Findings Spectral Gaps in Quasicrystals

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Quantissima sur Oise – Cergy 2025

Based on joint works with

Paul Hege and Massimo Moscolari

Physical Review B (2022)
Mathematics of Computation (2025)

LONG-RANGE INTERACTING
QUANTUM
SPIN SYSTEMS
OUT OF EQUILIBRIUM
EXPERIMENT, THEORY AND MATHEMATICS

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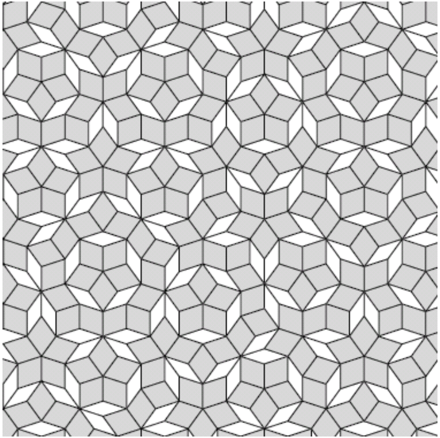
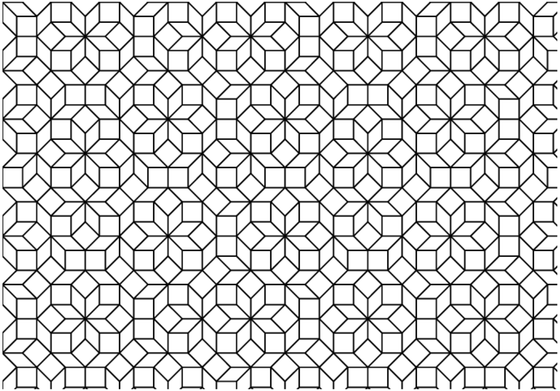
TRR
352

Introduction

Q: How to find the spectrum of a tight-binding operator on a quasicrystaline lattice?



Penrose tiling



Ammann-Beenker tiling

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He numerically computes eigenvalues and eigenfunctions of the $p_x + \mathrm{i}p_y$-thight-binding model on finite patches of the **Ammann-Beenker tiling**: For nearest neighbours the hoppings are

$$H_{xy} = -t\sigma_3 - \frac{\Delta}{2}\cos(\alpha_{xy})\sigma_1 - \frac{\mathrm{i}\Delta}{2}\sin(\alpha_{xy})\sigma_2$$

and with on-site term

$$H_{xx} = -\mu\sigma_3 \,.$$

Here $t, \mu, \Delta \in \mathbb{R}$ and α_{xy} is the signed angle between the line xy and the horizontal axis.

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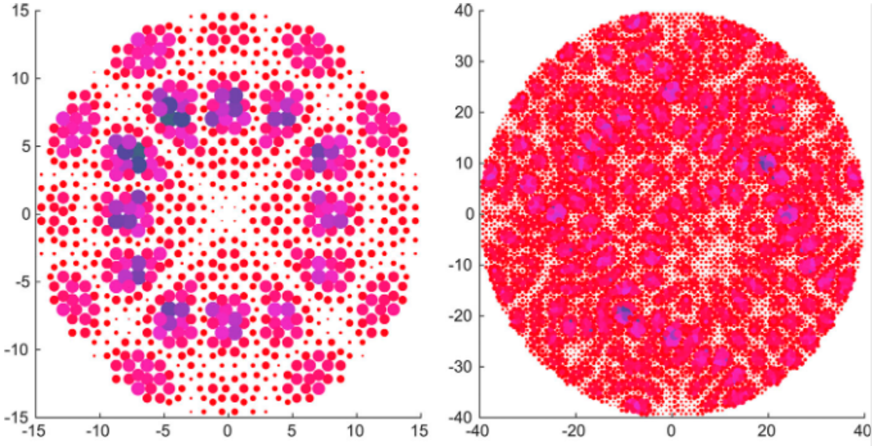
His goal is to understand the spectrum of the Hamiltonian on the infinite aperiodic domain within a parameter range in which the model is expected to exhibit topological non-triviality, where edge states lead to spectral pollution when the domain is restricted to a finite size.

