Probing the infinite: Computing spectral & transport properties in infinite dimensions

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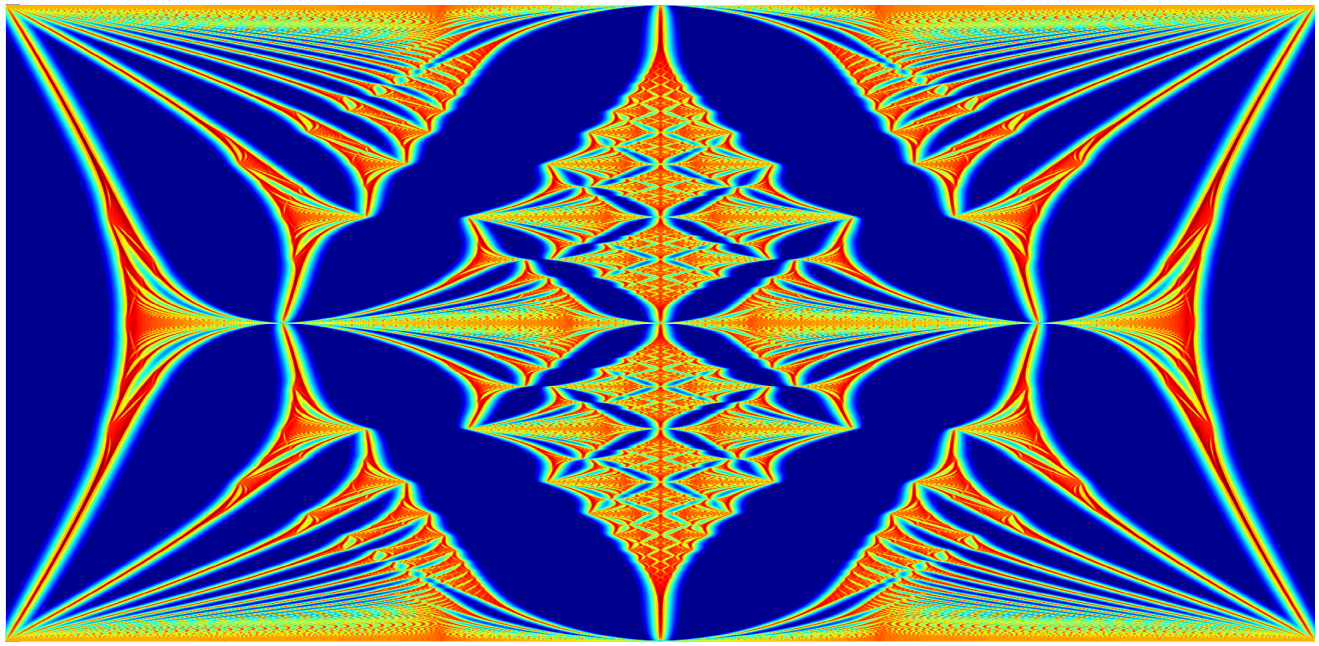

Outline

GOAL: compute spectral properties of operators in infinite-dimensions

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

BUT: typically much harder and more subtle than finite dimensions!

§	Problem	Main References for Algorithms
I	Spectra	"**How to compute spectra with error control**" C., Roman, Hansen, *Physical Review Letters*, 2019
II	Spectral Measures	"**Computing spectral measures of self-adjoint operators**" C., H., Townsend, *SIAM Review*, to appear "**Computing spectral measures and spectral types**" C., *Communications in Mathematical Physics*, to appear

Program on Infinite-Dimensional Spectral Computations

How: Deal with operator A directly, instead of 'truncate-then-solve'

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

Common tool: Compute properties of $(A - z)^{-1}$

$$\text{Finite-dimensional NLA} \rightsquigarrow \text{Infinite-dimensional NLA}$$

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

$\Rightarrow$ Optimal algorithms realising boundaries of what computers can achieve.

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, ...

[1] Papers and details: http://www.damtp.cam.ac.uk/user/mjc249/home.html

GOAL of this talk: convince you that these methods for infinite-dimensional problems can now be used in applications

Part I:
How to compute spectra with error control

With a case study on quasicrystals

The infinite-dimensional spectral problem

In many applications, we are given an operator acting on $\ell^2(\mathbb{N})$ ($\ell^2(\mathbb{N})$ = canonical infinite-dimensional Hilbert space):

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

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

GOAL: compute spectrum of A from matrix elements

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?

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Even if a method converges, still face:

- 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. ✓
- Avoids spectral pollution. ✓

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- Avoids spectral pollution. ✓
- Provides error control (guaranteed certificate of accuracy)
  $\Rightarrow$ computations reliable and useful in applications. ✓

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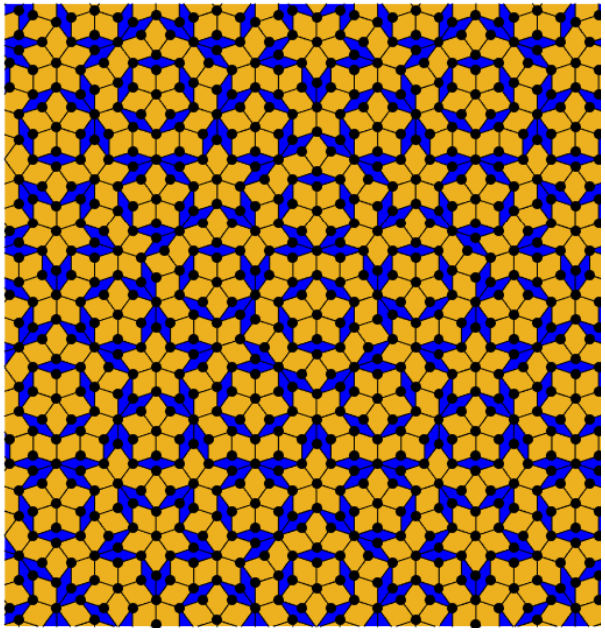
- Computationally efficient. ✓

Case study: Quasicrystals

Quasicrystals: aperiodic structures with long-range order.



Left: D. Shechtman, **Nobel Prize in Chem. 2011** for discovering quasicrystals.
Right: Penrose tile, a 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

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

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

$$[A\psi]_i = -\sum_{i\sim j} e^{\mathrm{i}\theta_{ij}(B)}\psi_j,$$

Model 2: Graph Laplacian (electronic properties)

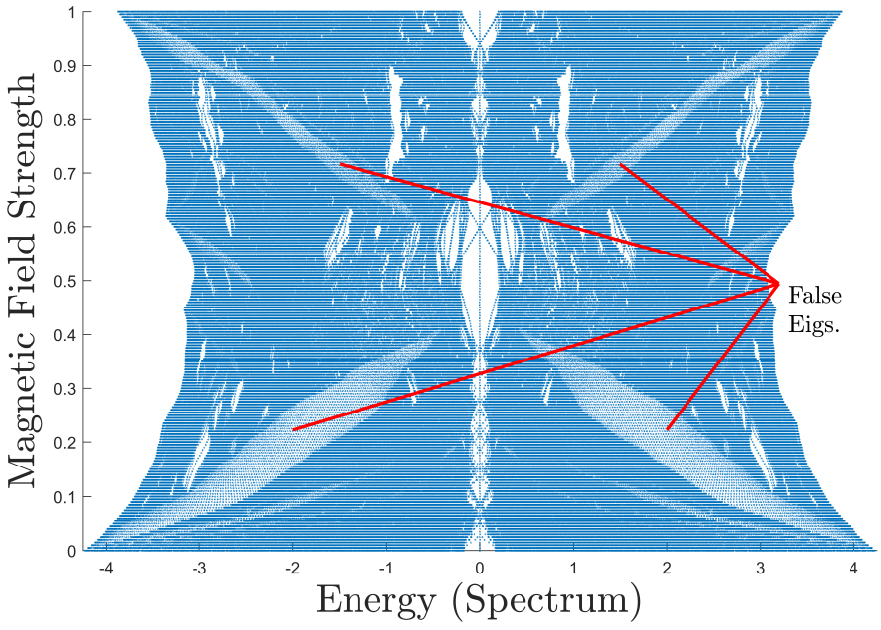
$$[A\psi]_i = \sum_{i\sim j} (\psi_j - \psi_i),$$

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

Model 1: Magnetic field

Finite truncations

Spectral pollution.



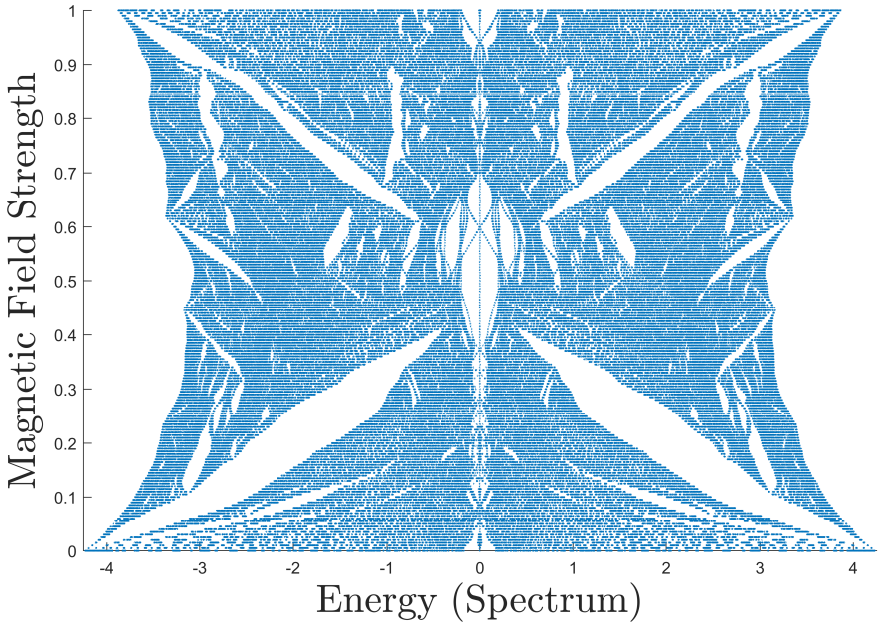
Unreliable

Does not converge

No error control

New method

First convergent computation.

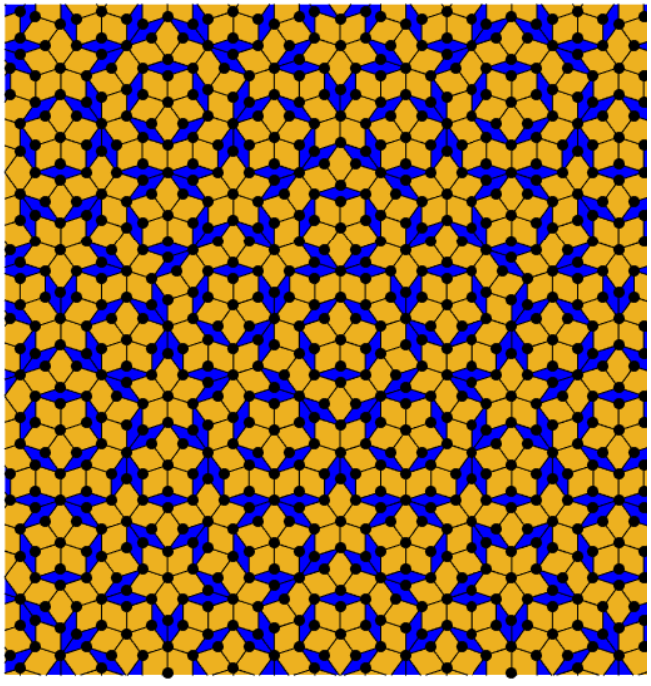


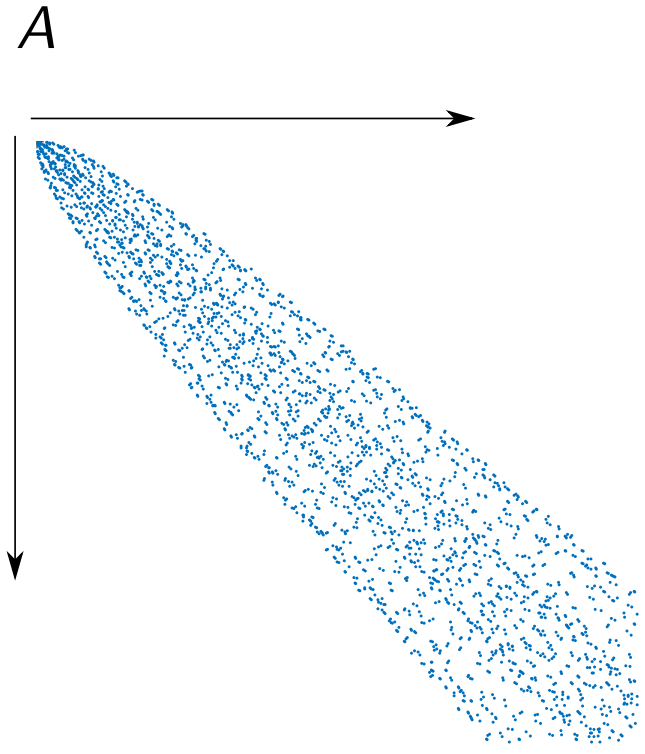
Reliable

Converges

Error control

Idea I: Rectangular truncations





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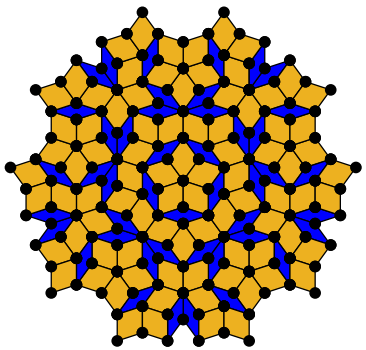

