What Can Be Computed in Infinite-Dimensional Spectral Problems?

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Papers and talks:
http://www.damtp.cam.ac.uk/user/mjc249/home.html

"The infinite! No other question has ever moved so profoundly the spirit of humankind; no other idea has so fruitfully stimulated the intellect; yet no other concept stands in greater need of clarification." – **David Hilbert**

Motivation: Szegő limit theorems

Beiträge zur Theorie der Toeplitzschen Formen.

(Erste Mitteilung.)

Von

G. Szegő in Budapest.

§ 8.

Ein Satz über die Eigenwerte der Toeplitzschen Formen.

21. Satz XVIII. *Es sei* $f(\theta)$ (L) *integrabel und* $m \leqq f(\theta) \leqq M$. *Es seien ferner*

$$\lambda_0^{(n)}, \lambda_1^{(n)}, \ldots, \lambda_n^{(n)} \qquad (n = 0, 1, 2, \ldots)$$

die zu $f(\theta)$ *gehörigen Eigenwerte. Dann ist*

$$m \leqq \lambda_\varkappa^{(n)} \leqq M \qquad (\varkappa = 0, 1, \ldots, n;\ n = 0, 1, 2, \ldots)$$

und wenn $F(\lambda)$ *eine für* $m \leqq \lambda \leqq M$ *definierte stetige Funktion bezeichnet,*

$$\lim_{n=\infty} \frac{F(\lambda_0^{(n)}) + F(\lambda_1^{(n)}) + \ldots + F(\lambda_n^{(n)})}{n+1} = \frac{1}{2\pi} \int_0^{2\pi} F[f(\theta)]\, d\theta. \text{ [37]}$$

Integrable real-valued function

$$c_n = \frac{1}{2\pi} \int_0^{2\pi} f(\theta)\, e^{in\Theta}\, d\theta$$

Eigenvalues

Continuous test function.

Asymptotic behavior of spectral measures!

Gábor Szegő (Stanford)

$$\begin{pmatrix} c_0 & c_{-1} & c_{-2} & \ldots & c_{-n} \\ c_1 & c_0 & c_{-1} & \ldots & c_{-n+1} \\ c_2 & c_1 & c_0 & \ldots & c_{-n+2} \\ & & & \ldots & . \\ c_n & c_{n-1} & c_{n-2} & \ldots & c_0 \end{pmatrix},$$

Self-adjoint Toeplitz matrix.

Motivation: Schwinger's approx. of quantum systems

Schwinger: approx. $-\Delta + V$ on $\mathbb{R}$ using periodic finite grids

$$X_N = \left\{ j\sqrt{2\pi/N} : j = 0, \pm 1, \dots, \pm N \right\}, \qquad q_N \text{ multiplication},$$

$$p_N \quad \text{F.T. of} \quad q_N, \qquad H_N = \frac{1}{2}\left(p_N^2 + V(q_N)\right)$$

Julian Schwinger
(Harvard,
Nobel Prize in Physics 1965)

Digernes, Varadarajan, and Varadhan: Schwinger's method converges to spectra of $-\Delta + V$ on $L^2(\mathbb{R}^d)$ for certain families with compact resolvent.

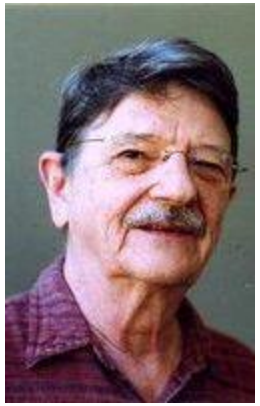
Given a self-adjoint Schrödinger operator $-\Delta + V$ on $\mathbb{R}^d$,
can we approximate its spectrum from sampling V?

- Schwinger, *"Unitary operator bases,"* **Proc. Natl. Acad. Sci. USA**, 1960.
- Weyl, *"The theory of groups and quantum mechanics,"* **Dover**, 1931.
- Digernes, Varadarajan, Varadhan, *"Finite approximations to quantum systems,"* **Rev. Math. Phys.**, 1994.

Arveson's work on C^*-algebras and finite sections of bounded operators

$$A \text{"="} \begin{pmatrix} a_{11} & a_{12} & \cdots \\ a_{21} & a_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}, \qquad A\left(\sum_{k=1}^{\infty} x_k e_k\right) = \sum_{j=1}^{\infty}\left(\sum_{k=1}^{\infty} a_{jk} x_k\right) e_j$$

Canonical basis vectors of $l^2(\mathbb{N})$



William Arveson (Berkeley)

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

Arveson's work on C^*-algebras and finite sections of bounded operators

$$A \text{"="} \begin{array}{c} \xrightarrow{\;\;n\;\;} \\ \underbrace{\begin{pmatrix} \boxed{\begin{matrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{matrix}} & \begin{matrix} \cdots \\ \cdots \end{matrix} \\ \begin{matrix} \vdots & \vdots \end{matrix} & \ddots \end{pmatrix}}_{A_n} \end{array}, \qquad A\left(\sum_{k=1}^{\infty} x_k e_k\right) = \sum_{j=1}^{\infty}\left(\sum_{k=1}^{\infty} a_{jk} x_k\right) e_j$$

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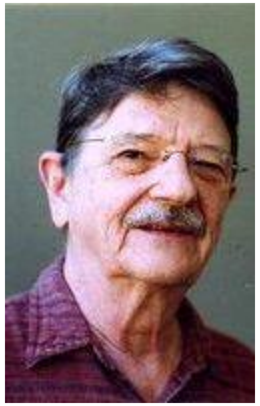

William Arveson (Berkeley)

When does $\mathrm{Sp}(A_n)$ converge? In what sense?
Can we compute $\mathrm{Sp}(A)$ from matrix entries?

Arveson's work on C^*-algebras and finite sections of bounded operators

n

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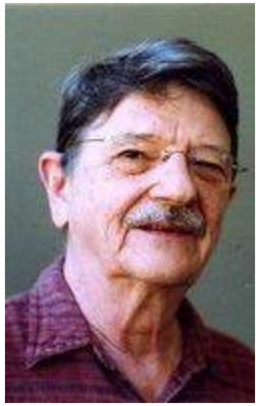
A_n

Canonical basis vectors of $l^2(\mathbb{N})$



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"Most operators that arise in practice are not presented in a representation in which they are diagonalized, and it is often very hard to locate even a single point in the spectrum. Thus, one often has to settle for numerical approximations. Unfortunately, there is a dearth of literature on this basic problem and, so far as we have been able to tell, ***there are no proven [general] techniques****."* W. Arveson, Berkeley (1994)

Arveson's work on C^*-algebras and finite sections of bounded operators

$$A \text{ "="} \begin{pmatrix} \boxed{\begin{matrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{matrix}} & \cdots \\ \vdots \quad \vdots & \ddots \end{pmatrix}, \qquad A\left(\sum_{k=1}^{\infty} x_k e_k\right) = \sum_{j=1}^{\infty}\left(\sum_{k=1}^{\infty} a_{jk} x_k\right) e_j$$

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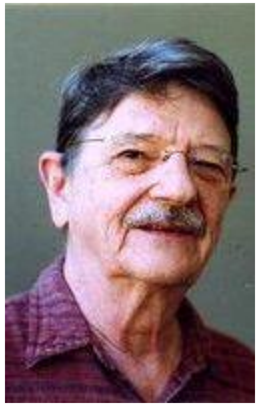

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Goal of talk: Explore mathematical foundations of computing $\mathrm{Sp}(A)$.

(NB: All operators in this talk are closed and densely defined.)

What can go wrong…

Spectral pollution

Definition: Let $\{S_n\} \subset \mathbb{C}$ be a sequence of closed sets (approximations of $\mathrm{Sp}(A)$). We say the sequence suffers from ***spectral pollution*** if there exists $\lambda \in \mathbb{C} \backslash \mathrm{Sp}(A)$ with

$$\liminf_{n \to \infty} \mathrm{dist}(\lambda, S_n) = 0.$$

Examples of $\{S_n\}$:

- **Matrix case ($l^2(\mathbb{N})$):** truncate to $\mathcal{P}_n A \mathcal{P}_n \in \mathbb{C}^{n \times n}, S_n = \mathrm{Sp}(\mathcal{P}_n A \mathcal{P}_n)$
- **PDE on unbounded domain:** truncate domain then discretise.

<u>Pervasive:</u> Dirac and Schrödinger operators, magnetohydrodynamics, matter physics, photonic waveguides, …

Spectral pollution

eigenvalues of infinite multiplicity: H is unitarily equivalent to a countable sum of harmonic oscillators

Magnetic Schrödinger on $L^2(\mathbb{R}^2)$:

$$H = (i\partial_x + y/2)^2 + \left(i\partial_y - x/2\right)^2, \qquad \mathrm{Sp}(H) = \{1,3,5,\ldots\}$$