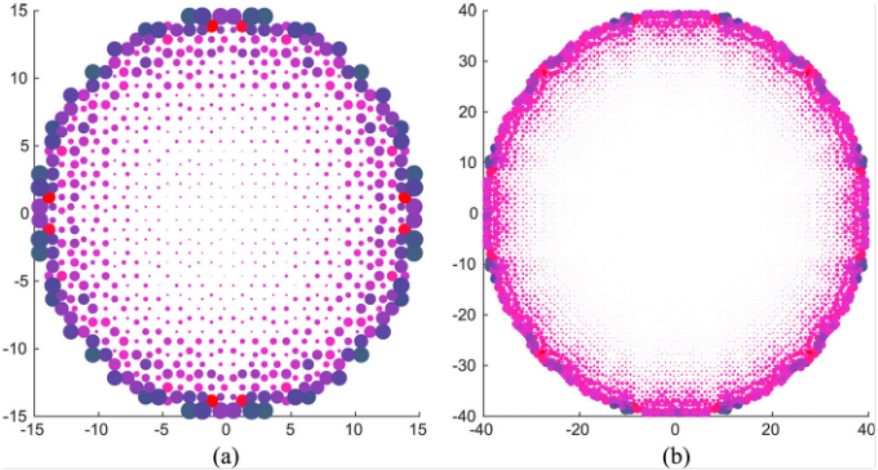
Introduction (figures from T. Loring)



(a) (b)

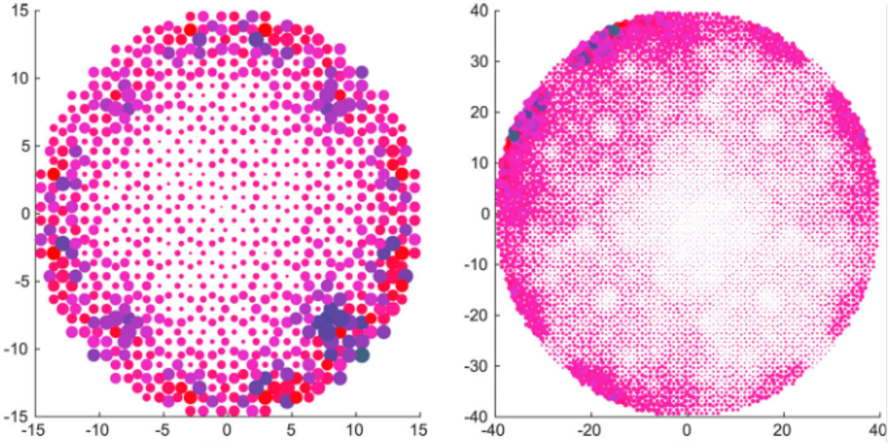
Bulk eigenfunctions at radius 15 and radius 40.

Introduction (figures from T. Loring)



Edge eigenfunctions at radius 15 and radius 40.

Introduction (figures from T. Loring)



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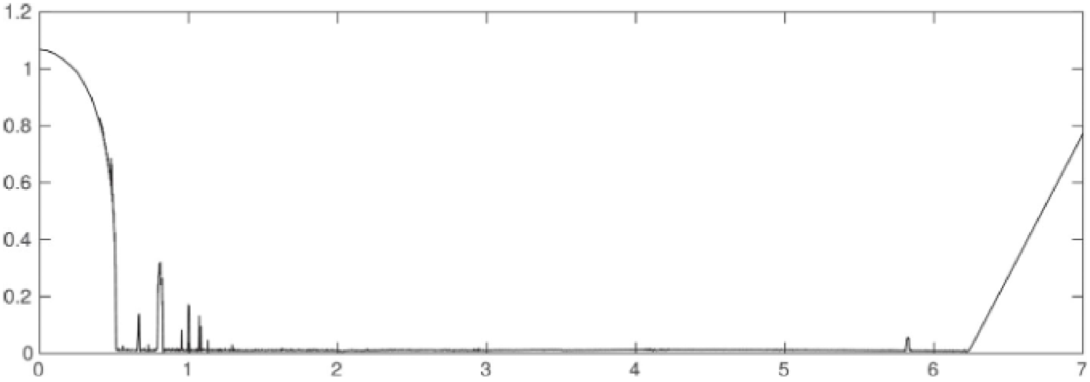
But also eigenfunctions that are neither clearly bulk nor clearly edge states appear at all scales.