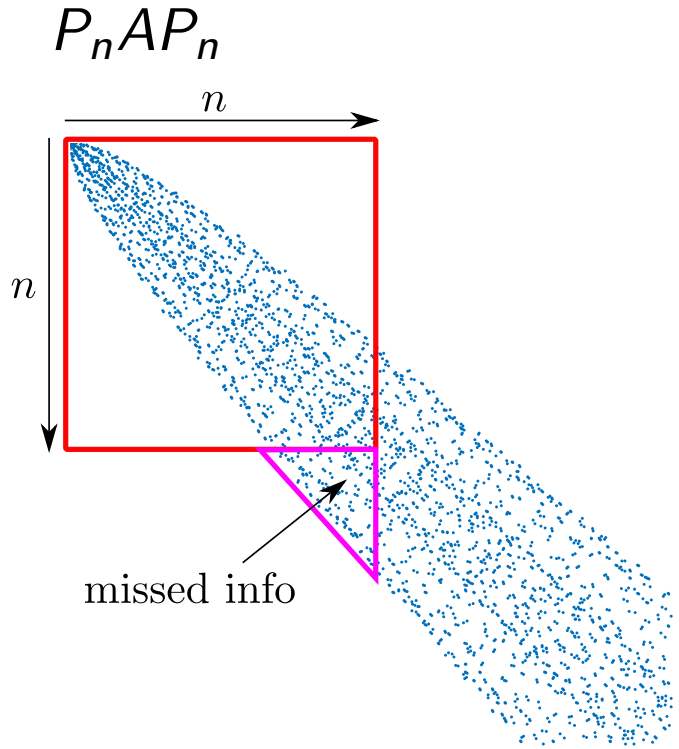

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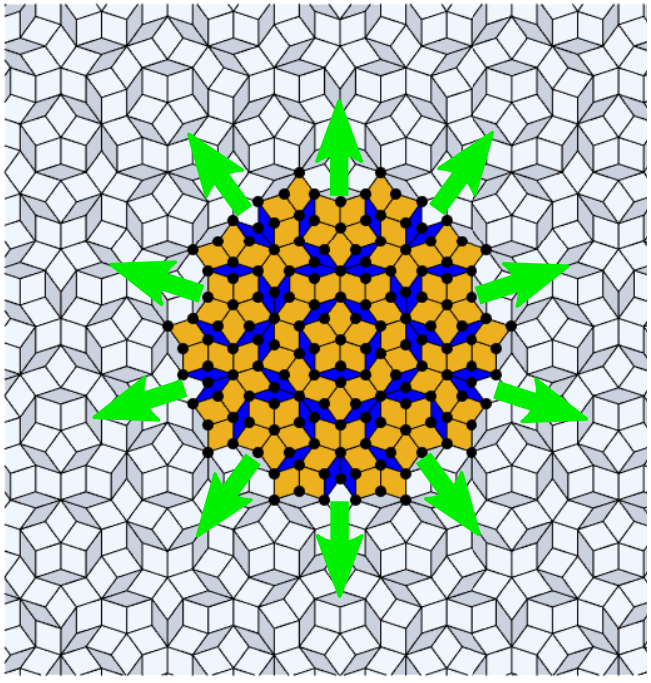
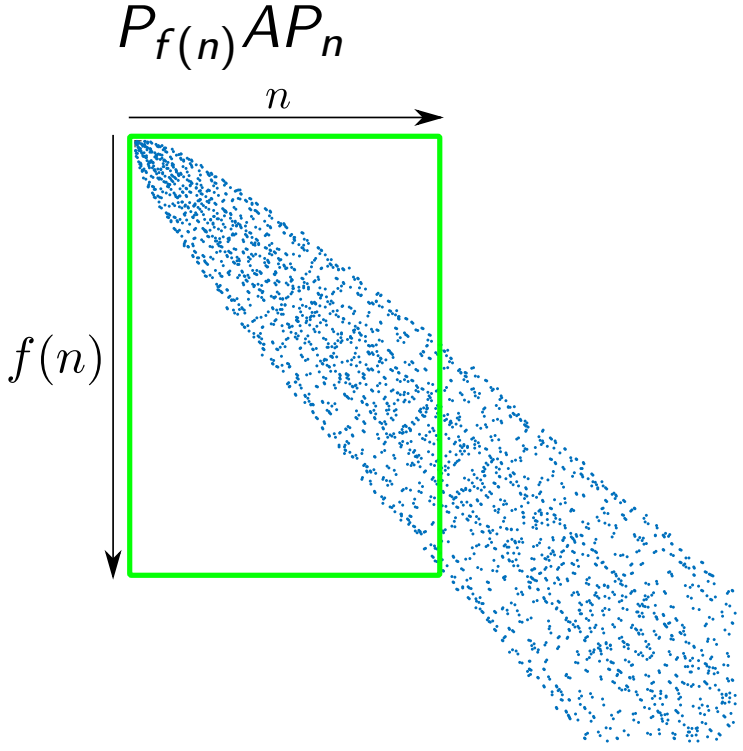




Idea II: Locally compute distance function and minimisers

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

$$\gamma_n(z) := \sigma_1(P_{f(n)}(A - zI)P_n).$$

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

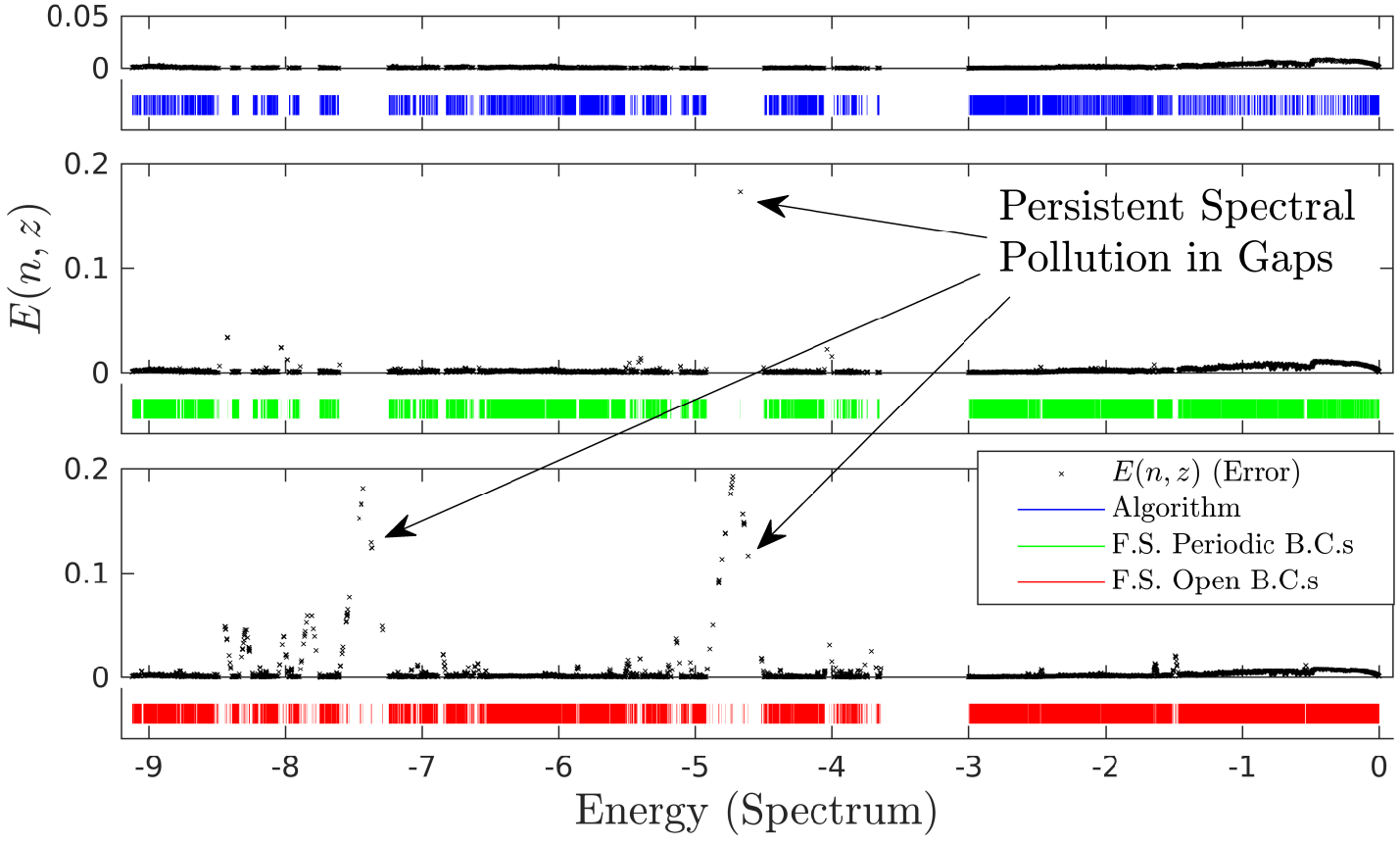
Step 2: Bound the distance to the spectrum:

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

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

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

Model 2: Graph Laplacian (electronic properties)



