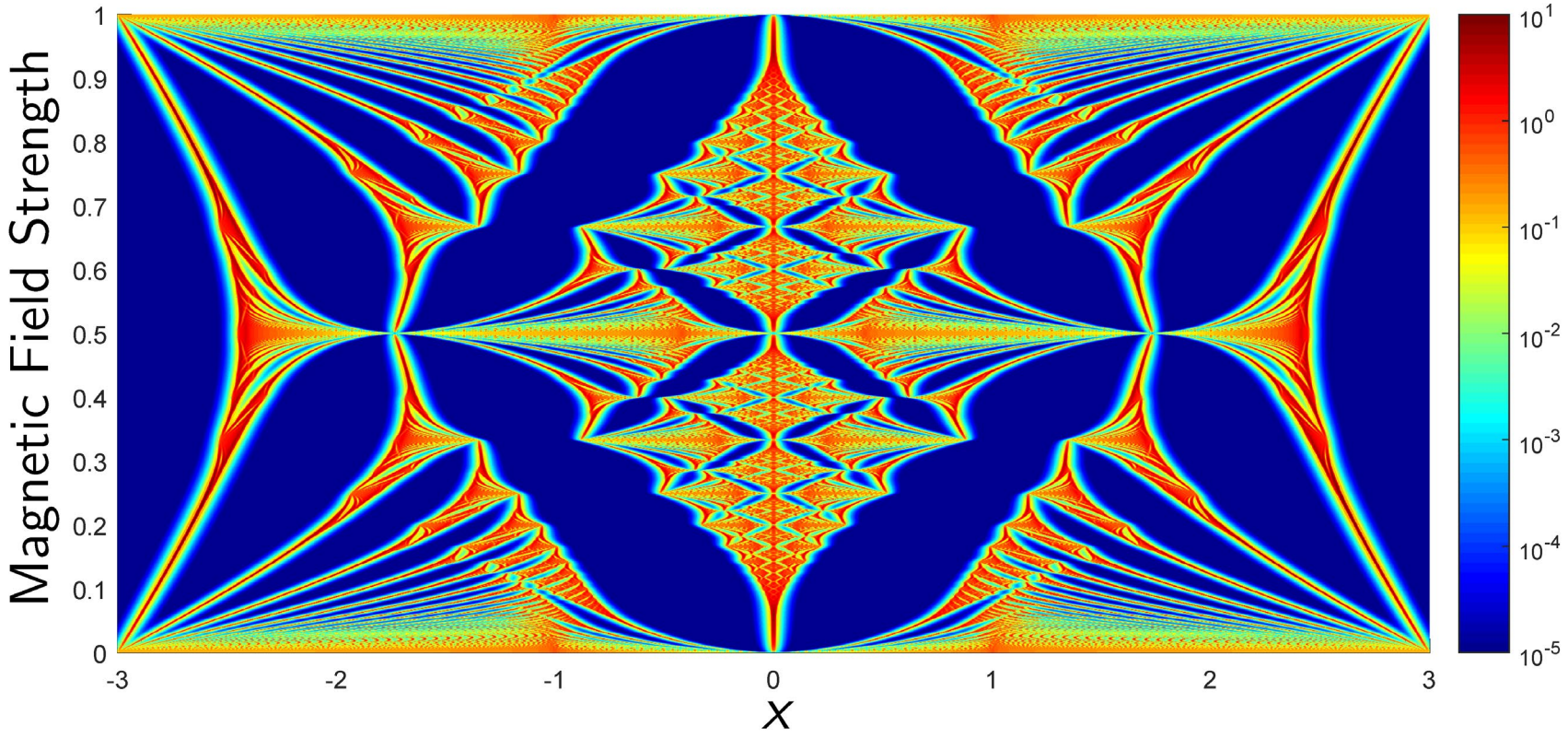
How to compute spectral properties of operators on Hilbert spaces with error control

Matthew Colbrook, DAMTP



Spectral measure of magnetic graphene, computed to high precision (see log scale).

Collaborators

Computing spectra (1st part of this talk):

Anders Hansen

Cambridge

Bogdan Roman

Cambridge

Computing spectral measures (2nd part of this talk):

Alex Townsend

Cornell

Andrew Horning

Cornell

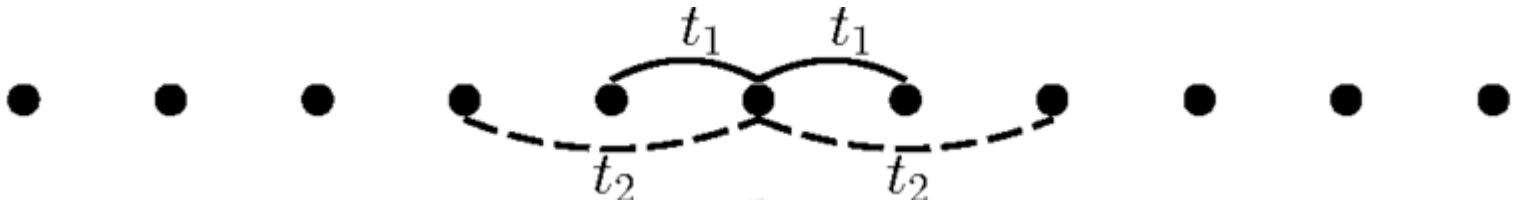
Infinite-dimensional operators: Example

Consider discrete Schrödinger operators acting on $l^2(\mathbb{Z})$

$$A = \begin{pmatrix} \ddots & \ddots & & & & \\ \ddots & v_{-1} & 1 & & & \\ & 1 & v_0 & 1 & & \\ & & 1 & v_1 & \ddots & \\ & & & \ddots & \ddots & \end{pmatrix}, \quad v_j \in \mathbb{R} \text{ for } j \in \mathbb{Z}.$$

Can we compute the spectrum for general potentials?

A rich problem in many areas of physics and (pure & applied) maths!



The infinite-dimensional problem

Finite Dimensions	**Infinite Dimensions**
Eigenvalues	Spectrum $\mathrm{Sp}(A) = \{z \in \mathbb{C} : A - z \text{ not invertible}\}$
Eigenvectors or states	Spectral Measure (includes states)

Goal: compute spectral properties of the operator from matrix elements

Can extend to PDEs (e.g. sample coefficients)

Much harder and more subtle than finite dimensions!

Computational Spectral Problem

Quantum mechanics and C^*algebras, structural mechanics, optics, acoustics, statistical physics, number theory, matter physics, analysis of PDEs, data analysis, neural networks and AI, nuclear scattering, computational chemistry…

Pretty much every area of physics and applied maths!

Physicists and mathematicians contributing to **computational spectral theory:**

D. Arnold (Minnesota), W. Arveson (Berkeley), A. Böttcher (Chemnitz), W. Dahmen (South Carolina), E. B. Davies (KCL), P. Deift (NYU), L. Demanet (MIT), C. Fefferman (Princeton), G. Golub (Stanford), A. Iserles (Cambridge), W. Schlag (Yale), E. Schrödinger (DIAS), J. Schwinger (Harvard), N. Trefethen (Oxford), V. Varadarajan (UCLA), S. Varadhan (NYU), J. von Neumann (IAS), M. Zworski (Berkeley),...

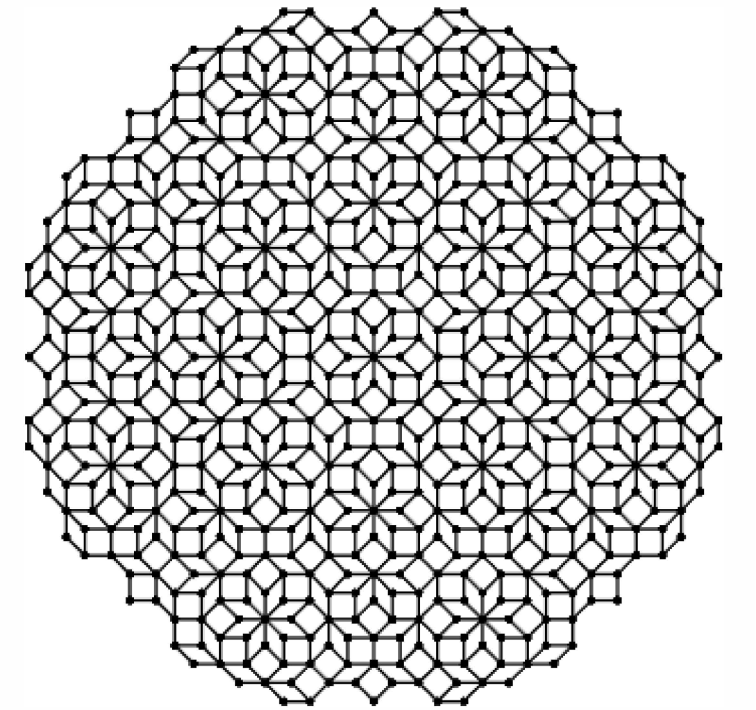
Extremely well studied for over 50 years by many “heavyweights”!