Introduction (figures from T. Loring)



Upper bound to the distance of the spectrum of the infinite volume operator obtained from computing eigenvalues on a finite sample.

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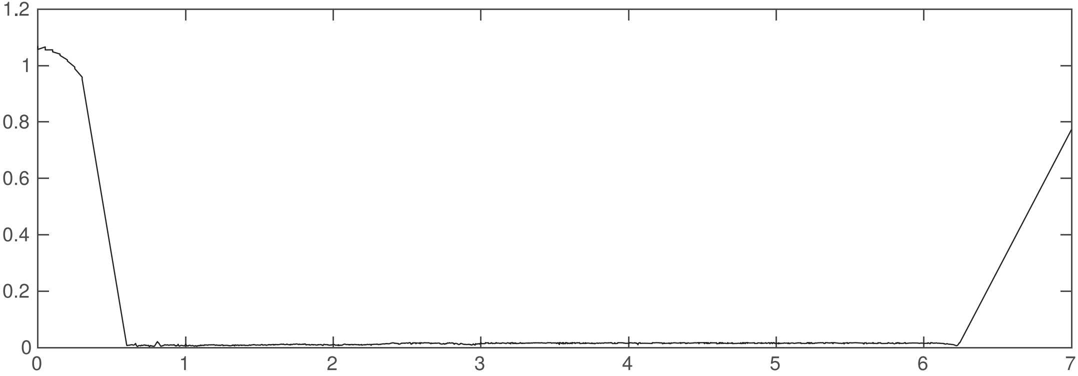


Upper bound obtained from his new spectral localizer method.

Introduction

PHYSICAL REVIEW LETTERS **122,** 250201 (2019)

How to Compute Spectra with Error Control

Matthew J. Colbrook, Bogdan Roman, and Anders C. Hansen
Department of Applied Mathematics and Theoretical Physics, University of Cambridge,
Wilberforce Road, Cambridge CB3 0WA, United Kingdom

(Received 28 November 2018; published 28 June 2019)

Computing the spectra of operators is a fundamental problem in the sciences, with wide-ranging applications in condensed-matter physics, quantum mechanics and chemistry, statistical mechanics, etc. While there are algorithms that in certain cases converge to the spectrum, no general procedure is known that (a) always converges, (b) provides bounds on the errors of approximation, and (c) provides approximate eigenvectors. This may lead to incorrect simulations. It has been an open problem since the 1950s to decide whether such reliable methods exist at all. We affirmatively resolve this question, and the algorithms provided are optimal, realizing the boundary of what digital computers can achieve. Moreover, they are easy to implement and parallelize, offer fundamental speed-ups, and allow problems that before, regardless of computing power, were out of reach. Results are demonstrated on difficult problems such as the spectra of quasicrystals and non-Hermitian phase transitions in optics.

DOI: 10.1103/PhysRevLett.122.250201

Introduction (Colbrook et al. continued)

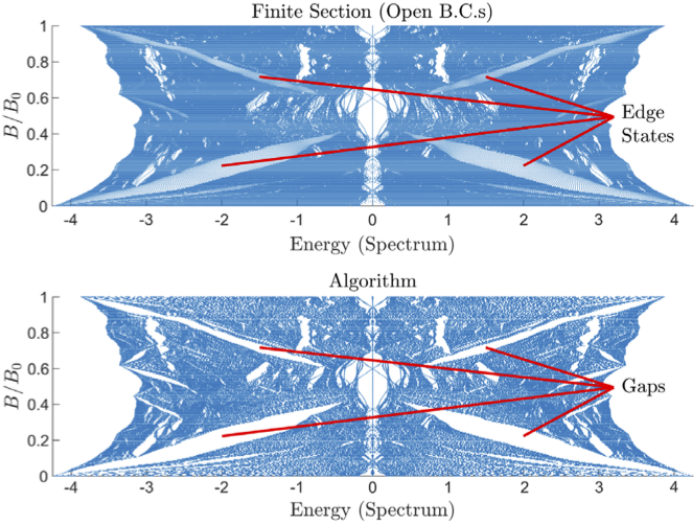
Introduction.—It is hard to overestimate the importance of computing the spectra of operators in mathematical physics, quantum chemistry, condensed-matter physics, statistical mechanics, Hermitian, as well as non-Hermitian, quantum mechanics, quasicrystals, optics, and many other fields. Motivated by the many applications, the topic has been intensely investigated, by both physicists [1–9] and mathematicians [10–17], since the 1950s. A reliable algorithm should converge and guarantee that any point of the output is close to the spectrum, up to a chosen arbitrary small error tolerance. A key question is whether such algorithms exist. Despite more than 90 years of quantum theory, the answer to this question has been unknown, even for Schrödinger operators.