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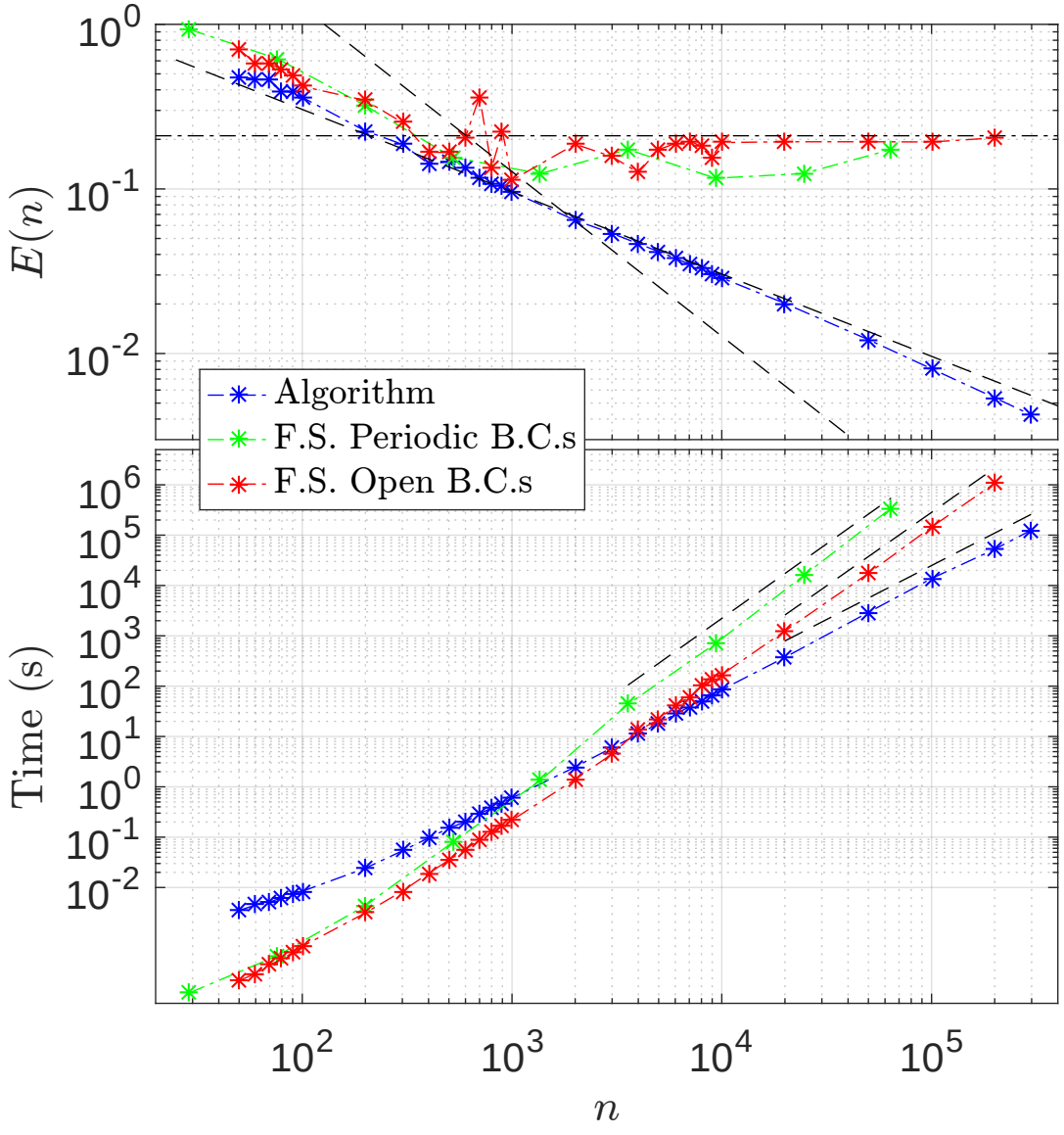
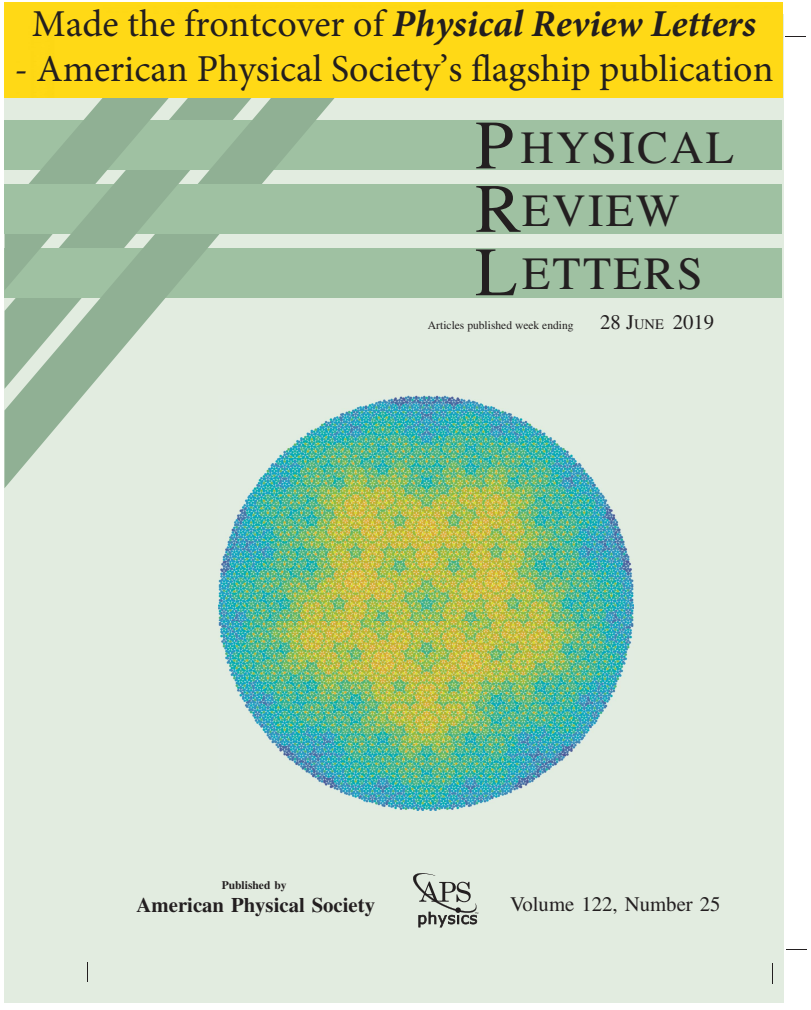


Advantages

- 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...



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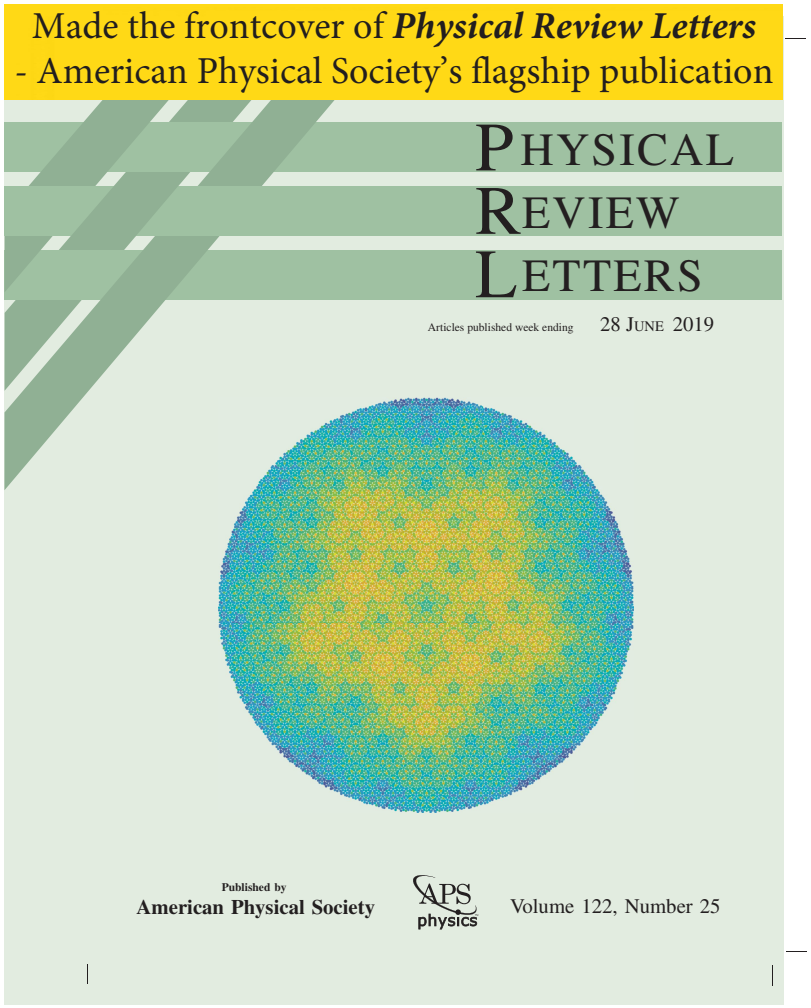
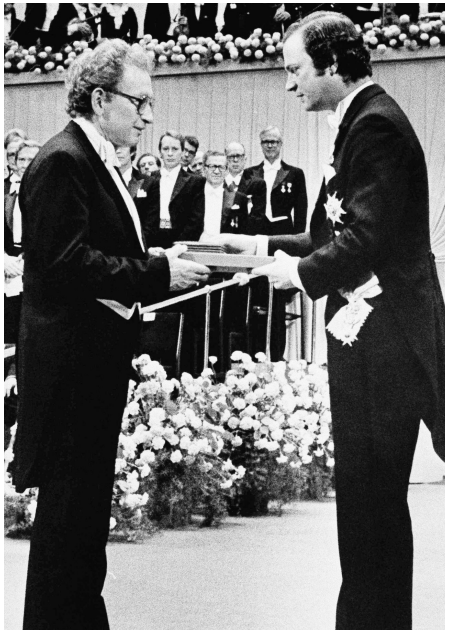


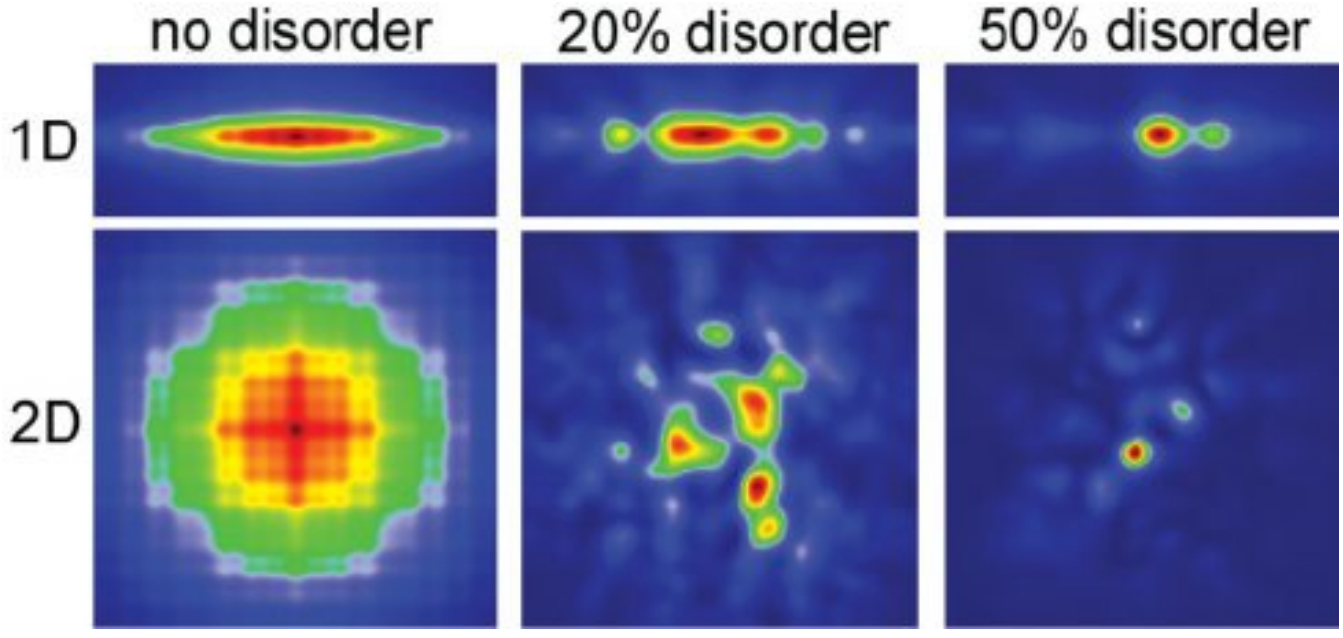
Extends to unbounded operators and PDEs with coefficients of locally bounded total variation (e.g. algorithms point sample coefficients).

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

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.

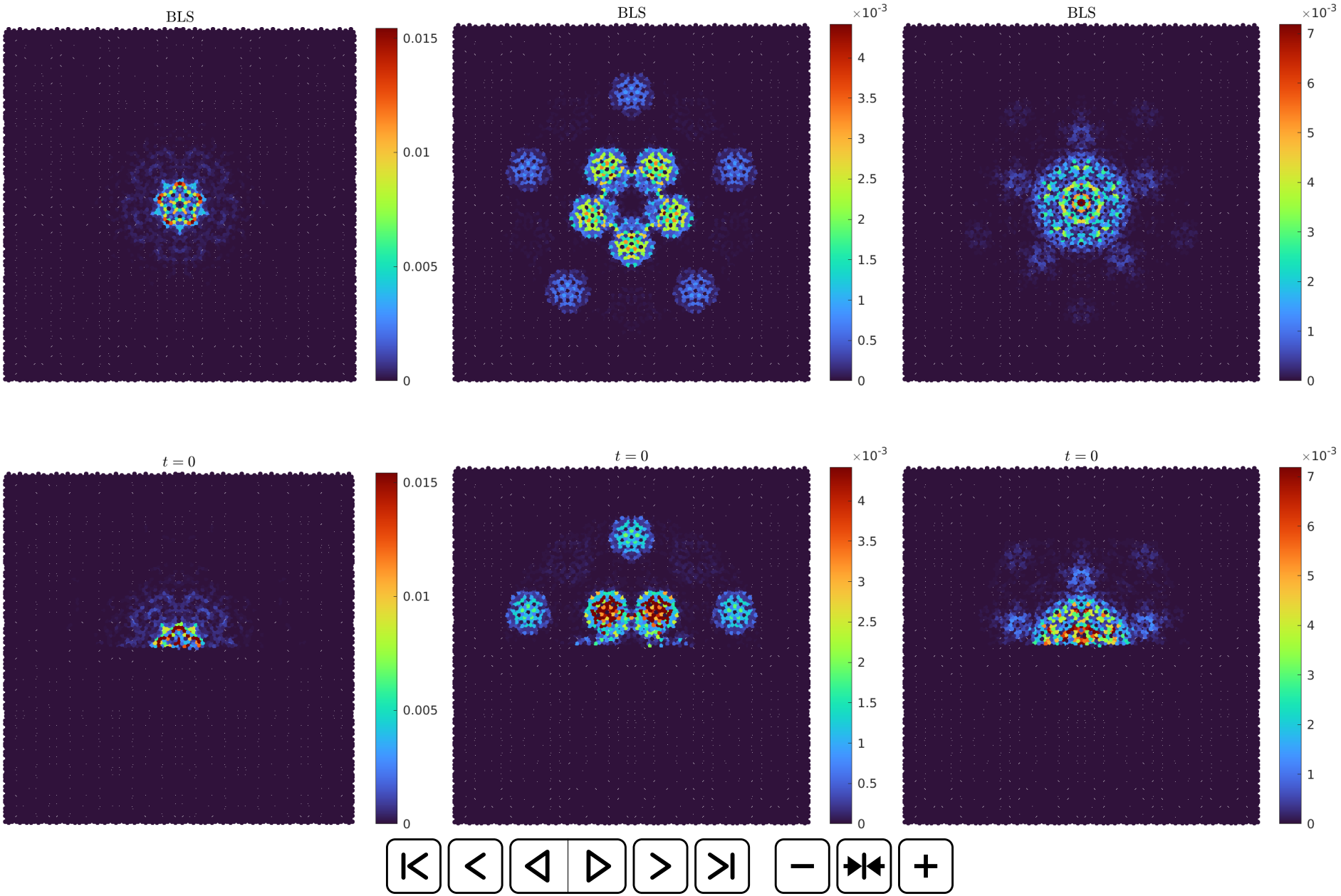
What happens in aperiodic systems? Do we need disorder?

