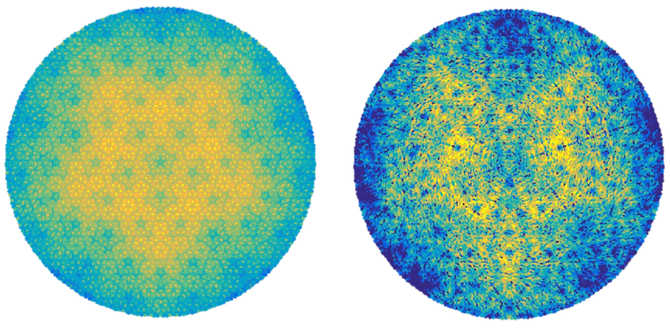

How to Compute Spectra with Error Control[1]

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The Problem

- Spectral computations are ubiquitous in the sciences with a vast number of applications.
- In general, infinite-dimensional spectral computations suffer from spectral pollution ("edge states" in physicists' terminology) – eigenvalues of finite truncations that have nothing to do with the infinite-dimensional spectrum.
- Non-normal case worse - often don't capture the whole spectrum via standard methods.

OPEN PROBLEM: Can we devise methods that converge and avoid spectral pollution?

- Despite more than 90 years of quantum theory, unknown even for general Schrödinger operators (both on discrete lattices and also in the continuum).

Results in Discrete Case

- Consider bounded self-adjoint operators A acting on the canonical Hilbert space $l^2(\mathbb{N})$.
- Assume we have a function $f\colon \mathbb{N} \to \mathbb{N}$ describing column decay in the sense that

$$\lim_{n\to\infty} \left\| (I - P_{f(n)}) A P_n \right\| = 0,$$

where P_n denotes the orthogonal projection onto the span of the first n basis vectors.

EXAMPLES: Sparse matrices, Jacobi operators, discrete Schrödinger operators, finite-range interaction Hamiltonians on lattices,…

RESULT: We devise an algorithm $\Gamma_n(A)$ with the following desirable properties [1]:

- **Converges** to the full spectrum $\mathrm{Sp}(A)$ in Hausdorff metric, **avoiding spectral pollution**.
- **Computes an error bound** $E(n,z)$ such that for any solution z in the output $\Gamma_n(A)$,

$$\mathrm{dist}(z, \mathrm{Sp}(A)) \leq E(n,z) \quad \text{and} \quad \lim_{n\to\infty} \max_{z\in\Gamma_n(A)} E(n,z) = 0.$$

- Algorithm is **fast**, completely **local and parallelisable**, avoiding direct diagonalisation.
- The algorithm is **optimal**, realising the boundaries of what computers can achieve.

IDEA OF ALGORITHM:

Step I: Given a region of interest $\mathcal{D}$ and a grid of points $\mathcal{G}$ over $\mathcal{D}$, approximate the function

$$\gamma_n(z) = \sigma_1\big(P_{f(n)}(A - zI)P_n\big) + \left\| (I - P_{f(n)}) A P_n \right\|$$

where $\sigma_1(C)$ denotes the smallest singular value of a rectangular matrix C. This can be done in parallel. We prove that

$$\gamma_n(z) \geq \mathrm{dist}\big(z, \mathrm{Sp}(A)\big), \qquad \lim_{n\to\infty} \gamma_n(z) = \mathrm{dist}\big(z, \mathrm{Sp}(A)\big).$$

Step II: For a given $z \in \mathcal{G}$, output the minimisers of $\gamma_n(z)$ over a disc of radius $\gamma_n(z)$ and centre z. This is an approximation of the spectrum locally near z.

Physical meaning: We compute the ground state energy of folded Hamiltonian

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

and this contains all of the interactions of the first n basis vectors without needing to apply boundary conditions (such as open, periodic etc.).

EXTENSIONS:

- Arbitrary graphs and lattices (instead of $\mathbb{N}$) through choice of basis.
- Can extend to unbounded operators with locally uniform convergence to spectra.
- Can compute approximate states and can be adapted to compute pseudospectra.
- Can be made to handle non-Hermitian operators.