However, computing spectra is **notoriously** hard…

London Millennium Bridge: When computing spectra goes badly wrong!

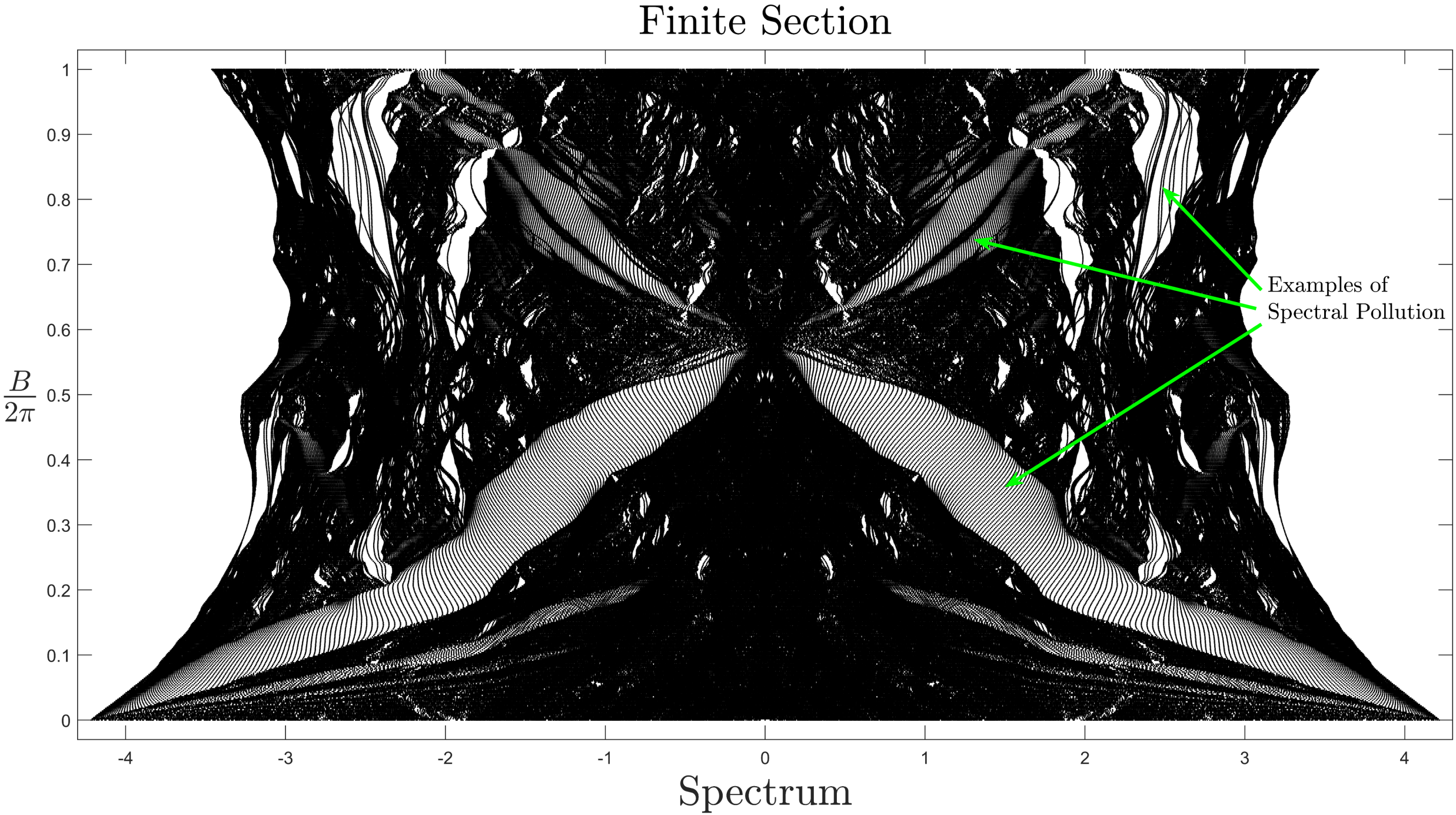
- Opened on **10 June** 2000.
- Spectra correspond to vibrations or “resonances” of bridge.
- Unexpected resonances caused bridge closure on **12 June**.
- Closed for **two years** and cost **several million pounds** to fix.

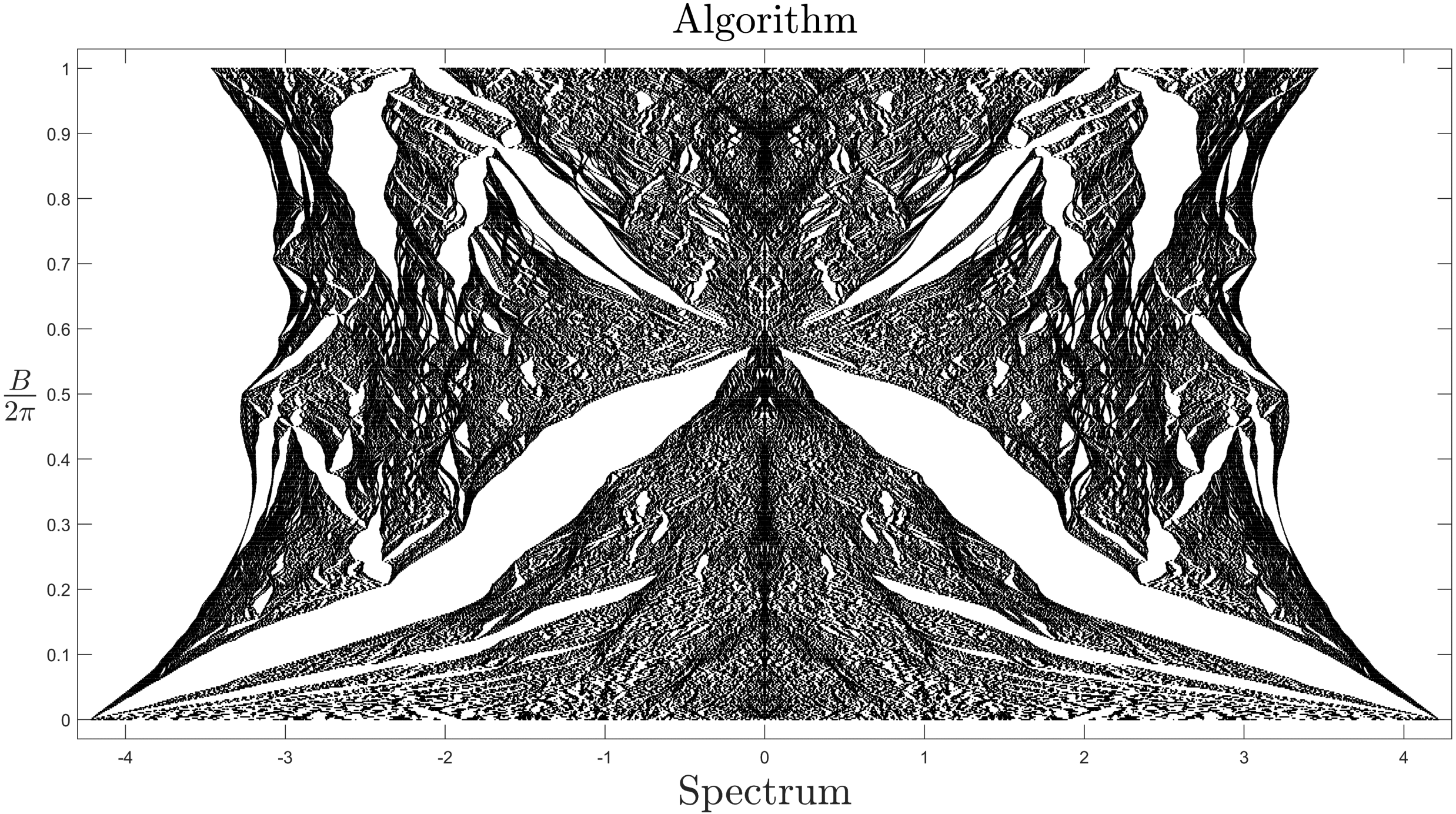
Quasicrystal example



Apply perpendicular magnetic field.

