Spectral analysis and new resolvent based methods

Matthew Colbrook
University of Cambridge

May 2, 2019

Outline

- Introduction and motivation.
- Schrödinger and PDEs.
- Resolvent I: computing the spectrum.
- Resolvent II: computing the measure.

Motivation

- Spectra of infinite-dimensional operators, vast number of applications.

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.**"

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.**"
- Situation even worse for the Schrödinger case:

$$H = -\Delta + V, \qquad V : \mathbb{R}^d \to \mathbb{C},$$

can we compute $\mathrm{Sp}(H)$ from sampling $V(x)$?

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.**"
- Situation even worse for the Schrödinger case:

$$H = -\Delta + V, \qquad V : \mathbb{R}^d \to \mathbb{C},$$

  can we compute $\mathrm{Sp}(H)$ from sampling $V(x)$?
- Naive discretisations can fail spectacularly even if $V(x) \in \mathbb{R}$.

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.**"
- Situation even worse for the Schrödinger case:

$$H = -\Delta + V, \qquad V : \mathbb{R}^d \to \mathbb{C},$$

  can we compute $\mathrm{Sp}(H)$ from sampling $V(x)$?
- Naive discretisations can fail spectacularly even if $V(x) \in \mathbb{R}$.
- Talk will present solution to this problem and how to compute spectra for much more general cases.

Computational Schrödinger Problem

Problem of algorithmically computing $\mathrm{Sp}(H)$ goes at least as far back as Schrödinger himself [1].

Computational Schrödinger Problem

Problem of algorithmically computing $\mathrm{Sp}(H)$ goes at least as far back as Schrödinger himself [1].

Studied by great scientists and mathematicians throughout 20th and 21st centuries.

Computational Schrödinger Problem

Problem of algorithmically computing $\mathrm{Sp}(H)$ goes at least as far back as Schrödinger himself [1].

Studied by great scientists and mathematicians throughout 20th and 21st centuries.

Very incomplete list: P.W. Anderson, J. Schwinger, H. Weyl, T. Digernes, V.S. Varadarajan and S.R.S. Varadhan, A. Böttcher, P.A. Deift, L.C. Li, C. Tomei, C. Fefferman, L. Seco, P. Hertel, E. Lieb, W. Thirring, L. Demanet, W. Schlag, M. Zworski...

Motivation: a curious case of limits

Problem: Given bounded operator

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

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

Motivation: a curious case of limits

Problem: Given bounded operator

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

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

Answer [2]: No! Best one can do is compute using three successive limits:

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

Motivation: Kepler's conjecture

400 year old problem

What's the best way to pack tennis balls (or if your Kepler, cannon balls) in 3D space?

Motivation: Kepler's conjecture

Flyspeck program (T. Hales) - fully computer assisted verification via 50000 linear programs with irrational inputs!

Motivation: Kepler's conjecture

Flyspeck program (T. Hales) - fully computer assisted verification via 50000 linear programs with irrational inputs!

Computational problem: is 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 $\langle x, c\rangle_K = \lfloor 10^K \langle x, c\rangle \rfloor 10^{-K}, \quad K \in \mathbb{N}, \quad M \in \mathbb{Q}.$

Motivation: Kepler's conjecture

Flyspeck program (T. Hales) - fully computer assisted verification via 50000 linear programs with irrational inputs!

Computational problem: is 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 $\langle x, c\rangle_K = \lfloor 10^K \langle x, c\rangle \rfloor 10^{-K}, \quad K \in \mathbb{N}, \quad M \in \mathbb{Q}.$

Irrational input means A and y only known approximately, to any precision one wants.

Motivation: Kepler's conjecture

Flyspeck program (T. Hales) - fully computer assisted verification via 50000 linear programs with irrational inputs!

Computational problem: is 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 $\langle x, c\rangle_K = \lfloor 10^K \langle x, c\rangle \rfloor 10^{-K}, \quad K \in \mathbb{N}, \quad M \in \mathbb{Q}.$

Irrational input means A and y only known approximately, to any precision one wants.

Not computable. But if $\leq M$ replaced by $< M$ then verifiable.