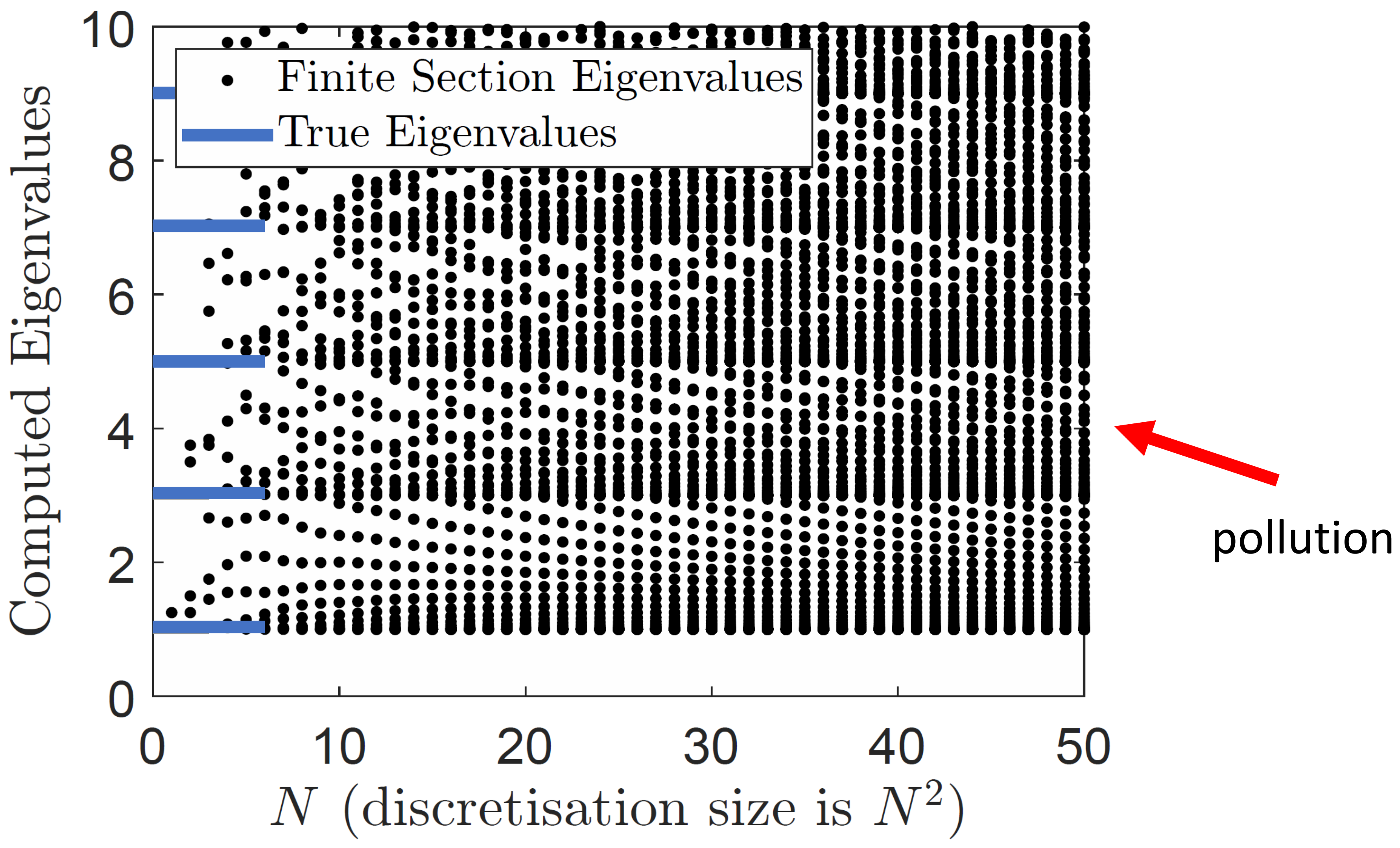
Use orthonormal basis $\psi_j(x) \otimes \psi_k(y)$,

$$\psi_k(x) = \frac{(-1)^k}{\sqrt{2^k k! \sqrt{\pi}}} e^{x^2/2} \frac{\mathrm{d}^k}{\mathrm{d}x^k} e^{-x^2}$$

Hermite functions

$\longrightarrow$ Sparse and self-adjoint “matrix”. BUT…

Spectral pollution



Where does spectral pollution occur?

Numerical range: $W(A) = \{\langle Ax, x\rangle : x \in \mathcal{D}(A), \|x\| = 1\}$

Essential numerical range: $W_e(A) = \bigcap_{B \text{ compact}} \mathrm{Cl}(W(A+B))$

Theorem (Pokrzywa): Let A be a bounded operator on a separable Hilbert space $\mathcal{H}$, $\{\mathcal{P}_n\}$ finite-rank orthogonal projections that converge strongly to I.

- If $z \notin W_e(A)$, $z \in \mathrm{Sp}(A)$ if and only if $\lim_{n\to\infty} \mathrm{dist}(z, \mathrm{Sp}(\mathcal{P}_n A \mathcal{P}_n)) = 0$.
- If $S \subset W_e(A)$ compact, $\exists$ finite-rank orth. project. $\{\mathcal{Q}_n\}$ with $\mathcal{P}_n \leq \mathcal{Q}_n$ and

$$\lim_{n\to\infty} \sup_{x \in \mathrm{Sp}(\mathcal{P}_n A \mathcal{P}_n) \cup S} \mathrm{dist}(x, \mathrm{Sp}(\mathcal{Q}_n A \mathcal{Q}_n)) + \sup_{x \in \mathrm{Sp}(\mathcal{Q}_n A \mathcal{Q}_n)} \mathrm{dist}(x, \mathrm{Sp}(\mathcal{P}_n A \mathcal{P}_n) \cup S) = 0$$

Spectral pollution occurs precisely on $W_e(A) \backslash \mathrm{Sp}(A)$.

Extensions to unbounded A, domain truncation (Bögli, Marletta, Tretter, 2020)

- Pokrzywa, *"Method of orthogonal projections and approximation of the spectrum of a bounded operator,"* **Studia Mathematica**, 1979.
- Bögli, Marletta, Tretter, *"The essential numerical range for unbounded linear operators,"* **Journal of Functional Analysis**, 2020

Spectral invisibility

Definition: Let $\{S_n\} \subset \mathbb{C}$ be a sequence of closed sets (approximations of $\mathrm{Sp}(A)$). We say the sequence suffers from ***spectral invisibility*** if there exists $\lambda \in \mathrm{Sp}(A)$ with

$$\limsup_{n\to\infty} \mathrm{dist}(\lambda, S_n) > 0.$$

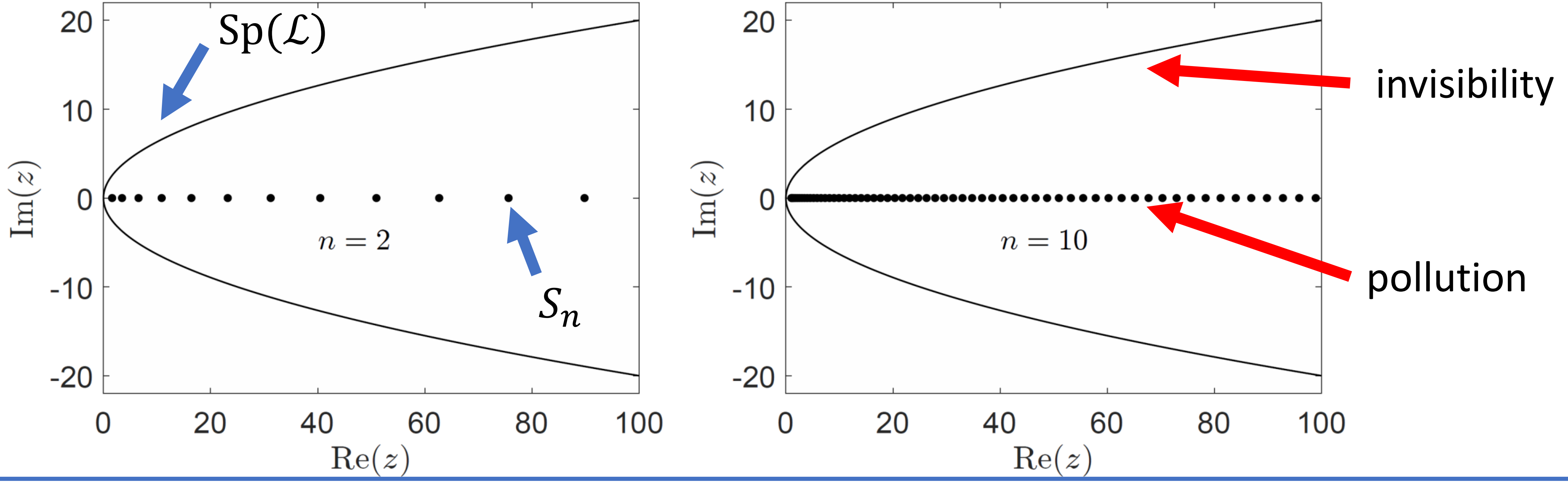
Currently no known characterization of invisibility (i.e., no analog to $W_e(A)$ for spectral pollution).

Spectral invisibility

- Convection-diffusion operator (normal) on $L^2(\mathbb{R})$:

$$\mathcal{L}u = -\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} - 2\frac{\mathrm{d}u}{\mathrm{d}x}, \qquad \mathrm{Sp}(\mathcal{L}) = \{k^2 + 2ki : k \in \mathbb{R}\}$$

- Truncate to $[-n, n]$ + Dirichlet BCs, $S_n = \left\{1 + \frac{m^2\pi^2}{4n^2} : m \in \mathbb{N}\right\}$



A method that <u>always</u> works…

Sketch of method

Spectra through injection moduli (smallest singular value)

Lipschitz-1 in z and A

$$\sigma_{\inf}(A) = \inf\{\|Av\|: v \in \mathfrak{D}(A), \|v\| = 1\}$$

$$\gamma(z, A) = \|(A - zI)^{-1}\|^{-1} = \min\{\sigma_{\inf}(A - zI), \sigma_{\inf}(A^* - \bar{z}I)\}$$

$$\mathrm{Sp}(A) = \{z \in \mathbb{C}: \gamma(z, A) = 0\}$$

Idea: $\mathcal{P}_n =$ orthog-projection onto span$\{e_1, \ldots, e_n\}$.

$$\gamma_{n,m}(z, A) = \min\{\sigma_{\inf}(\mathcal{P}_m(A - zI)\mathcal{P}_n), \underbrace{\sigma_{\inf}(\mathcal{P}_m(A^* - \bar{z})\mathcal{P}_n)}_{\text{Rectangular finite section.}}\}$$

$$\gamma_n(z, A) = \min\{\sigma_{\inf}(\,(A - zI)\mathcal{P}_n), \sigma_{\inf}(\,(A^* - \bar{z}))\mathcal{P}_n\}$$

Dini's theorem: $\gamma_{n,m} \uparrow_{m\to\infty} \gamma_n \downarrow_{n\to\infty} \gamma$ uniformly on compacts

- Hansen, *"On the solvability complexity index, the n-pseudospectrum and approximations of spectra of operators,"* **J. Amer. Math. Soc.**, 2011.

