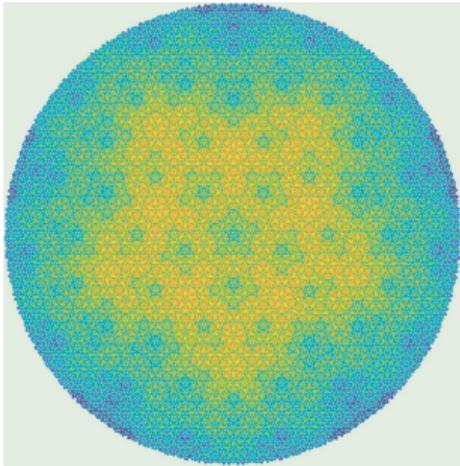


Infinite-Dimensional Spectral Computations

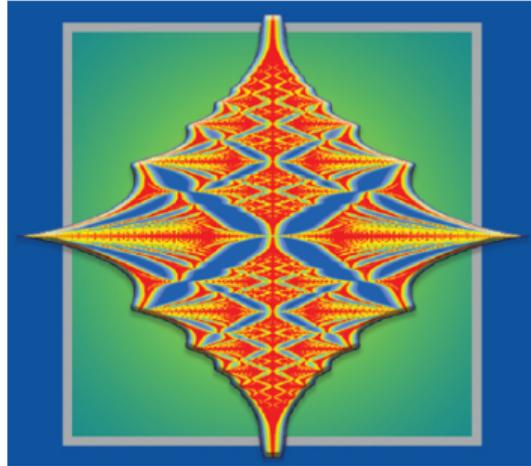
Matthew Colbrook

(University of Cambridge + École Normale Supérieure)

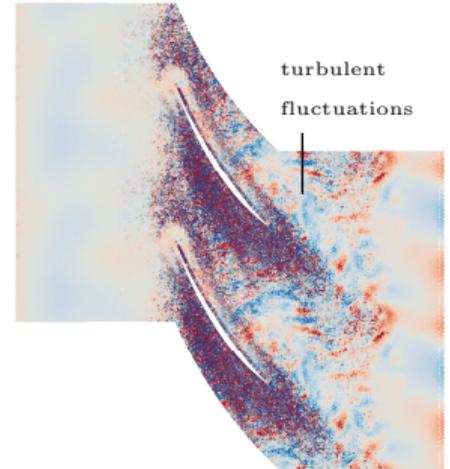
m.colbrook@damtp.cam.ac.uk



quantum state of quasicrystal



spectral measure of graphene



Koopman mode of turbulent flow

The infinite-dimensional spectral problem

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots \\ a_{21} & a_{22} & a_{23} & \cdots \\ a_{31} & a_{32} & a_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad \left[A \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \end{pmatrix} \right]_j = \sum_{k=1}^{\infty} a_{jk} x_k, \quad x \in l^2(\mathbb{N})$$

Finite Case ($B \in \mathbb{C}^{n \times n}$)	\Rightarrow	Infinite Case (operator A)
Eigenvalues	\Rightarrow	Spectrum, $\text{Sp}(A)$
$\{z \in \mathbb{C} : \det(B - z) = 0\}$	\Rightarrow	$\{z \in \mathbb{C} : A - z \text{ not invertible}\}$

GOAL: compute properties of $\text{Sp}(A)$ from matrix elements

Many applications: quantum mechanics, engineering, chemistry, matter physics, statistical mechanics, optics, number theory, PDEs, data science,...

The infinite-dimensional spectral problem

- 1920:** G. Szegő, "*Beiträge zur Theorie der Toeplitzschen Formen*" - finite section, Toeplitz operators, OPs, ...
- 1960:** J. Schwinger, "*Unitary operator bases*" - finite-dim. approx to Schrödinger operators in infinite-dim.
- 1983:** A. Böttcher & B. Silbermann, "*The finite section method for Toeplitz operators on the quarter-plane with piecewise continuous symbols.*" - C^* -algebra techniques (see also papers of W. Arveson and N. Brown).
- 1985:** P. Deift, L. C. Li, & C. Tomei, "*Toda flows with infinitely many variables*" - infinite-dimensional QR.
- 1994:** T. Digernes, V. S. Varadarajan & S. R. S. Varadhan, "*Finite approximations to quantum systems*" - convergence of Schwinger's method for Schrödinger operators with compact resolvent.
- 1996:** Fefferman & L. Seco, "*Interval arithmetic in quantum mechanics*" - computer-assisted proof of Dirac-Schwinger conjecture (ground state energy of atom).
- 2005:** L. N. Trefethen & M. Embree, "*Spectra and pseudospectra*" - pseudospectra of non-normal operators.

Mathematicians and physicists contributing to inf. dim. spectral computations include:

D. Arnold (Minnesota), W. Arveson (Berkeley), A. Böttcher (Chemnitz), W. Dahmen (South Carolina), E. B. Davies (King's College London), P. Deift (NYU), L. Demanet (MIT), C. Fefferman (Princeton), H. Goldstone (IAS), G. Golub (Stanford), A. Iserles (Cambridge), D. Jerison (MIT), T. Kato (Berkeley), A. Laptev (Imperial), E. Lieb (Princeton), S. Mayboroda (Minnesota), 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), ...

Things that typically go wrong

Fundamental challenges:

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

Even if a method converges,

- How do we know what part of the approximation to trust?

“In practice, 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 [general] techniques.”

W. Arveson, Berkeley (1994)

Things that typically go wrong

Fundamental challenges:

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

Even if a method converges,

- How do we know what part of the approximation to trust?

Method of this talk:

Things that typically go wrong

Fundamental challenges:

- ~~Miss parts of the spectrum.~~
- Approximate false $z \notin \text{Sp}(A)$ - “spectral pollution”.

Even if a method converges,

- How do we know what part of the approximation to trust?