Informal description

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

Informal description

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

(i) Δ_0 problems that can be computed in finite time.

Informal description

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

(i) Δ_0 problems that can be computed in finite time.

(ii) Δ_1 problems that can be computed using one limit with error control.

Informal description

SCI =number of limits needed to solve problem.

(i) Δ_0 problems that can be computed in finite time.
(ii) Δ_1 problems that can be computed using one limit with error control.
(iii) Δ_2 problems that can be computed using one limit, but error control may not be possible.

Informal description

SCI =number of limits needed to solve problem.

(i) Δ_0 problems that can be computed in finite time.

(ii) Δ_1 problems that can be computed using one limit with error control.

(iii) Δ_2 problems that can be computed using one limit, but error control may not be possible.

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

More Structure (Monotone)

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

More Structure (Monotone)

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

If computational problem maps to a totally ordered metric space:

More Structure (Monotone)

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

If computational problem maps to a totally ordered metric space:

Σ_m - problems requiring m limits but final limit from below.

More Structure (Monotone)

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

If computational problem maps to a totally ordered metric space:

Σ_m - problems requiring m limits but final limit from below.

Π_m - problems requiring m limits but final limit from above.

More Structure (Monotone)

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

If computational problem maps to a totally ordered metric space:

Σ_m - problems requiring m limits but final limit from below.

Π_m - problems requiring m limits but final limit from above.

One side version of error control.

More Structure (Monotone)

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

If computational problem maps to a totally ordered metric space:

Σ_m - problems requiring m limits but final limit from below.

Π_m - problems requiring m limits but final limit from above.

One side version of error control.

What about other spaces such as Hausdorff metric?

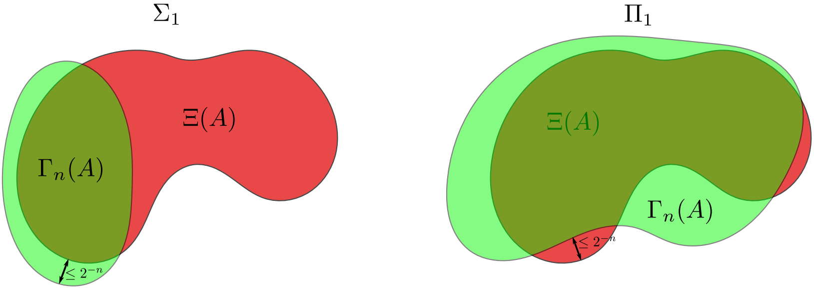


Figure: Meaning of Σ_1 and Π_1 convergence for problem function Ξ. The red area represents $\Xi(A)$ whereas the green areas represent the output of the algorithm $\Gamma_n(A)$.

Why study the non-computable and why care?

- Lower bounds stop us looking for algorithms that don't exist. Many everyday problems in numerical analysis are not computable!

Why study the non-computable and why care?

- Lower bounds stop us looking for algorithms that don't exist. Many everyday problems in numerical analysis are not computable!
- Sharp classification of many real-world problems of interest. E.g. Schrödinger operators, PDEs,...

Why study the non-computable and why care?

- Lower bounds stop us looking for algorithms that don't exist. Many everyday problems in numerical analysis are not computable!
- Sharp classification of many real-world problems of interest. E.g. Schrödinger operators, PDEs,...
- Construction of towers of algorithms give us info on assumptions needed to lower SCI $\Rightarrow$ new algorithms.

Why study the non-computable and why care?

- Lower bounds stop us looking for algorithms that don't exist. Many everyday problems in numerical analysis are not computable!
- Sharp classification of many real-world problems of interest. E.g. Schrödinger operators, PDEs,...
- Construction of towers of algorithms give us info on assumptions needed to lower SCI $\Rightarrow$ new algorithms.
- **Crucial** in rigorous numerical analysis to understand the difference between Δ_1, Σ_1 and Δ_2.

Why study the non-computable and why care?