The importance of this question is highlighted by the current interest in the spectral properties of systems with complicated spectra. The study of aperiodic systems, such as quasicrystals [18,19], often leads to complicated, even fractal-like spectra [20–24], which can make current a computer can achieve regarding limits of finite-dimensional systems.

In this Letter, we establish the boundaries for spectral problems in infinite dimensions. We show that it is *impossible* to design an algorithm for computing the spectra of Schrödinger operators which, given $\epsilon > 0$, halts and produces an output that is ϵ away from the true spectrum as measured in the Hausdorff metric. In other words, using information from a finite patch (truncation) of an operator A, it is impossible to produce an approximation $\Gamma(A)$ to the spectrum $\mathrm{Sp}(A)$, which satisfies the two inequalities (I) $\mathrm{dist}(z, \mathrm{Sp}(A)) \leq \epsilon$, for all $z \in \Gamma(A)$, and also (II) $\mathrm{dist}(w, \Gamma(A)) \leq \epsilon$, for all $w \in \mathrm{Sp}(A)$, simultaneously. However, we show that it is *possible* to create approximations, converging to the spectrum, that satisfy inequality (I). Indeed, we know the approximation is sound or reliable, but we do not know if we have got everything yet.

Namely, we provide an algorithm $\Gamma_n(\cdot)$, which both

Introduction (Colbrook et al. continued)



One application in their paper is the Hofstadter Hamiltonian on the hexagonal lattice.

Teaser

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Applying this algorithm to the $p_x + \mathrm{i}p_y$-model on the Ammann-Beenker tiling allows us to prove, for example, that the spectral gap at 0.804, which was conjectured by Loring to be "a mirage", remains open in the infinite system.

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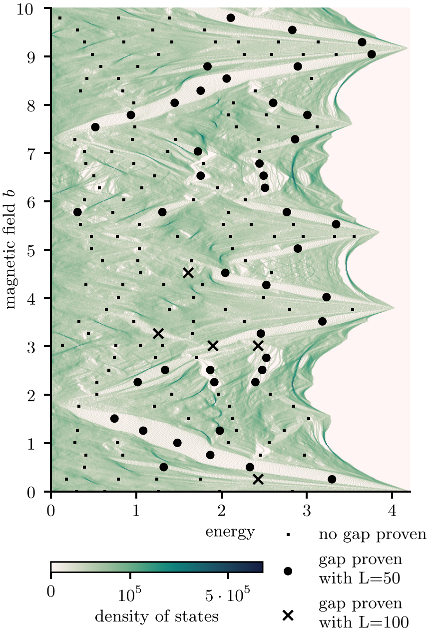
We also proved a number of gaps for the Hofstadter model on the Ammann-Beenker tiling.



The setting: short-range discrete operators

Definition

A subset $\Gamma \subset \mathbb{R}^n$ is called uniformly discrete if there exists $q > 0$, the packing radius, such that $d(x, y) \geq q$ for all $x, y \in \Gamma$ with $x \neq y$. Here and in the following $d(\cdot, \cdot)$ denotes the maximum distance and $B_r(x)$ the corresponding open "ball" of radius $r > 0$ around $x \in \mathbb{R}^n$.

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Definition

A discrete operator H in dimension $n \in \mathbb{N}$ is a bounded operator on a seperable Hilbert space $\mathcal{H}$, together with an orthonormal basis $(e_x)_{x \in \Gamma}$ indexed by a uniformly discrete subset $\Gamma \subset \mathbb{R}^n$. Its matrix elements at points $x, y \in \Gamma$ are $H_{xy} := \langle e_x, He_y \rangle$.