Sketch of method (in bounded case)

Hausdorff metric captures avoidance of pollution/invisibility:

$$d_{\mathrm{H}}(X,Y) = \max\left\{\sup_{x\in X}\inf_{y\in Y}|x-y|, \sup_{y\in Y}\inf_{x\in X}|x-y|\right\}$$

Algorithm that converges in **3 limits**:

$$\Gamma_{n_3,n_2,n_1}(A) = \left\{z \in \frac{1}{n_2}(\mathbb{Z}+i\mathbb{Z}) \colon |z| \leq n_2, \gamma_{n_2,n_1}(z,A) + \frac{1}{n_2} \leq \frac{1}{n_3}\right\}$$

$$\lim_{n_2\to\infty}\lim_{n_1\to\infty}\Gamma_{n_3,n_2,n_1}(A) = \mathrm{Sp}_{\frac{1}{n_3}}(A), \qquad \lim_{n_3\to\infty}\mathrm{Sp}_{\frac{1}{n_3}}(A) = \mathrm{Sp}(A)$$

$$\boxed{\mathrm{Sp}_{\epsilon}(A) = \{z\in\mathbb{C} \colon \gamma(z,A) \leq \epsilon\}}$$

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Can we do better (than 3 limits)?

$$\boxed{\mathrm{Sp}_\epsilon(A) = \{z \in \mathbb{C} : \gamma(z,A) \le \epsilon\}}$$

- Hansen, *"On the solvability complexity index, the n-pseudospectrum and approximations of spectra of operators,"* **J. Amer. Math. Soc.**, 2011.

A mathematical structure…

Computational problem

Definition: A ***computational problem*** is a collection $\{\Xi, \Omega, \mathcal{M}, \Lambda\}$ consisting of:

- Input class Ω;
- Metric space $(\mathcal{M}, d)$;
- Problem function $\Xi: \Omega \to \mathcal{M}$;
- Evaluation set, Λ, of $\mathbb{C}$-valued functions on Ω;

such that for $A, B \in \Omega$:

$$f(A) = f(B) \;\; \forall f \in \Lambda \quad \Rightarrow \quad \Xi(A) = \Xi(B).$$

E.g., $\Omega = \mathcal{B}(l^2(\mathbb{N}))$

E.g., $\mathcal{M} = \mathcal{M}_H$ (Hausdorff metric)

Thing we want to compute E.g., $\Xi = \mathrm{Sp}$

Info available to algorithms
E.g. Matrix entries

$\Xi(A)$ determined by $\{f(A): f \in \Lambda\}$

General algorithm (consistency)

Info algorithm reads on input A.

Definition: Given $\{\Xi, \Omega, \mathcal{M}, \Lambda\}$, a general algorithm is a map $\Gamma: \Omega \to \mathcal{M}$ such that for any $A \in \Omega$, there exists $\Lambda_\Gamma(A) \subset \Lambda$ finite and non-empty such that for $A, B \in \Omega$,

$$f(A) = f(B) \quad \forall f \in \Lambda_\Gamma(A) \quad \Rightarrow \quad \Lambda_\Gamma(A) = \Lambda_\Gamma(B), \Gamma(A) = \Gamma(B)$$

Can also consider restrictions (e.g., Turing or BSS machine)

Impossibility result for gen. alg. $\Longrightarrow$ impossibility result in any model

Solvability Complexity Index Hierarchy

- Δ_0: Solved in finite time (v. rare for cts problems).
- Δ_1: Solved in "one limit" with full error control:

$$d(\Gamma_n(A), \Xi(A)) \leq 2^{-n}$$

- Δ_2: Solved in "one limit":

$$\lim_{n\to\infty} \Gamma_n(A) = \Xi(A)$$

- Δ_3: Solved in "two successive limits":

$$\lim_{n\to\infty} \lim_{m\to\infty} \Gamma_{n,m}(A) = \Xi(A)$$

$\vdots$

Can work in *any* model. E.g., BSS machine, Turing machine, interval arithmetic, inexact input etc.

- Ben-Artzi, C., Hansen, Nevanlinna, Seidel, "*On the solvability complexity index hierarchy and towers of algorithms,*" preprint.
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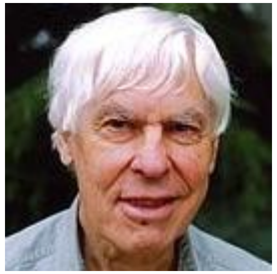

Steve Smale
(Berkeley,Fields Medal 1966)

Smale: *"Is there any purely rational iterative generally convergent algorithm for polynomial zero finding?"*

Curt McMullen
(Harvard, Fields Medal 1998)

McMullen: *"Yes, if the degree is three; no, if the degree is higher."*

Doyle & McMullen: *"The problem can be solved using successive limits for the quartic and quintic, but not the sextic."*

Peter Doyle
(Dartmouth)

Can work in *any* model. E.g., BSS machine, Turing machine, interval arithmetic, inexact input etc.

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- McMullen, *"Families of rational maps and iterative root-finding algorithms,"* **Ann. of Math.**, 1987.
- Doyle, McMullen, *"Solving the quintic by iteration,"* **Acta Math.**, 1989.
- Smale, *"The fundamental theorem of algebra and complexity theory,"* **Bull. Amer. Math. Soc.**, 1981.

Why no proven techniques (Arveson)?

Ξ': $B \in \{0,1\}^{\mathbb{N}\times\mathbb{N}} = \Omega'$, does B have finitely many cols with finitely many 1s?

Descriptive set theory + SCI $\implies \{\Xi', \Omega', \{0,1\}, \Lambda\} \notin \Delta_3$

- C., *"On the computation of geometric features of spectra of linear operators on Hilbert spaces,"* **Found. Comput. Math.**, 2022.

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For $\alpha \in \{0,1\}^{\mathbb{Z}}$ define

$$[C(\alpha)]_{k,l} = \begin{cases} 1, & k < l, \alpha_k = \alpha_l = 1, \alpha_n = 0 \text{ for } k < n < l \\ 0, & \text{otherwise.} \end{cases}$$

shift on $\mathrm{span}\{e_i : \alpha_i = 1\}$

Given $B \in \{0,1\}^{\mathbb{N}\times\mathbb{N}}$ set

$$A(B) = \oplus_{j=1}^{\infty} C(\alpha_i^{(j)}), \qquad \alpha_i^{(j)} = \begin{cases} 1, & |i| \leq j \\ B_{|i|-j,j}, & \text{otherwise.} \end{cases}$$

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If $\Xi'(B) = 1$, $\mathrm{Sp}(B) = \{0\} \cup \mathbb{T}$. Otherwise $\mathrm{Sp}(B) = \{z : |z| \le 1\}$.

If classical spectral problem $\in \Delta_3$, so is $\{\Xi', \Omega', \{0,1\}, \Lambda\}$, contradiction!

• C., *"On the computation of geometric features of spectra of linear operators on Hilbert spaces,"* **Found. Comput. Math.**, 2022.

What about additional structure?
Computing spectra with error control…

Reasons it's hard I

$$A = \bigoplus_{r=1}^{\infty} J_{l_r}, \qquad J_{l_r} = \begin{pmatrix} 0 & 1 & & \\ & 0 & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{pmatrix} \in \mathbb{C}^{l_r \times l_r}$$

$\boxed{\text{Instability}}$

$$\mathrm{Sp}(A) = \begin{cases} \{0\}, & \sup l_r < \infty \\ \{z : |z| \leq 1\}, & \text{otherwise} \end{cases}$$

No $\{\Gamma_n\}$ when given $\{l_r\}_{r=1}^{\infty}$ can determine if it is bounded.

$\Longrightarrow$ No $\{\Gamma_n\}$ computes spectra of gen. tridiagonal operators.

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$\Longrightarrow$ No $\{\Gamma_n\}$ computes spectra of gen. tridiagonal operators.

Always have: $\|(A - zI)^{-1}\|^{-1} \leq \mathrm{dist}(z, \mathrm{Sp}(A))$

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

known cts. bijection
$g: \mathbb{R}_{>0} \to \mathbb{R}_{>0}$

Reasons it's hard II

$$A = \bigoplus_{r=1}^{\infty} A_{l_r}, \qquad A_{l_r} = \begin{pmatrix} 1 & & & & 1 \\ & 0 & & & \\ & & \ddots & & \\ & & & 0 & \\ 1 & & & & 1 \end{pmatrix} \in \mathbb{C}^{l_r \times l_r}$$

Info at ∞

$$\mathrm{Sp}(A) = \{0,2\}, \qquad \mathrm{Sp}\big(\mathrm{diag}(1,0,\dots)\big) = \{0,1\}$$

More involved: Suppose for a contradiction $\{\Gamma_n\}$ converges, choose $\{l_r\}_{r=1}^{\infty}$ so $\Gamma_n(A)$ does not converge (try it!)

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Assume access to $\langle Ae_j, e_i\rangle$, $\langle Ae_j, Ae_i\rangle$, $\langle A^* e_j, A^* e_i\rangle$

Motivation: bounded diagonal operators

$$A = \begin{pmatrix} a_1 & & \\ & a_2 & \\ & & \ddots \end{pmatrix}$$

$\boldsymbol{\Lambda}$**:** Matrix entries of A *(readable info)*

Algorithm: $\Gamma_n(A) = \{a_1, a_2, \dots, a_n\} \to \mathrm{Sp}(A) = \overline{\{a_1, a_2, \dots\}}$ in Haus. Metric.