Hard problem - no previous method converges to spectrum.


Finite Section
$\frac{B}{2\pi}$
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-4
-3
-2
-1
0
1
2
3
4
Spectrum
Examples of
Spectral Pollution


Algorithm
$\frac{B}{2\pi}$
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-4
-3
-2
-1
0
1
2
3
4
Spectrum

Example I: Diagonal (very easy)

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

If $\Gamma_n(A) = \{a_1, \ldots, a_n\}$, then $\Gamma_n(A) \longrightarrow \mathrm{Sp}(A)$ in the Hausdorff metric.

Also have $\Gamma_n(A) \subseteq \mathrm{Sp}(A)$.

This is optimal from a foundations point of view.

Example II: Compact (still easy)

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

If $\Gamma_n(A) = \mathrm{Sp}(P_n A P_n)$, then $\Gamma_n(A) \longrightarrow \mathrm{Sp}(A)$ in the Hausdorff metric.

Known for decades.

BUT no error control possible (even for self-adjoint).

Example III: Jacobi (hard?!)

$$A = \begin{pmatrix} a_1 & b_1 & & \\ b_1 & a_2 & b_2 & \\ & b_2 & a_3 & \ddots \\ & & \ddots & \ddots \end{pmatrix}$$

This problem has been open for decades.

What about sparse normal operators? Surely this is even harder?!

Paradox

New result: Large class Ω (covering arguably most applications and including sparse normal) such that we can compute $\Gamma_n(A) \longrightarrow \mathrm{Sp}(A)$ and $\mathrm{E}_n(A) \downarrow 0$ for $A \in \Omega$

$$\mathrm{dist}\big(z, \mathrm{Sp}(A)\big) \leq \mathrm{E}_n(A), \text{ for all } z \in \Gamma_n(A).$$

Paradox: Easier problem than compact operators! Up to controllable error bound – as easy as diagonal operators.

Also for each $z \in \Gamma_n(A)$, compute approximate state $v_{n,z}$ with

$$\|v_{n,z}\| = 1, \qquad \|(A - z)v_{n,z}\| \leq \mathrm{E}_n(A)$$

What about Schrödinger operators?

Consider self-adjoint Schrödinger operators $-\nabla^2 + \mathrm{V}$ on $L^2(\mathbb{R}^d)$.
Can we compute spectra from sampling V?

NB: Open problem since Schwinger in1960s to do this for general case.

New result: If V has locally bounded total variation and grows at most polynomially at infinity then yes! And with error control as before.

Paradox: Easier problem than compact operators!

Can also be extended to many non-self-adjoint Schrödinger operators, singular potentials, more general partial differential operators etc.

New Algorithm (discrete case)

Consider matrix representation of general bounded operator

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots \\ a_{21} & a_{22} & a_{23} & \dots \\ a_{31} & a_{32} & a_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad (Ax)_j = \sum_{k \in \mathbb{N}} a_{jk} x_k.$$

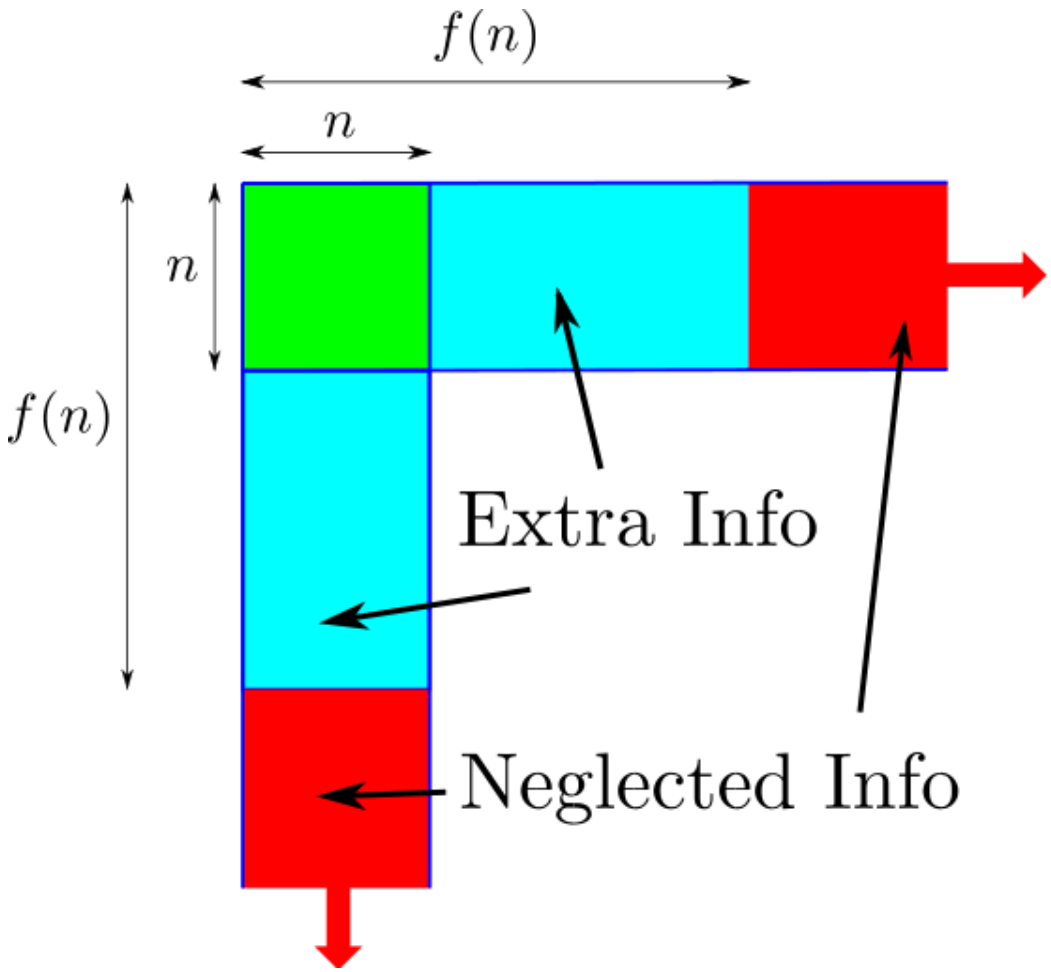
Dispersion bounded by $f : \mathbb{N} \to \mathbb{N}$ and null sequence $\{c_n\}$ if

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

What does this mean?

Rectangular truncations

- No need to apply boundary conditions
- Algorithm captures the correct interactions of the first n basis sites



Treats **infinite** dimensional operator directly via **finite** dimensional numerical linear algebra techniques!

Continuous increasing function $g : [0, \infty) \to [0, \infty)$ with $g(x) \leq x$.

Controlled growth of the resolvent by g if

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

Measures conditioning of the problem

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

Normal operators well-conditioned with

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

Theorem: Know f and g $\Rightarrow$ compute spectrum with error control!

Step 1: Approximate locally via smallest singular value:

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

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

Step 2: Bound the distance to the spectrum:

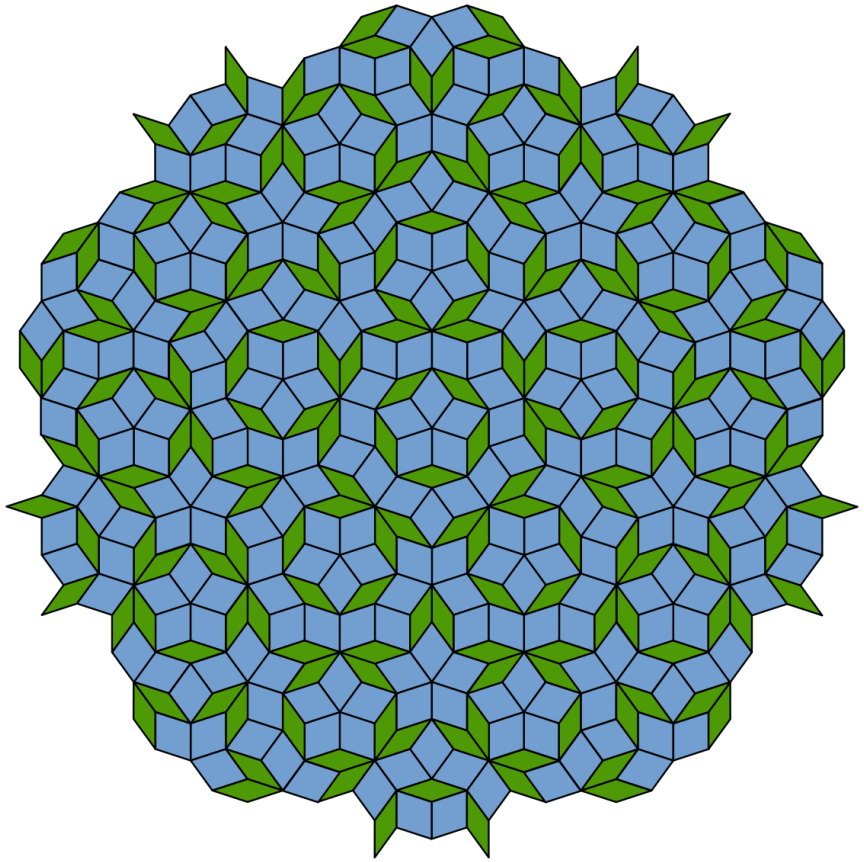
$$\gamma(z) \leq \mathrm{dist}(z, \mathrm{Sp}(A)) \leq g^{-1}(\gamma(z)) \leq g^{-1}(\gamma_n(z)).$$

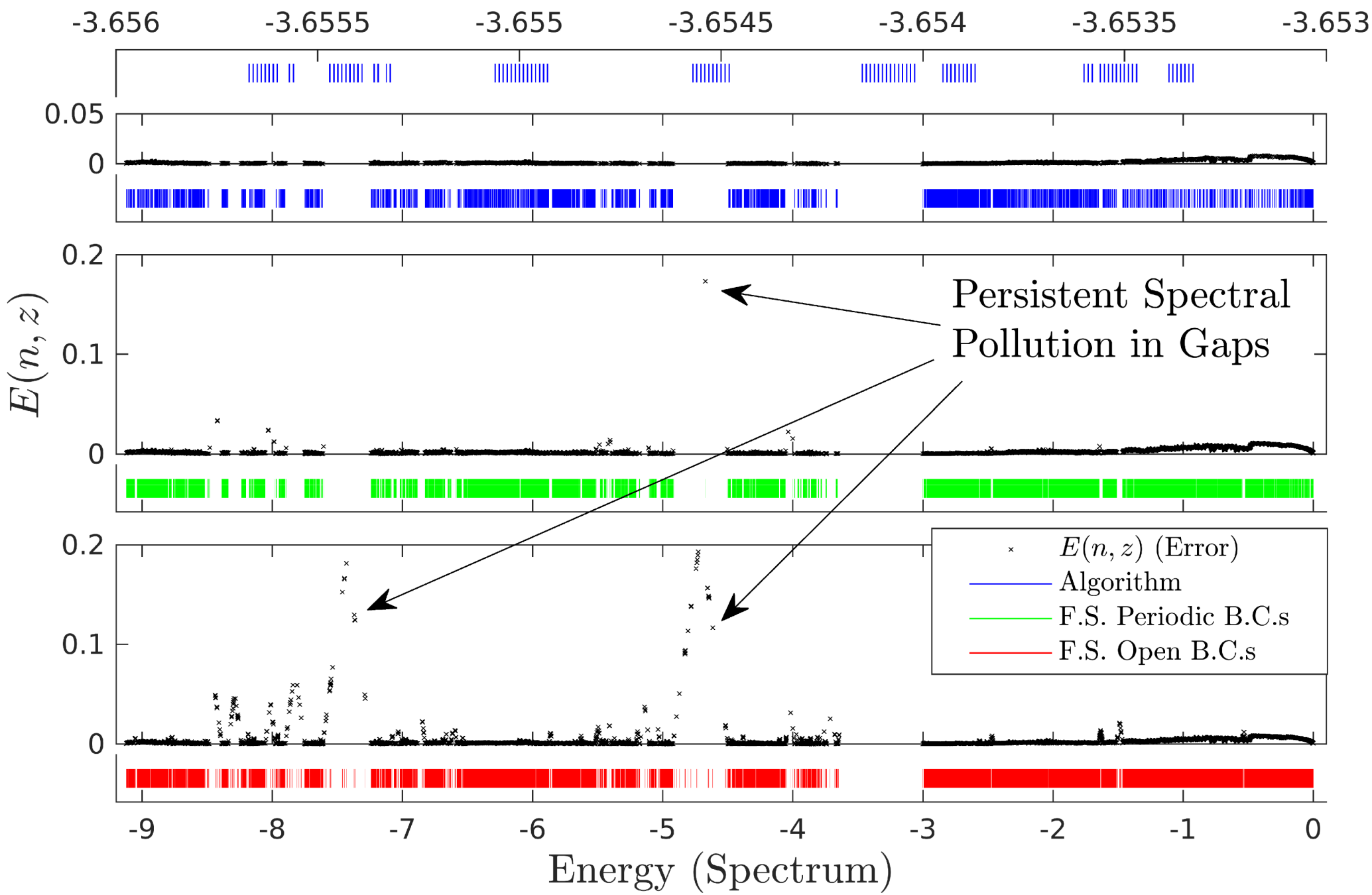
Step 3: Find (almost) local minimisers and output $\Gamma_n(A)$ with

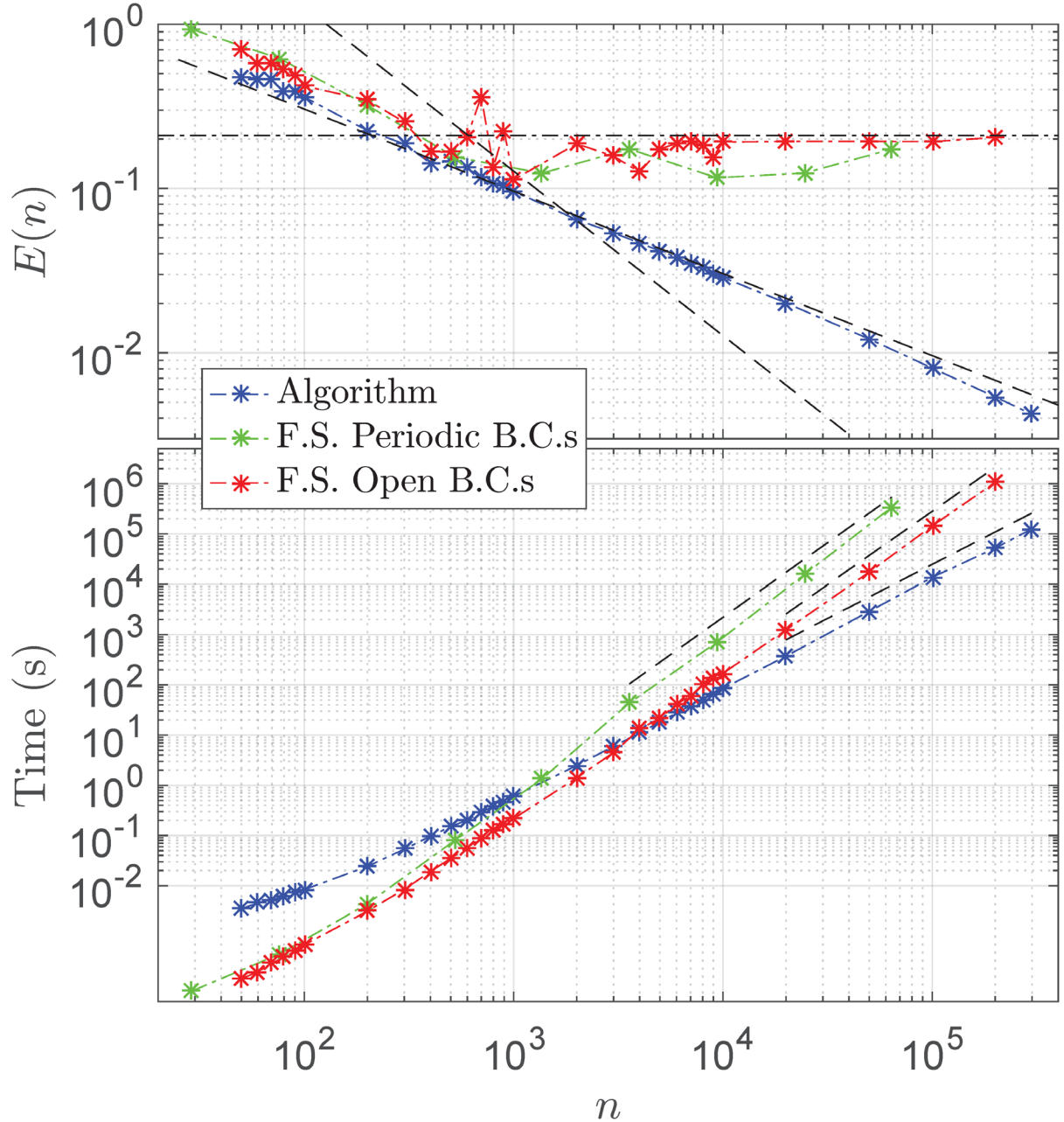
$$\Gamma_n(A) \to \mathrm{Sp}(A), \quad \mathrm{dist}(z, \mathrm{Sp}(A)) \leq g^{-1}(\gamma_n(z)), \quad \sup_{z \in \Gamma_n(A)} g^{-1}(\gamma_n(z)) \to 0$$

NB: Without either f or g, constructing an algorithm convergent to the spectrum is impossible (even dropping error control).

