Diagonalising the infinite:
How to compute spectra with error control

With a case study on quasicrystals

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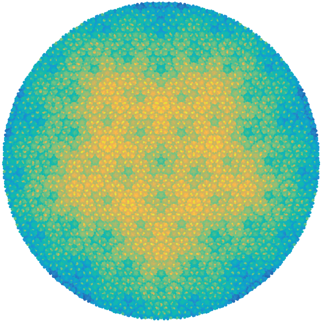
IMA Lighthill-Thwaites Session



Paper:
M.J. Colbrook, B. Roman, and A.C. Hansen
"How to compute spectra with error control"
Physical Review Letters 122.25 (2019)

The infinite-dimensional spectral problem

In many applications, we are given an operator acting on $\ell^2(\mathbb{N})$ ($\ell^2(\mathbb{N})$ = canonical inner product space in infinite dimensions):

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots \\ a_{21} & a_{22} & a_{23} & \dots \\ a_{31} & a_{32} & a_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad \left[A \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \end{pmatrix} \right]_j = \sum_{k \in \mathbb{N}} a_{jk} x_k.$$

Finite Case	$\Rightarrow$	Infinite Case
Eigenvalues	$\Rightarrow$	Spectrum, $\mathrm{Sp}(A)$
$\{z \in \mathbb{C} : \det(A - zI) = 0\}$	$\Rightarrow$	$\{z \in \mathbb{C} : A - zI \text{ not invertible}\}$

GOAL: compute spectrum of A from matrix elements

Many applications: quantum mechanics, chemistry, matter physics, stat. mechanics, optics, number theory, PDEs, math. of info., **quasicrystals**,...

MUCH harder and more subtle than finite dimensions!

London Millennium Bridge:
When computing spectra goes badly wrong!

- Opened on 10 June 2000.
- Spectra correspond to vibrations or “resonances” of bridge.
- Unexpected resonances caused bridge closure on 12 June.
- Closed for two years and cost several million pounds to fix.

Things that typically go wrong

Fundamental challenges:

- Miss parts of the spectrum.
- Approximate false $z \notin \mathrm{Sp}(A)$ - "spectral pollution".

Open problem (even for Schrödinger operators) for > 50 years:
Can we overcome these issues in the general case?

"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 to compute the spectra of infinite dimensional operators. 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 techniques."

W. Arveson, Berkeley (1994)

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- How do we know what part of approximation to trust?
- Methods can be inefficient and slow to converge.

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- Converges without missing parts of spectrum. ✓

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- Converges without missing parts of spectrum. ✓
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- Provides error control (guaranteed certificate of accuracy)
  $\Rightarrow$ computations reliable and useful in applications. ✓

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- Provides error control (guaranteed certificate of accuracy)
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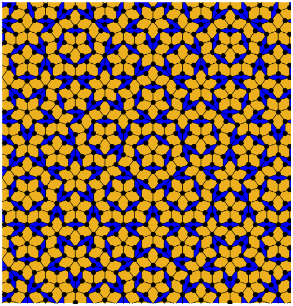
- Computationally efficient. ✓

Case study: Quasicrystals

Quasicrystals: aperiodic structures with long-range order.

Left: D. Shechtman, **Nobel Prize in Chem. 2011** for discovering quasicrystals.
Right: Penrose tile, canonical model used in physics.

Vertex model: site at each vertex and bonds along edges of tiles.

Case study: Quasicrystals

Motivation:

- We understand periodic systems really well but not aperiodic.
- Long range order & short range disorder everywhere in nature.
- What's the analogy of periodic physics for aperiodic systems?
- Many exotic physical properties and beginning to be used in
  - heat insulation
  - LEDs, solar absorbers, and energy coatings
  - reinforcing materials, e.g. low-friction gears
  - bone repair (hardness, low friction, corrosion resistance)...
- Understanding spectral properties key for physical insight.

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BUT: Aperiodic nature of quasicrystals has made it a considerable challenge to approximate spectrum of full infinite-dimensional operator!