Method of this talk:

- Converges without missing parts of spectrum. ✓

Things that typically go wrong

Fundamental challenges:

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

Even if a method converges,

- How do we know what part of the approximation to trust?

Method of this talk:

- Converges without missing parts of spectrum. ✓
- Avoids spectral pollution. ✓

Things that typically go wrong

Fundamental challenges:

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

Even if a method converges,

- ~~How do we know what part of the approximation to trust?~~

Method of this talk:

- Converges without missing parts of spectrum. ✓
- Avoids spectral pollution. ✓
- Provides error control (guaranteed certificate of accuracy)
⇒ computations reliable and useful in applications. ✓

Things that typically go wrong

Fundamental challenges:

- ~~Miss parts of the spectrum.~~
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Method of this talk:

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⇒ computations reliable and useful in applications. ✓

Numerical linear algebra: Finite-dimensional ⇒ Infinite-dimensional

Background programme: foundations of infinite-dimensional spectral computations

Key Question: What is possible in infinite-dimensional spectral computations?

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

⇒ Compute many spectral properties for the first time.

Framework: Classify problems in a computational hierarchy measuring intrinsic difficulty.

⇒ Algorithms realise boundaries of what computers can achieve.

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

-
- M. Colbrook, "*The Foundations of Infinite-Dimensional Spectral Computations*," PhD diss., 2020.
 - M. Colbrook, V. Antun , A. Hansen "Can stable and accurate neural networks be computed? - On the barriers of deep learning and Smale's 18th problem," Proc. Natl. Acad. Sci. USA, to appear.

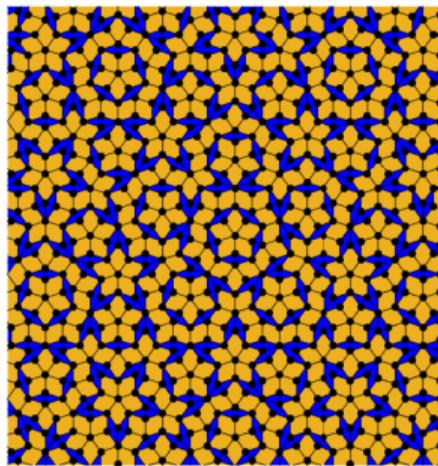
Talk structure: three problems

- **Part 1:** Computing spectra with error control.
- **Part 2:** Computing spectral measures.
- **Part 3:** Data driven computations and Koopman operators.

Part 1: Computing spectra with error control.

-
- M. Colbrook, B. Roman, A. Hansen "*How to compute spectra with error control*" Physical Review Letters, 2019.
 - M. Colbrook, A. Hansen "*The foundations of spectral computations via the solvability complexity index hierarchy*," Journal of the European Mathematical Society, under revisions.

Example: quasicrystals



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

Aperiodicity \Rightarrow interesting physics

Aperiodicity \Rightarrow considerable challenge to approximate S_p

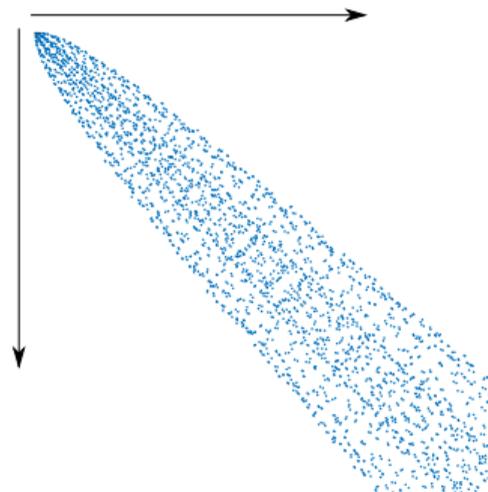
Example: quasicrystals

Model: Perpendicular magnetic field (of strength B).

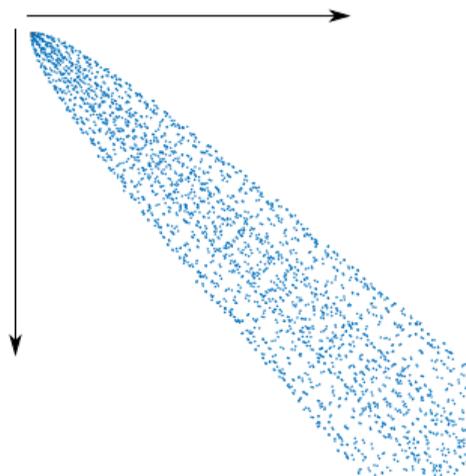
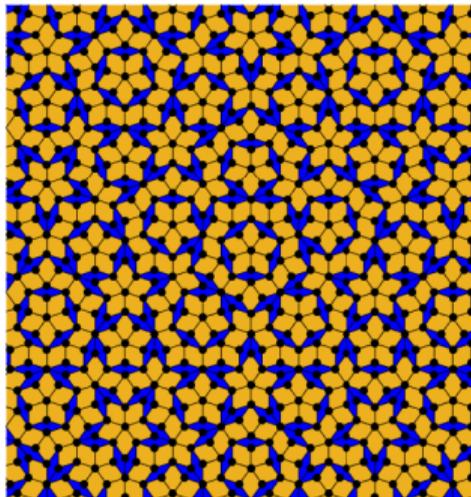
Matrix equation

