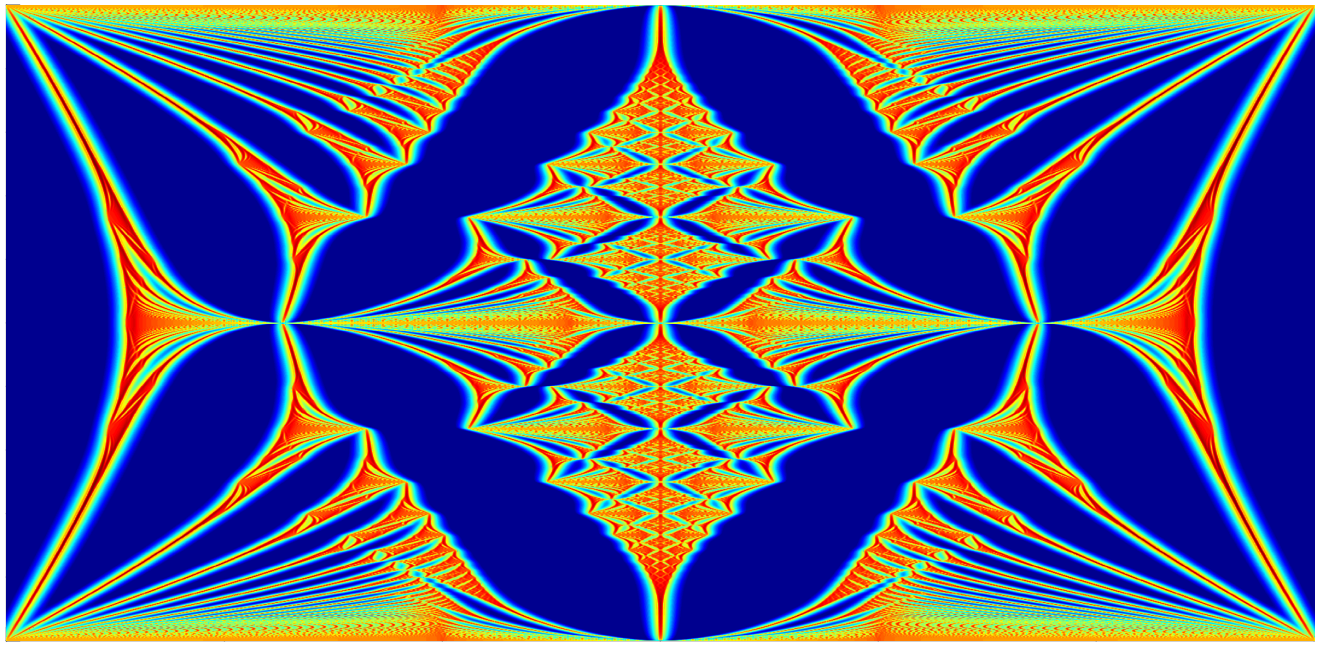
Infinite-Dimensional Spectral Computations

Student Mechanics Seminar 26th March

Matthew Colbrook
University of Cambridge

Andrew Horning
Cornell University



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 harder and more subtle than finite dimensions!

§	Problem	Main References
I	Spectra	"**How to compute spectra with error control**" C., Roman, Hansen, *Physical Review Letters*, 2019
II	Discrete Spectra	"**FEAST for differential eigenvalue problems**" H., Townsend, *SIAM J. on Num. Analysis*. 2020
III	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'

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

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

Finite-dimensional NLA $\rightsquigarrow$ Infinite-dimensional NLA

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

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

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 inner product space in infinite dimensions):

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

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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Method of this talk:

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- Converges without missing parts of spectrum. ✓

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- 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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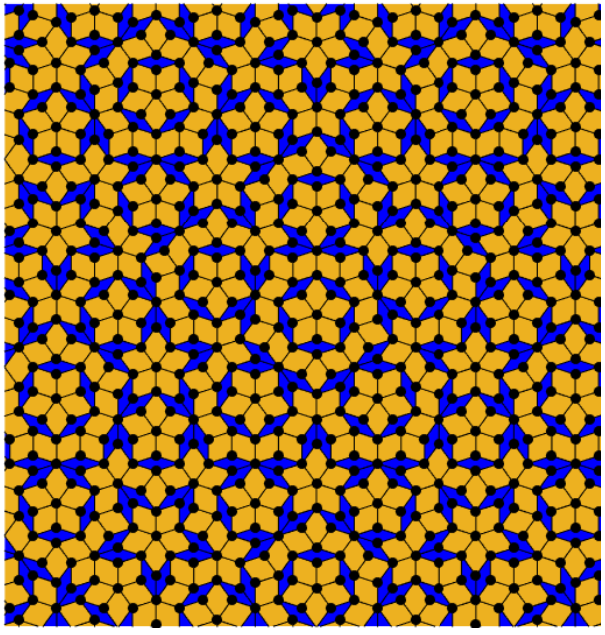
- Computationally efficient. ✓

Case study: Quasicrystals

Quasicrystals: aperiodic structures with long-range order.



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

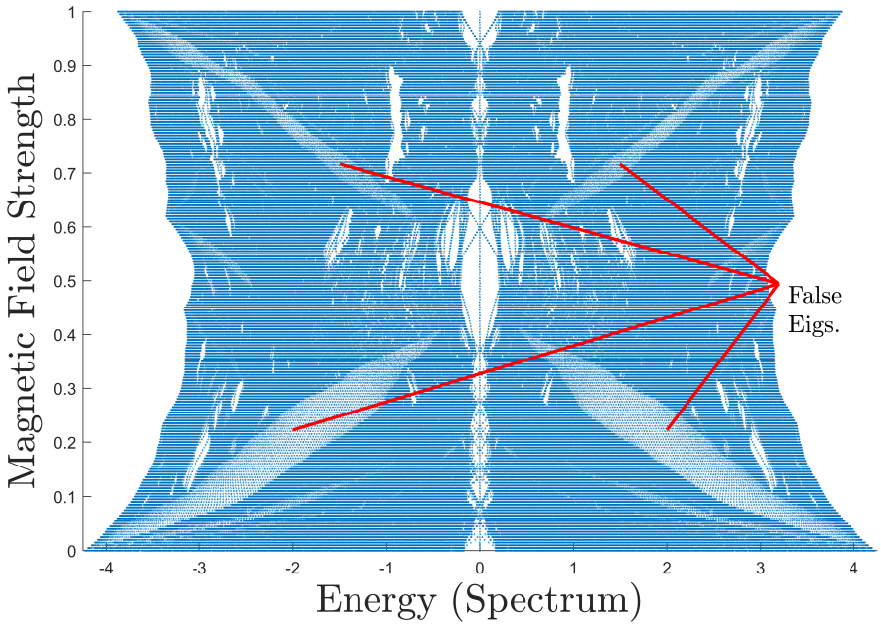
$$[A\psi]_i = \sum_{i\sim j} (\psi_j - \psi_i),$$

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

Model 1: Magnetic field

Finite truncations

Spectral pollution.



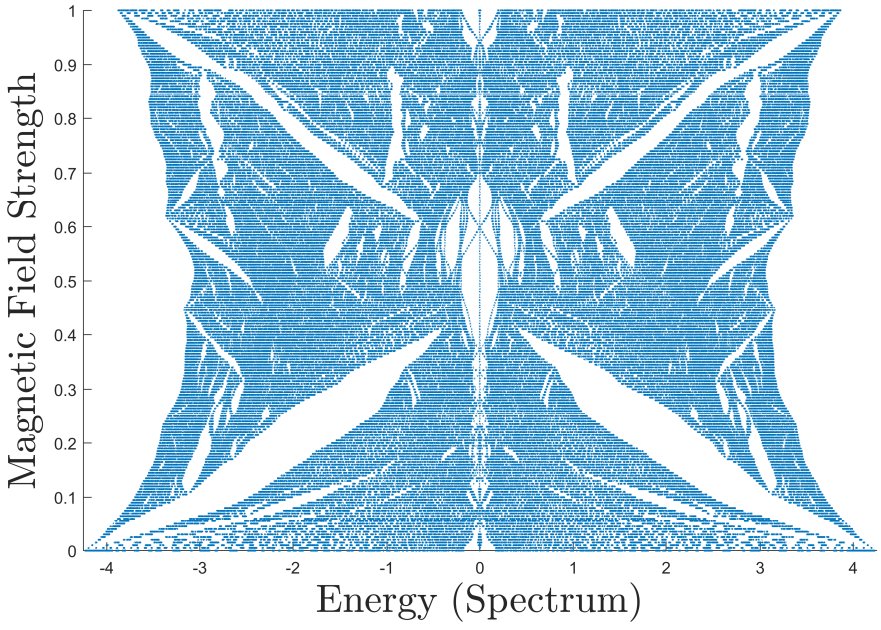
Unreliable

Does not converge

No error control

New method

First convergent computation.

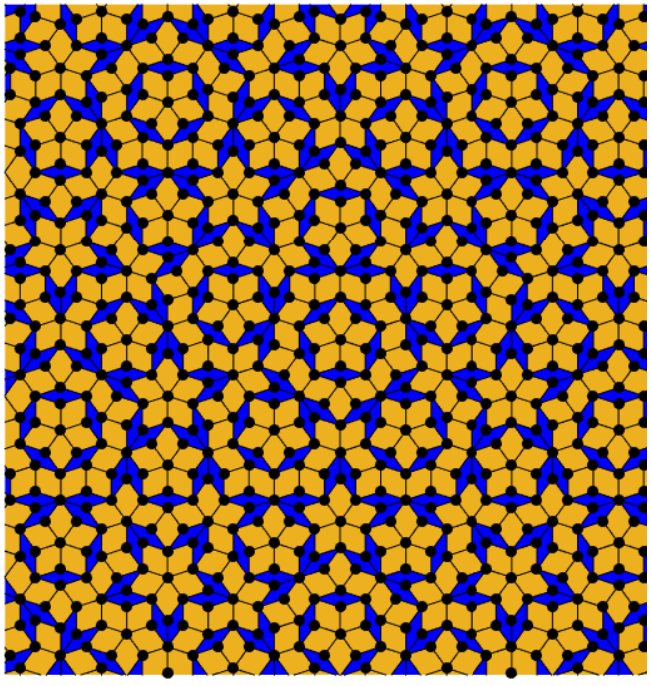


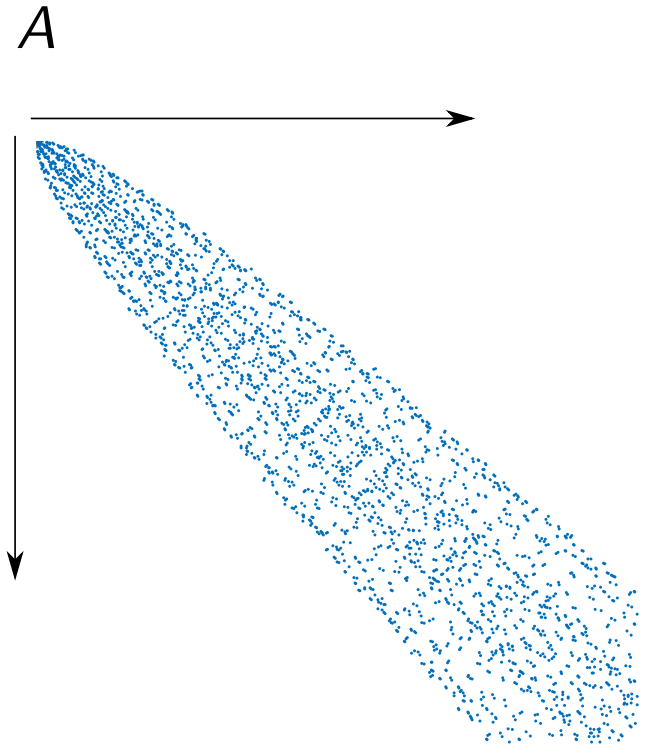
Reliable

Converges

Error control

Idea I: Rectangular truncations





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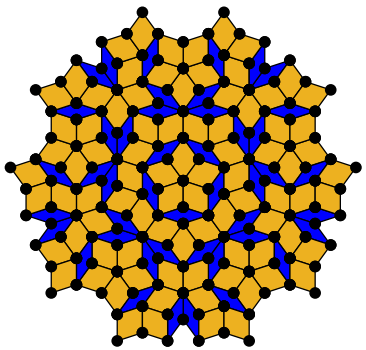

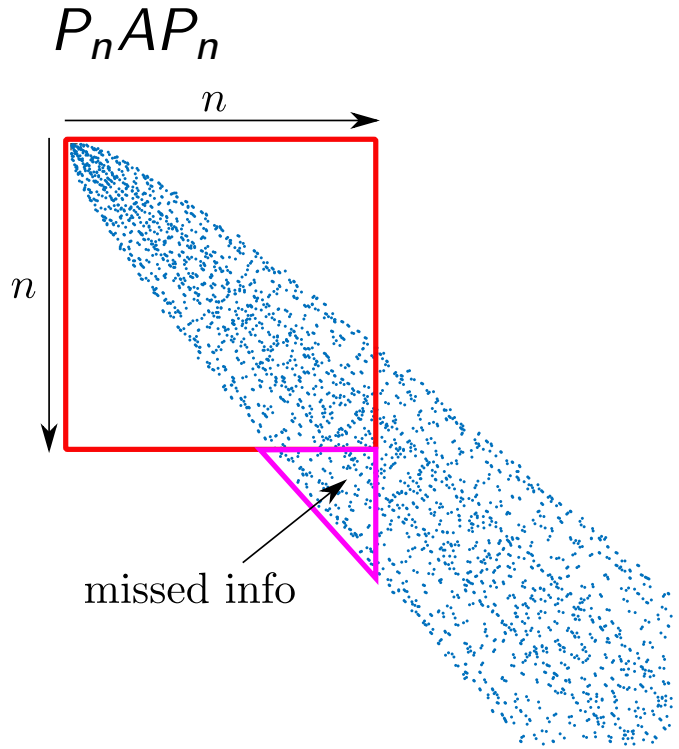

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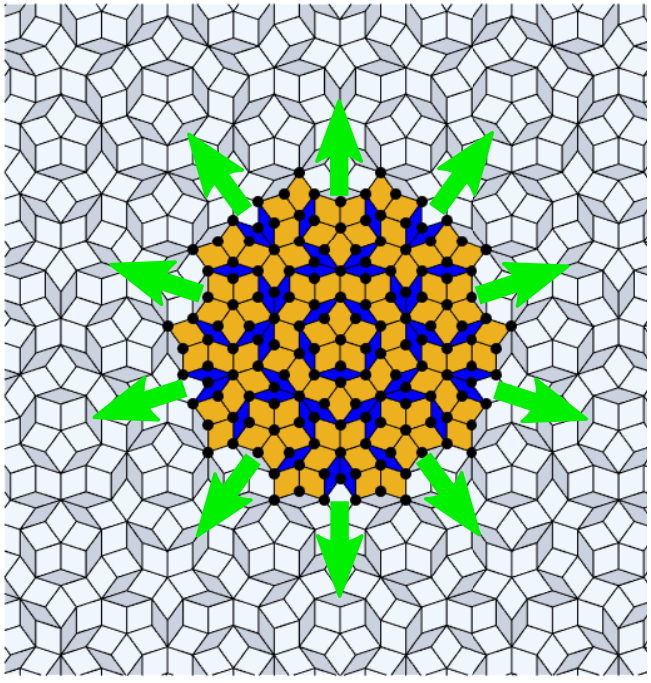
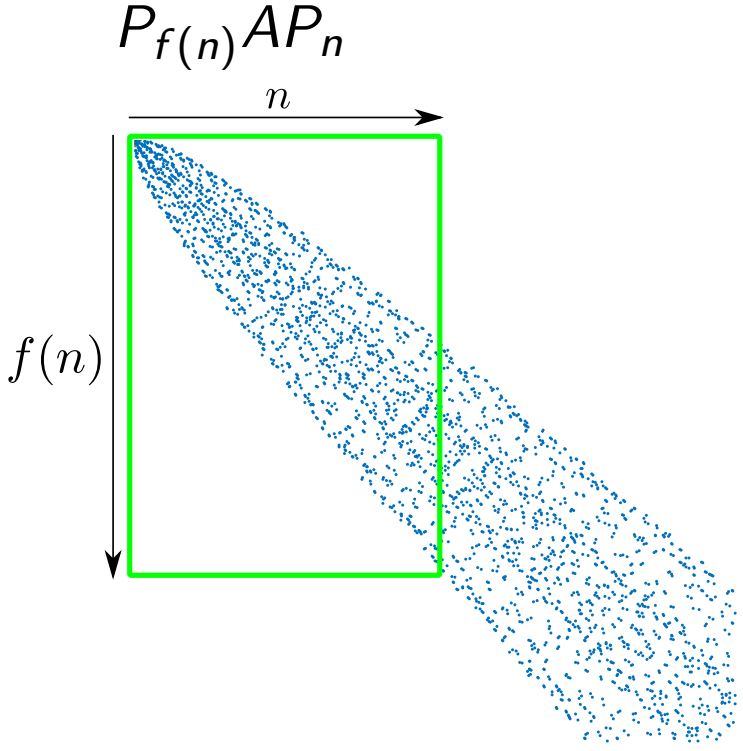