Case study: Quasicrystals

Model 1: Perpendicular magnetic field (of strength B).

$$\left[A \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \end{pmatrix} \right]_j = -\sum_{j \sim k} e^{\mathrm{i}\theta_{jk}(B)} x_k ,$$

Model 2: Graph Laplacian (electronic/vibrational properties)

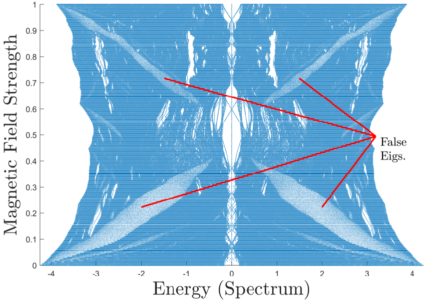
$$\left[A \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \end{pmatrix} \right]_j = \sum_{j \sim k} (x_k - x_j) ,$$

Very hard problems - no previous method even converges to spectrum.

Model 1: Magnetic field

Finite truncations

Spectral pollution.



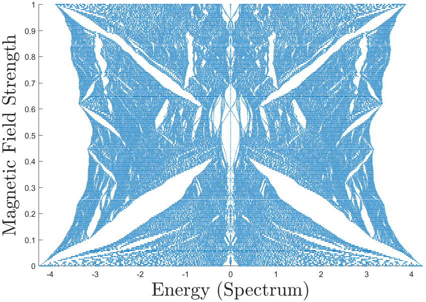
Unreliable

Does not converge

No error control

New method

First convergent computation.

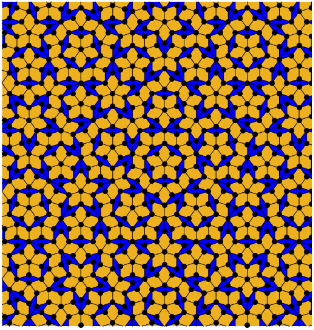


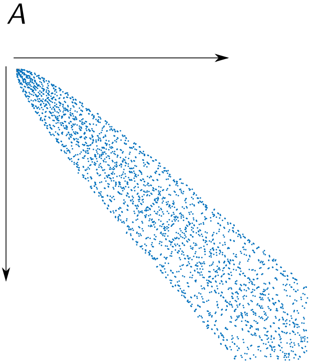
Reliable

Converges

Error control

Idea: Rectangular truncations





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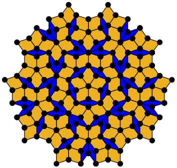
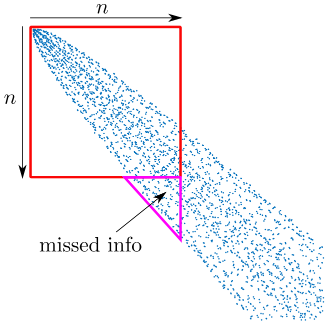


$P_n A P_n$



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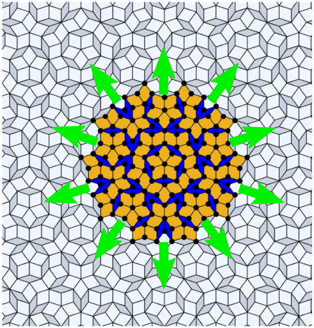
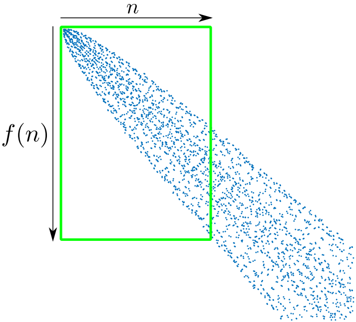


$P_{f(n)}AP_n$



Locally compute distance function and minimisers

Rectangular truncation $P_{f(n)}(A - zI)P_n$

$\Downarrow$ smallest singular values $\sigma_1(P_{f(n)}(A - zI)P_n)$

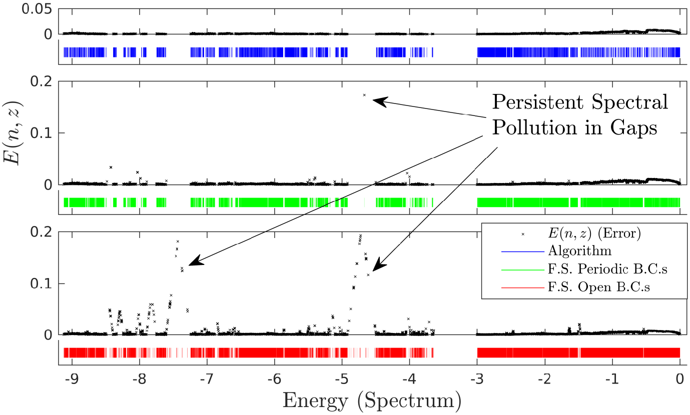
Approximate distance function $\mathrm{dist}(z, \mathrm{Sp}(A))$

$\Downarrow$ local minimisers

Output $\Gamma_n(A) \to \mathrm{Sp}(A)$ and error bound $\sup_{z\in\Gamma_n(A)} E(n, z) \to 0$

Provably **OPTIMAL**: no algorithm or method can do better.