We say that a discrete operator H in dimension $n \in \mathbb{N}$ is short-range, if there exist $C, \varepsilon > 0$ such that

$$|H_{xy}| \leq C \, d(x, y)^{-(n+\varepsilon)} \qquad \text{for all } x, y \in \Gamma.$$

It has finite range $m > 0$ if

$$d(x, y) > m \quad \Rightarrow \quad H_{xy} = 0 \, .$$

The setting: finite local complexity (flc)

Definition

For a discrete operator H two sets $A, B \subset \Gamma$ are said to be equivalent w.r.t. the action of H, if there is a $t \in \mathbb{R}^n$ such that $B = A + t$ and if there exists $U : A \to S^1 \subset \mathbb{C}$ such that for all $a_1, a_2 \in A$ it holds that

$$H_{b_1 b_2} = U(a_1) H_{a_1 a_2} U(a_2)^* \,,$$

where $b_1 = a_1 + t$ and $b_2 = a_2 + t$.

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Definition

A discrete operator H is said to have finite local complexity (flc) if for any $L > 0$ the set of subsets

$$\{\Gamma \cap B_L(x) \mid x \in \mathbb{R}^n\}$$

is contained in finitely many equivalence classes with respect to equivalent action.

The (flc) spectral problem is solvable with explicit error control

Definition

The flc spectral problem is the computational problem $(\Omega, \Lambda, (\mathcal{M}, d_{\mathrm{H}}), \Xi)$, where

- Ω is the set of **normal** discrete operators with (flc) and short-range;
- Λ is a family of evaluation functions $(f_i)_{i \in \mathcal{I}}$ satisfying ...;
- $\mathcal{M}$ is the set of all compact subsets of $\mathbb{C}$ and d_{H} the Hausdorff distance;
- Ξ is the map which assigns to every operator H its spectrum, $\Xi(H) = \mathrm{Spec}(H)$.

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Theorem (Hege, Moscolari, T., MOC 2025)

Let $(\Omega, \Lambda, (\mathcal{M}, d_{\mathrm{H}}), \Xi)$ be the flc spectral problem. Then for every $k \in \mathbb{N}$ there exists a Blum-Shub-Smale (BSS) algorithm $\Gamma_k : \Omega \to \mathcal{M}$, using the family Λ of evaluation functions, such that

$$d_{\mathrm{H}}(\Gamma_k(H), \Xi(H)) \leq 2^{-k}$$

for all $H \in \Omega$.

The lower norm function and quasi-modes

The key steps in the proof are upper and lower bounds on the lower norm function

$$\rho_H : \mathbb{C} \to [0, \infty) , \qquad \lambda \mapsto \rho_H(\lambda) \ := \inf_{\psi \in \mathcal{H} \setminus \{0\}} \frac{\|(H - \lambda)\psi\|}{\|\psi\|} .$$

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It is also used to define the δ-pseudospectrum of an operator H as

$$\mathrm{Spec}_\delta(H) := \{ \lambda \in \mathbb{C} \,|\, \rho_H(\lambda) \leq \delta \} .$$

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For normal operators H it holds that

$$\rho_H(\lambda) = d(\lambda, \mathrm{Spec}(H))$$

and for general operators one still has

$$\rho_H(\lambda) \leq d(\lambda, \mathrm{Spec}(H)) \,.$$

Uneven sections and the upper bound

Following Colbrook et al. we use so called uneven local sections to avoid spectral pollution.

Definition

Let H be a discrete operator with finite range m, let $x \in \mathbb{R}^n$, $L > 0$, and $\lambda \in \mathbb{C}$. The uneven section for these data is the rectangular matrix

$$Q_{L,\lambda,x} : \mathcal{H}_{B_L(x)} \to \mathcal{H}_{B_{L+m}(x)}\,, \quad Q_{L,\lambda,x}(\psi) := 1_{B_{L+m}(x)}(H-\lambda)1_{B_L(x)}\psi\,,$$

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Theorem: The upper bound

Let H be a discrete operator with finite range m, and let $\lambda \in \mathbb{C}$, $L > 0$, and $x \in \mathbb{R}^n$ be arbitrary. Let

$$\varepsilon_{L,\lambda,x} := s_1(Q_{L,\lambda,x})$$

be the smallest singular value of $Q_{L,\lambda,x}$. Then

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Proof: The singular value decomposition allows us to write

$$Q_{L,\lambda,x} = USV^* = \sum_{i=1}^{k} |u_i\rangle s_i \langle v_i|\,,$$

where $(u_i)_{i=1,\ldots,k}$ are the first k columns of U, $(v_i)_{i=1,\ldots,k}$ the columns of V, and $(s_i)_{i=1,\ldots,k}$ the diagonal elements of S.