Extensions to Partial Differential Operators

- The above result can be extended [2], with locally uniform convergence to spectra, to compute spectra of closed partial differential operators acting on $L^2(\mathbb{R}^d)$ of the form

$$T = \sum_{|k|\leq N} a_k(x)\partial^k.$$

- Assume coefficients are polynomially bounded and of locally bounded total variation.
- Idea is to approximate $\|(T - zI)^{-1}\|^{-1}$ locally through point samples of the coefficients and the theory of quasi-Mote Carlo numerical integration.
- This result can be extended to domains other than $\mathbb{R}^d$.
- Treats Schrödinger operators considerably more general than previous results [2,3].

Results Beyond [1]

- A wealth of spectral problems can be solved [4,5,6,7,8,9]. For example:

a) Spectral measures, decompositions and spectral types (pure point, abs. cts, sing, cts).
b) Discrete spectra, spectral gap, geometrical features such as capacity, generalised radii.
c) Lebesgue measure and fractal dimensions of spectra (applications in wavepackets).

- These computational problems can be classified into a hierarchy, precisely measuring their difficulty and proving optimality of the new algorithms.
- Error control allows applications in computer-assisted proofs.

Numerical Examples and Applications

QUASICRYSTALS

- An important topic (2011 Nobel prize in chemistry) with many interesting physical properties and potential applications.
- Few known analytic results, very difficult theoretically (particularly in dimensions larger than one), with often fractal-like spectra.
- We study the canonical 2D model – a Penrose tile.

Example 1: Graphical Laplacian (Fig. 1) which models an electronic Hamiltonian. We compare against standard truncation methods (finite section) with open boundary conditions and periodic approximations of the tiling. The new method is much faster, and converges, avoiding spectral pollution. Top right of poster: ground state (left) and state nearest -5 (right) computed by the method without direct diagonalisation.

Example 2: Magnetic Hamiltonian (Fig. 2) with constant perpendicular magnetic force. The new algorithm is able to cope with the fractal-like butterfly spectrum and correctly leave out the gaps. The new algorithm can also cope with non-constant magnetic fields (which cannot be dealt with using standard methods, even for periodic crystals).

Future work: Using the algorithm for 3D quasicrystals models.

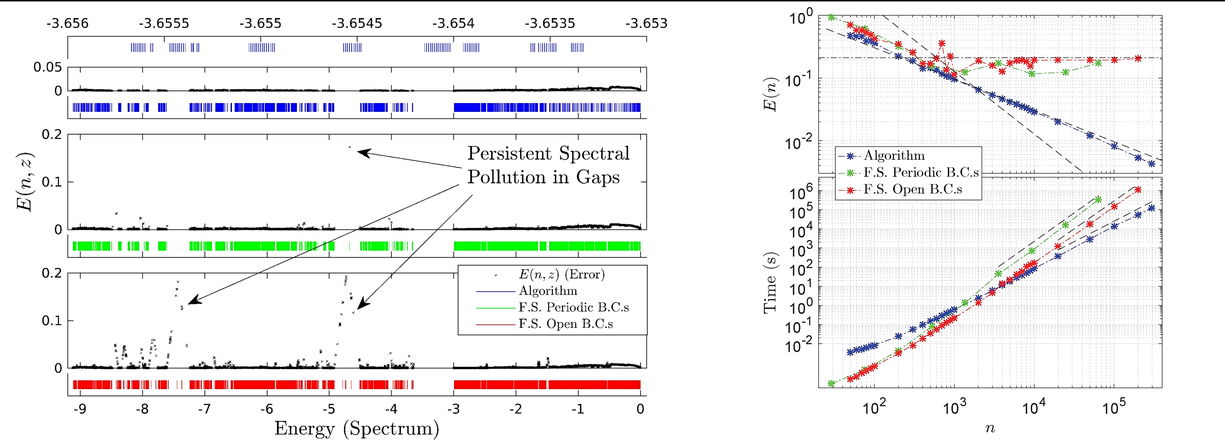


Fig. 1: Left: Computed spectrum of graphical Laplacian. Right: Computational times and errors of methods.