Example: Laplacian on Penrose tiling




-3.656
-3.6555
-3.655
-3.6545
-3.654
-3.6535
-3.653
0.05
0
0.2
0.1
0
$E(n,z)$
Persistent Spectral
Pollution in Gaps
0.2
0.1
0
$E(n,z)$ (Error)
Algorithm
F.S. Periodic B.C.s
F.S. Open B.C.s
-9
-8
-7
-6
-5
-4
-3
-2
-1
0
Energy (Spectrum)


10^0
10^{-1}
10^{-2}
$E(n)$
Algorithm
F.S. Periodic B.C.s
F.S. Open B.C.s
10^6
10^5
10^4
10^3
10^2
10^1
10^0
10^{-1}
10^{-2}
Time (s)
10^2
10^3
10^4
10^5
n

Example: $\mathcal{PT}$ symmetry breaking

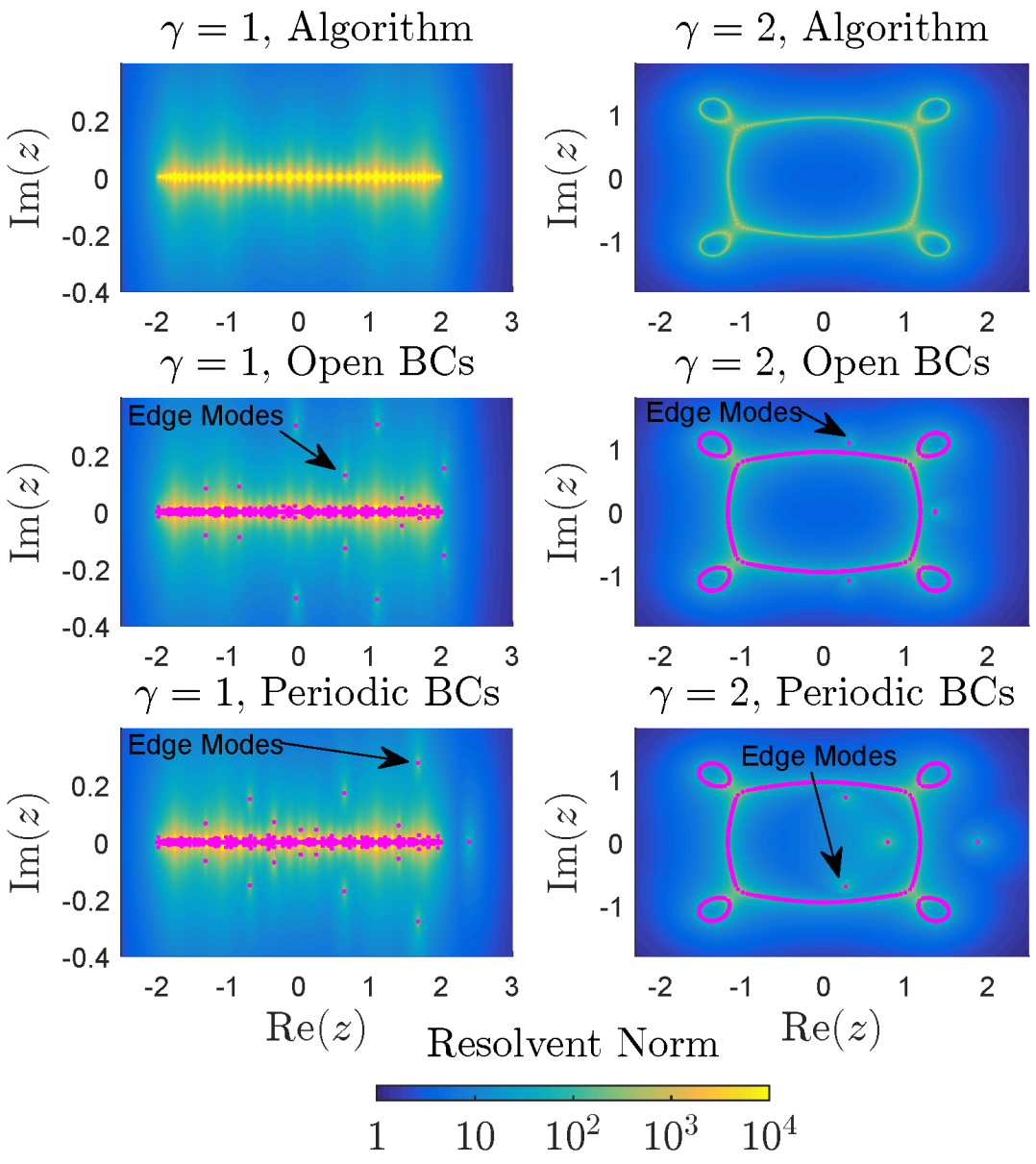
- Aperiodic Hamiltonian:

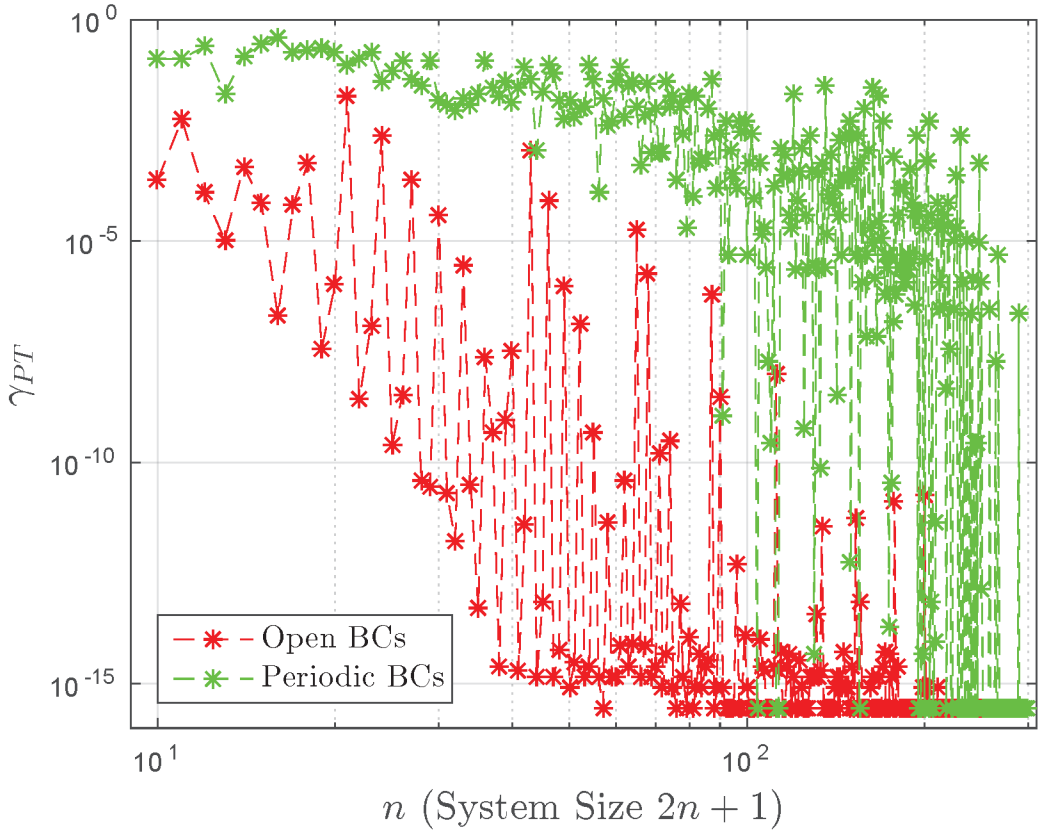
$$(Hx)_n = x_{n-1} + x_{n+1} + (\cos(n) + i\gamma\sin(n))\, x_n,\ n \in \mathbb{Z}$$

