Computing the spectrum of aperiodic infinite-volume operators with error control

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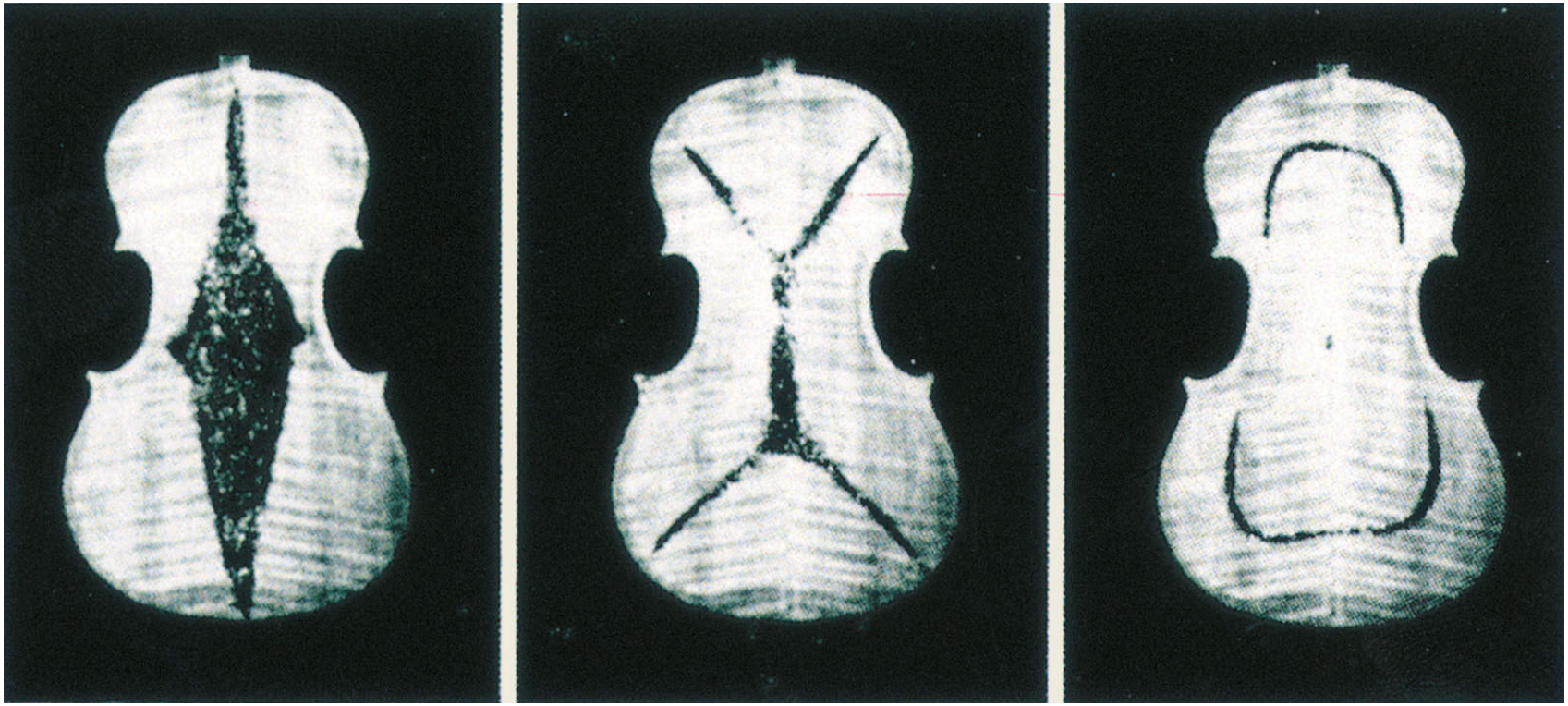


Computing the spectrum of different linear operators is important across physics

Algorithms which provide **rigorous error control** are preferable and used for **computer proofs** in math

We develop algorithms to compute the spectrum with error control for **infinite-volume operators** with **finite local complexity**

Image source: https://physicsworld.com/a/science-and-the-stradivarius/

Error control for matrix eigenvalues

Consider a matrix like

$$A = \begin{pmatrix} 1.5 & -1 & -0.5 \\ -1 & 3 & -1.5 \\ -0.5 & -1.5 & 2 \end{pmatrix}$$

If you just call `eigh` in Python or Matlab, you get

$$\mathrm{Spec}(A) \approx \{-3.64958989, 1.6742044, 2.47538548\}\,.$$

But **what is the precision** of this approximation, how many digits are significant? With interval arithmetic, we would instead get something like

$$\mathrm{Spec}(A) \subseteq (-3.7, -3.6) \cup (1.6, 1.7) \cup (2.4, 2.5)$$

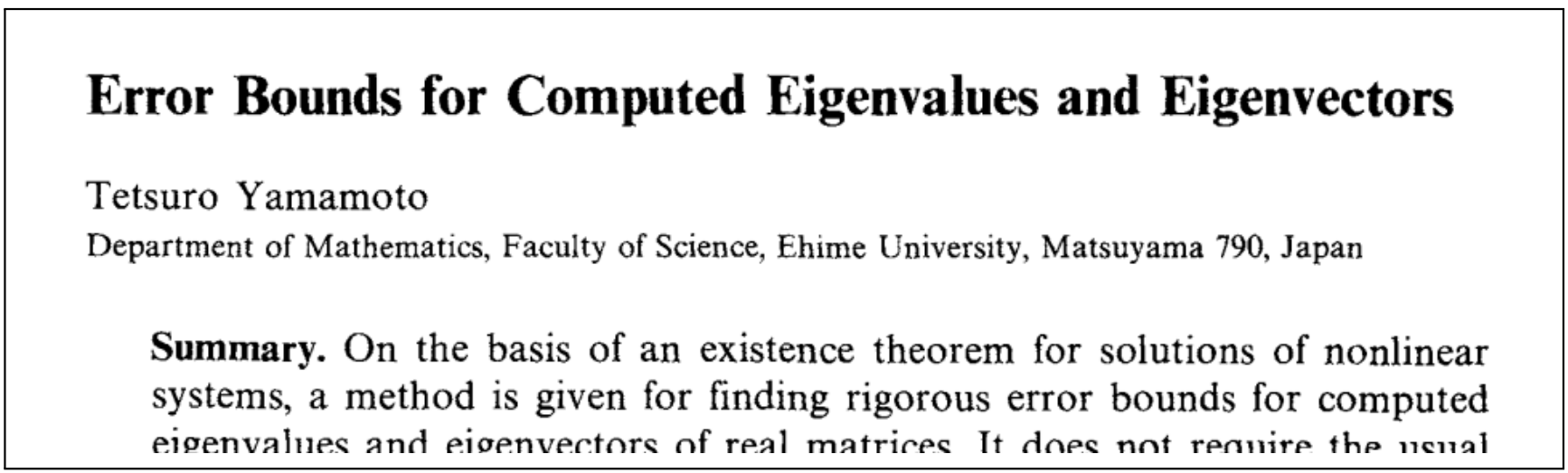
This is also known as **validated numerics**.

Error control for finite-dimensional eigenvalue computations

Most eigenvalue algorithms are **iterative** (power iteration, Lanczos, Arnoldi, . . .)

How many steps should we iterate until we have a good enough approximation of the eigenvalues and eigenbasis?

Solution by Yamamoto (1980, 1981) using interval arithmetic



Error Bounds for Computed Eigenvalues and Eigenvectors

Tetsuro Yamamoto
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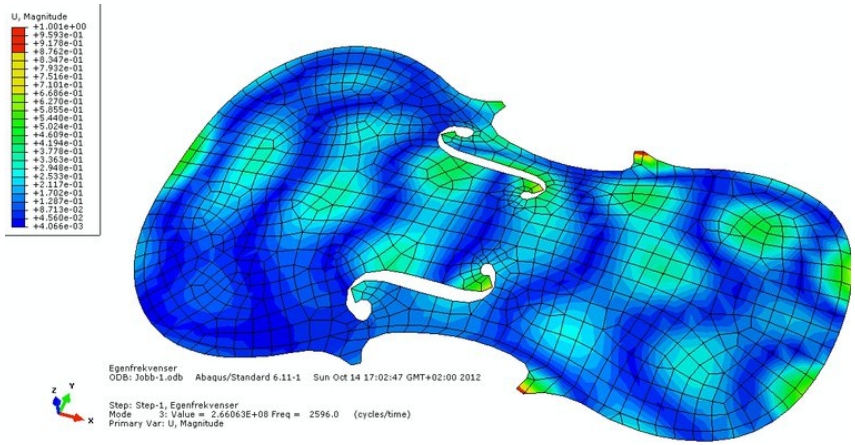
Summary. On the basis of an existence theorem for solutions of nonlinear systems, a method is given for finding rigorous error bounds for computed eigenvalues and eigenvectors of real matrices. It does not require the usual

Error control for continuous systems

If instead of a matrix we have a **differential operator**, the problem of **discretization** needs to be solved additionally



For general *infinite-dimensional systems*, the *Rayleigh–Ritz method* can be used to get an upper bound on eigenvalues:

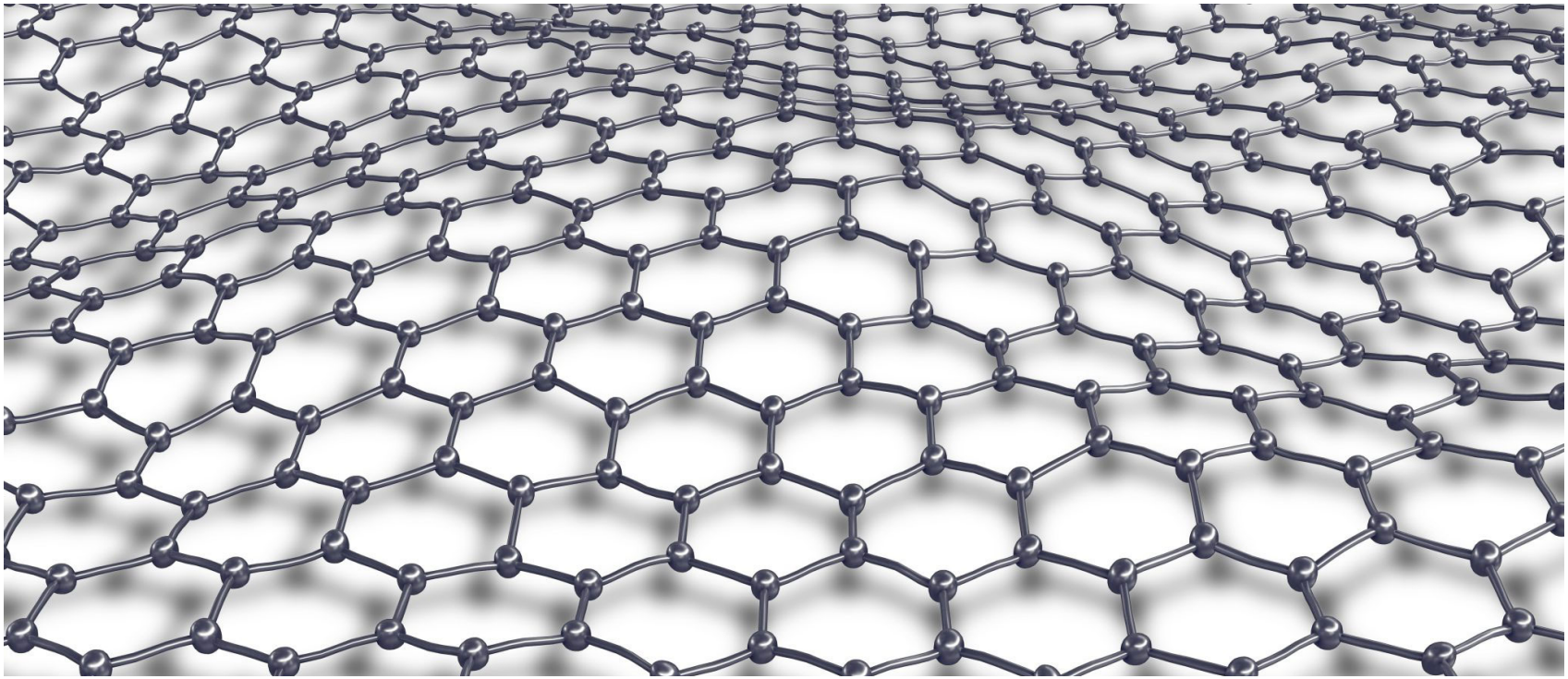
$$\lambda_1 \leq \frac{\|Hv\|}{\|v\|}, \ \lambda_2 \leq \cdots$$

Obtaining **lower bounds** on eigenvalues is usually much more involved – see Kato 1949, Weyl 1950, Bazley and Fox 1961. There are even integrated FE methods (Carstensen 2014, . . .)