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 ($|\psi|^2$ shown)



Conclusion of Part I

- 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.
- (Method extends to computing semigroups with error control.)
- New type of Bulk Localised State (BLS) for magnetic quasicrystals that support localised transport within the bulk.

We'll investigate BLSs further in part II...

Part II:
Computing spectral measures and projections

Spectral measures

Finite-dimensional: $A \in \mathbb{C}^{n\times n}$ self-adjoint, o.n. basis of e-vectors $\{v_j\}_{j=1}^n$

$$v = \left(\sum_{k=1}^{n} v_k v_k^*\right) v, \quad v \in \mathbb{C}^n \qquad Av = \left(\sum_{k=1}^{n} \lambda_k v_k v_k^*\right) v, \quad v \in \mathbb{C}^n.$$

Infinite-dimensional: Self-adjoint operator $\mathcal{L} : \mathcal{D}(\mathcal{L}) \to \mathcal{H}$ with spectrum

$$\Lambda(\mathcal{L}) = \{z \in \mathbb{C} : \mathcal{L} - z \text{ not bounded invertible}\}.$$

Bad news: Typically, no longer an o.n. basis of e-vectors.

Spectral Theorem: Projection-valued spectral measure $\mathcal{E}$ (assigns an orthogonal projector to each Borel-measurable set) with

$$f = \left(\int_{\mathbb{R}} d\mathcal{E}(y)\right) f, \quad f \in \mathcal{H} \qquad \mathcal{L}f = \left(\int_{\mathbb{R}} y\, d\mathcal{E}(y)\right) f, \quad f \in \mathcal{D}(\mathcal{L}).$$

Intuition: Diagonalises an infinite-dimensional operator.

GOAL: Compute (scalar versions of) $\mathcal{E}$.

Motivation

Scalar-valued measures (action of projections):

$$\mu_f(\Omega) = \langle \mathcal{E}(\Omega) f, f \rangle$$

Lebesgue decomposition theorem:

$$d\mu_f(y) = \underbrace{\sum_{\lambda \in \Lambda^{\mathrm{P}}} \langle \mathcal{P}_\lambda f, f \rangle \, \delta(y-\lambda) dy}_{\text{discrete part}} + \underbrace{\rho_f(y)\, dy + d\mu_f^{(\mathrm{sc})}(y)}_{\text{continuous part}}.$$

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,...

Example: in quantum mechanics, μ_f describes the likelihood of different outcomes when the observable $\mathcal{L}$ is measured. Can also solve SE

$$i\frac{df}{dt} = \mathcal{L}f, \quad f(0) = f_0, \quad \text{via} \quad f(t) = \left(\int_{\mathbb{R}} \exp(-ity)\, d\mathcal{E}(y) \right) f_0.$$

A very hard problem!

"Most operators that arise in practice are not presented in a representation in which they are diagonalized... this raises the question of how to implement the methods of finite dimensional numerical linear algebra 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)

Some methods do exist, but treat cases with a lot of structure (e.g. compact perturbations of tridiagonal Toeplitz, some classes of singular Sturm–Liouville problems, etc.)

In contrast, want a **general** method to resolve spectral measures of $\mathcal{L}$ (e.g. PDEs, integral operators, infinite matrices,...) and not an underlying discretisation or truncation.

Finite-dimensional NLA $\Rightarrow$ Infinite-dimensional NLA

Ideas from physics

Idea: For $z = x + i\epsilon$, use

$$\mu_f^\epsilon(x) = \langle \frac{(\mathcal{L} - z)^{-1} - (\mathcal{L} - \overline{z})^{-1}}{2\pi i} f, f \rangle = \frac{1}{\pi} \int_{\Lambda(\mathcal{L})} \frac{\epsilon}{(x-\lambda)^2 + \epsilon^2} d\mu_f(\lambda).$$

Convolution with Poisson kernel: smoothed measure.

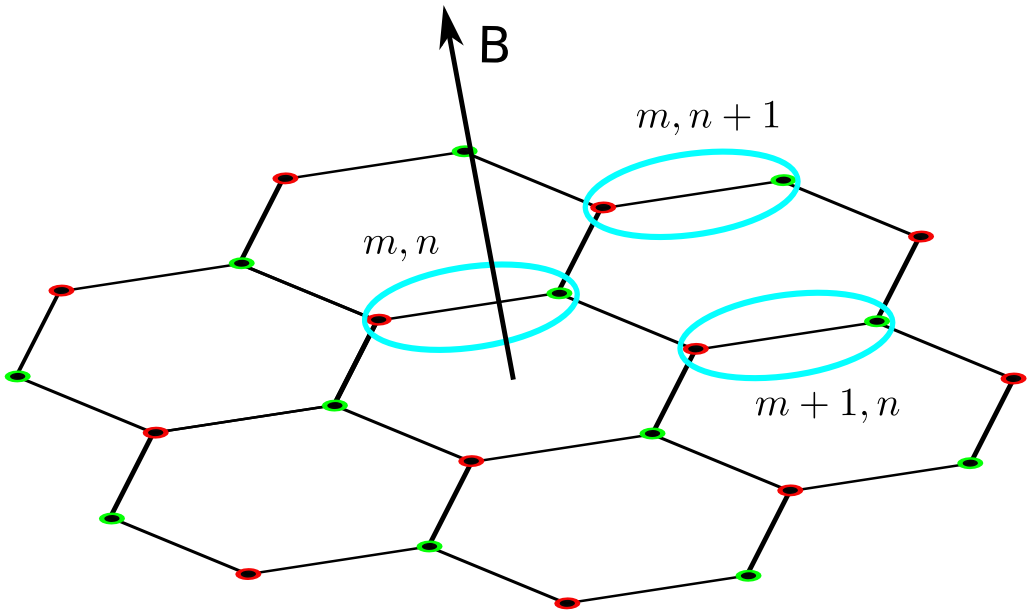
Converges weakly to measure as $\epsilon \downarrow 0$:

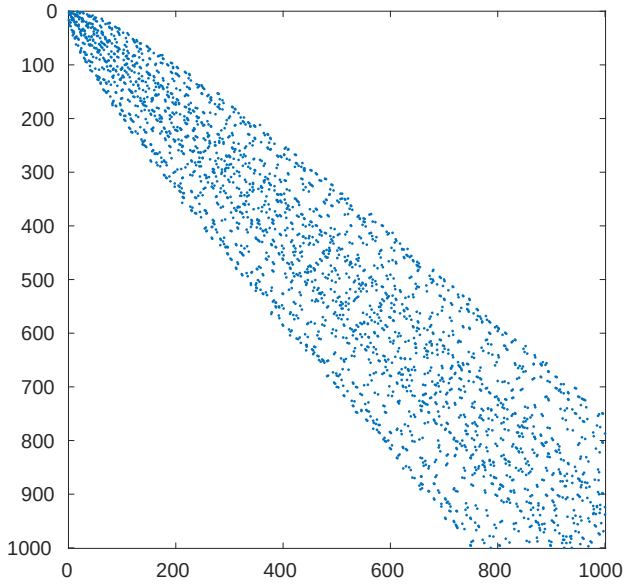
$$\int_{\mathbb{R}} \phi(y) \mu_f^\epsilon(y)\, dy \to \int_{\mathbb{R}} \phi(y)\, d\mu_f(y), \qquad \text{as} \qquad \epsilon \downarrow 0,$$

for any bounded, continuous function ϕ.

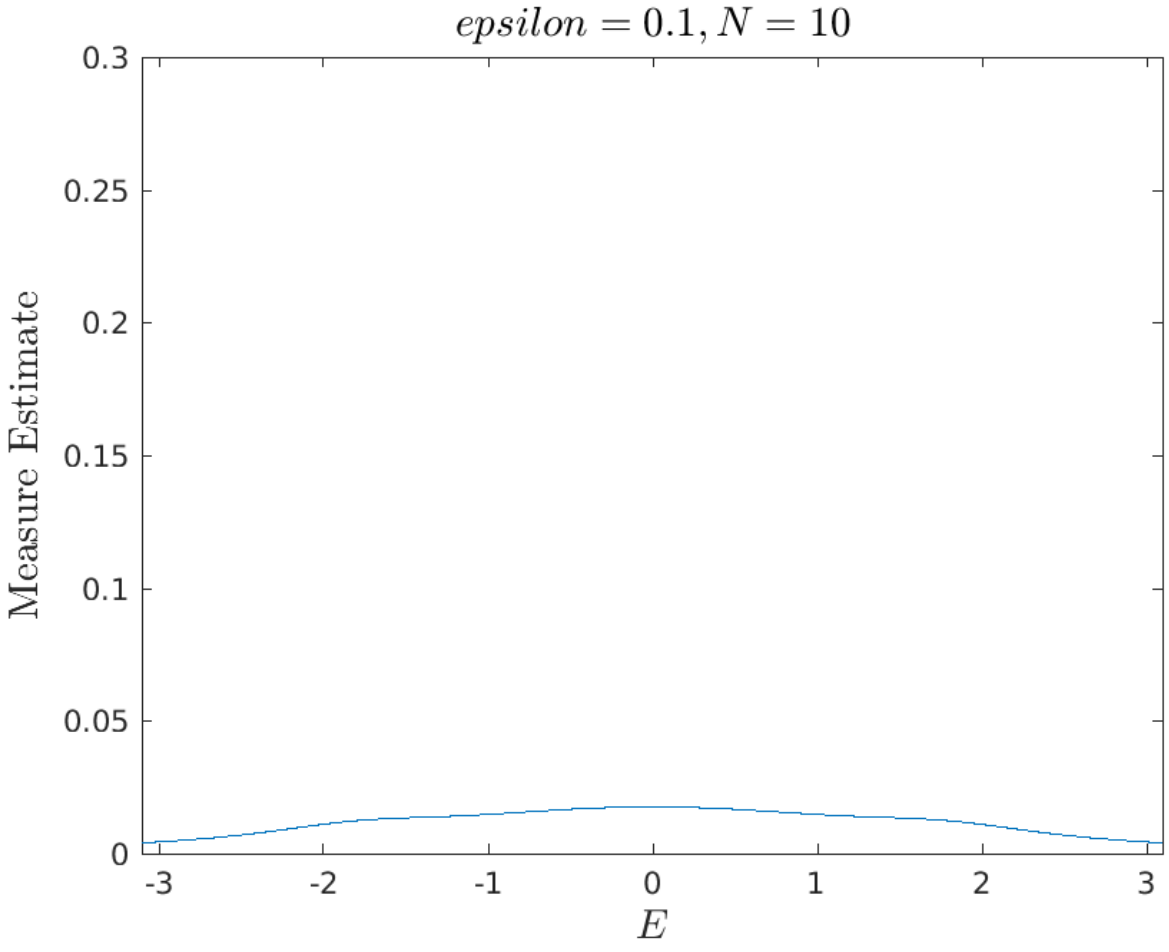
Approximate μ_f^ϵ via $\mu_{f,N}^\epsilon$ ($N =$ truncation parameter).