One-sided error control: $\Gamma_n(A) \subset \mathrm{Sp}(A)$

$$d_{\mathrm{H}}(\Gamma_n(A), \mathrm{Sp}(A)) = \max\left\{ \sup_{x \in \Gamma_n(A)} d(x, \mathrm{Sp}(A)), \sup_{y \in \mathrm{Sp}(A)} d(y, \Gamma_n(A)) \right\}$$

Motivation: bounded diagonal operators

$$A = \begin{pmatrix} a_1 & & \\ & a_2 & \\ & & \ddots \end{pmatrix}$$

$\boldsymbol{\Lambda}$**:** Matrix entries of A *(readable info)*

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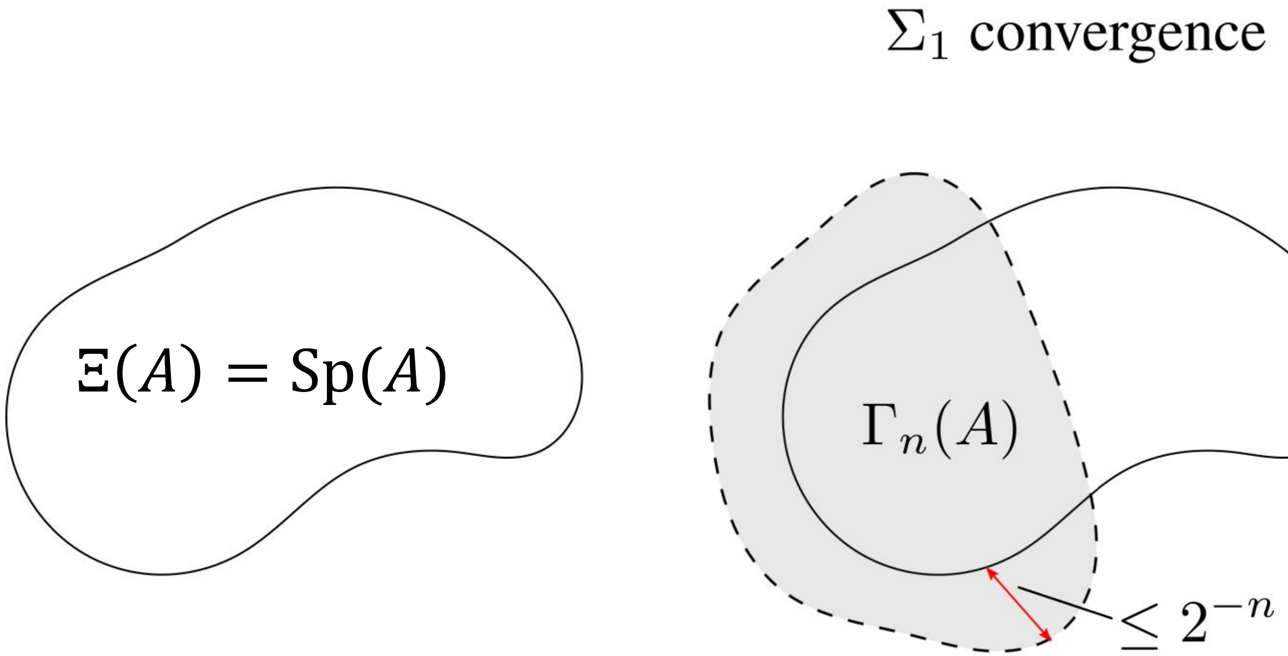
But: No algorithm with $\hat{\Gamma}_n(A) \to \mathrm{Sp}(A)$ with $\mathrm{Sp}(A) \subset \hat{\Gamma}_n(A)$.

Error control for spectral problems

$$d_{\mathrm{H}}(X,Y) = \max\left\{\sup_{x\in X} d(x,Y), \sup_{y\in Y} d(y,X)\right\}$$



- Σ_1: $\exists$ alg. $\{\Gamma_n\}$ s.t. $\lim_{n\to\infty} \Gamma_n(A) = \Xi(A)$, $\max_{z\in\Gamma_n(A)} \mathrm{dist}\big(z, \Xi(A)\big) \leq 2^{-n}$

- C., *"The foundations of infinite-dimensional spectral computations,"* **PhD diss., University of Cambridge**, 2020.

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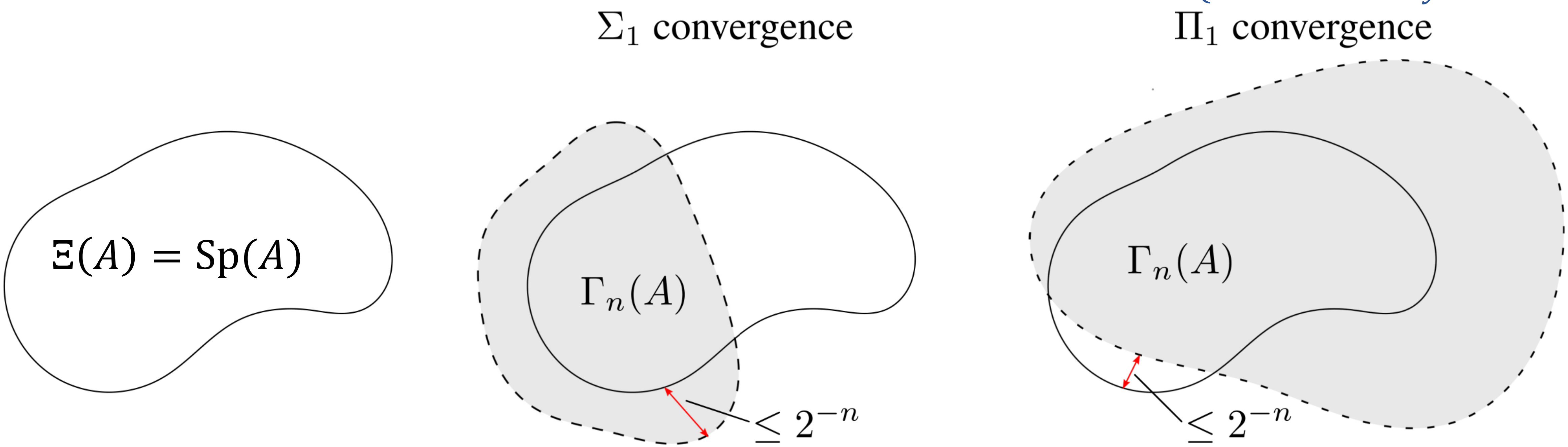

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Such problems can be used in a proof!

- C., *"The foundations of infinite-dimensional spectral computations,"* **PhD diss., University of Cambridge**, 2020.

CompSpec: Method with error control ($\in \Sigma_1$)

$$\sigma_{\inf}(A) = \inf\{\|Av\| : v \in \mathfrak{D}(A), \|v\| = 1\}$$

$$\gamma(z, A) = \|(A - zI)^{-1}\|^{-1} = \min\{\sigma_{\inf}(A - zI), \sigma_{\inf}(A^* - \bar{z}I)\}$$

$$\mathcal{P}_n = \text{orthog-projection onto span}\{e_1, \ldots, e_n\}$$

Idea: $\sqrt{\sigma_{\inf}(\mathcal{P}_n(A - zI)^*(A - zI)\mathcal{P}_n)} = \sigma_{\inf}([A - zI]\mathcal{P}_n) \downarrow \sigma_{\inf}(A - zI)$

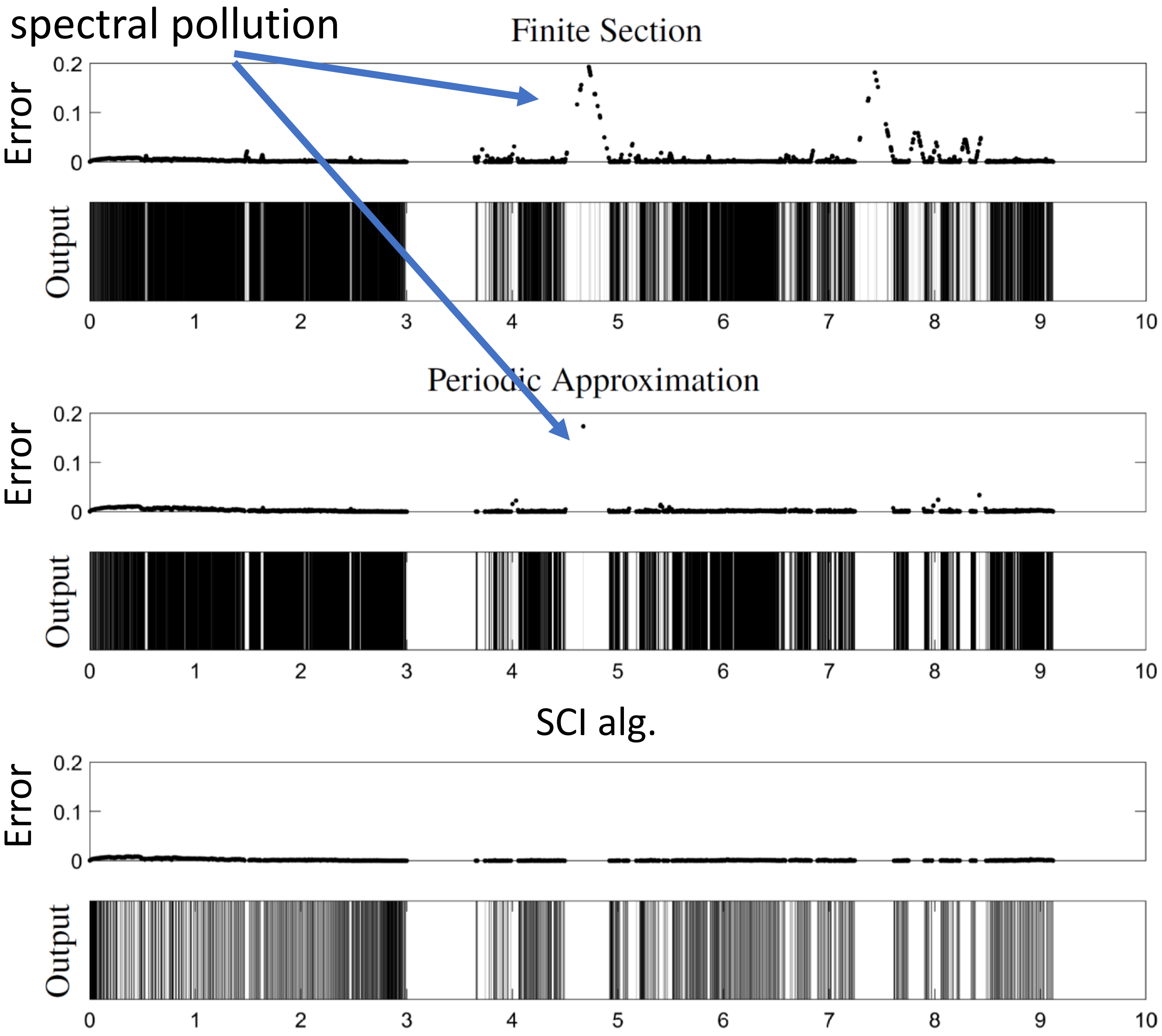
$$g^{-1}(\min\{\sigma_{\inf}([A - zI]\mathcal{P}_n), \sigma_{\inf}([A^* - \bar{z}I]\mathcal{P}_n)\}) \downarrow g^{-1}(\|(A - zI)^{-1}\|^{-1}) \geq \text{dist}(z, \text{Sp}(A))$$