Locally compute distance function and minimisers

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

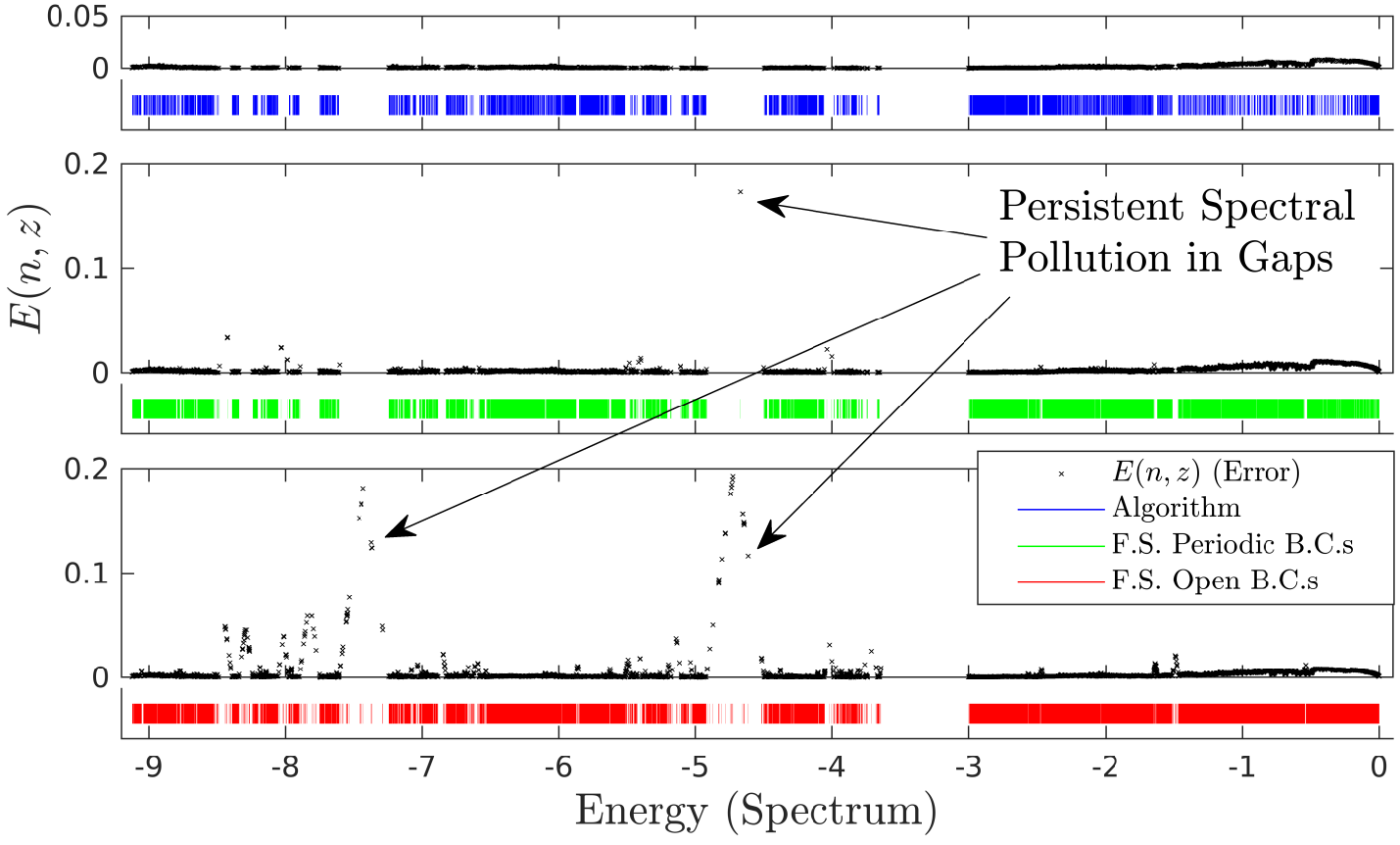
$\Downarrow$ smallest singular values $\sigma_1(P_{f(n)}(A - zI)P_n)$

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

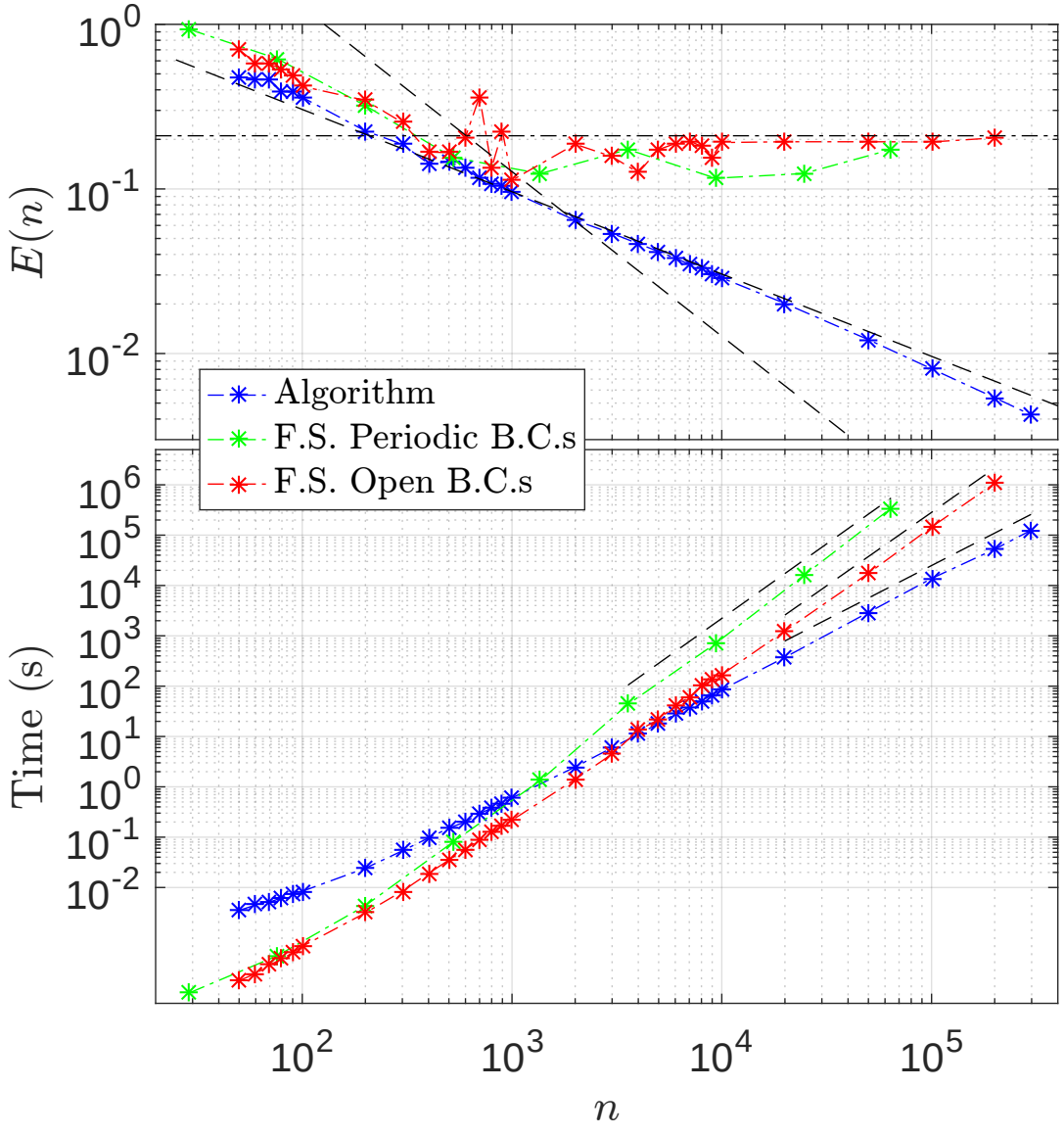
$\Downarrow$ local minimisers

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

Model 2: Graph Laplacian (electronic properties)



Model 2: Graph Laplacian (electronic properties)



Advantages

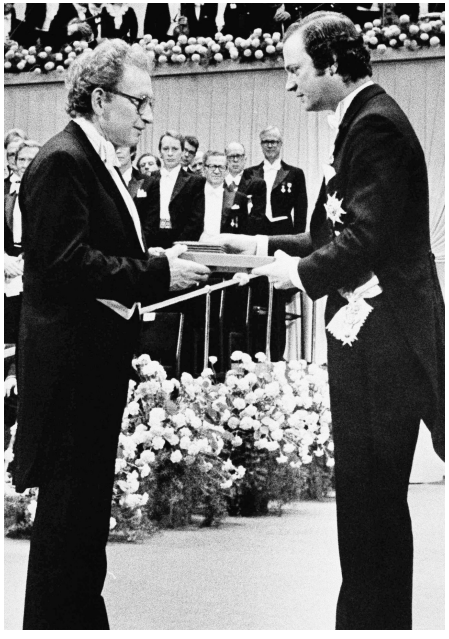
- First method that always converges to correct solution.
  (e.g. no spectral pollution)
- Local and parallelisable $\Rightarrow$ FAST!
- Explicitly bounds the error:

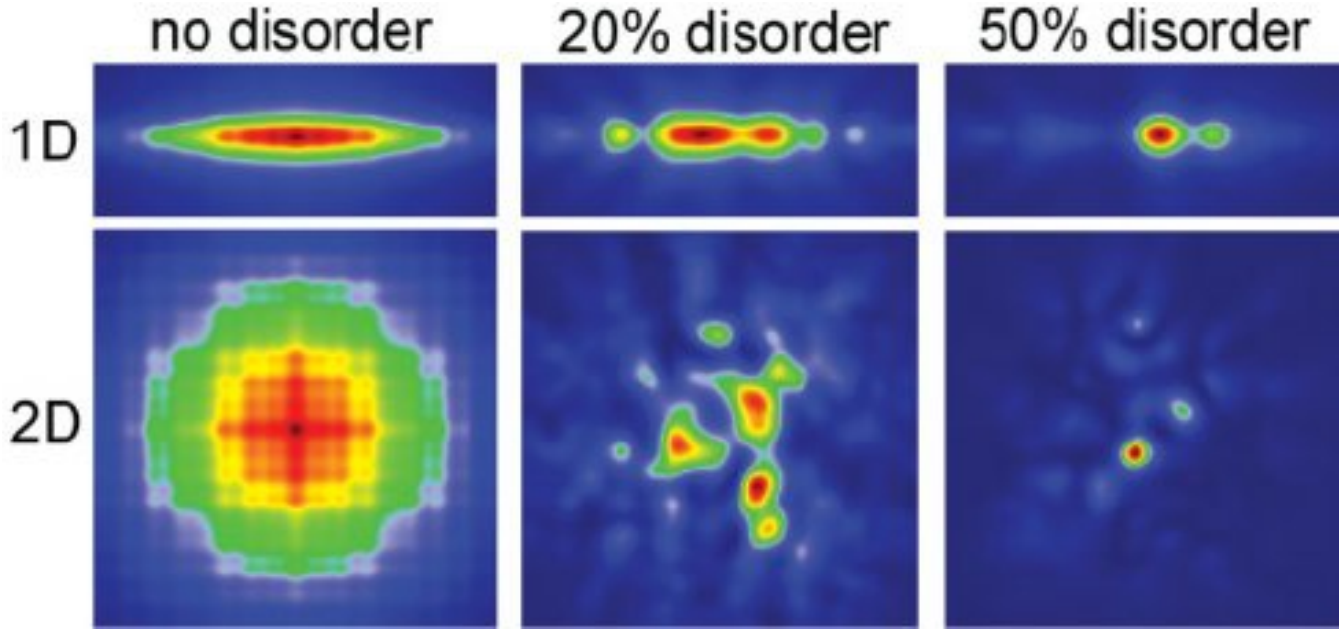
$$\text{Error} \leq E_n \downarrow 0.$$

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

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.