Numerical balancing act: Magnetic graphene





Numerical balancing act: Magnetic graphene



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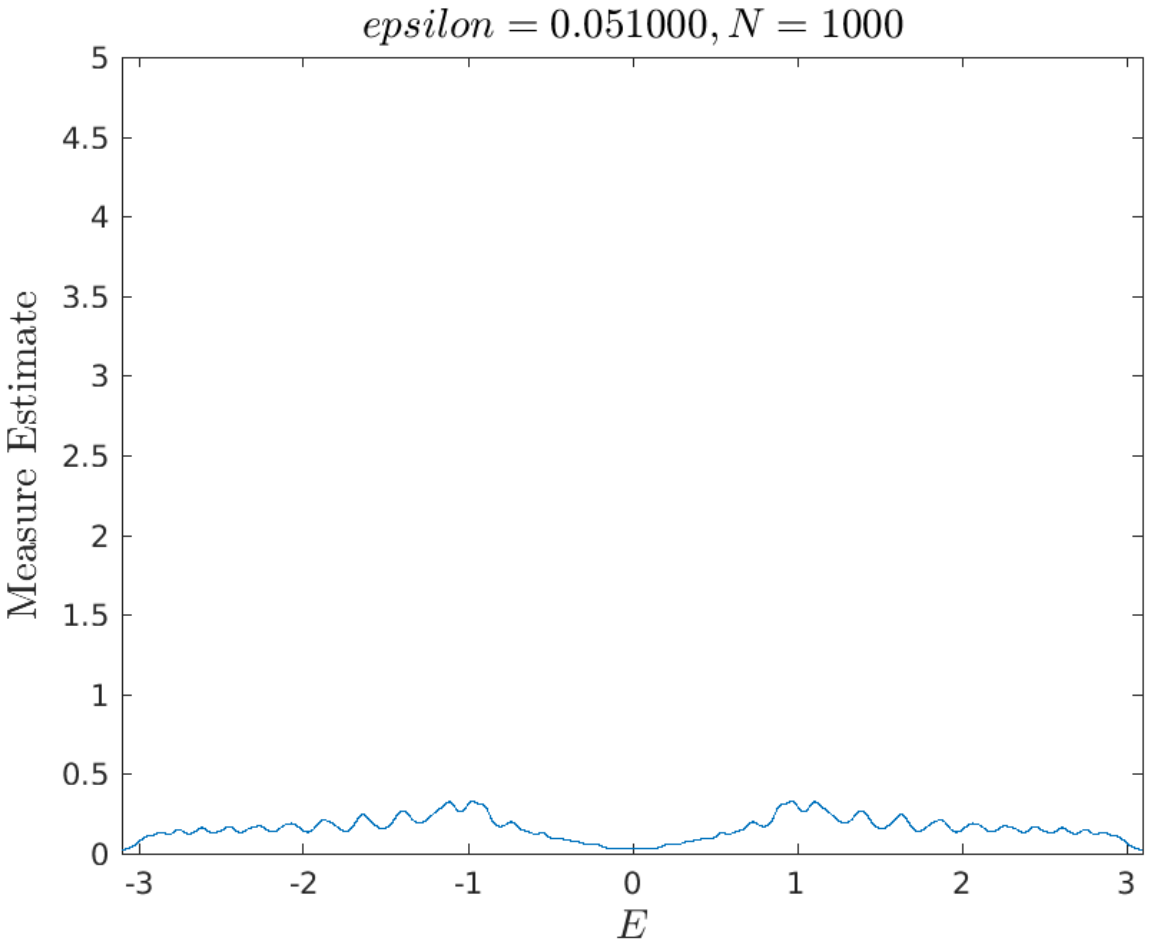
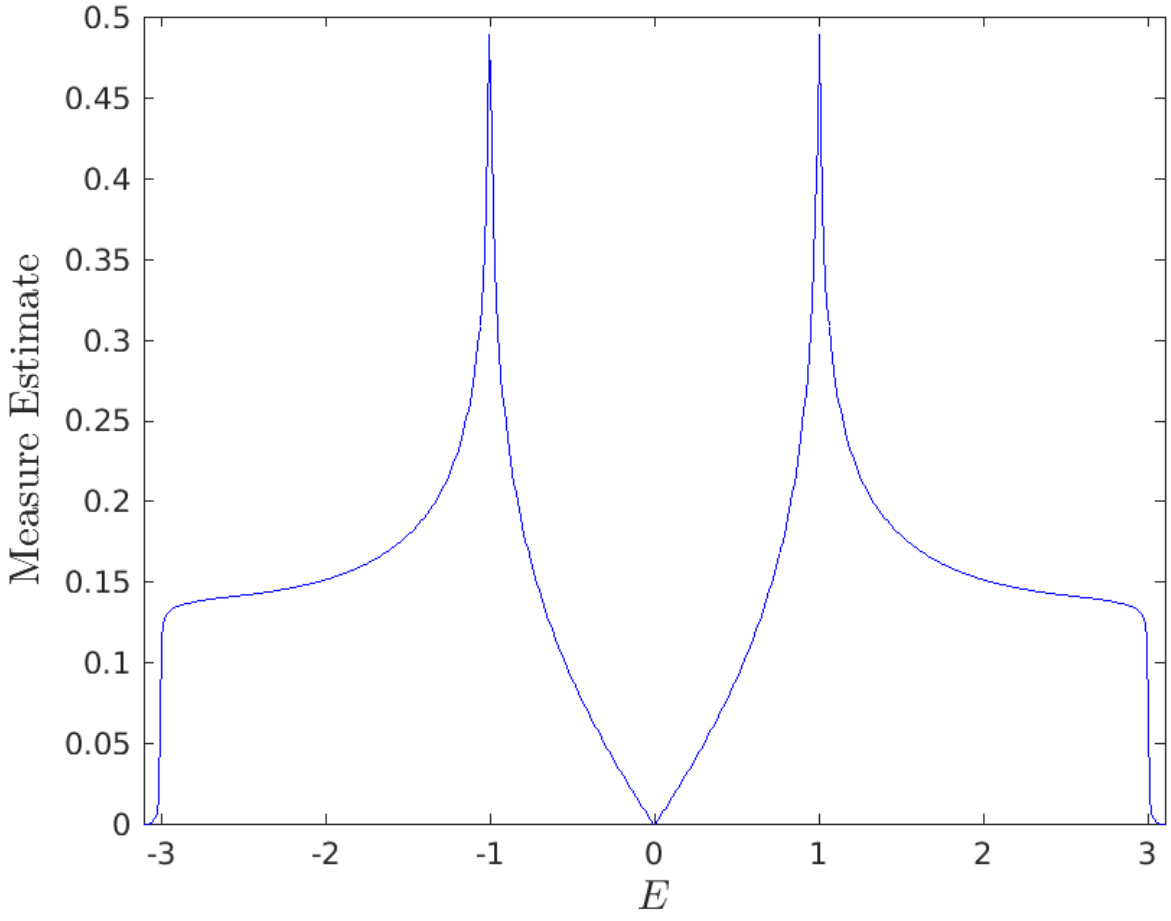


Theorem

If we know rate of off-diagonal decay of infinite matrix, can compute measure in one limit. Extends to other operators such as PDEs.

This is through a rectangular least squares type problem that computes $(\mathcal{L} - z)^{-1} f$ with (asymptotic) error control. $N(\epsilon)$ chosen **adaptively**.

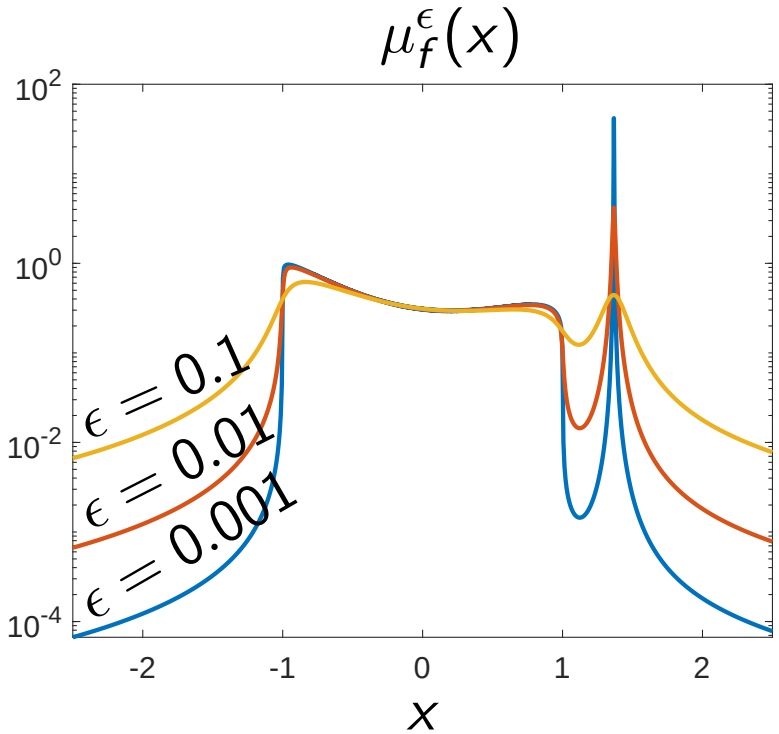


Example: Integral operator

$$\mathcal{L}u(x) = xu(x) + \int_{-1}^{1} e^{-(x^2+y^2)} u(y)\, dy, \qquad x \in [-1, 1].$$

Discretise using adaptive Chebyshev collocation method.

Look at μ_f with $f(x) = \sqrt{3/2}\, x$.



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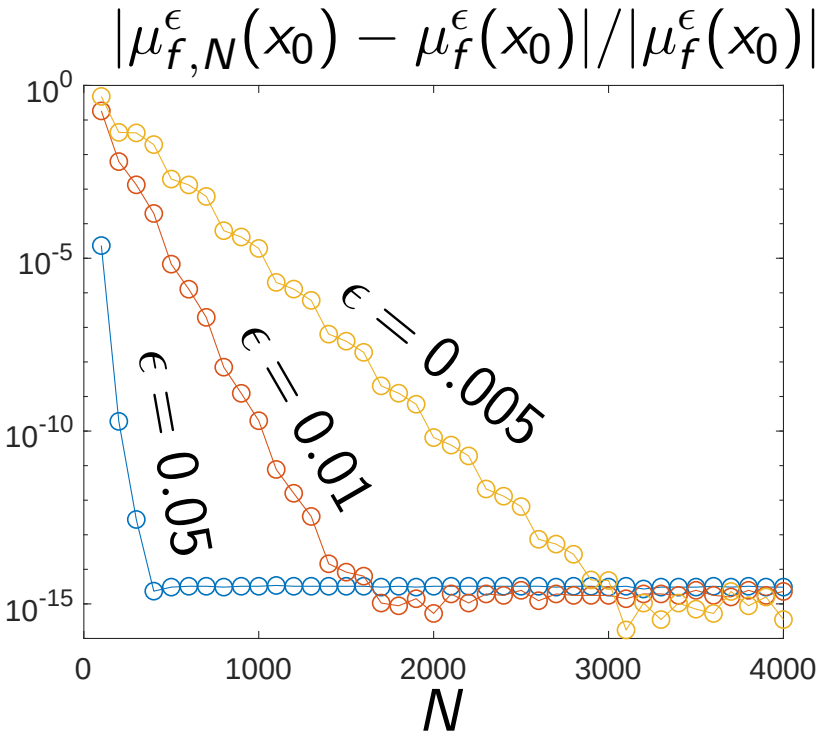
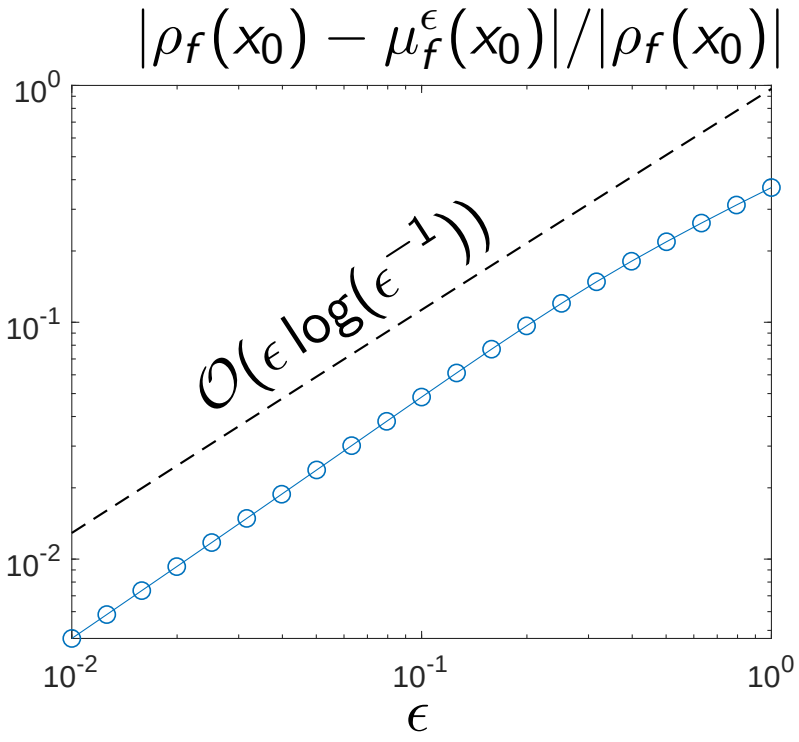




$|\rho_f(x_0) - \mu^\epsilon_f(x_0)| = \mathcal{O}(\epsilon \log(\epsilon^{-1}))$ and need $N \approx 20/\epsilon$.

$\Rightarrow$ Infeasible to get more than five or six digits!

Q: Can we do better?