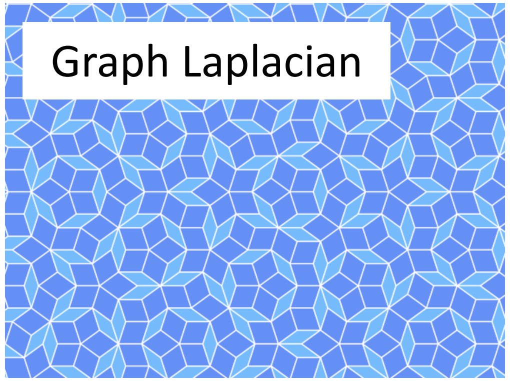
$$\boxed{\|(A - z)^{-1}\|^{-1} \geq g(\text{dist}(z, \text{Sp}(A)))}$$

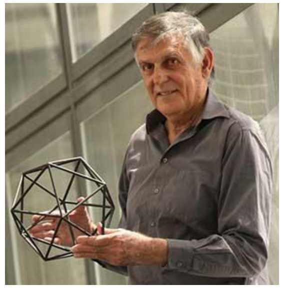
Final ingredient: adaptive search for local minimisers.

- C., Roman, Hansen, "*How to compute spectra with error control*," **Phys. Rev. Lett.**,2019.

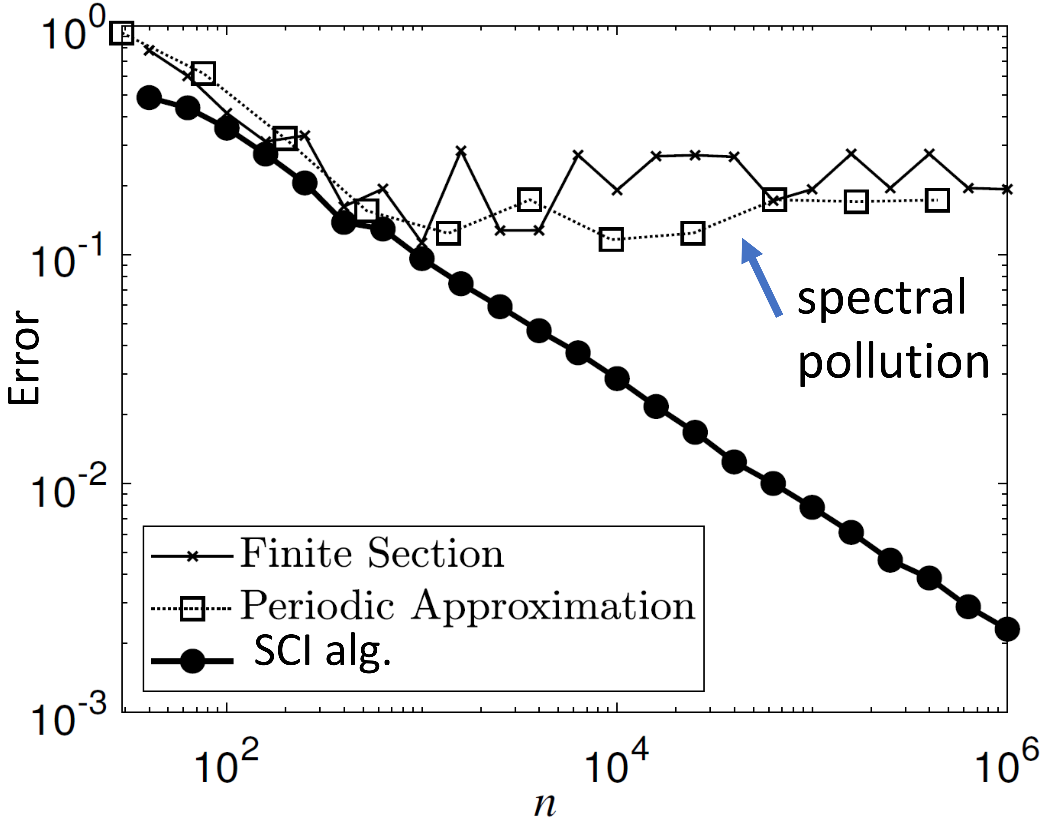
Example: Quasicrystal







Dan Shechtman
(Iowa State, Nobel Prize in Chemistry 2011)



Non-self-adjoint example with non-trivial g

$$T = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + ix^3 \text{ on } \mathbb{R}$$

j	E_j to 30 digits with interval arithmetic
1	1.156 267 071 988 113 293 799 219 177 999 9
2	4.109 228 752 809 651 535 843 668 478 561 3
3	7.562 273 854 978 828 041 351 809 110 631 4
4	11.314 421 820 195 804 402 233 783 948 426 9
5	15.291 553 750 392 532 388 181 630 791 751 9
6	19.451 529 130 691 728 314 686 111 714 104 4
7	23.766 740 435 485 819 131 558 025 968 789 9
8	28.217 524 972 981 193 297 595 053 878 268 9
9	32.789 082 781 862 957 492 447 371 485 046 3
10	37.469 825 360 516 046 866 428 873 594 530 5
100	627.694 712 248 436 511 352 673 702 901 153 6

- Drysdale, C., Woodley, *"Computation and Verification of Spectra for Non-Hermitian Systems,"* **Phys. Rev. Lett.**, 2025.

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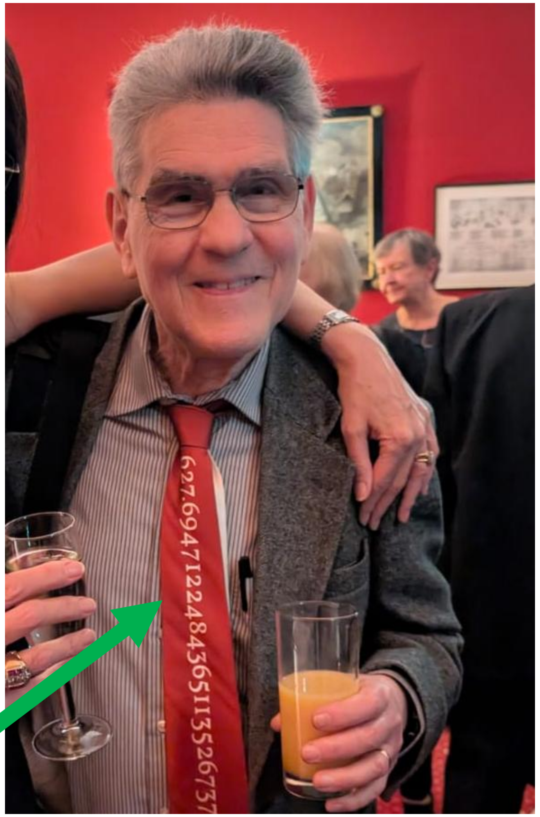

Carl Bender
(Washington, MIT,
Heineman Prize 2017)

- Drysdale, C., Woodley, *"Computation and Verification of Spectra for Non-Hermitian Systems,"* **Phys. Rev. Lett.**, 2025.

Schwinger's problem

Theorem: Ω: class of self-adjoint diff. operators on $L^2(\mathbb{R}^d)$

$$T = \sum_{k\in\mathbb{Z}^d_{\geq 0},|k|\leq N} c_k(x)\,\partial^k$$

- $C_0^\infty(\mathbb{R}^d)$ a core of T.
- $\{c_k\}$ poly bounded, locally bounded total variation.

Can access:

- $\{c_k(q)\}$ for $q \in \mathbb{Q}^d$.
- Polynomial that bounds $\{c_k\}$ on $\mathbb{R}^d$.

(a) Know $\|c_k\|_{\mathrm{TV}([-n,n]^d)} \leq b_n \Longrightarrow \{\mathrm{Sp},\Omega\} \in \Sigma_1$.