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

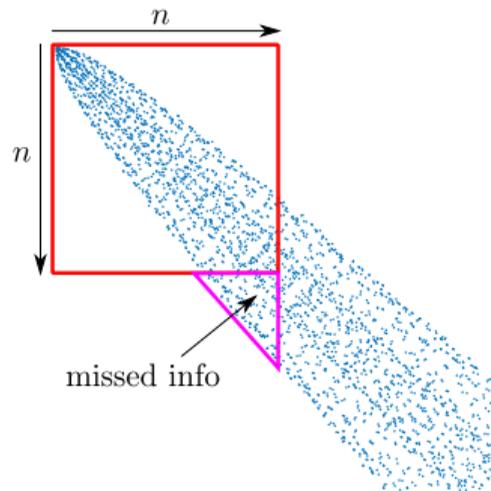
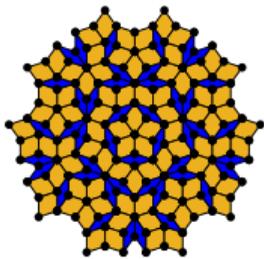
Matrix sparsity



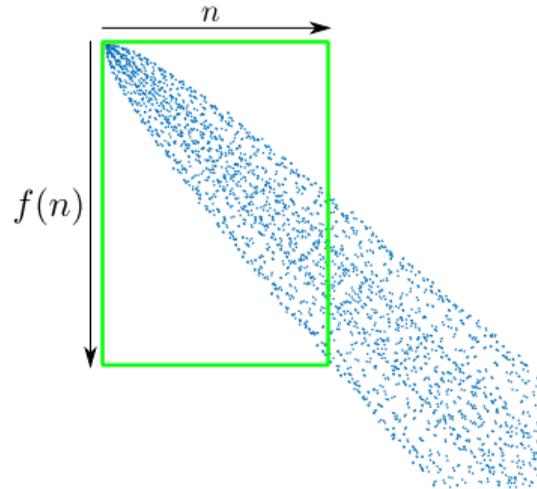
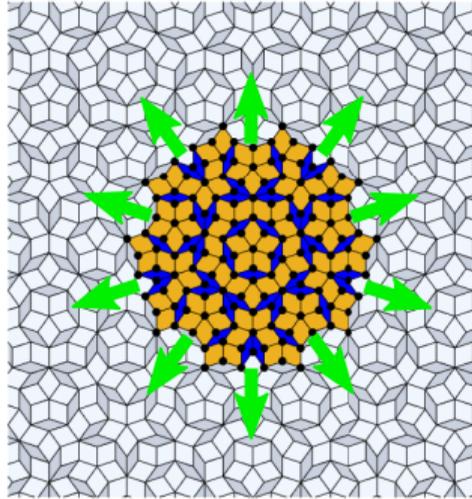
Example: quasicrystals



Previous approaches: square truncations



Idea: rectangular truncations

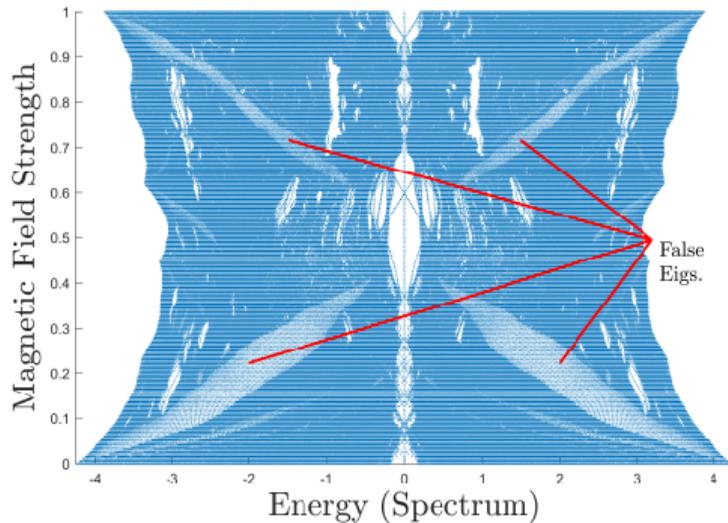


- ⇒ Computation of $\|(A - z)^{-1}\|^{-1} = \text{dist}(z, \text{Sp}(A))$ from above.
- ⇒ Computation of $\text{Sp}(A)$ via adaptive local minimisers.

Example: quasicrystals

Square truncations

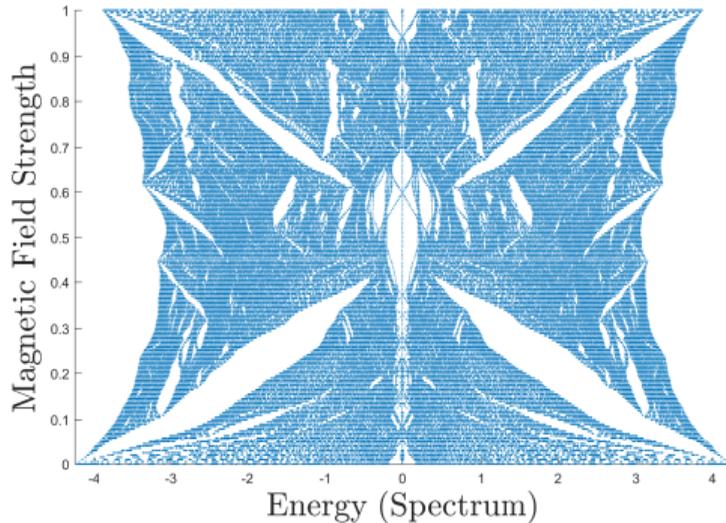
Spectral pollution.



