Stable Approximation and Spectral Theory

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Summary

This work is devoted to the study of band-dominated operators on ℓ^p spaces with $p \in [1, \infty]$. When studying equations involving such operators, a common approach is to approximate the equation involving the infinite dimensional operator through a system of finite equations. However, approximating the operator does not necessarily mean that also the solution of the equation, or even the solvability, is well approximated. This work presents conditions under which the approximation of such operators leads to a useful approximation of solvability and solutions.

The spectral behavior of band-dominated operators, that are in general non-normal, is captured by pseudospectra. Pseudospectra are supersets of the spectrum that, in contrast to the spectrum, are robust under small perturbations. They are closely related to the lower norm, a function that maps operators to positive real numbers. In this work, we show that the lower norm of an operator A is determined by the set of submatrices that consist of consecutive columns of A. This leads to sufficient conditions for methods that approximate pseudospectra avoiding spectral pollution.

Moreover, approximation methods for band-dominated operators are studied. The emphasis is on two methods: the finite section method (FSM) and the periodic finite section method (PFSM). Both methods use a projection-based truncation method to approximate infinite dimensional equations by finite dimensional ones. The most important property of such methods is the applicability: an approximation method is called applicable if the finite dimensional systems are eventually solvable and the solutions converge to the solutions of the infinite dimensional system for all right-hand sides. The applicability of the FSM can be characterized by the elementwise invertibility of a set of operators, the so-called stability indicators. In this work, a new characterization through stability indicators of the applicability of the PFSM is proven.

Additionally, one-dimensional discrete Schrödinger operators are studied. The relation of the spectrum of a discrete Schrödinger operator H is compared to the spectrum of its half-line compression H^+ and conditions for the applicability of the FSM are given.

In the case of integer-valued potentials, it is proven that the invertibility of H already implies the invertibility of H^+ and the applicability of the FSM.

The spectra of Schrödinger operators with periodic potentials are described by Floquet-Bloch theory. For such operators, the spectrum of H^+ is the union of the spectrum of H and so-called Dirichlet eigenvalues. In this work, a method is derived that allows the explicit computation of Dirichlet eigenvalues by a computer algebra system for periodic binary valued potentials with small periods. As a result, conditions for the applicability of the FSM for smaller periods are given.

The third class of potentials considered in this work are Sturmian potentials. This work focuses on the approximation of the spectra of H and H^+ using Schrödinger operators with periodic potential. It is proven that this leads to spectral convergence. Subsequently, conditions for the applicability of the FSM for discrete Schrödinger operators with Sturmian potentials are given, including an algorithm that can be carried out by a computer algebra system. An interlacing structure of so-called Dirichlet eigenvalue candidates of the approximants, a superset of the Dirichlet eigenvalues, is established. This result allows for a fine localization of the Dirichlet eigenvalues of the approximants, and consequently also for the Dirichlet eigenvalues of H^+.

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Chapter 1

Introduction

This work is devoted to the study of bounded linear operators on the spaces $\ell^p(\mathbb{I})$ for $\mathbb{I} \subset \mathbb{Z}$ and $p \in [1, \infty]$. We study operators that have a matrix representation with finite bandwidth. These are usually referred to as band operators. Additionally, we investigate band-dominated operators, characterized be their ability to be uniformly approximated by band operators. Band-dominated operators can be found in many fields of mathematics and physics, from neural networks [15] and quantum mechanics [49] to signal processing [82]. Examples of these operators include discrete Schrödinger operators, Jacobi operators or convolution-type operators. In many cases, equations involving such operators cannot be solved analytically. Hence, a common approach is to approximate the equation involving the infinite dimensional operator through a system of finite equations. However, approximating the operator does not necessarily mean that also the solution of the equation, or even the solvability, is well approximated. The aim of this work is to find conditions under which the approximation of such operators leads to a useful approximation of solvability and solutions.

The first part of this thesis deals with general band-dominated operators. When studying the spectral behavior of such operators, that are in general non-normal, pseudospectra are introduced. Pseudospectra are supersets of the spectrum that, in contrast to the spectrum, are robust under small perturbations. The most famous work on pseudospectra is the book by Trefethen and Embree [104].

Our approach to the study of pseudospectra makes use of the lower norm ν which is the function that maps an operator A to

$$\inf\{\|Ax\| : x \in \ell^p(\mathbb{I}), \|x\| = 1\}. \tag{1.1}$$

Then the ε-pseudospectrum of an operator A is the sublevel set of the function $\lambda \mapsto \min(\nu(A - \lambda I), \nu(A^* - \lambda I))$ where A^* denotes the Banach space adjoint. Our main tool is a result by Chandler-Wilde, Chonchaiya and Lindner [16, 17, 20] that yields a uniform approximation of the function ν on sets of operators with uniform norm bound and bandwidth by functions that are defined similarly to (1.1) but only consider finitely supported vectors. Using this, we find that the lower norm of an operator A is determined by the set of submatrices that consist of consecutive columns of A. This leads to sufficient conditions for methods that approximate pseudospectra avoiding spectral pollution.

Moreover, approximation methods for operators on $\ell^p(\mathbb{I})$ are studied. The emphasis is on two methods: the finite section method (FSM) and the periodic finite section method (PFSM). Both methods use a projection-based truncation method to approximate infinite dimensional equations by finite dimensional ones. The most important property of such methods is the applicability: an approximation method is called applicable if the finite dimensional systems are eventually solvable and the solutions converge to the solutions of the infinite dimensional system for all right-hand sides. An overview over the well-known theory of the FSM is given, in particular results by Rabinovich, Roch, Silbermann, Lindner and Seidel [65, 67, 71, 86] that characterize the applicability of the FSM by the elementwise invertibility of a set of operators, the so-called stability indicators. For the PFSM, however, the methods of the authors mentioned above could not be applied directly since the finite matrices are not subject to a uniform band structure. Using the approximation of the lower norm via the approximation of column-submatrices, a proof for the stability indicators of the PFSM is presented in this work.

In the second part of this work, discrete Schrödinger operators on the space $\ell^2(\mathbb{Z})$ are studied. Such operators arise from the discretization of the one-dimensional time-independent Schrödinger equation in quantum physics. The relation of the spectrum of a discrete Schrödinger operator H on $\ell^2(\mathbb{Z})$ is compared to the spectrum of its half-line compression H^+ on $\ell^2(\mathbb{N})$. Additionally, conditions for the applicability of the FSM are given.

We distinguish between different classes of potentials. In the case of integer-valued potentials, it is proven that the invertibility of H already implies the invertibility of H^+, and it is shown that such operators are FSM-simple, meaning that the invertibility of H already implies the applicability of the FSM.

The spectra of Schrödinger operators with periodic potentials are described by Floquet-Bloch theory. An overview on this approach can be found in the book by Teschl [102]. For such operators, the spectrum of H^+ is the union of the spectrum of H and so-called Dirichlet eigenvalues. In this work, a method is derived that allows the explicit computation of Dirichlet eigenvalues by a computer algebra system for periodic binary valued potentials with small periods. As a result, conditions for the applicability of the FSM for smaller periods are given.

The third class of potentials considered in this work are aperiodic potentials, more specifically Sturmian potentials. Discrete Schrödinger operators with Sturmian potentials can be used as a one-dimensional model of quasicristals, which is an ordered structure without any periodicity in it. Quasicristals were first discovered by Shechtman in 1982 [95], for which he received the Nobel Prize in Chemistry in 2011. After the discovery, the spectral analysis of discrete Schrödinger operators with Sturmian potentials rose in popularity. Sütő [100] and Bellissard [10] proved that the spectrum of such operators is a Cantor set.

This work focuses on the approximation of the spectra of H and H^+ using Schrödinger operators with periodic potential, H_m and H_m^+. It is proven that $\sigma(H_m) \to \sigma(H)$ and $\sigma(H_m^+) \to \sigma(H^+)$ in Hausdorff distance as $m \to \infty$. Subsequently, conditions for the applicability of the FSM for discrete Schrödinger operators with Sturmian potentials are given, including an algorithm that can be carried out by a computer algebra system. An interlacing structure of so-called Dirichlet eigenvalue candidates of H^+, a superset of the Dirichlet eigenvalues, is established. This result allows for a fine localization of the Dirichlet eigenvalues of the approximants H_m^+, and consequently also for the location of elements of $\sigma(H^+) \setminus \sigma(H)$.

Chapter 2

Preliminaries

2.1 Basic Notation

Numbers, sets and sequences

As usual, by $\mathbb{N}$, $\mathbb{Z}$, $\mathbb{Q}$, $\mathbb{R}$ and $\mathbb{C}$ we denote the sets of natural, integer, rational, real and complex numbers. The set of non-negative integers is denoted by $\mathbb{Z}_+$ and the set of non-positive integers is denoted by $\mathbb{Z}_-$. Similarly, $\mathbb{R}_+$ and $\mathbb{R}_-$ are the non-negative and non-positive real numbers, respectively. The unit circle in the complex plane, that is $\{z \in \mathbb{C} : |z| = 1\}$ is denoted by $\mathbb{T}$. We call a set $\mathbb{I} \subset \mathbb{Z}$ a discrete interval if it is the intersection of a real interval with $\mathbb{Z}$.

Subsets and proper subsets are denoted by $\subset$ and $\subsetneq$, respectively. Whenever we want to emphasize that a union of sets is disjoint we use $\uplus$ instead of $\cup$. The cardinality of a set M is denoted by $|M|$ and the characteristic function by χ_M. For a set M in a topological space we write $\operatorname{clos}(M)$ for the closure and $\operatorname{int}(M)$ for the interior.

We define $|x|_\infty := \max\limits_{1\le i\le n} |x_i|$ for a vector $x \in \mathbb{C}^n$. For $M \subset \mathbb{C}^n$ and $x \in \mathbb{C}^n$ we denote $\operatorname{dist}(x, M) := \inf\limits_{m\in M} |x - m|_\infty$. The distance for two sets $M, N \subset \mathbb{C}^n$ is then defined by

$$\operatorname{dist}(M, N) := \min\left\{ \inf_{m\in M} \operatorname{dist}(m, N), \inf_{n\in N} \operatorname{dist}(n, M)\right\}. \tag{2.1}$$

We denote sequences of objects by $(x_n)_{n\in\mathbb{I}}$ where $\mathbb{I} \subset \mathbb{C}$. For a set M we sometimes write $(x_n)_{n\in\mathbb{I}} \subset M$, meaning $x_n \in M$ for all $n \in \mathbb{I}$. If the choice of the set $\mathbb{I}$ is clear form context then we sometimes omit the subscript and just write (x_n).

For $a, b \in \mathbb{R}$ and $\varepsilon > 0$, let us write $a \overset{\varepsilon}{\approx} b$ if $b \in (a - \varepsilon, a + \varepsilon)$ and $a \overset{\varepsilon}{\preceq} b$ if $b \in [a, a + \varepsilon)$. In particular, if $a \overset{\delta}{\approx} b$ and $b \overset{\varepsilon}{\approx} c$ then $a \overset{\delta+\varepsilon}{\approx} c$. The same holds for the relation $\overset{\varepsilon}{\preceq}$.

Banach spaces and operators

We will denote Banach spaces by X and Y, their corresponding norms by $\|\cdot\|_X$ and $\|\cdot\|_Y$ and the dual spaces by X^* and Y^*. Whenever there is no ambiguity about the space we just use $\|\cdot\|$ for the norm. Unless stated otherwise Banach spaces are always complex. In case X is also a Hilbert space we write $\langle\cdot,\cdot\rangle_X$ or just $\langle\cdot,\cdot\rangle$ for the inner product.

We define $\mathcal{L}(X, Y)$ to be the set of all bounded linear operators mapping from X to Y. $\mathcal{L}(X, Y)$ is a Banach space when equipped with the usual addition and scalar multiplication as well as the operator norm

$$\|A\|_{\mathcal{L}(X,Y)} := \sup_{\substack{x\in X \\ \|x\|_X=1}} \|Ax\|_Y.$$

We abbreviate $\mathcal{L}(X) := \mathcal{L}(X,X)$. With the usual composition of operators, $\mathcal{L}(X)$ is a unital Banach algebra. The identity operator in $\mathcal{L}(X)$ is denoted by I_X or just I when the space is clear from context.

For an operator $A \in \mathcal{L}(X,Y)$ we denote the inverse by A^{-1}, and we say that A is invertible whenever such an inverse exists in $\mathcal{L}(Y,X)$.

We define the kernel and the image of A by

$$\ker A := \{x \in X : Ax = 0\} \quad \text{and} \quad \operatorname{im} A := \{Ax : x \in X\}.$$

Sometimes the image of A is also called the range. By the bounded inverse theorem A is invertible if and only if A is bijective, i.e. $\ker A = \{0\}$ and $\operatorname{im} A = Y$.

For $A \in \mathcal{L}(X,Y)$ the (Banach space) adjoint operator $A^* \in \mathcal{L}(Y^*,X^*)$ is defined by $(A^*f)(x) := f(Ax)$ for all $f \in Y^*$ and $x \in X$.

In the case that X and Y are Hilbert spaces we define the adjoint differently. The (Hilbert space) adjoint $A^H \in \mathcal{L}(Y,X)$ is the unique operator that satisfies $\langle Ax, y\rangle_Y = \langle x, A^H y\rangle_X$ and does not coincide with the Banach space adjoint. If $A = A^H$ then A is called self-adjoint and if $AA^H = A^H A$ then A is called normal.

When a sequence $(A_n)_{n\in\mathbb{N}} \subset \mathcal{L}(X,Y)$ converges to some $A \in \mathcal{L}(X,Y)$ with respect to the operator norm we write $A_n \rightrightarrows A$ and say that A_n norm-converges to A. A sequence $(A_n)_{n\in\mathbb{N}} \subset \mathcal{L}(X,Y)$ converges strongly to $A \in \mathcal{L}(X,Y)$ if for all $x \in X$ holds

$$\|A_n x - Ax\| \to 0 \quad \text{as } n \to \infty.$$

Every norm-converging sequence also converges strongly. In a reflexive Banach space strong converge is equivalent to strong convergence of the adjoint operator in the dual space [62, Cor. 1.16].

An important result on the strong convergence of linear operators is the Banach-Steinhaus theorem, which is a consequence of the principle of uniform boundedness [31, Theorem 1.3.4].

Proposition 2.1. *([31, Corollary 1.3.5]) Let X, Y be Banach spaces and let $(A_n)_{n\in\mathbb{N}} \subset \mathcal{L}(X,Y)$. If $A_n \to A$ then $\sup_{n\in\mathbb{N}} \|A_n\| < \infty$.*

A bounded linear operator $K \in \mathcal{L}(X,Y)$ is compact if it maps bounded sets to precompact sets. We denote the set of all compact operators from X to Y by $\mathcal{K}(X,Y)$ which again forms a Banach space since it is a closed subspace of $\mathcal{L}(X,Y)$. Moreover, $\mathcal{K}(X) := K(X,X)$ is a closed two-sided ideal of $\mathcal{L}(X)$ meaning that it is a closed subspace such that for all $K \in \mathcal{K}(X)$ and $A \in \mathcal{L}(X)$ we have $KA \in \mathcal{K}(X)$ and $AK \in \mathcal{K}(X)$.

A notable property of compact operators is that they turn strong convergence into norm convergence: $A_n \to A$ is equivalent to $A_n K \rightrightarrows AK$ for all $K \in \mathcal{K}(X)$ [85, Thm. 1.1.3]. In a reflexive Banach space, both statements are also equivalent to $KA_n \rightrightarrows KA$ for all $K \in \mathcal{K}(X)$ [62, Prop. 1.14].

Let X be a Banach space and $Y \subset X$ a subspace. Then we denote the quotient space by X/Y. If Y is closed then

$$\|x + Y\|_{X/Y} := \inf_{y\in Y} \|x + y\|_X$$

is a norm, turning $(X/Y, \|\cdot\|_{X/Y})$ into a Banach space. If Y is also reflexive then the infimum is always attained.

Similarly, if X is a Banach algebra and Y is a closed two-sided ideal then X/Y is again a Banach algebra. The most important quotient algebra throughout this work is the Calkin algebra $\mathcal{L}(X)/\mathcal{K}(X)$.

Sequence spaces

Let $d \in \mathbb{N}$, $p \in [1, \infty)$ and $\mathbb{I} \subset \mathbb{Z}^d$. Then we define

$$\ell^p(\mathbb{I}) := \Big\{(x_n)_{n\in\mathbb{I}} \subset \mathbb{C} : \sum_{n\in\mathbb{I}} |x|^p < \infty\Big\},$$
$$\|(x_n)_{n\in\mathbb{I}}\|_{\ell^p(\mathbb{I})} := \Big(\sum_{n\in\mathbb{I}} |x|^p\Big)^{1/p},$$

and

$$\ell^\infty(\mathbb{I}) := \Big\{(x_n)_{n\in\mathbb{I}} \subset \mathbb{C} : \sup_{n\in\mathbb{I}} |x| < \infty\Big\},$$
$$\|(x_n)_{n\in\mathbb{I}}\|_{\ell^\infty(\mathbb{I})} := \sup_{n\in\mathbb{I}} |x|.$$

We usually abbreviate $\|\cdot\|_p := \|\cdot\|_{\ell^p(\mathbb{I})}$. Note that for all $p \in [1, \infty]$ the spaces $\ell^p(\mathbb{I})$ are Banach spaces and $\ell^2(\mathbb{I})$ is a Hilbert space with inner product

$$\langle (x_n)_{n\in\mathbb{I}}, (y_n)_{n\in\mathbb{I}}\rangle_{\ell^2(\mathbb{I})} = \sum_{n\in\mathbb{I}} x_n\overline{y_n}.$$

If $1 < p < \infty$ then the dual space of $\ell^p(\mathbb{I})$ can be identified with $\ell^q(\mathbb{I})$, where $\frac{1}{p} + \frac{1}{q} = 1$. In particular, these spaces are reflexive Banach spaces. The dual space of $\ell^1(\mathbb{I})$ can be identified with $\ell^\infty(\mathbb{I})$, but for infinite $\mathbb{I}$ the dual space of $\ell^\infty(\mathbb{I})$ is strictly larger than $\ell^1(\mathbb{I})$, see [62, Example 1.26].

We additionally define $\operatorname{supp}(x) = \{n \in \mathbb{I} : x_n \neq 0\}$ and

$$c_{00}(\mathbb{I}) := \{(x_n)_{n\in\mathbb{I}} \subset \mathbb{C} : |\operatorname{supp}(x_n)| < \infty\}.$$

Note that $c_{00} \subset \ell^\infty(\mathbb{I})$ and together with the norm $\|\cdot\|_{c_{00}(\mathbb{I})} := \|\cdot\|_\infty$ the space $c_{00}(\mathbb{I})$ forms a normed vector space.

For infinite $\mathbb{I}$ the closure of $c_{00}(\mathbb{I})$ w.r.t. $\|\cdot\|_\infty$ is the Banach space

$$c_0 := \big\{(x_n)_{n\in\mathbb{I}} : \lim_{|n|\to\infty} x_n = 0\big\}.$$

For all of the above spaces we refer to the sequences $e_i := (e_i)_{j\in\mathbb{I}}$ with $(e_i)(j) = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{else} \end{cases}$ as the canonical basis vectors.

2.2 Spectral analysis

In this section let X be a complex Banach space.

2.2.1 The spectrum

Given a bounded linear operator $A \in \mathcal{L}(X)$, we denote its *spectrum* by

$$\sigma(A) \ := \ \{\lambda \in \mathbb{C} : A - \lambda I \text{ is not invertible}\}.$$

The spectrum is always non-empty and compact. The invertibility of $A - \lambda I$ can fail if one of the following is satisfied:

(a) $A - \lambda I$ is not injective

(b) $\operatorname{im}(A - \lambda I)$ is not dense in X

(c) $\operatorname{im}(A - \lambda I)$ is not closed in X.

Condition (a) means that λ is an eigenvalue of A. We call the set of all eigenvalues the *point spectrum* and denote it by $\sigma_p(A)$. The set of all $\lambda \in \mathbb{C}$ that are not eigenvalues but (b) holds is called the *residual spectrum* and denoted by $\sigma_r(A)$. Lastly, $\sigma_c(A) := \sigma(A) \setminus (\sigma_p(A) \cup \sigma_r(A))$ is called the continuous spectrum and consists of $\lambda \in \mathbb{C}$ for which (c) holds but neither (a) nor (b). We thus have divided the spectrum in a disjoint union

$$\sigma(A) = \sigma_p(A) \mathbin{\dot\cup} \sigma_r(A) \mathbin{\dot\cup} \sigma_c(A).$$

The complement of the spectrum is the resolvent set $\rho(A) := \mathbb{C} \setminus \sigma(A)$. For $\lambda \in \rho(A)$ we call $(A - \lambda I)^{-1}$ the resolvent of A.

For finite square matrices $A \in \mathbb{C}^{n \times n}$ injectivity is equivalent to surjectivity and the spectrum therefore only consists of eigenvalues which are given by

$$\sigma(A) = \{\lambda \in \mathbb{C} : \det(A - \lambda I) = 0\}.$$

Definition 2.2. (Spectral radius) The spectral radius of an operator $A \in \mathcal{L}(X)$ is defined as

$$r(A) := \lim_{n \to \infty} \|A^n\|^{1/n}.$$

It follows from the submultiplicativity of the operator norm that $r(A) \leq \|A\|$. The name spectral radius is justified by the following result, known as Gelfand's formula.

Proposition 2.3. *[31, Theorem 4.1.3] Let $A \in \mathcal{L}(X)$ then*

$$r(A) = \max_{\lambda \in \sigma(A)} |\lambda|.$$

In order to compare spectra of different operators we introduce the Hausdorff distance on subset of $\mathbb{C}$.

Definition 2.4. Let $M, N \subset \mathbb{C}$ then the Hausdorff distance between M and N is given by

$$d_H(M, N) := \max\left\{ \sup_{m \in M} \operatorname{dist}(m, N), \sup_{n \in M} \operatorname{dist}(n, M) \right\}.$$

Recall that the Hausdorff distance differs from the notion of $\operatorname{dist}(M,N)$ from (2.1). For instance,

$$\begin{aligned} \operatorname{dist}(M,N) = 0 &\iff \operatorname{clos}(M) \cap \operatorname{clos}(N) \neq \emptyset, \qquad \text{while} \\ d_H(M,N) = 0 &\iff \operatorname{clos}(M) = \operatorname{clos}(N). \end{aligned}$$

The set of non-empty compact subspaces of $\mathbb{C}$ becomes a metric spaces when equipped with d_H.

Definition 2.5. Then for a sequence $(M_n)_{n\in\mathbb{N}}$ of subsets of a topological space we define the topological limes superior as

$$\limsup_{n\to\infty} M_n := \bigcap_{n_0\in\mathbb{N}} \operatorname{clos}\Bigg(\bigcup_{n\geq n_0} M_n \Bigg).$$

In a metric space $\limsup_{n\to\infty} M_n$ coincides with the set of all partial limits of sequences $(x_n)_{n\in\mathbb{N}}$ with $x_n \in M_n$. We denote the set of all limit points of sequences $(x_n)_{n\in\mathbb{N}}$ with $x_n \in M_n$ by $\liminf_{n\to\infty} M_n$. Then

$$\liminf_{n\to\infty} M_n = \limsup_{n\to\infty} M_n \qquad \iff \qquad M_n \text{ converges w.r.t. } d_H,$$

in which case the closure of a Hausdorff limit of (M_n) is given by the set $\limsup_{n\to\infty} M_n = \limsup_{n\to\infty}$, see e.g. [46, §3.1.2].

We will need the following properties of the eigenvalues of finite Hermitian matrices.

Lemma 2.6. *(Courant-Fischer, e.g. [50, p. 16-4]) Let $A \in \mathbb{C}^{n\times n}$ be Hermitian with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ and let $\mathcal{F}^n_m$ denote the set of m-dimensional subspaces of $\mathbb{C}^n$ for $m \in \mathbb{N}$. Then for $k \in \{1,\dots,n\}$*

$$\begin{aligned} \lambda_k &= \max_{D\in\mathcal{F}^n_{k-1}} \min\Big\{ \langle y, Ay\rangle : y \in \mathbb{C}^n\,,\ y \perp D\,,\ \|y\| = 1 \Big\} \\ &= \min_{D\in\mathcal{F}^n_{n-k}} \max\Big\{ \langle y, Ay\rangle : y \in \mathbb{C}^n\,,\ y \perp D\,,\ \|y\| = 1 \Big\}. \end{aligned}$$

Lemma 2.7. *(Weyl's inequality, e.g. [50, p. 16-4]) Let $n \in \mathbb{N}$ and $A, B \in \mathbb{C}^{n\times n}$ be Hermitian. We denote the i-th eigenvalue of a Hermitian matrix M by $\lambda_i(M)$, arranged in descending order. Then the following hold:*

(a) For every pair $j,k \in \{1,\dots,n\}$ such that $j+k \geq n+1$,

$$\lambda_{j+k-n}(A+B) \geq \lambda_j(A) + \lambda_k(B).$$

(b) For every pair $j,k \in \{1,\dots,n\}$ such that $j+k \leq n+1$,

$$\lambda_j(A) + \lambda_k(B) \geq \lambda_{j+k-1}(A+B).$$

2.2.2 The lower norm and pseudospectra

Let us define the lower norm – a quantity that is closely related to the invertibility of an operator.

Definition 2.8. For $A \in \mathcal{L}(X, Y)$ the lower norm is defined by

$$\nu(A) := \inf_{\substack{x \in X \\ \|x\|=1}} \|Ax\|.$$

The definition of ν is very similar to the definition of $\|\cdot\|_{\mathcal{L}(X,Y)}$, in fact, one only replaces the $\sup$ by a $\inf$. This explains the name *lower norm*, even though ν is not a norm on $\mathcal{L}(X, Y)$.