Image source: http://www.violin-analysis.com/

Spectral computations for infinite-volume systems

Instead of continuous systems, we will consider discrete operators **on infinite domains** – for example, the tight-binding approximation for an electron in a material.



Similar to the continuous case, we provide error control to the usually ad-hoc methods of reducing these systems to **finite-dimensional parts**

What kind of systems will we consider?

We consider **tight binding models** (discrete Hamiltonians) H on a discrete subset $\Gamma \subseteq \mathbb{R}^n$.

That is, we assume that H is a bounded operator on a Hilbert space $\mathcal{H}$ with a basis $(e_i)_{i\in\Gamma}$ indexed by Γ.

Furthermore, we assume that the operator has **short range**, that is, its matrix entries H_{xy} decay like

$$|H_{xy}| \leq C \frac{1}{d(x,y)^{n+\varepsilon}}$$

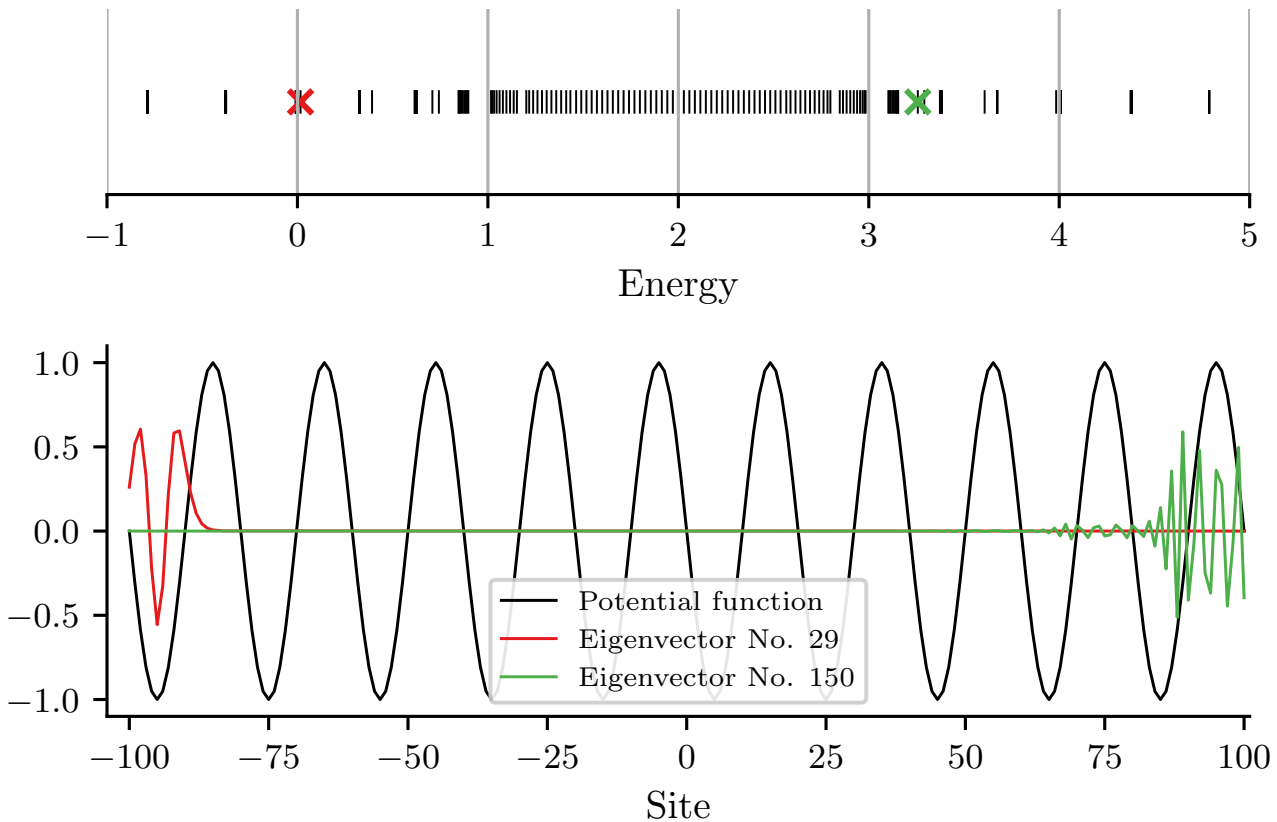
for some $C, \varepsilon > 0$.

In addition, we will require **finite local complexity** – more on that later.

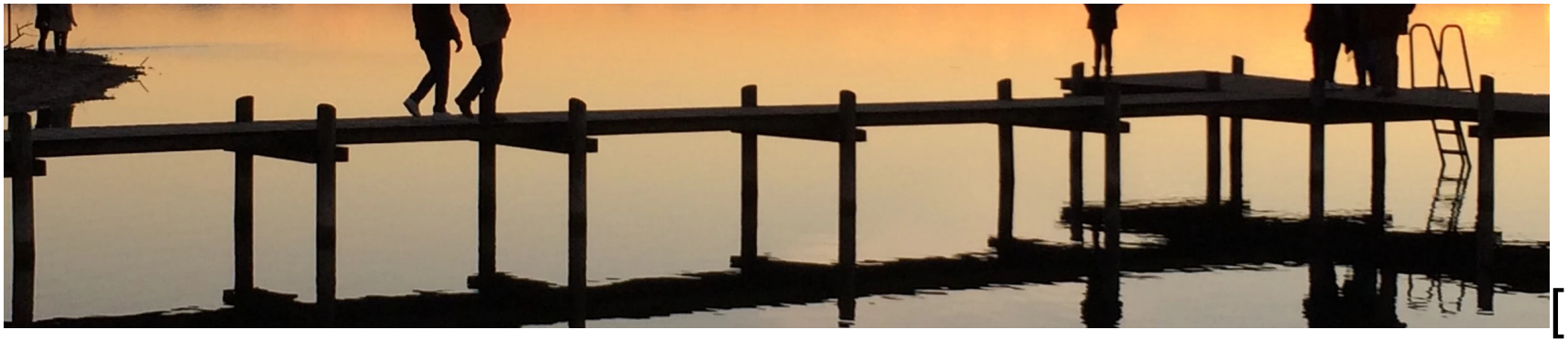
What do physicists usually do?

One can obviously not pass infinite matrices into Numpy's `eigh`... Therefore physicists often just **cut off** to produce a finite-dimensional matrix and approximate the spectrum

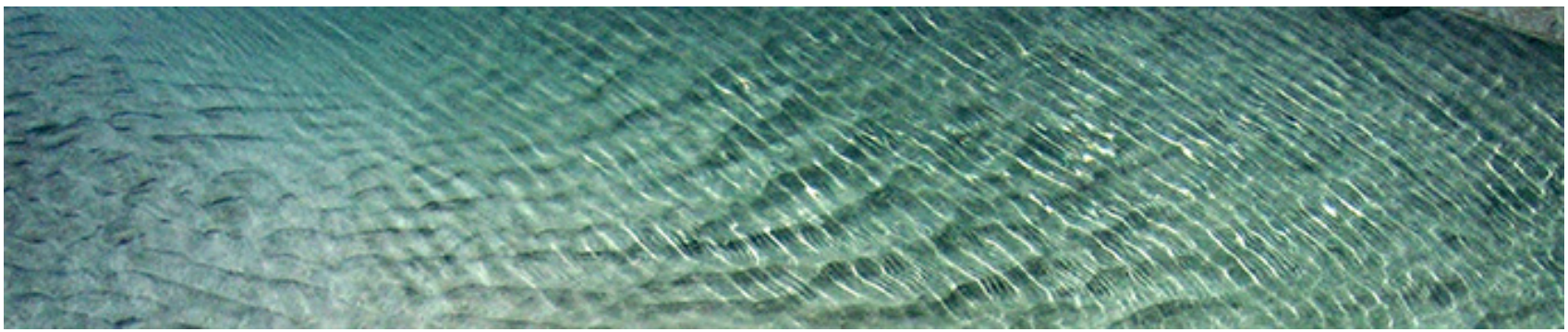
However, this approach **can lead to wrong results** due to **edge states**



Periodic and aperiodic infinite-volume systems

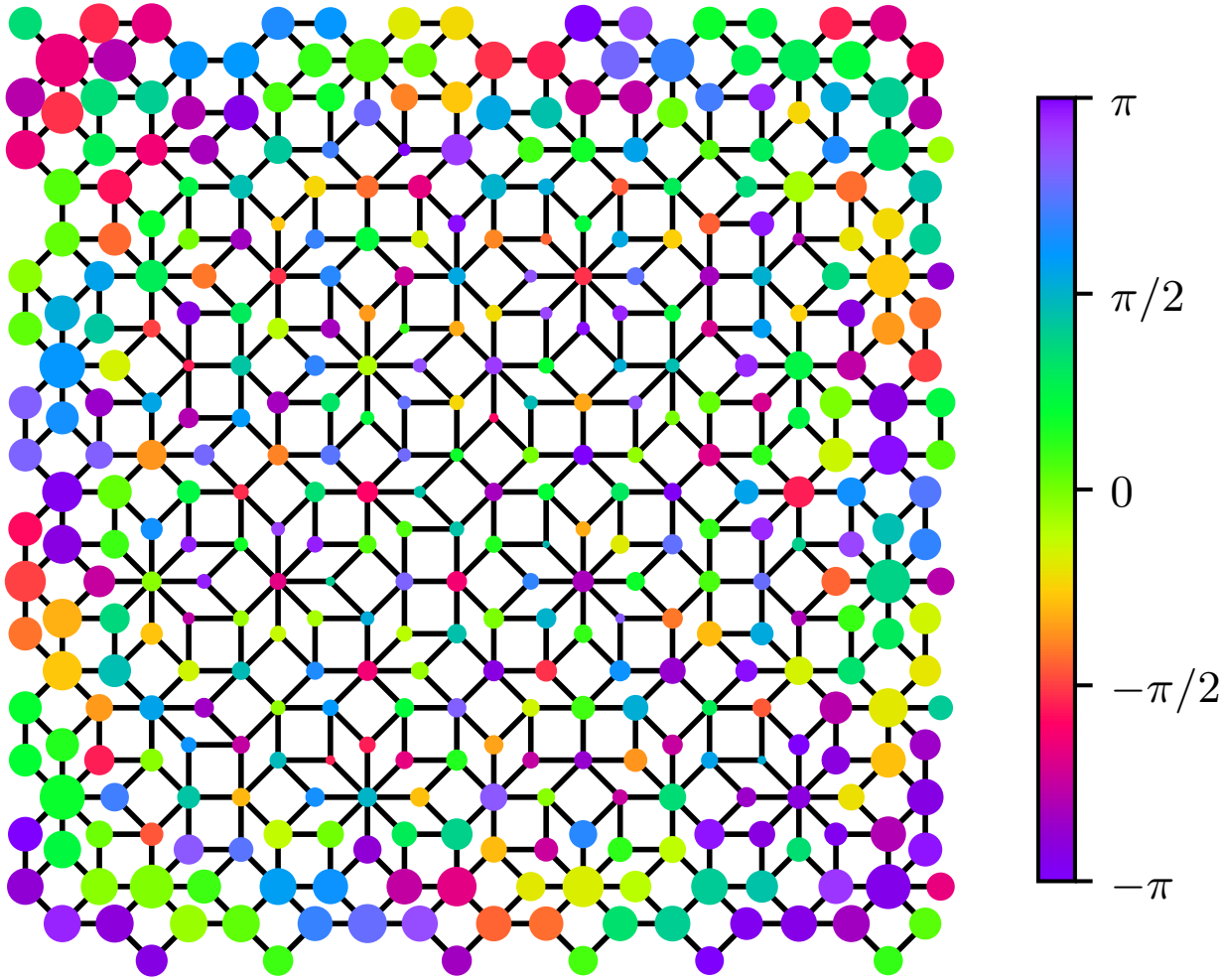


For *periodic Hamiltonians*, the spectrum can be computed using the Bloch-Floquet transform (Bloch 1928).