Does not converge
No error control

New method

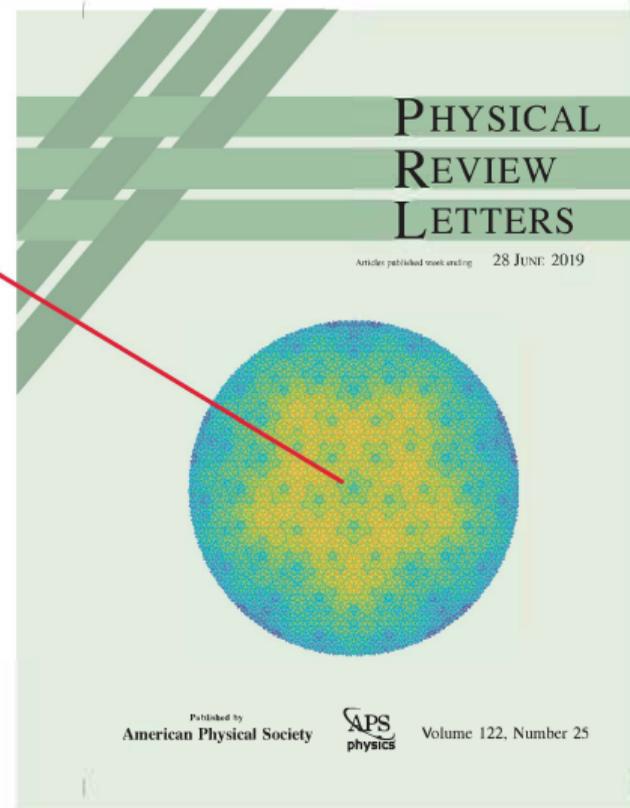
Convergent computation.



Converges
Error control

Remarks

- Rigorously compute approximate states.
e.g. quasicrystals
- Error control, output $\Gamma_n(A)$ & computed bound E_n :
 - $\Gamma_n(A) \rightarrow \text{Sp}(A)$
 - $\sup_{z \in \Gamma_n(A)} \text{dist}(z, \text{Sp}(A)) \leq E_n \downarrow 0$.
- Local, parallelisable and fast.
- Extends to non-sparse matrices.
- Extends to (certain) non-normal ($AA^* \neq A^*A$) operators.



Similar ideas work for PDEs...

PDEs on unbounded domains

$$[\mathcal{L}u](x) = \sum_{k \in \mathbb{Z}_{\geq 0}^d: |k| \leq N} a_k(x) \partial^k u(x) \quad \text{on } L^2(\mathbb{R}^d).$$

Coefficients $a_k(x)$:

- polynomially bounded
- bounded total variation on compact balls

⇒ Compute $\text{Sp}(\mathcal{L})$ with error control!

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

· J. Schwinger, "*The special canonical group*," Proc. Nat. Acad. Sci. U.S.A, 1960.

· J. Schwinger, "*Unitary operator bases*," Proc. Nat. Acad. Sci. U.S.A, 1960.

Part 2: Computing spectral measures.

-
- M. Colbrook, "*Computing spectral measures and spectral types*" Communications in Mathematical Physics, 2021.
 - M. Colbrook, A. Horning, A. Townsend "*Computing spectral measures of self-adjoint operators*" SIREV, 2021.

Spectral measures

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

$$v = \left(\sum_{j=1}^n v_j v_j^* \right) v, \quad v \in \mathbb{C}^n \quad Bv = \left(\sum_{j=1}^n \lambda_j v_j v_j^* \right) v, \quad v \in \mathbb{C}^n.$$

Infinite-dimensional: Self-adjoint operator $\mathcal{L} : \mathcal{D}(\mathcal{L}) \rightarrow \mathcal{H}$, (\mathcal{H} = Hilbert space).

Bad news: Typically, no longer a basis of e-vectors.

Spectral Theorem: Projection-valued spectral measure \mathcal{E}

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

Diagonalises infinite-dimensional operator \mathcal{L} .

Spectral measures

Scalar-valued measures: $\nu_g(U) = \langle \underbrace{\mathcal{E}(U)}_{\text{projection}} g, g \rangle$ ($U \subset \mathbb{R}$).

QM example: ν_g describe likelihood of different outcomes when Hamiltonian \mathcal{L} is measured.

Lebesgue decomposition theorem:

$$d\nu_g(\lambda) = \underbrace{\sum_{\text{eigenvalues } \lambda_j} \langle \mathcal{P}_{\lambda_j} g, g \rangle \delta(\lambda - \lambda_j) d\lambda}_{\text{discrete part}} + \underbrace{\rho_g(\lambda) d\lambda + d\nu_g^{(\text{sc})}(\lambda)}_{\text{continuous part}}.$$

Stone's formula

$$\nu_g^\epsilon(x) = \frac{-1}{2\pi i} \langle [(\mathcal{L} - (x - i\epsilon))^{-1} - (\mathcal{L} - (x + i\epsilon))^{-1}]g, g \rangle = \frac{1}{\pi} \int_{\mathbb{R}} \frac{\epsilon}{(x - \lambda)^2 + \epsilon^2} d\nu_g(\lambda).$$

Convolution with Poisson kernel: smoothed measure.