Sometimes ν is also called the injectivity modulus, suggesting that it somehow indicates the injectivity of an operator. If A is not injective then $\nu(A) = 0$ follows immediately. However, the converse is not true: consider the operator $M \in \mathcal{L}(\ell^2(\mathbb{N}))$ defined by $(Mx)_n = \frac{1}{n} x_n$. Then M is injective, but $\nu(A) = 0$. This is due to the fact that M_a does not have closed range:

Lemma 2.9. *(e.g. [62, Lemma 2.32])*
Let $A \in \mathcal{L}(X, Y)$. Then $\nu(A) > 0$ if and only if A is injective and $\operatorname{im} A$ is closed.

If $\nu(A) > 0$ we also say that A is bounded below. Boundedness from below is not quite enough to ensure that an operator is invertible. Consider the right shift S on $\ell^2(\mathbb{N})$. Then S is injective and $\operatorname{im}(S) = \{(x_i)_{i \in \mathbb{N}} \in \ell^2(\mathbb{N}) : x_1 = 0\}$ is closed. In fact, S is isometric, meaning both $\nu(S) = 1$ and $\|S\| = 1$. However, S is not surjective. More precisely, $\operatorname{im} S$ is closed but not dense. By Theorem 2.24 this implies that $\nu(A^*) = 0$. Therefore, it is also necessary for the invertibility of A that A^* is bounded from below.

Lemma 2.10. *(e.g. [62, Lemma 2.35])*
Let $A \in \mathcal{L}(X, Y)$. Then A is invertible if and only if A and A^* are bounded below. Moreover, if A is invertible then

$$\nu(A) = \|A^{-1}\|^{-1}. \tag{2.2}$$

We introduce the quantity $\mu(A) := \min(\nu(A), \nu(A^*))$ in order to check if A and A^* are bounded below simultaneously. In the case that A is invertible then (2.2) yields $\nu(A) = \nu(A^*)$. We can generalize (2.2) to all operators in $\mathcal{L}(X, Y)$ by writing

$$\mu(A) = \|A^{-1}\|^{-1}.$$

using the convention that $\|A^{-1}\|^{-1} = 0$ if A is not invertible.

Furthermore, the lower norm is Lipschitz continuous as function from $\mathcal{L}(X, Y)$ to $\mathbb{R}_+$.

Lemma 2.11. *(e.g. [62, Lemma 2.38])*
For $A, B \in \mathcal{L}(X, Y)$ it holds that $|\nu(A) - \nu(B)| \leq \|A - B\|$.

This property directly transfers to $\mu : \mathcal{L}(X, Y) \to \mathbb{R}_+$.

If X and Y are finite dimensional then the lower norm coincides with the smallest singular value. The singular values of $A \in \mathbb{R}^{m \times n}$ are given by the square roots of the eigenvalues of A^*A if $m \geq n$ and by the square roots of the eigenvalues of AA^* if $m < n$. In the case that $X = Y$ is a Hilbert space and $A \in \mathcal{L}(X, Y)$ is normal and invertible then $\|A^{-1}\| = \max_{\lambda \in \sigma(A^{-1})} |\lambda|$. Therefore, $\nu(A - \lambda I) = \operatorname{dist}(\lambda, \sigma(A))$ holds for normal operators. Hence, for normal operators the map $\mu(A - \cdot I)$ from $\mathbb{C} \to \mathbb{R}_+$ determines the spectrum of A and vice versa. Moreover, $\nu(A) = \mu(A)$.

If A is not normal then only $\mu(A - \lambda I) \leq \operatorname{dist}(\lambda, \sigma(A))$ holds [104, Thm. 4.2]. In this case, the spectrum usually fails to capture important properties of A and pseudospectra are introduced.

Definition 2.12. Let $A \in \mathcal{L}(X)$ and $\varepsilon > 0$. The ε-pseudospectrum $\sigma_\varepsilon(A)$ is the set of all $\lambda \in \mathbb{C}$ satisfying $\mu(A - \lambda I) < \varepsilon$.

From above considerations it is clear that $\sigma_\varepsilon(A) = \sigma(A) \cup \{\lambda \in \mathbb{C} : \nu(A - \lambda) < \varepsilon\}$. An element $x \in X$ with $\|x\| = 1$ and $\|(A - \lambda I)x\| < \varepsilon$ is called a pseudoeigenvector of A for the pseudoeigenvalue λ. The pseudospectrum can also be characterized via perturbations:

Lemma 2.13. *([104, p. 31]) Let $A \in \mathcal{L}(X)$ and $\varepsilon > 0$. Then $\lambda \in \sigma_\varepsilon(A)$ if and only if $\lambda \in \sigma(A+E)$ for some $E \in \mathcal{L}(X)$ with $\|E\| < \varepsilon$.*

We describe some more well-known properties of the pseudospectrum.

Lemma 2.14. *([104, Theorem 4.3])*
Let $A \in \mathcal{L}(X)$ and $\varepsilon > 0$. Then the following holds:

(a) $\sigma_\varepsilon(A)$ is a non-empty open subset of $\mathbb{C}$ and every bounded component has a non-empty intersection with $\sigma(A)$.

(b) The pseudospectra are strictly nested supersets of the spectrum, i.e. $\sigma_{\varepsilon_1}(A) \subsetneq \sigma_{\varepsilon_2}(A)$ for $0 < \varepsilon_1 < \varepsilon_2$ and

$$\sigma(A) = \bigcap_{\varepsilon > 0} \sigma_\varepsilon(A).$$

Lemma 2.14(b) states that $\sigma_\varepsilon(A)$ is nowhere constant in ε. Using the continuity of μ and the fact that $\mu(A - \lambda I) \to \infty$ as $|\lambda| \to \infty$ we even get that the level set $\{\lambda \in \mathbb{C} : \mu(A - \lambda I) = \varepsilon\}$ is non-empty. We can ask a related question: can this set contain any open subsets of $\mathbb{C}$? This question plays a role when considering the set

$$\sigma_\varepsilon^{\leq}(A) := \{\lambda \in \mathbb{C} : \mu(A - \lambda I) \leq \varepsilon\} = \sigma_\varepsilon(A) \cup \{\lambda \in \mathbb{C} : \mu(A - \lambda I) = \varepsilon\}.$$

Since μ is continuous it is clear that $\operatorname{clos}(\sigma_\varepsilon(A)) \subset \sigma_\varepsilon^{\leq}(A)$. If the level $\{\lambda \in \mathbb{C} : \mu(A - \lambda I) = \varepsilon\}$ does not contain any open subsets of $\mathbb{C}$ then also $\operatorname{clos}(\sigma_\varepsilon(A) = \sigma_\varepsilon^{\leq}(A))$ holds. Interestingly, this is not always the case [94, Theorem 3.1]. However, Globevnik[42] and Shargorodsky[94] showed that for bounded operators on $\ell^p(\mathbb{I})$ with $\mathbb{I} \subset \mathbb{Z}^d$ we do indeed have $\operatorname{clos}(\sigma_\varepsilon(A) = \sigma_\varepsilon^{\leq}(A))$.

2.3 Bounded linear operators on sequence spaces

Throughout this section, let $\mathbb{I}, \mathbb{J} \in \{\mathbb{Z}^d, \mathbb{Z}_+, \mathbb{Z}_-, \mathbb{N}\}$ and $p \in [1, \infty]$.

Basic operators

We define basic operators acting on $\ell^p(\mathbb{I})$.

Definition 2.15. (Multiplication operator) For $a = (a_n)_{n \in \mathbb{I}} \in \ell^\infty(\mathbb{I})$ the multiplication by a is denoted by M_a and defined by

$$\begin{aligned} M_a : \quad \ell^p(\mathbb{I}) \quad &\to \ell^p(\mathbb{I}) \\ (x_n)_{n \in \mathbb{I}} &\mapsto (a_n x_n)_{n \in \mathbb{I}}. \end{aligned}$$

It is easy to see that $\|M_a\| = \|a\|_\infty$.

Definition 2.16. (Projection) For $U \subset \mathbb{I}$ we define the projection on U as $P_U := M_{\chi_U}$.

Since $P_U^2 = P_U$, this operator is indeed a projection. In the Hilbert space $\ell^2(\mathbb{I})$ it is orthogonal. Moreover, if U is finite then $\operatorname{im} P_U$ is isomorphic to $\mathbb{C}^{|U|}$.

Definition 2.17. (Shift operator) For $i \in \mathbb{Z}^d$ the shift operator by i is defined by

$$\begin{aligned} S_i : \quad \ell^p(\mathbb{I}) \quad &\to \ell^p(\mathbb{I}) \\ (x_n)_{n\in\mathbb{I}} &\mapsto (x_{n-i})_{n\in\mathbb{I}}, \end{aligned}$$

where we set $x_n = 0$ if $n \notin \mathbb{I}$.

For $d = 1$ the shift operator by 1 is called the (right) shift and the shift operator by -1 is called the left shift. We sometimes abbreviate $S := S_1$. If $\mathbb{I} = \mathbb{Z}$ then the left shift is the inverse of the right shift.

Matrix representation

Let $A \in \mathcal{L}(\ell^p(\mathbb{I}), \ell^p(\mathbb{J}))$. Then we can identify $P_{\{i\}}AP_{\{j\}}|_{\operatorname{im} P_{\{j\}}}$ with a complex number

$$P_{\{i\}}AP_{\{j\}}|_{\operatorname{im} P_{\{j\}}} =: A_{i,j} \in \mathbb{C}.$$

For $p = 2$ this corresponds to $a_{i,j} = \langle Ae_j, e_i \rangle$, where $(e_i)_{i\in\mathbb{I}}$ denotes the canonical basis. Now the matrix $(A_{i,j})_{i\in\mathbb{I}, j\in\mathbb{J}}$ defines also an operator $\hat{A}$ from $\ell^p(\mathbb{I})$ to $\ell^p(\mathbb{J})$ by the usual matrix-vector multiplication:

$$(\hat{A}x)_i = \sum_{j\in\mathbb{J}} A_{i,j} x_j.$$

For $p < \infty$ it is known that A and $\hat{A}$ coincide, see [62, Section 1.3.5]. This does not need to be the case for $p = \infty$. However, this work will only be concerned with operators for which $A = \hat{A}$ also holds in the case $p = \infty$, see also next section.

For an operator $A \in \mathcal{L}(\ell^p(\mathbb{Z}^d), \ell^p(\mathbb{Z}^d))$ and $\mathbb{I} \subset \mathbb{Z}^d$, we abbreviate the restriction of A to $\ell^p(\mathbb{I})$,

$$A|_{\ell^p(\mathbb{I})} \; : \; \ell^p(\mathbb{I}) \to \ell^p(\mathbb{Z}^d),$$

by $A|_{\mathbb{I}}$ and call it the restriction of A to $\mathbb{I}$. Furthermore, the operator $\ell^2(\mathbb{N}^d) \to \ell^2(\mathbb{N}^d)$, corresponding to the matrix $A^+ := (A_{ij})_{i,j\in\mathbb{N}^d}$, is called the compression of A to $\mathbb{N}^d$. Similarly, A^- is the compression on $(\mathbb{Z}_-)^d$

Throughout most of this thesis we will work in one dimension, meaning that $d = 1$. In that context, we use the following abbreviations for discrete intervals. Given $a, b \in \mathbb{Z}$, we write

$$\begin{aligned} a..b \quad &:= \quad \{n \in \mathbb{Z} : a \leq n \leq b\}, \\ a.. \quad &:= \quad \{n \in \mathbb{Z} : a \leq n\}, \\ ..b \quad &:= \quad \{n \in \mathbb{Z} : n \leq b\}. \end{aligned}$$

Together with the abbreviations above, this explains the notations $A|_{a..b}$, $A|_{a..}$ and $A|_{..b}$. Moreover, let $A_{a..b}$ denote the matrix $(A_{i,j})_{i,j\in a..b}$.

For $A \in \mathcal{L}(\mathbb{I}, \mathbb{J})$ and $i \in \mathbb{I}$ we call the sequence $(A_{i,j})_{j\in\mathbb{J}}$ the i-th row of A. For $j \in \mathbb{J}$ we call $(A_{i,j})_{i\in\mathbb{I}}$ the j-th column of A. When $\mathbb{I} = \mathbb{J}$ then for $k \in \mathbb{I}$ the sequence $(A_{i+k,i})$ is called the k-th diagonal of A. The diagonals for $k = -1$, $k = 0$ and $k = 1$ are called superdiagonal, the main diagonal and the subdiagonal, respectively.

For $p \in [1, \infty)$ the matrix representation of the adjoint of $A \in \mathcal{L}(\ell^p(\mathbb{I}))$ is given by the transpose, that is $(A_{i,j})^* = (A_{j,i})$, while for $p = 2$ the Hilbert space adjoint is given by the Hermitian adjoint $A^H_{i,j} = \overline{A_{j,i}}$.

Convention on projections and embeddings

We will often be concerned with the interplay of finite and infinite matrices and we will therefore need to map operators into different spaces. In order to reduce the notational effort we make the following conventions. For $U \subset \mathbb{I}$ let $T : \operatorname{im} P_U \to \ell^p(U)$ be the canonical embedding. We want to interpret $P_U A P_U$ as an operator on $\ell^p(U)$. Technically, we are considering $T P_U A P_U T^{-1}$, but we usually drop the expressions T and T^{-1}. In the case that U is finite we may write "as a finite matrix" or something similar to recall that this identification takes place.

We are also interested in the converse: if $B \in \mathcal{L}(\ell^p(U))$ then for $c \in \mathbb{C}$ the extension $\widetilde{B} = T^{-1}AT + c(I - P_U)$ is an operator on $\ell^p(\mathbb{I})$. When we write that a sequence $(A_n)_{n\in\mathbb{N}}$ of finite matrices converges to an infinite matrix $A \in \mathcal{L}(\ell^p(\mathbb{I}))$ we actually mean that $(\widetilde{A_n})_{n\in\mathbb{N}}$ converges to A. Thereby we usually set $c = 0$ in order to have $\|\widetilde{B}\| = \|B\|$. However, if we are interested in quantities regarding the inverses, for example $\|A_n^{-1}\|$, we choose $c \neq 0$ appropriately. For finite square matrices $\det$ and tr denote the determinant and the trace, respectively.

Band operators

Definition 2.18. An operator on $\ell^p(\mathbb{I})$ is called a band operator if it is a finite sum of finite products of shift and multiplication operators, that is,

$$A = \sum_{|k|_\infty \leq w} M_{a^{(k)}} S_k$$

with all $a^{(k)} \in \ell^\infty(\mathbb{I})$. The number $w \in \mathbb{N}$ is called the bandwidth of A. The set of all band operators on $\ell^p(\mathbb{I})$ with bandwidth w is denoted by $\mathrm{BO}_p^w(\mathbb{I})$. We set $\mathrm{BO}_p(\mathbb{I}) := \bigcup_{w\in\mathbb{Z}_+} \mathrm{BO}_p^w(\mathbb{I})$. We omit the argument $\mathbb{I}$ whenever it is clear from context.

Let us present some equivalent characterizations:

Lemma 2.19. *([62, Proposition 1.36]) Let $A \in \ell^p(\mathbb{I})$. Then the following are equivalent:*

(i) A is a band operator with bandwidth w,

(ii) $A_{ij} = 0$ for $|i - j|_\infty > w$,

(iii) $P_U A P_W = 0$ for all set $U, W \subset \mathbb{Z}^n$ with $\operatorname{dist}(U, V) > w$.

This means that band operators exactly correspond to infinite matrices with bounded diagonals, of which only finitely many are not zero.

For operators $A \in \mathcal{L}(\ell^p(\mathbb{I}), \ell^p(\mathbb{J}))$ we define band operators and bandwidth via (ii). For $d = 1$ and a band operator with bandwidth 1 the only three non-zero diagonals are the main diagonal, the sub- and the superdiagonal. They are therefore called tridiagonal operators.

A band operator can be interpreted as a bounded operator on every $\ell^p(\mathbb{I})$ with $p \in [1, \infty]$. Even its invertibility is independent of p:

Proposition 2.20. *([58, 5.27], [85, Cor. 2.5.4]). Let A be a band operator on $\ell^p(\mathbb{I})$ for some $p \in [1, \infty]$. If A is invertible, then A is also invertible as an operator on $\ell^q(\mathbb{I})$ for all $q \in [1, \infty]$.*

This justifies the notations $\mathrm{BO}(\mathbb{I}) := \mathrm{BO}_p(\mathbb{I})$ and $\mathrm{BO} := \mathrm{BO}_p$. Since BO is closed under addition, multiplication and scalar multiplication it forms a subalgebra of $\mathcal{L}(\ell^p(\mathbb{I}))$. The closure of BO w.r.t. $\|\cdot\|_p$ forms a Banach algebra that depends on $p \in [1, \infty]$ and is denoted by BDO_p. We call operators in BDO_p band-dominated operators. The subalgebra BDO_p is inverse closed in $\mathcal{L}(\ell^p(\mathbb{I}))$, meaning that if a band-dominated operator is invertible its inverse is again band-dominated [62, Prop. 1.46].

We state some results on sequences of band operators with a uniform bound on their bandwidth and their limits.

Lemma 2.21. *Let $w \in \mathbb{Z}_+$ and $(A_n)_{n\in\mathbb{N}} \subset \mathrm{BO}^w(\mathbb{I})$. If for some $A \in \mathcal{L}(\ell^p(\mathbb{I}))$ we have $A_n \to A$ then $A \in \mathrm{BO}^w(\mathbb{I})$.*

Proof. Let $U, W \subset \mathbb{I}$ with $\operatorname{dist}(U, W) > w$. Then $P_U A_n P_W = 0$ for all $n \in \mathbb{N}$. Thus, for all $x \in \ell^p(\mathbb{I})$ we have that

$$P_U A P_W x = \lim_{n\to\infty} P_U A_n P_W x = 0$$

which proves the claim. □

The following result shows that on $\ell^\infty(\mathbb{I})$ strong convergence is equivalent to uniform converge when the operators are uniformly banded.

Proposition 2.22. *Let $w \in \mathbb{Z}_+$ and $(A_n)_{n\in\mathbb{N}} \subset \mathrm{BO}^w(\mathbb{I})$. Then for $A \in \mathcal{L}(\ell^\infty(\mathbb{I}))$ the following are equivalent:*

(i) $A_n \to A$ in $\mathcal{L}(\ell^\infty(\mathbb{I}))$,

(ii) $A_n \rightrightarrows A$ in $\mathcal{L}(\ell^\infty(\mathbb{I}))$.

Proof. Clearly, uniform convergence implies strong convergence.

For the other direction we use Lemma 2.21 and find that A is also banded with bandwidth w. The same holds for $A_n - A$. We only show the statement for $\mathbb{I} = \mathbb{Z}^d$ since for all other cases the operators can be extended to $\ell^\infty(\mathbb{Z})$ by zero.

Take $x = \sum_{k\in\mathbb{Z}^d} e_{k(2w+1)} \in \ell^\infty(\mathbb{Z}^d)$. Then, due to the bandedness of $(A_n - A)$, $\|(A_n - A)x\|_\infty = \sup_{k\in\mathbb{Z}^d} \|(A - A_n)e_{k(2w+1)}\|_\infty$. For every $\varepsilon > 0$ the strong convergence allows us to find an $n_0 \in \mathbb{N}$ such that for all $n \geq n_0$ we have that

$$\max_{j\in\{0,\dots,2w\}^d} \|(A - A_n)S_j x\|_\infty < \frac{\varepsilon}{(2w+1)^d}.$$

We conclude that

$$\sup_{i\in\mathbb{Z}^d} \|(A - A_n)e_i\|_\infty < \frac{\varepsilon}{(2w+1)^d},$$

meaning that every matrix entry of $A_n - A$ is bounded by $\frac{\varepsilon}{2w+1}$ in modulus. For every $y \in \ell^\infty(\mathbb{Z}^d)$ this yields that $\|(A_n - A)y\|_\infty \leq (2w+1)^d \frac{\varepsilon}{(2w+1)^d} \|y\|_\infty = \varepsilon \|y\|_\infty$ and therefore the uniform convergence follows. □

2.4 Fredholm theory

Sometimes it is not enough to know whether an operator is invertible or not, but we also want to know how far it is from being invertible. For example, consider the multiplication operators M_a and M_b on $\ell^2(\mathbb{N})$ with the sequences $a = (0, 1, 1, 1, \dots)$ and $b = (1, 0, 0, 0, \dots)$. Both operators are clearly not invertible, but 0 is only an eigenvalue of multiplicity 1 for M_a, while that kernel of M_b is almost the entire space. Likewise, changing only one entry in a would make M_a invertible, while the invertibility of M_b cannot be achieved by changing finitely many entries in b. We therefore have the intuition that M_a is closer to invertibility than M_b. With the theory of Fredholm operators we are able to formalize this intuition. We start with the theory of Fredholm operators on Banach spaces X and will later focus on the case of band-dominated operators on sequence spaces.

2.4.1 Fredholm operators

For a Banach space X and $A \in \mathcal{L}(X)$ we define the numbers

$$\alpha(A) := \dim(\ker(A)), \quad \beta(A) := \dim(X/\operatorname{im}(A)).$$

Thus $\alpha(A)$ and $\beta(A)$ give an indication on how much the injectivity and surjectivity fail, respectively.

Definition 2.23. An operator $A \in \mathcal{L}(X)$ is called Fredholm if $\alpha(A)$ and $\beta(A)$ are finite. If A is Fredholm then the index of A is given by $\operatorname{ind}(A) := \alpha(A) - \beta(A)$.

Due to the open mapping theorem Fredholm operators have a closed range. By Banach's closed range theorem this property transfers to the adjoint [5]:

Theorem 2.24. *For $A \in \mathcal{L}(X)$ the following are equivalent:*

(i) $\operatorname{im}(A)$ *is closed*

(ii) $\operatorname{im}(A^*)$ *is closed*

(iii) $\operatorname{im}(A) = \{x \in X : f(x) = 0 \text{ for all } f \in \ker(A^*)\}$

(iv) $\operatorname{im}(A^*) = \{f \in X^* : f(x) = 0 \text{ for all } x \in \ker(A)\}$.

As a consequence, A is Fredholm if and only if A^* is Fredholm. Moreover,

$$\alpha(A) = \beta(A^*), \quad \beta(A) = \alpha(A^*), \quad \operatorname{ind}(A) = -\operatorname{ind}(A^*).$$

The following theorem, known as Atkinson's theorem, establishes a link between the Fredholm property and compact operators. Roughly speaking, it states that Fredholmness is invertibility up to compact operators.

Theorem 2.25. *([3])*
An operator $A \in \mathcal{L}(X)$ is Fredholm if and only if the coset $A + \mathcal{K}(X)$ is invertible in the Calkin algebra $\mathcal{L}(X)/\mathcal{K}(X)$. Moreover, if A and B are Fredholm and $K \in \mathcal{K}(X)$ then

(a) AB *and* BA *are Fredholm as well and* $\operatorname{ind}(AB) = \operatorname{ind}(BA) = \operatorname{ind}(A) + \operatorname{ind}(B)$.

(b) $A + K$ *is Fredholm and* $\operatorname{ind}(A + K) = \operatorname{ind}(A)$.

(c) The map $\operatorname{ind} : \{A \in \mathcal{L}(X) : A \text{ Fredholm}\} \to \mathbb{Z}$ *is continuous w.r.t. the topology of* $\mathcal{L}(X)$. *In particular,* ind *is constant on connected components.*

Note that invertibility in the Calkin algebra is not equivalent to being a compact perturbation of an invertible operator on $\mathcal{L}(X)$. A Fredholm operator A with non-zero index cannot be written as $A = B + K$ for B invertible and K compact since part (b) of above theorem yields $\operatorname{ind}(A) = \operatorname{ind}(B) = 0$. However, the condition $\operatorname{ind}(A) = 0$ is sufficient for a Fredholm operator to be a compact perturbation of an invertible operator:

Proposition 2.26. *(e.g. [44, Chapter XV, Cor. 2.4])*
Let $A \in \mathcal{L}(X)$ *be Fredholm. Then there exists a* $K \in \mathcal{K}(X)$ *with* $A + K$ *invertible if and only if* $\operatorname{ind}(A) = 0$.

Definition 2.27. The set of all complex numbers λ for which $A - \lambda I$ is not Fredholm is called the essential spectrum of A and is denoted by $\sigma_{\text{ess}}(A)$.

Clearly $\sigma_{\text{ess}}(A) \subset \sigma(A)$ and by Atkinson's theorem $\sigma_{\text{ess}}(A) = \sigma(A + \mathcal{K}(X))$. Therefore, $\sigma_{\text{ess}}(A)$ is also always non-empty and compact. The notion of the essential spectrum goes back to Weyl [106] who defined it as the part of the spectrum of a certain differential operator that is independent of boundary conditions.

2.4.2 Notions of convergence

In the Fredholm theory of band-dominated operators the limit operator method plays an important role. This method has a telling name: the limit operators of a band-dominated operator A are obtained via limits. The obvious question is: what kind of convergence do we consider here. Neither strong nor uniform convergence are the right choice for limit operators for all $p \in [1, \infty]$. Most literature that deals with limit operators uses $\mathcal{P}$-convergence, such as [85, 62, 90, 47]. We say (A_n) $\mathcal{P}$-converges to A and write $A_n \overset{\mathcal{P}}{\to} A$ as $n \to \infty$ if (A_n) is bounded and

$$\|P_{\{-m,\dots,m\}^d}(A_n - A)\| \to 0 \qquad \text{and} \qquad \|(A_n - A)P_{\{-m,\dots,m\}^d}\| \to 0 \tag{2.6}$$

as $n \to \infty$ for every fixed $m \in \mathbb{N}$. For simplicity, we defined $\mathcal{P}$-convergence differently than how it was first introduced in [88] and then adopted by other authors. But our definition is equivalent when we choose the approximate projection $\mathcal{P} = (P_{\{-m,\dots,m\}^d})_{m\in\mathbb{N}}$, see e.g. [62, Proposition 1.65]. For a detailed survey on the theory around $\mathcal{P}$-convergence, the so-called $\mathcal{P}$-theory, see [91].