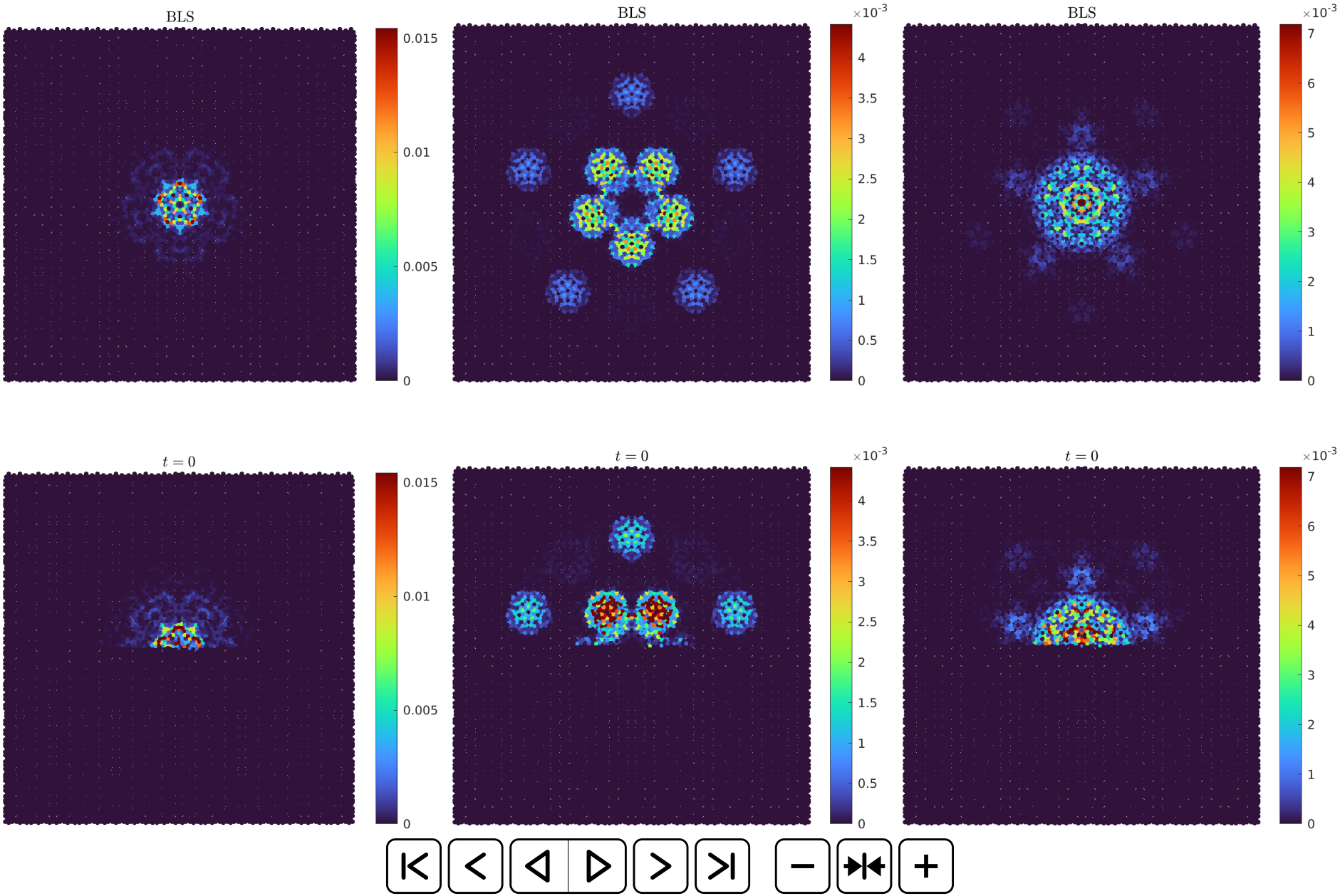
What happens in aperiodic systems? Do we need disorder?

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 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.
- New type of Bulk Localised State (BLS) for magnetic quasicrystals that support localised transport within the bulk.

Part II: Discrete Spectrum

H. and Townsend, **FEAST for differential eigenvalue problems**, *SIAM Journal on Numerical Analysis*, 2020.

The infinite-dimensional *eigenvalue* problem (IDEP)

$$\mathcal{L}u = \lambda u, \qquad u \in \mathcal{D}(\mathcal{L}) \subset \mathcal{H}$$

For example…

Integral operator

$$[\mathcal{L}u](x) = a(x)u(x) + \int_{-1}^{1} k(x,y)u(y)\,dy$$

Ordinary differential operator

$$[\mathcal{L}u](x) = a_K(x)u^{(k)}(x) + \cdots + a_1(x)u'(x) + a_0(x)u(x)$$

Partial differential operator

$$[\mathcal{L}u](x) = -\nabla \cdot (A(x)\nabla u) + \mathbf{b}(x) \cdot \nabla u + c(x)u$$

*Domain $\mathcal{D}(\mathcal{L})$ usually encodes smoothness, integrability, and/or boundary conditions

Droplet formation

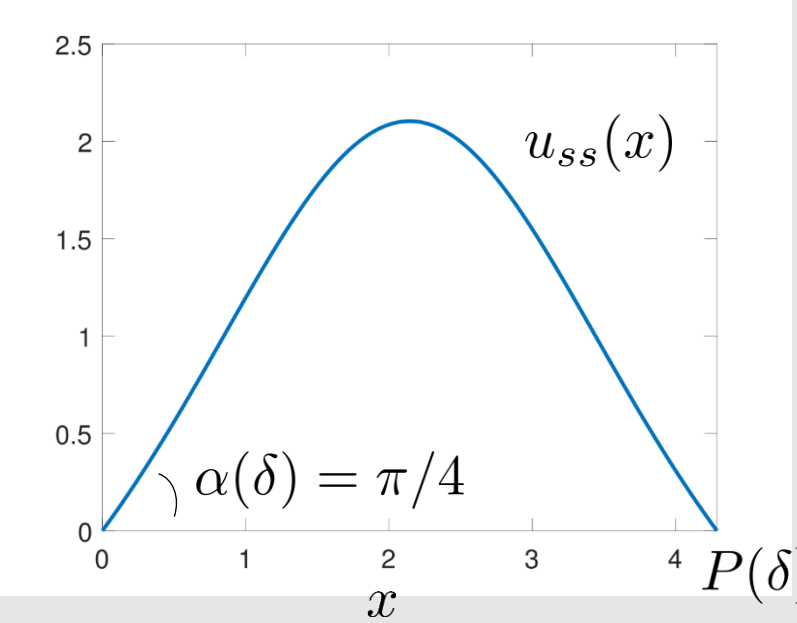
$$u_t = \partial_x^4 u + \partial_x(u\partial_x u)$$

Linear

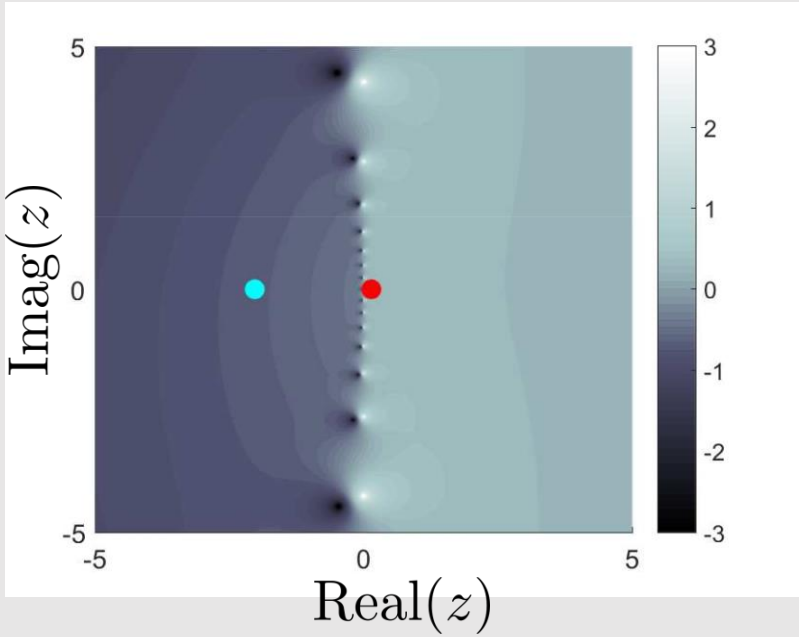
stability

$$-\frac{d^4u}{dx^4} - \frac{d}{dx}\left(u_{ss}\frac{du}{dx}\right) = \lambda u,$$

$$u(0) = u(l) = 0, \quad u''(0) = u''(l) = 0$$



$P(\delta) = 4.2891$

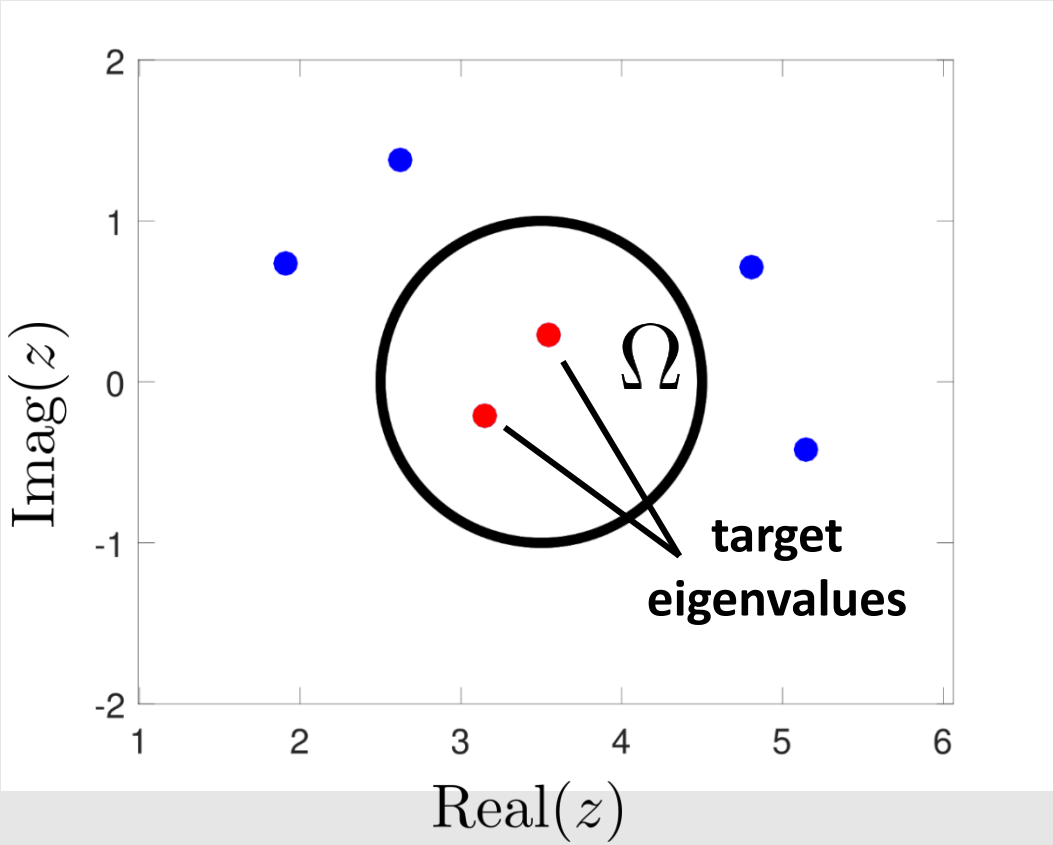



```
L=chebop(0,P);
L.op=@(x,u) -diff(u,4)-diff(uss(x)*diff(u));
L.lbc=@(u) [u; diff(u,2)];
L.rbc=@(u) [u; diff(u,2)];
[V,D]=contFEAST(L,'half_plane','right');
```

Laugesen and Pugh (2000), H. and Townsend (2019)

contFEAST() – a computational framework for IDEP

$$\mathcal{L}u = \lambda u, \qquad u \in \mathcal{D}(\mathcal{L}) \subset \mathcal{H}$$



GOAL: Given a search region Ω, compute all eigenvalues of L in Ω, and associated eigenfunctions.

Key ingredients:

1) Solve shifted linear equations

$$(\mathcal{L} - z)v = f \quad \text{where} \quad v \in \mathcal{D}(\mathcal{L}), f \in \mathcal{H}$$

2) Compute inner products

$$\langle f, g \rangle_{\mathcal{H}} \quad \text{where} \quad f, g \in \mathcal{H}$$

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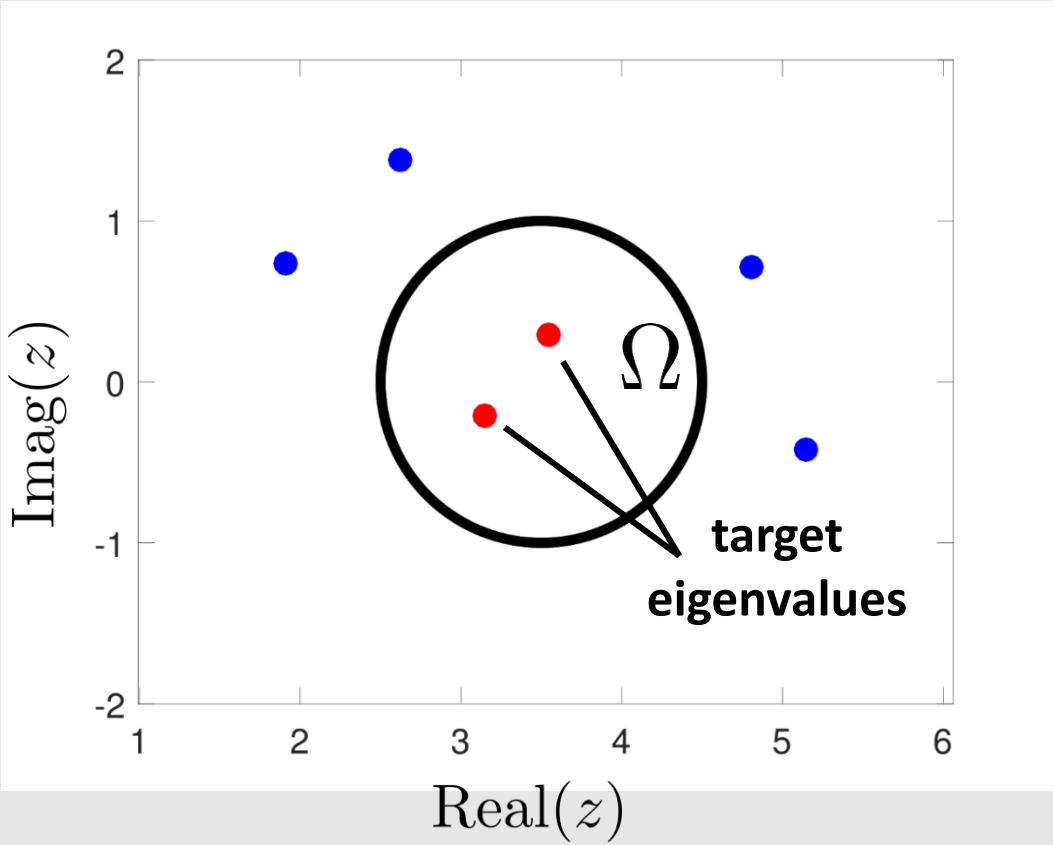

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Key results:

1) If solutions to linear systems and inner products are computed with accuracy $0 < \epsilon < 1$, then*

$$|\lambda_k - \hat{\lambda}_k| \leq C\epsilon\,|\lambda_k|$$

2) Constant C depends only on $\mathcal{L}$ and $\partial\Omega$, but is **independent** of underlying discretization or approximation scheme

*See [H. and Townsend, 2020]

How it works: a continuous analogue of FEAST

contFEAST() – Compute eigenvalues of operator in target region.