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$$(H-\lambda)v_1 = (H-\lambda)1_{B_L(x)}v_1 = 1_{B_{L+m}(x)}(H-\lambda)1_{B_L(x)}v_1 = Q_{L,\lambda,x}v_1 = s_1 u_1 .$$

Hence, $\|(H-\lambda)v_1\| = s_1\|u_1\| = s_1$. $\square$

The lower bound

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Let H be a discrete operator with finite range m, $L > m$, and $\lambda \in \mathbb{C}$. Set

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

and $M := \sup_{x,y \in \Gamma} |H_{xy}|$. Then

$$\rho_H(\lambda) \geq \varepsilon_{L,\lambda} - \frac{C}{L} \qquad \text{with} \qquad C := mM \left(\frac{36m}{q}\right)^{n/2} .$$

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Strategy of the proof: Show that if H has a δ-quasi-mode ψ at some energy λ, then it must be detectable on sufficiently large scales $L > m$, i.e. that a suitable restriction of ψ to a suitable box $B_L(x)$ is a $\delta + \frac{C}{L}$-quasi-mode.

Proof of the lower bound

For $x \in \mathbb{R}^n$ and $L > 0$ define the tent function $V_{L,x} : \mathbb{R}^n \to \mathbb{R}$ with Lipschitz const. $\frac{1}{L}$ by

$$V_{L,x}(y) := \max\left(0, 1 - \frac{\|x - y\|}{L}\right) .$$

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Lemma 1

For all $\psi \in \mathcal{H}$ we have

$$\int_{x\in\mathbb{R}^n} \|[V_{L,x}, H]\,\psi\|_{\mathcal{H}}^2 \,\mathrm{d}x^n \le \frac{m^2 M^2}{L^2}\left(\frac{36m}{q}\right)^n \|V_{L,0}\|_{L^2(\mathbb{R}^n)}^2 \|\psi\|_{\mathcal{H}}^2$$

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Lemma 2

Assume that $\psi \in \mathcal{H}$ is a δ-quasi-mode of H at $\lambda \in \mathbb{C}$. Then there exists $x \in \mathbb{R}^n$ such that

$$\|(H-\lambda)V_{L,x}\psi\| \leq \left(\delta + \tfrac{C}{L}\right)\|V_{L,x}\psi\|$$

and thus

$$\varepsilon_{L,\lambda} \leq \varepsilon_{L,\lambda,x} \leq \delta + \tfrac{C}{L} .$$

Proof of Lemma 2

Proof of Lemma 2: We trivially have

$$\int \|V_{L,x}\phi\|_{\mathcal{H}}^2 \, \mathrm{d}x^n = \|\phi\|_{\mathcal{H}}^2 \|V_{L,0}\|_{L^2(\mathbb{R}^n)}^2 .$$

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Using this and Minkowski's inequality in $L^2(\mathbb{R}^n)$

$$\int_{\mathbb{R}^n} \|(H-\lambda)V_{L,x}\psi\|_{\mathcal{H}}^2 \, \mathrm{d}x^n \quad = \quad \int_{\mathbb{R}^n} \|V_{L,x}(H-\lambda)\psi - [V_{L,x}, H]\psi\|_{\mathcal{H}}^2 \, \mathrm{d}x^n$$

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$$\begin{aligned}
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\end{aligned}$$

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&\le \Big(\underbrace{\sqrt{\textstyle\int_{\mathbb{R}^n} \|V_{L,x}(H-\lambda)\psi\|_{\mathcal{H}}^2 \,\mathrm{d}x^n}}_{=\|(H-\lambda)\psi\|_{\mathcal{H}}\|V_{L,0}\|_{L^2(\mathbb{R}^n)}} + \underbrace{\sqrt{\textstyle\int_{\mathbb{R}^n} \|[V_{L,x}, H]\psi\|_{\mathcal{H}}^2 \,\mathrm{d}x^n}}_{\le \frac{C}{L}\|\psi\|_{\mathcal{H}}\|V_{L,0}\|_{L^2(\mathbb{R}^n)}} \Big)^2 \\
&\le \left(\delta + \tfrac{C}{L}\right)^2 \|V_{L,0}\|_{L^2(\mathbb{R}^n)}^2 \|\psi\|_{\mathcal{H}}^2
\end{aligned}$$