- Increase γ to get complex spectrum
- Phase transition depends on boundary conditions
- Rigorously compute phase transition ($\gamma_{PT} \approx 1$) and pseudospectrum:

$$\mathrm{Sp}_\varepsilon(H) = \{z \in \mathbb{C}: \|(H - z)^{-1}\| \geq \varepsilon^{-1}\} = \cup_{\|B\| \leq \varepsilon} \mathrm{Sp}(H + B)$$

- Algorithm computes this with error control (no g required)


$\gamma = 1$, Algorithm
$\gamma = 2$, Algorithm
$\gamma = 1$, Open BCs
$\gamma = 2$, Open BCs
$\gamma = 1$, Periodic BCs
$\gamma = 2$, Periodic BCs
Edge Modes
Im(z)
Re(z)
Resolvent Norm
1
10
10^2
10^3
10^4


γ_{PT}
Open BCs
Periodic BCs
n (System Size $2n+1$)

New exemplar of spectral computation?

Problems with previous methods (general case open >50 years):

- Spurious modes or false solutions
- Not detecting all of spectrum (bridge example)
- Dealing with unbounded domains
- Figuring out if we have converged yet (only have heuristics)

New method:

- Local and parallelisable.
- Convergent for first time.
- Faster than previous methods.
- Explicitly bounds the error of the output.
- Optimal (prove no method can do better).

Extends to unbounded operators and PDEs with coefficients of locally bounded total variation (e.g. point sample coefficients).

Made the front cover of ***Physical Review Letters***

Programme: The Foundations of Infinite-Dimensional Spectral Computations

- Deal with operators directly, instead of previous “truncate-then-solve”
- Classify problems in a computational hierarchy (the SCI hierarchy) measuring their intrinsic difficulty and the optimality of algorithms.*
- 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 spectrum (e.g. capacity), spectral gap problem, spectral measures, ...

*This holds regardless of model of computation (Turing, analog,…) – some nice links with descriptive set theory.

Spectral measures

Spectral measure

- "Diagonalise":

$$Ax = \int_{\mathrm{Sp}(A)} \lambda d\mathcal{E}(\lambda)x.$$

- Many applications have a continuous spectral component.
- **Crucial in:** quantum mechanics, scattering in particle physics, correlation in stochastic processes/signal-processing, fluid stability, resonances, density-of-states in materials science, orthogonal polynomials, random matrix theory, evolution PDEs,…
- **Problem:** current methods restricted to operators with lots of structure (typically small perturbations of trivial cases)

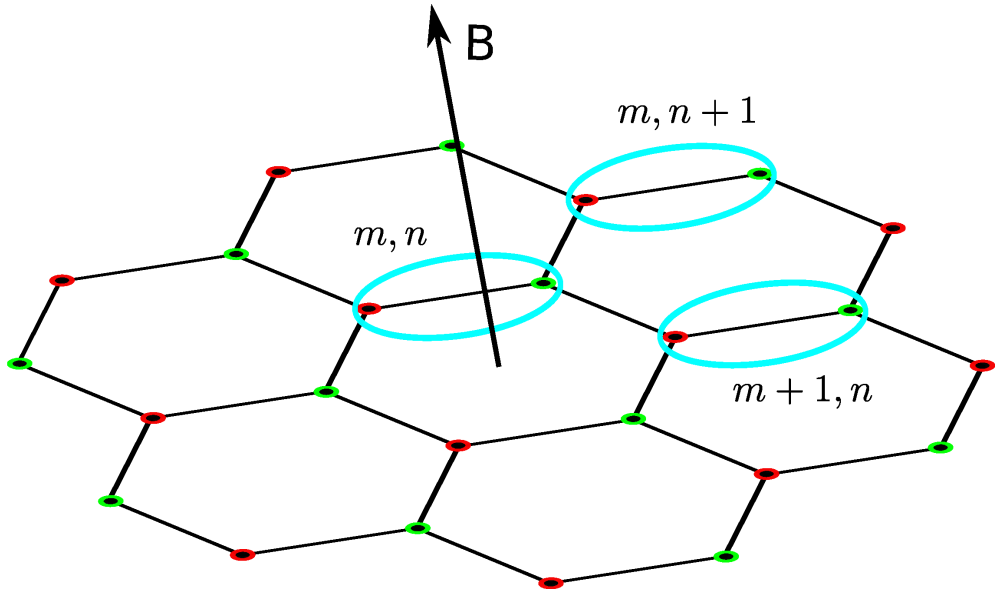
Extending ideas from physics

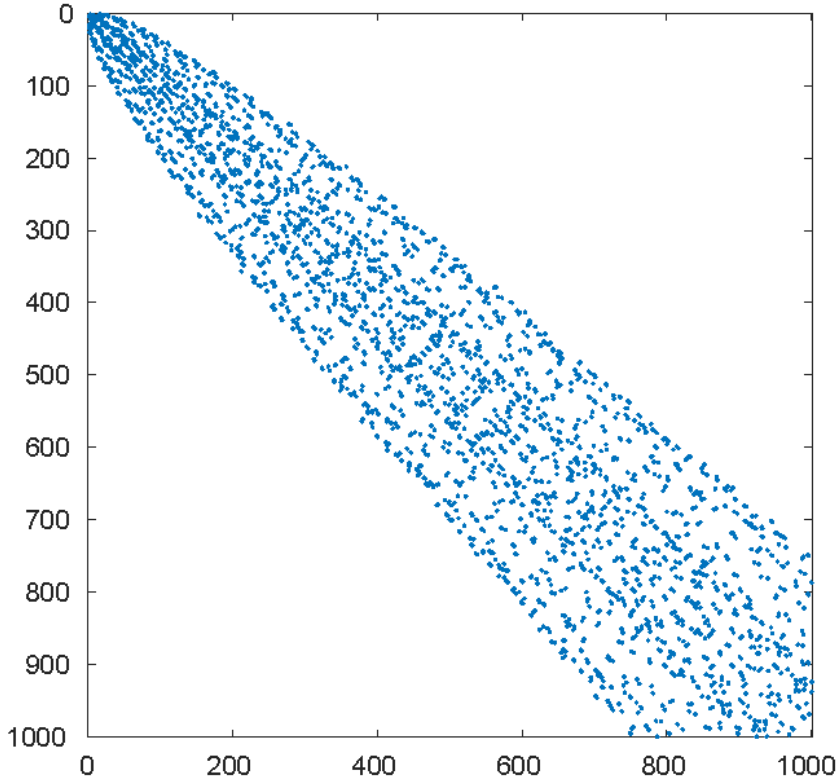
- For $z = x + i\epsilon$

$$\frac{(A - z)^{-1} - (A - \overline{z})^{-1}}{2\pi i} = \frac{1}{\pi} \int_{\mathrm{Sp}(A)} \frac{\epsilon}{(x - \lambda)^2 + \epsilon^2} d\mathcal{E}(\lambda).$$