Spectral Projection **Range Sketching** **Rayleigh—Ritz Step**

Build basis for target eigenspace

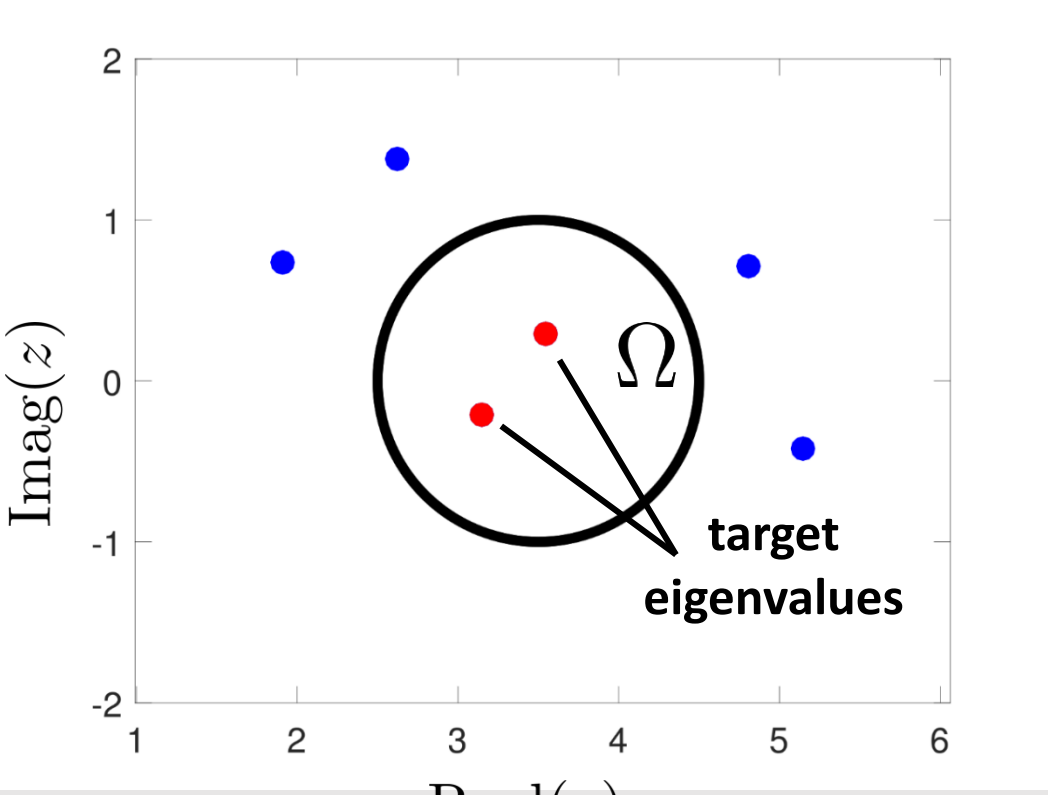
Small eigenvalue problem for target eigenvalues and eigenvectors

How it works: a continuous analogue of FEAST

contFEAST() – Compute eigenvalues of operator in target region.

Spectral Projection **Range Sketching** **Rayleigh—Ritz Step**

$$P_\Omega(\mathcal{L}) = \sum_{\ell=1}^{M} w_k(\mathcal{L} - z_k)^{-1}$$



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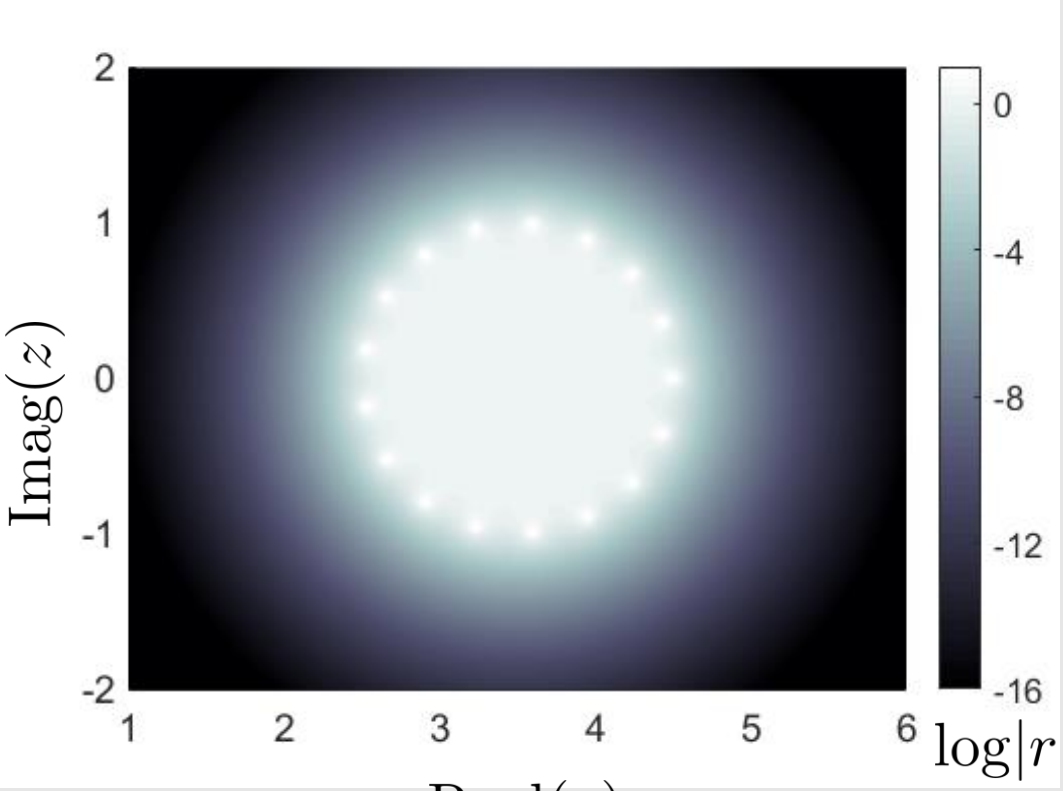


scalar filter $$r(\lambda) = \sum_{\ell=1}^{M} w_k(\lambda - z_k)^{-1}$$

op. filter $$r(\mathcal{L}) = \sum_{k=1}^{\infty}\sum_{\ell=1}^{M} w_\ell(\lambda_k - z_\ell)^{-1} P_k$$

$$= \sum_{\ell=1}^{M} w_\ell(\mathcal{L} - z_\ell)^{-1}$$

How it works: a continuous analogue of FEAST

contFEAST() – Compute eigenvalues of operator in target region.

Spectral Projection **Range Sketching** **Rayleigh—Ritz Step**

$$V = P_\Omega(\mathcal{L})Y$$

$v_i \in \mathrm{range}(P_\Omega(\mathcal{L}))$ ← $P_\Omega(\mathcal{L})$ ← $y_i \in \mathcal{H}$

$V = [v_1 \ \cdots \ v_m]$

Filters out unwanted eigencomponents

$Y = [y_1 \ \cdots \ y_m]$

$v_1, \ldots, v_m$ approximates a basis for the target eigenspace

How it works: a continuous analogue of FEAST

contFEAST() – Compute eigenvalues of operator in target region.

Spectral Projection **Range Sketching** **Rayleigh—Ritz Step**

$$L = Q^* \mathcal{L} Q$$

Orthonormalize basis $v_1, \ldots, v_m$ using $\langle \cdot, \cdot \rangle$

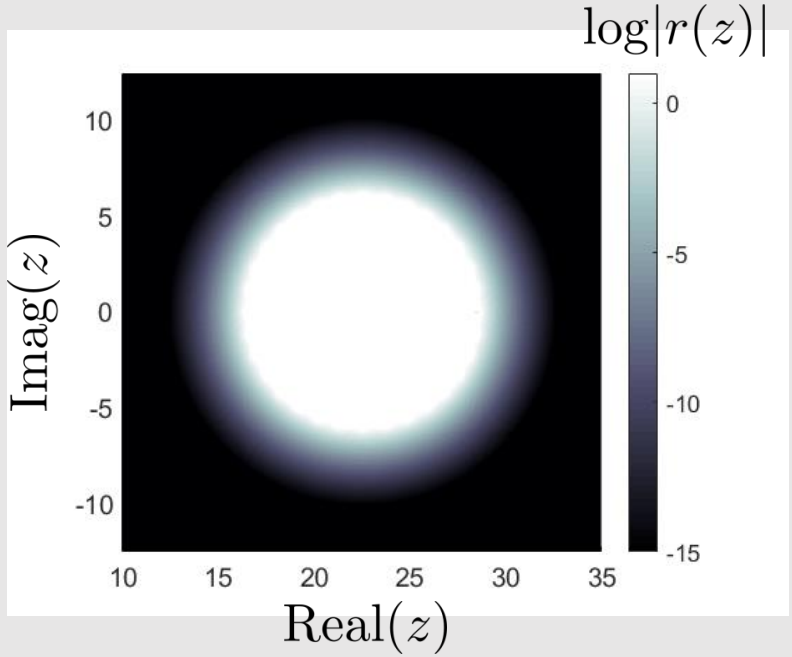
New orthonormal basis $q_1, \ldots, q_m$

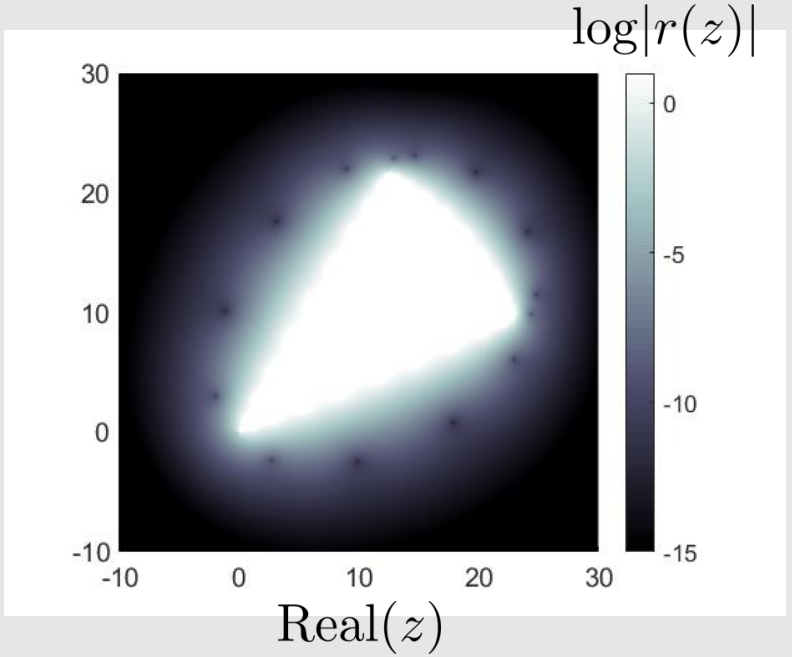
$$u_j = \sum_{i=1}^{m} c_k^{(j)} q_k$$

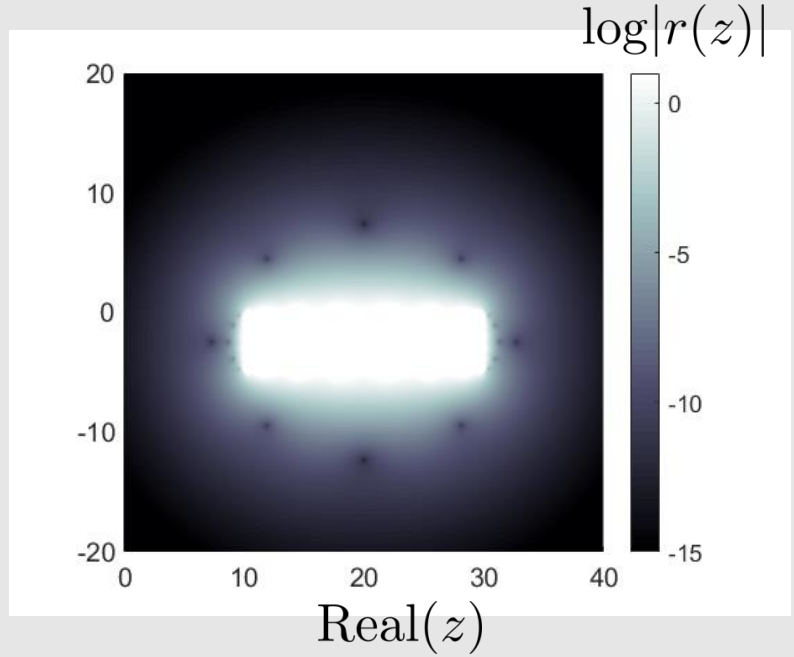
Eigenvector coordinates satisfy

$$\underbrace{\begin{pmatrix} L_{1,1} & \cdots & L_{1,m} \\ \vdots & \ddots & \vdots \\ L_{m,1} & \cdots & L_{m,m} \end{pmatrix}}_{L_{i,j} = \langle q_i, \mathcal{L} q_j \rangle} \begin{pmatrix} c_1^{(j)} \\ \vdots \\ c_m^{(j)} \end{pmatrix} = \lambda_j \begin{pmatrix} c_1^{(j)} \\ \vdots \\ c_m^{(j)} \end{pmatrix}$$

Target regions and rational filters



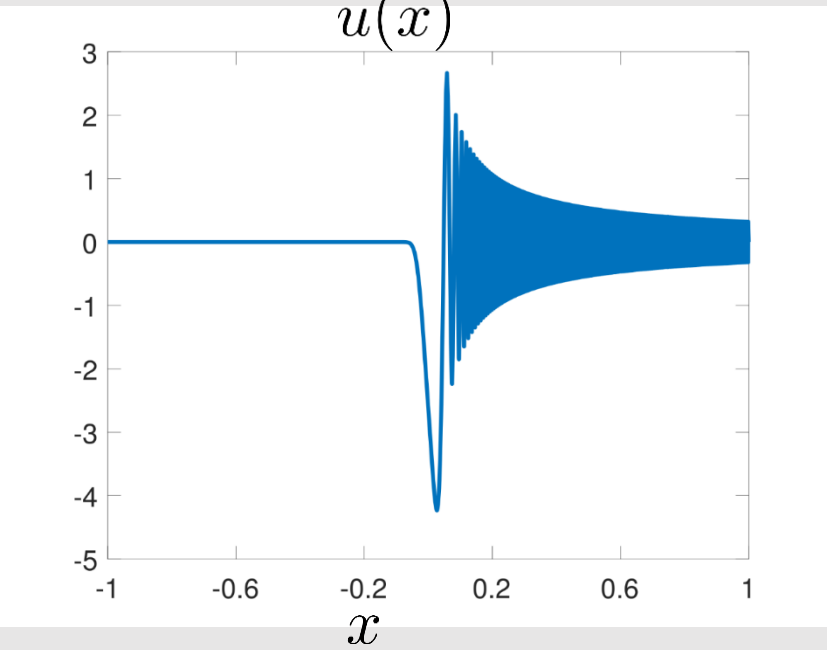




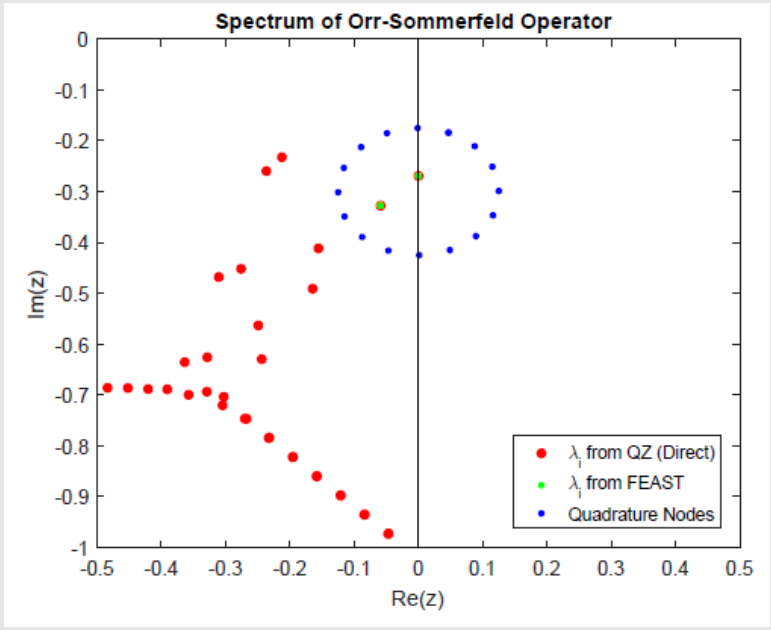
Use any closed, piecewise-smooth curve. For example…

```
%FEAST with a circular search region
cntr=22.5; rad=6;
circle=chebfun(@(t) cntr+rad*exp(2*pi*1i*t),[0 1]);
[V,D]=contFEAST(L,circle);
```

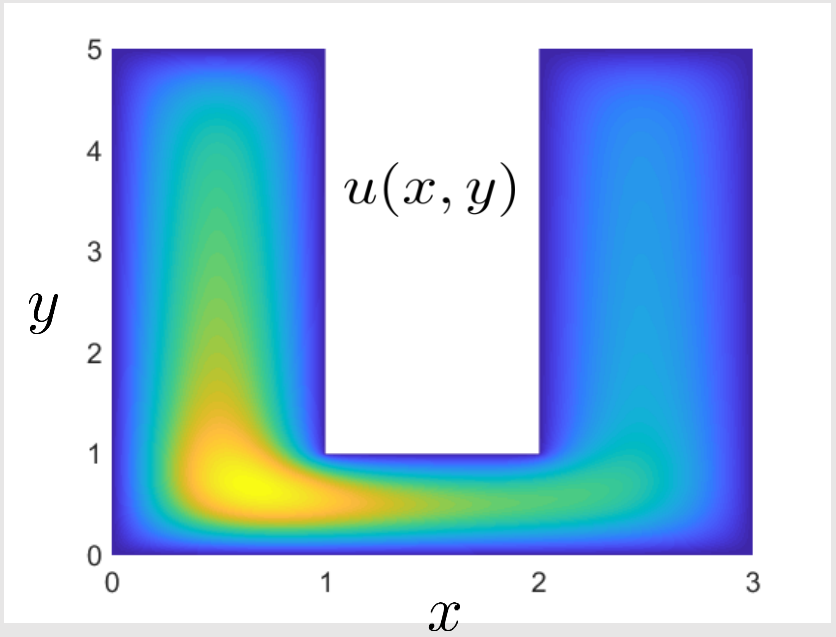
Leveraging adaptive spectral methods



ApproxFun (Julia)



Chebfun (Matlab)



ultraSEM (Matlab)

Part III: Spectral Measures

Colbrook, H., and Townsend, **Computing spectral measures of self-adjoint operators**, *SIAM Review* (to appear).