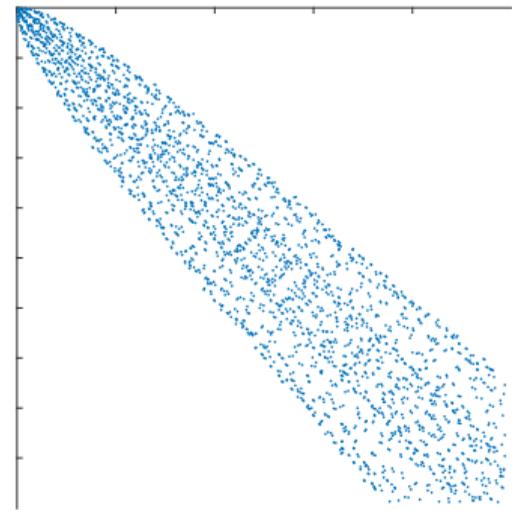
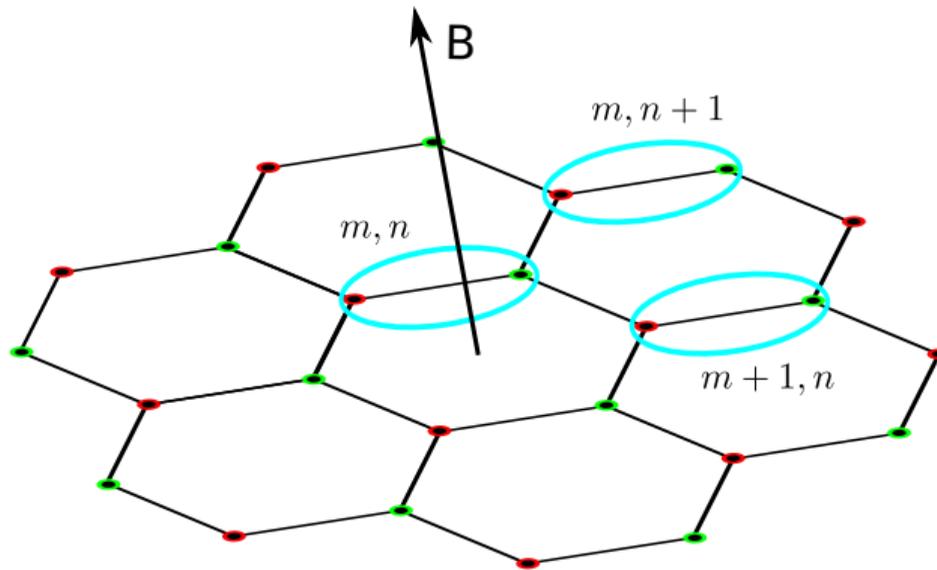
Approximate via truncation of $(\mathcal{L} - z)^{-1}$ ($N =$ truncation parameter).

· R. Haydock, H. Volker, M. Kelly, “*Electronic structure based on the local atomic environment for tight-binding bands*” Journal of Physics C, 1972.

· L. Lin, Y. Saad, C. Yang, “*Approximating spectral densities of large matrices*” SIAM Review, 2016.

· M. Webb, S. Olver. “*Spectra of Jacobi operators via connection coefficient matrices.*” Communications in Mathematical Physics, 2021.

Numerical balancing act with graphene



Numerical balancing act with graphene

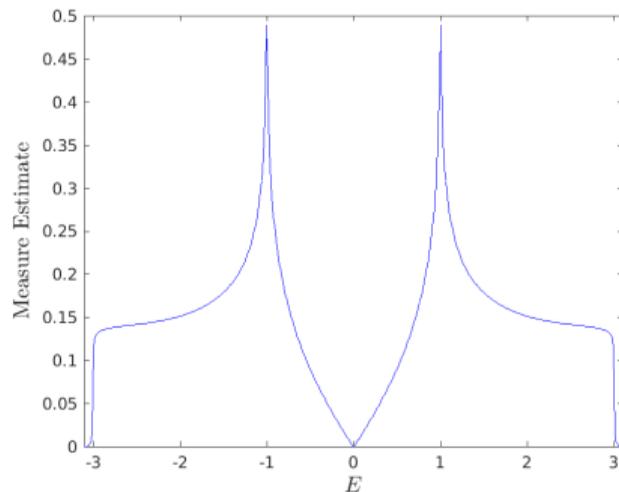
Numerical balancing act with graphene

Numerical balancing act

Theorem (C. (2021))

Can compute measure if known rate of off-diagonal decay of infinite matrix. Extends to PDEs.

$(\mathcal{L} - z)^{-1}g$ computed using rectangular truncations and least squares with adaptive $N(\epsilon)$.



Problem: As $\epsilon \downarrow 0$, $N(\epsilon) \rightarrow \infty$ and $\nu_g^\epsilon - \nu_g = \mathcal{O}(\epsilon \log(\epsilon^{-1}))$ (slow convergence).

Idea: rational kernels

Idea: $K(x) = \frac{1}{2\pi i} \sum_{j=1}^m \frac{\alpha_j}{x - a_j} - \frac{\bar{\alpha}_j}{x - \bar{a}_j}$ $K_\epsilon(x) = \epsilon^{-1} K(x\epsilon^{-1})$

$\{a_j\}_{j=1}^m$ distinct points in upper half plane and
$$\begin{pmatrix} 1 & \dots & 1 \\ a_1 & \dots & a_m \\ \vdots & \ddots & \vdots \\ a_1^{m-1} & \dots & a_m^{m-1} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_m \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

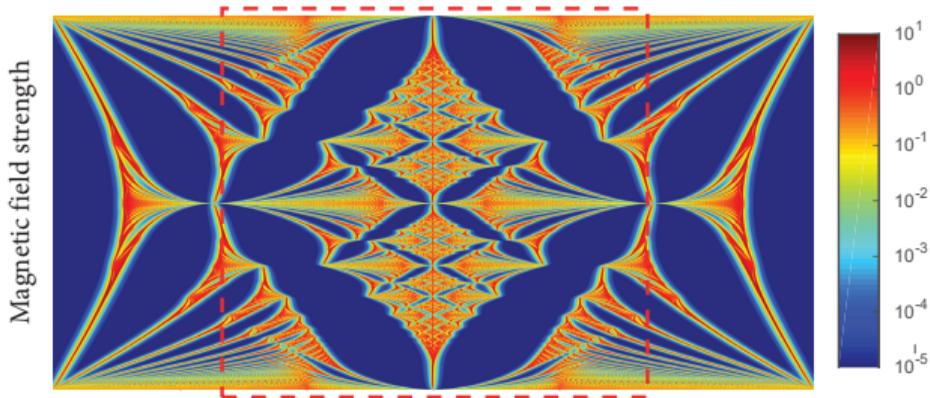
Gen. Stone's f.: $[K_\epsilon * \nu_g](x) = \frac{-1}{2\pi i} \sum_{j=1}^m \langle [\alpha_j(\mathcal{L} - (x - \epsilon a_j))^{-1} - \bar{\alpha}_j(\mathcal{L} - (x - \epsilon \bar{a}_j))^{-1}] g, g \rangle$

Stone's formula: $\frac{-1}{2\pi i} \langle [(\mathcal{L} - (x - i\epsilon))^{-1} - (\mathcal{L} - (x + i\epsilon))^{-1}] g, g \rangle$

Theorem (C., Horning, Townsend (2021))

If ν_g "sufficiently regular" locally near x_0 , then $|[K_\epsilon * \nu_g](x_0) - \rho_g(x_0)| = \mathcal{O}(\epsilon^m \log(\epsilon^{-1}))$

Beautiful fractal structure!