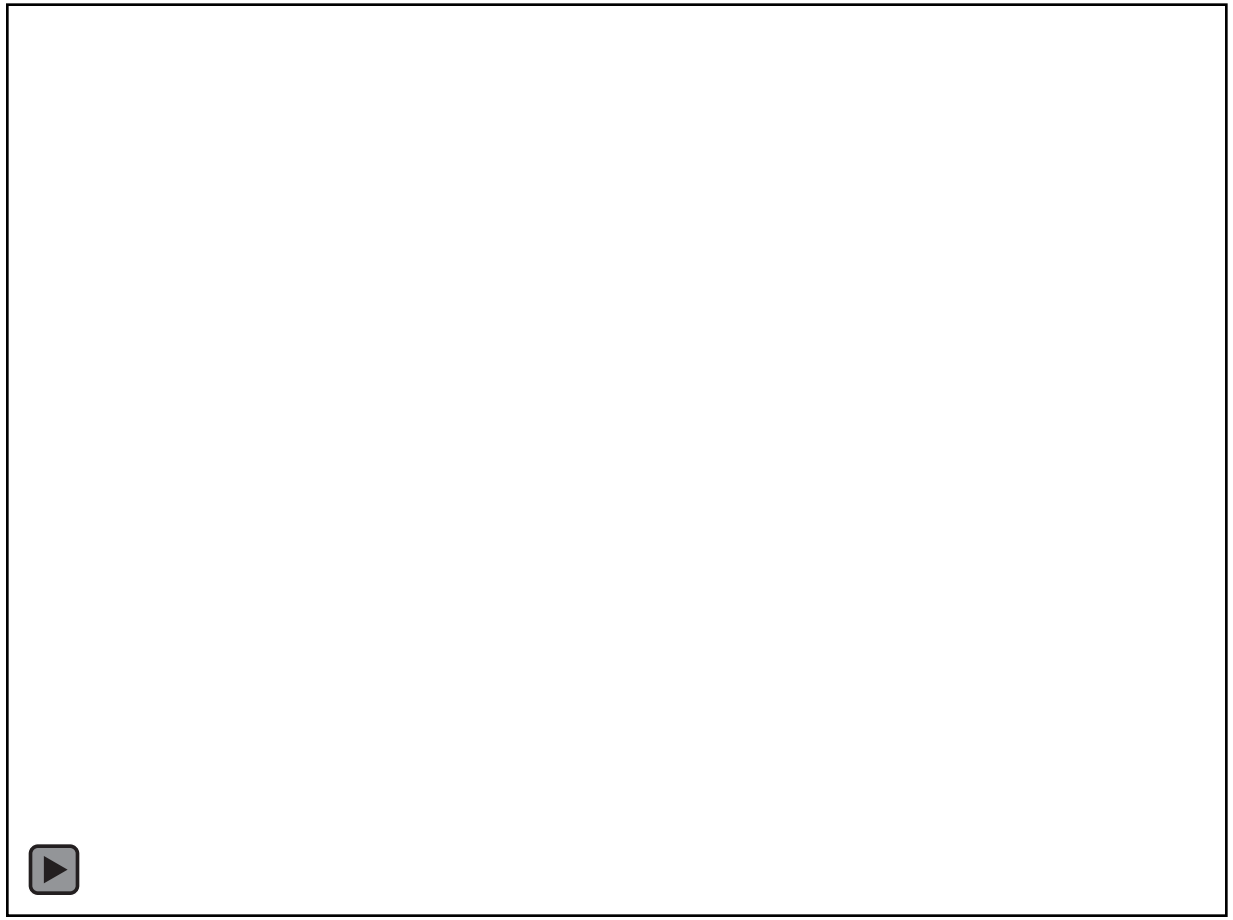
- **Smoothed** convolution with Poisson kernel (cf. Stone's formula).
- Converges weakly as $\epsilon \downarrow 0$
- This idea is used in condensed matter physics (e.g. "Lorentz" kernel), DOS calculations, autocorrelation functions, plasma physics, etc.

Example: Magnetic Graphene

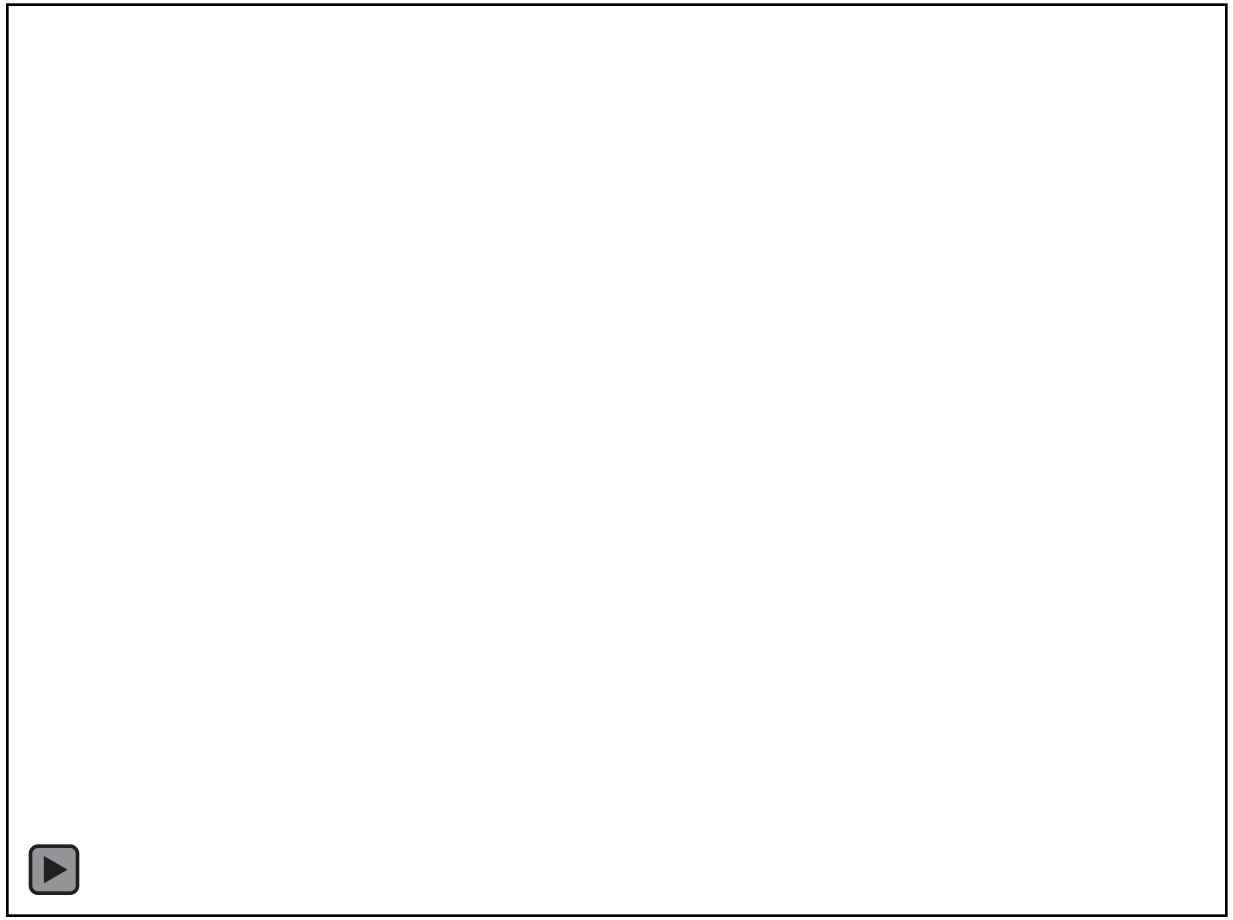




Square truncation 1: Fix N, decrease ε

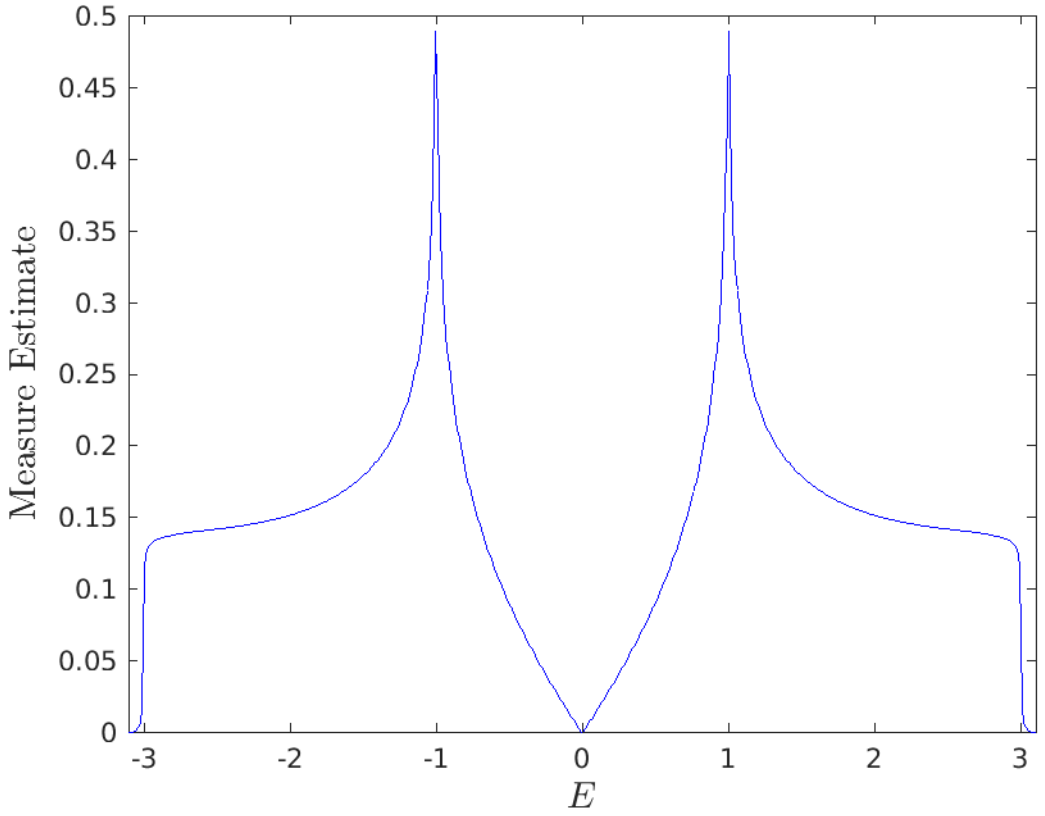


Square truncation 2: Fix ε, increase N



Theorem: If we know f, we can compute in one limit!