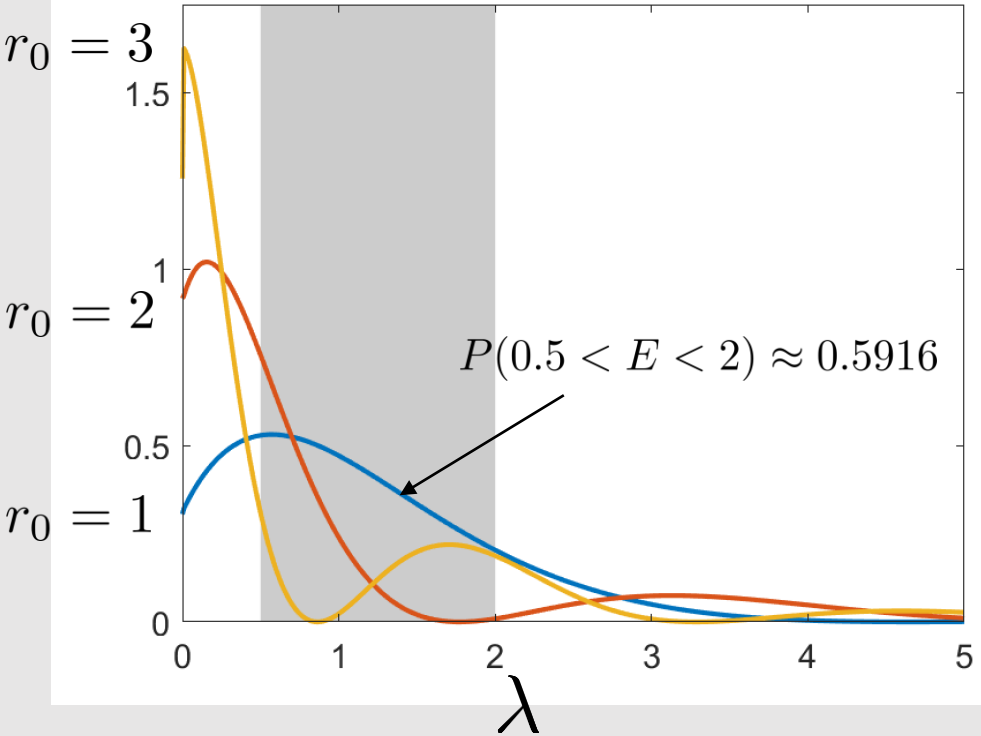
Spectral measures in QM

Hellman potential

$$\mathcal{L}u = -\frac{d^2u}{dr^2} + \left(\frac{\ell(\ell+1)}{r^2} + \frac{1}{r}\left(e^{-r} - 1\right) \right) u$$

centrifugal term

continuous spectral measures



$$f_{r_0}(r) = C_{r_0} e^{-(r-r_0)^2}$$

Wave function

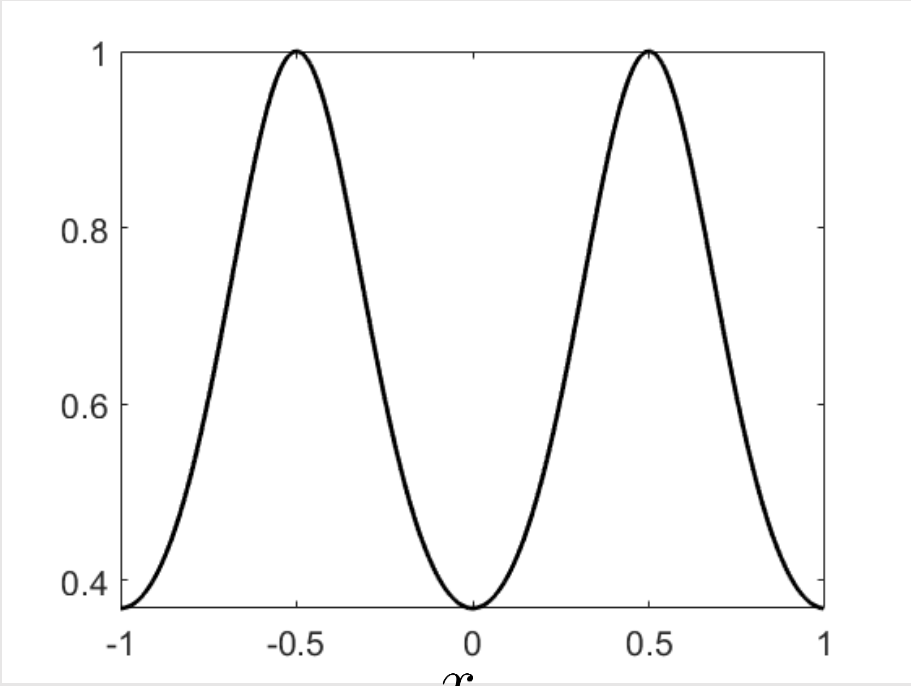
Specsolve code

```
normf = sqrt(pi/8)*(2-igamma(1/2,8)/gamma(1/2)); % Normalization
f = @(r) exp(-(r-2).^2)/sqrt(normf);             % Measure wrt f(r)
V={@(r) 0, @(r) exp(-r)-1, 1};                   % Potential, l=1
[xi, wi] = chebpts(20,  [1/2 2]);                % Quadrature rule
mu = rseMeas(V, f, xi, 0.1, 'Order', 4)          % epsilon=0.1, m=4
ion_prob = wi * mu;                              % Ionization prob
```

Diagonalizing an operator

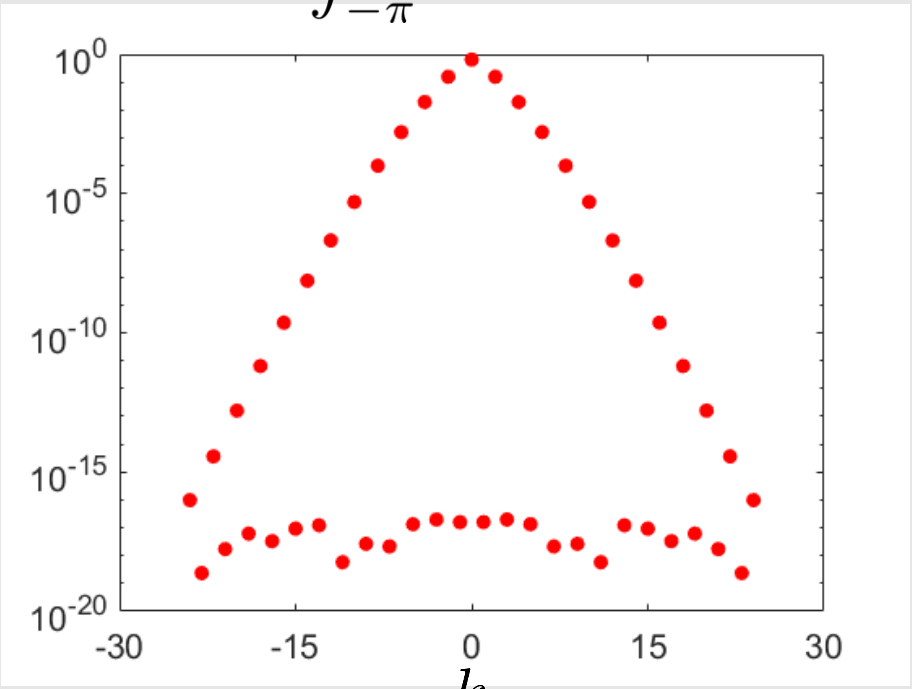
$$-u''(x) = f(x), \qquad u(\pm 1) = 0$$

$$f(x) = \exp(-\cos^2(\pi x))$$



Switch to eigenvector coordinates

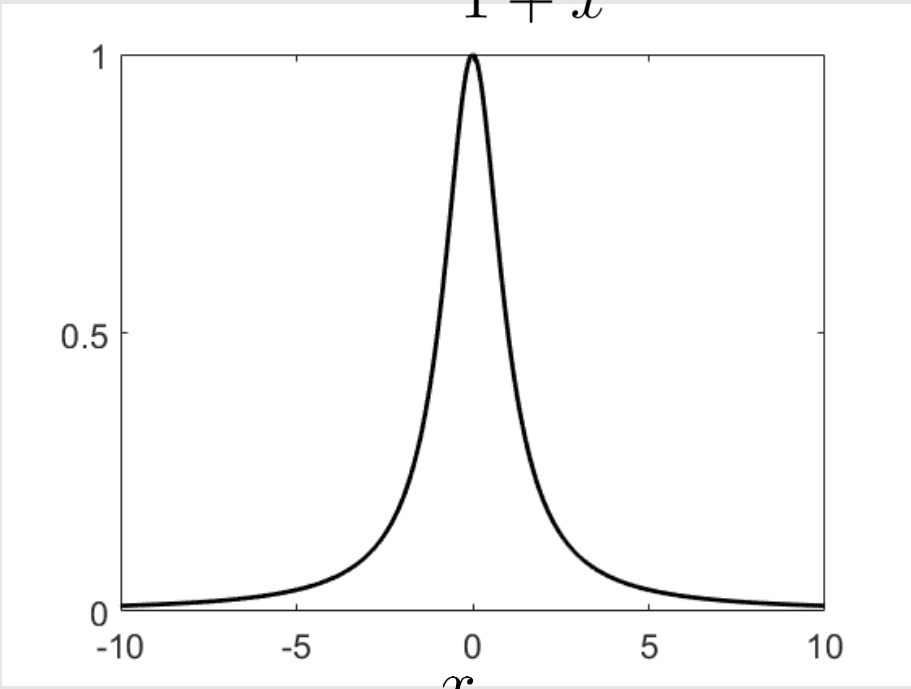
$$\hat{f}(k) = \int_{-\pi}^{\pi} f(x) e^{-2\pi i k x}\, dx$$



Diagonalizing an operator

$$-u''(x) = f(x), \qquad \int_{-\infty}^{\infty} |u'(x)|^2 \, dx < \infty$$

$$f(x) = \frac{1}{1+x^2}$$



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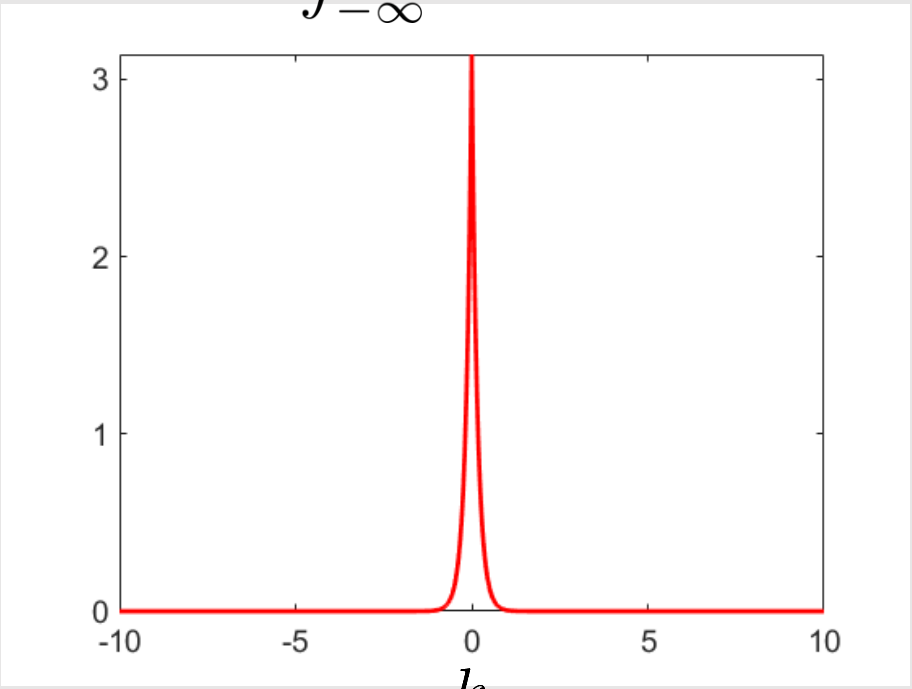


Spectral measures

$\mathcal{L} : \mathcal{D}(\mathcal{L}) \to \mathcal{H}$

self-adjoint operator

Spectral Theorem

$\mathcal{E}(\Omega)$

projection-valued measure

$-u''(x), \qquad -1 \le x \le 1$

discrete spectrum

$$\mathcal{E}([a,b])f = \sum_{a \le \lambda_k \le b} \hat{f}_k \, e^{2\pi i k x}$$

$-u''(x), \qquad -\infty < x < \infty$

continuous spectrum

$$\mathcal{E}([a,b])f = \int_{a \le 2\pi k^2 \le b} \hat{f}(k) \, e^{2\pi i k x} \, dk$$