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Using this and Minkowski's inequality in $L^2(\mathbb{R}^n)$

$$\begin{aligned}
\int_{\mathbb{R}^n} \|(H-\lambda)V_{L,x}\psi\|_{\mathcal{H}}^2 \,\mathrm{d}x^n &= \int_{\mathbb{R}^n} \|V_{L,x}(H-\lambda)\psi - [V_{L,x},H]\psi\|_{\mathcal{H}}^2 \,\mathrm{d}x^n \\
&\leq \Bigg(\underbrace{\sqrt{\textstyle\int_{\mathbb{R}^n} \|V_{L,x}(H-\lambda)\psi\|_{\mathcal{H}}^2 \,\mathrm{d}x^n}}_{=\|(H-\lambda)\psi\|_{\mathcal{H}}\|V_{L,0}\|_{L^2(\mathbb{R}^n)}} + \underbrace{\sqrt{\textstyle\int_{\mathbb{R}^n} \|[V_{L,x},H]\psi\|_{\mathcal{H}}^2 \,\mathrm{d}x^n}}_{\leq \frac{C}{L}\|\psi\|_{\mathcal{H}}\|V_{L,0}\|_{L^2(\mathbb{R}^n)}} \Bigg)^2 \\
&\leq \left(\delta + \tfrac{C}{L}\right)^2 \|V_{L,0}\|_{L^2(\mathbb{R}^n)}^2 \|\psi\|_{\mathcal{H}}^2 \\
&= \int_{\mathbb{R}^n} \left(\delta + \tfrac{C}{L}\right)^2 \|V_{L,x}\psi\|_{L^2(\mathbb{R}^n)}^2 \,\mathrm{d}x^n
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Thus, there exists $x \in \mathbb{R}^n$ such that $\|(H-\lambda)V_{L,x}\psi\| \leq \left(\delta + \frac{C}{L}\right) \|V_{L,x}\psi\|$.

Proof of Lemma 2 continued

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Thus, there exists $x \in \mathbb{R}^n$ such that $\|(H-\lambda)V_{L,x}\psi\|_{\mathcal{H}} \le \left(\delta + \frac{C}{L}\right) \|V_{L,x}\psi\|_{\mathcal{H}}$.

Since $\tilde{\psi} := V_{L,x}\psi$ is supported in $B_L(x)$ we obtain

$$\|Q_{L,\lambda,x}\tilde{\psi}\|_{\mathcal{H}} = \|(H-\lambda)\tilde{\psi}\|_{\mathcal{H}} \le \left(\delta + \tfrac{C}{L}\right) \|\tilde{\psi}\|_{\mathcal{H}}\,,$$

and hence $\varepsilon_{L,\lambda} \le \varepsilon_{L,\lambda,x} \le \delta + \frac{C}{L}$. $\square$

Proof of the lower bound

Proof of the lower bound: Let $\lambda \in \mathbb{C}$. For any $\delta > \rho_H(\lambda)$, by definition of the lower norm function, there exists a δ-quasi-mode $\psi \in \mathcal{H}$, i.e.

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$$\varepsilon_{L,\lambda} \leq \delta + \tfrac{C}{L} \,.$$

As this holds for all $\delta > \rho_H(\lambda)$, we obtain

$$\varepsilon_{L,\lambda} - \tfrac{C}{L} \leq \rho_H(\lambda) \,. \qquad \square$$

Computability of the (pseudo-)spectrum for flc-operators

Assuming that for an flc-operator H one can find an algorithm that yields all finitely many inequivalent realizations $(Q_{L,\lambda,i})_{i=1}^{k}$ of $Q_{L,\lambda,x}$ at a given spectral value $\lambda \in \mathbb{C}$ and scale L, one can (numerically) compute