Moreover, we say a sequence $(A_n)_{n\in\mathbb{N}} \subset \mathcal{L}(\ell^p(\mathbb{I}))$ converges $*$-strongly to $A \in \mathcal{L}(\ell^p(\mathbb{I}))$ if $A \to A$ and $A^* \to A^*$ in the dual space. In this case, we write $A_n \overset{*}{\to} A$ as $n \to \infty$. If the operators $A, A_1, A_2, \dots$ all have a matrix representation then we say (A_n) converges entrywise to A if $\lim\limits_{n\to\infty} (A_n)_{ij} = A_{ij}$ for all $i, j \in \mathbb{I}$ at write $A_n \overset{ij}{\to} A$ as $n \to \infty$.

The following implications follow directly from the definition:

- Uniform convergence implies $*$-strong convergence.
- $*$-strong convergence implies strong convergence and $\mathcal{P}$-convergence.
- Strong convergence implies entrywise convergence.
- $\mathcal{P}$-convergence implies entrywise convergence.

We sketch above observations in Figure 2.1.

$$\begin{tikzcd}
 & & \to \arrow[dr, Rightarrow] & \\
\rightrightarrows \arrow[r, Rightarrow] & \overset{*}{\to} \arrow[ur, Rightarrow] \arrow[dr, Rightarrow] & & \overset{ij}{\to} \\
 & & \overset{\mathcal{P}}{\to} \arrow[ur, Rightarrow] &
\end{tikzcd}$$

Figure 2.1: Hierarchy of convergences. For the entrywise convergence we assume that all operators have a matrix representation.

Depending on the choice of $p \in [1, \infty]$ we can find additional implications.

Proposition 2.28. *([47, Proposition 2.23])*

(a) If $p < \infty$ then $\mathcal{P}$-convergence implies strong convergence.

(b) If $p \in (1, \infty)$ then $\mathcal{P}$-convergence is equivalent to $*$-strong convergence.

Recall from Proposition 2.22 that for a sequence of operators with uniformly bounded bandwidth and $p = \infty$ strong convergence is equivalent to uniform convergence. Hence, that same holds for $p = 1$ and $*$-strong convergence instead of strong convergence. Also, for $p \in (1, \infty)$ the condition of uniformly bounded bandwidth yields additional equivalences of notions of convergence.

Proposition 2.29. *([47, Proposition 2.24]) Let $p \in (1, \infty)$, $w \in \mathbb{Z}_+$ and $(A_n)_{n \in \mathbb{N}} \subset \mathrm{BO}^w$. Then for $A \in \mathrm{BO}$ the following are equivalent:*

(i) $A_n \overset{*}{\to} A$ as $n \to \infty$,

(ii) $A_n \to A$ as $n \to \infty$,

(iii) $A_n \overset{\mathcal{P}}{\to} A$ as $n \to \infty$,

(iv) $A_n \overset{ij}{\to} A$ as $n \to \infty$.

We summarize the previous results is Figure 2.2.

2.4.3 Limit operators

In Section 2.4.1 we presented several characterizations of Fredholmness. Firstly, the finiteness of the dimensions of kernel and cokernel, where the latter could be replaced by the kernel of the adjoint. Additionally, we found that Fredholmness is equivalent to invertibility in the Calkin algebra which, as a factor algebra, is often complicated to work with.

The Fredholmness of a band-dominated operator on $X = \ell^p(\mathbb{I})$ can also be characterized via the invertibility of a certain set of operators in $\mathcal{L}(\ell^p(\mathbb{Z}^d))$, namely the limit operators. The statement

“A band-dominated operator is Fredholm if and only if all its limit operators are invertible.” (2.7)

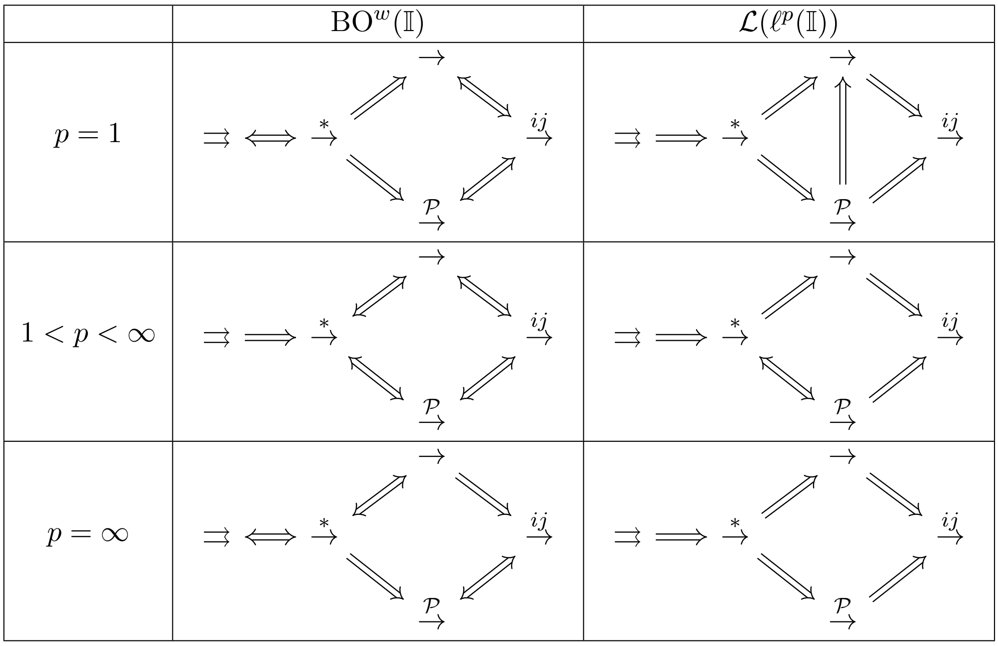

Figure 2.2: Updated hierarchy of convergences for different values of p. In the column labeled $\mathrm{BO}^w(\mathbb{I})$ we assume that $(A_n) \subset \mathrm{BO}^w$ for some $w \in \mathbb{Z}_+$. For the entrywise convergence we assume that all operators have a matrix representation. The implications shown are discussed in Propositions 2.22, 2.28 and 2.29.

is the main theorem of limit operator theory. While the first ideas concerning limit operators go back to J. Favard [35], it was in the 1980s when E.M. Muhamadiev [77] who proved a result similar to the above for certain elliptic differential operators. B.V. Lange and V.S. Rabinovich [60] could generalize these ideas to band-dominated operators on $\ell^p(\mathbb{Z}^d)$ for $p \in (1, \infty)$. However, they also required that the inverses of the limit operators are uniformly bounded. It took until 2013 when M. Lindner and M. Seidel were able to show that the uniform boundedness condition is redundant.

Remark 2.30. ($\mathcal{P}$-Theory)
A lot of work in limit operator theory was done in order to generalize the setting from scalar sequence spaces $\ell^p(\mathbb{Z}^d)$ to Banach space valued sequence spaces

$$\ell^p(\mathbb{Z}^d, X) := \Big\{ (x_n)_{n \in \mathbb{Z}^d} \subset X : \sum_{n \in \mathbb{Z}^d} \|x\|_X^p < \infty \Big\},$$

where X is a Banach space. The space $\ell^p(\mathbb{Z}^d, X)$ is also a Banach space when equipped with the norm

$$\|(x_n)_{n \in \mathbb{Z}^d}\|_{\ell^p(\mathbb{Z}^d, X)} := \Big(\sum_{n \in \mathbb{Z}^d} \|x\|_X^p \Big)^{\frac{1}{p}}.$$

It were Rabinovich, Roch and Silbermann [83] who generalized the results of Lange and Rabinovich regarding (2.7) to $\ell^p(\mathbb{Z}^d, \mathbb{C}^d)$, to $\ell^2(\mathbb{Z}^d, H)$ for a Hilbert space H [84] and finally to $\ell^p(\mathbb{Z}^d, X)$ [85] for $p \in (1, \infty)$. Lindner [62] later proved the cases $p \in \{1, \infty\}$.

In order to obtain these results the authors mentioned above work in the co-called $\mathcal{P}$-framework. In particular, one has to replace notions of compactness and Fredholmness by $\mathcal{P}$-compactness and $\mathcal{P}$-Fredholmness, respectively. An overview over the $\mathcal{P}$-framework can be found in [91].

For $\dim X < \infty$ and $p \in (1, \infty)$ the $\mathcal{P}$-framework coincides with the classical framework, meaning that $\mathcal{P}$-compactness and compactness are equivalent. The notions of $\mathcal{P}$-Fredholmness and Fredholmness are equivalent also for the cases $p = 1$ and $p = \infty$, see [91, Corollary 12]. This work is only concerned with the spaces $\ell^p(\mathbb{Z}^d)$ for $p \in [1, \infty]$, Chapter 4 even requires $p = 2$. Therefore, we refrain from properly introducing the $\mathcal{P}$-framework here in order to keep the technical and notational effort to a minimum.

Definition 2.31 (Limit operators)**.** Let $A \in \mathrm{BDO}_p(\mathbb{Z}^d)$ and let further $h = (h_n)$ be a sequence in $\mathbb{Z}^d$ with $|h_n| \to \infty$ such that $S_{-h_n} A S_{h_n}$ $\mathcal{P}$-converges. Then the limit is called a limit operator of A associated to the sequence h and denoted by A_h.

Moreover, let $\mathrm{Lim}(A)$ denote the set of all limit operators of A, together with the following local versions: For a sequence $g = (g_n) \subset \mathbb{Z}^d$ with $|g_n| \to \infty$, we put

$$\mathrm{Lim}_g(A) := \{A_h : h \text{ is a subsequence of } g\}.$$

For $d = 1$ we set $\mathrm{Lim}_+(A) := \mathrm{Lim}_{(1,2,\dots)}(A)$ and $\mathrm{Lim}_-(A) := \mathrm{Lim}_{(-1,-2,\dots)}(A)$.

For $A \in \mathrm{BDO}_p(\mathbb{N})$ we extend A to an operator $\hat{A} \in \mathrm{BDO}_p(\mathbb{Z})$ by zero. Then we define the limit operators of A to be the limit operators of $\hat{A}$, but we only consider sequences that tend to $+\infty$. In particular, $\mathrm{Lim}(A) = \mathrm{Lim}_+(\hat{A})$. Similarly, we define limit operators for band-dominated operators on $\ell^p(\mathbb{Z}_+)$ and $\ell^p(\mathbb{Z}_-)$.

It can easily be seen that the extension by zero of $A \in \mathrm{BDO}_p(\mathbb{N})$ in the previous definition was arbitrary and that any other band-dominated extension would yield the same set of limit operators for A. For the rest of this section we restrict ourselves to $\mathbb{I} \in \{\mathbb{Z}^d, \mathbb{N}, \mathbb{Z}_+, \mathbb{Z}_-\}$. We sometimes rephrase the condition $|h_n| \to \infty$ as $n \to \infty$ by saying that h tends to infinity.

Now we can state the main theorem of limit operator theory.

Theorem 2.32. *[83, 71]*
A band-dominated operator A on $\ell^p(\mathbb{I})$ is Fredholm if and only if all limit operators of A are invertible.

As a consequence of Theorem 2.32,

$$\sigma_{\mathrm{ess}}(A) = \bigcup_{B \in \mathrm{Lim}(A)} \sigma(B). \tag{2.8}$$

It can even be shown that the injectivity of all limit operators is sufficient for Fredholmness. This condition originates from the analysis of differential equations, where Favard [35] proved the existence of almost periodic solutions for systems ODE's with almost periodic coefficients and right-hand side. Therefore, the following is known as Favard's condition.

Proposition 2.33. *[18, 19] A band operator A on $\ell^p(\mathbb{I})$ is Fredholm if and only if all limit operators of A are injective on $\ell^\infty(\mathbb{Z})$.*

The sufficiency of Favard's condition for Fredholmness is a peculiarity of the one-dimensional setting. In higher dimension an analogue of Proposition 2.33 does not hold. For a counterexample in two-dimension see [91, Example 30].

Next we summarize well-known properties of the relation between A and its limit operators. For instance, as an immediate consequence of the definition the set of limit operators is shift-invariant.

Proposition 2.34. *([62, Proposition 3.94]) Let* $A \in \mathrm{BDO}_p(\mathbb{I})$*,* $B \in \mathrm{Lim}(A)$ *and* $n \in \mathbb{N}$*. Then* $S_{-n}BS_n$ *is also a limit operator of* A*.*

Proposition 2.35. *(e.g. [19, Theorem 5.12], [62, Proposition 3.4]) Let* $A, A' \in \mathrm{BDO}_p(\mathbb{I})$*. Let* g *be a sequence of integers tending to infinity such that* $B = A_g$ *and* $B' = A'_g$*. Then the following hold:*

(a) $(A + A')_g$ *exists and is equal to* $B + B'$*,*

(b) $(AA')_g$ *and* $(A'A)_g$ *exist and are equal to* BB' *and* $B'B$*, respectively,*

(c) $\|B\| \leq \|A\|$*,*

(d) $\nu(B) \geq \nu(A)$*,*

(e) $\mathrm{Lim}(B) \subset \mathrm{Lim}(A)$*,*

(f) $B^* = (A^*)_g$*.*

Further, let $(A_n)_{n\in\mathbb{N}} \subset \mathrm{BDO}_p(\ell^p(\mathbb{I}))$ *and* $h \subset \mathbb{Z}$ *with* $|h_m| \to \infty$ *as* $m \to \infty$ *such that the limit operators* $(A_n)_h$ *exist for sufficiently large* n*. If, in addition,* $A_n \rightrightarrows A$ *as* $n \to \infty$ *then the limit operator* A_h *exists and* $(A_n)_h \rightrightarrows A_h$ *holds as* $n \to \infty$*.*

In Proposition 2.29 we saw the equivalence of different notions of convergence for uniformly banded operators. In the following we will see that we can also use other notions of convergence in Definition 2.31 even for band-dominated operators.

Proposition 2.36. *Let* $A \in \mathrm{BDO}_p(\mathbb{I})$ *and let* $h = (h_n)$ *be a sequence of integers with* $|h_n| \to \infty$*. Then* $\mathrm{Lim}_h(A)$ *is non-empty. Moreover, for* $L \in \mathrm{BDO}_p(\mathbb{Z})$ *and* $p \in (1, \infty)$ *the following are equivalent:*

(i) $S_{-g_n}AS_{g_n} \xrightarrow{*} L$ *as* $n \to \infty$ *for some* $(g_n) \subset h$*,*

(ii) $S_{-g_n}AS_{g_n} \to L$ *as* $n \to \infty$ *for some* $(g_n) \subset h$*,*

(iii) $S_{-g_n}AS_{g_n} \xrightarrow{\mathcal{P}} L$ *as* $n \to \infty$ *for some* $(g_n) \subset h$*,*

(iv) $S_{-g_n}AS_{g_n} \xrightarrow{ij} L$ *as* $n \to \infty$ *for some* $(g_n) \subset h$*.*

In particular, $L = A_g$ *is a limit operator of* A *if and only if one of the above holds.*

Proof. If $A \in \mathrm{BO}(\mathbb{I})$ then this is a direct application of Proposition 2.29. Since every matrix entry of A is bounded by $\|A\|$ we can conclude that for all i, j the sequence $(S_{-h_n}AS_{h_n})_{i,j} = A_{i+h_n,j+h_n}$ has a convergent subsequence. By passing to subsequence we can find a sequence $h' \subset h$ such that $S_{-h'_n}AS_{h'_n}$ converges entrywise to some $L \in \mathrm{BO}(\mathbb{Z})$. Since the entrywise convergence of uniformly banded operators is equivalent to $*$-strong convergence, we get that $L \in \mathrm{Lim}_h(A)$. This proves the statement for band operators.

Now let $A \in \mathrm{BDO}_p(\mathbb{I})$. We first check that $\mathrm{Lim}_h(A) \neq \emptyset$. Let (A_m) be a sequence of band operators such that $A_m \rightrightarrows A$. With above observations and the help of a diagonal argument we can find a sequence $h' \subset h$ such that $(A_m)_{h'}$ exists for every $m \in \mathbb{N}$. Now by the final part of Proposition 2.35 we find that also $A_{h'}$ exists and is equal to the limit of $(A_m)_{h'}$ in norm as $m \to \infty$.

A look at Figure 2.2 shows that it only remains to show that (iv) implies (iii). So let $S_{-h_n}AS_{h_n} \xrightarrow{ij} L$ as $n \to \infty$. Since we just proved that the set $\mathrm{Lim}_h(A)$ is not empty we can take an element L' of that set. By definition, there is a subsequence $h' \subset h$ such that $S_{-h'_n}AS_{h'_n}$ convergences P-strongly to L'. This implies that $L = L'$ and therefore (iii) holds. $\square$

We will also need the following property.

Proposition 2.37. *([61, Proposition 3.7]) Let* $A \in \mathrm{BDO}_p(\mathbb{Z})$ *and* g *be a sequence of integers tending to infinity. Then* $\mathrm{Lim}_g(A)$ *is sequentially compact with respect to* $\mathcal{P}$*-convergence, meaning that every sequence in* $\mathrm{Lim}_g(A)$ *has a* $\mathcal{P}$*-convergent subsequence with limit in* $\mathrm{Lim}_g(A)$*. In particular, this applies to the set* $\mathrm{Lim}(A)$.

2.4.4 Self-similar and recurrent operators

We define the class of self-similar operators on the axis. Self-similarity is an inherent property of operators which are periodic (see Section 2.5 and 4.2), aperiodic (in the sense of Section 4.3) or pseudoergodic (see Section 3.3).

Definition 2.38. An operator $A \in \mathrm{BDO}_p(\mathbb{Z})$ is called self-similar if $A \in \mathrm{Lim}(A)$. We call A left-self-similar if $A \in \mathrm{Lim}_-(A)$ and right-self-similar if $A \in \mathrm{Lim}_+(A)$.

In a broader mathematical context self-similarity usually means that an object is approximately similar to a part of itself. In our setting the object is a band-dominated operator A and the parts are finite one-sided cut-offs such as $P_{k..k+N}A$ or $AP_{k..k+N}$. Using the notion of $\mathcal{P}$-converge (2.6), one can see that these parts are captured approximately by the set of limit operators. Therefore, being appropriately similar to a part of itself can be understood as being its own limit operator. The latter property has immediate consequences for the relation of the spectrum and the essential spectrum:

Lemma 2.39. *Let* A *be a band-dominated operator on* $\ell^p(\mathbb{Z})$*. Then the following holds:*

(a) If A *is self-similar then* $\sigma(A) = \sigma_{\text{ess}}(A)$.

(b) If A *is left-self-similar then* $\sigma(A) = \sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(A^-)$.

(c) If A *is right-self-similar then* $\sigma(A) = \sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(A^+)$.

In particular, a self-similar operator A *is invertible if and only if* A *is Fredholm.*

Proof. Part (a) follows from (2.8). For part (b) recall that $\sigma_{\text{ess}}(A) \subset \sigma(A)$. The inclusion $\sigma_{\text{ess}}(A^-) \subset \sigma_{\text{ess}}(A)$ holds by (2.8) since $\mathrm{Lim}(A^-) = \mathrm{Lim}_-(A) \subset \mathrm{Lim}(A)$. Finally, $\sigma(A) \subset \sigma_{\text{ess}}(A^-)$ holds by (2.8) and the assumption that A is left-self-similar. Part (c) is proven analogously. □

Another interesting consequence for self-similar operators is that the boundedness from below already implies the boundedness from below for the adjoint and therefore invertibility.

Lemma 2.40. *If* A *is self-similar, then* $\nu(A) = \nu(A^*)$*. In particular, if* $\nu(A) > 0$ *then* A *is invertible.*

Proof. Assume that $\nu(A) > 0$ and $\nu(A^*) = 0$. Then A is injective and $\mathrm{im}(A)$ is closed by Lemma 2.9. Operators with closed range and either $\alpha(A) < \infty$ or $\beta(A) < \infty$ are called semi-Fredholm [92]. It is known that band-dominated semi-Fredholm operators on $\ell^p(\mathbb{Z})$ are always Fredholm [92, Theorem 4.3]. Hence, A is Fredholm and by Lemma 2.39 A is invertible. This contradicts $\nu(A^*) = 0$.

If we assume $\nu(A) = 0$ and $\nu(A^*) > 0$ we obtain a contradiction by arguing analogously that A^* is invertible for $p < \infty$. For $p = \infty$ we consider the operator $A^{\triangleleft} \in \mathcal{L}(\ell^1)$ given by the matrix representation $A^{\triangleleft}_{ij} = A_{ji}$. We find that $(A^{\triangleleft})^* = A$. Moreover, follows from approximation with band operators that $A^{\triangleleft} \in \mathrm{BDO}_1(\mathbb{Z})$ and it is self-similar. In particular, using the canonical embedding of $\ell^1(\mathbb{Z})$ into the dual space of ℓ^∞ we find that $\nu(A^*) > 0 \implies \nu(A^{\triangleleft}) > 0$. Now the first part of the proof can be applied to $A^{\triangleleft}$ in order to get a contradiction. Therefore, $\nu(A) = 0 \iff \nu(A^*) = 0$. Finally, if both $\nu(A)$ and $\nu(A^*)$ are positive then, due to Lemma 2.10, A is invertible and $\nu(A) = \nu(A^*) = \|A^{-1}\|^{-1}$. □

Recall from Proposition 2.35 that the set of limit operators $\mathrm{Lim}(B)$ of a limit operator $B \in \mathrm{Lim}(A)$ is contained in the set of limit operators of A itself. The inclusion might not be strict, i.e. it can happen that $\mathrm{Lim}(A) = \mathrm{Lim}(B)$. If this is the case for all $B \in \mathrm{Lim}(A)$ then the set $\mathrm{Lim}(A)$ is minimal in the sense that it cannot be made smaller by passing to the limit operators of an element. Minimal sets of limit operators occur for different classes of operators and have interesting consequences for the spectral quantities, see [66].

Definition 2.41. An operator $A \in \mathrm{BDO}_p(\mathbb{Z})$ is called recurrent if $\mathrm{Lim}(B) = \mathrm{Lim}(A)$ for every $B \in \mathrm{Lim}(A)$.

We summarize some results of [66] on the relation of self-similar and recurrent operators as well as the properties of their respective sets of limit operators:

- While the property that A is recurrent is invariant under compact perturbations, self-similarity is not.
- Neither of the two properties implies the other.
- If A is recurrent then each limit operator is self-similar.

Lemma 2.42. *([66, Lemma 3.4]) Let $A \in \mathrm{BO}(\mathbb{Z})$ be a recurrent operator. Then the following are equivalent:*

(i) one $B \in \mathrm{Lim}(A)$ is Fredholm,

(ii) one $B \in \mathrm{Lim}(A)$ is invertible on $\ell^p(\mathbb{Z})$,

(iii) all $B \in \mathrm{Lim}(A)$ are invertible on $\ell^p(\mathbb{Z})$,

(iv) all $B \in \mathrm{Lim}(A)$ are injective on $\ell^\infty(\mathbb{Z})$,

(v) A is Fredholm.

If, in addition, A is self-similar then each of the above conditions is equivalent to

(vi) A is invertible.

An application of 2.35 to recurrent operators yields the following proposition, see also [66, Proposition 3.7].

Lemma 2.43. *Let $A \in \mathrm{BDO}_p(\mathbb{Z})$ be a recurrent operator. Then the following hold:*

(a) all elements of $\mathrm{Lim}(A)$ are limit operators of each other, including themselves,

(b) *all elements of* $\operatorname{Lim}(A)$ *have the same norm, lower norm, spectrum (that is entirely essential spectrum) and pseudospectra,*

(c) *for all* $B \in \operatorname{Lim}(A)$ *one has* $\operatorname{Lim}_-(B) = \operatorname{Lim}_+(B) = \operatorname{Lim}(B)$.

An interesting application of Zorn's Lemma [18, Proposition 3.7] guarantees for any band-dominated operator A that there exists a self-similar and recurrent limit operator $B \in \operatorname{Lim}(A)$.

2.5 Periodic band-dominated operators

We introduce the class of periodic band-dominated operators, one of the few classes of non-compact operators for which the spectrum can be computed explicitly. Therefore, periodic band-dominated operators are a natural choice for the approximation of more complicated operators, as we will see in Sections 3.1, 3.5 and 4.3.

Definition 2.44. We call a sequence $(x_n)_{n\in\mathbb{Z}} \subset \mathbb{C}$ periodic with period K if $x_n = x_{n+K}$. A band-dominated operator A on $\ell^p(\mathbb{Z})$ is called periodic with period K if $A = S_{-K}AS_K$.

Sometimes we also say that A is K-periodic or just that A is periodic if the period K is not relevant. One easily sees that if A has a matrix representation then A is K-periodic if and only if $A_{i,j} = A_{i+K,j+K}$, i.e. all diagonals of A are K-periodic. We call an operator $A^+ \in \mathcal{L}(\ell^p(\mathbb{N}))$ one-sided K-periodic if it is the compression of a K-periodic operator B, that is, $A^+ = P_{\mathbb{N}}BP_{\mathbb{N}}$.

The limit operators of a K-periodic band-dominated operator are found easily, and there are only K of them. The consequences are not surprising.

Proposition 2.45. *(e.g. [66]) For a K-periodic $A \in \operatorname{BDO}_p(\mathbb{Z})$, $p \in (1,\infty)$, and its compression $A^+ = P_{\mathbb{N}}AP_{\mathbb{N}} \in \operatorname{BDO}_p(\mathbb{N})$ we have the following:*

(a) $\operatorname{Lim}(A) = \{S_{-k}AS_k, k \in 0..K-1\}$,

(b) *A is (right-) self-similar and recurrent.*

(c) $\sigma(A) = \sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(A^+) \subset \sigma(A^+)$,

(d) *if $A \in \operatorname{BO}(\mathbb{Z})$ then A is invertible if and only if A is injective on $\ell^\infty(\mathbb{Z})$.*

Proof. Since every element of $(S_{-n}AS_n)_{n\in\mathbb{N}}$ is an element of the finite set $\{S_{-k}AS_k, k \in 0..K-1\}$ the limits are also in that set. In particular, $A \in \operatorname{Lim}(A) = \operatorname{Lim}_+(A) = \operatorname{Lim}(B)$ for every $B \in \operatorname{Lim}(A)$. This proves the first two statements. Now the third follows from Lemma 2.39. The fourth statement is a combination of 2.42 with the observation that the injectivity of one element in $\operatorname{Lim}(A)$ already implies the injectivity of all elements in the set. □

The spectral analysis of periodic band-dominated operators is well known. We start with the case of 1-periodic operators which are known as Laurent operators. The one-sided 1-periodic operators are referred to as Toeplitz operators.