Model 2: Graph Laplacian (electronic properties)



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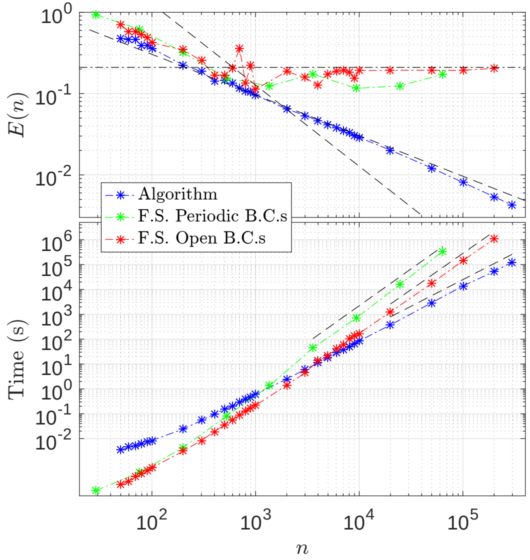


Advantages

- First method that always converges to correct solution.
  (e.g. no spectral pollution)
- Local and parallelisable $\Rightarrow$ FAST!
- Explicitly bounds the error:

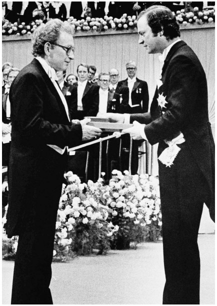
$$\text{Error} \leq E_n \downarrow 0.$$

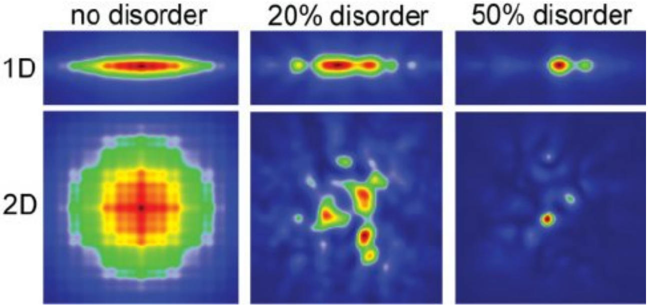
- Can prove it is OPTIMAL (see paper).
- Rigorously compute approximate states...

Made the frontcover of ***Physical Review Letters***
- American Physical Society's flagship publication

Background

Periodic systems have extended states (not localised), but add disorder...





Left: P. Anderson, **Nobel Prize in Phys. 1977** for discovering Anderson localisation. Right: Examples in 1D and 2D photonic lattices.

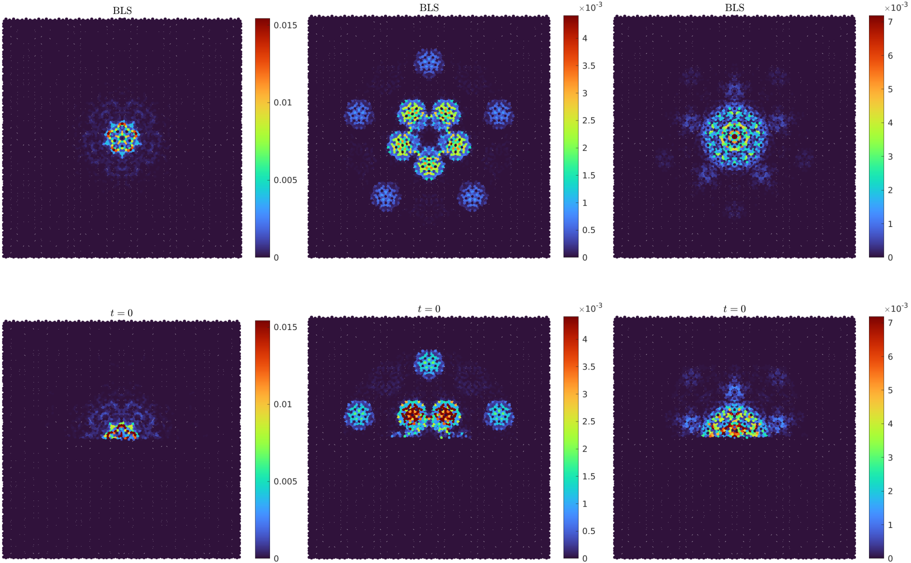
What happens in aperiodic systems? Do we need disorder?