- Lower bounds stop us looking for algorithms that don't exist. Many everyday problems in numerical analysis are not computable!
- Sharp classification of many real-world problems of interest. E.g. Schrödinger operators, PDEs,...
- Construction of towers of algorithms give us info on assumptions needed to lower SCI $\Rightarrow$ new algorithms.
- **Crucial** in rigorous numerical analysis to understand the difference between Δ_1, Σ_1 and Δ_2.
- Problems in Σ_1 and Π_1 can be used in computer assisted proofs in pure maths and mathematical physics.

Recall

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

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

Triple $\{\Xi, \Omega, \mathcal{M}\}$ 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

- Want to compute spectrum of a Schrödinger operator

$$H = -\Delta + V, \qquad V : \mathbb{R}^d \to \mathbb{C},$$

from sampling the potential V.

Schrödinger Operators

- Want to compute spectrum of a Schrödinger operator

$$H = -\Delta + V, \qquad V : \mathbb{R}^d \to \mathbb{C},$$

  from sampling the potential V.
- Unsolved for a long time when considering H acting on $\mathrm{L}^2(\mathbb{R}^d)$. Also allow non self-adjointness (complex potentials).

Schrödinger Operators

- Want to compute spectrum of a Schrödinger operator

$$H = -\Delta + V, \qquad V : \mathbb{R}^d \to \mathbb{C},$$

  from sampling the potential V.
- 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 closed A and B - generalises Hausdorff metric.

Schrödinger operators: Bounded potential

$\phi : [0, \infty) \to [0, \infty)$ some increasing function.

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

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

Theorem 1 (Bounded potential [2])

$$\Delta_1 \not\ni \{\mathrm{Sp}, \Omega_{\phi,g}\} \in \Sigma_1, \qquad \Delta_1 \not\ni \{\mathrm{Sp}_\epsilon, \Omega_{\phi,g}\} \in \Sigma_1.$$

Schrödinger operators: Unbounded sectorial potential

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

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

Theorem 2 (Unbounded potential [2])

$$\Sigma_1 \cup \Pi_1 \not\ni \{\mathrm{Sp}, \Omega_\infty\} \in \Delta_2, \quad \Sigma_1 \cup \Pi_1 \not\ni \{\mathrm{Sp}_\epsilon, \Omega_\infty\} \in \Delta_2.$$

Schrödinger operators: Unbounded sectorial potential

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

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

Theorem 2 (Unbounded potential [2])

$$\Sigma_1 \cup \Pi_1 \not\ni \{\mathrm{Sp}, \Omega_\infty\} \in \Delta_2, \quad \Sigma_1 \cup \Pi_1 \not\ni \{\mathrm{Sp}_\epsilon, \Omega_\infty\} \in \Delta_2.$$

Same classification as $\mathcal{K}(\ell^2(\mathbb{N}))$, harder than previous problem!

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

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

Coefficients of bounded total variation $\Rightarrow$ can compute Sp and Sp_ϵ with Σ_1 error control.

For simplicity, in rest of talk will consider discrete case on $l^2(\mathbb{N})$. Many of the results extend to continuous case also.

For simplicity, in rest of talk will consider discrete case on $l^2(\mathbb{N})$. Many of the results extend to continuous case also.

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 $\mathrm{Sp}(A)$.

For simplicity, in rest of talk will consider discrete case on $l^2(\mathbb{N})$. Many of the results extend to continuous case also.

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 $\mathrm{Sp}(A)$.

P_n denotes projection onto span of first n basis vectors.

For simplicity, in rest of talk will consider discrete case on $l^2(\mathbb{N})$. Many of the results extend to continuous case also.

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 $\mathrm{Sp}(A)$.

P_n denotes projection onto span of first n basis vectors.

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)...