But for *aperiodic systems*, there are no universal methods to compute the spectrum of infinite-volume systems.

2D quasicrystals edge state example



Error control using periodic approximants

One of the most highly developed approaches towards error control is to approximate H by a periodic operator H_{per} so that local patches in approximate one-to-one correspondence (Beckus and Bellissard 2016, Beckus and Takase 2021, . . .)

For this case, there exist statements of the form

$$d_H\left(\bigcup_{x\in X_1}\sigma(A_{x_1}),\ \bigcup_{x_2\in X_2}\sigma(A_{x_2})\right)\leq Cd_H(X_1,X_2)^{\alpha}\,,$$

for some dynamical systems X_1 and X_2.

Problem: *periodic approximations cannot always be found*.

Question

Can you think of a simple system with finite local complexity that cannot be approximated periodically?

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Answer

The string (or 0/1-valued potential)

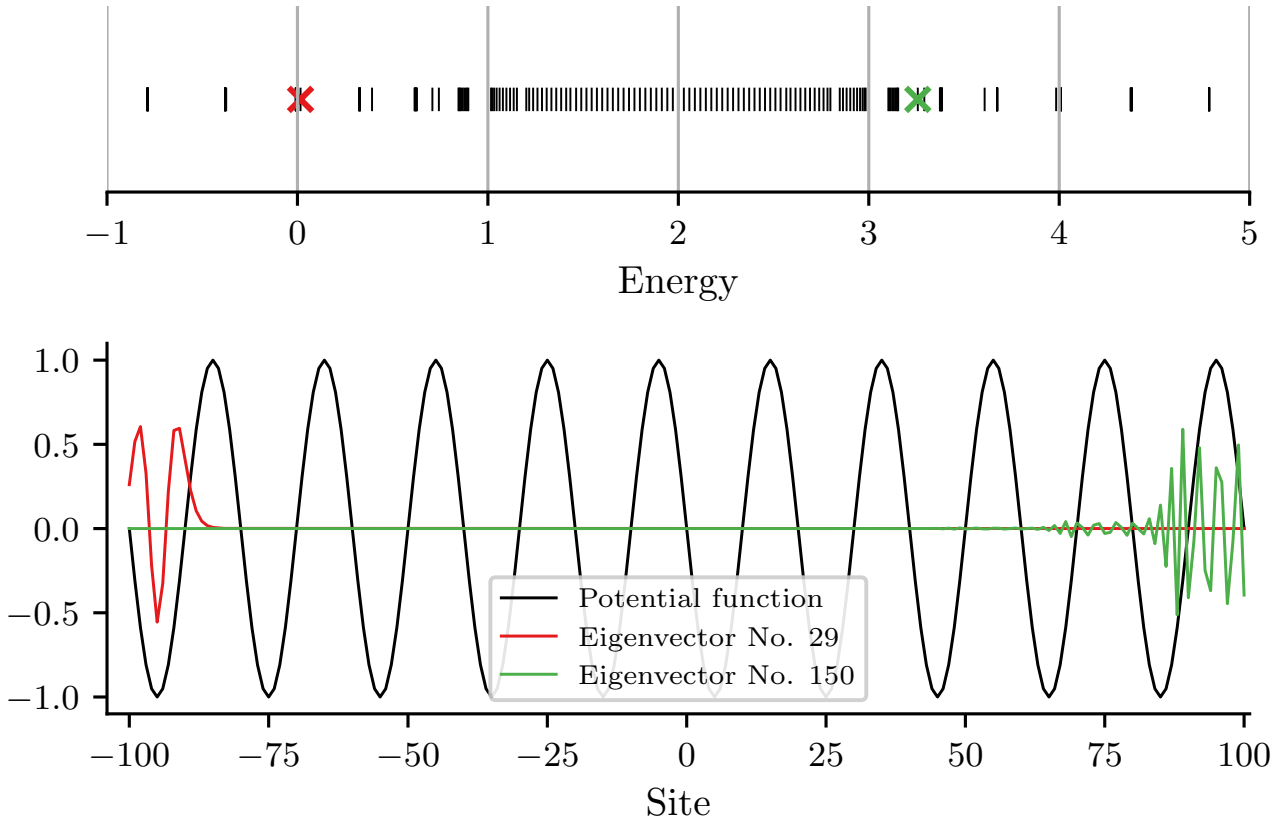
$$\ldots 000000000111111111\ldots$$

has subwords 0^*1^*, but any periodic approximant must also have the patch 10 if it has 01.

The method of uneven sections

Let H be a discrete operator with finite range m for simplicity.

If we compute the spectrum of $\mathbf{1}_{B_L(x)} H \mathbf{1}_{B_L(x)}$, the Dirichlet boundary conditions introduce possibly large errors in the spectrum *(spectral pollution)*



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Solution of *Colbrook, Roman, Hansen (2020)*: Compute the smallest singular value of

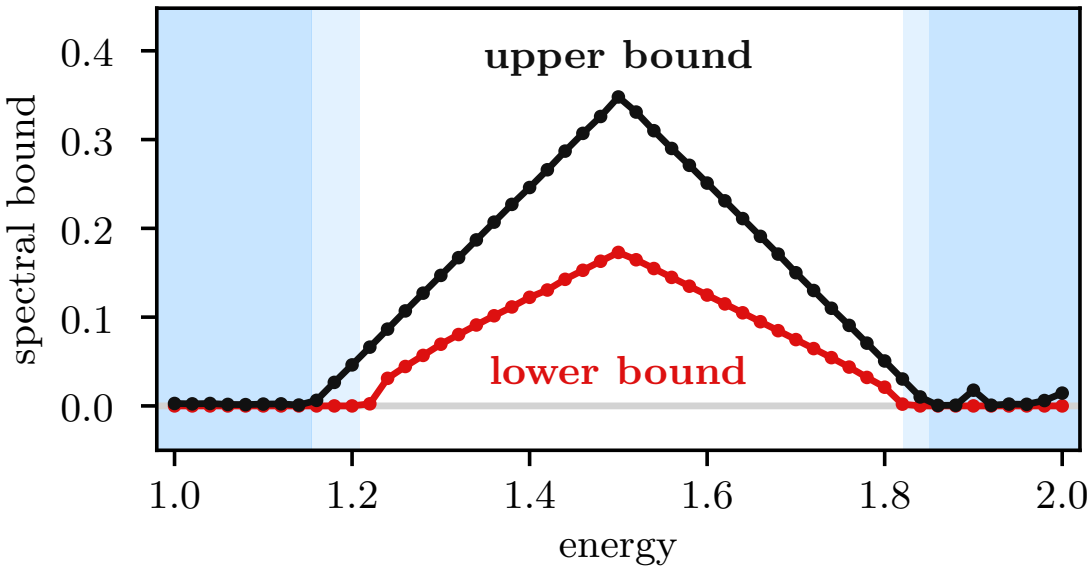
$$\mathbf{1}_{B_{L+m}(x)}(H - \lambda)\mathbf{1}_{B_L(x)}$$

for a set of $\lambda \in \mathbb{C}$. We will denote this as $\varepsilon_{L,\lambda,x}$. If $v \in \mathcal{H}_{B_L(x)}$ is the corresponding singular vector, then v is an $\varepsilon_{L,\lambda,x}$-quasimode of the infinite-volume H, and thus

$$d(\lambda, \mathrm{Spec}(H)) \leq \varepsilon_{L,\lambda,x}$$

for H self-adjoint. Thus, spectrum of H is guaranteed!

Advantages of uneven sections



- Easy to compute
- Converges quickly in practice
- Requires no spatial structure

Limitations of uneven sections – no-go theorem

The upper bound

$$d(\lambda, \mathrm{Spec}(H)) \leq \varepsilon_{L,\lambda,x}$$

is only a **one-sided** bound

Actually, Colbrook et al. provided a **no-go theorem**, saying that it is **impossible** to computationally bound $d(\lambda, \mathrm{Spec}(H))$ from below for general operators.

Their proof is very simple: the operators

$$I_1 = \begin{pmatrix} 2 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \\ \vdots & & & \ddots \end{pmatrix}, \quad I_2 = \begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 2 & 0 & \cdots \\ 0 & 0 & 1 & \\ \vdots & & & \ddots \end{pmatrix}, \quad \text{etc.}$$

cannot all be distinguished from 1 by looking at finitely many elements, but the spectra are $\{1, 2\}$ and $\{1\}$.

Circumventing the no-go theorem

The no-go theorem is so simple that is **even works for infinite diagonal matrices**!

I would argue that the no-go theorem **says more about the statement of the problem** than about the actual difficulty of spectral computation.

It has been suggested by *Colbrook, Hansen (2021)* that **adding structure can improve computability**. This is just what we do here: we add the structure of *finite local complexity (flc)*

Finite local complexity

For discrete operators, we say that H has *equivalent action* on $B_L(x)$ and $B_L(x+t)$ if

$$B_L(x+t) \cap \Gamma = (B_L(x) \cap \Gamma) + t$$

and for all $a_1, a_2 \in B_L(x) \cap \Gamma$, we have

$$H_{a_1+t,a_2+t} = H_{a_1 a_2}$$

up to a pointwise phase modification.

We say H has *finite local complexity* if there are finitely many $x_1, \ldots, x_N \in \mathbb{R}^n$ such that for any $y \in \mathbb{R}^n$, there is a $k \in \{1, \ldots, N\}$ such that H has equivalent action on $B_L(y)$ and $B_L(x_k)$.

Detectability of infinite volume spectrum

Question: Is the spectrum a “local” property or can it depend on the large scale structure of the Hamiltonian?

We show that *a fixed window size is sufficient* to detect any spectrum of the infinite-volume operator.

(Similar result: Beckus, Takase 2021, Lemma 3.1)

Detectability of infinite volume spectrum

Theorem 1 Let $n \in \mathbb{N}$, $\Gamma \subseteq \mathbb{R}^n$ a countable set, and H a discrete operator on Γ with finite range $m > 0$. Then for every $\lambda \in \mathbb{C}$ and $L > m$ it holds that

$$d(\lambda, \mathrm{Spec}(H)) \;\geq\; \varepsilon_{L,\lambda}\sqrt{1-\delta} - \|H - \lambda\|\sqrt{\delta}\,, \tag{1}$$

where

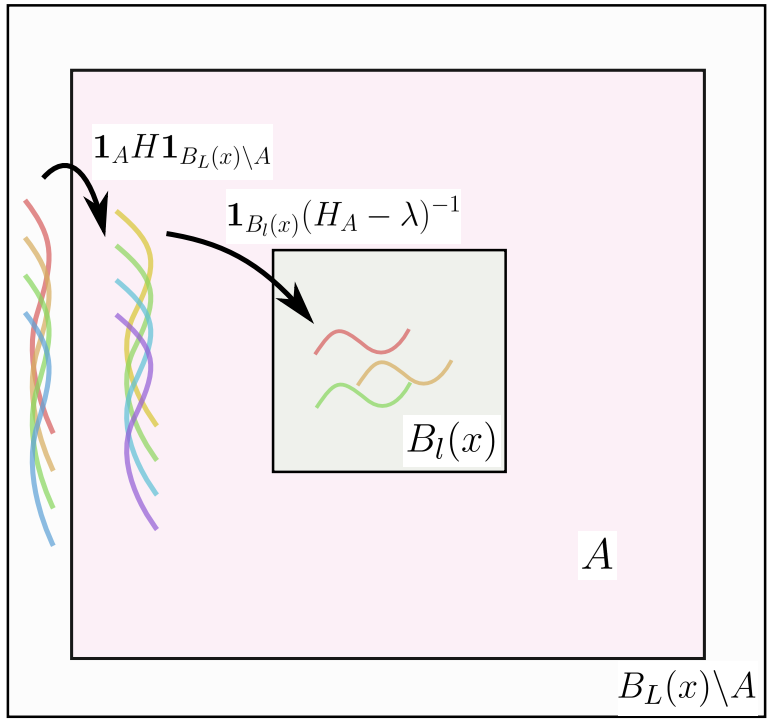
$$\varepsilon_{L,\lambda} := \inf_{x \in \mathbb{R}^n} \varepsilon_{L,\lambda,x} \tag{2}$$