(b) Know $\|c_k\|_{\mathrm{TV}([-n,n]^d)} = O(b_n) \Longrightarrow \{\mathrm{Sp},\Omega\} \in \Delta_2\backslash(\Sigma_1 \cup \Pi_1)$.

- C., Hansen, *"The foundations of spectral computations via the solvability complexity index hierarchy,"* **J. Eur. Math. Soc.**, 2022

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Sampling schemes to construct matrix.

Extends to other domains, singular coefficients etc.

Verifiable

Not verifiable

- C., Hansen, "*The foundations of spectral computations via the solvability complexity index hierarchy,*" **J. Eur. Math. Soc.**, 2022

Sampler of results for bounded op. on $l^2(\mathbb{N})$

increasing difficulty

Error control **1 limit** **2 limits** **3 limits**

$$\begin{tikzcd}[column sep=small]
\Pi_0 \arrow[d, phantom, "\shortparallel" description] & & & \Pi_1 \arrow[dr, phantom, "\subsetneq" sloped] & & & & \Pi_2 \arrow[dr, phantom, "\subsetneq" sloped] & & & & \Pi_3 \arrow[dr, phantom, "\cdots" sloped] & \\
\Delta_0 \arrow[d, phantom, "\shortparallel" description] \arrow[r, phantom, "\subsetneq"] & \Delta_1 \arrow[r, phantom, "\subsetneq"] \arrow[urr, phantom, "\subsetneq" sloped] \arrow[drr, phantom, "\subsetneq" sloped] & & \Sigma_1 \cup \Pi_1 \arrow[rr, phantom, "\subsetneq"] & & \Delta_2 \arrow[r, phantom, "\subsetneq"] \arrow[ur, phantom, "\subsetneq" sloped] \arrow[dr, phantom, "\subsetneq" sloped] & & \Sigma_2 \cup \Pi_2 \arrow[rr, phantom, "\subsetneq"] & & \Delta_3 \arrow[r, phantom, "\subsetneq"] \arrow[ur, phantom, "\subsetneq" sloped] \arrow[dr, phantom, "\subsetneq" sloped] & & \Sigma_3 \cup \Pi_3 \; \cdots & \\
\Sigma_0 & & & \Sigma_1 \arrow[ur, phantom, "\subsetneq" sloped] & & & & \Sigma_2 \arrow[ur, phantom, "\subsetneq" sloped] & & & & \Sigma_3 \arrow[ur, phantom, "\cdots" sloped] &
\end{tikzcd}$$

$$\Delta_0 \subsetneq \Delta_1 \subsetneq \Sigma_1 \cup \Pi_1 \subsetneq \Delta_2 \subsetneq \Sigma_2 \cup \Pi_2 \subsetneq \Delta_3 \subsetneq \Sigma_3 \cup \Pi_3 \cdots$$

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Compact operators

$$
\begin{array}{ccccccccccccccc}
\Pi_0 & & & & \Pi_1 & & & & & \Pi_2 & & & & \Pi_3 & \\
\| & & & \rotatebox{-45}{$\subsetneq$} & & \rotatebox{45}{$\subsetneq$} & & & \rotatebox{-45}{$\subsetneq$} & & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & \iddots \\
\Delta_0 & \subsetneq & \Delta_1 & \subsetneq & \Sigma_1 \cup \Pi_1 & \subsetneq & \Delta_2 & \subsetneq & & \Sigma_2 \cup \Pi_2 & \subsetneq & \Delta_3 & \subsetneq & \Sigma_3 \cup \Pi_3 & \cdots \\
\| & & & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & \rotatebox{45}{$\subsetneq$} & & \ddots \\
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\Delta_0 \arrow[d, phantom, "\parallel" sloped] \arrow[r, phantom, "\subsetneq"] & \Delta_1 \arrow[ur, phantom, "\subsetneq" sloped] \arrow[dr, phantom, "\subsetneq" sloped] & \subsetneq & \Sigma_1 \cup \Pi_1 \arrow[r, phantom, "\subsetneq"] & \Delta_2 \arrow[ur, phantom, "\subsetneq" sloped] \arrow[dr, phantom, "\subsetneq" sloped] & \subsetneq & \Sigma_2 \cup \Pi_2 \arrow[r, phantom, "\subsetneq"] & \Delta_3 \arrow[ur, phantom, "\subsetneq" sloped] \arrow[dr, phantom, "\subsetneq" sloped] & \subsetneq & \Sigma_3 \cup \Pi_3 & \cdots \\
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\end{tikzcd}$$

Normal operators

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Compact operators

"Sparse" operators

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\| & & & \rotatebox{-45}{$\subsetneq$} & & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & \rotatebox{45}{$\subsetneq$} & & \rotatebox{-45}{$\subsetneq$} & & \iddots & \\
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\Sigma_0 & & & & \Sigma_1 & & & & \Sigma_2 & & & & \Sigma_3 & &
\end{array}$$

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Normal operators

General operators

Sampler of results for bounded op. on $l^2(\mathbb{N})$

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Approx. sparse normal op

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\Sigma_0 & & & & \Sigma_1 & & & & \Sigma_2 & & & & \Sigma_3 \quad \cdot^{\cdot^{\cdot}}
\end{array}$$

Approx. sparse normal op

Normal operators

General operators

Zoo of problems: spectral type (pure point, absolutely continuous, singularly continuous), Lebesgue measure and fractal dimensions of spectra, discrete spectra, essential spectra, eigenspaces + multiplicity, spectral radii, essential numerical ranges, geometric features of spectrum (e.g., capacity), spectral gap problem, resonances ...

Example with larger SCI: Fine spectral features

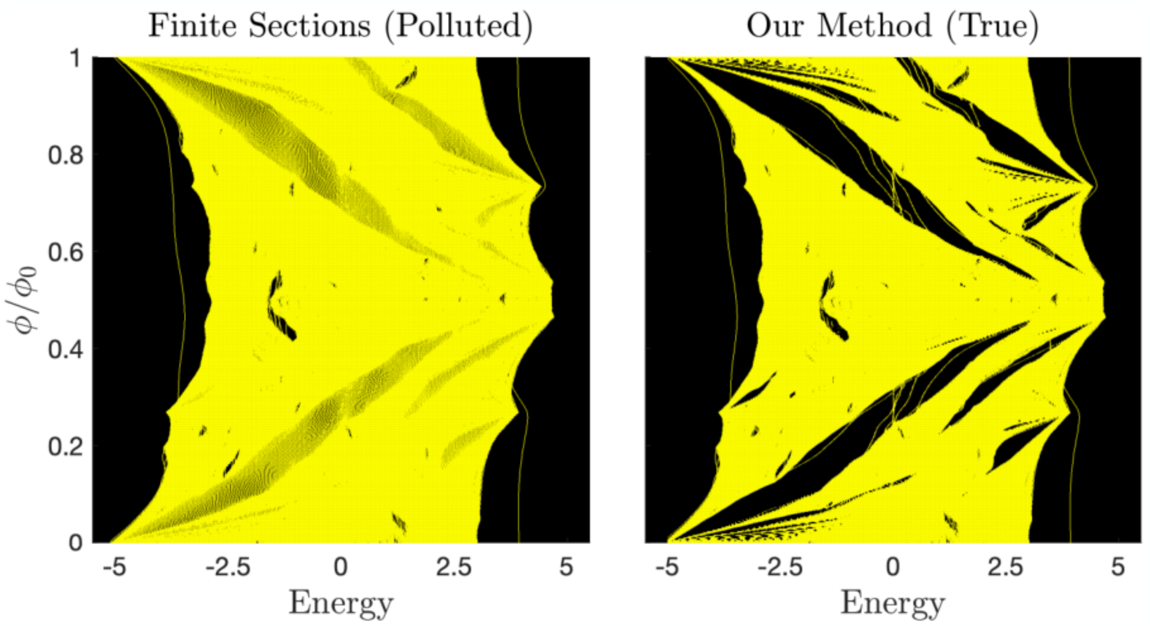


FIG. 1: Spectrum of twisted bilayer graphene modeled by the Stampfli tiling in a uniform magnetic field, with flux ϕ/ϕ_0 on the vertical axis. *Left:* Finite section approximation, which introduces spectral pollution. *Right:* Our algorithm produces a clean, pollution-free spectrum with certified error bounds, revealing the true spectral gaps and band structure, thereby enabling the accurate extraction of physically relevant features, such as gap locations, fractality, and localization regimes.

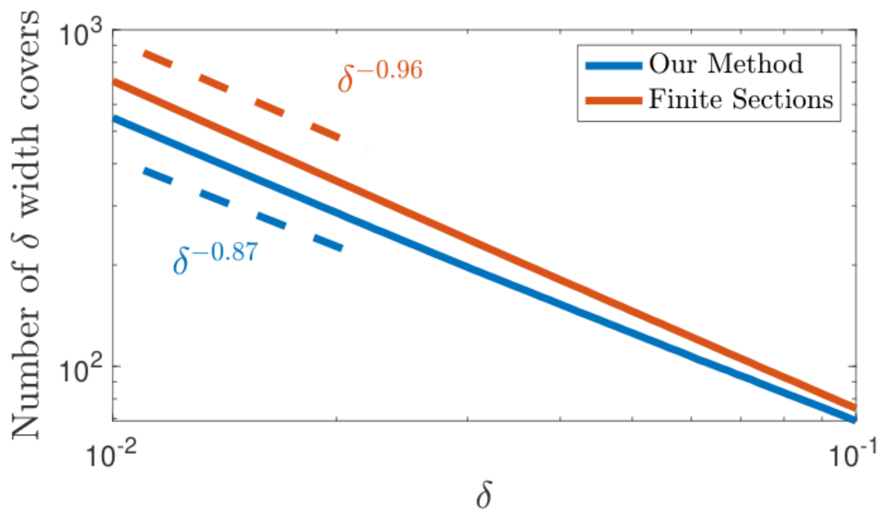


FIG. 3: Finite sections versus our method for computing the box-counting dimension of the Stampfli tiling. Due to pollution, finite sections fail to reach the scaling, whereas our method, with guaranteed error bounds, yields accurate estimates of the box-counting dimension.