Spectral measures

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

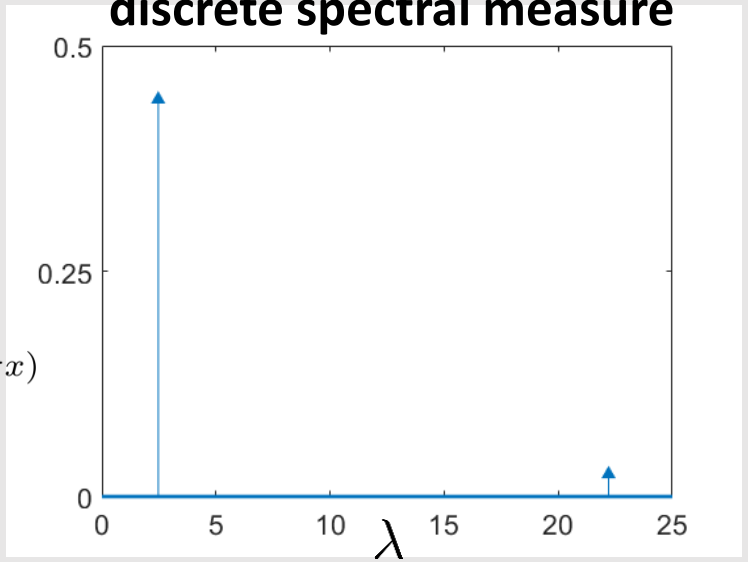
spectral measure w.r.t. f

$$-u''(x), \qquad -1 \le x \le 1$$

discrete spectrum

$$f(x) = e^{-\cos^2(\pi x)}$$

discrete spectral measure



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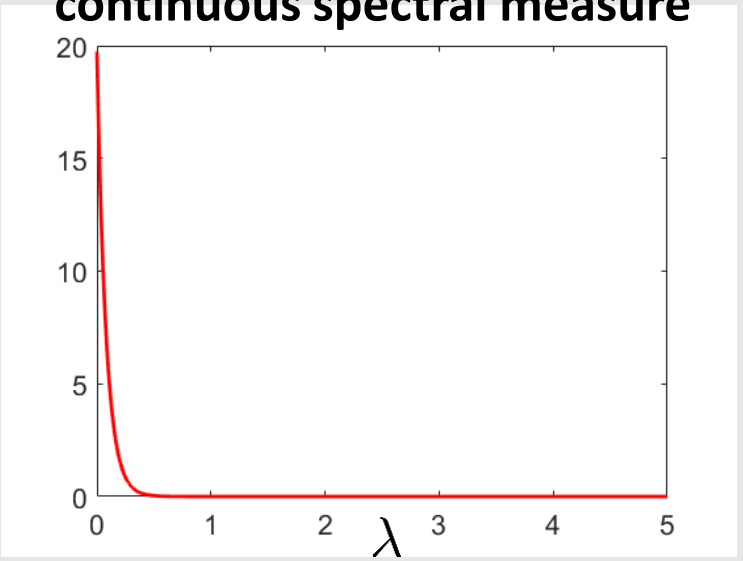
continuous spectrum

$$f(x) = \frac{1}{1+x^2}$$

continuous spectral measure



Smoothed spectral measures: Stone's theorem

$$\mathcal{R}_{\mathcal{L}}(z) = (\mathcal{L} - z)^{-1}$$

Spectral identity for resolvent

$$\langle \mathcal{R}_{\mathcal{L}}(z) f, f \rangle = \int_{\mathbb{R}} \frac{d\mu_f(\lambda)}{\lambda - z}$$

Look at "jump" across real axis

$$\frac{1}{\pi} \underbrace{\left(\langle \mathcal{R}_{\mathcal{L}}(x + i\epsilon) f, f \rangle - \langle \mathcal{R}_{\mathcal{L}}(x - i\epsilon) f, f \rangle \right)}_{\mathrm{Im} \langle \mathcal{R}_{\mathcal{L}}(z) f, f \rangle} = \int_{\mathbb{R}} \underbrace{\frac{1}{\pi} \frac{\epsilon^2}{(\lambda - x)^2 + \epsilon^2}}_{\text{Poisson kernel (shifted and scaled)}} d\mu_f(\lambda)$$

A simple framework

$$\mu_f^\epsilon(\lambda) = \frac{1}{\pi}\mathrm{Im}\langle \mathcal{R}(\lambda + i\epsilon, \mathcal{L})f, f\rangle$$

Given $\lambda_1, \ldots, \lambda_n \in \mathbb{R}$

Fix $\epsilon > 0$ and choose $f \in \mathcal{H}$

For $k = 1, \ldots, n$

1) Solve $(\mathcal{L} - (\lambda_k + i\epsilon)\mathcal{I})u_k = f$

2) Compute $\mu_f^\epsilon(\lambda_k) = \frac{1}{\pi}\mathrm{Im}\langle u_k, f\rangle$

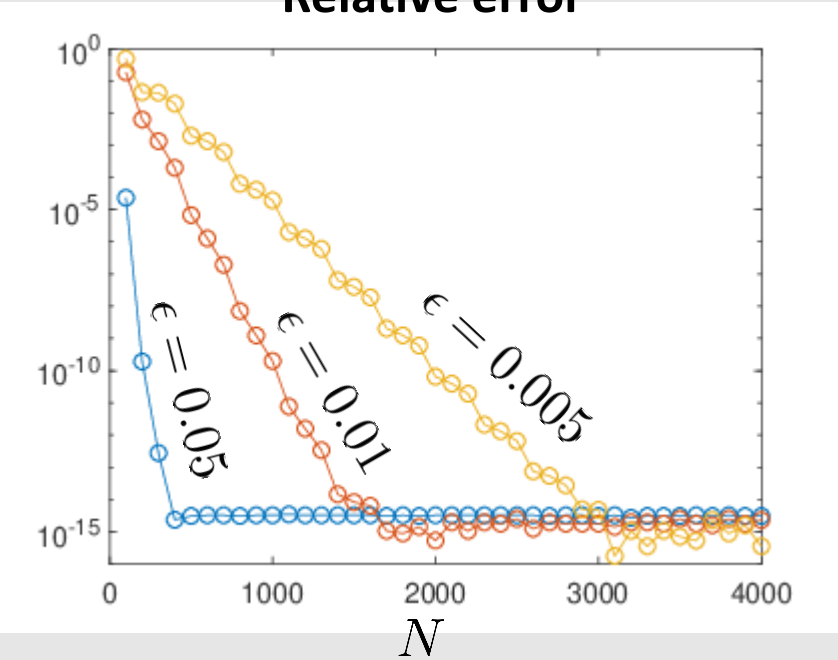
Convergence of smoothed measures

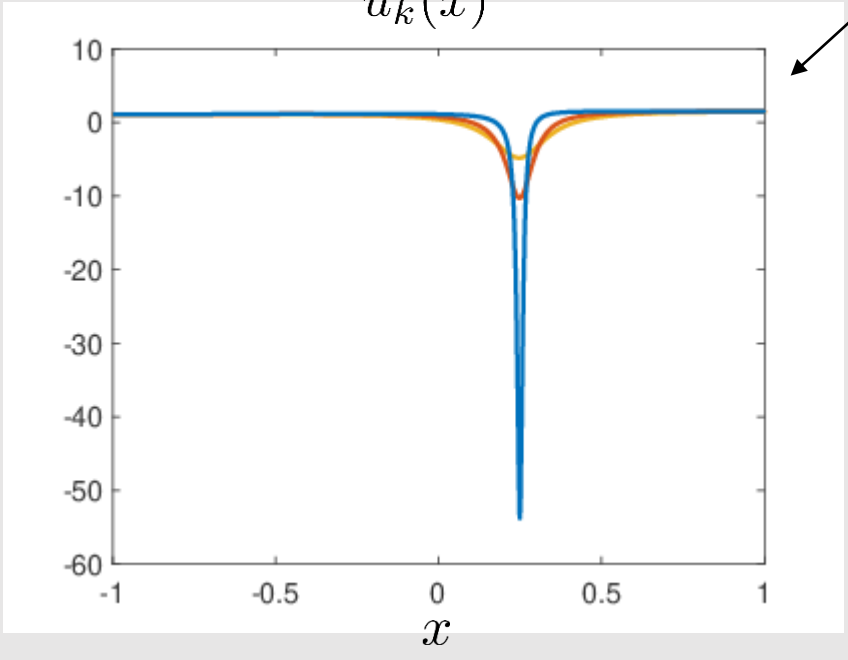
$$1)\ \text{Solve}\ (\mathcal{L} - (\lambda_k + i\epsilon)\mathcal{I})u_k = f$$

singular in the limit $\epsilon \to 0$

Integral operator

Relative error





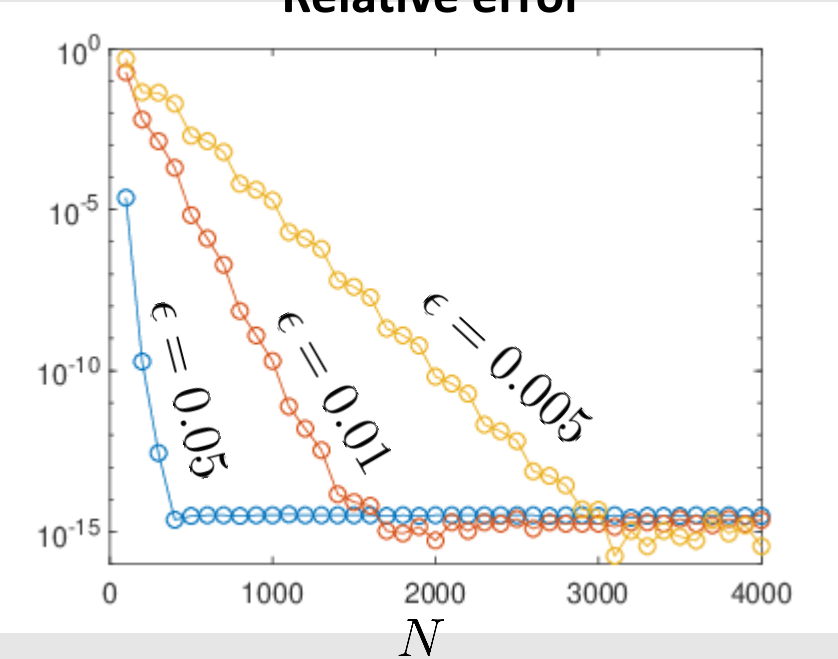
Convergence of smoothed measures

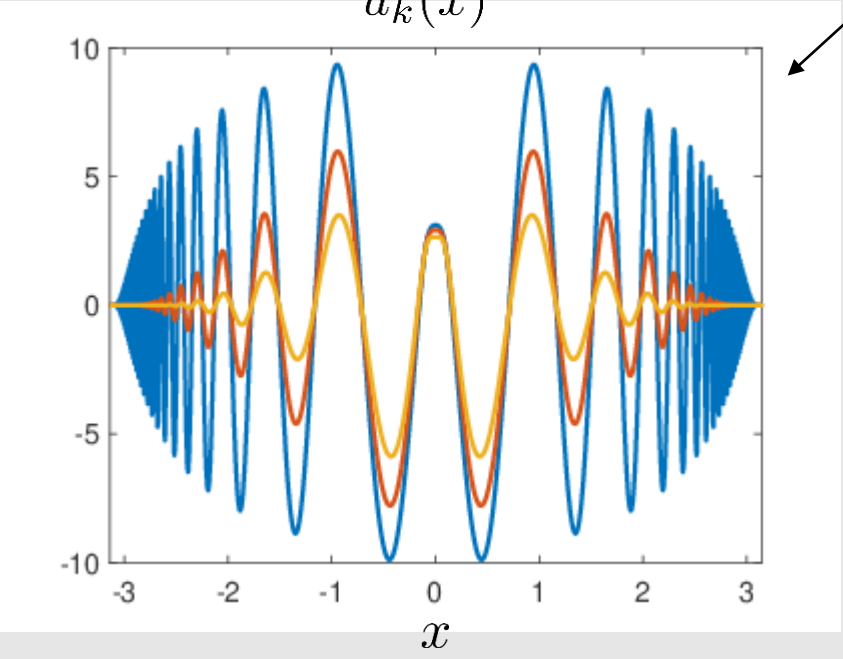
$$1)\ \text{Solve}\ (\mathcal{L} - (\lambda_k + i\epsilon)\mathcal{I})u_k = f$$

singular in the limit $\epsilon \to 0$

Differential operator

Relative error

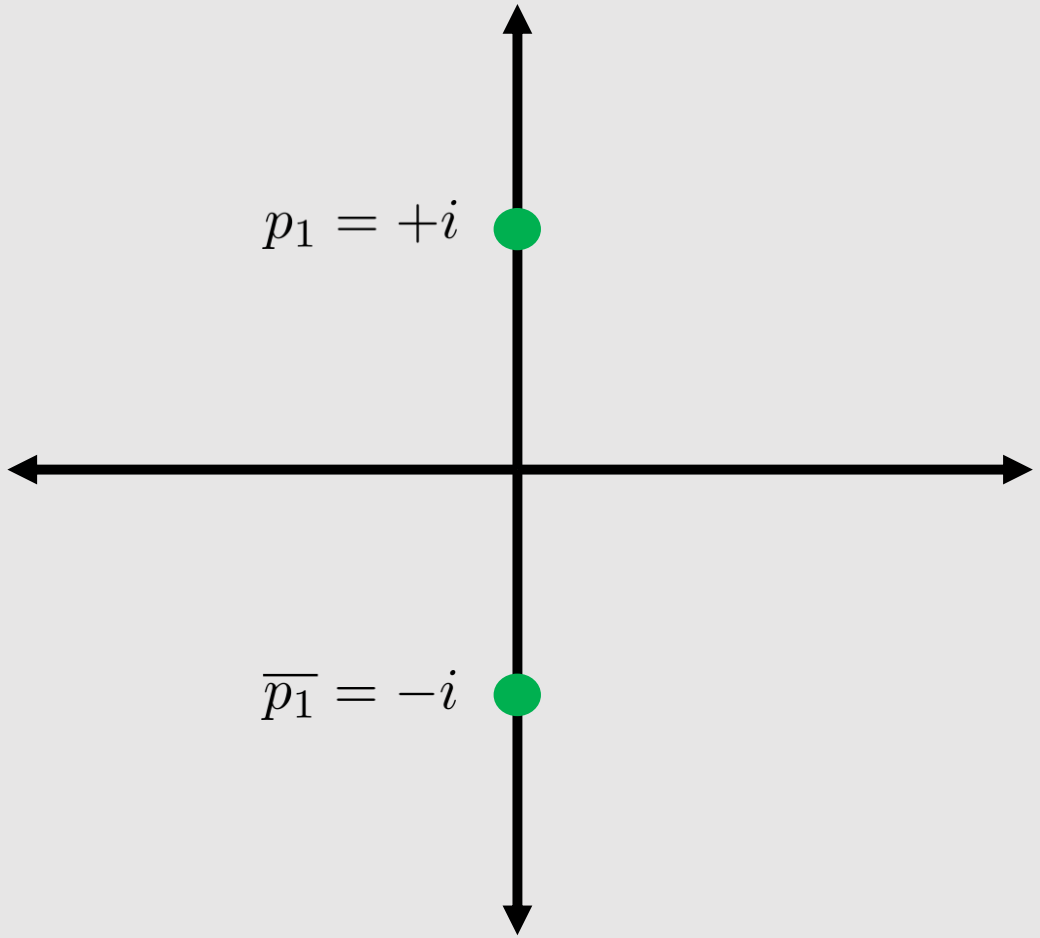




Rational kernels

Stone's theorem

$$\int_{\mathbb{R}} \frac{1}{\pi} \frac{\epsilon^2}{(\lambda - x)^2 + \epsilon^2} \, d\mu_f(\lambda) = \frac{1}{\pi} \mathrm{Im} \langle \mathcal{R}(x + i\epsilon, \mathcal{L}) f, f \rangle$$



"Generalized" Stone's theorem

$$[K_\epsilon^{(m)} * \mu_f](x) = \frac{-1}{\pi} \sum_{k=1}^{m} \mathrm{Im} \left(r_k \langle \mathcal{R}(x - \epsilon p_k), \mathcal{L}) f, f \rangle \right)$$