Bulk Localised States: A new state for quasicrystals

- **Bulk Localised States (BLSs):** New states for magnetic quasicrystals
  - localised
  - "in-gap" (confirmed via comp. of inf-dim (topological) Chern numbers)
  - support transport
- **Cause (also confirmed with toy models):** Interplay of magnetic field with incommensurate areas of building blocks of quasicrystal.
- Not due to an internal edge, impurity or defect in the system.

$\rightsquigarrow$ NEW EXCITING PHYSICS!

Transport: **Error control** allows us to be **certain** of this phenomenon.



Conclusion

- Can now compute spectra of large class of operators.
- Computation has explicit error control.
- New method does not suffer from spectral pollution.
- New algorithm is fast, local and parallelisable.
- Extensions: non-Hermitian operators, general infinite matrices, PDEs, etc.
- New type of Bulk Localised State (BLS) for magnetic quasicrystals that support localised transport within the bulk.

Future/ongoing work:

- What other spectral problems can be computed in infinite dimensions?
- Further applications in quantum mechanics.
- Further study of BLSs.

Contents of extra slides

- Extension to PDEs.
- Extension to non-Hermitian operators.
- BLSs without rotational symmetry.
- Chern number.
- Program on infinite-dimensional spectral problems.
- Fractal dimensions.
- Naive approximations for quasicrystals (e.g. periodic approximations)

Extensions to PDEs

Closed operator L on $\mathbb{R}^d$ of form

$$Lu(x) = \sum_{k \in \mathbb{Z}^d_{\geq 0} : |k| \leq N} a_k(x) \partial^k u(x)$$

Assume coefficient functions:

- polynomially bounded
- of bounded total variation on compact balls

($+$ some standard technical assumptions)

$\Rightarrow$ Compute $\mathrm{Sp}(L)$ locally uniformly on compact subsets with error control

NB: Open problem since Schwinger's work in the 1960s to do this for general Schrödinger operators (even without error control)

Executive summary

- Build matrix rep. w.r.t. basis of tensorised Hermite functions.
- Use bound on total variation and quasi-Monte Carlo integration to compute matrix entries of L, L^*L and LL^* with error control.
- Use these estimates to directly approximate $\mathrm{dist}(z, \mathrm{Sp}(L))$.
- Apply (roughly) the same algorithm as before.

NB: Can extend technique to other discretisation methods such as FEM.

Example: Eigenvalues with guaranteed error bounds

$$L = -\Delta + x^2 + V(x) \text{ on } L^2(\mathbb{R})$$

V	$\cos(x)$	$\tanh(x)$	$\exp(-x^2)$	$(1+x^2)^{-1}$
E_0	1.7561051579	0.8703478514	1.6882809272	1.7468178026
E_1	3.3447026910	2.9666370800	3.3395578680	3.4757613534
E_2	5.0606547136	4.9825969775	5.2703748823	5.4115076464
E_3	6.8649969390	6.9898951678	7.2225903394	7.3503220313
E_4	8.7353069954	8.9931317537	9.1953373991	9.3168983920

Extension to non-Hermitian operators

Definition (Known off-diagonal decay)

Dispersion of A bounded by function $f : \mathbb{N} \to \mathbb{N}$ and null sequence $\{c_n\}$ if

$$\max\{\|(I - P_{f(n)})AP_n\|, \|P_n A(I - P_{f(n)})\|\} \leq c_n.$$

Definition (Well-conditioned)

Continuous increasing function $g : [0, \infty) \to [0, \infty)$ with $g(x) \leq x$.
Controlled growth of the resolvent by g if

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

- Measures conditioning of the problem through

$$\{z \in \mathbb{C} : \|(A - z)^{-1}\|^{-1} \leq \epsilon\} =: \mathrm{Sp}_\epsilon(A) = \bigcup_{\|B\| \leq \epsilon} \mathrm{Sp}(A + B).$$

- Normal operators (A commutes with A^*) well-conditioned with

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

Idea II: Locally compute distance function and minimisers

Step 1: Smallest singular value of **rectangular** truncations:

$$\gamma_n(z) := \min\{\sigma_1(P_{f(n)}(A-z)P_n), \sigma_1(P_{f(n)}(A^*-\bar{z})P_n)\}.$$

This converges locally uniformly down to $\|(A-z)^{-1}\|^{-1}$.