Magneto-graphene

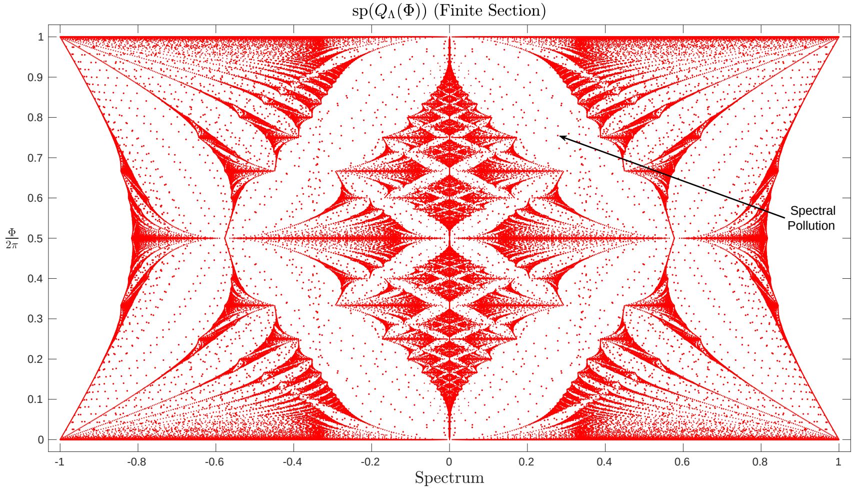


Figure: Finite section.

Can be turned into this

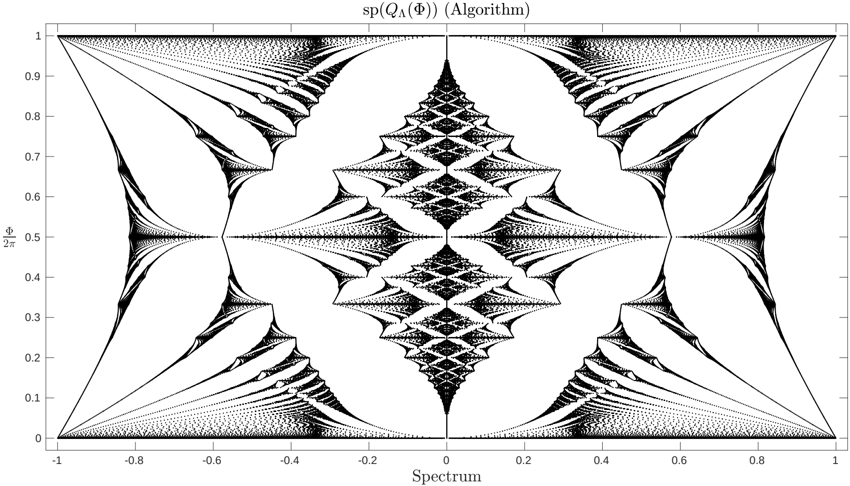


Figure: Guaranteed error bound of 10^{-5}.

First algorithm that computes Sp with error control

Definition 3 (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

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

First algorithm that computes Sp with error control

Definition 3 (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

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

Definition 4 (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

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

What does this mean?

- Dispersion - think banded matrices.

What does this mean?

- Dispersion - think banded matrices.
- Controlled resolvent - g is a measure of the conditioning of the problem of computing $\mathrm{Sp}(A)$ through the formula

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

What does this mean?

- Dispersion - think banded matrices.
- Controlled resolvent - 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

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

What does this mean?

- Dispersion - think banded matrices.
- Controlled resolvent - 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

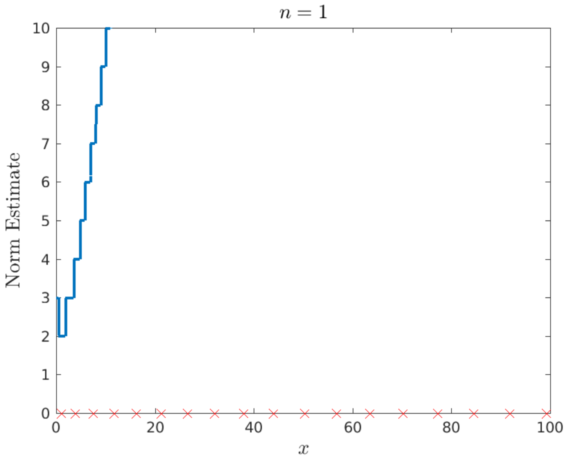
$$\left\|(A - zI)^{-1}\right\|^{-1} = \mathrm{dist}(z, \mathrm{Sp}(A)), \quad g(x) = x.$$

Know $f, g \Rightarrow$ can compute Sp with Σ_1 error control [3]!