Rational kernels

Stone's theorem

$$\int_{\mathbb{R}} \frac{1}{\pi} \frac{\epsilon^2}{(\lambda - x)^2 + \epsilon^2} \, d\mu_f(\lambda) = \frac{1}{\pi} \mathrm{Im} \langle \mathcal{R}(x + i\epsilon, \mathcal{L}) f, f \rangle$$

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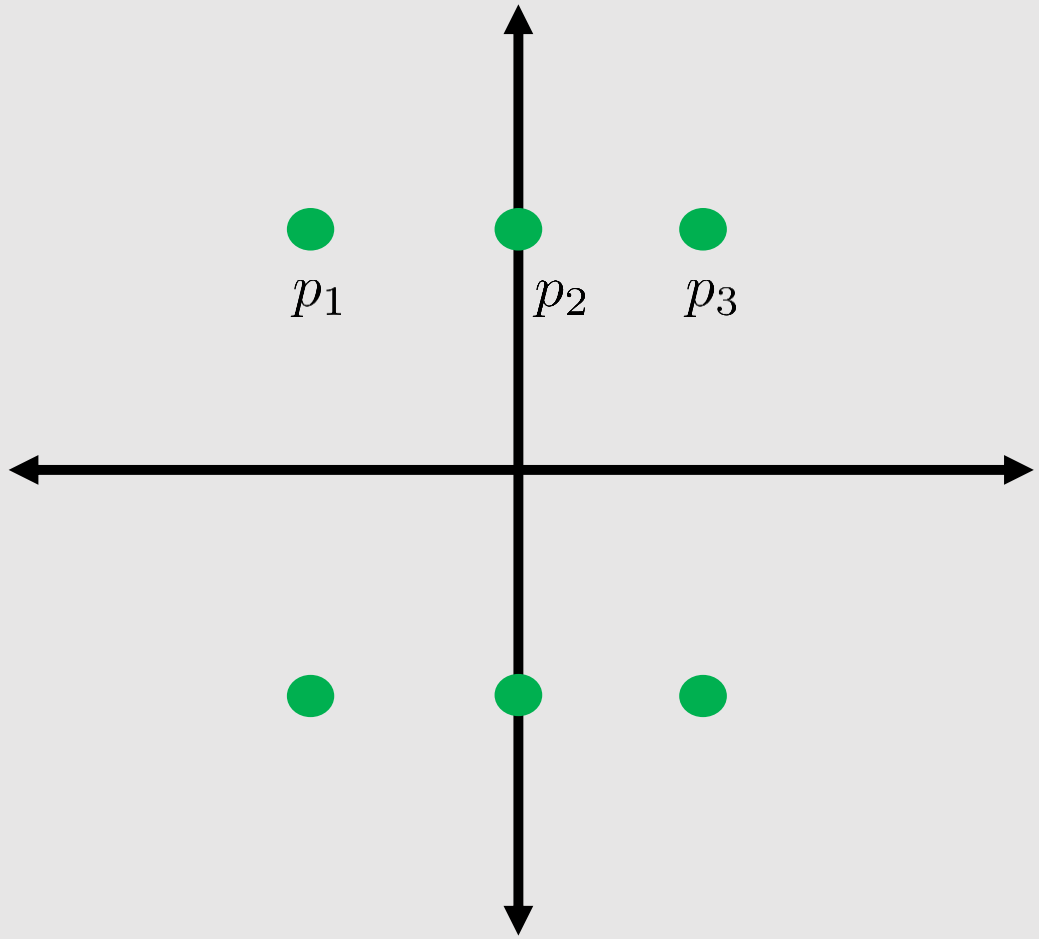
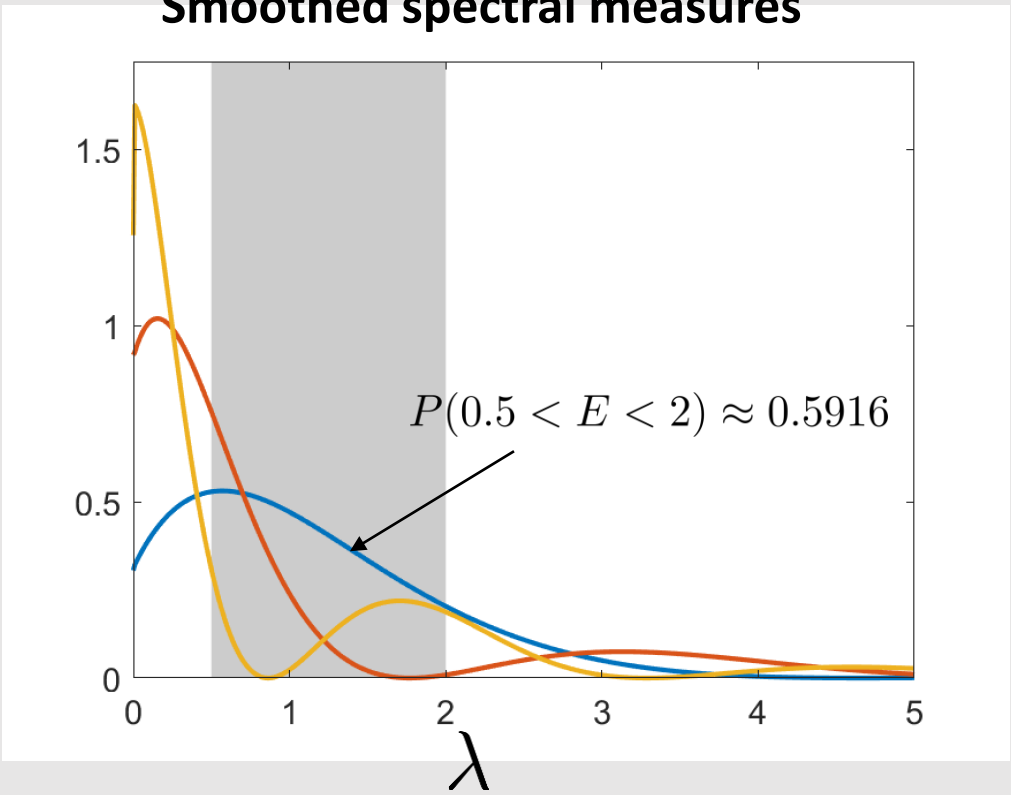
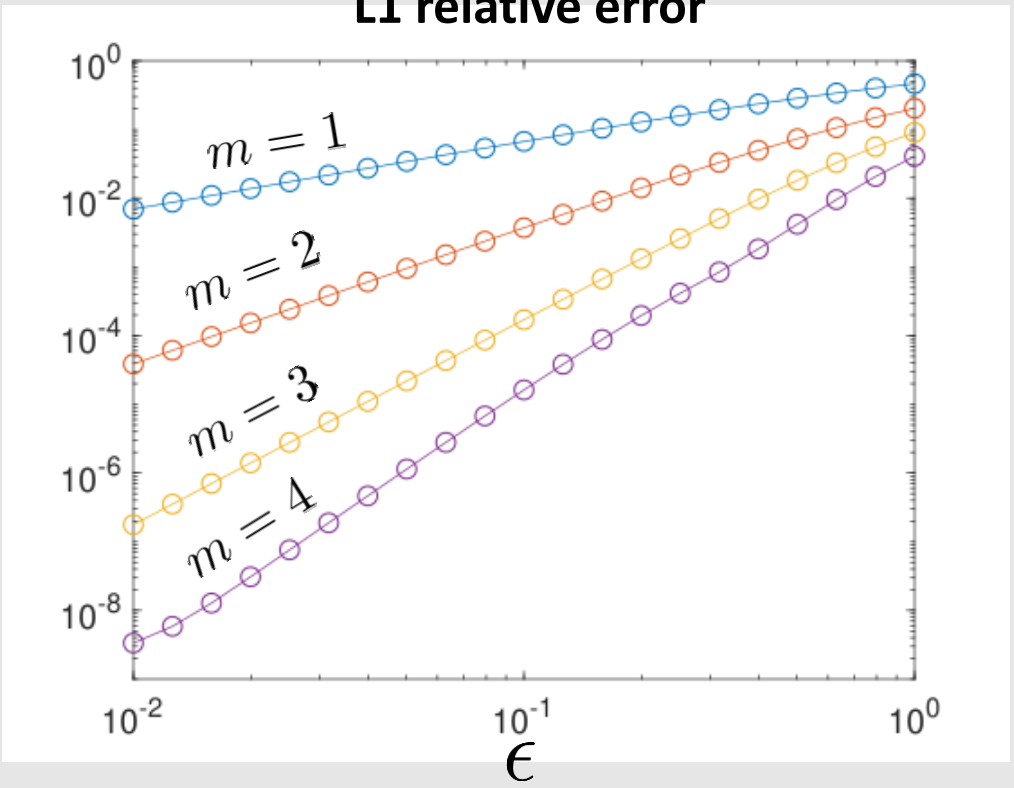


Rational kernels

Smoothed spectral measures



L1 relative error

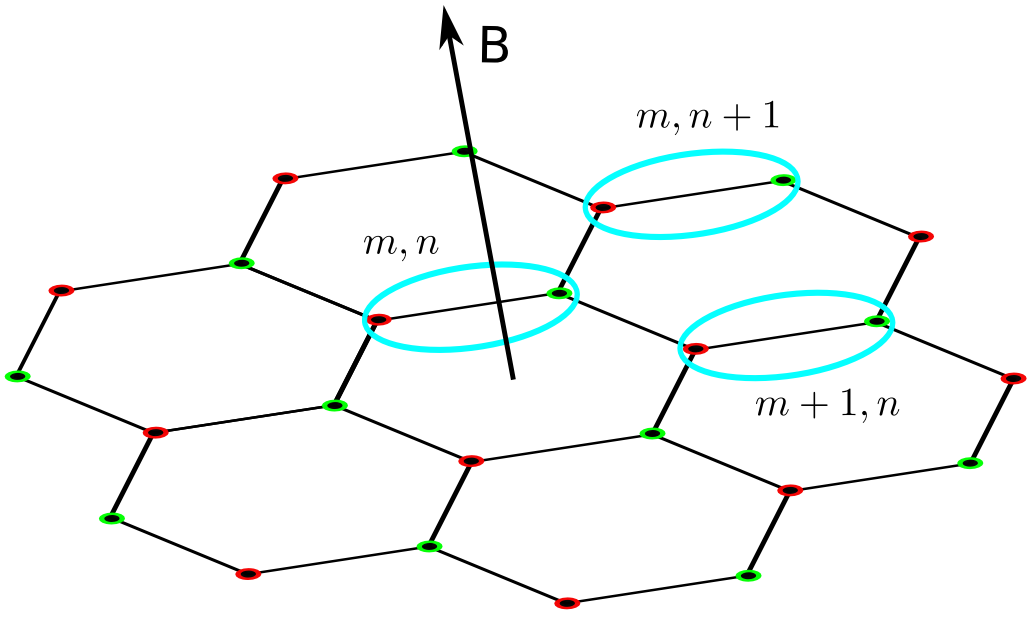


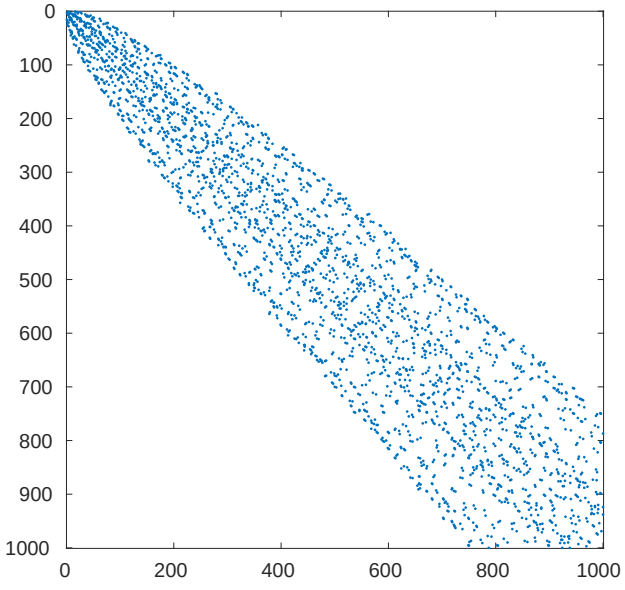
Theorem [Colbrook, H., and Townsend, 2020]

If μ_f is absolutely continuous in $I = [a - \delta, b + \delta]$ with Radon-Nikodym derivative $\rho_f \in W^{m,p}(I)$, then

$$\|\rho_f(x) - [K_\epsilon^{(m)} * \mu_f](x)\|_{L^p(a,b)} = \mathcal{O}(\epsilon^m \log(1/\epsilon)) \qquad \text{as} \qquad \epsilon \downarrow 0.$$