and

$$\delta := \frac{n}{\lceil L/m - 1 \rceil}\,. \tag{3}$$

Proof Idea 1: Lage mass in the „rim“

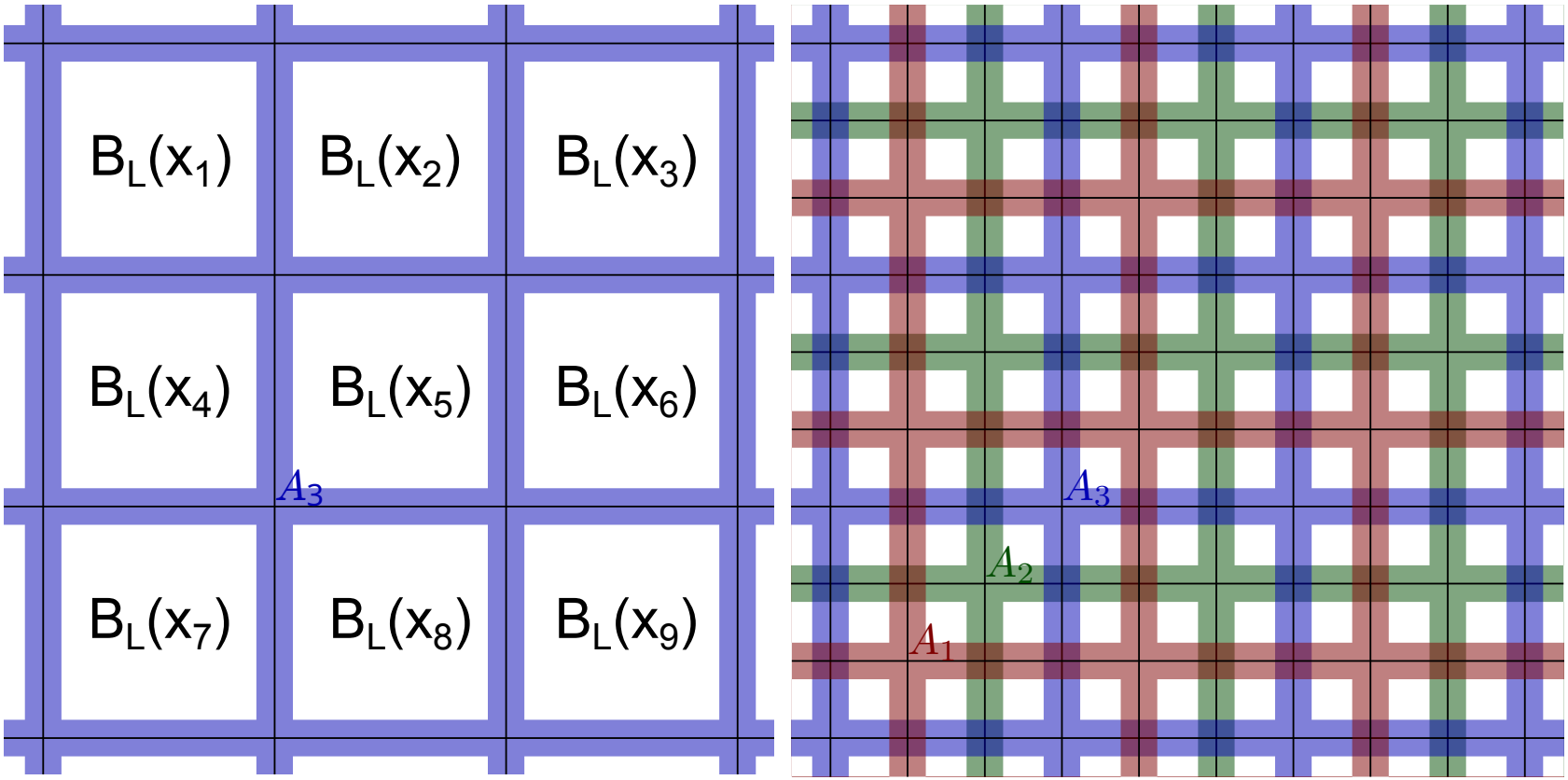
If $d(\lambda, \mathrm{Spec}(H)) = \rho$, we can find a ρ-quasimode (approximate eigenstate) ψ, in the infinite-volume system. If the restricton $\psi \mathbf{1}_{B_L(x)}$ is a quasimode of H, then we can bound $\varepsilon_{L,\lambda,x}$.



Actually, $\psi \mathbf{1}_{B_L(x)}$ *will* be a quasimode if $\|\psi\|_{B_{L+m}(x)\setminus B_{L-m}(x)}$ is small. That is, the only way $\psi \mathbf{1}_{B_L(x)}$ might not be a quasimode is if **a large fraction of the ℓ^2 mass is in the „rim“**.

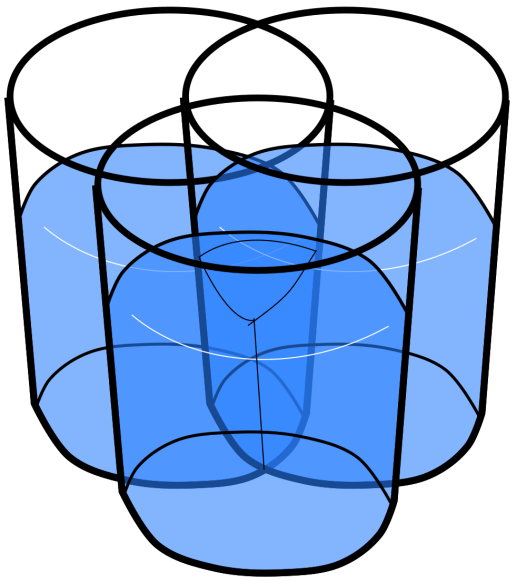
Proof Notion 2: Multiple overlapping coverings

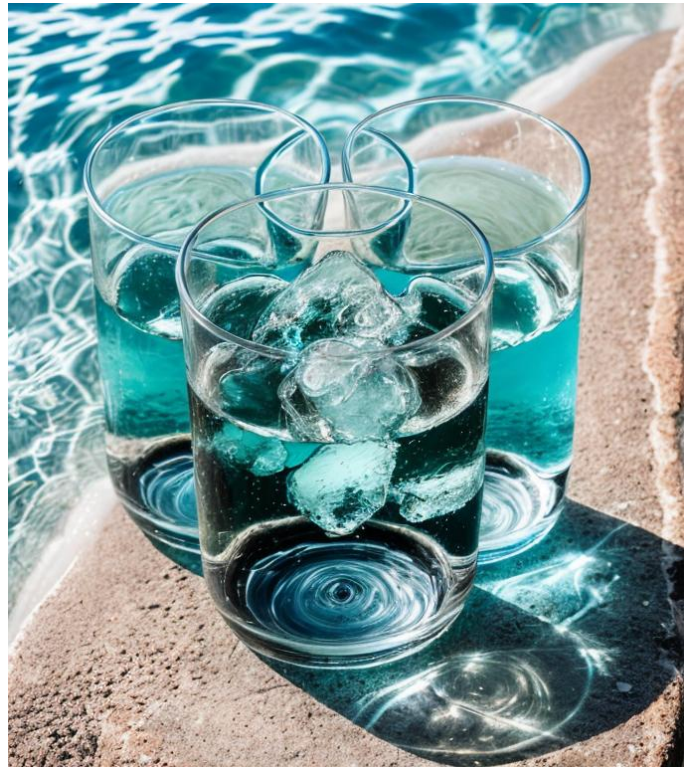
We construct a **grid of squares**. If the mass in the edges is small in any grid, this is sufficient

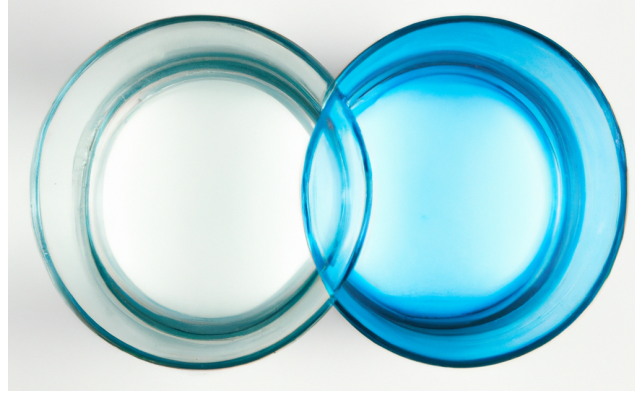


By constructing **multiple overlapping grids**, we can cover the edges of one covering with the interiors of another

Proof Notion 3: The mass cannot be in the edges for all the coverings







Computability of the *flc* spectral problem

We use a notion of computability from *Colbrook and Hansen (2021)*, together with the notion of *Blum-Shub-Smale* algorithms (like Turing machine with real numbers)

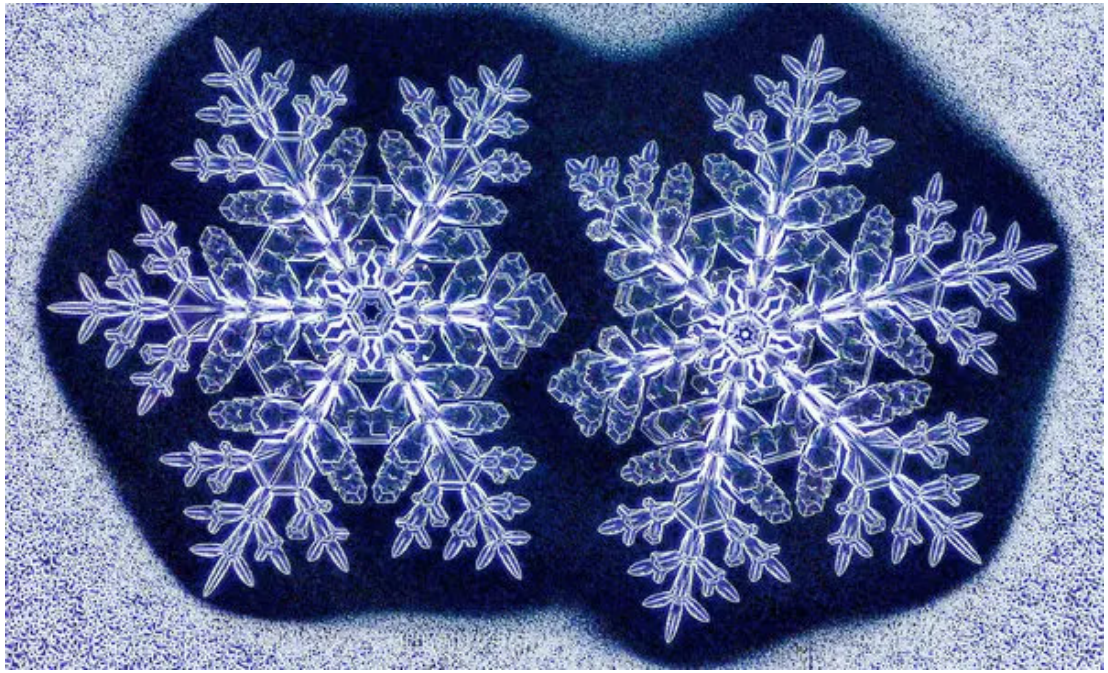
Colbroo and Hansen defined the computational problem using the matrix entries as evaluation functions and showed that it is **not solvable** with error control from this data

We show that by adding the very general notion of finite local complexity, **the problem becomes solvable with error control**

We show lower solvability complexity index (SCI, $\approx$ number of limits needed) with flc than in general

Application: Quasicrystals

Have you every seen a **five-pointed snowflake** or other crystal with fivefold symmetry?