Idea: can we approximate the quantity $\|(A - zI)^{-1}\|^{-1}$ locally? Then gain an upper bound:

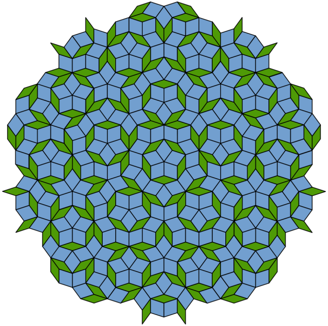
$$\|(A - zI)^{-1}\|^{-1} \leq \mathrm{dist}(z, \mathrm{Sp}(A)) \leq g^{-1}(\|(A - zI)^{-1}\|^{-1}).$$

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



Laplacian on Penrose Tile

Aperiodic, no known method for analytic study.

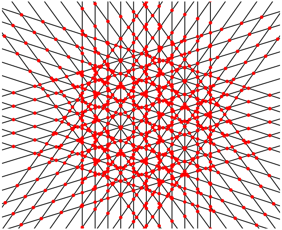
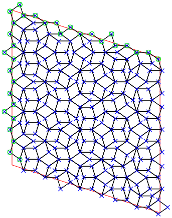


Naïve Approximations

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.

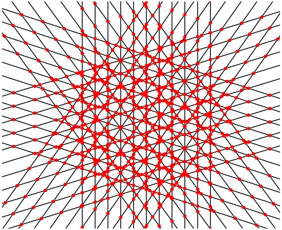
Naïve Approximations

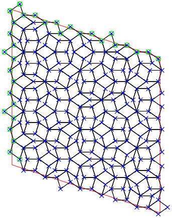
1. Finite section with open boundary conditions: compute eigenvalues of **truncated matrix** $P_n H_0 P_n$ for large n. Similar “Galerkin” methods - suffer from spectral pollution.
2. Can construct Penrose tile via ”Pentagrid” $\rightsquigarrow$ “Periodic Approximants”

Naïve Approximations

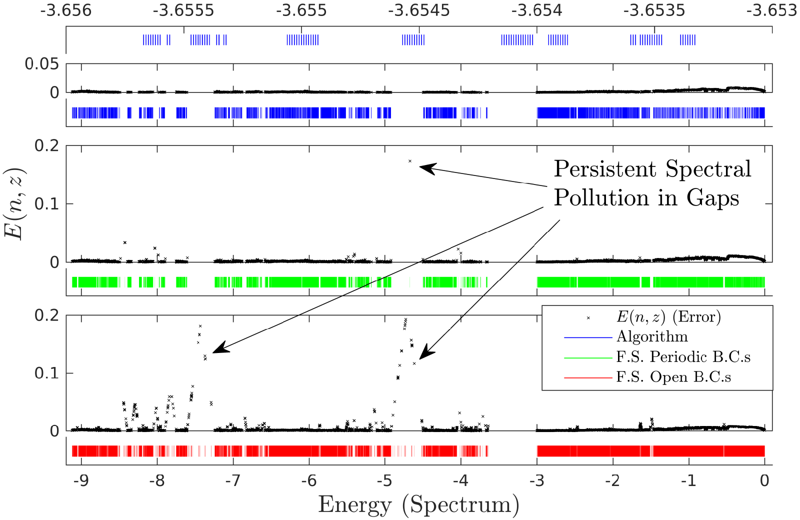
1. Finite section with open boundary conditions: compute eigenvalues of **truncated matrix** $P_n H_0 P_n$ for large n. Similar “Galerkin” methods - suffer from spectral pollution.
2. Can construct Penrose tile via ”Pentagrid” $\rightsquigarrow$ “Periodic Approximants”