2.5.1 Laurent and Toeplitz operators

For a 1-periodic operator $A \in \mathrm{BDO}(\ell^p(\mathbb{Z}))$ each diagonal is constant. For $j \in \mathbb{Z}$ let a_j denote the j-th diagonal of A, that is $a_j = A_{ik}$ for $i - k = j$. The spectral quantities of a Laurent operator can be derived with the help of the function

$$a : [0, 2\pi) \to \mathbb{C}, \qquad \varphi \mapsto a(\varphi) := \sum_{k=-\infty}^{\infty} a_k \mathrm{e}^{ik\varphi}. \tag{2.9}$$

Surprisingly, the condition that $A \in \mathcal{L}(\ell^p(\mathbb{Z}))$ is already sufficient for the convergence of the series in (2.9), see [13, Proposition 2.4] for $p \in (1, \infty)$ and [62, p. 23] for the cases $p = 1$ and $p = \infty$. If $A \in \mathrm{BDO}_p(\mathbb{Z})$ then its symbol is continuous and $\lim_{\varphi \to 2\pi} a(\varphi) = a(0)$, i.e. a describes a closed curve.

We see that A is invertible if and only if 0 is not in the range of a and then function $1/a$ is also the symbol of a Laurent operator B. In this case, B is the inverse of A, see [13, Proposition 2.46].

For band-dominated Laurent operators the second condition is redundant and by [13, Propostition 4.7] the statement can be simplified to

$$\sigma(A) = \operatorname{im} a. \tag{2.10}$$

For $p = 2$ consider the Fourier transform

$$\mathcal{F} : L^2([0, 2\pi)) \to \ell^2(\mathbb{Z}), \qquad a \mapsto \mathcal{F}(a) := (a_j)_{j \in \mathbb{Z}},$$

with

$$a_j := \frac{1}{2\pi} \int_0^{2\pi} a(\varphi) \mathrm{e}^{-ij\varphi} \, \mathrm{d}\varphi.$$

The sequence (a_j) is referred to as the Fourier coefficients of the function a. It is well known that $\mathcal{F}$ is an isometric isomorphism with inverse

$$\mathcal{F}^{-1} : \ell^2(\mathbb{Z}) \to L^2([0, 2\pi)), \qquad (a_j) \mapsto \sum_{j=-\infty}^{\infty} a_j \mathrm{e}^{ij\cdot}.$$

The entries a_k on the diagonal of A are therefore the Fourier coefficients of the symbol a of A. Note that the action of A on a vector x is given by

$$(Ax)_k = \sum_{j \in \mathbb{Z}} a_j x_{k-j},$$

which is the convolution of the sequences (a_j) and $x = (x_j)$. Recall the convolution of two Fourier series corresponds to the multiplication of the associated functions,

$$\mathcal{F}^{-1} A \mathcal{F} = M_a,$$

where M_a is the multiplication operator by a on $L^2([0, 2\pi))$ defined by $M_a(f) = af$. If $A \in \mathrm{BDO}_2(\mathbb{Z})$ then (2.10) is easy to see, and we also get

$$\|A\| = \|M_a\| = \max_{\varphi \in [0, 2\pi)} |a(\varphi)| \qquad \text{and} \qquad \nu(A) = \nu(M_a) = \min_{\varphi \in [0, 2\pi)} |a(\varphi)|.$$

For Toeplitz operators A^+ the symbol is the same as for the Laurent operator A with the same diagonals. If A^+ is band-dominated then limit operator theory yields that $\sigma_{\mathrm{ess}}(A^+) = \sigma(A) = \mathrm{im}(a)$. In order to describe the spectrum of A^+ we define the winding number $\mathrm{wind}(b, \lambda)$ of a closed curve b around $\lambda \in \mathbb{C}$.

Definition 2.46. [13, Section 2.41] Let $b : [0, 2\pi) \to \mathbb{C}$ be a closed curve and $0 \notin b([0, 2\pi))$. Let $\beta : (0, 2\pi) \to \mathbb{R}$ be a continuous function such that $b(\varphi) = |b(\varphi)|\mathrm{e}^{2\pi\beta(\varphi)i}$ for $\varphi \in (0, 2\pi)$. Then the winding number of b around 0,

$$\operatorname{wind}(b) := \lim_{\varphi\to 2\pi} \beta(\varphi) - \lim_{\varphi\to 0} \beta(\varphi),$$

exists and is an integer that does not depend on the choice of β. For $\lambda \in \mathbb{C} \setminus b(\mathbb{T})$ we define the winding number of b around λ by $\operatorname{wind}(b, \lambda) := \operatorname{wind}(b - \lambda)$.

Figuratively, the winding number is the number of rotations that the curve b makes around λ. If $b : \mathbb{T} \to \mathbb{C}$ is a continuously differentiable closed curve and $\lambda \notin b(\mathbb{T})$ then Cauchy's integral formula yields

$$\operatorname{wind}(b, \lambda) := \frac{1}{2\pi i} \int_{b(\mathbb{T})} \frac{\mathrm{d}z}{z - \lambda} = \frac{1}{2\pi i} \int_0^{2\pi} \frac{b'(\mathrm{e}^{i\theta})}{b(\mathrm{e}^{i\theta}) - \lambda} \mathrm{e}^{i\theta}\, \mathrm{d}\theta.$$

Now, for the spectrum of a Toeplitz operator we have

$$\sigma(A^+) = \operatorname{im} a \cup \{\lambda \in \mathbb{C} : \operatorname{wind}(a, \lambda) \neq 0\}, \tag{2.11}$$

and $\operatorname{ind}((A - \lambda I)^+) = -\operatorname{wind}(a, \lambda)$ for all $\lambda \notin \operatorname{im}(a)$, see [13, Theorem 2.47].

2.5.2 The spectrum of periodic operators

The approach for Laurent operators described above can be generalized to periodic operators by identifying them with block Laurent operators. Let A be a K-periodic operator on $\ell^p(\mathbb{Z})$. For $j \in \mathbb{Z}$ we then define

$$a_j := \begin{pmatrix} A_{jK+1,1} & \cdots & A_{jK+1,K} \\ \vdots & \ddots & \vdots \\ A_{(j+1)K,1} & \cdots & A_{(j+1)K,K} \end{pmatrix}.$$

Now the block Laurent structure of A can be described with the help of the sequence (a_j):

$$A = \left(\begin{array}{cc|ccc|ccc|cc}
\ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \\
\cdots & A_{K,K} & A_{0,1} & \cdots & A_{0,K} & A_{-K,1} & \cdots & A_{-K,K} & A_{-2K,1} & \cdots \\ \hline
\cdots & A_{K+1,K} & A_{1,1} & \cdots & A_{1,K} & A_{-K+1,1} & \cdots & A_{-K+1,K} & A_{-2K+1,1} & \cdots \\
\ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \\
\cdots & A_{2K,K} & A_{K,1} & \cdots & A_{K,K} & A_{0,1} & \cdots & A_{0,K} & A_{-K,1} & \cdots \\ \hline
\cdots & A_{2K+1,K} & A_{K+1,1} & \cdots & A_{K+1,K} & A_{1,1} & \cdots & A_{1,K} & A_{-K+1,1} & \cdots \\
\ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \\
\cdots & A_{3K,K} & A_{2K,1} & \cdots & A_{2K,K} & A_{K,1} & \cdots & A_{K,K} & A_{0,1} & \cdots \\ \hline
\cdots & A_{3K+1,K} & A_{2K+1,1} & \cdots & A_{2K+1,K} & A_{K+1,1} & \cdots & A_{K+1,K} & A_{1,1} & \cdots \\
\ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots
\end{array}\right)$$

$$= \begin{pmatrix}
\ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
\ddots & a_0 & a_{-1} & a_{-2} & a_{-3} & \ddots \\
\ddots & a_1 & a_0 & a_{-1} & a_{-2} & \ddots \\
\ddots & a_2 & a_1 & a_0 & a_{-1} & \ddots \\
\ddots & a_3 & a_2 & a_1 & a_0 & \ddots \\
\ddots & \ddots & \ddots & \ddots & \ddots & \ddots
\end{pmatrix}.$$

As for Laurent operators, we can compute the spectrum with the help of the symbol, which is now defined by

$$a : [0, 2\pi) \to \mathbb{C}^{m\times m}, \qquad \varphi \mapsto a(\varphi) := \sum_{k=-\infty}^{\infty} a_k \mathrm{e}^{ik\varphi}.$$

For $p = 2$ we introduce the vector-valued Fourier transform

$$\mathcal{F} : L^2([0, 2\pi), \mathbb{C}^K) \to \ell^2(\mathbb{Z}, \mathbb{C}^K), \qquad f \mapsto \mathcal{F}(f) := (f_k)_{k\in\mathbb{Z}},$$

with

$$f_k := \frac{1}{2\pi} \int_0^{2\pi} f(\varphi)\mathrm{e}^{-ik\varphi}\, \mathrm{d}\varphi.$$

Again, $\mathcal{F}$ is an isometric isomorphism which maps A to a multiplication operator by the symbol a, see e.g. [31, Theorem 4.4.9] and the proof thereof. More precisely, $\mathcal{F}^{-1}A\mathcal{F} = M_a$, where

$$M_a : L^2([0, 2\pi), \mathbb{C}^K) \to L^2([0, 2\pi), \mathbb{C}^K), \qquad f \mapsto af.$$

Theorem 2.47. *Let $A \in \mathrm{BDO}_2(\mathbb{Z})$ be K-periodic. Then*

$$\|A\| = \|M_a\| = \max_{\varphi\in[0,2\pi)} \|a(\varphi)\| \qquad \textit{and} \qquad \nu(A) = \nu(M_a) = \min_{\varphi\in[0,2\pi)} \nu(a(\varphi)), \tag{2.12}$$

where $\|a(\varphi)\|$ denotes the spectral norm of the matrix $a(\varphi)$.

For $A \in \ell^p(\mathbb{Z})$ with a matrix representation let $d_j := \sup_{i\in\mathbb{Z}} |A_{i+j,i}|$. We define

$$\|A\|_{\mathcal{W}} := \sum_{j\in\mathbb{Z}} d_j$$

and the Wiener algebra

$$\mathcal{W}(\mathbb{Z}) := \{A \in \mathcal{L}(\ell^p(\mathbb{Z})) : \|A\|_{\mathcal{W}} < \infty\}.$$

One can show that $\mathcal{W}(\mathbb{Z})$ equipped with the norm $\|\cdot\|_{\mathcal{W}}$ is a Banach algebra and is independent of p and we have

$$\mathrm{BO}(\mathbb{Z}) \subset \mathcal{W}(\mathbb{Z}) \subset \mathrm{BDO}_p(\mathbb{Z}), \qquad \forall p \in [1, \infty].$$

For further details see [62, Section 1.3.6]. Due to Wiener's theorem [85, Theorem 2.5.2], $\mathcal{W}(\mathbb{Z})$ is inverse closed. Therefore, the spectrum of $A \in \mathcal{W}(\mathbb{Z})$ is independent of p, which is a generalization of Proposition 2.20. The same can be said about the essential spectrum, see [63].

An interesting consequence of (2.12) is that the lower norm of an operator coincides with the lower norm of the adjoint.

Corollary 2.48. *Let $A \in \mathrm{BDO}_2(\mathbb{Z})$ be K-periodic. Then $\nu(A) = \nu(A^*)$.*

Proof. This is a direct consequence of Lemma 2.40. Nevertheless, we present an explicit proof in order to showcase the methods involved. Using that A^* is also a K-periodic operator we denote its symbol by b with coefficients b_k. Due to (2.12) it suffices to show that $\nu(a(\varphi)) = \nu(b(\varphi))$ for all $\varphi \in [0, 2\pi)$. The block Laurent structure of A^* is given by

$$A^* = \begin{pmatrix} \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \ddots & a_0^* & a_1^* & a_2^* & a_3^* & \ddots \\ \ddots & a_{-1}^* & a_0^* & a_1^* & a_2^* & \ddots \\ \ddots & a_{-2}^* & a_{-1}^* & a_0^* & a_1^* & \ddots \\ \ddots & a_{-3}^* & a_{-2}^* & a_{-1}^* & a_0^* & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix} = \begin{pmatrix} \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \ddots & b_0 & b_{-1} & b_{-2} & b_{-3} & \ddots \\ \ddots & b_1 & b_0 & b_{-1} & b_{-2} & \ddots \\ \ddots & b_2 & b_1 & b_0 & b_{-1} & \ddots \\ \ddots & b_3 & b_2 & b_1 & b_0 & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}.$$

Thus $b_k = a_{-k}^*$. For the symbols that means

$$b(\varphi) = \sum_{k=-\infty}^{\infty} b_k e^{ik\varphi} = \sum_{k=-\infty}^{\infty} a_{-k}^* e^{ik\varphi} = \sum_{k=-\infty}^{\infty} a_k^* e^{-ik\varphi} = \sum_{k=-\infty}^{\infty} (a_k e^{ik\varphi})^* = a(\varphi)^*.$$

Since $a(\varphi)$ and $a(\varphi)^*$ are finite-dimensional matrices their lower norms coincide with their respective smallest singular values. The identity of the singular values of $a(\varphi)$ and $a(\varphi)^*$ therefore implies $\nu(a(\varphi)) = \nu(a(\varphi)^*) = \nu(b(\varphi))$.

□

For periodic operators in the Wiener algebra and their one-sided compressions we can again express the spectrum with the help of the symbol.

Theorem 2.49. *([13, Theorem 2.93 b), Theorem 2.94 b)]) Let $A \in \mathcal{W}(\mathbb{Z})$ be K-periodic and a denote its symbol. Then*

$$\sigma(A) = \bigcup_{\varphi \in [0,2\pi)} \sigma(a(\varphi)) = \{\lambda \in \mathbb{C} : \det(a(\varphi) - \lambda I) = 0 \textit{ for some } \varphi \in [0, 2\pi)\}.$$

For the one-sided periodic operator $A^+ = P_{\mathbb{N}} A P_{\mathbb{N}} \in \mathcal{W}(\mathbb{N})$ we have that $\sigma_{\mathrm{ess}}(A^+) = \sigma(A)$ and $\mathrm{ind}((A - \lambda I)^+) = -\operatorname{wind}(\det(a), \lambda)$ for all $\lambda \notin \sigma_{\mathrm{ess}}(A^+)$.

Note that the analogue of (2.11) does not hold. Obviously, $\sigma(A^+) \supset \sigma(A) \cup \{\lambda \in \mathbb{C} : \mathrm{wind}(\det(a), \lambda) \neq 0\}$ but for periodic operators it can happen that $\mathrm{ind}(A_+ - \lambda) = 0$ but $\lambda \in \sigma(A_+) \setminus \sigma(A)$. We will study such cases extensively in Section 4.2, see e.g. Example 4.31. For Toeplitz operators, however, Coburn's lemma [21], guarantees that this is not the case.

For the tridiagonal case the set $\sigma(A^+)$ was analyzed by Hagger [47]. With the help of a variant of Coburn's lemma (see [47, Theorem 4.38]) he found different formulas for the spectra of one-sided periodic operators, depending on the existence and location of zero entries on the sub- and superdiagonal. We only consider the case where both of them are always non-zero.

Theorem 2.50. *([47, Theorem 4.42(i)]) Let A^+ be a tridiagonal one-sided K-periodic operator. Let $(a_j)_{j\in\mathbb{N}}$ denote the superdiagonal and $(c_j)_{j\in\mathbb{N}}$ denote the subdiagonal. If $a_j \neq 0$ and $c_j \neq 0$ for all $j \in \mathbb{N}$ then*

$$\begin{aligned}\sigma(A^+) = {} & \sigma_{\mathrm{ess}}(A^+) \cup \{\textit{holes of } \sigma_{\mathrm{ess}}(A^+)\} \\ & \cup \left\{ \lambda \in \sigma(A_{1..K-1}) : |\det(A_{1..K} - \lambda I)| < \min\left\{ \prod_{j=1}^{K} |a_j|, \prod_{j=1}^{K} |c_j| \right\} \right\}.\end{aligned}$$

With "holes of $\sigma_{\mathrm{ess}}(A^+)$" we mean the bounded connected components of the complement of $\sigma_{\mathrm{ess}}(A^+)$.

2.6 References

The general spectral and Fredholm theory presented in this chapter are standard results that can be found in most books about operator theory such as [31]. The results on limit operator theory are mostly from [62]. An excellent source for the theory of Laurent and Toeplitz operators, and for the theory of periodic operators as block Laurent and block Toeplitz operators is [13].

Chapter 3

Spectral Approximation via Approximation of Submatrices

In this chapter we consider methods to approximate spectra and lower norms of operators on $\ell^p(\mathbb{I})$. Unless mentioned otherwise we assume that $\mathbb{I} \subset \mathbb{Z}^d$ and $p \in [1, \infty]$. The main focus will be on the one-dimensional case $d = 1$.

3.1 Convergence of spectra and pseudospectra

In many applications one is interested in the spectrum of a band-operator on $\ell^p(\mathbb{Z})$. A prominent example are discrete Schrödinger operators which will be covered in Chapter 4. However, computing the spectrum of a band operator in $\ell^p(\mathbb{Z})$ or $\ell^p(\mathbb{N})$ is in general a hard task. A notable exception to this are periodic band operators for which the spectrum can be computed as described in Section 2.5. Instead of computing the spectra directly we can try to approximate spectra. The approach is the following: for a band operator A we find a sequence $(A_n)_{n\in\mathbb{N}}$ of operators, for which we can compute each $\sigma(A_n)$ and

$$\sigma(A_n) \to \sigma(A) \tag{3.1}$$

holds in Hausdorff metric. Typical choices for A_n are either finite matrices or periodic operators.

For non-normal operators the convergence of spectra is usually too much to ask for since not even convergence in operator norm implies (3.1), as the following example shows.

Example 3.1. *([52, Example 3.8]) For $\delta \geq 0$ define $T_\delta : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ by*

$$(T_\delta x)_j = \begin{cases} x_{j-1} & \text{if } j \neq 0 \\ \delta x_{j-1} & \text{if } j = 0 \end{cases}$$

For $\lambda \in \mathbb{C}$ with $|\lambda| < 1$ it can be seen that the sequence $(x_j)_{j\in\mathbb{Z}} \in \ell^2(\mathbb{Z})$ with $x_j = \lambda^{-j}\chi_{-\mathbb{N}}(j)$ is an eigenvector of T_0 for the eigenvalue λ. Indeed, for $j < 0$

$$((T_0 - \lambda I)x)_j = x_{j-1} - \lambda x_j = 0,$$

and for $j \geq 0$ both $(T_0 x)_j$ and λx_j are 0. Since the spectrum of T_0 is closed we can infer that the closed unit disk $\mathbb{D}$ lies in $\sigma(T_0)$. Together with $r(A) = 1$ and Proposition 2.3 we find that $\sigma(T_0) = \mathbb{D}$.

For $\delta > 0$, however, it follows that T_δ is invertible with the inverse

$$(T_\delta^{-1}x)_j = \begin{cases} x_{j+1} & \textit{if } j \neq -1 \\ \frac{1}{\delta}x_{j+1} & \textit{if } j = -1 \end{cases}.$$

The matrix representations of T_δ and T_δ^{-1} are

$$T_\delta = \begin{pmatrix} \ddots & \ddots & & & & \\ \ddots & 0 & 0 & & & \\ & 1 & 0 & 0 & & \\ & & \delta & 0 & 0 & \\ & & & 1 & 0 & \ddots \\ & & & & \ddots & \ddots \end{pmatrix}, \quad T_\delta^{-1} = \begin{pmatrix} \ddots & \ddots & & & & \\ \ddots & 0 & 1 & & & \\ & 0 & 0 & \frac{1}{\delta} & & \\ & & 0 & 0 & 1 & \\ & & & 0 & 0 & \ddots \\ & & & & \ddots & \ddots \end{pmatrix}.$$

Both T_δ and T_δ^{-1} have spectral radius 1. Together with $\sigma(A^{-1}) = \{\lambda^{-1} : \lambda \in \sigma(A)\}$, see e.g. [52, Theorem III 6.15], it follows that $\sigma(A) \subset \mathbb{T}$. In fact, for $\lambda \in \mathbb{T}$ it is not hard to see that $\nu(T_\delta - \lambda I) = 0$ and therefore, $\sigma(T_\delta) = \mathbb{T}$. In particular, we find that $T_\delta \rightrightarrows T_0$ as $\delta \to 0$ but $\mathbb{T} = \sigma(T_\delta) \not\to \sigma(T_0) = \mathbb{D}$.

For non-normal operators it is more fruitful to look for conditions such that

$$\sigma_\varepsilon(A_n) \to \sigma_\varepsilon(A) \tag{3.2}$$

for all $\varepsilon > 0$. It can be shown that on $\ell^p(\mathbb{I})$ (3.2) is equivalent to the convergence of the lower norms [68]:

$$\nu(A_n - \lambda I) \to \nu(A - \lambda I) \tag{3.3}$$

for all $\lambda \in \mathbb{C}$.

We will mainly focus on (3.3) which for normal operators also implies (3.1). Note that due to Lemma 2.11 uniform converge is sufficient for the convergence of the lower norms. In particular, (3.2) and (3.3) hold for the operators in Example 3.1.

Usually, convergence in operator norm is a harsh restriction. For instance, if we want to use approximations of finite rank, we can only reach compact operators since $K(\ell^p(\mathbb{Z}))$ is norm-closed. Operators that are uniform limits of periodic operators are called limit-periodic, see [24]. In this work, we will consider operators that are neither compact nor limit-periodic. Thus, from now on our goal is to obtain weaker conditions for the convergence of the lower norm.

3.2 The local lower norm

Throughout this section let $\mathbb{I} \in \{\mathbb{Z}, \mathbb{N}, \mathbb{Z}_+, \mathbb{Z}_-\}$. We define the diameter of a set $S \subset \mathbb{Z}$ as $\operatorname{diam}(S) = \sup_{s,t \in S} |s - t|$. Let us now introduce a localized version of the lower norm.

Definition 3.2. For $A \in \mathrm{BO}(\ell^p(\mathbb{I}))$ and $N \in \mathbb{N}$ we call

$$\nu_N(A) := \inf \big\{ \|Ax\| : x \in \ell^p(\mathbb{I}), \|x\| = 1, \operatorname{diam}(\operatorname{supp}(x)) < N \big\} \tag{3.4}$$

the local lower norm of A.

We find for all $A \in \mathrm{BO}(\ell^p(\mathbb{I}))$ that $\nu_N(A)$ is monotonically decreasing and

$$\nu_N(A) \to \nu(A) \quad \text{as} \quad N \to \infty. \tag{3.5}$$

Together with (2.2) we get, as $N \to \infty$,

$$\min\left\{\nu_N(A), \nu_N(A^*)\right\} \searrow \min\left\{\nu(A), \nu(A^*)\right\} \;=\; 1 / \|A^{-1}\|. \tag{3.6}$$

For the approximation of spectral quantities, it is important to know that (3.5) holds in a very uniform sense, as follows:

Lemma 3.3 ([71, Prop. 6]). *Let $\varepsilon > 0$, $r > 0$ and $w \in \mathbb{N}$. Then there is an $N \in \mathbb{N}$ such that, for all band operators A on $\ell^p(\mathbb{I})$ with bandwidth less than w and $\|A\| < r$,*

$$\nu(A) \le \nu_N(A) \le \nu(A) + \varepsilon\,.$$

One can explicitly quantify the relation of N and ε:

$$N > 4w\left(\frac{2r}{\varepsilon}\right)^p$$

for $p \in (1, \infty)$ and

$$N > \frac{2wr}{\varepsilon}$$

for $p = 1$ and $p = \infty$. An analogous localization of the operator norm can be found in [48, Prop. 3.4].

For an even finer localization of the lower norm, put,

$$\nu_{\mathbb{J}}(A) \;:=\; \inf\{\|Ax\| : \mathrm{supp}(x) \subseteq \mathbb{J}, \|x\| = 1\}. \tag{3.7}$$

Corollary 3.4. *For every $A \in \mathrm{BO}(\mathbb{I})$ and all $\varepsilon > 0$, there are $l, r \in \mathbb{Z}$ such that $\nu_{l..r}(A) \le \nu(A) + \varepsilon$.*

Proof. With the help of Lemma 3.3 choose N large enough that

$$\nu(A) + \varepsilon \ge \nu_N(A) + \frac{\varepsilon}{2} \le \inf_j \nu_{j..j+N-1}(A) + \frac{\varepsilon}{2}$$

and then j such that $\nu_{j..j+N-1}(A)$ is in the $\frac{\varepsilon}{2}$ neighborhood of the infimum. Then $l := j$ and $r := j + N - 1$ satisfy the statement. □

Definition 3.5. Let A be a band matrix with bandwidth w. For $N \in \mathbb{N}$, we say that C is an N-column submatrix of A if C consists of N consecutive columns of A. For simplicity and comparability, restrict C to size $(N + 2w) \times N$, capturing the banded part of $AP_{k+1..k+N}$, that is $C = P_{k+1-w..k+N+w}AP_{k+1..k+N}$. Further, let $\mathcal{C}_N(A)$ denote the set of all N-column submatrices of A and set $\mathcal{C}(A) := \cup_{N\in\mathbb{N}} \mathcal{C}_N(A)$.