- Chok, C., Embree, Fillman, "*Cantor-Set Physics in Quasicrystals: Fractal Spectra and Transport Without Contamination,*" **under review at Phys. Rev. Lett.**

New magic angle for twisted bilayer Penrose tilings

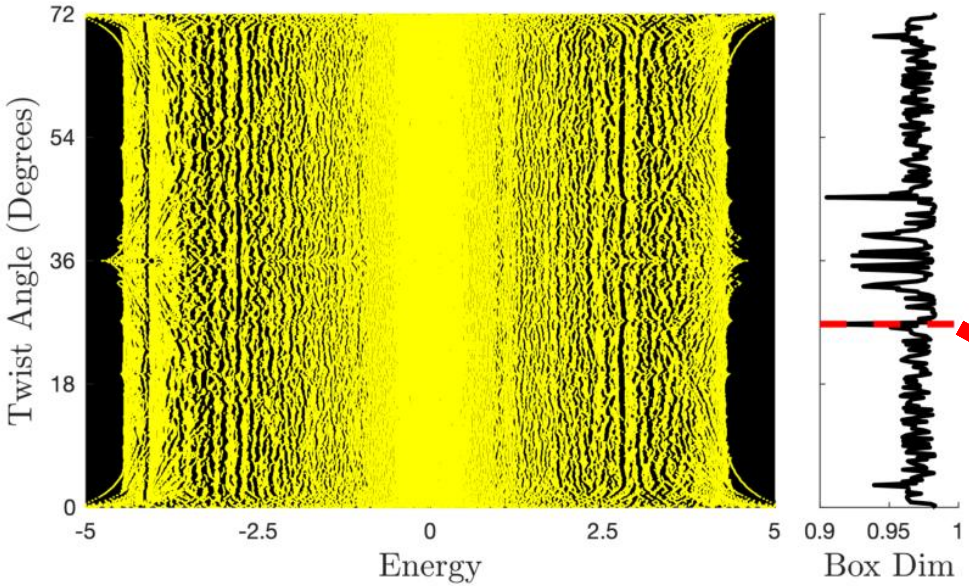


FIG. 8: Angle-resolved spectrum and fractal dimension of the twisted bilayer Penrose quasicrystal. *Left:* Energy spectrum versus twist angle $\theta \in [0, 72^\circ]$ (one fivefold period). *Right:* Box-counting dimension, showing a dip near the straight-worm angle $\theta = 36^\circ$ and a pronounced minimum at the ring-worm angle $\theta = 27.228^\circ$ (red line).

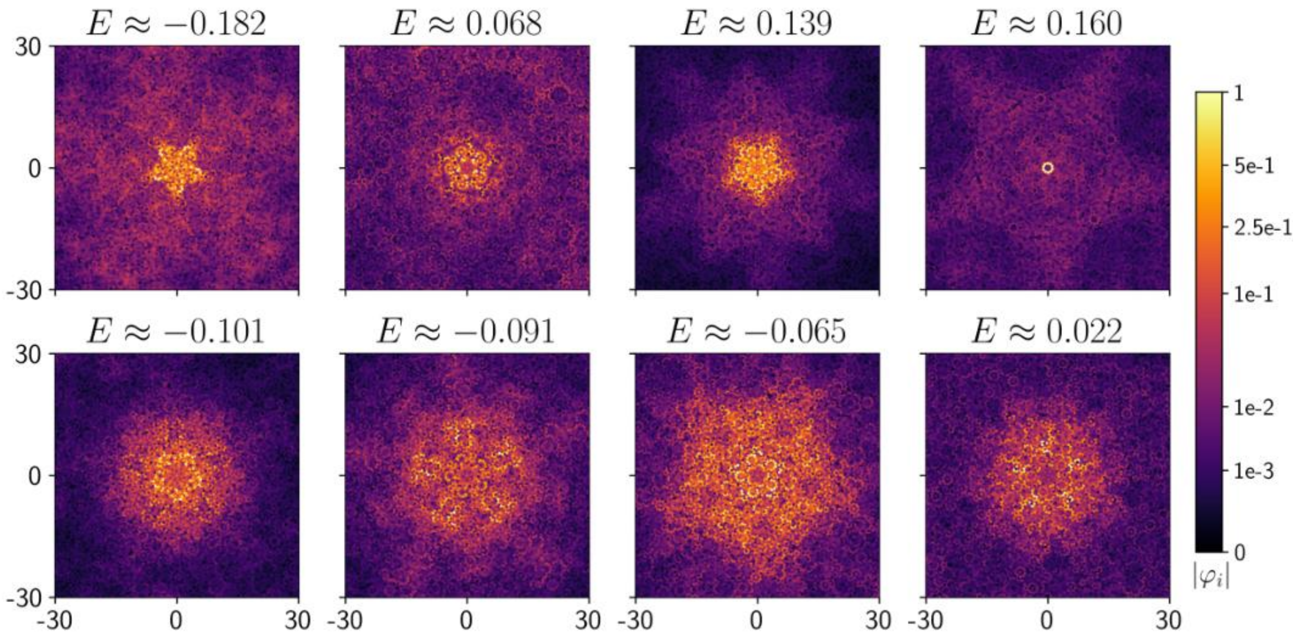
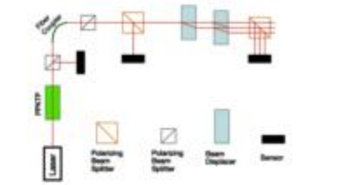
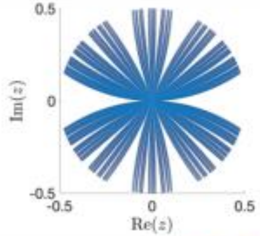


FIG. 10: Eigenstate localization in the twisted bilayer Penrose quasicrystal at $\theta = 27.228^\circ$. *Top:* Eigenmodes resonant with the surrounding ring-worms, producing strong central confinement. *Bottom:* Eigenmodes that partially leak through the ring-worm barrier but remain confined to the central region.

- Chok, C., Embree, Fillman, "*Cantor-Set Physics in Quasicrystals: Fractal Spectra and Transport Without Contamination,*" **under review at Phys. Rev. Lett.**

<table>
<tr><th>Operator</th><th>Application</th><th>Spectrum</th><th>Box Dim</th></tr>
<tr>
<td>Unitary Fibonacci
$|n,\uparrow\rangle \mapsto C^{11}_{\omega_n}|n+1,\uparrow\rangle + C^{21}_{\omega_n}|n-1,\downarrow\rangle$
$|n,\downarrow\rangle \mapsto C^{12}_{\omega_n}|n+1,\uparrow\rangle + C^{22}_{\omega_n}|n-1,\downarrow\rangle$</td>
<td>Single-Photon Quantum Walks
</td>
<td>
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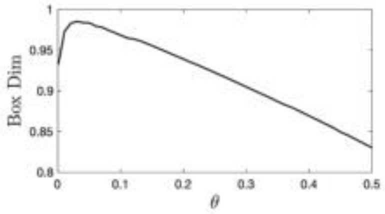
<td>
</td>
</tr>
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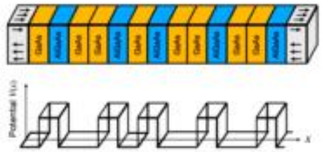
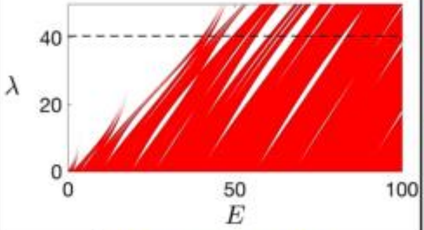
<td>Continuum Quasicrystal
(Kronig—Penney Models)
$H_{\omega,\lambda} = -\frac{d^2}{dx^2} + \lambda \sum_{n\geq 0} \omega_n 1_{x\in[n,n+1)}$</td>
<td>Superlattice of Semiconductors
</td>
<td>
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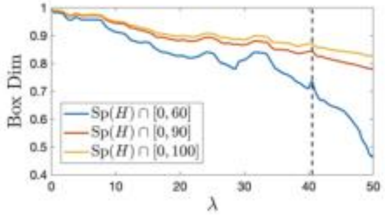
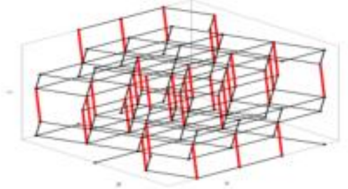
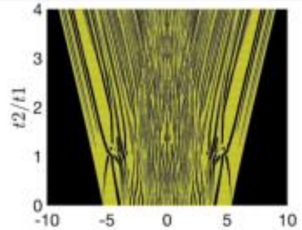
<td>
</td>
</tr>
<tr>
<td>Three-Dimensional Quasicrystals
$H = \sum_{\langle j,k\rangle} t_{jk} \left(|j\rangle\langle k| + |k\rangle\langle j|\right)$</td>
<td>Acoustic Metamaterial
</td>
<td>
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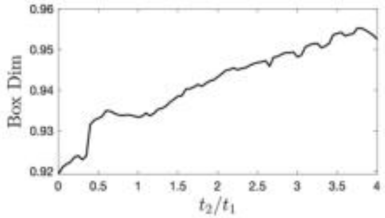
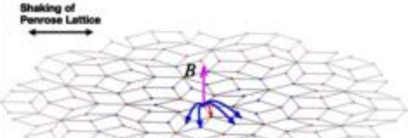
<td>
</td>
</tr>
<tr>
<td>Haldane Model
$H_\lambda = \sum_{\langle j,k\rangle} e^{i\varphi_{jk}} |j\rangle\langle k| + \sum_{\langle\langle j,k\rangle\rangle} \lambda e^{i\varphi_{jk}} |j\rangle\langle k|$</td>
<td>Vibration of Lattice

