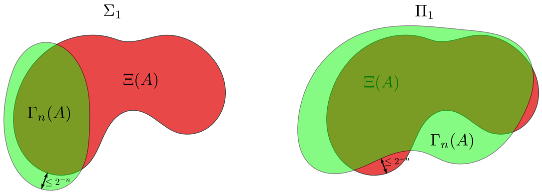

Figure: Meaning of Σ_1 and Π_1 convergence for problem function Ξ. The red area represents $\Xi(A)$ whereas the green areas represent the output of the algorithm $\Gamma_n(A)$. Σ_1 convergence means convergence as $n \to \infty$ but each output point in $\Gamma_n(A)$ is at most distance 2^{-n} from $\Xi(A)$.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

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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

$$\phi : [0,\infty) \to [0,\infty) \text{ some increasing function and } M > 0$$
$$\Omega_\phi := \{H : \mathcal{D}(H) = \mathrm{W}^{2,2}(\mathbb{R}^d), V \in \mathrm{BV}_\phi(\mathbb{R}^d), \|V\|_\infty \leq M\},$$
$$\Omega_{\phi,g} := \{H \in \Omega_\phi : \|(-\Delta + V - zI)^{-1}\|^{-1} \geq g(\mathrm{dist}(z, \mathrm{Sp}(H)))\},$$

- 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 $g(x) \leq x$, $\lim_{x\to\infty} g(x) = \infty$.

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Theorem 1 (Bounded potential [22])

$$\Delta_1^G \not\ni \{\mathrm{Sp}(\cdot), \Omega_\phi\} \in \Pi_2^A, \quad \Delta_1^G \not\ni \{\mathrm{Sp}(\cdot), \Omega_{\phi,g}\} \in \Sigma_1^A.$$

Extensions

Can extend the above to

- Unbounded potentials.
- PDEs $Tu(x) = \sum_{|k|\leq N} a_k(x)\partial^k u(x)$ with polynomially bounded coefficients.
- 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?
Simply taking square truncations $\mathrm{Sp}(P_nAP_n)$ (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 2 (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

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

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Definition 3 (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

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

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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 [23].

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

- Quantum mechanics, quasicrystals

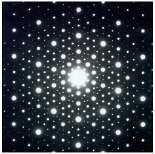

Figure: Left: Dan Shechtman, Nobel Prize in Chemistry 2011.
Right: Electron diffraction pattern of quasicrystal.

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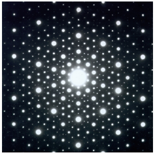

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- Intensely investigated since the 1950s, still very active today.

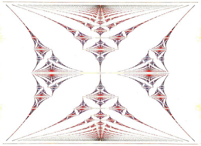
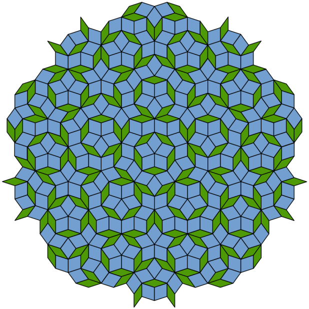


Figure: Left: Artur Avila, Fields Medal 2014. Right: Hofstadter butterfly.

Laplacian on Penrose Tile



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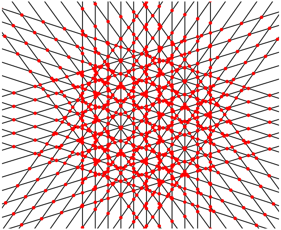
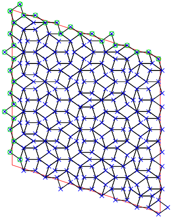
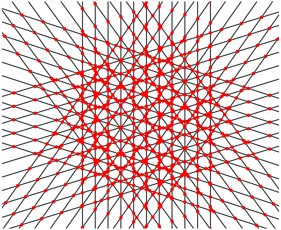
2. Can construct Penrose tile via "Pentagrid" $\rightsquigarrow$ "Periodic Approximants"

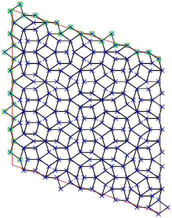




Naïve Approximations

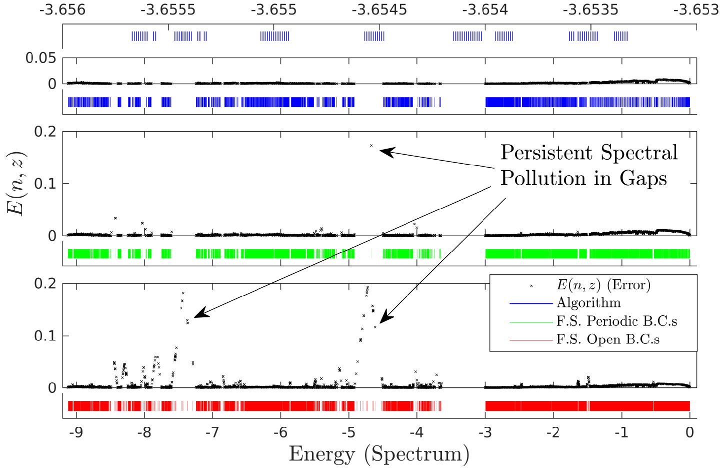
1. Finite section with open boundary conditions: compute eigenvalues of **truncated matrix** $P_n H_0 P_n$ for large n. Similar "Galerkin" methods - suffer from spectral pollution.
2. Can construct Penrose tile via "Pentagrid" $\rightsquigarrow$ "Periodic Approximants"



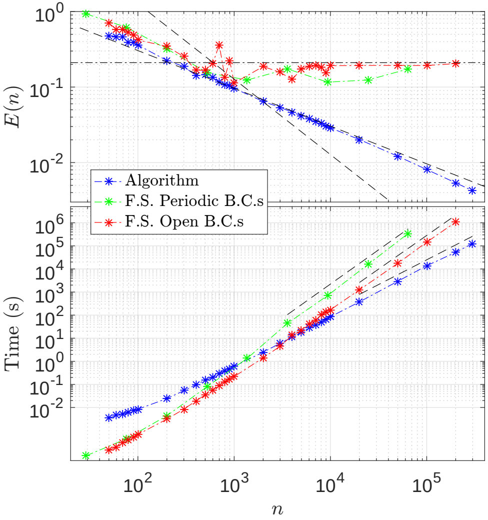


These represent state of art in (vast physics/maths) literature. Can we beat this?

Laplacian on Penrose Tile



Laplacian on Penrose Tile



Open Problems

- Sharp classification for continuous non-Hermitian Schrödinger operators (recall only know $\in \Pi_2^A$) and more general PDEs - applications in rigorous numerics for resonances in arbitrary dimension etc.

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- Non-linear eigenvalue problems, extensions to Banach spaces...
- 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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Solvability Complexity Index (SCI) [24, 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 4 (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 5 (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 6 (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 7 (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

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

as well as

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