We call a band operator A self-contained if every $C \in \mathcal{C}(A)$ appears infinitely often in A.

Corollary 3.6. *For $A \in \mathrm{BO}(\mathbb{Z})$, the statements*

(i) A is self-contained,

(ii) A is self-similar and

(iii) A is invertible if and only if it is Fredholm

are related as follows: (i) $\Rightarrow$ (ii) $\Rightarrow$ (iii).
If the set of all entries of A as a matrix is finite then (i) $\Leftrightarrow$ (ii).

Proof. This is immediate from Lemmas 4.3 and 2.2 in [66]. ☐

Examples of self-contained operators are operators with periodic and aperiodic matrix diagonals, see Sections 4.2 and 4.3. For self-contained operators, many of our formulas and arguments simplify due to Lemma 2.40. We can discard $\nu(A^*)$ and $\nu_N(A^*)$ from (3.6), i.e.

$$\nu_N(A) \searrow \nu(A) = \frac{1}{\|A^{-1}\|} \quad \text{as } N \to \infty.$$

3.3 Column submatrices, spectra and approximation

Because the column submatrices $C \in \mathcal{C}_N(A)$ determine the effect of A on vectors x with $\operatorname{diam}(\operatorname{supp}(x)) < N$, the set $\mathcal{C}_N(A)$ has obvious connections to $\nu_N(A)$:

Lemma 3.7. *([41, Lemma 4.1]) Let $A \in \mathrm{BO}(\mathbb{I})$ with a discrete interval $\mathbb{I} \subseteq \mathbb{Z}$. Then, for every $N \in \mathbb{N}$,*

$$\nu_N(A) \;=\; \inf\{\nu_{j..j+N-1}(A) : j..j+N-1 \subseteq \mathbb{I}\} \;=\; \inf\{\nu(C) : C \in \mathcal{C}_N(A)\}.$$

Proof. Rewriting the definition (3.4) in terms of (3.7), gives the first equality. The second equality is by the definition of N-column submatrices and $\mathcal{C}_N(A)$. ☐

With the error estimates from Lemma 3.3 one can get bounds for the pseudospectra from the sets $\mathcal{C}_N(A)$ [16, 70].

The connection between $\mathcal{C}_N(A)$ and $\nu_N(A)$ can also be lifted to a connection between $\mathcal{C}(A)$ and $\nu(A)$, which again is closely connected to the resolvent norm and the spectrum of A.

Proposition 3.8. *([41, Proposition 4.2]) Let $\mathbb{I}_A, \mathbb{J}_A, \mathbb{I}_B, \mathbb{J}_B \subseteq \mathbb{Z}$ be finite or infinite discrete intervals and let $A : \ell^p(\mathbb{J}_A) \to \ell^p(\mathbb{I}_A)$ and $B : \ell^p(\mathbb{J}_B) \to \ell^p(\mathbb{I}_B)$ be band operators, associated with matrices $(A_{ij})_{i\in\mathbb{I}_A, j\in\mathbb{J}_A}$ and $(B_{ij})_{i\in\mathbb{I}_B, j\in\mathbb{J}_B}$ with the same bandwidth w.*

- *(a) If, for some $N \in \mathbb{N}$, $\mathcal{C}_N(A) \subseteq \mathcal{C}_N(B)$ then $\nu_N(A) \geq \nu_N(B)$.*
- *(b) If $\mathcal{C}(A) \subseteq \mathcal{C}(B)$ then $\nu(A) \geq \nu(B)$.*
- *(c) If $p < \infty$, $N \in \mathbb{N}$ and $\mathcal{C}_{N+2w}(A) \subseteq \mathcal{C}_{N+2w}(B)$ then also $\mathcal{C}_N(A^*) \subseteq \mathcal{C}_N(B^*)$.*
- *(d) If $\mathcal{C}(A) \subseteq \mathcal{C}(B)$ then also $\mathcal{C}(A^*) \subseteq \mathcal{C}(B^*)$.*

Now suppose $\mathbb{I}_A = \mathbb{J}_A$ and $\mathbb{I}_B = \mathbb{J}_B$, so that A and B are endomorphisms of $\ell^p(\mathbb{I}_A)$ and $\ell^p(\mathbb{I}_B)$, respectively.

- *(e) If $\mathcal{C}(A) \subseteq \mathcal{C}(B)$ then*

$$\nu(A-\lambda) \;\geq\; \nu(B-\lambda), \quad \forall \lambda \in \mathbb{C} \tag{3.8}$$

and

$$\|(A-\lambda)^{-1}\| \;\leq\; \|(B-\lambda)^{-1}\|, \quad \forall \lambda \in \mathbb{C},$$

whence

$$\sigma(A) \subseteq \sigma(B) \qquad \textit{and} \qquad \sigma_\varepsilon(A) \subseteq \sigma_\varepsilon(B), \quad \varepsilon > 0.$$

Proof. (a) This is immediate from Lemma 3.7.

(b) If $\mathcal{C}(A) \subseteq \mathcal{C}(B)$, i.e. $\mathcal{C}_N(A) \subseteq \mathcal{C}_N(B)$ holds for all $N \in \mathbb{N}$, then, by (a) and (3.5), it follows that $\nu(A) \geq \nu(B)$.

(c) Let $\mathcal{C}_{N+2w}(A) \subseteq \mathcal{C}_{N+2w}(B)$ and take $C \in \mathcal{C}_N(A^*)$. Then C has N columns and $N + 2w$ rows. So C^* is contained in $N + 2w$ consecutive columns of A and, hence, in a matrix $D \in \mathcal{C}_{N+2w}(A) \subseteq \mathcal{C}_{N+2w}(B)$. Using the same arguments backwards, $C \in \mathcal{C}_N(B^*)$.

(d) If $\mathcal{C}(A) \subseteq \mathcal{C}(B)$ then $\mathcal{C}_{N+2w}(A) \subseteq \mathcal{C}_{N+2w}(B)$, and, by (c), $\mathcal{C}_N(A^*) \subseteq \mathcal{C}_N(B^*)$ for all $N \in \mathbb{N}$, so that $\mathcal{C}(A^*) \subseteq \mathcal{C}(B^*)$.

(e) From $\mathcal{C}(A) \subseteq \mathcal{C}(B)$ it follows that $\mathcal{C}(A - \lambda) \subseteq \mathcal{C}(B - \lambda)$ for all $\lambda \in \mathbb{C}$, so that (3.8) follows in analogy. By (d), we also have $\mathcal{C}((A - \lambda)^*) \subseteq \mathcal{C}((B - \lambda)^*)$ for all $\lambda \in \mathbb{C}$, so that (3.8) also holds for the adjoints, i.e.,

$$\nu(A - \lambda) \; \geq \; \nu(B - \lambda) \quad \text{and} \quad \nu((A - \lambda)^*) \; \geq \; \nu((B - \lambda)^*)$$

for all $\lambda \in \mathbb{C}$. Now the inequality of the resolvent norms follows from (2.2). The inclusion of spectra and pseudospectra is now immediate, by their definition. □

The next result shows how the lower norm and the pseudospectrum of an operator can be approximated via its column submatrices.

Theorem 3.9. *([41, Theorem 4.3]) Let $A \in \mathrm{BO}^w(\mathbb{Z})$ and $(A_n)_{n\in\mathbb{N}} \subset \mathrm{BO}^w(\mathbb{Z})$ with a uniform upper bound on their norms. If*

$$\forall N \in \mathbb{N}\; \exists m_0 \in \mathbb{N} : \; \forall m \geq m_0 : \quad \mathcal{C}_N(A_m) \; = \; \mathcal{C}_N(A) \tag{3.9}$$

then $\nu(A_m) \to \nu(A)$ and, in fact,

$$\nu(A_m - \lambda) \; \to \; \nu(A - \lambda), \qquad \lambda \in \mathbb{C}.$$

If, additionally, $p = 2$ and $A, A_1, A_2, \ldots$ are normal then

$$\sigma(A_m) \to \sigma(A).$$

Proof. Let $\varepsilon > 0$ and take $N \in \mathbb{N}$ so that Lemma 3.3 applies, with $\frac{\varepsilon}{2}$ in place of ε, to A and all A_m with $m \in \mathbb{N}$. This is possible since we have a uniform upper bound on their norms and on their bandwidths.

Now, in accordance with N, take m large enough that (3.9) holds. Then, by Lemma 3.3, Proposition 3.8 (a) and again Lemma 3.3, in this order,

$$\nu(A_m) \overset{\varepsilon/2}{\approx} \nu_N(A_m) = \nu_N(A) \overset{\varepsilon/2}{\approx} \nu(A), \quad \text{so that} \quad \nu(A_m) \overset{\varepsilon}{\approx} \nu(A).$$

Since ε was arbitrary, it follows that $\nu(A_m) \to \nu(A)$ as $m \to \infty$. Repeating the same argument for $A_m - \lambda$ and $A - \lambda$ in place of A_m and A proves the claim. The spectral convergence for self-adjoint operators then follows from the identity $\nu(A - \lambda) = \mathrm{dist}(\lambda, \sigma(A))$. □

Remark 3.10. It is noteworthy that Theorem 3.9 requires neither $A_n \rightrightarrows A$ nor $A_n \to A$, but we still obtain the convergence of lower norms. One can think of condition (3.9) as "convergence of column submatrices", which can be formalized with the following pseudometric:

$$d_{\mathrm{col}}(A,B) := \min\left\{ \inf\left\{ \frac{1}{r} : r \in [1,\infty), d(\mathcal{C}_{\lfloor r \rfloor}(A), \mathcal{C}_{\lfloor r \rfloor}(B)) \leq \frac{1}{r} \right\}, 1 \right\},$$

where d denotes the Hausdorff-distance for subsets of $\mathbb{C}^{(N+2w)\times N}$. Note that for any band operator A we have that $d_{\mathrm{col}}(A, S_{-1}AS) = 0$ and therefore d_{col} is not a metric. However, symmetry and the triangle inequality follow from the properties of the Hausdorff metric. By Theorem 3.9, the map $A \mapsto \nu(A)$ is continuous with respect to the pseudometric d_{col} on BO^w. This extends the results of Beckus [7] for self-adjoint Schrödinger operators on $\ell^2(\mathbb{Z})$ to uniformly banded operators on $\ell^p(\mathbb{Z})$.

Clearly, $A_n \rightrightarrows A$ implies that $d_{\mathrm{col}}(A_n, A) \to 0$ but the converse does not hold true. Neither of $A_n \to A$ and $d_{\mathrm{col}}(A_n, A) \to 0$ implies the other: Consider the multiplication operator $A_n = M_{\chi_{-n..n}}$. Then $A_n \to I$ for $p < \infty$, but each A_n contains a zero column, and therefore $d_{\mathrm{col}}(A_n, A) = 1$. Conversely, for periodic but not Laurent operator B the sequence $(S_{-n}BS_n)_{n\in\mathbb{N}}$ does not converge while $d_{\mathrm{col}}(A_n, A_m) = 0$ for all $m, n \in \mathbb{N}$.

Note that (3.9) implies convergence of column submatrices, but if the set of all matrix entries is finite then it is even equivalent to it. Since we will mostly work with such operators we will use (3.9) instead of d_{col}.

For sequences of operators that are not subject to condition (3.9), that is the eventual equality of all column-submatrices, we cannot expect convergence of the lower norms – and therefore also not convergence of the pseudospectra, let alone the spectra. We aim to obtain bounds on the limes inferior of the lower norm for sequences that do not satisfy 3.9.

Recall that for a band operator A with bandwidth w the elements of $\mathcal{C}_N(A)$ are $(2w+N) \times N$ matrices with 2-norm $\|\cdot\|$. Let $N \in \mathbb{N}$ and $(A_m)_{m\in\mathbb{N}} \subset \mathrm{BO}^w$ for some $w \in \mathbb{Z}_+$. According to Definition 2.5, the topological limes superior is given by

$$\limsup_{m\to\infty} \mathcal{C}_N(A_m) := \bigcap_{m_0\in\mathbb{N}} \mathrm{clos}\Bigg(\bigcup_{m\geq m_0} \mathcal{C}_N(A_m) \Bigg)$$

where the closure is taken with respect to the topology induced by the matrix norms from above. The topological limes superior of the sequence $(\mathcal{C}_N(A_m))_{m\in\mathbb{N}}$ is the set of all accumulation points of sequences $(M_m)_{m\in\mathbb{N}}$ with $M_m \in \mathcal{C}_N(A_m)$.

Theorem 3.11. *Let $w \in \mathbb{Z}_+$ and $(A_n)_{n\in\mathbb{N}} \subset \mathrm{BO}^w(\mathbb{Z})$ and $\Phi \subset \mathrm{BO}^w(\mathbb{Z})$ such that all operators in (A_n) and Φ have a uniform upper bound on their norms. If*

$$\limsup_{m\to\infty} (\mathcal{C}_N(A_m)) = \bigcup_{B\in\Phi} \mathcal{C}_N(B) \tag{3.10}$$

holds for all $N \in \mathbb{N}$ then

$$\liminf_{m\to\infty} \nu(A_m) = \inf_{B\in\Phi} \nu(B). \tag{3.11}$$

In case all operators in Φ are invertible then there is an $m_0 \in \mathbb{N}$ such that (A_m) is invertible for all $m > m_0$ and

$$\limsup_{m\geq m_0} \|A_m^{-1}\| = \sup_{B\in\Phi} \|B^{-1}\|. \tag{3.12}$$

Proof. Let us first prove for fixed $N \in \mathbb{N}$ that

$$\liminf_{j\to\infty}\left(\inf\left\{\nu(M) : M \in \mathcal{C}_N(A_j)\right\}\right) = \min\left\{\nu(\widetilde{M}) : \widetilde{M} \in \limsup_{m\in\mathbb{N}} \mathcal{C}_N(A_m)\right\}. \tag{3.13}$$

Note that we can write the minimum on the right-hand side since $\limsup_{m\in\mathbb{N}} \mathcal{C}_N(A_m)$ is a bounded and closed subset of $\mathbb{C}^{(2w+N\times N)}$, therefore it is compact and the continuous function ν attains its minimum. In order to prove (3.13), let $\varepsilon > 0$ and take $\widetilde{M} \in \limsup\limits_{m\to\infty} \mathcal{C}_N(A_m)$. Then, for each $j_0 \in \mathbb{N}$ there exists a $j \geq j_0$ and $M \in \mathcal{C}_N(A_j)$ such that $\|\widetilde{M} - M\| < \varepsilon$. Due to the Lipschitz continuity of ν we get that $\nu(\widetilde{M}) \overset{\varepsilon}{\approx} \nu(M)$ and therefore the inequality "$\leq$" holds in (3.13).

For the other direction, consider a sequence $(M_j)_{j\in\mathbb{N}}$ with $M_j \in \mathcal{C}_N(A_j)$ such that the left-hand side of (3.13) equals $\liminf\limits_{j\to\infty} \nu(M_j)$. We pass to a subsequence, again denoted by (M_j), such that $\lim\limits_{j\to\infty} \nu(M_j)$ exists and also equals the left-hand side of (3.13). With a compactness argument we find that (M_j) has at least one accumulation point $\widetilde{M} \in \mathbb{C}^{(2w+N)\times N}$. Then $\widetilde{M} \in \limsup\limits_{m\to\infty} \mathcal{C}_N(A_m)$ and we can use the continuity of the lower norm again to obtain the inequality "$\leq$" in (3.13).

We continue with the proof of (3.11). Recall that we can express the lower norm as the limit of the local lower norms: $\nu(A_m) = \lim_{N\to\infty} \nu_N(A_m)$. With the help of Lemma 3.7 we can express the local lower norm with the column-submatrices and obtain

$$\liminf_{m\to\infty} \nu(A_m) = \liminf_{m\to\infty} \lim_{N\to\infty} \inf\{\nu(M) : M \in \mathcal{C}_N(A_m)\}.$$

Since a uniform bound on the operator norms and bandwidths exists we can apply Lemma 3.3 and find that $\inf\{\nu(M) : M \in \mathcal{C}_N(A_m)\}$ converges uniformly as $N \to \infty$. This allows us to swap the limits in N and m, since the Moore-Osgood theorem [101, p. 139-140] applies. We thus have

$$\liminf_{m\to\infty} \nu(A_m) = \lim_{N\to\infty} \liminf_{m\to\infty} \inf\{\nu(M) : M \in \mathcal{C}_N(A_m)\}.$$

Now we can apply (3.13) and then use condition (3.10) from the theorem:

$$\begin{aligned}
\liminf_{m\to\infty} \nu(A_m) &= \lim_{N\to\infty} \liminf_{m\to\infty} \inf\{\nu(M) : M \in \mathcal{C}_N(A_m)\} \\
&= \lim_{N\to\infty} \min\left\{\nu(\widetilde{M}) : \widetilde{M} \in \limsup_{m\in\mathbb{N}} \mathcal{C}_N(A_m)\right\} \\
&= \lim_{N\to\infty} \min\left\{\nu(\widetilde{M}) : \widetilde{M} \in \bigcup_{B\in\Phi} \mathcal{C}_N(B)\right\}.
\end{aligned}$$

Using Lemma 3.7 again we get

$$\liminf_{m\to\infty} \nu(A_m) = \lim_{N\to\infty} \min_{B\in\Phi} \nu_N(B).$$

Recall that $\nu_N(D)$ decreases monotonically and therefore the limit on the right-hand side can be replaced with an infimum. In particular, it commutes with the infimum over Φ. Finally, we obtain

$$\liminf_{m\to\infty} \nu(A_m) = \inf_{B\in\Phi}\left\{\lim_{N\to\infty} \nu_N(B)\right\} = \inf_{B\in\Phi}\left\{\nu(B)\right\}.$$

It remains to show that the invertibility of all operators in Φ implies the stability of (A_n). For $p < \infty$ we observe that $M \in \limsup_{m\to\infty}(\mathcal{C}_N(A_m^*))$ implies that there is an $\widetilde{M} \in \limsup_{m\to\infty}(\mathcal{C}_{N+2w}(A_m))$ such that M is the restriction of $\widetilde{M}^*$ to the columns $2w+1..N+w$. Due to condition 3.10 we also have that $\widetilde{M} \in \mathcal{C}_{N+2w}(B)$ for some $B \in \Phi$ and therefore $M \in \bigcup_{B\in\Phi} \mathcal{C}_N(B^*)$.

In other words, condition 3.10 implies that it automatically holds for the adjoints of all operators involved. Therefore, we obtain (3.11) also for the adjoint operators. The rest follows from Lemma 2.10. The invertibility of A_n for n large enough carries over to the case $p = \infty$ due to Lemma 2.20. Since for invertible operators $\nu(A) = \nu(A^*)$ we also get (3.12) for $p = \infty$. ☐

The reader might wonder whether the infimum in (3.11) is attained as a minimum. This is not true in general, but the following Proposition gives a sufficient condition.

Proposition 3.12. *Let $\Phi \subset \mathrm{BDO}_p(\mathbb{Z})$ with the following properties:*

(a) All operators in Φ have a uniform upper bound on their norms.

(b) For each $\varepsilon < 0$ there is a $w \in \mathbb{N}$ such that for every $B \in \Phi$ there is a $B^{(w)} \in \mathrm{BO}^w$ with $\|B - B^{(w)}\| < \varepsilon$.

(c) The set $\Psi = \{S_k B S_{-k} : B \in \Phi, k \in \mathbb{Z}\}$ is sequentially compact with respect to $\mathcal{P}$-convergence.

Then there is a $B' \in \Phi$ such that $\nu(B') = \inf_{B\in\Phi} \nu(B)$.

Proof. We follow the ideas of Lindner and Seidel [71, Theorem 8], who proved a similar statement for the set of limit operators of a band-dominated operator, answering the long-standing question whether the elementwise invertibility of limit operators in sufficient for the Fredholmness of a band-dominated operator.

For $\mathbb{I} \subset \mathbb{Z}$ and $A \in \mathrm{BDO}_p(\mathbb{Z})$ we write $A|_{\mathbb{I}} := AP_{\mathbb{I}}$ and understand $A|_{\mathbb{I}}$ as an operator from $\ell^p(\mathbb{I})$ to $\ell^p(\mathbb{Z})$.

We set $\varepsilon_k := 2^{-k}$. First, we show that we can find numbers $D_k \in \mathbb{N}$ with $D_{k+1} > 2D_k$ such that

$$\nu_{D_k}(B) \le \nu(B) + \varepsilon_k \le \nu(B|_{\mathbb{I}}) + \varepsilon_k \tag{3.14}$$

holds for all $B \in \Psi$ and $k \in \mathbb{N}$. To do so, we use condition (b) and choose $w \in \mathbb{N}$ such that we can approximate every $B \in \Phi$ with operators $B^{(w)}$ of bandwidth w up to a distance of $\varepsilon_k/3$. Note that, due to (a), also all $B^{(w)}$ are uniformly bounded. With Lemma 3.3 we can choose D_k such that $\nu_{D_k}(B^{(w)}) \le \nu(B^{(w)}) + \varepsilon_k/3$. Thus, with the Lipschitz continuity of the lower norm we get

$$\nu_{D_k}(B) \le \nu_{D_k}\left(B^{(w)}\right) + \frac{\varepsilon}{3} \le \nu\left(B^{(w)}\right) + \frac{2\varepsilon_k}{3} \le \nu(B) + \varepsilon_k,$$

which proves (3.14) since $\nu(B) \le \nu(B|_{\mathbb{I}})$ is straightforward.

Now choose a sequence $(B_n)_{n\in\mathbb{N}} \subset \Phi$ such that $\lim_{n\to\infty} \nu(B_n) = \inf_{B\in\Phi}(\nu(B))$. Our strategy is to construct a sequence $(C_n) \subset \Phi$ by shifting the elements of (B_n) such that the column-submatrices that almost attain the lower norm are localized near 1. Then we use the sequential compactness of Ψ in order to obtain an accumulation point C of (C_n) which will attain the minimum.

For each $n \in \mathbb{N}$ we can find a shift $j_n^0 \in \mathbb{Z}$ such that $\nu_{1..D_n}(S_{-j_n^0} B_n S_{j_n^0}) = \nu_{D_n}(B_n)$ and set $C_n^{(0)} := S_{j_n^0} B_n S_{-j_n^0}$. Consequently,

$$\nu_{1..D_n}(C_n^{(0)}) \le \nu(B_n) + \varepsilon_k. \tag{3.15}$$

Now for $k \in 1..n$ we recursively define $C_n^{(k)} := S_{-j_n^k} C_n^{(k-1)} S_{j_n^k}$ for $j_n^k \in 0..D_{n-k+1}$ such that

$$\nu_{1..D_{n-k}}(C^{(k)}) = \nu_{D_{n-k}}(C_n^{(k-1)}|_{1..D_{n-k+1}}).$$

Figuratively, we find the most critical column-submatrix M (meaning the one with the smallest lower norm) of size D_{n-k} that appears in the first D_{n-k+1} columns of the predecessor $C_n^{(k-1)}$. Then we obtain $C_n^{(k)}$ by shifting $C_n^{(k-1)}$ such that M appears exactly in the columns 1 to D_{n-k}.

Now we apply (3.14) to the operators $C_n^{(k)} \in \Psi$:

$$\nu_{1..D_{n-k}}(C_n^{(k)}) \le \nu(C_n^{(k-1)}|_{1..D_{n-k+1}}) + \varepsilon_{n-k} = \nu_{1..D_{n-k+1}}(C_n^{(k-1)}) + \varepsilon_{n-k}. \tag{3.16}$$

Finally, we set $C_n := C_n^{(n)}$. By construction, $C_n = S_{-(j_n^n + \dots + j_n^{n-l+1})} C_n^{(n-l)} S_{(j_n^n + \dots + j_n^{n-l+1})}$ and for the shift distance we get $0 \le j_n^n + \dots + j_n^{n-l+1} \le D_1 + \dots + D_l \le 2D_l$. Therefore,

$$\begin{aligned}
\nu_{-2D_l..D_l}(C_n) \le \nu_{1..D_l}(C_n^{(n-l)}) &\overset{(3.16)}{\le} \nu_{1..D_{l+1}}(C_n^{(n-l-1)}) + \varepsilon_l \\
&\overset{(3.16)}{\le} \dots \overset{(3.16)}{\le} \nu_{1..D_n}(C_n^{(0)}) + \sum_{m=l}^{n-1} \varepsilon_m \\
&\overset{(3.15)}{\le} \nu(B_n) + \sum_{m=l}^{n} \varepsilon_m \\
&\le \nu(B_n) + 2^{-l+1}.
\end{aligned}$$

Since $(C_n) \subset \Psi$ we can, by assumption, pass to a subsequence (C_{h_n}) that $\mathcal{P}$-converges to some $C \in \Psi$. In particular, this means that $\|(C_{h_n} - C)P_{-2D_l..D_l}\| \to 0$ for each $l \in \mathbb{N}$ as $n \to \infty$. Now for any given $\varepsilon > 0$ first choose l sufficiently large such that $2^{-l+1} < \varepsilon/2$ and then n sufficiently large such that $\|(C_{h_n} - C)P_{-2D_l..D_l}\| < \varepsilon/2$. Then

$$\nu(C) \le \nu_{-2D_l..D_l}(C) < \nu_{-2D_l..D_l}(C_n) + \varepsilon/2 \le \nu(B) + 2^{-l+1} + \varepsilon/2 \le \nu(B) + \varepsilon,$$

which means that $\nu(C) = \inf_{B \in \Phi} \nu(B)$. This concludes the proof since $C \in \Psi$ is a finite shift of some operator $B' \in \Phi$ that, of course, has the same lower norm. $\square$

Since the proof of Proposition 3.12 is based on the work of Lindner and Seidel [71] for limit operators it is no surprise that it also applies to the choice $\Phi = \operatorname{Lim}(A)$ for $A \in \mathrm{BDO}_p$. This is due to the fact that $\operatorname{Lim}(A)$ is shift-invariant by Proposition 2.34 and sequentially compact with respect to $\mathcal{P}$-convergence by Proposition 2.37. We therefore recover the one-dimensional case of [71, Theorem 8].

