A New Class of Algorithms for Computing Spectra with **Error Control**

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Background

- Hilbert space $l^2(\mathbb{N})$ with $\|x\|_2 = \sqrt{\sum_{j=1}^{\infty} |x_j|^2}$, $\langle x, y \rangle = \sum_{j=1}^{\infty} x_j \bar{y}_j$
- Bounded linear operator $A : l^2(\mathbb{N}) \to l^2(\mathbb{N})$ realised as matrix

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

  Denote these by $\mathcal{B}(l^2(\mathbb{N}))$.
- Want to compute spectrum (generalistion of eigenvalues)

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

  from the matrix elements.

Motivation

- Quantum mechanics, quasicrystals

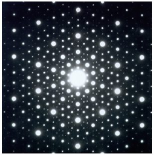

Figure: Left: Dan Shechtman, Nobel Prize in Chemistry 2011. Right: Electron diffraction pattern of quasicrystal.

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

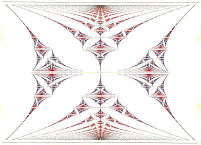

Figure: Left: Artur Avila, Fields Medal 2014. Right: Hofstadter butterfly.

Our computational problem

- Convergence in $\mathcal{M}$, set of all compact subsets of $\mathbb{C}$ provided with the Hausdorff metric $d = d_{\mathrm{H}}$

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

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4. Error control?

Hierarchy of complexity

Definition 1 (Tower of Algorithms)

A *tower of algorithms of height k* is a family of sequences of functions

$$\Gamma_{n_k,\ldots,n_1} : \Omega \to \mathcal{M},$$

where $n_k, \ldots, n_1 \in \mathbb{N}$ and $\Gamma_{n_k,\ldots,n_1}$ are "algorithms". Moreover,

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

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Definition 2 (Solvability Complexity Index (SCI))

Solvability Complexity Index, $\mathrm{SCI}(\mathrm{Sp}, \Omega)$ is the smallest integer k for which there exists a tower of algorithms of height k. If no such tower exists then $\mathrm{SCI}(\mathrm{Sp}, \Omega) = \infty$.

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Solution: restrict to smaller subclass. Large subclass $\Omega \subset \mathcal{B}(l^2(\mathbb{N}))$ with $\mathrm{SCI}(\mathrm{Sp}, \Omega) = 1$. What's more can gain error control, an algorithm such that

$$z \in \Gamma_n(A) \Rightarrow \mathrm{dist}(z, \mathrm{Sp}(A)) < 2^{-n}.$$

Call this class Σ_1 - "output is reliable".

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Some notation:

- If $z \notin \mathrm{Sp}(A)$ write

$$R(z, A) := (A - zI)^{-1} \in \mathcal{B}(l^2(\mathbb{N})).$$

- Operator norm: $\|A\| := \sup_{x:\|x\|=1} \|Ax\|$.

Main Result

Theorem 3

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Corollary 4

Let G *be a countable, locally finite, connected graph and* Ω_G *be class of finite range interaction Hamiltonians on vertices of* G*.*

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Application: Laplacian on Quasi-crystals

G a graph, V set of vertices. $x \sim y$ if sites x, y connected by edge. Laplacian H_0 acts on $\psi \in l^2(V) \cong l^2(\mathbb{N})$ by

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- Calculating the spectrum currently an open problem in the quasicrystal community - 2D cases very hard!
- Vast physics literature on Hamiltonians on aperiodic structures.

Applications of Quasicrystals

- Reinforce steel via coating - e.g. machinery, surgical instruments...
- Heat insulation
- LEDs
- Solar absorbers
- Unique electrical properties, optical properties, hardness and nonstick properties...

Constructing Penrose Tile

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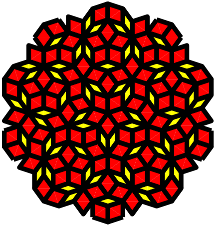

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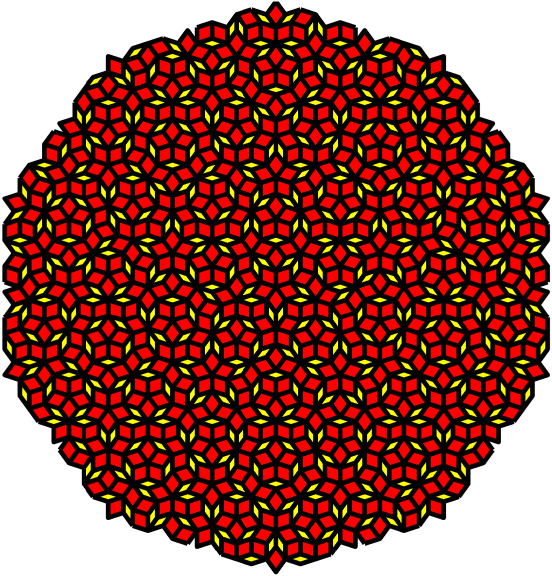

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1. Finite section with open boundary conditions: compute eigenvalues of **truncated matrix** $P_n H_0 P_n$ for large n. Similar "Galerkin" methods - suffer from spectral pollution.