Accelerating convergence

Let $m \in \mathbb{N}$, $K \in L^1(\mathbb{R})$. We say K is an mth order kernel if:

(i) Normalised: $\int_{\mathbb{R}} K(x)dx = 1$,

(ii) Zero moments: $K(x)x^j$ integrable, $\int_{\mathbb{R}} K(x)x^j dx = 0$ for $0 < j < m$,

(iii) Decay at $\pm\infty$: There is a constant C_K, independent of x, such that

$$|K(x)| \leq C_K(1 + |x|)^{-(m+1)}, \qquad x \in \mathbb{R}.$$

Theorem

If K is mth order, $K_\epsilon(x) = \epsilon^{-1}K(x\epsilon^{-1})$ and μ_f locally absolutely continuous near x_0 with density ρ_f then

- *Pointwise: If ρ_f locally $\mathcal{C}^{n,\alpha}$ near x_0 then*

$$|[K_\epsilon * \mu_f](x_0) - \rho_f(x_0)| = \mathcal{O}(\epsilon^{n+\alpha}) + \mathcal{O}(\epsilon^m \log(\epsilon^{-1}))$$

- *L^p: If ρ_f locally $\mathcal{W}^{n,p}$ near x_0 $(1 \leq p < \infty)$ then*

$$\|[K_\epsilon * \mu_f] - \rho_f\|_{L^p_{loc}} = \mathcal{O}(\epsilon^n) + \mathcal{O}(\epsilon^m \log(\epsilon^{-1}))$$

Rational kernels $\rightsquigarrow$ high-order generalised Stone's formula

Idea: Replace Poisson kernel with rational kernel

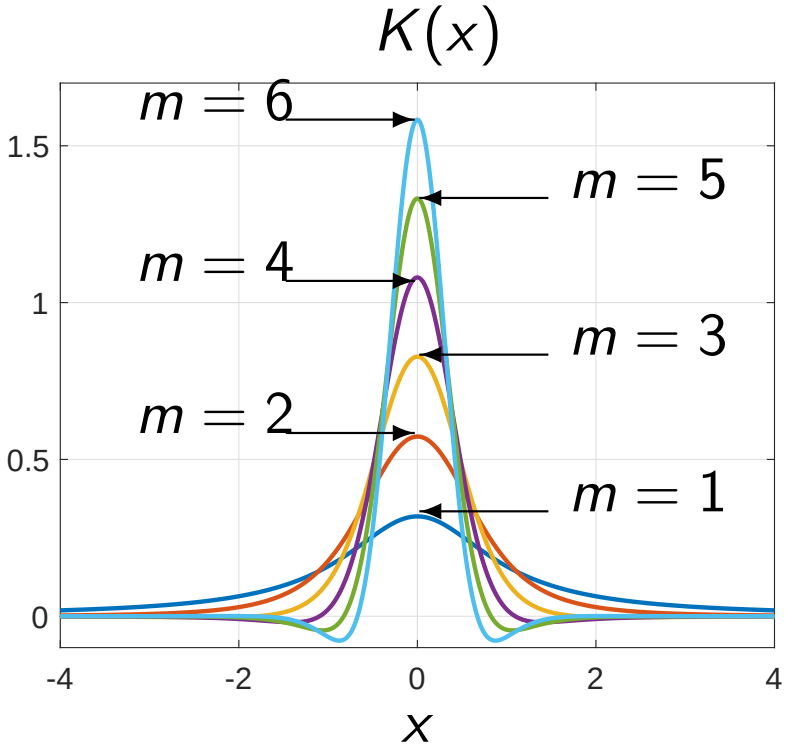
$$K(x) = \frac{1}{2\pi i} \sum_{j=1}^{m} \frac{\alpha_j}{x - a_j} - \frac{1}{2\pi i} \sum_{j=1}^{m} \frac{\beta_j}{x - b_j}.$$

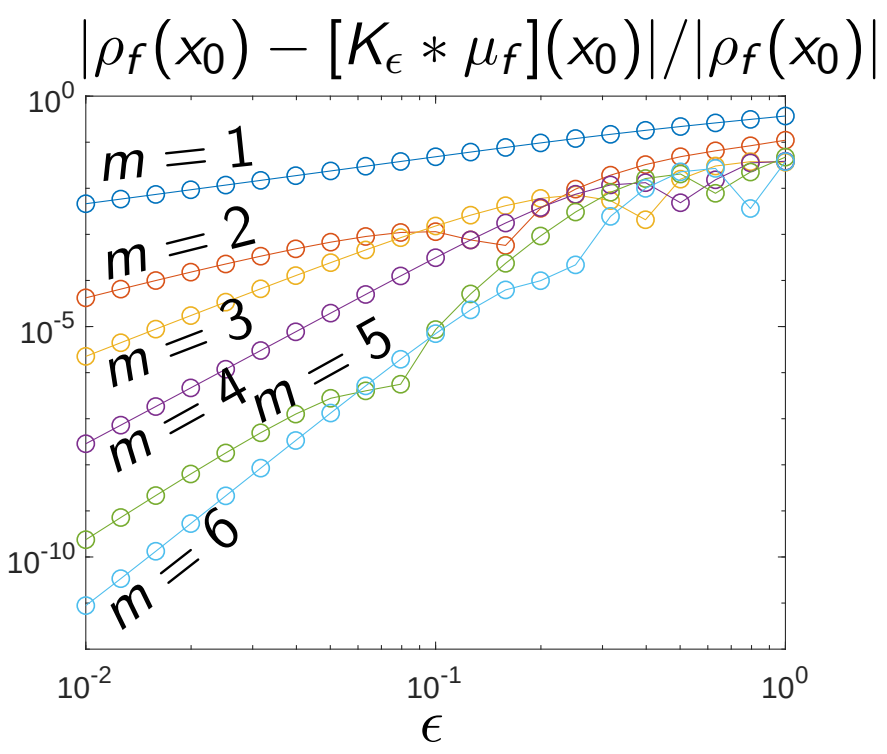
Can compute convolution with error control using resolvent

$$[K_\epsilon * \mu_f](x)$$
$$= \frac{-1}{2\pi i} \left[\sum_{j=1}^{m} \alpha_j \langle (\mathcal{L} - (x - \epsilon a_j))^{-1} f, f \rangle - \sum_{j=1}^{m} \beta_j \langle (\mathcal{L} - (x - \epsilon b_j))^{-1} f, f \rangle \right].$$

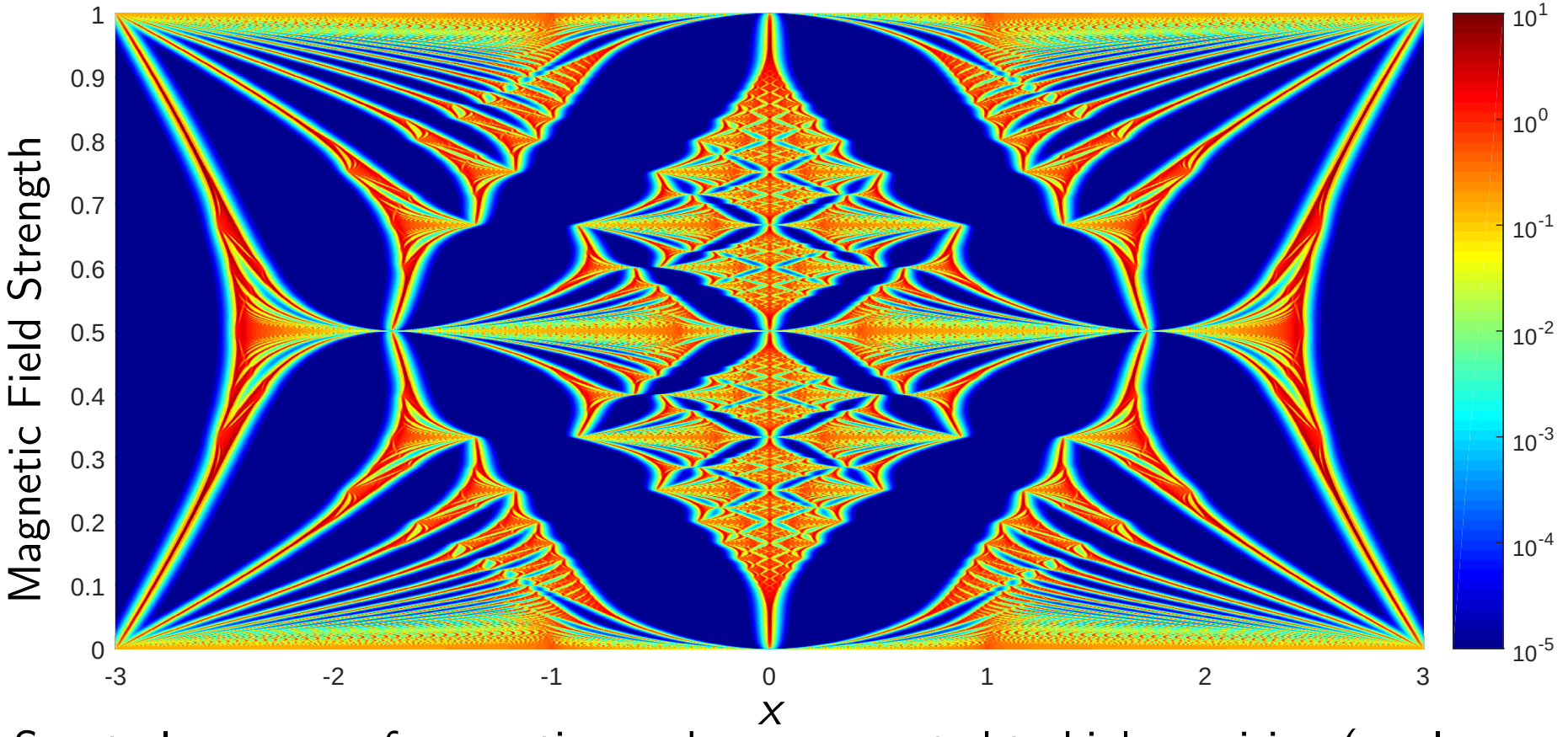
Fix a_j in UHP, b_j in LHP $\Rightarrow$ unique $\{\alpha_j, \beta_j\}$ s.t. K an mth order kernel.

Integral operator revisited





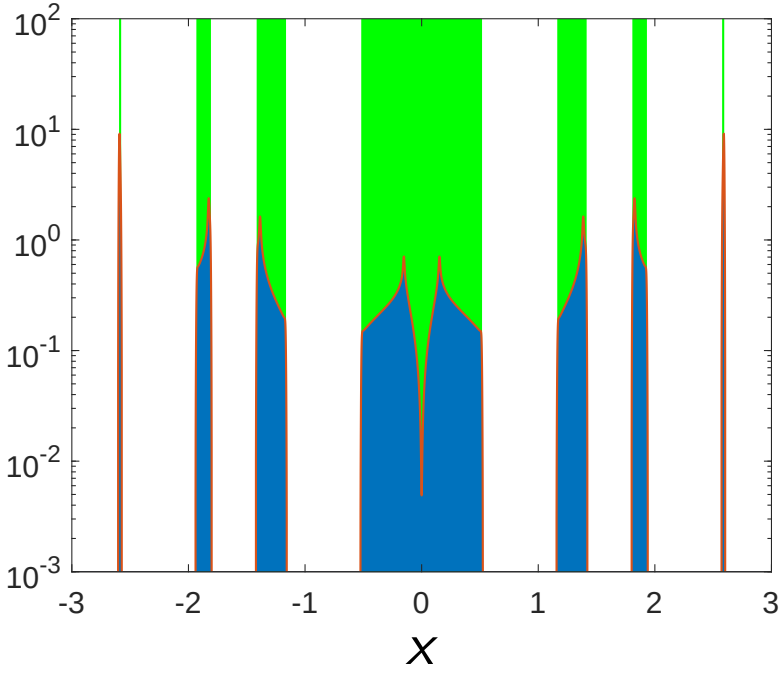
Example I: Back to graphene

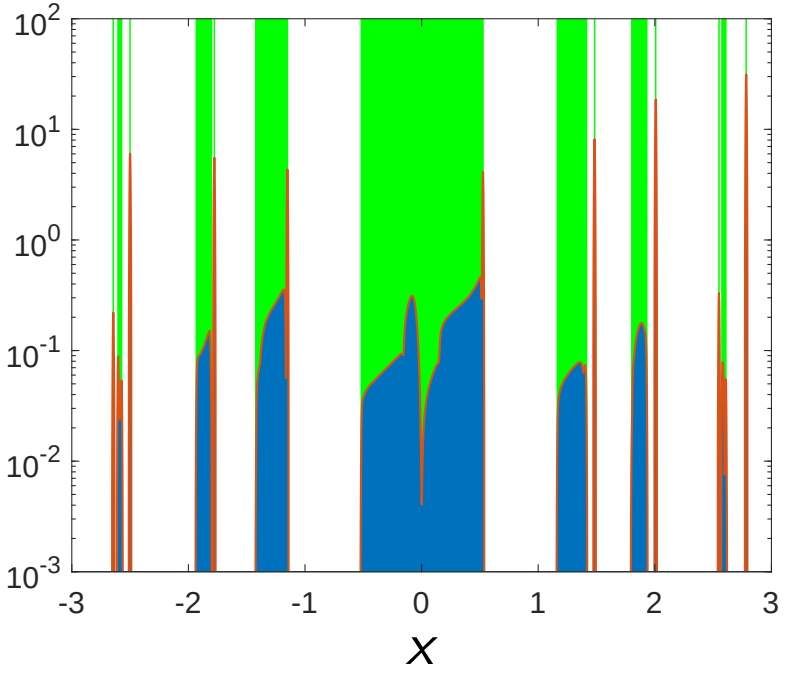


Spectral measure of magnetic graphene, computed to high precision (see log scale - sorry Callum!) using $m = 4$ kernel.