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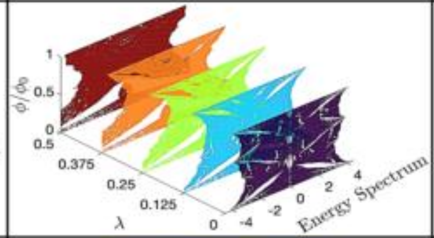
<td>
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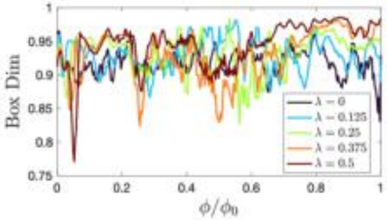
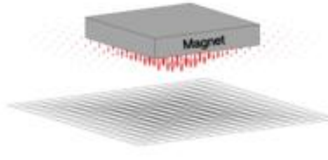
<td>
</td>
</tr>
<tr>
<td>Inhomogeneous Magnetic Field
$H = \sum_{\langle j,k\rangle} e^{i\theta_{jk}} |j\rangle\langle k|$</td>
<td>Gaussian Magnetic Field

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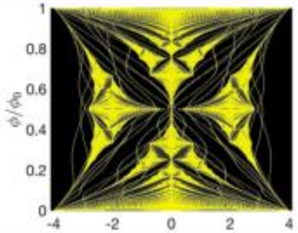
<td>
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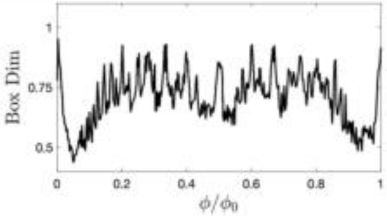
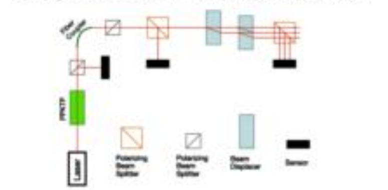
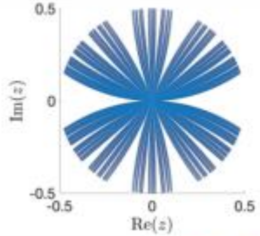
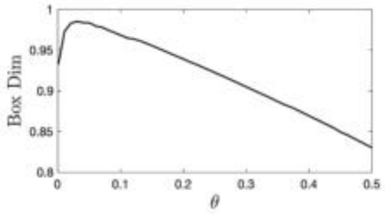
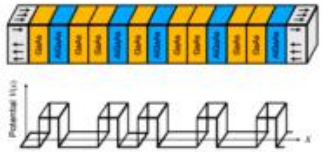
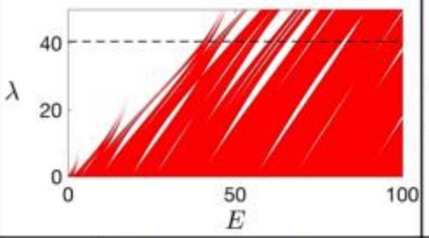
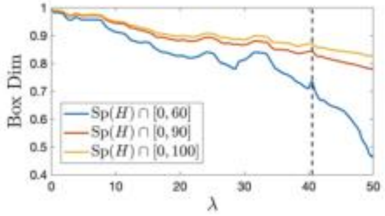
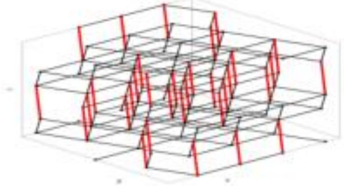
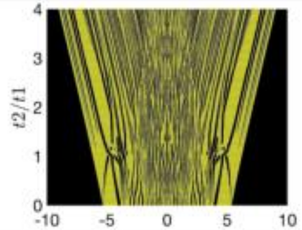
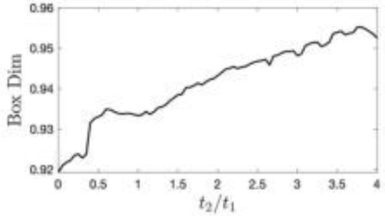
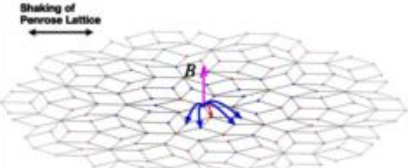
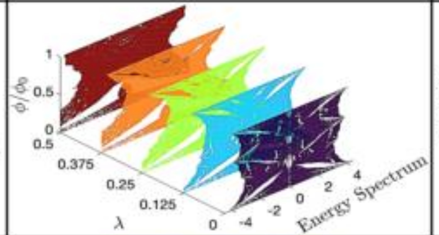
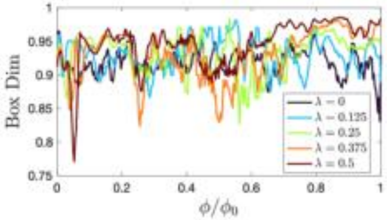
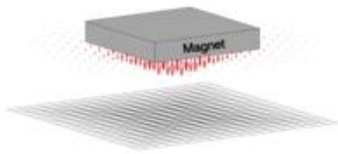
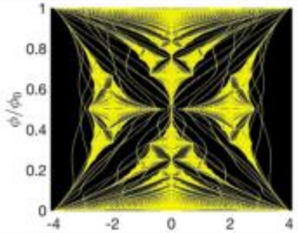
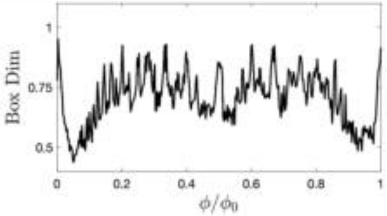
<td>
</td>
</tr>
</table>

- Chok, C., Embree, Fillman, "*Cantor-Set Physics in Quasicrystals: Fractal Spectra and Transport Without Contamination*," **under review at Phys. Rev. Lett.**

Operator	Application	Spectrum	Box Dim
Unitary Fibonacci $\lvert n,\uparrow\rangle \mapsto C^{11}_{\omega_n}\lvert n+1,\uparrow\rangle + C^{21}_{\omega_n}\lvert n-1,\downarrow\rangle$ $\lvert n,\downarrow\rangle \mapsto C^{12}_{\omega_n}\lvert n+1,\uparrow\rangle + C^{22}_{\omega_n}\lvert n-1,\downarrow\rangle$	Single-Photon Quantum Walks 		
Continuum Quasicrystal (Kronig—Penney Models) $H_{\omega,\lambda} = -\frac{d^2}{dx^2} + \lambda \sum_{n\geq 0} \omega_n 1_{x\in[n,n+1)}$	Superlattice of Semiconductors 		
Three-Dimensional Quasicrystals $H = \sum_{\langle j,k\rangle} t_{jk}\left(\lvert j\rangle\langle k\rvert + \lvert k\rangle\langle j\rvert\right)$	Acoustic Metamaterial 		
Haldane Model $H_\lambda = \sum_{\langle j,k\rangle} e^{i\varphi_{jk}}\lvert j\rangle\langle k\rvert + \sum_{\langle\langle j,k\rangle\rangle} \lambda e^{i\varphi_{jk}}\lvert j\rangle\langle k\rvert$	Vibration of Lattice 		
Inhomogeneous Magnetic Field $H = \sum_{\langle j,k\rangle} e^{i\theta_{jk}}\lvert j\rangle\langle k\rvert$	Gaussian Magnetic Field 		

James Chok
- On the postdoc market!

- Chok, C., Embree, Fillman, "*Cantor-Set Physics in Quasicrystals: Fractal Spectra and Transport Without Contamination*," **under review at Phys. Rev. Lett.**

Shameless final plug...

Upcoming book with CUP:

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Matthew J. Colbrook

100s of: classifications, algorithms, examples (webpage: full code), figures, exercises (webpage: full solutions).

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Foundations, Algorit

Applica

Matthew J.

Connections with harmonic analysis. Main tool is computing $(A, z, u) \mapsto (A - zI)^{-1}u$ Lower bounds through things like Anderson localization.

100s of: classifications

examples (webpage: full code), figures, exercises (webpage: full solutions).

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Foundations, Algorithms, and Modern

Main tool is essential injection moduli (Edmunds & Evans 1987):

$$\tau_{\inf}(A) = \inf\left\{\liminf_{n\to\infty}\|Ax_n\| : x_n \in \mathcal{D}(A), \|x_n\| = 1, x_n \xrightarrow{w} 0\right\}$$

Typically incurs and extra limit. $W_e(A)$ *is universally* Π_2

100s of: classifications, algorithms, examples (webpage: full code), figures, exercises (webpage: full solutions).

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Injection moduli for $T(z)$. Contour methods for discrete spectra of holomorphic familes.

100s of: classifications, algorithms, examples (webpage: full code), figures, exercises (webpage: full solutions).

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Contents

Conclusion: FOUNDATIONS $\longleftrightarrow$ METHODS

- $\exists$ interesting mathematical structure in inf.-dim. spectral computations.
- Many spectral problems in inf. dim. are impossible. *Some harder than others.*
- ***SCI hierarchy*** is a tool for discovering the foundations of computation.

  Lower bounds $\Longrightarrow$ spot assumptions needed to lower SCI.

  Upper bounds $\Longrightarrow$ new "inf.-dim." algorithms. <u>*Rigorous, optimal, practical.*</u>
- $\Sigma_1 \cup \Pi_1 \Longrightarrow$ computer-assisted proofs

Could this framework be useful in your area?

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