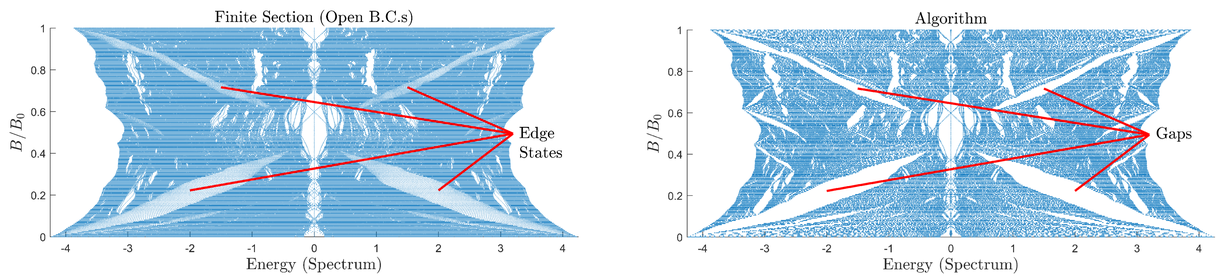


Fig. 2: Spectra of magnetic model (strength B). The algorithm correctly leaves out the gaps and is able to capture the complicated Structure.

PHASE TRANSITIONS (PT-Symmetric Hamiltonians)

- Non-self-adjoint yet can have real spectra, typically for small imaginary part of potential.
- Symmetry breaking: complex spectra when imaginary part of potential increased beyond threshold. These types of operators used in open systems in optics.
- Study phase transition for aperiodic operator

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

- Fig. 3 shows pseudospectra of algorithm and finite section (open and periodic boundary conditions). The algorithm predicts the phase transition at $\gamma_{PT} \approx 1$, whereas edge states cause the phase transition to be fragile in the thermodynamic limit (suggesting $\gamma_{PT} \to 0$).

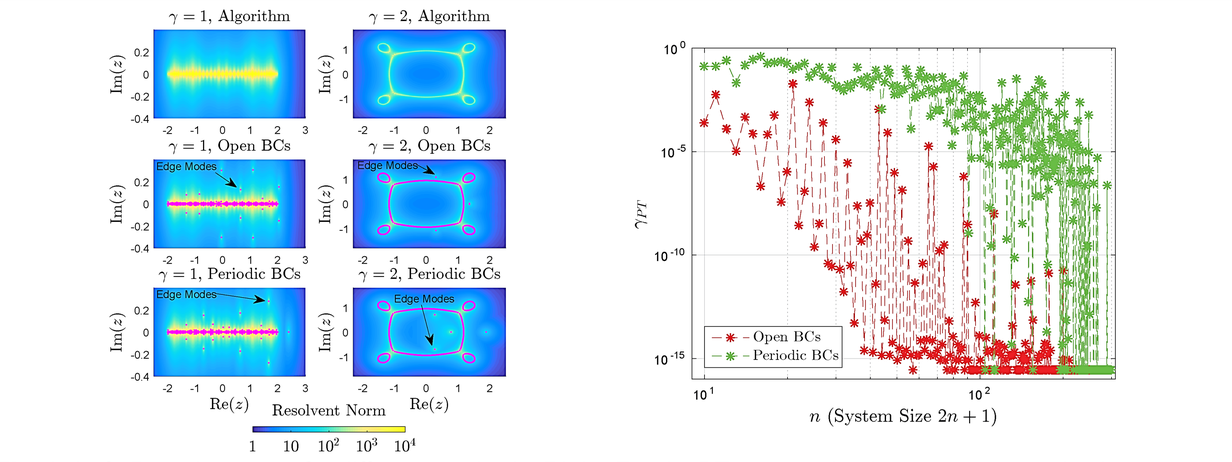
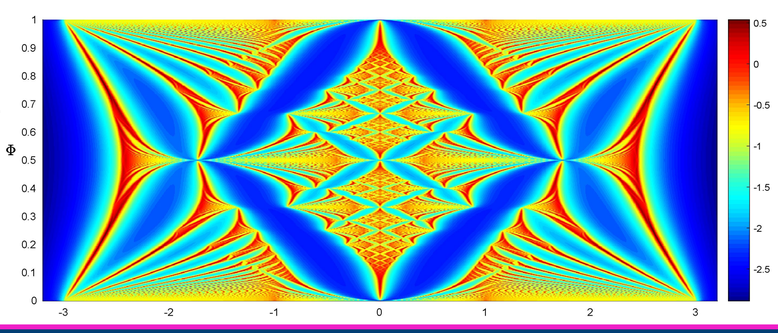


Fig. 3: Left: Pseudospectra for different methods. Right: Fragile PT-symmetric phase as system size increases.

FOR DISCUSSION:

SPECTRAL MEASURES [6]

- Can be used to solve infinite-dimensional evolution PDEs with error control.
- Right: Visualisation of spectral measure for magneto-graphene (field strength Φ).



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