Example: the non-self-adjoint Anderson model

The results of previous section, namely Theorem 3.9 and Theorem 3.11 can be used to derive a method to approximate pseudospectra. We demonstrate this method for a specific model from physics.

The famous Anderson model [1, 2] of 1958 studies localization and delocalization of eigenvectors for a better understanding of electric conductivity in 1D disordered media. In this model, one looks at the self-adjoint Schrödinger operator H on $\ell^2(\mathbb{Z})$ defined by

$$(Hx)_i = x_{i-1} + x_{i+1} + b(i)x_i, \tag{3.17}$$

where $b : \mathbb{Z} \to \mathbb{R}$ is called the potential. In the Anderson model, the potential is almost surely pseudoergodic – a notion introduced by Davies [30] in order to capture spectral properties of random operators while eliminating stochastic details. For a finite set of real numbers Σ, a pseudoergodic potential $b : \mathbb{Z} \to \Sigma$ contains all possible finite subsequences over Σ. More precisely, b is pseudoergodic if for every $m \in \mathbb{N}$ and $w : \{1, \dots, m\} \to \Sigma$ there is a $k \in \mathbb{Z}$ such that $b(k + j) = w(j)$ for $j \in \{1, \dots, m\}$. It is straightforward to prove that any operator H as in (3.17) with $b : \mathbb{Z} \to \Sigma$ pseudoergodic is self-similar but not recurrent and the spectrum is given by $\sigma(H) = \Sigma + [-2, 2]$, see e.g. [67].

In the late 1990s, the Anderson model reemerged in a non-self-adjoint (nsa) setting: The only change is that now

$$(Hx)_i = e^g x_{i-1} + e^{-g} x_{i+1} + b(i)x_i,$$

where $g > 0$ is the strength of an external magnetic field. The now also famous paper of Hatano and Nelson [49] looks at flux lines in type II superconductors under the influence of a tilted external magnetic field. Within short time, the nsa Anderson model reappeared in population dynamics [78] and other areas.

Mathematicians from stochastics [45] and spectral theory [29, 30, 76] studied its spectrum and how it invades the complex plane, and the subject of pseudospectra (see [104] and the references therein) received an additional uplift.

For pseudoergodic potentials we can construct approximants as follows. For $m \in \mathbb{N}$, let b_m be the periodic extension of a concatenation of all elements of Σ^m. Listing those $|\Sigma|^m$ words of length m takes $m|\Sigma|^m$ letters if done naively and $|\Sigma|^m$ in a clever condensed arrangement as a de Bruijn sequence [32]. For example, the word $u = 000001010011100101110111$ and the cyclic word $v = 00010111$ both contain all $w \in \{0, 1\}^3$.

For either arrangement, let H_m be the Schrödinger operator defined by (3.17) with potential b_m. Then Theorem 3.9 applies, so that $\sigma_\varepsilon(H_m) \to \sigma_\varepsilon(H)$, in particular, condition (3.9) holds with $m_0 := N$. Moreover, the operators H_m are periodic by construction, and therefore we can apply Theorem 2.47 to compute their pseudospectra. In Figure 3.1 we plot the pseudospectrum of the approximant described above with the choices $m = 14$, $\Sigma = \{-3, 3\}$ and $e^g = \frac{1}{2}$. Hence, we approximate the spectrum of an operator H given by

$$(Hx)_i = \frac{1}{2} x_{i-1} + 2x_{i+1} + b(i)x_i, \tag{3.18}$$

with $b : \mathbb{Z} \to \{-3, 3\}$ pseudoergodic. Note that also in this case the spectra of all such operators are independent of the specific choice of the pseudoergodic word b, see e.g. [30]. The non-self-adjoint Anderson model is a special case of a tridiagonal operator with pseudoergodic diagonals. Such operators have been studied extensively in [47].

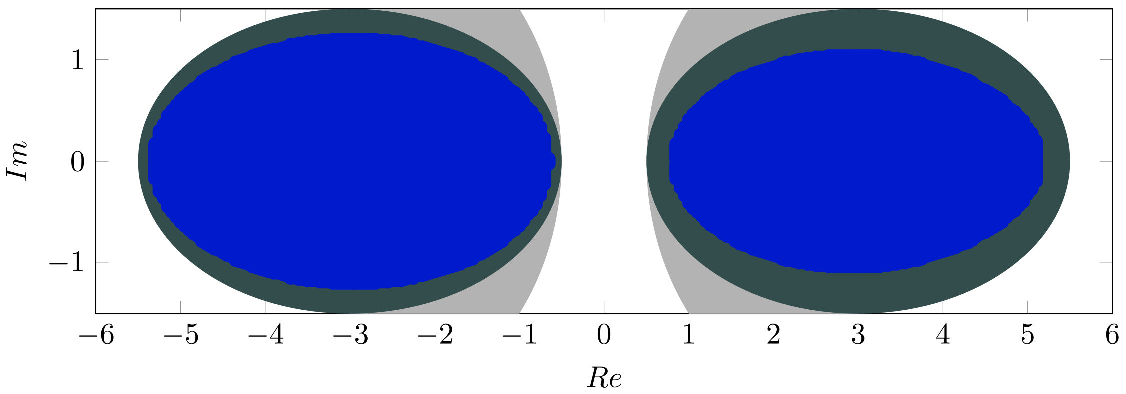

Figure 3.1. ([41, Figure 2]) Here is an approximation of the pseudospectrum of the nsa Anderson model H with parameters chosen as in (3.18). In blue, we see the ε-pseudospectrum of H_{14} [38], with a periodic potential containing all subwords of b of length 14, for $\varepsilon = 10^{-4}$. By Theorem 3.9, $\sigma_\varepsilon(H_m)$ approximates $\sigma_\varepsilon(H)$ in Hausdorff distance as $m \to \infty$. For the spectrum, known bounds, e.g. from Theorem 14 in [30], are displayed: dark gray is guaranteed to be spectrum, bright gray shows how far the spectrum could go at most.

3.4 Compressions of band operators

Let $A \in \mathrm{BO}(\mathbb{Z})$ and let w denote its bandwidth. We want to compare the inverses, resolvent norms and spectra of A and its compressions A^+, given by

$$A^+ := P_{\mathbb{N}} A P_{\mathbb{N}} \ : \ \ell^p(\mathbb{N}) \to \ell^p(\mathbb{N}),$$

where we embed $\operatorname{im} P_{\mathbb{N}}$ into $\ell^p(\mathbb{N})$ canonically. The compression A^- is defined analogously via $P_{\mathbb{Z}_-} A P_{\mathbb{Z}_-}$.

As an intermediate operator between A and A^+, look at its restriction

$$A|_{\mathbb{N}} \ := \ AP_{\mathbb{N}} \ : \ \ell^p(\mathbb{N}) \to \ell^p(\mathbb{Z})$$

to $\ell^p(\mathbb{N})$. The matrix of $A|_{\mathbb{N}}$ is $\mathbb{Z} \times \mathbb{N}$ and consists of the columns of A with index in $\mathbb{N}$; the matrix of A^+ is $\mathbb{N} \times \mathbb{N}$ and consists of the rows of $A|_{\mathbb{N}}$ with index in $\mathbb{N}$:

$$A \ = \ \left(\begin{array}{ccc|ccccc}
\ddots & \ddots & \ddots & & & & & \\
\ddots & + & * & * & & & & \\
\ddots & * & + & * & * & & & \\
\hline
 & * & * & + & * & * & & \\
 & & * & * & + & * & * & \ddots \\
 & & & * & * & + & * & \ddots \\
 & & & & * & * & + & \ddots \\
 & & & & & \ddots & \ddots & \ddots
\end{array}\right)$$

The bandwidth here is $w = 2$,
"$+$" marks the main diagonal,

the right half is $A|_{\mathbb{N}}$,
the lower right quarter is A^+.

Let us start with the assumption that

$$\mathcal{C}(A) \ = \ \mathcal{C}(A|_{\mathbb{N}}), \tag{3.19}$$

so that no other patterns appear on the columns with index $j \in \mathbb{Z}_-$ of A and the only aspect here is what effect the truncation, from A to A^+, has on the resolvent and the spectrum. Before we come to this, let us study some further implications of (3.19).

Lemma 3.13. *([41, Lemma 4.4]) Let* $A \in \mathrm{BO}(\mathbb{Z})$*. If* A *satisfies* (3.19) *then*

- *(a) A is self-contained,*
- *(b) also A^* is subject to* (3.19) *in place of A, and*
- *(c) one also has $\mathcal{C}(A) = \mathcal{C}(A|_{k..})$ for all $k \in \mathbb{Z}$.*

Self-containedness of a band operator B can even be characterized via the restrictions $B|_{\mathbb{N}}$ and $B|_{-\mathbb{N}}$ in the following sense:

- *(d) B is self-contained if and only if $\mathcal{C}(B) = \mathcal{C}(B|_{\mathbb{N}}) \cup \mathcal{C}(B|_{-\mathbb{N}})$.*

Proof. (a) Let $C \in \mathcal{C}(A|_{\mathbb{N}})$ and let $l..r$ be the corresponding column numbers. We show that C can be found in infinitely many positions of A:

By (3.19), the submatrix $D \in \mathcal{C}(A)$ at columns $-r..r$ of A can be found in $A|_{\mathbb{N}}$, and hence at columns $1..2r+1$ or later. In particular, the rightmost $r-l+1$ columns of D, forming C, are found at columns $l+r+1..2r+1$ or later, which is disjoint from the location, $l..r$, (it is further to the right) of the original $C \in \mathcal{C}(A|_{\mathbb{N}})$. Now keep repeating the argument for the newly found copy of C in $A|_{\mathbb{N}}$ to find a further copy of C, even further to the right. Hence, C appears infinitely many times in A, i.e. A is self-contained.

(b) Follows from Proposition 3.8 (c).

(c) Follows from (a).

(d) Since self-containedness of B implies that every $C \in \mathcal{C}(B)$ appears infinitely often, it is clear that C also appears in $B|_{\mathbb{N}}$ or in $B|_{-\mathbb{N}}$. Hence, it remains to show that $\mathcal{C}(B) = \mathcal{C}(B|_{\mathbb{N}}) \cup \mathcal{C}(B|_{-\mathbb{N}})$ implies that B is self-contained. But this can be done via similar arguments as in (a). □

A first quick judgement on the spectrum of A^+ compared to that of A: The step from A to $A|_{\mathbb{N}}$ does not change the lower norm, by the assumption (3.19) and Proposition 3.8 (b). But the step from $A|_{\mathbb{N}}$ to A^+, chopping off some nonzero rows and hence deleting the entries $y_{1-w}, \dots, y_0$ of every $y := A|_{\mathbb{N}}x$, decreases the lower norm and hence increases the inverse, resolvent and spectrum.

The proper analysis is straightforward: For $x \in \ell^p(\mathbb{N})$,

$$\|A^+x\| = \|P_{\mathbb{N}}AP_{\mathbb{N}}\hat{x}\| \le \|AP_{\mathbb{N}}\hat{x}\| = \|A\hat{x}\|,$$

where $\hat{x} \in \ell^p(\mathbb{Z})$ is x, extended by zeros. But $P_{\mathbb{N}}AP_{\mathbb{N}}x = AP_{\mathbb{N}}x$ if $\operatorname{supp}(x) \subseteq w+1..$. So, for all $N \in \mathbb{N}$,

$$\nu_{j..j+N-1}(A^+) \le \nu_{j..j+N-1}(A|_{\mathbb{N}}) = \nu_{j..j+N-1}(A), \quad j \in 1..w, \tag{3.20}$$

$$\nu_{j..j+N-1}(A^+) = \nu_{j..j+N-1}(A|_{\mathbb{N}}) = \nu_{j..j+N-1}(A), \quad j \in w+1.. . \tag{3.21}$$

Columns with index in $1..w$ might have lost some nonzero entries when passing from A via $A|_{\mathbb{N}}$ to A^+; columns in $w+1..$ did not. With this preparation, we prove:

Proposition 3.14. *([41, Proposition 4.5]) Let* $A \in \mathrm{BO}(\mathbb{Z})$ *with bandwidth* w*. Then, for all* $T \in \{A-\lambda, (A-\lambda)^* : \lambda \in \mathbb{C}\}$ *and all* $N \in \mathbb{N}$*,*

$$\nu_N(T^+) \;=\; \min\left\{ \min_{j=1}^{w} \nu_{j..j+N-1}(T^+)\ ,\ \nu_N(T|_{\mathbb{N}}) \right\}, \tag{3.22}$$

where $\nu_{l..r}(T^+)$ *is the smallest singular value of the rectangular submatrix*

$$(T^+_{ij})_{i\in 1..r+w,\, j\in l..r}, \qquad l, r \in \mathbb{N},$$

of T^+*. If, additionally,* (3.19) *holds for* A*, then* $\nu_N(T|_{\mathbb{N}}) = \nu_N(T)$*, so that*

$$\nu_N(T^+) \;=\; \min\left\{ \min_{j=1}^{w} \nu_{j..j+N-1}(T^+)\ ,\ \nu_N(T) \right\}. \tag{3.23}$$

In particular,

$$\nu(T^+) \;\le\; \nu(T) \qquad \textit{and} \qquad \|(T^+)^{-1}\| \;\ge\; \|T^{-1}\|,$$

so that,

$$\sigma(A) \subseteq \sigma(A^+) \qquad \textit{and} \qquad \sigma_\varepsilon(A) \subseteq \sigma_\varepsilon(A^+), \quad \varepsilon > 0.$$

Proof. We fix $N \in \mathbb{N}$, apply (3.20) and (3.21) to $T = A - \lambda$, and conclude (3.22) via Lemma 3.7:

$$\begin{aligned}
\nu_N(T^+) \;&=\; \inf_{j\in\mathbb{N}} \nu_{j..j+N-1}(T^+) \\
&=\; \min\left\{ \min_{j=1}^{w} \nu_{j..j+N-1}(T^+)\ ,\ \inf_{j\ge w+1} \nu_{j..j+N-1}(T^+) \right\} \\
&\overset{(3.21)}{=}\; \min\left\{ \min_{j=1}^{w} \nu_{j..j+N-1}(T^+)\ ,\ \inf_{j\ge w+1} \nu_{j..j+N-1}(T) \right\} \\
&\overset{(3.20)}{=}\; \min\left\{ \min_{j=1}^{w} \left\{ \nu_{j..j+N-1}(T^+),\ \nu_{j..j+N-1}(T) \right\}\ ,\ \inf_{j\ge w+1} \nu_{j..j+N-1}(T) \right\} \\
&=\; \min\left\{ \min_{j=1}^{w} \nu_{j..j+N-1}(T^+)\ ,\ \inf_{j\in\mathbb{N}} \nu_{j..j+N-1}(T) \right\} \\
&=\; \min\left\{ \min_{j=1}^{w} \nu_{j..j+N-1}(T^+)\ ,\ \nu_N(T|_{\mathbb{N}}) \right\}.
\end{aligned}$$

Since also (3.19) transfers from A to all $A - \lambda$, we get $\nu_N(T) = \nu_N(T|_{\mathbb{N}})$. Now (3.23) follows from Proposition 3.8. By Lemma 3.13 and Corollary 3.6 T is self-similar. Thus, the rest follows from Lemma 2.40. □

Remark 3.15. Letting $N \to \infty$ in (3.22) yields $\nu(T^+) = \min\{c, \nu(T|_{\mathbb{N}})\}$, where

$$c \;:=\; \lim_{N\to\infty} \min_{j=1}^{w} \nu_{j..j+N-1}(T^+) \;=\; \min_{j=1}^{w} \nu_{j..}(T^+) \;=\; \nu_{1..}(T^+) \;=\; \nu(T^+)$$

since $\nu_{l..r}(T^+) \to \nu_{l..}(T^+)$ as $r \to \infty$ by monotonicity and Corollary 3.4. This equality shows that the second term in the minimum of (3.22) and (3.23) is asymptotically irrelevant.

3.5 Stability of approximation methods

In addition to the computation of spectra discussed in the previous sections, a common problem in functional analysis is the solution of systems of equations with infinitely many variables, such as

$$Ax = b \tag{3.24}$$

for a given $b \in \ell^p(\mathbb{I})$. Our aim is to use approximation methods to transfer the problem to the finite dimensional setting. This field of mathematics that builds the bridge between functional analysis and linear algebra has, for example, been studied in [46, 64]

3.5.1 Projection methods

We say a sequence (b_n) of elements of $\ell^p(\mathbb{I})$ converge entrywise to some $b \in \ell^p(\mathbb{I})$ if $\|P_{-m..m}(b_n - b)\| \to 0$ as $n \to \infty$ for all $m \in \mathbb{N}$.

We approximate (3.24) by a sequence of equations given by

$$A_n x_n = b_n \quad \text{for} \quad n \in \mathbb{N}. \tag{3.25}$$

If we have that $A_n \xrightarrow{\mathcal{P}} A$ and b_n converges to b entrywise as $n \to \infty$ for all $m \in \mathbb{N}$ then we call (3.25) an approximation method. Technically, this requires that all A_n and b_n are chosen from the same spaces as A and b, that is $\mathcal{L}(\ell^p(\mathbb{I}))$ and $\ell^p(\mathbb{I})$, respectively. However, if $A_n \in \mathcal{L}(\operatorname{im} P_{\mathbb{J}_n})$ for some sequence of finite discrete intervals $\mathbb{J}_n$ we will treat each A_n as finite matrix and each b_n as a finite dimensional vector in order to solve (3.25) numerically. Hence, we will understand (3.25) as finite dimensional equations and for the convergence $A_n \xrightarrow{\mathcal{P}} A$ we use the embedding of A_n into $\mathcal{L}(\ell^p(\mathbb{I}))$ by continuation with zero. The vectors b_n can be seen as elements of $\ell^p(\mathbb{I})$ through continuation by zero. In accordance with Figure 2.2 we can replace $A_n \xrightarrow{\mathcal{P}} A$ with $A_n \to A$ if $p < \infty$ and all operators have a uniform bound on their norm and bandwidth.

A natural way to obtain A_n and b_n from A and b, respectively is by using projections, which leads to the following definition.

Definition 3.16. (Projection method) Let $(\Pi_n^L)_{n\in\mathbb{N}}$ and $(\Pi_n^R)_{n\in\mathbb{N}}$ be sequences of projections on $\ell^p(\mathbb{I})$ and let $A \in \mathcal{L}(\ell^p(\mathbb{I}))$. Then the sequence $(A_n)_{n\in\mathbb{N}}$ defined by $A_n := \Pi_n^L A \Pi_n^R$ is called a projection method for A if $A_n \xrightarrow{\mathcal{P}} A$ and $\Pi_n^L \xrightarrow{\mathcal{P}} I$ as $n \to \infty$.

Clearly, every projection method is an approximation method.

Definition 3.17. An approximation method is called $\mathcal{P}$-applicable if there is an n_0 such that A_n is invertible for all $n \geq n_0$ and their inverses $\mathcal{P}$-converge.

We introduce the concept of stable sequences which is linked directly to the applicability of projection methods by what is known as Polski's Theorem, see Theorem 3.19 below.

Definition 3.18. A sequence (A_n) is called stable if there exists an $n_0 \in \mathbb{N}$ such that A_n is invertible for all $n \geq n_0$ and $\sup_{n\geq n_0} \|A_n^{-1}\| < \infty$.

Usually, the operators A_n are not invertible on $\ell^p(\mathbb{I})$, hence we interpret A_n as an operator $\operatorname{im}\Pi_n^R \to \operatorname{im}\Pi_n^L$. In particular, if $\operatorname{im}\Pi_n^L, \operatorname{im}\Pi_n^R \subset \operatorname{im} P_{\mathbb{J}_n}$ for some sequence of finite discrete intervals $(\mathbb{J}_n)$ then A_n is a finite matrix. In that case, a necessary condition for (A_n) to be stable is that $\dim \operatorname{im} \Pi_n^L = \dim \operatorname{im} \Pi_n^R$. Sometimes projection methods that result in rectangular matrices are also considered, see e.g. [64, Section 6.4]. Then one can still try to solve over-determined systems with least squares. However, throughout this thesis we will only consider projection methods that obey $\dim \operatorname{im} \Pi_n^L = \dim \operatorname{im} \Pi_n^R$. Therefore, we assume this condition for the rest of this section.

Theorem 3.19. *[85, Theorem 6.1.3] Let (P_n) be a sequence of projections that $\mathcal{P}$-converges to the identity. Let $(A_n)_{n\in\mathbb{N}}$ with $A_n \in \mathcal{L}(\operatorname{im} P_n)$ be a projection method for $A \in \mathrm{BDO}_p(\mathbb{I})$ such that $A_n = A_n P_n = P_n A_n$. If additionally*

$$\sup_{n\in\mathbb{N}} \|P_{-m..m} A_n (I - P_{-k..k})\| \to 0 \quad \textit{as} \quad k \to \infty \tag{3.26}$$

holds for all $m \in \mathbb{N}$ then this method is applicable if and only if A is invertible and the sequence (A_n) is stable.

Proof. We first show that the stability of the sequence (A_n) and the invertibility of A implies the applicability of the method. Due to the stability of (A_n) we can choose n_0 such that A_n is invertible for all $n \geq n_0$. Thus, it remains to show that (A_n) $\mathcal{P}$-converges. For $m \in \mathbb{N}$ we compute

$$\begin{aligned}\|(A_n^{-1} - A^1)P_{-m..m}\| &\leq \|(A_n^{-1}P_n - P_n A^{-1})P_{-m..m}\| + \|(P_n - I)A^{-1}P_{-m..m}\| \\ &\leq \|A_n^{-1}P_n\| \|(A - A_n P_n)A^{-1}P_{-m..m}\| + \|(P_n - I)A^{-1}P_{-m..m}\|.\end{aligned}$$

Note that $\mathcal{P}$-convergence is not affected by the multiplication by a bounded operator, see e.g. [62, Proposition 1.70]. Hence, together with the stability we find that both summands go to 0 as $n \to \infty$. Similarly, we compute

$$\|P_{-m..m}(A_n^{-1} - A^1)\| \leq \|P_{-m..m}A^{-1}(A - A_n P_n)\| \|A_n^{-1}P_n\| + \|P_{-m..m}A^{-1}(P_n - I)\|,$$

and find the same limit. Therefore, we have shown that $A_n^{-1} \xrightarrow{\mathcal{P}} A^{-1}$, which implies applicability.

Let us now show the other direction. The applicability implies the invertibility of A_n for all n sufficiently large. Since $\mathcal{P}$-convergent sequences are bounded by definition we directly obtain stability.

For any $m \in \mathbb{N}$ we check that

$$\begin{aligned}\|P_{-m..m}(AA_n^{-1}P_n - I)\| &\leq \|P_{-m..m}(AA_n^{-1}P_n - A_n A_n^{-1}P_n)\| \\ &\leq \|P_{-m..m}(A - A_n)\| \|A_n^{-1}\| \to 0\end{aligned}$$

as $n \to \infty$. Therefore, for any given right-hand side $b \in \ell^p(\mathbb{I})$ we have that the entrywise limit of $A_n^{-1}P_n$ is a solution of $Ax = b$ which proves the injectivity of A.

In order to show the injectivity of A choose n_0 sufficiently large such that A_n is invertible for $n \geq n_0$. Then for $k, m \in \mathbb{N}$, $n \in \mathbb{N}$ sufficiently large and some $C \in \mathbb{R}_+$

$$\begin{aligned}\|P_{-m..m}x\| &= \|P_{-m..m}A_n^{-1}A_n P_n x\| \\ &\leq \|P_{-m..m}A_n^{-1}P_{-k..k}A_n P_n x\| + \|P_{-m..m}A_n^{-1}(I - P_{-k..k})A_n P_n x\| \\ &\leq \|P_{-m..m}A_n^{-1}\| \|P_{-k..k}A_n P_n x\| + \|P_{-m..m}A_n^{-1}(I - P_{-k..k})\| \|A_n P_n x\| \\ &\leq C(\|P_{-k..k}A_n P_n x\| + \|P_{-m..m}A_n^{-1}(I - P_{-k..k})\|)\end{aligned} \tag{3.27}$$

For $k \to \infty$ the second summand will vanish uniformly in n due to (3.26) and therefore $\nu(A) \geq C$. This means A is bounded from below and therefore injective, see Lemma 2.9.

□

The proof of previous theorem shows that applicability means that $A_n^{-1} \xrightarrow{\mathcal{P}} A^{-1}$. Taking a closer look at (3.27) we have shown that the stability of A_n implies the boundedness from below of A. This is not a special feature of projection methods, it holds for any strongly converging sequence, see also Proposition 2.36 in [62]. If, in addition, also $A_n^* \to A^*$ then the stability of (A_n) implies the invertibility of A ([62, Corollary 2.37]). Recall from Proposition 2.28 that for band operators with a uniform bound on the bandwidth this condition is redundant.

Proposition 3.20. *[62, Corollary 2.37] Let* $(A_n)_{n\in\mathbb{N}} \subset \mathrm{BDO}_p(\mathbb{I})$ *and* $A_n \xrightarrow{*} A$ *as* $n \to \infty$ *for some* $A \in \mathrm{BO}(\mathbb{I})$. *Then the following hold:*

(a) $\nu(A) \geq \limsup_{n\to\infty} \nu(A_n)$.

(b) If (A_n) *is stable then* A *is invertible and* $\|A^{-1}\| \leq \liminf_{n\to\infty} \|A_n^{-1}\|$.

Theorem 3.19 and Proposition 3.20 show for projection methods and also for strongly convergent sequences of operators in BO^{w} that the stability of the sequence $\mathcal{A} := (A_n)_{n\in\mathbb{N}}$ does imply the invertibility of the limit, but the converse is in general not true, as we will see in Example 3.23.