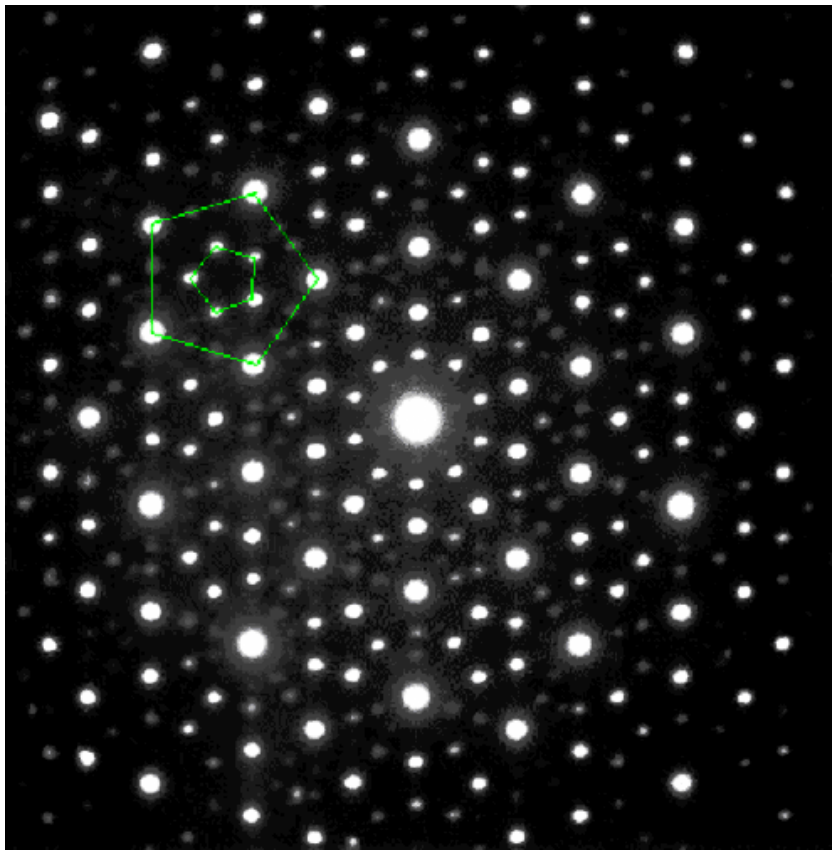


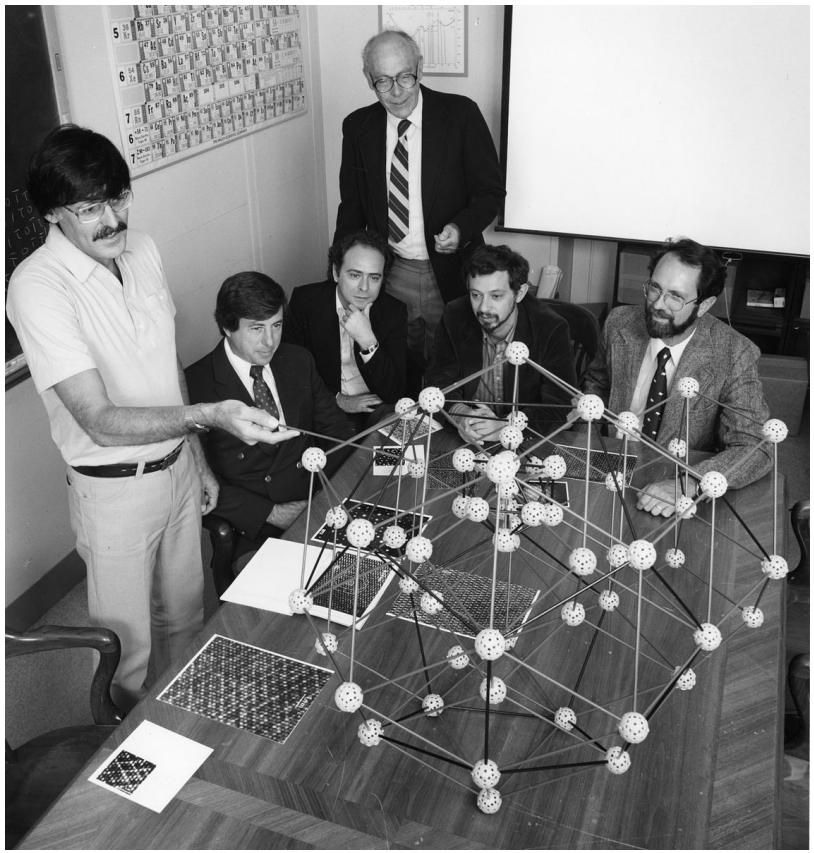
Using lattice theory, one can show that only 2-, 3-, 4- and 6-fold symmetries are possible. This is known as **crystallographic restriction** (Kepler 1611).

But crystals with fivefold symmetries **exist!** (Shechtman 1984)

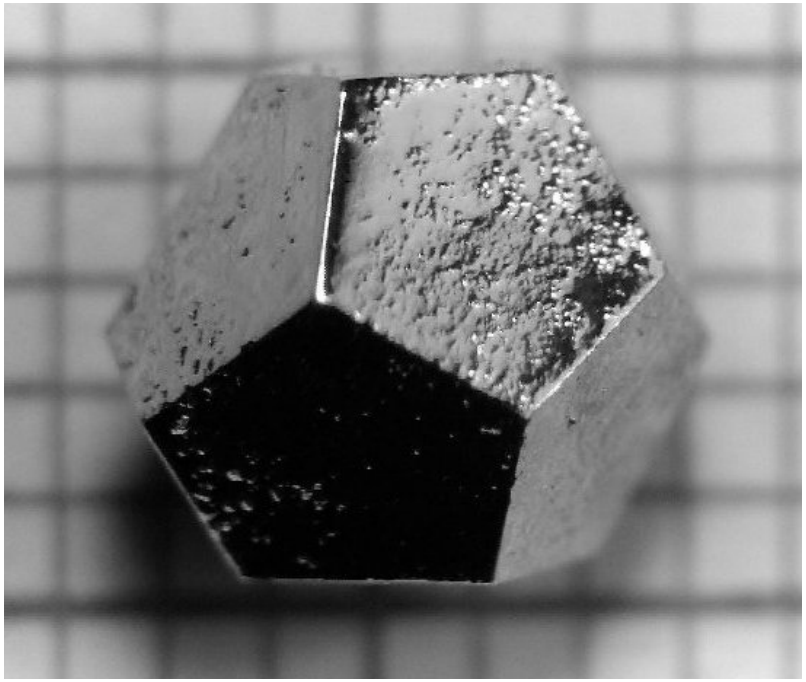
Discovery of quasicrystals (nonperiodic crystals)

"Forbidden" symmetries were unexpectedly discovered in artificial crystals by Dan Schechtman in 1982



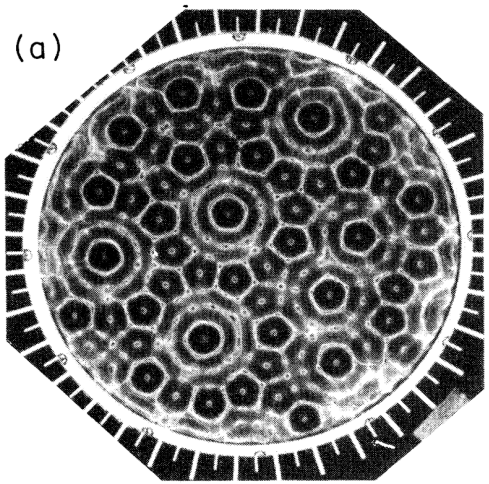


Images of quasicrystals



Ho-Mg-Zn dodecahedral quasicrystal

(https://commons.wikimedia.org/wiki/File:Ho-Mg-ZnQuasicrystal.jpg)



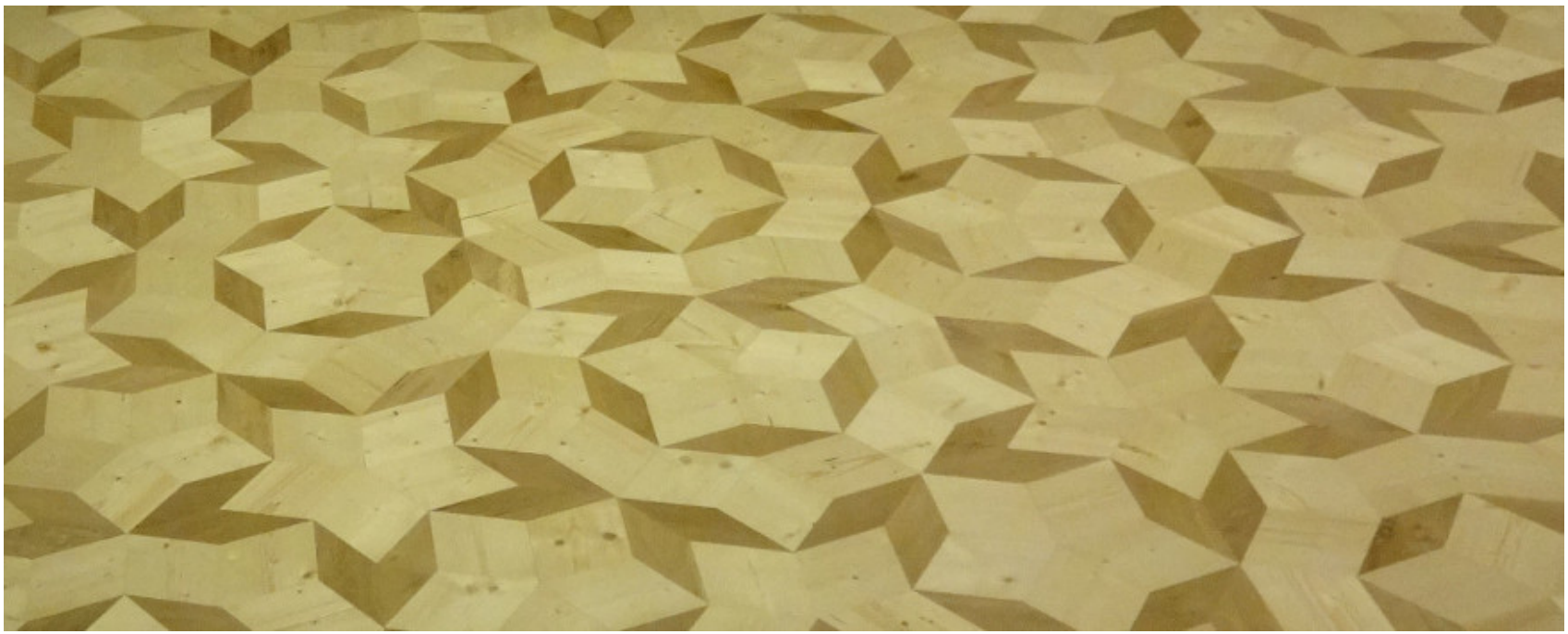
Standing water wave quasicrystal

(https://doi.org/10.1103/PhysRevE.47.R788)

The math behind quasicrystals

Quasicrystals have **a strong long-distance structure** without being periodic

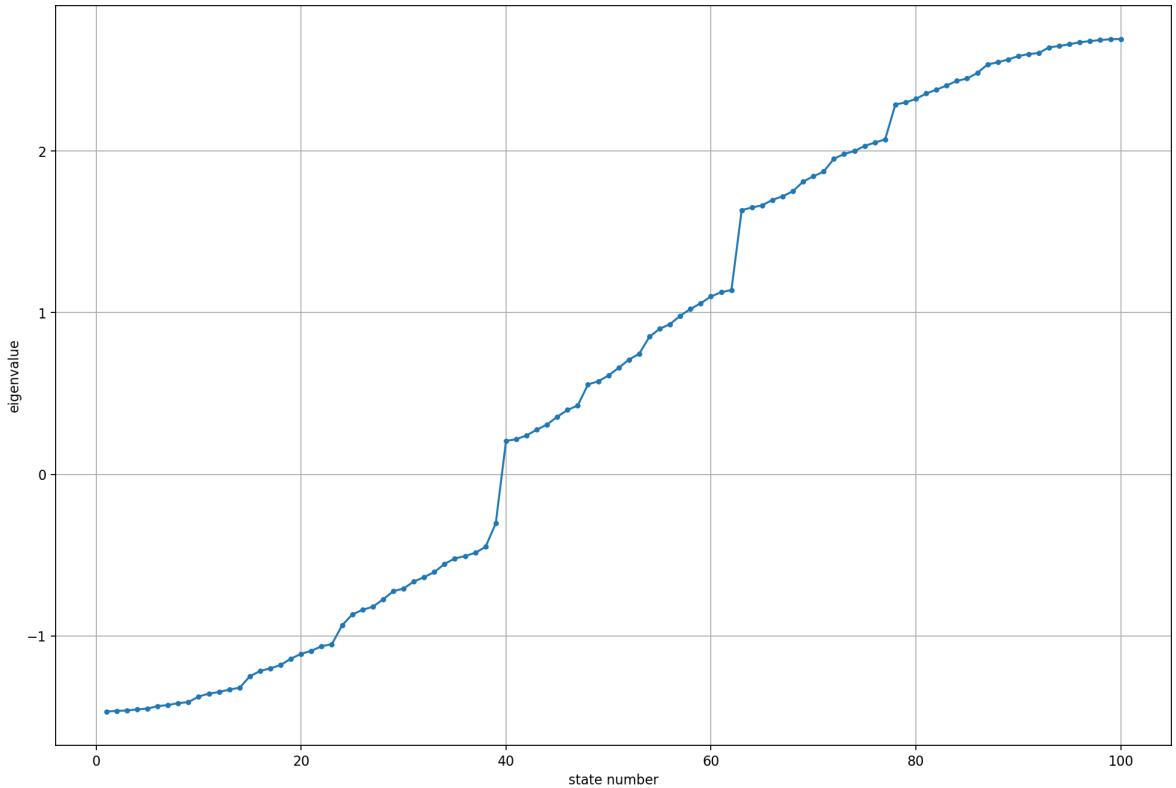
The mathematical theory is given by self-similar **aperiodic tilings**, such as the famous **Penrose tilings** (i.e., math predates physics!)