Horizontal slice = spectral measure at constant magnetic field strength.

Software package (developed with Andrew Horning):

SpecSolve available at <https://github.com/SpecSolve>

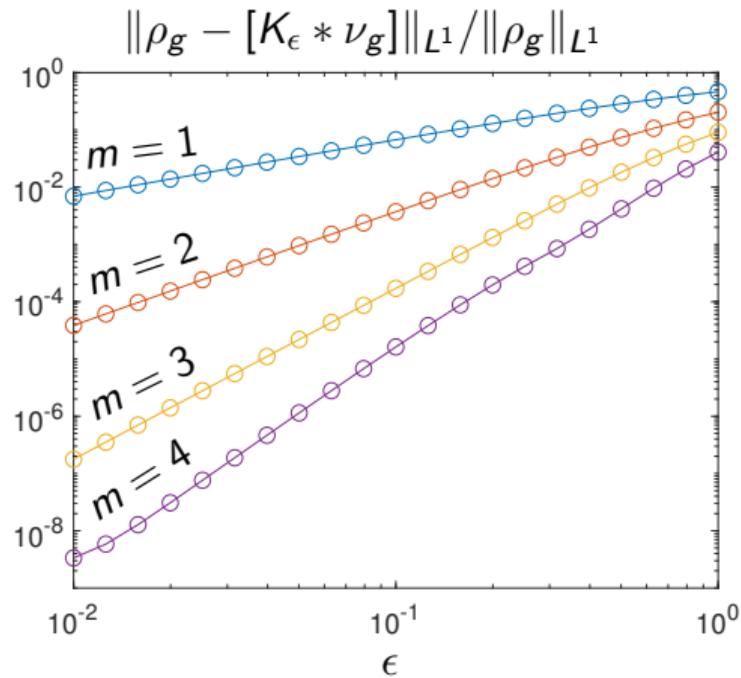
Current capabilities include: ODEs on real line & half-line, integral operators, and discrete operators.

Demo: radial Schrödinger operator

$$[\mathcal{L}u](r) = -\frac{d^2u}{dr^2}(r) + \left(\frac{\ell(\ell+1)}{r^2} + \frac{1}{r}(e^{-r} - 1) \right) u(r), \quad r > 0.$$

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

Demo: radial Schrödinger operator



Part 3: Data driven computations and Koopman operators.

New algorithm: ResDMD!

The setup: discrete dynamical system

Dynamical system: Statespace $\Omega \subset \mathbb{R}^d$, $F : \Omega \rightarrow \Omega$, $\mathbf{x}_{n+1} = F(\mathbf{x}_n)$.

Given snapshot data: $\{\mathbf{x}^{(m)}, \mathbf{y}^{(m)}\}_{m=1}^M$ with $\mathbf{y}^{(m)} = F(\mathbf{x}^{(m)})$.

Goal: Learn properties of the dynamical system.

Challenges:

- F is unknown
- F is typically nonlinear
- system could be chaotic
- snapshot data could be noisy

Koopman operators in one slide



Vol. 17, 1931 *MATHEMATICS: B. O. KOOPMAN* 315

HAMILTONIAN SYSTEMS AND TRANSFORMATIONS IN HILBERT SPACE

By B. O. KOOPMAN

DEPARTMENT OF MATHEMATICS, COLUMBIA UNIVERSITY

Communicated March 23, 1931

In recent years the theory of Hilbert space and its linear transformations has come into prominence.¹ It has been recognized to an increasing extent that many of the most important departments of mathematical



DYNAMICAL SYSTEMS OF CONTINUOUS SPECTRA

By B. O. KOOPMAN AND J. v. NEUMANN

DEPARTMENTS OF MATHEMATICS, COLUMBIA UNIVERSITY AND PRINCETON UNIVERSITY

Communicated January 21, 1932

1. In a recent paper by B. O. Koopman,¹ classical Hamiltonian mechanics is considered in connection with certain self-adjoint and unitary operators in Hilbert space Φ ($= \mathfrak{E}_2$). The corresponding canonical resolution of the identity $E(\lambda)$, or "spectrum of the dynamical system," is introduced, together with the conception of the spectrum revealing in its structure

Let $g : \Omega \rightarrow \mathbb{C}$, define

$$[\mathcal{K}g](\mathbf{x}) = g(F(\mathbf{x})), \quad \mathbf{x} \in \Omega.$$

\mathcal{K} is a linear, so system determined by spectral information of $\mathcal{K} : L^2(\Omega) \rightarrow L^2(\Omega)$

\Rightarrow infinite-dimensional spectral computation from snapshot data!