The stability of $\mathcal{A}$ can also be put in an algebraic context, see e.g. [14, 85, 90]. Let $\mathcal{F}$ denote the set of all bounded sequences of operators in $\mathcal{L}(\ell^p(\mathbb{I}))$. This set becomes a Banach algebra when provided with elementwise operations and the supremum norm. This Banach algebra is unital since the sequence of identity operators serves as identity. Furthermore, denote by $\mathcal{G}$ the set of all sequences (G_n) for which $\|G_n\| \to 0$ as $n \to \infty$. It is easily seen that $\mathcal{G}$ forms a closed ideal in $\mathcal{F}$ and therefore $\mathcal{F}/\mathcal{G}$ is again a unital Banach algebra. Then for $\mathcal{A} \in \mathcal{F}$ one can show [85, Lemma 6.1.4]

$$\{\lambda \in \mathbb{C} : (A_n - \lambda I)_{n\in\mathbb{N}} \text{ is stable}\} = \sigma(\mathcal{A} + \mathcal{G}). \tag{3.28}$$

In order to apply this to the setting of a projection method (A_n) for $A \in \mathcal{L}(\ell^p(\mathbb{I}))$ we assume that $\operatorname{im} \Pi_n^L = \operatorname{im} \Pi_n^R = \operatorname{im} P_{\mathbb{J}_n}$ for some discrete interval $\mathbb{J}$. Then we extend all operators A_n by the identity to the whole space $\ell^p(\mathbb{I})$. Let $\mathcal{A}$ denote the sequences of those extensions. Then $\mathcal{A} \in \mathcal{F}$ and therefore (3.28) holds.

Let us compare the sets $\sigma(A)$ and $\sigma(\mathcal{A} + \mathcal{G})$. Due to Proposition 3.20, $\sigma(\mathcal{A} + \mathcal{G}) \supseteq \sigma(A)$. Ideally, $\sigma(\mathcal{A} + \mathcal{G}) = \sigma(A)$ holds because this implies:

(a) the projection method is applicable to $A - \lambda I$ whenever the operator is invertible, and

(b) we can approximate the spectrum: $\sigma(A) = \lim_{\varepsilon\searrow 0} \lim_{n\to\infty} \sigma_\varepsilon(A_n)$.

In many cases, however, $\sigma(\mathcal{A} + \mathcal{G}) \setminus \sigma(A) \neq \emptyset$. The set $\sigma(\mathcal{A} + \mathcal{G}) \setminus \sigma(A)$ is often referred to as spectral pollution.

Before discussing some examples of projection methods we mention that in the case of uniform convergence there is no spectral pollution. This follows from the fact that $A_n \rightrightarrows A$ implies $\nu(A_n) \to \nu(A)$ and that the same holds for the adjoint operators.

Lemma 3.21. *Let* $(A_n)_{n\in\mathbb{N}} \subset \mathcal{L}(\ell^p(\mathbb{I}))$ *and* $A_n \rightrightarrows A$ *as* $n \to \infty$ *for some* $A \in \mathcal{L}(\ell^p(\mathbb{I}))$. *Then* (A_n) *is applicable to* A *if and only* A *is invertible.*

3.5.2 The finite section method

The most straightforward projection method on $\ell^p(\mathbb{Z})$ is to choose the projections $\Pi_n^R := \Pi_n^L := P_{-n..n}$. This corresponds to cutting finite square matrices out of the infinite matrix A, centered around 0. Therefore, this method is called the finite section method.

The first rigorous treatment of the FSM goes back to Baxter [6] and Gohberg & Feldman [43] who studied Wiener-Hopf and Toeplitz operators. For a rigorous treatment of the FSM see [86].

Definition 3.22. Let $(l_n)_{n\in\mathbb{N}}$ and $(r_n)_{n\in\mathbb{N}}$ be integer sequences with $l_n < r_n$ for all $n \in \mathbb{N}$ and $l_n \to -\infty$ and $r_n \to \infty$ as $n \to \infty$. Then the finite section method (short FSM) for the operator $A \in \mathcal{L}(\ell^p(\mathbb{Z}))$ is the projection method for A given by $\Pi_n^L = \Pi_n^R = P_{l_n..r_n}$. The sequences (l_n) and (r_n) are called cut-off sequences. If $l_n = -n$ and $r_n = n$ then (A_n) is called the standard FSM. We say A is FSM-simple if the invertibility of A implies the applicability of the standard FSM.

For the FSM the sequence of finite submatrices is given by $A_n = (A_{i,j})_{i,j=l_n}^{r_n}$ for $n \in \mathbb{N}$. A simple example that shows the problems of the FSM arises from the application to the shift operator. In the cases that $\mathbb{I}$ is a half-line, such as $\mathbb{N}$, $\mathbb{Z}_+$ or $\mathbb{Z}_-$ only specify one cut-off sequence and fix the other to the end of the half-line. In case of $\mathbb{I} = \mathbb{N}$ this means that for the cut-off sequence $(r_n)_{n\in\mathbb{N}}$ the sequence is given by $(P_{1..r_n} A P_{1..r_n})_{n\in\mathbb{N}}$.

Example 3.23. *Let $A = S$ be the right shift and $(A_n)_{n\in\mathbb{N}}$ be the standard FSM. Then A is invertible but no A_n is invertible for any $n \in \mathbb{N}$, since the finite matrices are given by*

$$A_n = \begin{pmatrix} 0 & & & \\ 1 & \ddots & & \\ & \ddots & \ddots & \\ & & 1 & 0 \end{pmatrix}.$$

In the notion of spectral pollution we have that $0 \in \sigma_{stab}(\mathcal{A}) \setminus \sigma(A)$.

For band-dominated operators, the stability of (A_n) can be analyzed via limit operators thanks to the following result.

Theorem 3.24. *[65, 67, 86] The FSM with cut-off sequences $l = (l_n)_{n\in\mathbb{N}}$ and $r = (r_n)_{n\in\mathbb{N}}$ as above is applicable to $A \in \mathrm{BDO}_p(\mathbb{Z})$ if and only if the following operators are invertible:*

- *(S1) the operator A itself,*
- *(S2) all operators L^+ with $L \in \mathrm{Lim}_{l-1}(A)$,*
- *(S3) all operators R^- with $R \in \mathrm{Lim}_r(A)$.*

We sketch a proof that revolves around an operator called the stacked operator. For a sequence $(A_n)_{n\in\mathbb{N}}$ of finite matrices the stacked operator $\oplus_{n\in\mathbb{Z}} A_n : \ell^p(\mathbb{Z}^2) \to \ell^p(\mathbb{Z}^2)$ (see [85, p. 308] or [62, p. 60]) is defined by

$$\left(\underset{n\in\mathbb{Z}}{\oplus} A_n x\right)(k,n) := \begin{cases} (A_n^{\text{ext}} x_n)(k) & \text{if } n \in \mathbb{N} \\ x_n(k) & \text{else,} \end{cases}$$

where $x_k = x(\cdot, k) \in \ell^p(\mathbb{Z})$ and A_n^{ext} is the extension of the finite matrix A_n to on operator on $\ell^p(\mathbb{Z})$ by the identity.

Proof. The following properties hold for the stacked operator of the FSM, see [85, Theorem 6.1.6, Lemma 6.1.7] or [62, Proposition 2.22, Theorem 2.28]:

(a) if A is band-dominated then the stacked operator $\oplus_{n\in\mathbb{Z}} A_n$ is also band-dominated,

(b) (A_n) is stable if and only if the stacked operator $\oplus_{n\in\mathbb{Z}} A_n$ is Fredholm.

Recall that the stability of (A_n) together with the invertibility of A is equivalent to the applicability of the FSM, see Theorem 3.19. Due to the assumption of the theorem property (a) yields that $\oplus_{n\in\mathbb{Z}} A_n$ is band-dominated and by (b) we have to investigate its Fredholm property in order to find conditions for the stability of (A_n). This is where limit operators come into play: recall from Theorem 2.32 that $\oplus_{n\in\mathbb{Z}} A_n$ is Fredholm if and only if all its limit operators are invertible. The limit operators of the stacked operator $\oplus_{n\in\mathbb{Z}} A_n$ are again stacked operators $\oplus_{n\in\mathbb{Z}} B_n$, meaning they have the structure $(\oplus_{n\in\mathbb{Z}} B_n x)(k,n) := (B_n x_n)(k)$ where the B_n are one of the following (see e.g. [64, 65, 85]):

(L1) the operator A itself and its shifts $S_{-k}AS_k$, $k \in \mathbb{Z}$,

(L2) all limit operators of A,

(L3) the identity I operator on $\ell^p(\mathbb{Z})$,

(L4) operators $L^+ + I^-$ for $L \in \mathrm{Lim}_{l-1}(A)$ and their shifts,

(L5) operators $R^- + I^+$ for $R \in \mathrm{Lim}_r(A)$ and their shifts.

Due to the layered structure of $\oplus_{n\in\mathbb{Z}} B_n$, it is not hard to see that all limit operators of $\oplus_{n\in\mathbb{Z}} A_n$ are invertible if and only if all the operators above are invertible. There are some redundancies concerning the invertibility of all operators in (L1)-(L5). Of course the identity operator is invertible and the invertibility of A implies the invertibility of its shifts and, due to Fredholmness, also the invertibility of its limit operators. With these considerations, the set of operators in (L1)-(L5) boils down to the set of operators (S1)-(S3) from the statement of the theorem. ☐

For operators on $\ell^p(\mathbb{N})$ we directly get a similar result by extending them to $\ell^p(\mathbb{Z})$ by the identity.

Corollary 3.25. *(a) The FSM with cut-off sequence $r = (r_n)_{n\in\mathbb{N}}$ as above is applicable to a band-dominated operator A on $\ell^p(\mathbb{N})$ if and only if the following operators are invertible:*

(1) the operator A itself, *(2) all operators R^- with $R \in \mathrm{Lim}_r(A)$.*

(b) The FSM with cut-off sequence $l = (l_n)_{n\in\mathbb{N}}$ as above is applicable to a band-dominated operator A on $\ell^p(-\mathbb{Z})$ if and only if the following operators are invertible:

(1) the operator A itself, *(2) all operators L^+ with $L \in \mathrm{Lim}_{l-1}(A)$.*

We see that the set of operators that need to be invertible for the applicability of the FSM shrinks when moving from the two-sided to the one-sided case. Accordingly, we get the following result.

Corollary 3.26. *If $A \in \mathrm{BDO}_p(\mathbb{Z})$ be right-self-similar. If A is FSM simple then A^+ is also FSM simple.*

Proof. Let A be FSM simple and let A^+ be invertible. in order to show that the FSM is applicable to A^+ we first use that $A \in \operatorname{Lim}(A^+)$ is invertible. Therefore, the FSM is applicable to A and by Theorem 3.24 all operators R^- with $R \in \operatorname{Lim}_r(A)$ are invertible. Now Corollary 3.25 does the rest. □

In most of the literature that deals with Theorem 3.24 or variants thereof (e.g. [86, 65, 64]) the operators (S1)-(S3) are called the stability spectrum since it encodes the stability of the sequence (A_n). There, the stability spectrum is usually denoted by $\sigma^{\text{stab}}(A)$ or $\sigma_{\text{stab}}(A)$. This naming might be confusing since, in contrast to the spectrum, the stability spectrum is not a subset of $\mathbb{C}$ but a set of operators. In more recent literature on the topic, such as [48, 69], the term is less used. In this work we will instead refer to this set of operators as stability indicators and denote it by $\mathcal{I}_{\text{stab}}(A)$. By Theorem 3.24 we have

$$\mathcal{I}_{\text{stab}}(A) = \{A\} \cup \{L^+ : L \in \operatorname{Lim}_l(A)\} \cup \{R^- : R \in \operatorname{Lim}_r(A)\}.$$

We continue with some more direct consequences of Theorem 3.24.

Corollary 3.27. *An operator $A \in \mathcal{L}(\ell^p(\mathbb{Z}))$ is FSM-simple if and only if*

$$A \textit{ invertible} \quad \Longrightarrow \quad \begin{cases} L^+ \textit{ invertible} & \textit{for all } L \in \operatorname{Lim}_{l-1}(A) \\ R^- \textit{ invertible} & \textit{for all } R \in \operatorname{Lim}_r(A) \end{cases}.$$

Note that when passing to a subsequence the set of associated limit operators becomes smaller, that is $\operatorname{Lim}_{l'}(A) \subset \operatorname{Lim}_l(A)$ and $\operatorname{Lim}_{r'}(A) \subset \operatorname{Lim}_r(A)$. Hence, Theorem 3.24 implies the following.

Corollary 3.28. *Let l and r are cut-off sequences in the sense of Definition 3.22 and let $l' \subset l$ and $r' \subset r$ be subsequences. If the corresponding FSM with cut-off sequences l and r is applicable to $A \in \mathcal{L}(\ell^p(\mathbb{Z}))$ then also the FSM with cut-off sequences l' and r' is applicable to A.*

In particular, the applicability of the standard FSM implies the applicability of the FSM for any cut-off sequences.

On top of the qualitative result in Theorem 3.24 there is also a quantitative version that yields bounds on the inverses of the finite sections.

Proposition 3.29. *[48, Theorem 6.6] Let $A \in \mathcal{L}(\ell^p(\mathbb{Z}))$ and the FSM be applicable to A for the cut-off sequences l and r. Then*

$$\limsup_{n\to\infty} \|A_n^{-1}\| = \max_{B \in \mathcal{I}_{stab}(A)} \|B^{-1}\|,$$

where $\mathcal{I}_{stab}(A)$ is the set of stability indicators for A, that is $B = \{A, L^+, R^- : L \in \operatorname{Lim}_l(A), R \in \operatorname{Lim}_r(A)\}$.

3.5.3 Periodic finite sections

Recall from Example 3.23 that the FSM for the shift operator is not applicable for any cut-off sequences. There is a quick fix to this problem: we take the matrix entry A_{r_n+1,r_n}, which is a 1 that is barely not contained in A_n and move it to the top-right corner of our matrix A_n. This resulting matrix is then a circular shift:

$$\hat{A}_n = \begin{pmatrix} 0 & & & 1 \\ 1 & \ddots & & \\ & \ddots & \ddots & \\ & & 1 & 0 \end{pmatrix} : \quad \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \mapsto \begin{pmatrix} x_n \\ x_1 \\ \vdots \\ x_{n-1} \end{pmatrix}.$$

Each $\hat{A}_n$ is an isometry and thus $(\hat{A}_n)$ is stable. For a finite vector x we find that $\hat{A}_n x = P_{l_n..r_n} A\widetilde{x}$, where $\widetilde{x}$ is the periodic continuation of x to $\ell^\infty(\mathbb{Z})$. Therefore, the matrices $\hat{A}_n$ are referred to as finite sections of A with periodic boundary conditions.

For cut-off sequences (l_n) and (r_n) we define $d_n := r_n - l_n + 1$ for $n \in \mathbb{N}$ and set $\hat{P}_n = S_{-d_n} P_{l_n..r_n} + P_{l_n..r_n} + S_{d_n} P_{l_n..r_n}$. It is straightforward to show that $\hat{P}_n$ is a projection. Now we can define the periodic finite section method.

Definition 3.30. Let $(l_n)_{n\in\mathbb{N}}$ and $(r_n)_{n\in\mathbb{N}}$ be integer sequences with $l_n < r_n$ for all $n \in \mathbb{N}$ and $l_n \to -\infty$ and $r_n \to \infty$ as $n \to \infty$. Then the periodic finite section method (short PFSM) for the operator $A \in \mathcal{L}(\ell^p(\mathbb{Z}))$ is the projection method $\hat{A}_n := \Pi_n^L A \Pi_n^R$ for A with $\Pi_n^L = P_{l_n..r_n}$ and $\Pi_n^R = \hat{P}_n$. The sequences (l_n) and (r_n) are called cut-off sequences.

The matrix representation of $\hat{P}_n$ is given by

$$\begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \iddots \\ \dots & 0 & I_{d_n} & 0 & \dots \\ \dots & 0 & I_{d_n} & 0 & \dots \\ \dots & 0 & I_{d_n} & 0 & \dots \\ \iddots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

where I_{d_n} is the identity matrix on $\mathbb{C}^{d_n}$.

In the definition above we already claimed that $(\hat{A}_n)$ is a projection method, but we still have to prove that the periodic finite sections of $A \in \mathrm{BDO}_p(\mathbb{Z})$ $\mathcal{P}$-converge to A, since $\hat{P}_n \not\to I$.

Lemma 3.31. *Let* $A \in \mathrm{BDO}_p(\mathbb{Z})$. *Then* $\hat{A}_n \xrightarrow{\mathcal{P}} A$ *as* $n \to \infty$.

Proof. We abbreviate $P_n = P_{l_n..r_n}$. First assume that A is a band operator with bandwidth w. Then $P_{l_n+w..r_n-w} P_n A \hat{P}_n = P_{l_n+w..r_n-w} A$ and we have

$$\|P_{-m..m}(A - P_n A \hat{P}_n)\| = \|P_{-m..m}(I - P_{l_n+w..r_n-w})(A - P_n A \hat{P}_n)\| \to 0 \qquad \text{as } n \to \infty$$

for all $m \in \mathbb{N}$. For $n > m + w$ we also find $P_n A \hat{P}_n P_{-m..m} = P_n A P_{-m..m} = A P_{-m..m}$, and therefore also

$$\|(A - P_n A \hat{P}_n) P_{-m..m}\| \to 0 \quad \text{as } n \to \infty.$$

This proves $\hat{A}_n \xrightarrow{\mathcal{P}} A$ as $n \to \infty$ for $A \in \mathrm{BO}(\mathbb{Z})$ For band-dominated operators the statement follows via approximation by band operators and the uniform boundedness of P_n and $\hat{P}_n$. □

The entries of the matrix $\hat{A}_n$ from the PFSM are given by

$$(\hat{A}_n)_{i,j} = A_{i,j} + A_{i,j+d_n} + A_{i,j-d_n}. \tag{3.29}$$

From the matrix perspective it is easy to see that if A has bandwidth w then $\hat{A}_{i,j} = 0$ if $\operatorname{dist}(i, \{j - d_n, j, j + d_n\}) > w$.

Analogously to Theorem 3.24, our goal is to find stability indicators for the PFSM. We cannot follow the proof of Theorem 3.24 directly. The major problem is that if we build the stacked operator $\oplus_{n\in\mathbb{Z}} A_n$ of the periodic finite sections A_n then the property that A is band-dominated does not imply that $\oplus_{n\in\mathbb{Z}} A_n$ is also band-dominated. This means that the Fredholm property of $\oplus_{n\in\mathbb{Z}} A_n$ cannot be characterized by its limit operators.

We will nevertheless show that the following operators act as stability indicators for the PFSM for A with cut-off sequences (l_n) and (r_n):

$$\mathcal{I}^{\text{per}}_{\text{stab}}(A) := \{A\} \cup \{P_{\mathbb{Z}_-}R + P_{\mathbb{N}}L : L = A_{l_h-1}, R = A_{r_h}\}. \tag{3.30}$$

As for the FSM, the operator A itself is again a stability indicator. Instead of the compressions of the limit operators the stability indicators for the PFSM are supplemented by operators that act on the whole axis. These consist of restrictions of two limit operators L and R, one on the positive half-axis and the other one on the negative half-axis including 0. Note that L and R are not just any limit operators associated to subsequences of the left and right cut-off sequences, respectively. Indeed, L and R are coupled via one sequence h tending to infinity such that both $L = A_{l_h-1}$ and $R = A_{r_h}$.

In order to show that the set (3.30) deserves the name stability indicators we first consider another sequence of operators that approximates $A \in \mathrm{BDO}_p(\mathbb{Z})$. Let the cut-off sequences (l_n) and (r_n) be given. Then define the n-th periodic approximation $(\widetilde{A}_n)$ of A by the infinite matrix

$$(\widetilde{A}_n)_{i,j} := A_{i+kd_n, j+kd_n}, \qquad i, j \in \mathbb{Z}$$

where $k = k(i)$ is the unique integer such that $l_n \leq i + kd_n \leq r_n$. It is clear that $\widetilde{A}_n$ is a d_n-periodic operator and that $P_n A = P_n \widetilde{A}_n$.

We first consider the PFSM for band operators.

Theorem 3.32. *Let $A \in \mathrm{BO}(\mathbb{Z})$. Then the following are equivalent:*

(i) The PFSM $(\hat{A}_n)$ for A is stable.

(ii) The sequence $(\widetilde{A}_n)$ is stable.

(iii) All operators in $\mathcal{I}^{per}_{stab}(A)$ are invertible.

In the case that one of the above holds then

$$\limsup_{n\to\infty} \|\hat{A}_n^{-1}\| = \limsup_{n\to\infty} \|\widetilde{A}_n^{-1}\| = \max_{B\in\mathcal{I}^{per}_{stab}(A)} \|B^{-1}\|.$$

Proof. We will show the statement by proving

$$\liminf_{n\to\infty} \nu(\hat{A}_n) = \liminf_{n\to\infty} \nu(\widetilde{A}_n) = \min_{B\in\mathcal{I}^{\text{per}}_{\text{stab}}(A)} \nu(B). \tag{3.31}$$

Let $x \in \ell^p(\mathbb{Z})$ with $\|x\| = 1$ and $\operatorname{supp} x \subset [l_n, r_n]$ such that $\nu(\hat{A}_n) = \|\hat{A}_n x\|$. Then

$$\nu(\hat{A}_n) = \|P_n A \hat{P}_n x\| = \|P_n \widetilde{A}_n \hat{P}_n x\|. \tag{3.32}$$

Let w denote the bandwidth of A and assume $n > w$. For $p = \infty$ we can continue x periodically to $x^\infty \in \ell^\infty(\mathbb{Z})$ and find that $\widetilde{A}_n x_n^\infty$ is a periodic continuation of $\hat{A}_n x$, which directly yields $\liminf\limits_{n\to\infty} \nu(\widetilde{A}_n) \le \liminf\limits_{n\to\infty} \nu(\hat{A}_n)$. If $p < \infty$ take the vector $x^K := \sum_{j=0}^K S_{jd_n} x$ with $\|x^K\| = K^{\frac{1}{p}}$ and

$$\begin{aligned}
\left\|\widetilde{A}_n x_n^K\right\| &= \left\| \sum_{i=-1}^{K+1} P_{l_n+id_n..r_n+id_n} \sum_{j=0}^{K} \widetilde{A}_n S_{jd_n} x \right\| \\
&\le \left\| P_n \sum_{j=-1}^{K+1} \widetilde{A}_n S_{jd_n} x \right\| + \left\| \widetilde{A}_n S_{-d_n} x \right\| + \left\| \widetilde{A}_n S_{(N+1)d_n} x \right\| \\
&\le (K)^{\frac{1}{p}} \left\| P_n \widetilde{A_n} \hat{P}_n x \right\| + 2\|\widetilde{A}_n\| \overset{(3.32)}{=} (K)^{\frac{1}{p}} \nu(\hat{A}_n) + 2\|\widetilde{A}_n\|.
\end{aligned}$$

Sending $K \to \infty$ we see that

$$\nu(\widetilde{A}_n) \le \frac{(K)^{\frac{1}{p}} \nu(\hat{A}_n) + 2\|\widetilde{A}_n\|}{(K)^{\frac{1}{p}}} \to \nu(\hat{A}_n),$$

and therefore $\liminf\limits_{n\to\infty} \nu(\widetilde{A}_n) \le \liminf\limits_{n\to\infty} \nu(\hat{A}_n)$.

In order to see the converse inequality, note that all operators $\widetilde{A}_n$ have a uniform bound on their norms and their bandwidths. Therefore, we can use Lemma 3.3 and choose N sufficiently large such that $\nu_N(\widetilde{A}_n) \le \nu(\widetilde{A}_n) + \varepsilon$ holds for all $n \in \mathbb{N}$. Now let n be large enough such that $d_n > N + 2w$, where w denotes the bandwidth of A. Then choose $\widetilde{x} \in \ell^p(\mathbb{Z})$ with $\operatorname{diam} \operatorname{supp} \widetilde{x} \le N$ such that $\|\widetilde{A}_n \widetilde{x}\| \le \nu(\widetilde{A}_n) + \varepsilon$. Due to the periodicity of $\widetilde{A}_n$ we can assume without loss of generality that $\operatorname{supp} \widetilde{x} \subset (l_n - N, r_n]$. We define $\hat{x} := P_n(I + S_{d_n})\widetilde{x}$. Then $\|\hat{x}\| = 1$ and

$$\|\hat{A}_n \hat{x}\| = \|P_n A \hat{P}_n (I + S_{d_n})\widetilde{x}\| = \|P_n \widetilde{A}_n (S_{-d_n} + I + S_{d_n}) P_n (I + S_{d_n})\widetilde{x}\|. \tag{3.33}$$

Note that $\widetilde{x} = (P_n + S_{-d_n} P_n S_{d_n})\widetilde{x}$. Moreover, $d_n > w$ implies that $P_n \widetilde{A}_n S_{2d_n} P_n = 0$ and $P_n \widetilde{A}_n S_{-2d_n} P_n = 0$. Hence, we can rewrite (3.33) as

$$\begin{aligned}
\|\hat{A}_n \hat{x}\| &= \|P_n \widetilde{A}_n (S_{-d_n} + I + S_{d_n})\widetilde{x}\| \\
&= \|P_n (S_{d_n} + I + S_{-d_n}) \widetilde{A}_n \widetilde{x}\| \\
&\le \|\widetilde{A}_n \widetilde{x}\| \le \nu(\widetilde{A}_n) + \varepsilon,
\end{aligned}$$

where we used the periodicity of $\widetilde{A}_n$ and that the supports of $S_{d_n} \widetilde{A}_n \widetilde{x}$, $\widetilde{A}_n \widetilde{x}$ and $S_{-d_n} \widetilde{A}_n \widetilde{x}$ are disjoint. We thus get $\liminf\limits_{n\to\infty} \nu(\hat{A}_n) \le \liminf\limits_{n\to\infty} \nu(\widetilde{A}_n)$ which proves the first identity in (3.31).