Spectra of quasicrystals

The spectra of quasicrystalline operators have gaps just like periodic ones, but are **often fractal**.

One of the first studies was Kohmoto (1983), „Mapping and Escape“



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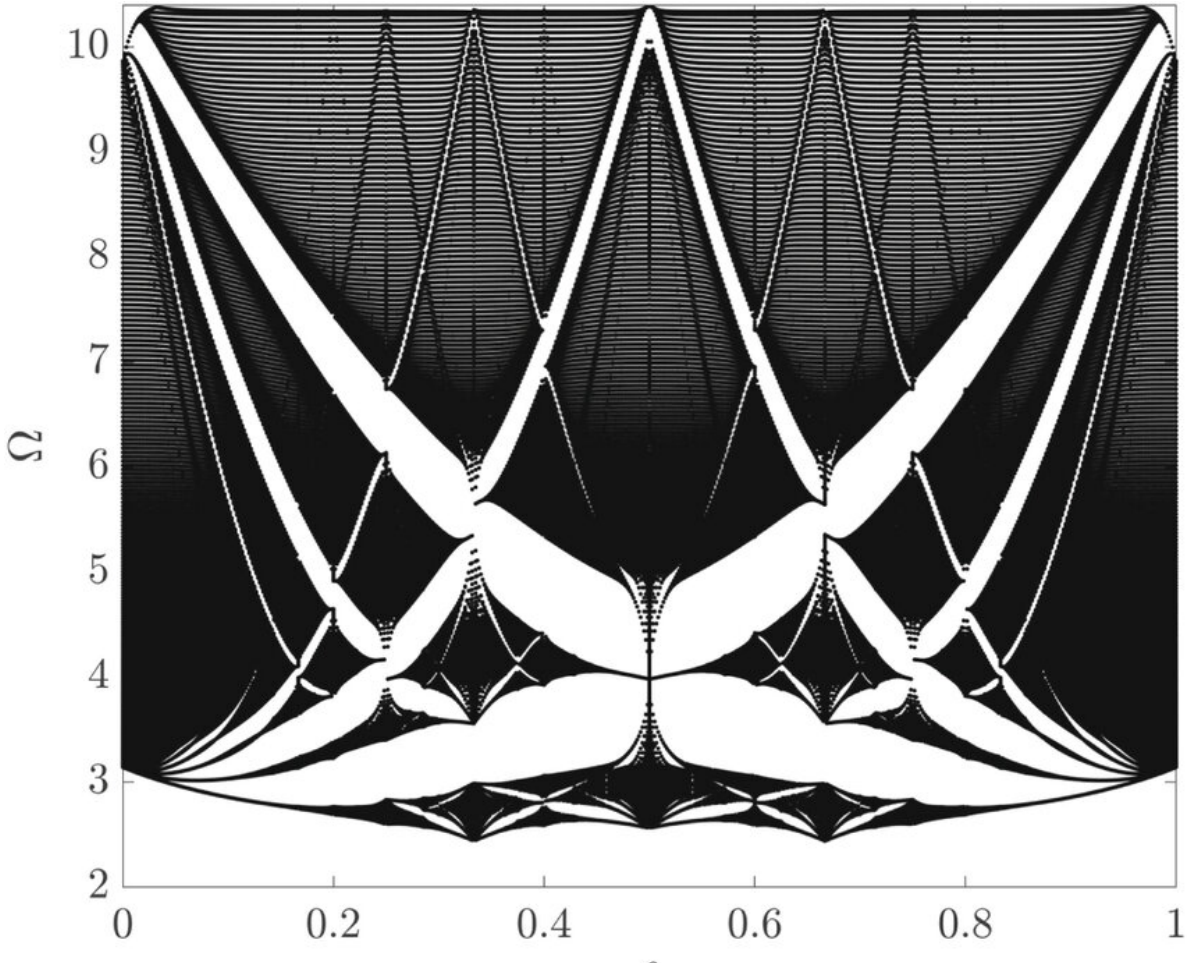


Computing spectral gaps in quasicrystals

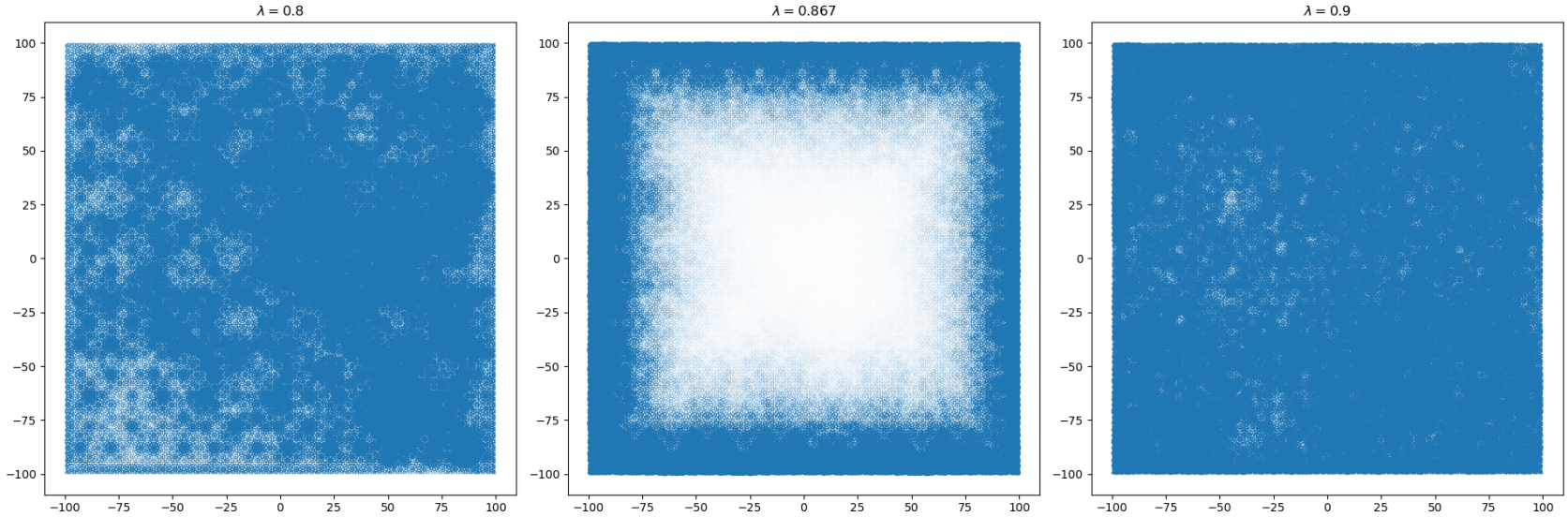
Quasicrystals are a great class to study because they have **low local complexity** (few patches)

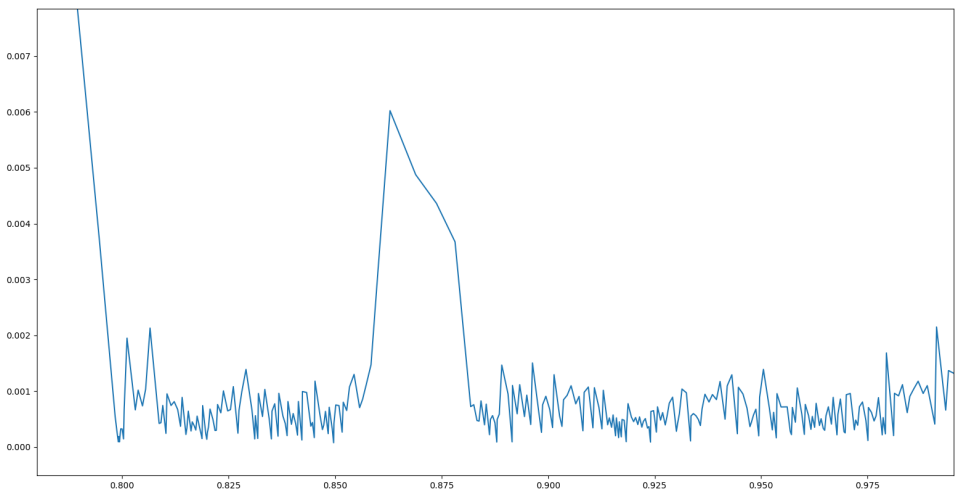
The previously described approach **converges slowly**, the size of the patches growing like $1/\varepsilon$, where ε is the required precision.

For practically computing the spectral gaps, we have developed a **method based on Dirichlet boundary conditions** which converges more quickly

Normally, Dirichlet bc introduce possibly many edge states. We formulate an **edge state criterion** to distinguish edge states from bulk states

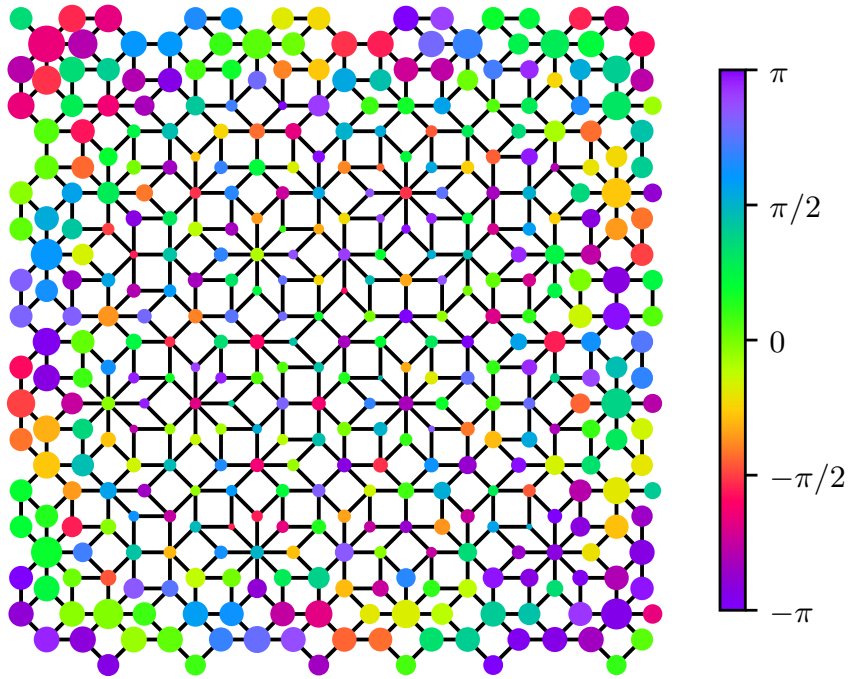
Evidence for a gap at $\lambda \approx 0.867$





Edge state criterion

We define an *edge state criterion* to distinguish edge states from bulk states among the eigenvectors of $\mathbf{1}_{B_L(x)} H \mathbf{1}_{B_L(x)}$.



The edge state criterion is simply based on the ℓ^2 mass in a certain distance from the edge.