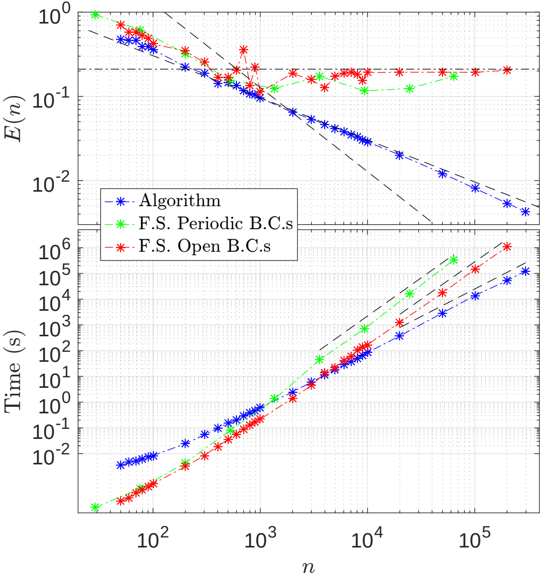


These represent state of art in (vast physics/maths) literature. Can we beat this?

Laplacian on Penrose Tile



Laplacian on Penrose Tile



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...
- 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.

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...
- 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.

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

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...
- 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.

Each problem tends to have a different algorithm and 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.

QUIZ

1. What's the classification of detecting if spectral pollution occurs on an interval (for banded self-adjoint operators)?

QUIZ

1. What's the classification of detecting if spectral pollution occurs on an interval (for banded self-adjoint operators)?
   Answer [4]: Σ_3 - two limits more than computing spectrum, which the finite section method was designed for!

QUIZ

1. What's the classification of detecting if spectral pollution occurs on an interval (for banded self-adjoint operators)?
   Answer [4]: Σ_3 - 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 $\mathrm{Sp}(A)$?

QUIZ

1. What's the classification of detecting if spectral pollution occurs on an interval (for banded self-adjoint operators)?
   Answer [4]: Σ_3 - 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 [4]: Σ_4 (but Σ_3 for Schrödinger case). Non trivial and uses ideas from descriptive set theory (Baire/Borel hierarchies).

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.
- We can compute $\mathrm{Sp}(T)$ but not the measure. Thus the current state of affairs in infinite dimensional spectral computations is analogous in finite dimensions to being able to compute the location of eigenvalues but not eigenvectors!

Idea: Use the formula

$$(T - zI)^{-1} = \int_{\mathrm{Sp}(T)} \frac{1}{\lambda - z} dE^T(\lambda),$$

Cauchy transform. A load of complex analysis and careful approximation theory...

Idea: Use the formula

$$(T - zI)^{-1} = \int_{\mathrm{Sp}(T)} \frac{1}{\lambda - z} dE^T(\lambda),$$

Cauchy transform. A load of complex analysis and careful approximation theory...

Know $f \Rightarrow$ can compute measure in one limit [5]!

Idea: Use the formula

$$(T - zI)^{-1} = \int_{\mathrm{Sp}(T)} \frac{1}{\lambda - z} dE^T(\lambda),$$

Cauchy transform. A load of complex analysis and careful approximation theory...

Know $f \Rightarrow$ can compute measure in one limit [5]!

But impossible to gain any form of error control, even for discrete Schrödinger operators.

Extensions

Can extend this to get SCI classifications for:

- Pure point, absolutely continuous, singular continuous parts of measure.
- Pure point, absolutely continuous, singular continuous parts of spectrum (as sets in complex plane).
- Functional calculus.
- Radon–Nikodym derivative of absolutely continuous part (very useful in physics).

Example 1

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

Measure associated with the orthonormal polynomials. 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

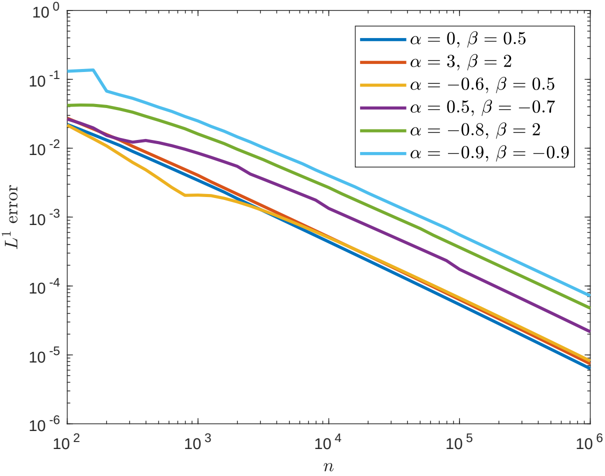


Figure: Convergence in L^1 for various parameters α, β as we increase the matrix size n. Fast $\mathcal{O}(n)$ solver!