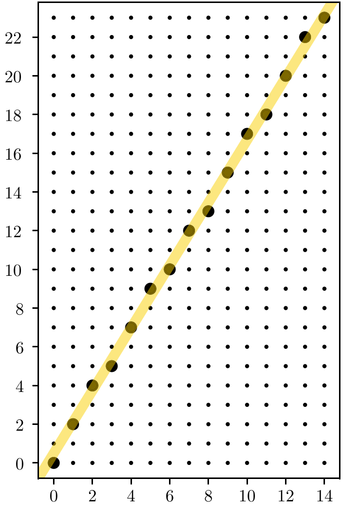
$$\varepsilon_{L,\lambda} = \inf_{x \in \mathbb{R}^n} \varepsilon_{L,\lambda,x} = \min_{i=1,\dots,k} s_1(Q_{L,\lambda,i}) \,.$$

Example: the $1d$-Fibonacci crystal

Let $\Gamma = \mathbb{Z}$ and

$$(H\psi)(j) = -\psi(j-1) - \psi(j+1) + \lambda V(j)\psi(j)$$

be the discrete Laplacian with an aperiodic potential, where $V(j)$ is either 0 or 1 according to the jth letter in the Fibonacci string.



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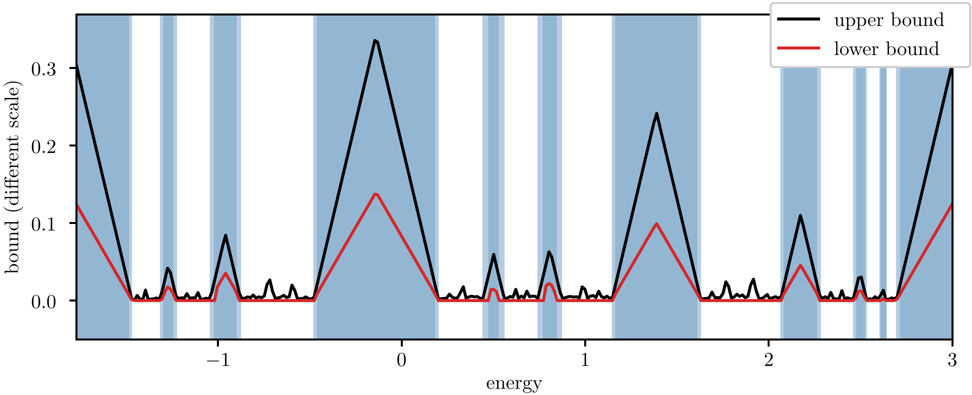
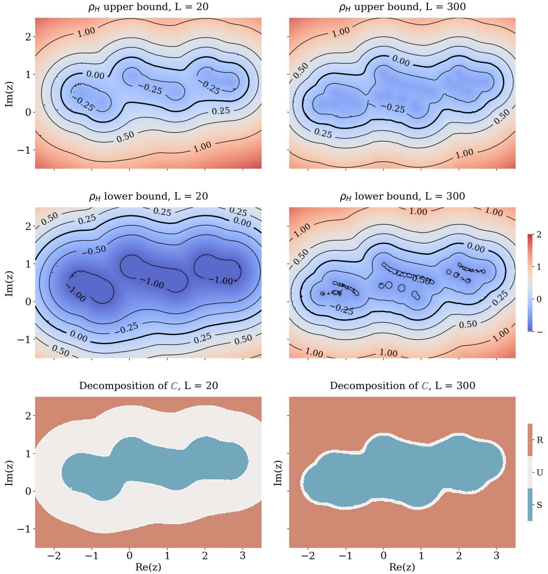


Results for $\lambda = 2$ and $L = 500$. The blue strips show the minimal resp. maximal sizes of the gaps compatible with our bounds.

Example: the 1d-Fibonacci crystal



Approximations to the 0.5-pseudospectrum for $\lambda = 1 + \mathrm{i}$.

Summary and conclusion

There is no algorithm that computes the spectrum of any general infinite-volume, discrete one-body operator to a given precision – this is obvious.

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As a consequence, for operators with finite local complexity – that is, if there is only a finite number of inequivalent actions of the operator on each scale – the spectrum is computable. More precisely, there is an algorithm that provides an approximation of the spectrum with arbitrary precision and two-sided error control in Hausdorff distance.

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Thanks for your attention!