Example I: Add a defect

Add potential $V(\mathbf{x}) = \frac{\cos(\|\mathbf{x}\|_2 \pi)}{(\|\mathbf{x}\|_2+1)^2}$. Slice at $\Phi = 0.25$, $\epsilon = 0.01$:





Example II: Eigenvalue hunting

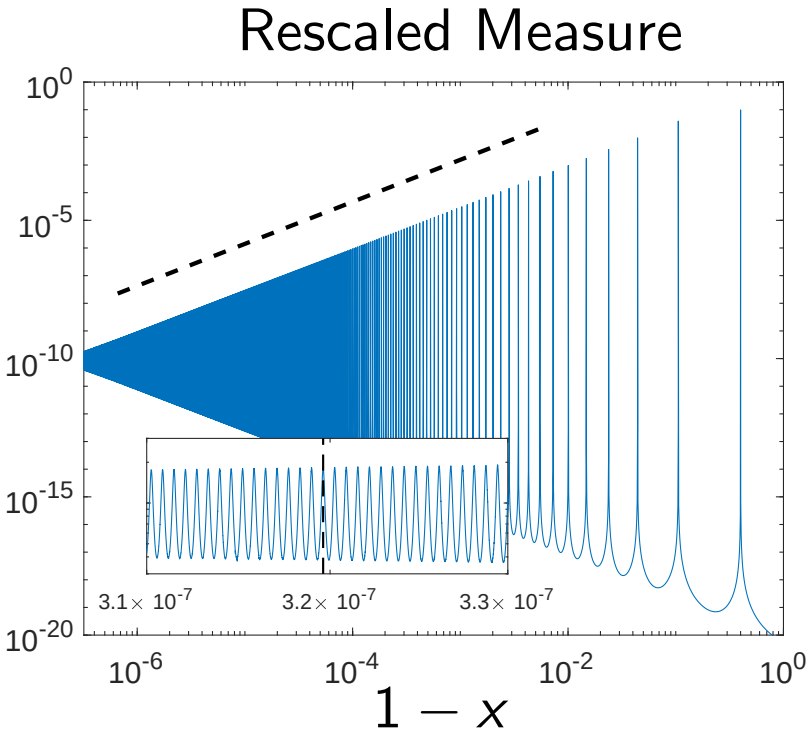
Example: Dirac operator.

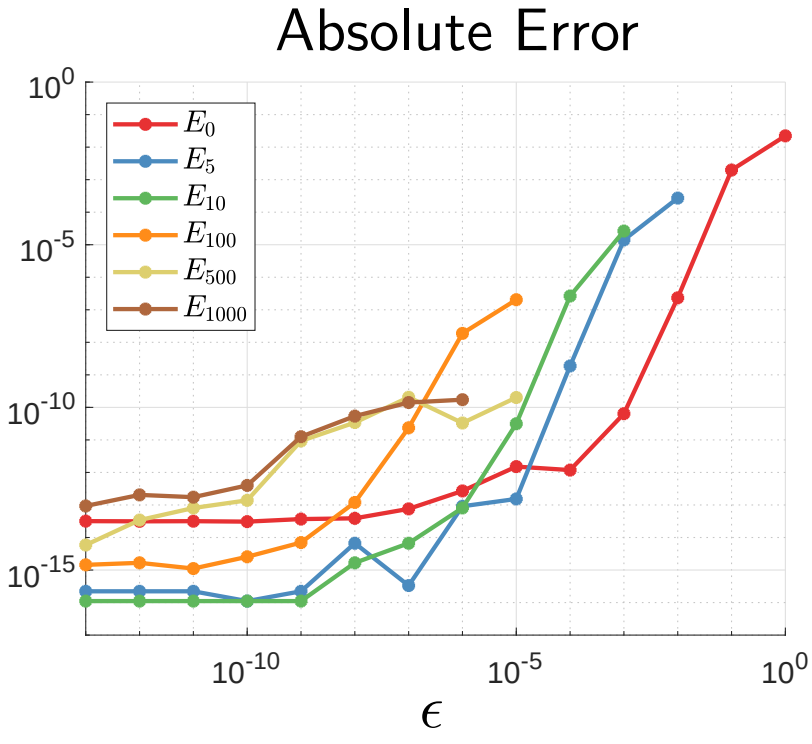
- Describes the motion of a relativistic electron.
- Essential spectrum given by $\mathbb{R}\backslash(-1,1) \Rightarrow$ spectral pollution!
- Consider radially symmetric potential, coupled system on half-line:

$$\mathcal{D}_V = \begin{pmatrix} 1+V(r) & -\frac{d}{dr}+\frac{-1}{r} \\ \frac{d}{dr}+\frac{-1}{r} & -1+V(r) \end{pmatrix}, \quad V(r) = \frac{\gamma}{r}.$$

- Map to $[-1,1]$ and solve shifted linear systems using sparse spectral methods.

Example II: Eigenvalue hunting





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

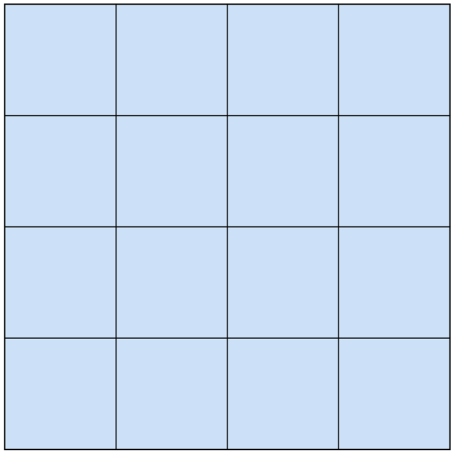
Example III: Chern numbers

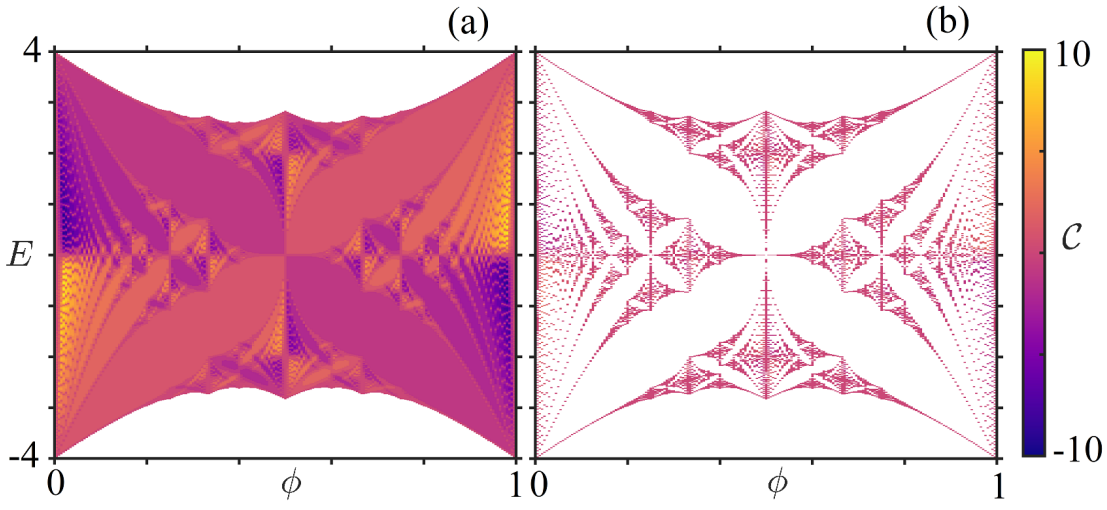
Finite dimensions	**Infinite dimensions**
$\hat{P}^n = \sum_{m=1}^{n} \lvert m\rangle\langle m\rvert, \;\; \hat{Q}^n = I - \hat{P}^n$	$\hat{P}^E = \int_{(-\infty, E]} d\mathcal{E}(\lambda)$
	$\hat{P}^E_\epsilon = \int_{-\infty}^{E} [K_\epsilon * \mathcal{E}](\lambda) d\lambda, \;\; \hat{Q}^E_\epsilon = I - \hat{P}^E_\epsilon$
$\hat{x}^n = \hat{Q}^n \hat{x} \hat{P}^n, \;\; \hat{y}^n = \hat{P}^n \hat{y} \hat{Q}^n$	$\hat{x}^E_\epsilon = \hat{Q}^E_\epsilon \hat{x} \hat{P}^E_\epsilon, \;\; \hat{y}^E_\epsilon = \hat{P}^E_\epsilon \hat{y} \hat{Q}^E_\epsilon$
$\mathcal{C}^n_i = -\frac{4\pi}{A_c^2} \mathrm{Im}\left\{\langle i \rvert \hat{x}^n \hat{y}^n \lvert i\rangle\right\}$	$\mathcal{C}^E_i = \frac{-4\pi}{A_c^2} \mathrm{Im}\left\{\langle i \rvert \hat{x}^E_\epsilon \hat{y}^E_\epsilon \lvert i\rangle\right\}$

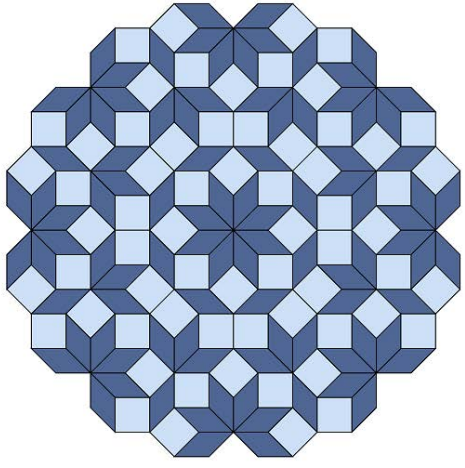
Take maximal count over site i.

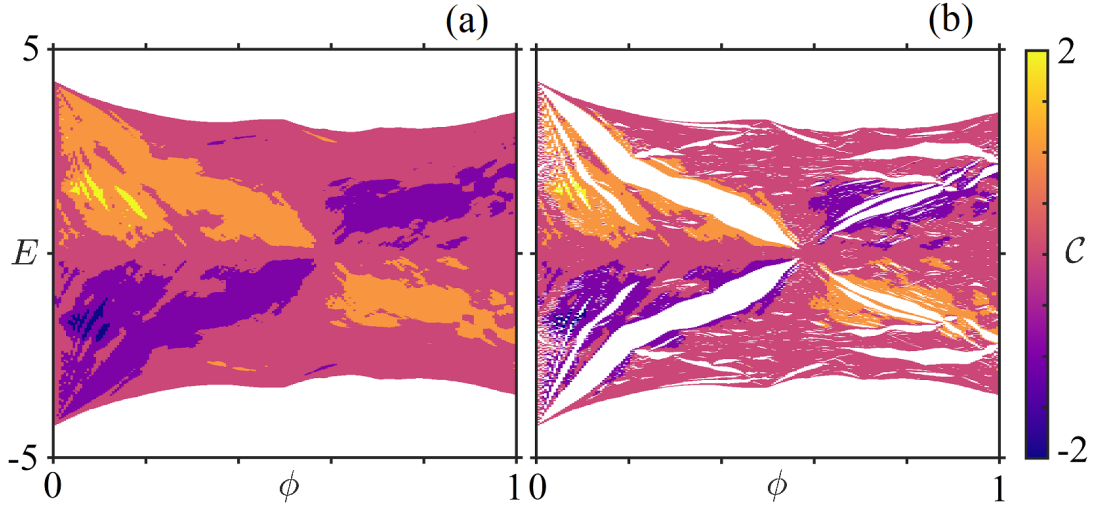
Intuition: Topological index to detect in-gap (conducting) state.

Example III: Chern numbers









Conclusion of Part II

- **Diagonalisation:** General framework for computing spectral measures and projections of self-adjoint operators.
- Convolution with **rational kernels**:
  - Can be evaluated using resolvent. ALL you need to be able to do is solve linear systems and compute inner products.
  - High-order kernels $\Rightarrow$ high-order convergence.
- Fast, local and parallelisable $\Rightarrow$ State-of-the-art results for PDEs, integral operators and discrete operators.
- Example: Chern numbers of BLSs showing they are in-gap.

Code: https://github.com/SpecSolve (written with Andrew Horning).

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, A.C. Hansen. "The foundations of spectral computations via the Solvability Complexity Index hierarchy: Part I." *arXiv preprint*.
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- M.J. Colbrook. "Computing spectral measures and spectral types." *Communications in Mathematical Physics*, to appear.
- M.J. Colbrook, A. Horning, and A. Townsend. "Computing spectral measures of self-adjoint operators." *SIAM Review*, to appear.
- M.J. Colbrook. "Computing semigroups with error control." *preprint*.