Example 2: Point Spectrum

Charlier polynomials are generated by

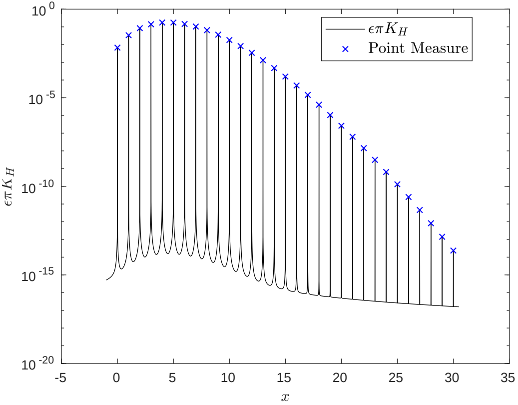
$$a_k = \sqrt{\alpha k}, \quad b_k = k + \alpha - 1$$

for $\alpha > 0$ and have measure

$$d\mu_J = \exp(-\alpha) \sum_{m=0}^{\infty} \frac{\alpha^m}{m!} \delta_m,$$

where δ_x denotes a Dirac measure located at the point x.

Example 2: Point Spectrum



Error $\approx 10^{-13}$. Could be used to compute embedded eigenvalues (very hard problem).

Example 3: Back to Graphene

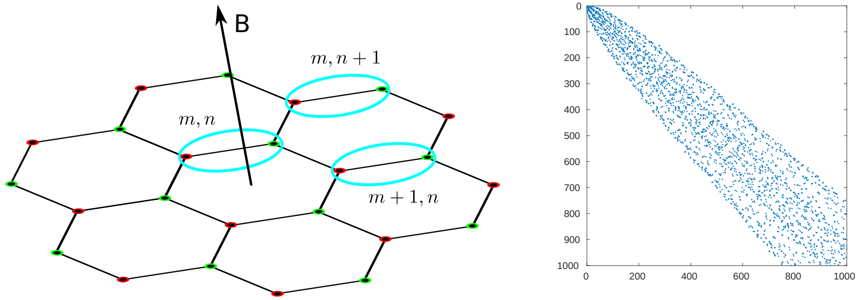
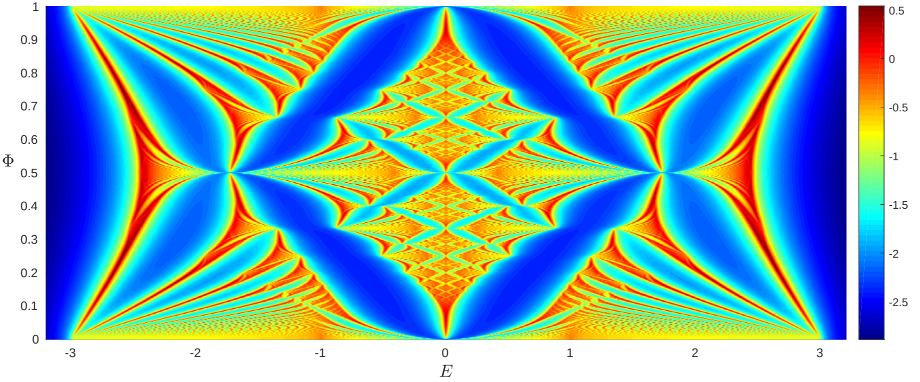


Figure: Left: Honeycomb structure of graphene with the spinor structure shown via the circled lattice vertices. Right: Sparsity structure of the first $10^3 \times 10^3$ block of the infinite matrix.

Example 3: Back to Graphene

Beautiful fractal structure!



Example 3: Back to Graphene

Add random potential of strength W, study time evolution of the Schrödinger equation

$$\frac{du}{dt} = -iHu, \quad u_{t=0} = e_1.$$

Increase $W \Rightarrow$ localisation. Consider the moments of the evolution given by

$$M_p(t;W) = \left\langle \sum_x |x|^p |u(x,t)|^2 \right\rangle.$$

Different power law scalings $M_p \propto t^{\alpha_p}$.