Extended Dynamic Mode Decomposition (EDMD) as a Galerkin method

Subspace $\text{span}\{\psi_j\}_{j=1}^N \subset L^2(\Omega)$, $\Psi(\mathbf{x}) = [\psi_1(\mathbf{x}) \cdots \psi_N(\mathbf{x})] \in \mathbb{C}^{1 \times N}$.

$$\Psi_X = [\Psi(\mathbf{x}^{(1)})^\top \cdots \Psi(\mathbf{x}^{(M)})^\top]^\top, \Psi_Y = [\Psi(\mathbf{y}^{(1)})^\top \cdots \Psi(\mathbf{y}^{(M)})^\top]^\top$$

$$\mathbf{g} = \sum_{j=1}^N \psi_j \mathbf{g}_j = \Psi \mathbf{g}, \quad \text{seek } K_{\text{DMD}} \in \mathbb{C}^{N \times N} \text{ with } \mathcal{K} \mathbf{g} \approx \Psi K_{\text{DMD}} \mathbf{g}$$

$$\min_{B \in \mathbb{C}^{N \times N}} \int_{\Omega} \max_{\|\mathbf{g}\|=1} |[\mathcal{K} \mathbf{g}](\mathbf{x}) - \Psi(\mathbf{x}) B \mathbf{g}|^2 d\omega(\mathbf{x}) \approx \sum_{m=1}^M w_m \left\| \Psi(\mathbf{y}^{(m)}) - \Psi(\mathbf{x}^{(m)}) B \right\|_2^2.$$

$$K_{\text{DMD}} = (\Psi_X^* W \Psi_X)^\dagger (\Psi_X^* W \Psi_Y) \quad (W = \text{diag}(w_1, \dots, w_M))$$
$$\lim_{M \rightarrow \infty} [\Psi_X^* W \Psi_X]_{jk} = \langle \psi_k, \psi_j \rangle \quad \text{and} \quad \lim_{M \rightarrow \infty} [\Psi_X^* W \Psi_Y]_{jk} = \langle \mathcal{K} \psi_k, \psi_j \rangle$$

-
- P. Schmid “*Dynamic mode decomposition for numerical and experimental data*,” J. Fluid. Mech, 2010.
 - M. Williams, I. Kevrekidis, C. Rowley “*A data-driven approximation of the koopman operator: Extending dynamic mode decomposition*,” J. Nonlin. Sci., 2015.

Idea: matrix capturing the residual (ResDMD)

If $g = \Psi \mathbf{g} \in \text{span}\{\psi_j\}_{j=1}^N$ and λ are a candidate eigenvector-eigenvalue pair then

$$\begin{aligned} \|\mathcal{K}g - \lambda g\|_{L^2(\Omega)}^2 &= \sum_{j,k=1}^N \mathbf{g}_k \bar{\mathbf{g}}_j [\langle \mathcal{K}\psi_k, \mathcal{K}\psi_j \rangle - \lambda \langle \psi_k, \mathcal{K}\psi_j \rangle - \bar{\lambda} \langle \mathcal{K}\psi_k, \psi_j \rangle + |\lambda|^2 \langle \psi_k, \psi_j \rangle] \\ &\approx \sum_{j,k=1}^N \mathbf{g}_k \bar{\mathbf{g}}_j \left[\underbrace{\Psi_Y^* W \Psi_Y}_{\text{additional matrix}} - \lambda \Psi_Y^* W \Psi_X - \bar{\lambda} \Psi_X^* W \Psi_Y + |\lambda|^2 \Psi_X^* W \Psi_X \right]_{jk} \end{aligned}$$

In large data limit (as $M \rightarrow \infty$), matrices $\Psi_Y^* W \Psi_Y$, $\Psi_X^* W \Psi_Y$, $\Psi_X^* W \Psi_X$ allow us to:

- (1) Rigorously avoid spectral pollution.
- (2) Compute spectra.

Spectral measures and Koopman mode decomposition

Measure-preserving dynamical system \Rightarrow spectral measures ν_g on $[-\pi, \pi]_{\text{per}}$.

Koopman mode decomposition:

$$f \in L^2(\Omega), \quad f(\mathbf{x}_n) = [\mathcal{K}^n f](\mathbf{x}_0) = \sum_{\text{e-vals } \lambda_j} c_{\lambda_j} \lambda_j^n \underbrace{\varphi_{\lambda_j}(\mathbf{x}_0)}_{\text{e-functions}} + \underbrace{\int_{[-\pi, \pi]_{\text{per}}} e^{in\theta} \phi_{\theta, f}(\mathbf{x}_0) d\theta}_{\text{ctsly param e-functions}}.$$

ν_g can be computed using ResDMD:

- High-order convergence.
- Rigorous error control.
- Practical and parallel $\mathcal{O}(N^2)$ computation using QZ algorithm.

Kernelized version for large state space dimension

Curse of dimensionality: 16×16 resol. of scalar, deg. 5 polys $\Rightarrow N = 10^{10}$ basis functions!

Kernelized EDMD \Rightarrow learns implicit basis in $\mathcal{O}(d)$ operations.

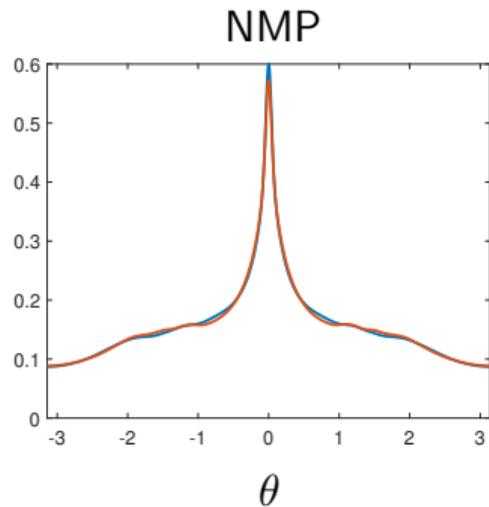
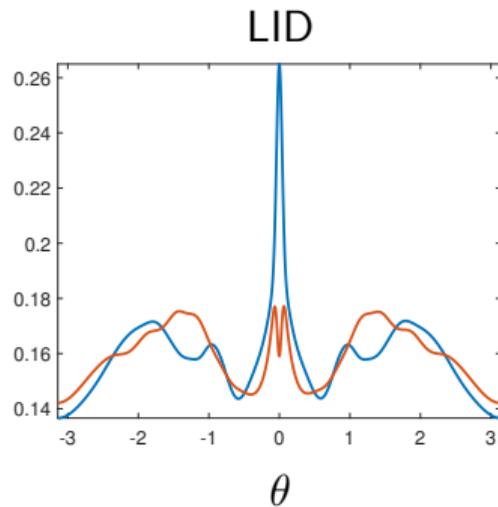
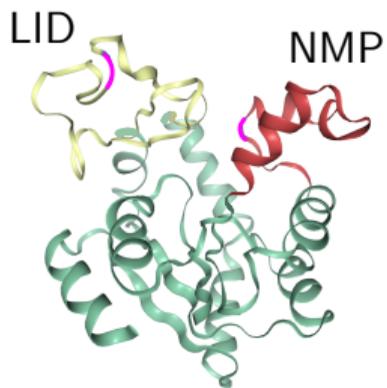
New method:

- 1 Apply kernelized EDMD to subset of data, select N dominant eigenfunctions as basis.
- 2 Apply ResDMD with this basis and the remaining M data.