- Rectangular least squares type problem that computes $(A - z)^{-1}$
- Need to choose $N(\varepsilon)$ **adaptively.**



Accelerating Convergence

- **New idea:** Replace Poisson kernel with general rational function for full infinite-dimensional operator through computing $(A - z)^{-1}$

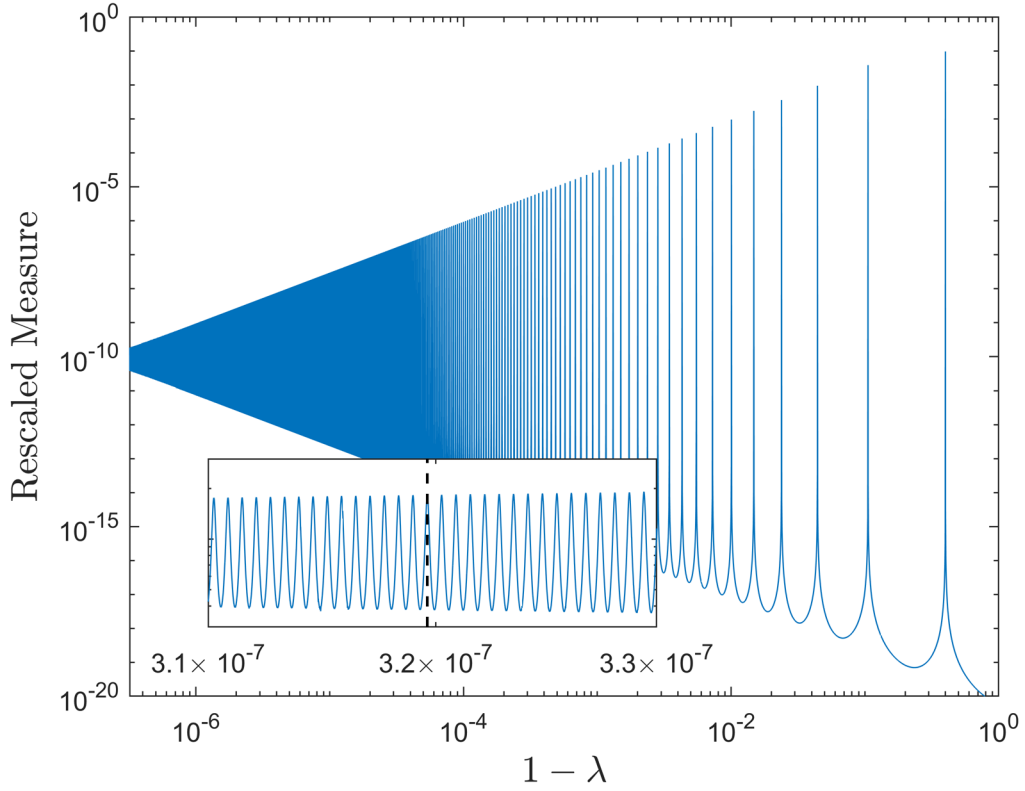
⇒ Compute measures with **error control** and **high order of convergence** for **general operators**! Even PDEs, integral operators,…

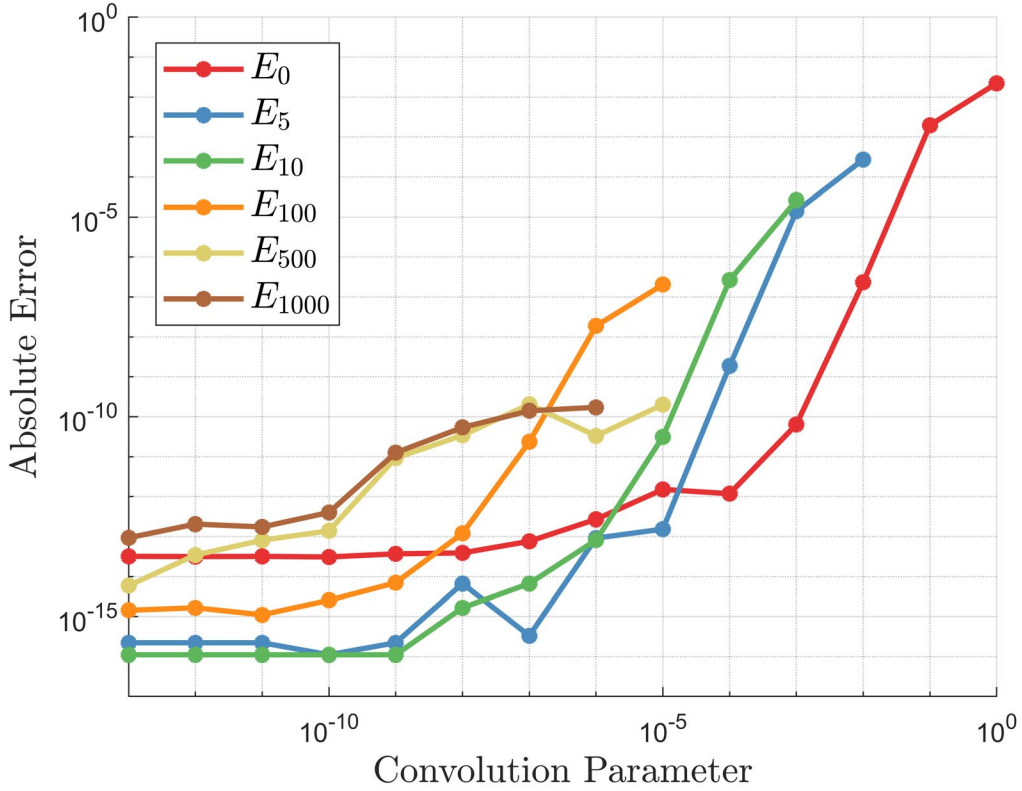
- Machinery of high order rational kernels
  - (Pointwise) If measure is locally $C^{n+\alpha}$, get pointwise rate of $O(\varepsilon^{n+\alpha})$.
  - (Average) If measure is locally $W^{n,p}$, get L^p_{loc} rate of $O(\varepsilon^n)$.

Example: Dirac operator

Describes relativistic electron, gap in essential spectrum

⇒ spurious solutions with current methods.





Conclusion

- Can compute spectra of a large class of operators with error control.
- New algorithm is fast, local and parallelisable.
- Methods extend to other problems (e.g. spectral measures) and classify problems into a hierarchy telling us what is possible.

Ongoing and future work:

- Applications in physics, e.g. materials science
- Other problems in QM: DFT etc.?
- Infinite back to finite? E.g. can acceleration be applied to DOS?
- Foundations of computational PDEs (e.g. Schrödinger equations)

One reason I wanted to give talk was to discuss other future directions

References

- M.J. Colbrook, B. Roman, and A.C. Hansen. “How to compute spectra with error control.” *Physical Review Letters* 122.25 (2019).
- M.J. Colbrook, A.C. Hansen. “On the infinite-dimensional QR algorithm.” *Numerische Mathematik* 143.1 (2019).
- M.J. Colbrook. “Computing spectral measures and spectral types.” *Submitted*.
- M.J. Colbrook, A. Horning, and A. Townsend. “Computing spectral measures of self-adjoint operators.” *Submitted*.

For further papers in this program, classifications in the SCI hierarchy and numerical code: http://www.damtp.cam.ac.uk/user/mjc249/home.html

If you have further ideas or problems for collaboration, please get in touch!