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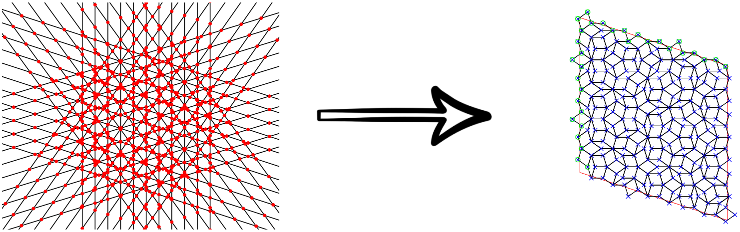

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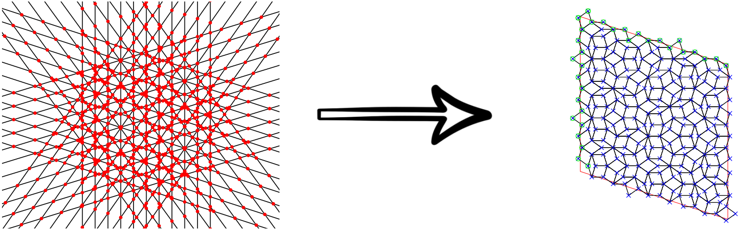
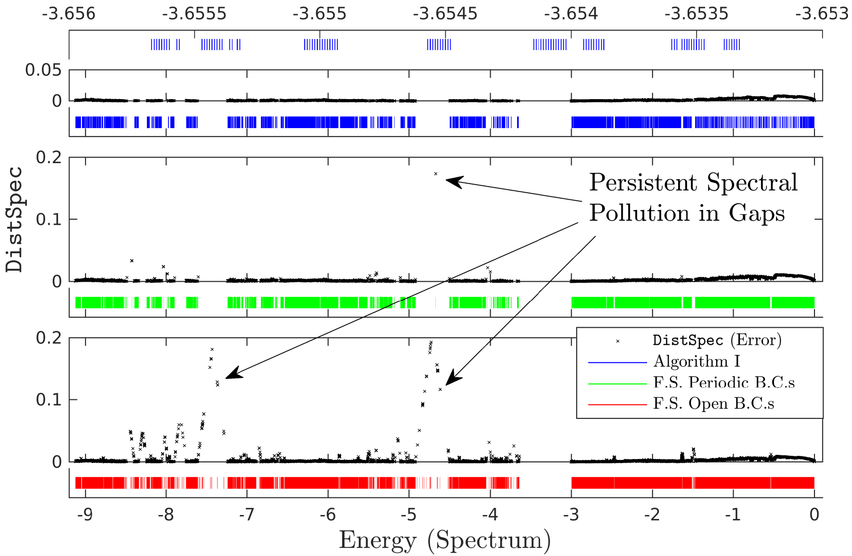


These represent state of art in literature. Can we beat this?

Numerical Results



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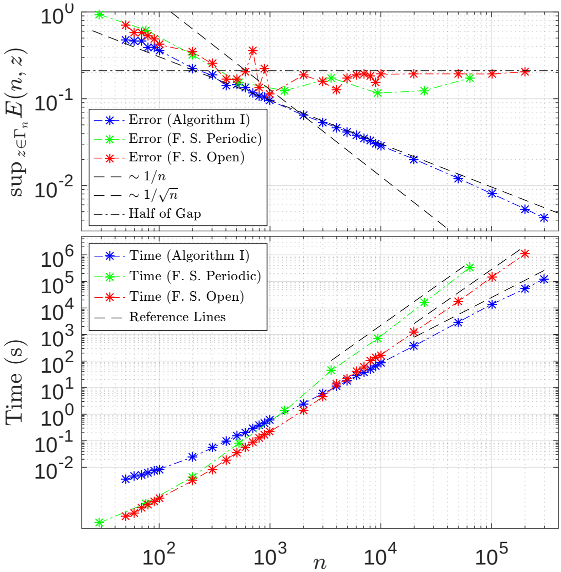
First algorithm that realises the sharp Σ_1 classification - logically impossible to do better.

Error and Speed Results



Thanks for Listening!