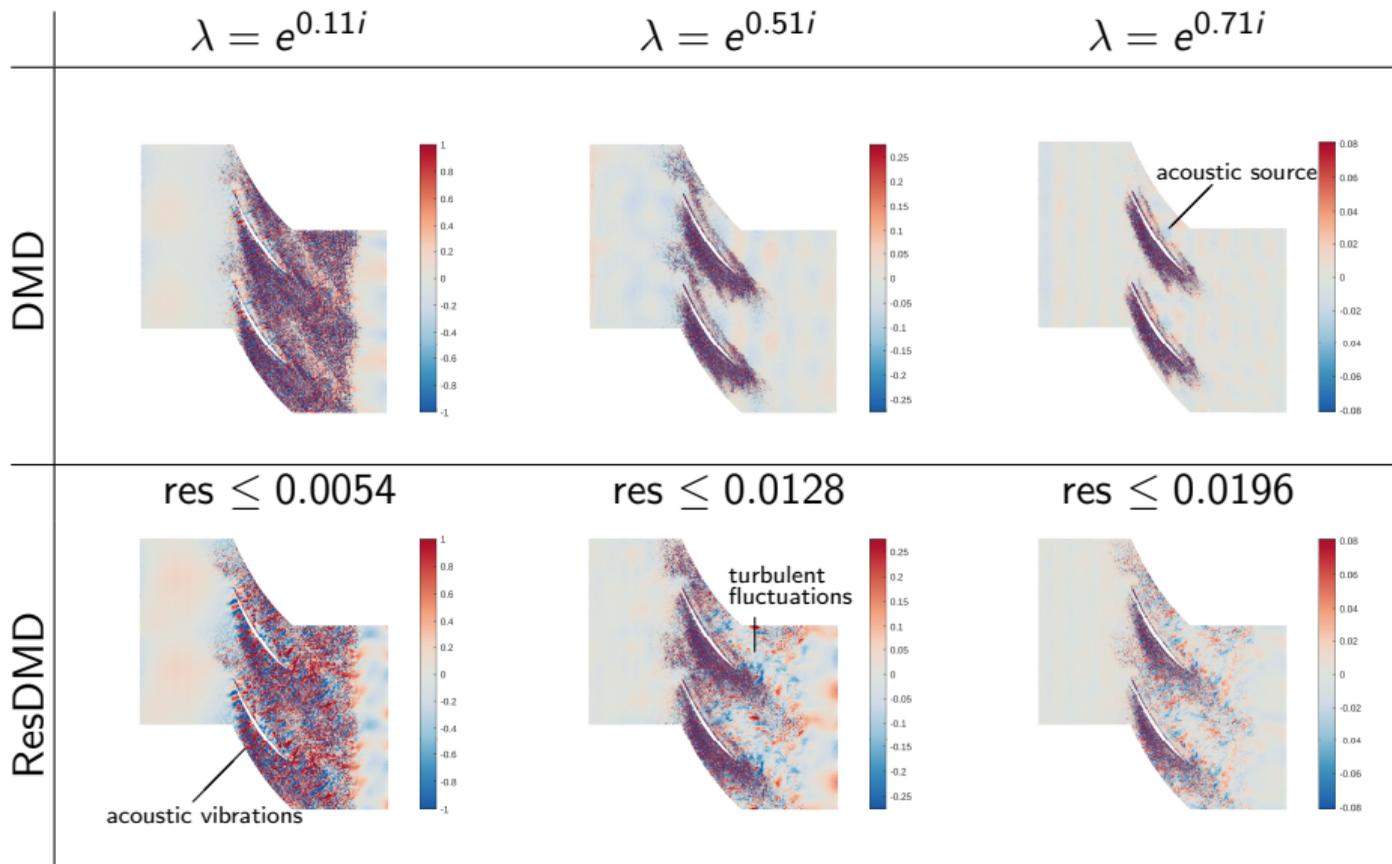
Rigorous and practical convergence as $M \rightarrow \infty$.

Can also check the basis a posteriori!

Spectral measures in molecular dynamics, $d = 20,046$



Turbulent flow past a cascade of aerofoils, $d = 295,122$



Concluding remarks

Algorithmic results in a programme on foundations of inf.-dim. spectral computations.

- **Part 1:** Computing spectra with error control.

Idea: Rectangular truncations to compute $\text{dist}(z, \text{Sp}(A))$.

- **Part 2:** Computing spectral measures.

Idea: Convolution with rational kernels through the resolvent.

All you need: Solve linear systems and compute inner products.

- **Part 3:** Data driven computations and Koopman operators.

Idea: New matrix for residual \Rightarrow ResDMD.

Further examples not in talk: spectral type (pure point, absolutely continuous, singularly continuous), Lebesgue measure and fractal dimensions of spectra, discrete & essential spectra, geometric features of spectra (e.g. radii, capacity etc.), spectral gap problem, ...

Details & code: <http://www.damtp.cam.ac.uk/user/mjc249/home.html>

If you have additional comments, questions, problems for collaboration, please get in touch!