Dirichlet based gap detection

Definition 2 Let $\varepsilon, L > 0$ and $\lambda \in \mathbb{R}$. We say that a Hamiltonian H is **locally ε-bulk-gapped at energy λ and scale L** if there exist constants $N \in \mathbb{N}$, $N \geq 2$, and $C < 1/N^d$ such that for any $x \in \Gamma$ and any $\psi \in \ell^2(\Gamma; \mathcal{H})$ we have the following implication: Whenever

$$\|(H - \lambda)\psi\|_{B_L(x)} \leq \varepsilon \|\psi\|_{B_L(x)}\,, \tag{4}$$

then for $l := \frac{L+r}{N} + r$ it holds that

$$\|\psi\|^2_{B_l(x)} \leq C\|\psi\|^2_{B_L(x)}\,. \tag{5}$$

Theorem 3 If a Hamiltonian H on $\ell^2(\Gamma; \mathcal{H})$ is locally ε-bulk-gapped at energy λ on some scale $L > 0$, then the interval $(\lambda - \varepsilon, \lambda + \varepsilon)$ is a gap in the spectrum of H, that is, $\sigma(H) \cap (\lambda - \varepsilon, \lambda + \varepsilon) = \varnothing$.

Resolvent criterion for ε-bulk-gappedness

Proposition 4 Let $L > 0$, $N \in \mathbb{N}$, $N \geq 2$, $l := \frac{L+r}{N} + r$, and $\lambda \in \mathbb{R}$. Assume that for every $x \in \Gamma$, we have

$$D(x) := \|\mathbf{1}_{\overline{B_l}(x)}(H_{B_{L-m}(x)} - \lambda)^{-1}\mathbf{1}_{B_{L-m}(x)}H\mathbf{1}_{B_L(x)\setminus B_{L-m}(x)}\| < N^{-d/2}$$

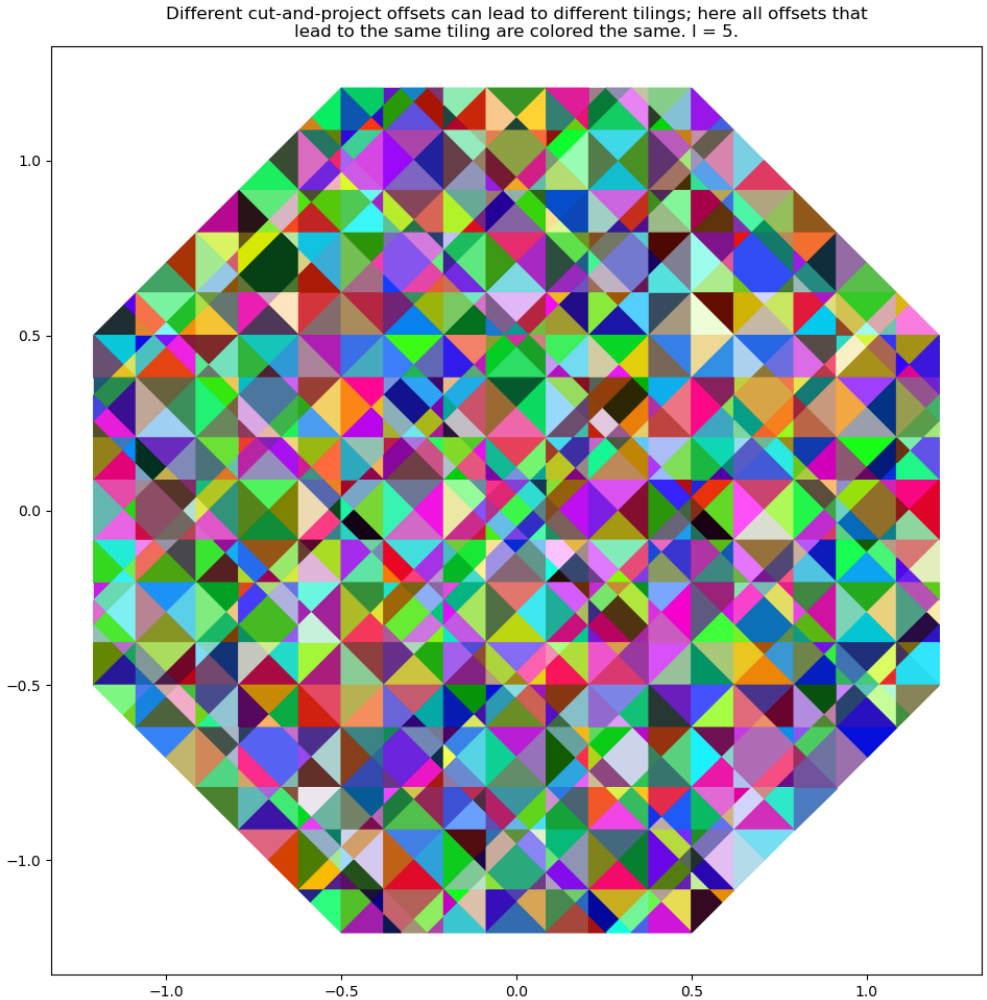
Then H is locally ε-bulk-gapped at energy λ and scale L for any $\varepsilon > 0$ with

$$\varepsilon < \inf_{x\in\Gamma} \frac{N^{-d/2} - D(x)}{\|\mathbf{1}_{\overline{B_l}(x)}(H_{B_{L-m}(x)} - \lambda)^{-1}\mathbf{1}_{B_{L-m}(x)}\|_{\mathrm{op}}} \,. \tag{6}$$

This means that spectral gaps can be checked **using the resolvent only**, which is much more efficient and can be done using sparse numerics.

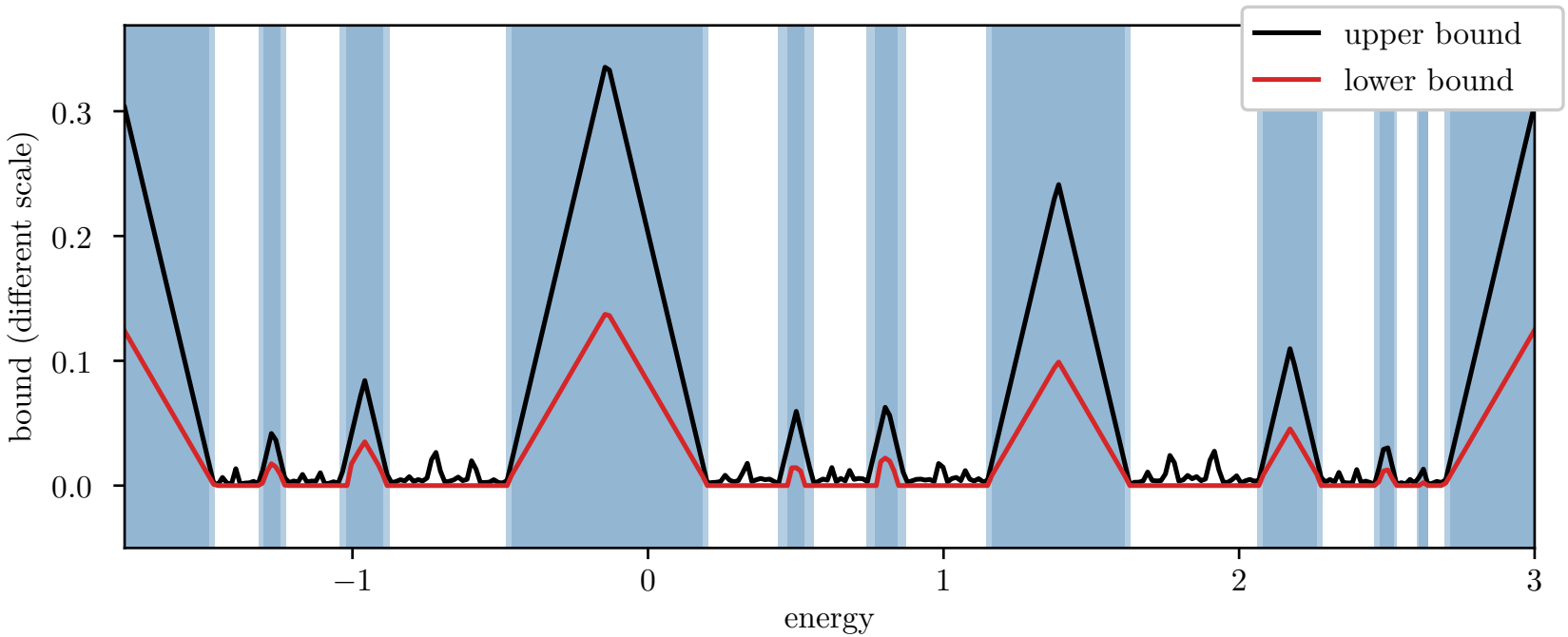
Application to quasicrystals: enumerating local patches

We enumerate local patches using the *cut-and-project method*.