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

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

Contents of extra slides

- Extension to PDEs.
- Extension to non-Hermitian operators.
- BLSs without rotational symmetry.
- 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 $\gamma_n(z)$.
- 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

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

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

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

- Measures conditioning of the problem through

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

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

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

Idea II: Locally compute distance function and minimisers

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

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

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

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

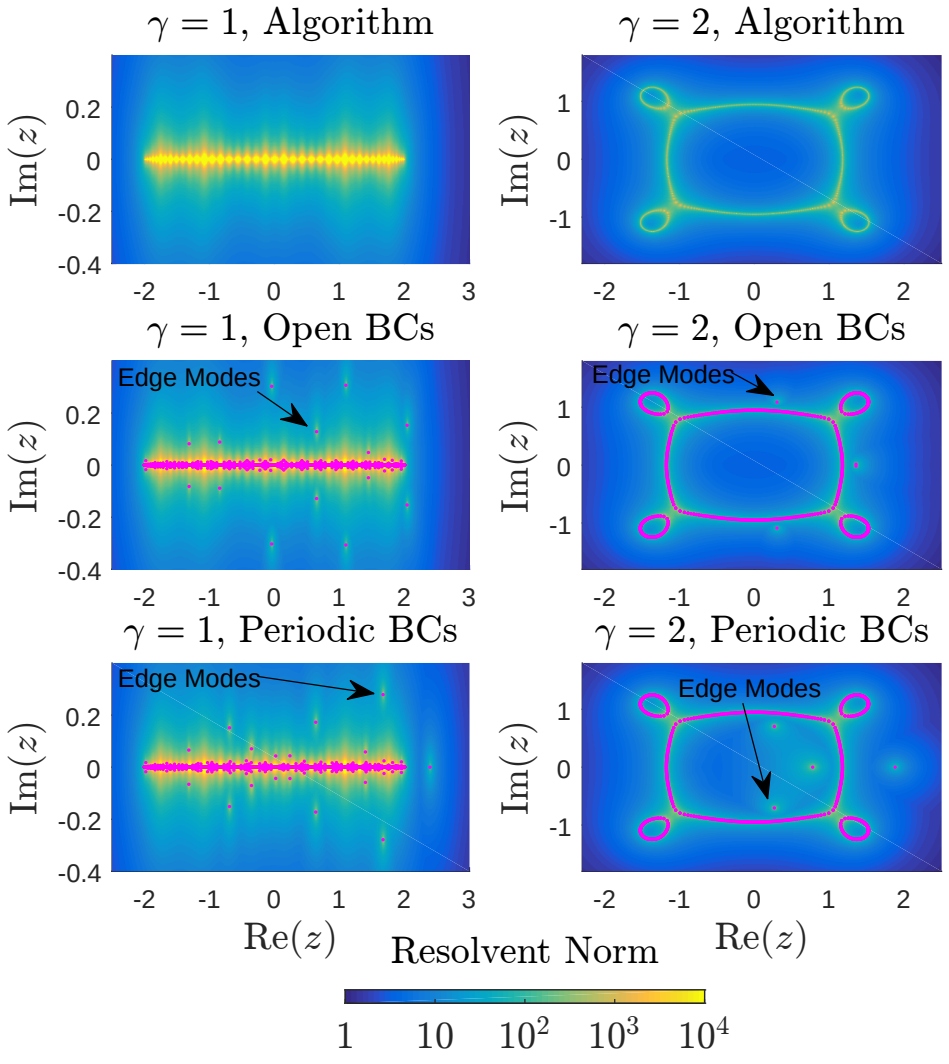
Example: PT symmetry (non-Hermitian QM)

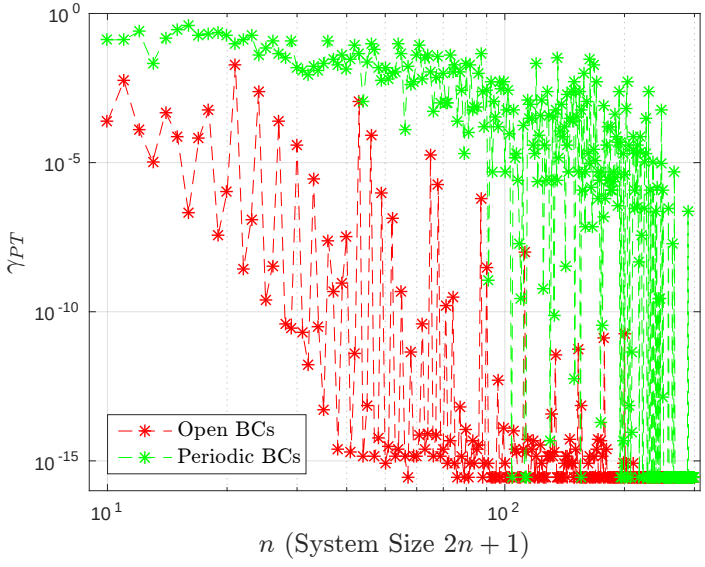
- PT symmetry: invariance w.r.t. simultaneous action of parity-inversion and time reversal.
- Operators with unbroken PT symmetry may poses real spectra, unitary time evolution etc.

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

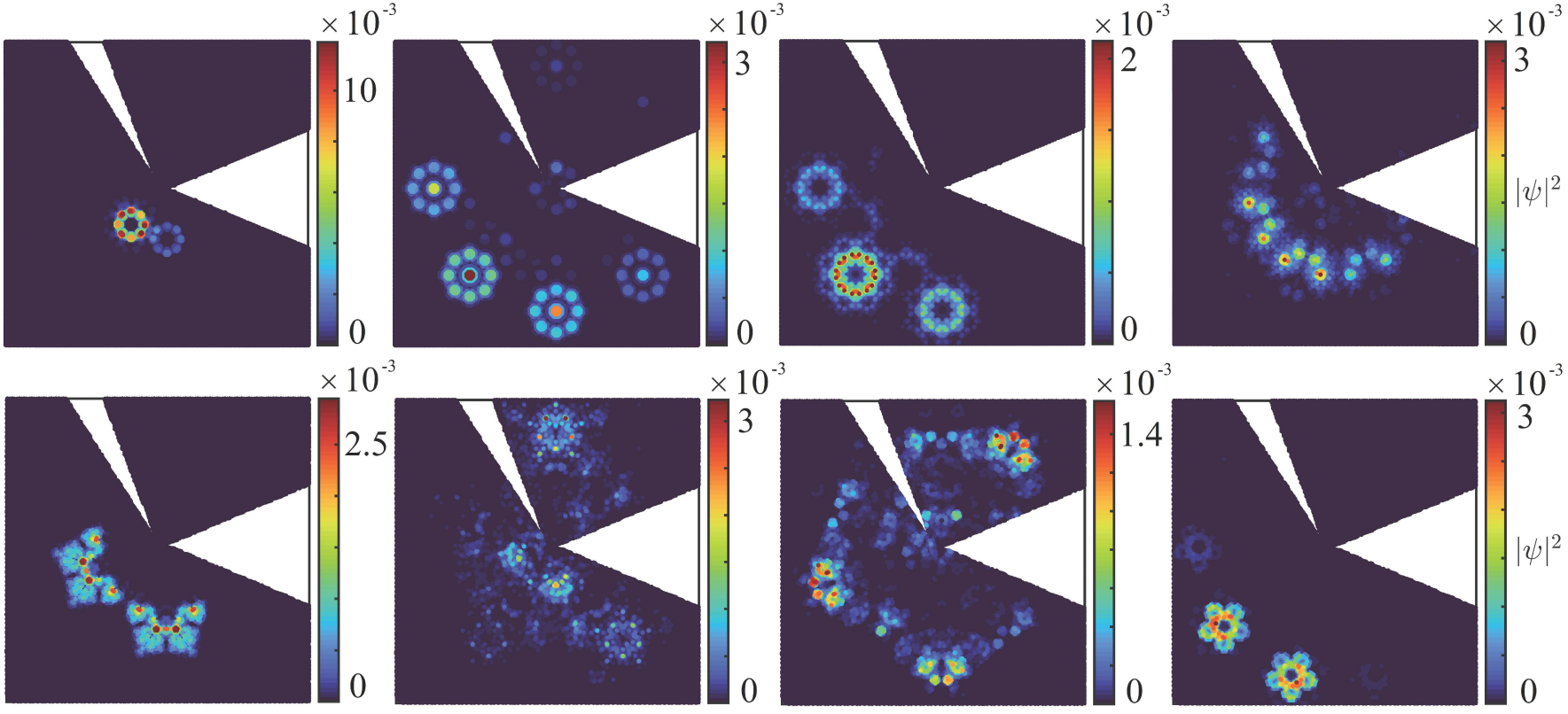
- Increase γ to get complex spectrum.
- Phase transition depends on boundary conditions.
- Rigorously compute this at $\gamma_{PT} \approx 1$.

Example: *PT* symmetry (non-Hermitian QM)

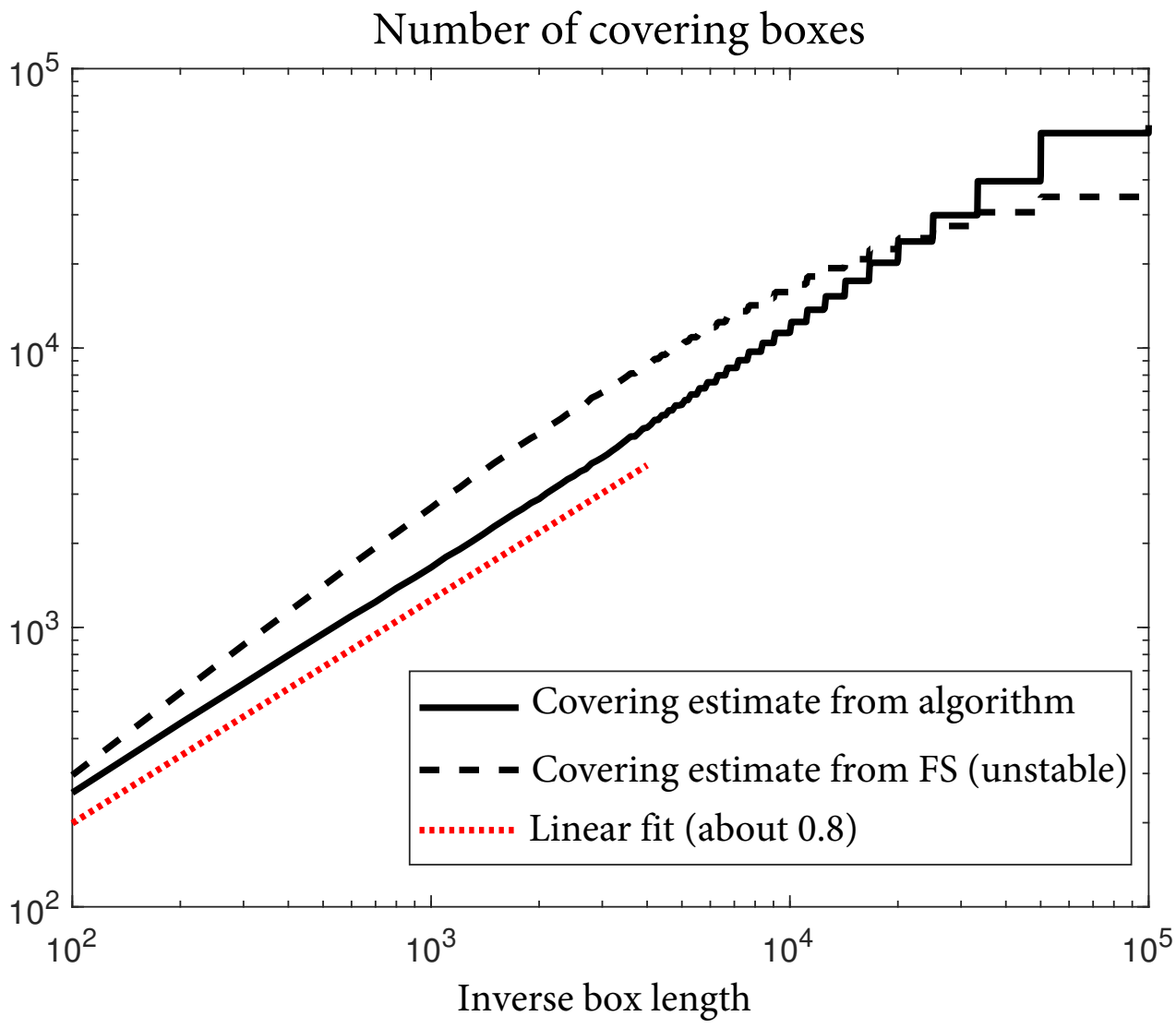




BLS for symmetry broken tilings



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"