Step 2: Bound the distance to the spectrum:

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

For Hermitian operators: take $g(z) = z$.

Step 3: Find 'local minimisers' and output $\Gamma_n(A)$ with

$$\Gamma_n(A) \to \mathrm{Sp}(A), \quad \mathrm{dist}(z, \mathrm{Sp}(A)) \leq \underbrace{g^{-1}(\gamma_n(z))}_{E(n,z)\text{ (error bound)}}, \quad \sup_{z\in\Gamma_n(A)} E(n,z) \to 0$$

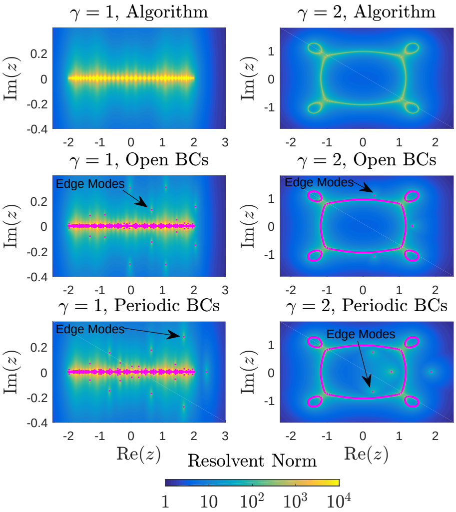
Example: PT symmetry (non-Hermitian QM)

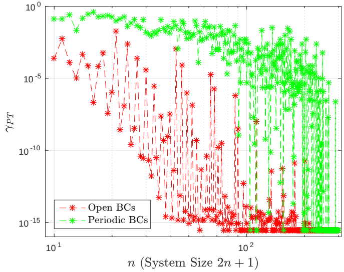
- PT symmetry: invariance w.r.t. simultaneous action of parity-inversion and time reversal.
- Operators with unbroken PT symmetry may poses real spectra, unitary time evolution etc.

$$[Ax]_n = x_{n-1} + x_{n+1} + (\cos(n) + \mathrm{i}\gamma \sin(n)), \quad n \in \mathbb{Z}$$

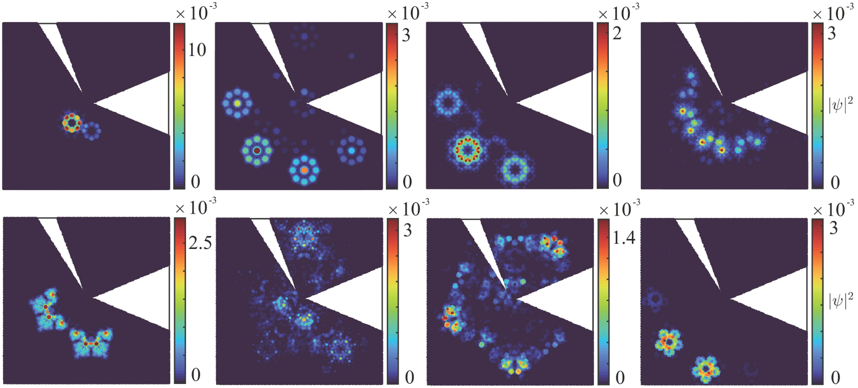
- Increase γ to get complex spectrum.
- Phase transition depends on boundary conditions.
- Rigorously compute this at $\gamma_{PT} \approx 1$.

Example: PT symmetry (non-Hermitian QM)





BLS for symmetry broken tilings



PhD Program: Foundations of Infinite-Dimensional Spectral Computations

How: Deal with operators directly, instead of previous 'truncate-then-solve'

$\Rightarrow$ Compute many spectral properties for the first time.

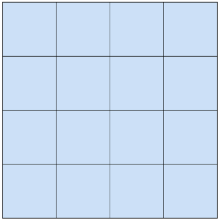
Framework: Classify problems in a computational hierarchy measuring their intrinsic difficulty and the optimality of algorithms.[1]

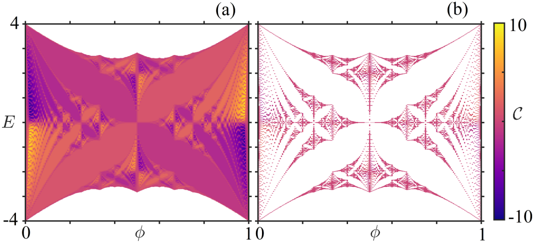
$\Rightarrow$ Algorithms that realise the boundaries of what computers can achieve.