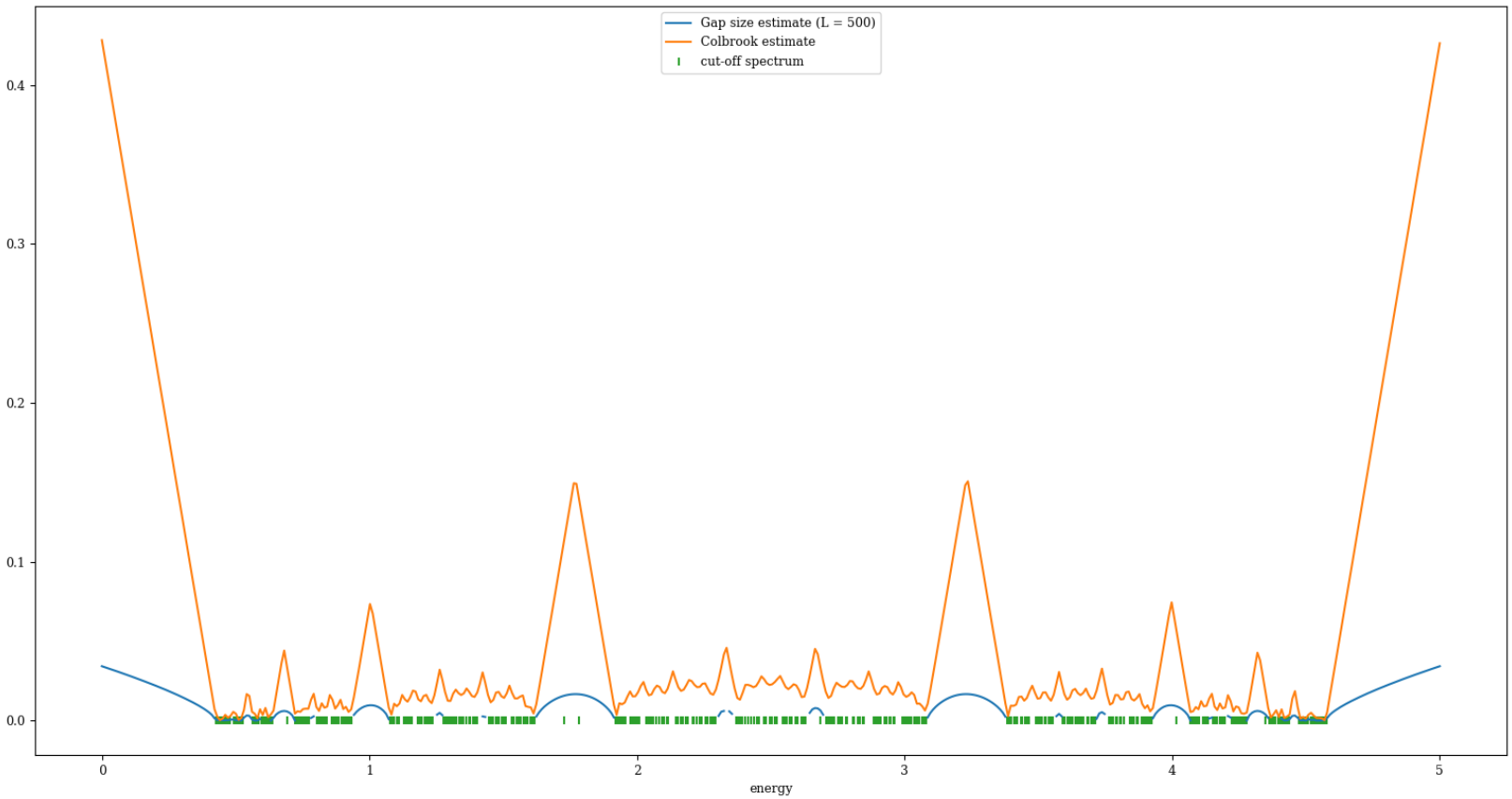


Decomposition of “acceptance region” to enumerate patches

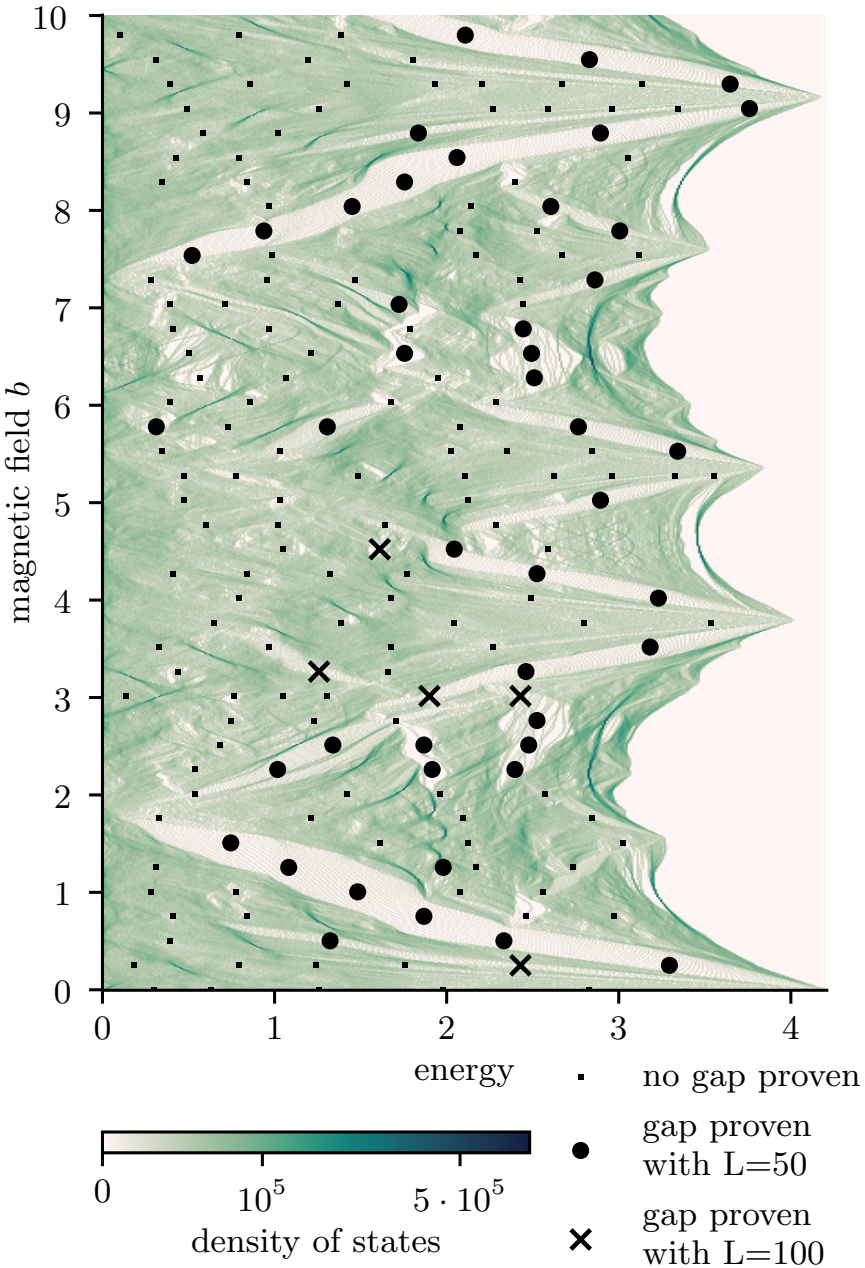
Quasicrystal results – Fibonacci



Quasicrystal results – Ammann-Beenker



Quasicrystal results – Ammann-Beenker



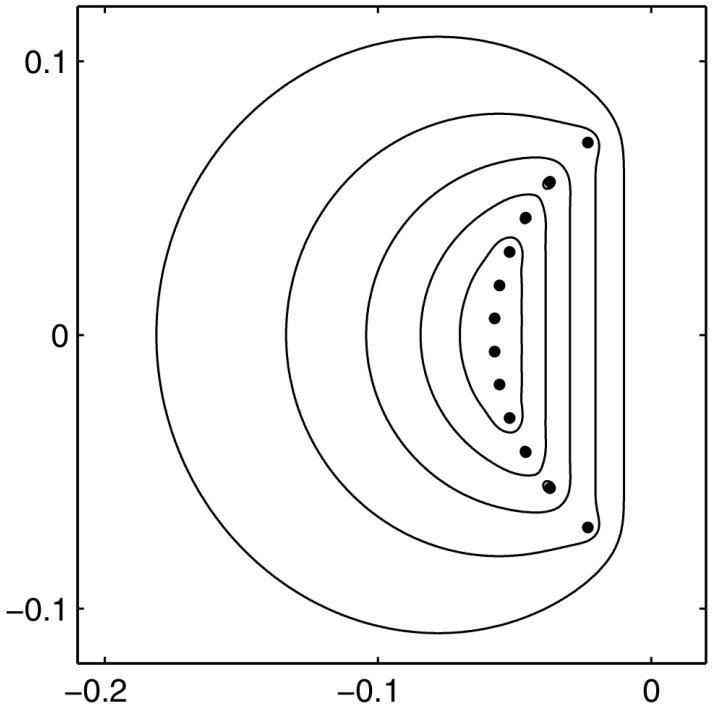
Extension – the pseudospectrum

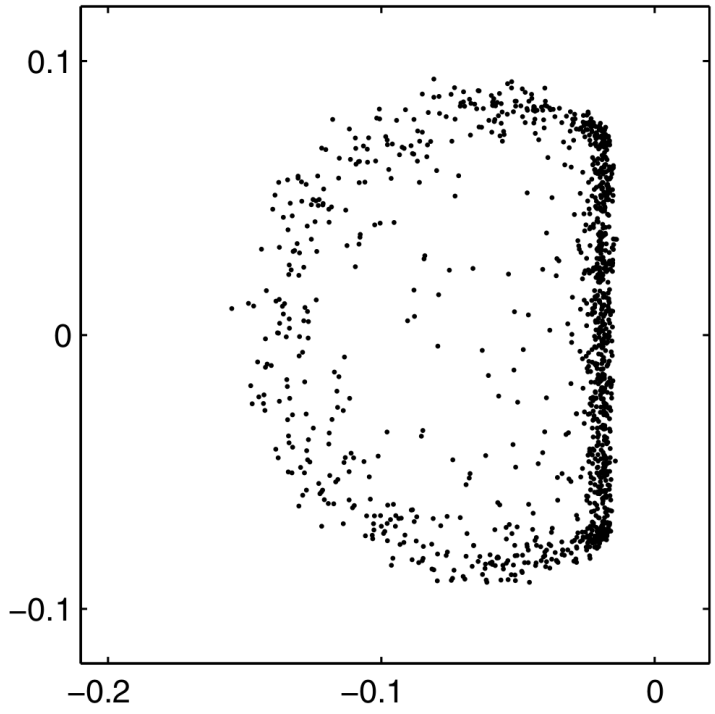
For **non-self-adjoint** operators, computing the spectrum is not continuous function. Thus, the spectrum of non-self-adjoint operators is not computable.

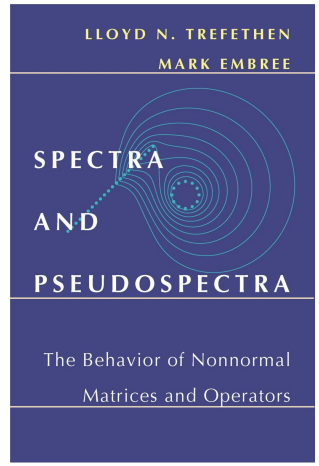
A different measure for non-self-adjoint operators is the ε-**pseudospectrum**.

$$\mathrm{Spec}_\varepsilon(H) = \left\{\lambda \in \mathbb{C} \;\middle|\; \|(H-\lambda)^{-1}\| \geq \varepsilon^{-1}\right\}$$

The pseudospectrum

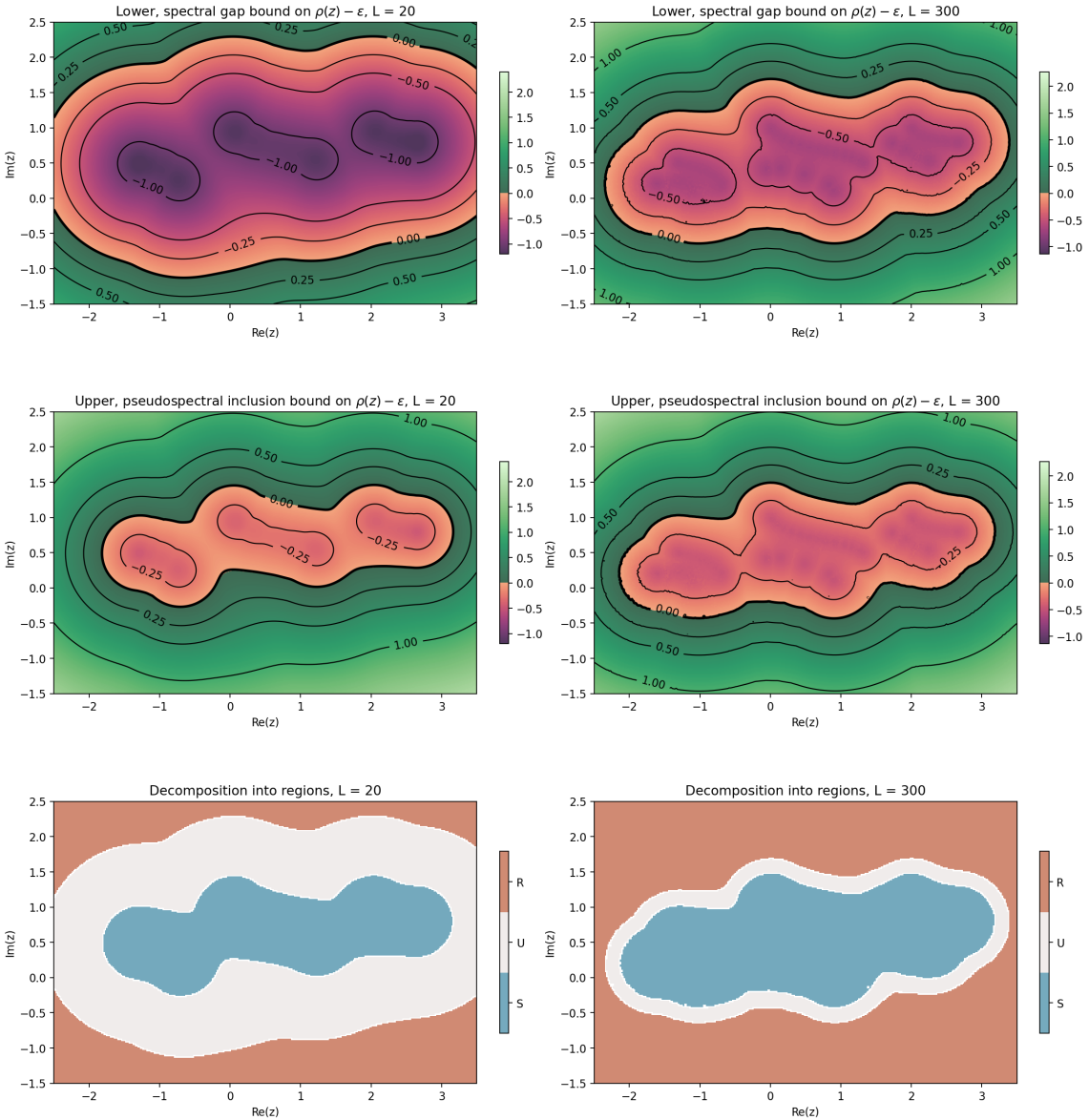






Upper and lower bounds on the pseudospectral radius

$$H\psi(n) = -\psi(n-1) + (1+i)F(n)\psi(n) - \psi(n+1)$$



Pseudospectrum **is computable** with error control in Hausdorff distance for non-self-adjoint operators