Example 3: Back to Graphene

Add random potential of strength W, study time evolution of the Schrödinger equation

$$\frac{du}{dt} = -iHu, \quad u_{t=0} = e_1.$$

Increase $W \Rightarrow$ localisation. Consider the moments of the evolution given by

$$M_p(t; W) = \left\langle \sum_x |x|^p \, |u(x,t)|^2 \right\rangle.$$

Different power law scalings $M_p \propto t^{\alpha_p}$.

Can compute time evolution efficiently with error control with new class of algorithms. No diagonalisation needed and completely parallelisable.

Example 3: Back to Graphene

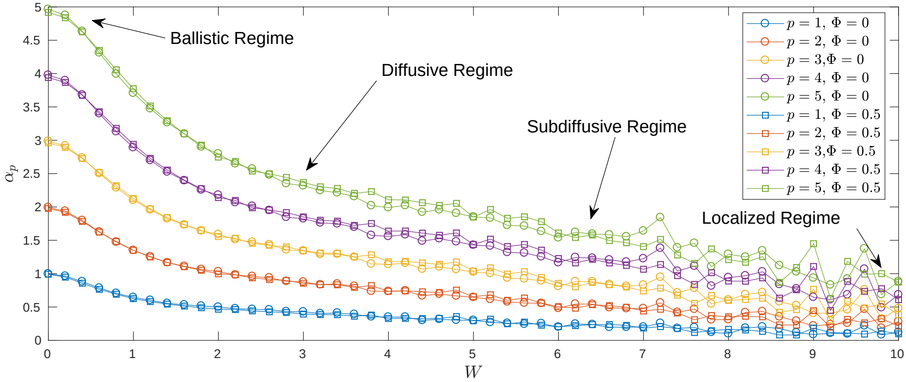


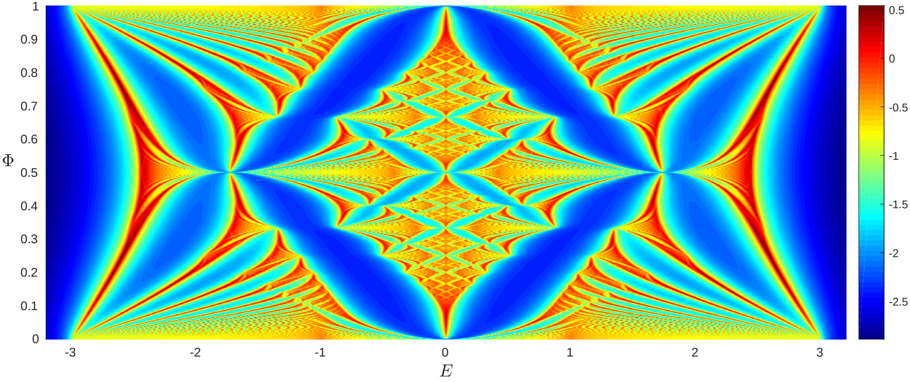
Figure: Exponent α_p as a function of W for $p = 1, 2, 3, 4$ and 5 with labelled the different transport regimes. Similar curves were noted for different values of Φ.

Open Problems

- 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).

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

Thank you for listening!



Erwin Schrödinger.
A method of determining quantum-mechanical eigenvalues and eigenfunctions.
In *Proceedings of the Royal Irish Academy. Section A: Mathematical and Physical Sciences*, volume 46, pages 9–16. JSTOR, 1940.

Jonathan Ben-Artzi, Matthew Colbrook, Anders Hansen, Olavi Nevanlinna, and Markus Seidel.
On the solvability complexity index hierarchy and towers of algorithms.

Matthew Colbrook, Bogdan Roman, and Anders Hansen.
How to compute spectra with error control.

Matthew Colbrook.
The foundations of spectral computations via the solvability complexity index hierarchy: Part II.

Matthew Colbrook.
Computing spectral measures and spectral types: new algorithms and classifications.