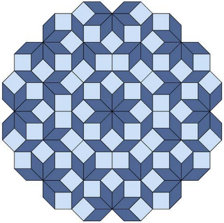
Also have foundations for: spectral type (pure point, absolutely continuous, singularly continuous), Lebesgue measure and fractal dimensions of spectra, discrete spectra, essential spectra, eigenvectors + multiplicity, spectral radii, essential numerical ranges, geometric features of spectra (e.g. capacity), spectral gap problem, spectral measures, ...

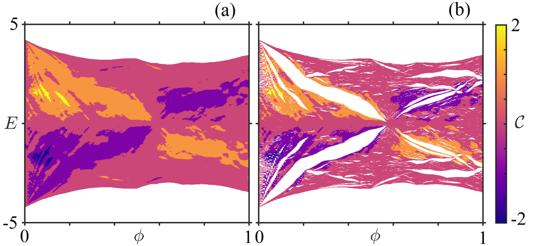
[1]Holds regardless of model of computation (Turing, analog,...).

Chern numbers

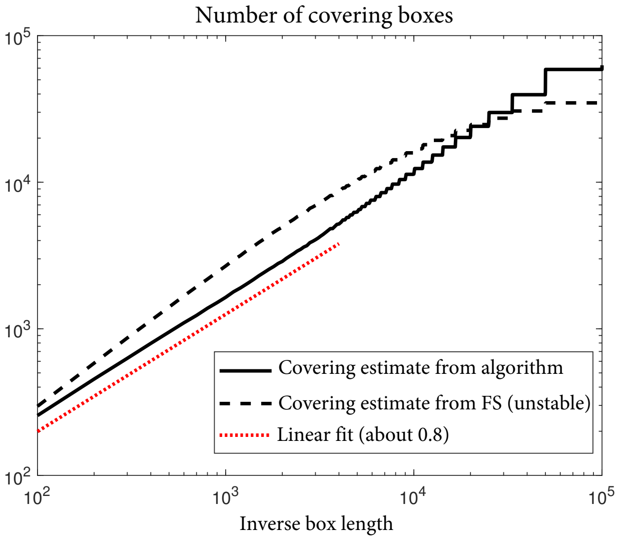






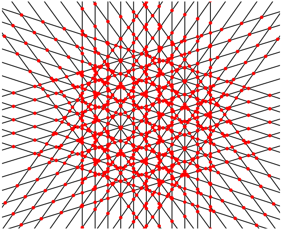


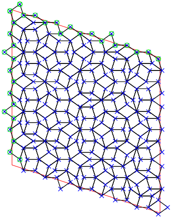
Fractal dimension of spectrum (Model 1)



Naive Approximations

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



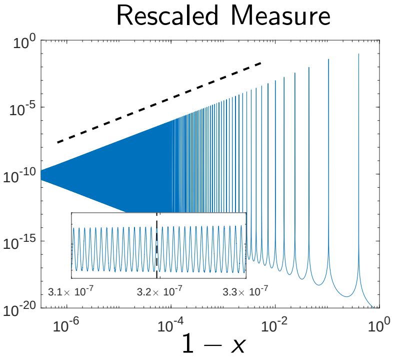


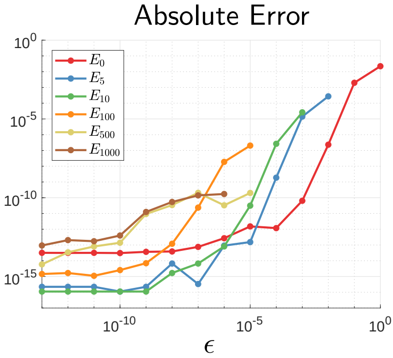
Eigenvalue hunting without spectral pollution

Example: Dirac operator.

- Describes the motion of a relativistic spin-1/2 particle.
- Essential spectrum given by $\mathbb{R} \backslash (-1, 1) \Rightarrow$ spectral pollution!
- Consider radially symmetric potential...

Eigenvalue hunting without spectral pollution





NB: Previous state-of-the-art achieves a few digits for a few excited states.