Example I: Magnetic graphene





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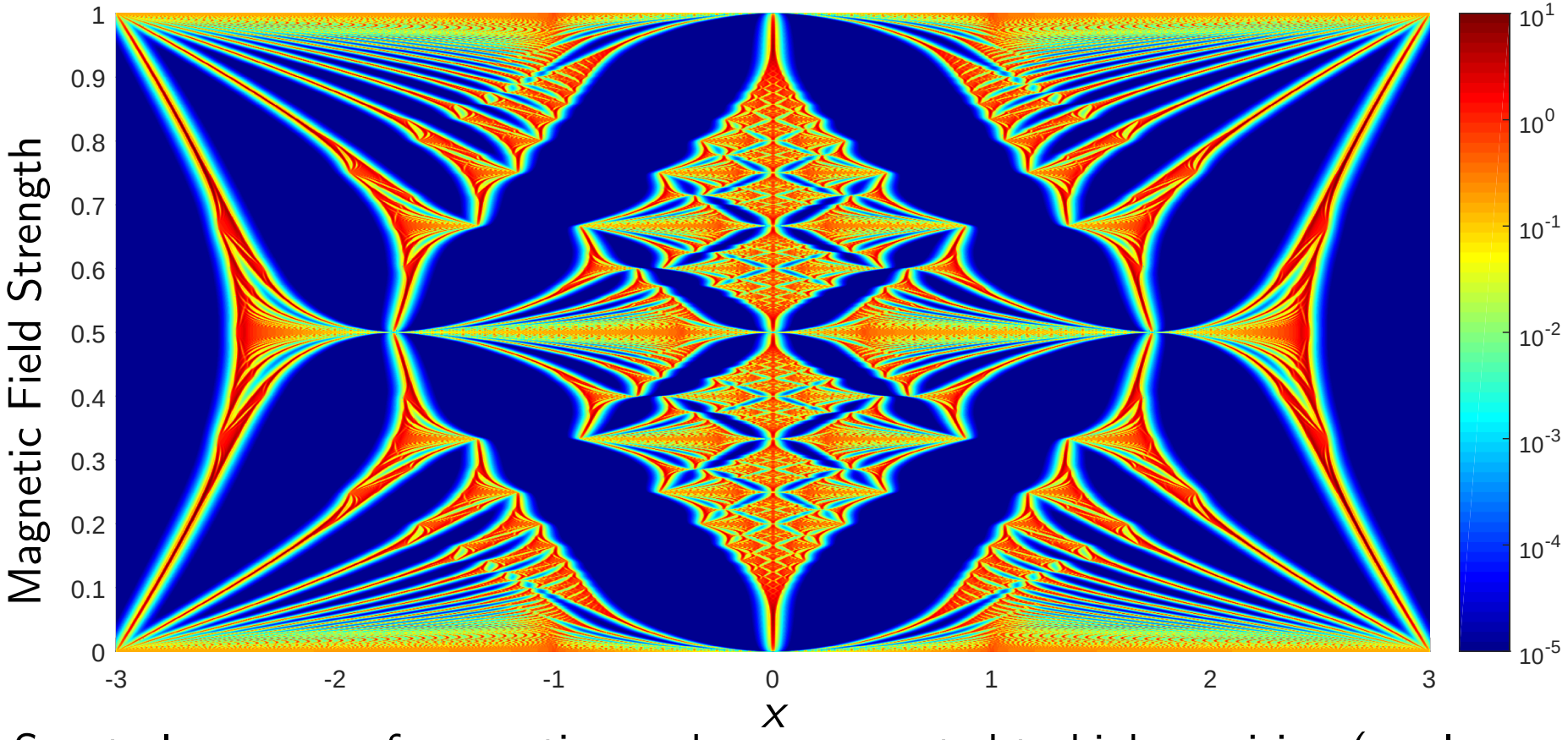
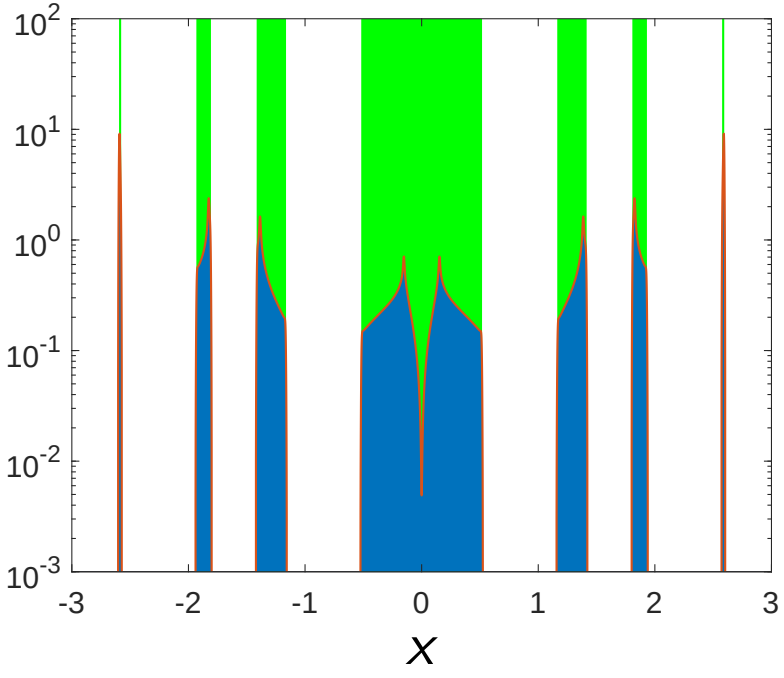
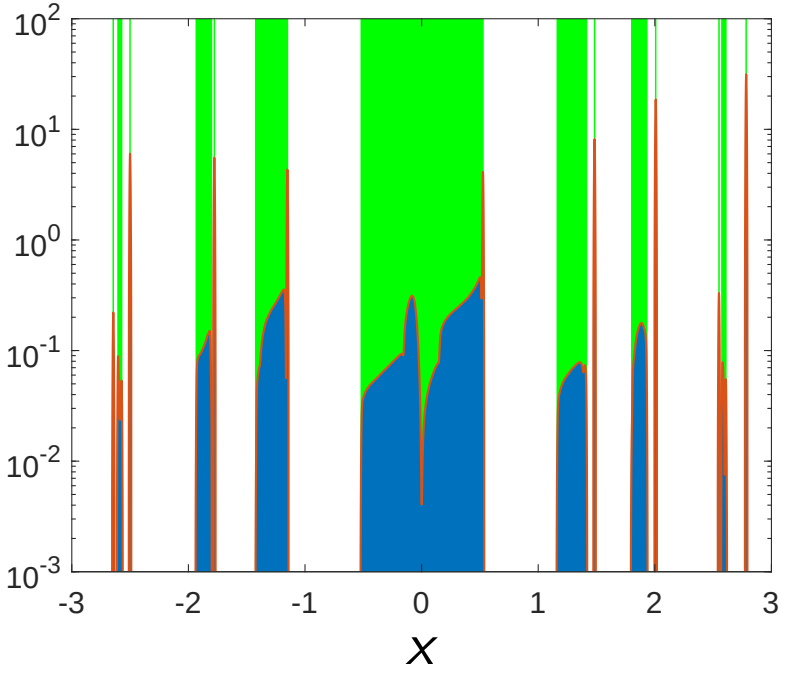


Spectral measure of magnetic graphene, computed to high precision (see log scale) using $m = 4$ kernel.

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

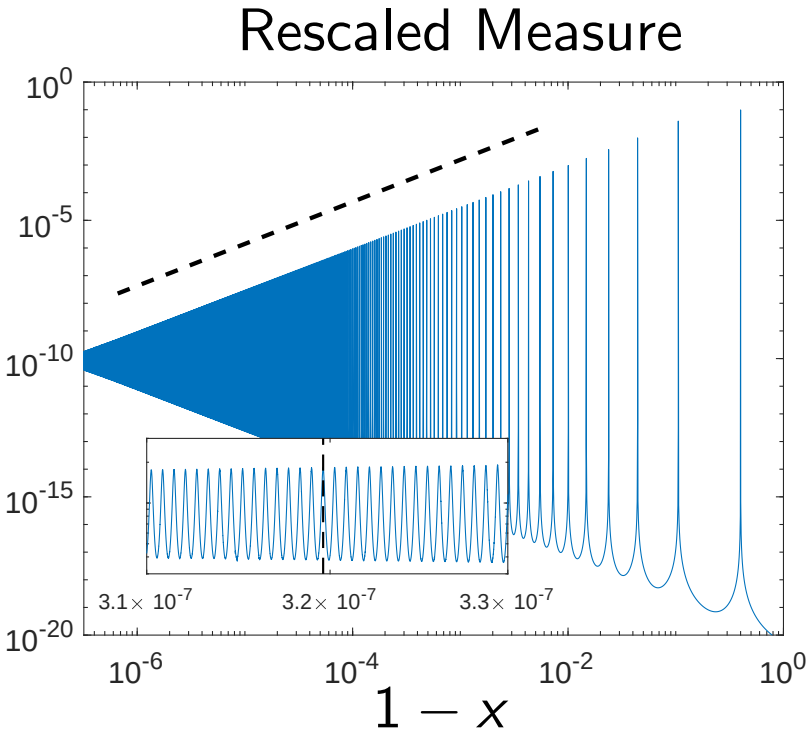
Example: Dirac operator.

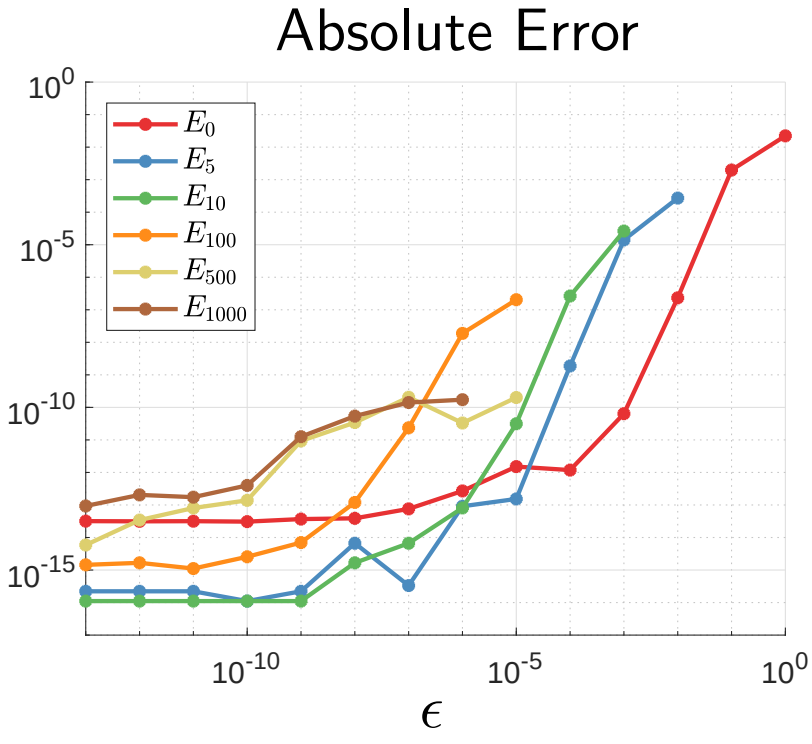
- Describes the motion of a relativistic electron.
- Essential spectrum given by $\mathbb{R}\backslash(-1,1) \Rightarrow$ spectral pollution!
- Consider radially symmetric potential, coupled system on half-line:

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

- 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.

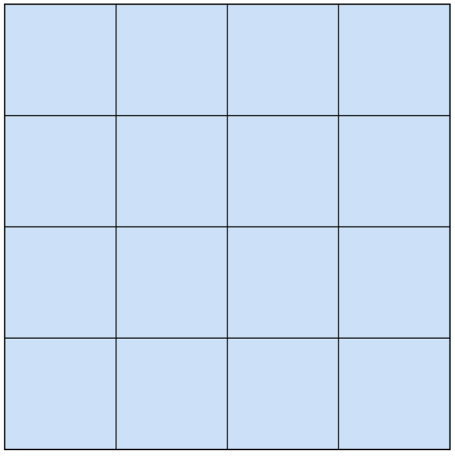
Example III: Chern numbers

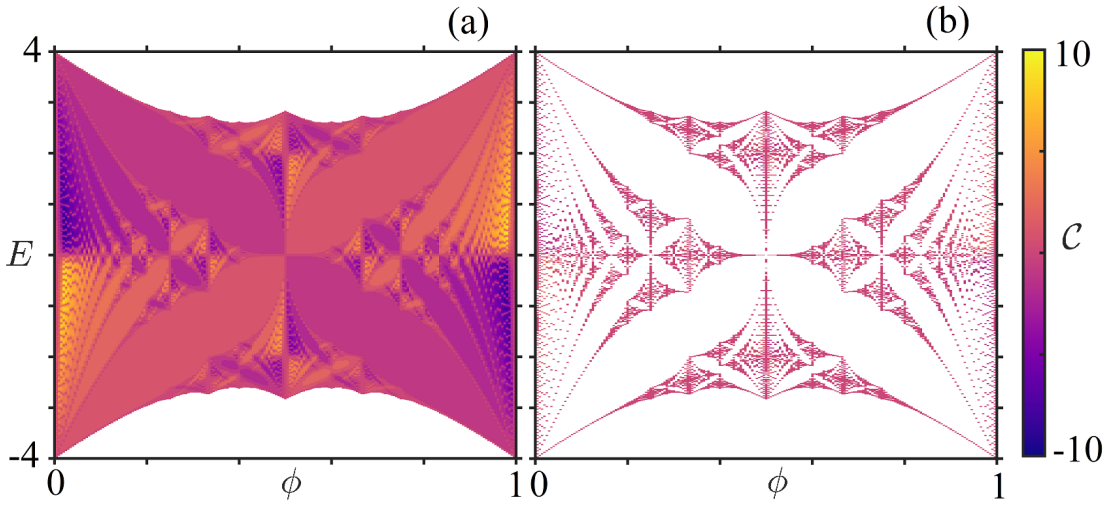
Finite dimensions	**Infinite dimensions**
$\hat{P}^n = \sum_{m=1}^{n} \lvert m\rangle\langle m\rvert, \;\; \hat{Q}^n = I - \hat{P}^n$	$\hat{P}^E = \int_{(-\infty, E]} d\mathcal{E}(\lambda)$
	$\hat{P}^E_\epsilon = \int_{-\infty}^{E} [K_\epsilon * \mathcal{E}](\lambda) d\lambda, \;\; \hat{Q}^E_\epsilon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

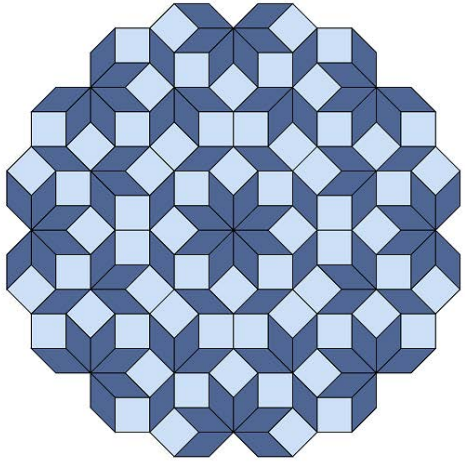
Round and take maximal count over site i.

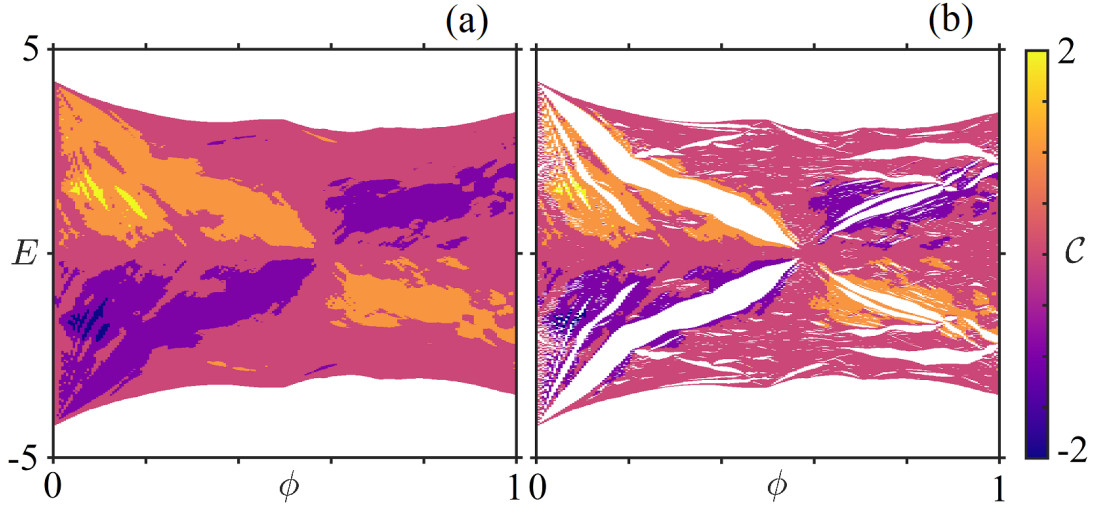
Intuition: Topological index to detect in-gap (conducting) state.

Example III: Chern numbers









Conclusion of Part III

- **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.

References

- M.J. Colbrook, B. Roman, and A.C. Hansen. "How to compute spectra with error control." *Physical Review Letters* 122.25 (2019).
- A. Horning, and A. Townsend. "FEAST for differential eigenvalue problems." *SIAM Journal on Numerical Analysis* 58.2 (2020).
- A. Horning, and Y. Nakatsukasa. "Twice is enough for dangerous eigenvalues." *preprint*.
- M.J. Colbrook, A. Horning, and A. Townsend. "Computing spectral measures of self-adjoint operators." *SIAM Review*, to appear.
- M.J. Colbrook. "Computing spectral measures and spectral types." *Communications in Mathematical Physics*, to appear.
- M.J. Colbrook, A.C. Hansen. "The foundations of spectral computations via the Solvability Complexity Index hierarchy." *preprint*.
- M.J. Colbrook. "On the computation of geometric features of spectra of linear operators on Hilbert spaces." *preprint*.
- M.J. Colbrook, A.C. Hansen. "On the infinite-dimensional QR algorithm." *Numerische Mathematik* 143.1 (2019).
- M.J. Colbrook. "Computing semigroups with error control." *preprint*.