The second identity in (3.31) is an application of Theorem 3.11. We need to show that

$$\limsup_{n\to\infty} \mathcal{C}_N(\widetilde{A}_n) = \bigcup_{D \in \mathcal{I}^{\text{per}}_{\text{stab}} A} \mathcal{C}_N(D) \tag{3.34}$$

holds for each $N \in \mathbb{N}$. Fix $N \in \mathbb{N}$ and let $B \in \limsup\limits_{n\to\infty} \mathcal{C}_N(\widetilde{A}_n)$. Then there is a sequence (B_n) with $B_n \in \mathcal{C}_N(\widetilde{A}_n)$ such that a subsequence converges to B. We can pass to a subsequence $(B_{h_n})_{n\in\mathbb{N}}$ such that B_{h_n} consists of the columns $j_n + 1..j_n + N$ of $\widetilde{A}_n$ and one of the following holds for all $n \in \mathbb{N}$:

(a) $j_n \in l_{h_n} + w - 1..r_{h_n} - N - w$.

(b) $j_n \in r_{h_n} - N - w + 1..r_{h_n} + w - 2$ and both limit operators associated to $(l_{h_n} - 1)$ and (r_{h_n}), respectively, exist.

In the first case, B_{h_n} consists of columns where $\widetilde{A}_n$ and A agree. Thus, we have $B_{h_n} \in \mathcal{C}_N(A)$ and therefore also $B \in \mathcal{C}_N(A)$ or $B \in \mathcal{C}_N(D)$ for some $D \in \operatorname{Lim}(A)$. In particular, $B \in \bigcup\limits_{D\in\mathcal{I}^{\text{per}}_{\text{stab}}A} \mathcal{C}_N(D)$.

In the second case the matrix B_{h_n} captures an area where two periods are glued together: the first few rows of B_{h_n} coincide with rows of A that are above r_{h_n} while the remaining rows coincide those of A that are below l_{h_n}. Since $j_h - r_{h_n}$ is bounded we can pass to a further subsequence, again denoted by h, such that $j_n = r_{h_n} + \tau$ for some constant $\tau \in -N - w..w$. Then the $N + 2w$ rows of B_{h_n} are given by

$$(B_{h_n})_{i+w,\cdot\cdot} = \widetilde{A}_{j_n+i,\cdot\cdot} = \widetilde{A}_{r_{h_n}+\tau+i,\cdot\cdot} = \begin{cases} A_{r_{h_n}+\tau+i,\cdot\cdot} & \text{if } \tau + i \leq 0 \\ A_{l_{h_n}+\tau+i-1,\cdot\cdot} & \text{if } \tau + i > 0 \end{cases},$$

for $i \in -w + 1..N + w$. Sending $n \to \infty$ we get

$$B_{i+w,\cdot\cdot} = \begin{cases} R_{\tau+i,\cdot\cdot} & \text{if } \tau + i \leq 0 \\ L_{\tau+i,\cdot\cdot} & \text{if } \tau + i > 0 \end{cases},$$

where L and R denote the limit operators associated to $(l_{h_n} - 1)$ and (r_{h_n}), respectively. In particular, $B \in \mathcal{C}_N(P_{-\mathbb{Z}}R + P_{\mathbb{N}}L)$. This proves the direction "$\subseteq$" in (3.34).

For the other inclusion in (3.34) we immediately find that each $B \in \mathcal{C}_N(A)$ is contained in $\mathcal{C}_N(\widetilde{A}_n)$ for sufficiently large n. Also, the submatrices of $P_{-\mathbb{Z}}R + P_{\mathbb{N}}L$ with $L = A_{l_h-1}$ and $R = A_{r_h}$ are readily found to be limits of the column-submatrices of $\widetilde{A}_n$ near the r_{h_n}-th column as $n \to \infty$. Thus, Theorem 3.11 applies and we have $\liminf_{n\to\infty} \nu(\widetilde{A}_n) = \inf_{B\in\mathcal{I}^{\text{per}}_{\text{stab}}(A)} \nu(B)$. In order to obtain (3.31) it only remains to show that the infimum is indeed a minimum. We outsource this proof to Lemma 3.33.

Lastly, in order to get from the lower norms to stability, invertibility and norms of the inverses, we check that $\nu(\hat{A}_n) = \nu(\hat{A}_n^*)$ since each $\hat{A}_n$ is a finite matrix. Also, by Corollary 2.48, $\nu(\widetilde{A}_n) = \nu(\widetilde{A}_n^*)$ holds for $p = 2$. With Proposition 2.20 and Lemma 2.10 this carries over to the other cases for $p \in [1, \infty]$. Then the rest follows from Lemma 2.10 and (3.12). □

Lemma 3.33. *For $A \in \operatorname{BDO}_p(\mathbb{Z})$ the stability indicators of the PFSM satisfy*

$$\inf_{B\in\mathcal{I}^{per}_{stab}(A)} \nu(B) = \min_{B\in\mathcal{I}^{per}_{stab}(A)} \nu(B).$$

Proof. We check that properties (a)-(c) of Proposition 3.12 are fulfilled for the set $\Phi = \mathcal{I}^{\text{per}}_{\text{stab}}(A) \cup \operatorname{Lim}(A)$ and therefore the proposition applies. The uniform boundedness property (a) is straightforward.

In order to check property (b) we use that A is band dominated and choose $w \in \mathbb{N}$ and $A \in \mathrm{BO}^{\mathrm{w}}$ such that $\|A - A'\| < \varepsilon/2$. By Proposition 2.35 we find that the same holds for the limit operators of A and A', and for the remaining operators $B \in \mathcal{I}_{\text{stab}}^{\text{per}}(A)$ we get that there is a $B' \in \mathcal{I}_{\text{stab}}^{\text{per}}(A') \subset \mathrm{BO}^{\mathrm{w}}$ with $\|B - B'\| < \varepsilon$ and therefore all operators in Φ can be uniformly approximated with band operators.

It only remains to show property (c), the sequential compactness of the set $\Psi = \{S_k B S_{-k} : B \in \Phi, k \in \mathbb{Z}\}$. Consider $(B_n) \subset \Phi$ and $(C_n) = (S_{k_n} B_n S_{-k_n})$ for $(k_n) \subset \mathbb{Z}$. If $(B_{h_n}) \subset \mathrm{Lim}(A)$ for any subsequence $(B_{h_n}) \subset (B_n)$ then the existence of an accumulation point in Φ follows from the shift invariance and the sequential compactness of $\mathrm{Lim}(A)$, see Proposition 2.34 and Proposition 2.37. In fact, the same can be said if $B_n = A$ holds for infinitely many n.

It remains to check the case where $B_n = P_{-\mathbb{Z}} R_n + P_{\mathbb{N}} L_n$ for all but finitely many n, where R_n and L_n are the limit operators associated to $r_{h^{(n)}}$ and $l_{h^{(n)}} - 1$ for some sequence $h^{(n)}$ tending to infinity, respectively. Without loss of generality we assume that this is the case for all n. If any subsequence of (k_n) tends to infinity then we again obtain an accumulation point in $\mathrm{Lim}(A)$. So assume that (k_n) is bounded. Then we can restrict us to a constant subsequence, again denoted by k_n, so that we have $k_n = k$ for some $k \in \mathbb{N}$. Then $(C_n) = (S_k B_n S_{-k})$ contains a $\mathcal{P}$-convergent subsequence if and only if (B_n) contains one. We construct the sequence $g = (g(n))_{n \in \mathbb{N}}$ with $g(n) := h_{j_n}^{(n)}$ with a choice of j_n such that the following are fulfilled for all $n \in \mathbb{N}$:

- $\|P_n(S_{-l_{g(n)}+1} A S_{l_{g(n)}-1} - L_n)\| < \frac{1}{n}$,
- $\|P_n(S_{-r_{g(n)}} A S_{r_{g(n)}} - R_n)\| < \frac{1}{n}$,
- $\lim\limits_{m \to \infty} g(m) = \infty$.

We pass to a subsequence g', $g'(n) = g(r(n))$, such that both limit operators $L = A_{l_{g'}-1}$ and $R = A_{r_{g'}}$ exist. In order to avoid the introduction of another subsequence assume that g' and r are chosen in a way such that $L_{(r(n))} \xrightarrow{\mathcal{P}} L' \in \mathrm{Lim}_l(A)$ and $R_{(p(n))} \xrightarrow{\mathcal{P}} R' \in \mathrm{Lim}_r(A)$. This can be done due to Proposition 2.37. For $m \in \mathbb{N}$ we have

$$\begin{aligned} \|P_m(L' - L)\| \leq\, & \|P_m(L' - L_{r(n)})\| \\ & + \|P_m(L_{r(n)} - S_{-l_{g'(n)}+1} A S_{l_{g'(n)}-1})\| \\ & + \|P_m(S_{-l_{g'(n)}+1} A S_{l_{g'(n)}-1} - L)\|. \end{aligned}$$

This first and the third summand converge to 0 as $n \to \infty$ by the choice of L and R. The second summand can be bounded from above by $\|P_n(S_{-l_{g'(n)}+1} A S_{l_{g'(n)}-1} - L_n)\|$ for sufficiently large n. By construction of g', this bound is equal to $1/n$ and therefore also goes to 0 as $n \to \infty$. This means that $L = L'$. The same can be done to show that $R = R'$.

Thus, $P_{-\mathbb{Z}} R_{r(n)} + P_{\mathbb{N}} L_{r(n)} \to P_{-\mathbb{Z}} R + P_{\mathbb{N}} L$ as $n \to \infty$. By construction, L and R are associated to the same subsequences of $l - 1$ and r, respectively, namely $l_{g'} - 1$ and $r_{g'}$. In particular, $P_{-\mathbb{Z}} R + P_{\mathbb{N}} L$ is again a stability indicator. Therefore, we found a converging subsequence of (B_n):

$$B_{r(n)} \to P_{-\mathbb{Z}} R + P_{\mathbb{N}} L \in \mathcal{I}_{\text{stab}}^{\text{per}}(A) \subset \Psi.$$

As discussed above, this implies that also $(C_{(m(n))})$ converges with limit in Ψ, which proves condition (c).

Now Proposition 3.12 yields that the lower norm attains its minimum on the set $\Phi = \mathcal{I}_{\text{stab}}^{\text{per}}(A) \cup \mathrm{Lim}(A)$. Using that $\nu(B) \geq \nu(A)$ for all $B \in \mathrm{Lim}(A)$, see Proposition 2.35, we find that $\min_{B \in \Phi}(\nu(B)) = \min_{B \in \mathcal{I}_{\text{stab}}^{\text{per}}(A)}(\nu(B))$, which concludes the proof. □

Even though the proof of Theorem 3.32 uses the bandedness of A heavily, the result regarding the stability indicators of the PFSM extends to band-dominated operators.

Theorem 3.34. *Let $A \in \mathrm{BDO}_p(\mathbb{Z})$. Then the following are equivalent:*

(i) The PFSM for A is stable.

(ii) All operators in $\mathcal{I}^{per}_{stab}(A)$ are invertible.

In the case that one of the above holds then

$$\limsup_{n\to\infty} \|\hat{A}_n^{-1}\| = \max_{B\in\mathcal{I}^{per}_{stab}(A)} \|B^{-1}\|.$$

Proof. Our goal is to show that

$$\liminf_{n\to\infty} \nu(\hat{A}_n) = \min_{B\in\mathcal{I}^{\text{per}}_{\text{stab}}(A)} \nu(B) \tag{3.35}$$

holds. We already know from the proof of Theorem 3.32 that (3.35) holds for band operators, see (3.31). In order to use this, we approximate A by a band operator C such that $\|A - C\| < \varepsilon$ for any given $\varepsilon > 0$. For the periodic finite sections we get $\|\hat{A}_m - \hat{C}_m\| < 3\varepsilon$, since $\|P_m\| = 1$ and $\|\hat{P}_m\| \leq 3\|P_m\| = 3$.

Regarding the stability indicators, we can find for each $B \in \mathcal{I}^{\text{per}}_{\text{stab}}(A)$ a $B' \in \mathcal{I}^{\text{per}}_{\text{stab}}(C)$ with $\|B - B'\| < 2\varepsilon$ and vice versa. In order to see this, consider $B \in \mathcal{I}^{\text{per}}_{\text{stab}}(A)$. If $B = A$ then $B' = C$ satisfies the claim. In any other case we have $B = P_{\mathbb{Z}_-}A_{r_h} + P_{\mathbb{N}}A_{l_h-1}$. Then pass to a subsequence $h' \subset h$ such that the limit operators $C_{r_{h'}}$ and $C_{l_{h'}-1}$ exist and set $B' = P_{\mathbb{Z}_-}C_{r_{h'}} + P_{\mathbb{N}}C_{l_{h'}-1} \in \mathcal{I}^{\text{per}}_{\text{stab}}(C)$. Then, by Proposition 2.35 (c), $\|B - B'\| \leq 2\varepsilon$. The same argument can be done when starting with $B' \in \mathcal{I}^{\text{per}}_{\text{stab}}(C)$ to find a $B \in \mathcal{I}^{\text{per}}_{\text{stab}}(A)$ with $\|B - B'\| \leq \varepsilon$.

All in all, we get

$$\liminf_{n\to\infty} \nu(\hat{A}_n) \overset{3\varepsilon}{\approx} \liminf_{n\to\infty} \nu(\hat{C}_n) = \inf_{B'\in\mathcal{I}^{\text{per}}_{\text{stab}}(C)} \nu(B') \overset{2\varepsilon}{\approx} \inf_{B\in\mathcal{I}^{\text{per}}_{\text{stab}}(A)} \nu(B).$$

Since $\varepsilon > 0$ was arbitrary we arrive at (3.35). The fact that the infimum is a minimum is by Lemma 3.33, as it is formulated for $A \in \mathrm{BDO}_p(\mathbb{Z})$. For $p < \infty$ we can do the same for the adjoint operators and arrive at the statement of the theorem with the help of Lemma 2.10. For $p = \infty$ we consider the operators $B^{\lhd} \in \mathrm{BDO}_1(\mathbb{Z})$ with $(B^{\lhd})^* = B$ for $B \in \mathcal{I}^{\text{per}}_{\text{stab}}(A)$ instead. We then find that (3.35) also holds for $(\hat{A}_n^T)$ in place of $(\hat{A}_n)$ and $B^{\lhd}$ in place of B for $B \in \mathcal{I}^{\text{per}}_{\text{stab}}(A)$. Thus we can pass from the lower norm to the norms of the inverses also in this case.

□

Remark 3.35. In contrast to the banded case, we omitted the sequence $(\widetilde{A}_m)$ in Theorem 3.34. This is due to the fact that the periodic continuation $\widetilde{C}$ of a banded approximation C is not necessarily a good banded approximation for the periodic continuation. In other words, $\|\widetilde{A}_m - \widetilde{C}_m\|$ cannot be bounded by a multiple of $\|A - C\|$. In order to see this, consider a closed curve a on $[0, 2\pi)$ and let $L(a)$ denote the Laurent operator on $\ell^2(\mathbb{Z})$ with symbol a. We define the operator $A = L(a)P_{l_m..r_m}$ and let C_h be the restriction of A to the first h diagonals around the main diagonal. Then $\|A - C_h\| \leq d_m\|(I - P_{-h..h})a\| \to 0$ as $h \to \infty$. However, the d_m-periodic continuation $\widetilde{A} = L(a)$ is a Laurent operator and in general $C_h \not\to A$ as $h \to \infty$, see Remark 1.40 in [62].

Having established stability indicators for both the FSM and PFSM, it makes sense to compare both sets. In order to facilitate comparability we first restructure the stability indicators for the FSM. Let $A \in \mathrm{BDO}_p(\mathbb{Z})$. Recall that

$$\mathcal{I}_{\text{stab}}(A) = \{A\} \cup \{L^+ : L \in \mathrm{Lim}_{l-1}(A)\} \cup \{R^- : R \in \mathrm{Lim}_r(A)\}.$$

We can combine operators from the last two sets: let h be a sequence tending to infinity such that the limit operator $L = A_{l_h-1}$ exists. By passing to a subsequence, again denoted by h, we can ensure that also $R = A_{r_h}$ exists. Then both L^+ and R^- are invertible if and only if the operator $\begin{pmatrix} R^- & 0 \\ 0 & L^+ \end{pmatrix}$ is invertible on $\ell^p(\mathbb{Z})$. Therefore, we can write both sets of stability indicators as

$$\mathcal{I}_{\text{stab}}(A) = \{A\} \cup \{B_{L,R} : L = A_{l_h-1}, R = A_{r_h}\}$$

and

$$\mathcal{I}^{\text{per}}_{\text{stab}}(A) = \{A\} \cup \{B^{\text{per}}_{L,R} : L = A_{l_h-1}, R = A_{r_h}\}$$

with

$$B_{L,R} = \left(\begin{array}{c|c} R^- & 0 \\ \hline 0 & L^+ \end{array}\right) \qquad \text{and} \qquad B^{\text{per}}_{L,R} = \left(\begin{array}{c} P_{\mathbb{Z}_-}R \\ \hline P_{\mathbb{N}}L \end{array}\right) = \left(\begin{array}{c|c} R^- & P_{\mathbb{Z}_-}RP_{\mathbb{N}} \\ \hline P_{\mathbb{N}}LP_{\mathbb{Z}_-} & L^+ \end{array}\right).$$

A first application of the previous theorems can be made, unsurprisingly, to periodic operators.

Corollary 3.36. *Let $A \in \mathrm{BDO}_p(\mathbb{Z})$ be K-periodic and invertible. Then the PFSM with cut-off sequences (l_n) and (r_n) such that each d_n is a multiple of K is applicable to A.*

Proof. For band operators this is a direct consequence of Theorem 3.32, where the sequence $(\widetilde{A}_n)$ is constant and equal to A, whence stable. For the band-dominated case we use Theorem 3.34 and examine the stability indicators. Since $d_n = r_n - l_n + 1 = jK$ for some $j \in \mathbb{N}$ we write $l_n = r_n - jK + 1$. Then, using periodicity, (3.30) yields

$$\begin{aligned} \mathcal{I}^{\text{per}}_{\text{stab}}(A) &= \{A\} \cup \{P_{\mathbb{Z}_-}R + P_{\mathbb{N}}L : L = A_{l_h-1}, R = A_{r_h}\} \\ &= \{A\} \cup \{P_{\mathbb{Z}_-}R + P_{\mathbb{N}}L : L = A_{r_h-jK}, R = A_{r_h}\} \\ &= \{A\} \cup \{R : R = A_{r_h}\}. \end{aligned}$$

A is invertible by assumption and therefore also its limit operators A_{r_h}, which concludes the proof. □

The reader might wonder about the alternative choice $\Pi^L_n := \hat{P}^*_n$ and $\Pi^L_n := P_n$, compare Definition 3.30. We refer to this method as left periodic finite sections, or short LPFSM. It turns out that the LPFSM can be treated as a PFSM, since

$$\hat{P}^*_n A P_n = (P_n A^* \hat{P}_n)^* = (\hat{A}^*_n)^*.$$

Of course taking the adjoint has no effect on the norms, invertibility and applicability. With the help of Proposition 2.35 we can even recycle $\mathcal{I}^{\text{per}}_{\text{stab}}(A^*)$ for the LPFSM:

Proposition 3.37. *The LPFSM is applicable to $A \in \mathrm{BDO}_p(\mathbb{Z})$ if and only if the PFSM is applicable to A^*. The stability indicators of the LPFSM are given by*

$$\mathcal{I}^{lper}_{stab} = \{A\} \cup \{RP_{-\mathbb{Z}} + LP_{\mathbb{N}} : L = A_{l_h-1}, R = A_{r_h}\}.$$

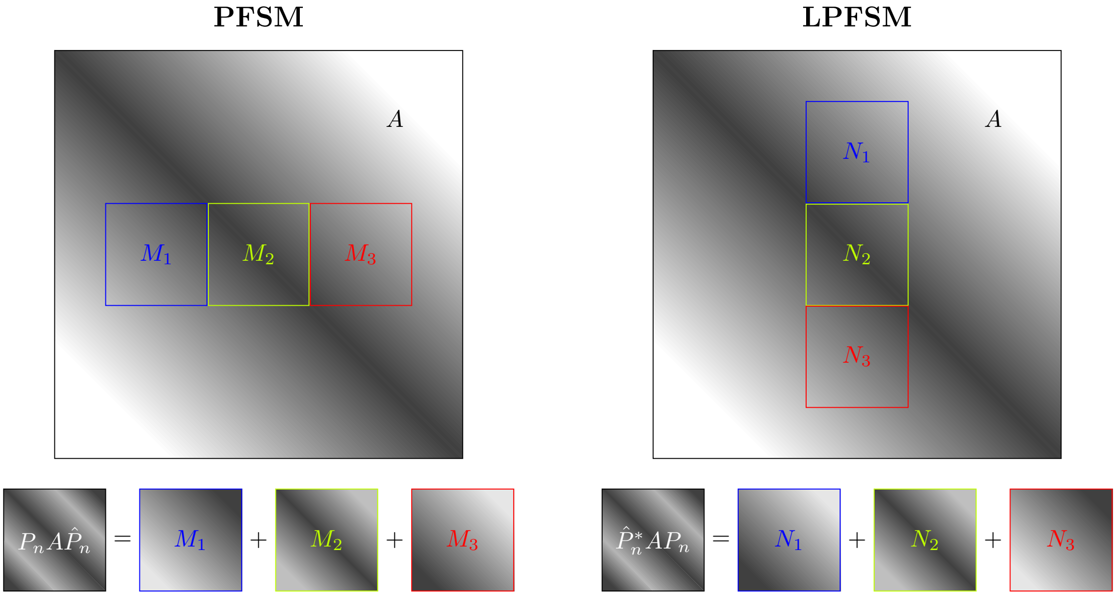

Figure 3.2: Sketch of the construction of the PFSM and LPFSM matrices for a band-dominated operator A.

The matrix entries of the LPFSM are given by

$$(\hat{P}_n^* A P_n)_{i,j} = A_{i,j} + A_{i+d_n,j} + A_{i-d_n,j}. \tag{3.36}$$

We schematically compare (3.36) with (3.29) for the FSM in Figure 3.2.

Recall from the beginning of this section our motivation was to fix the FSM so that it is still applicable for the shift operator S. The PFSM is not only applicable to the shift itself, the applicability is even invariant under shifts:

Proposition 3.38. *Let $A \in \mathrm{BDO}_p(\mathbb{Z})$. Then the PFSM is applicable to A if and only if it is applicable to AS.*

Proof. It is easy to see that if $B \in \mathrm{Lim}(A)$ then $BS \in \mathrm{Lim}(AS)$. Therefore,

$$\begin{aligned}\mathcal{I}^{\text{per}}_{\text{stab}}(AS) &= \{AS\} \cup \{P_{-\mathbb{Z}}RS + P_{\mathbb{N}}LS : L = A_{l_h - 1}, R = A_{r_h}\} \\ &= \bigcup_{B \in \mathcal{I}^{\text{per}}_{\text{stab}}(A)} \{BS\}.\end{aligned}$$

Since each $B \in \mathcal{I}^{\text{per}}_{\text{stab}}(A)$ is an operator on the axis, B is invertible if and only BS is invertible. ☐

Despite the merits of the shift-invariance, we do not want to give that impression that the PFSM is a strictly better version of the FSM. The following example shows that there are invertible operators for which the FSM is applicable but the PFSM is not.

Example 3.39. *Consider the sequence $a = (a_n)_{n \in \mathbb{Z}}$ with a_n is 0 if n is odd and $a_n = 1$ if n is even. We define the operator $A \in \mathrm{BO}(\mathbb{Z})$as $A = I + P_{\mathbb{Z}_-} S M_a P_{\mathbb{Z}_-} + P_{\mathbb{N}} M_a S_{-1} P_{\mathbb{N}}$. Then A has* *the matrix representation*

$$A = \begin{pmatrix} \ddots & & & & & \\ & M_1 & & & & \\ & & M_1 & & & \\ & & & M_2 & & \\ & & & & M_2 & \\ & & & & & \ddots \end{pmatrix}$$

with

$$M_1 = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \qquad \text{and} \qquad M_2 = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}.$$

From the matrix perspective it is easy to see that A is invertible and that the sequence (A_m) of finite sections in stable for any choice of cut-off sequences. Thus, the full FSM is applicable. However, for the periodic finite sections with cut-off sequences $l_m = -2m$ and $r_m = 2m+1$ we have

$$\hat{A}_m = \begin{pmatrix} 1 & & & & & 1 \\ & M_1 & & & & \\ & & M_1 & & & \\ & & & M_2 & & \\ & & & & M_2 & \\ 1 & & & & & 1 \end{pmatrix}.$$

We see that $\hat{A}_m$ is not invertible for any $m \in \mathbb{N}$ and therefore $(\hat{A}_m)$ is not stable and the PFSM is not applicable. As an illustration of Theorem 3.32 we additionally state the stability indicators of the PFSM. There is only one limit operator each in $\operatorname{Lim}_l(A)$ and $\operatorname{Lim}_r(A)$. They are given as block diagonal operators with the matrices M_1 and M_2, respectively. We denote them by L and R The cut-off sequences were chosen such that $P_{\mathbb{N}}L$ and $P_{-\mathbb{Z}}R$ cuts the blocks in half:

$$\mathcal{I}^{per}_{stab}(A) = \{A, B\} \quad \text{with} \quad B = \begin{pmatrix} \ddots & & & & & & & \\ & M_2 & & & & & & \\ & & M_2 & & & & & \\ & & & 1 & 1 & & & \\ & & & 1 & \mathbf{1} & & & \\ & & & & & M_1 & & \\ & & & & & & M_1 & \\ & & & & & & & \ddots \end{pmatrix}.$$

Here the bold $\mathbf{1}$ marks the entry $B_{0,0}$. Since B is not invertible also Theorem 3.32 yields that the PFSM is not applicable.

It will also show that the shift-invariance does not hold for shifts applied from the left, meaning that we cannot replace the operator AS in Proposition 3.38 by SA.

Example 3.40. *Let A, L and R be as in Example 3.39 and consider the PFSM for SA for the same* *cut-off sequences* (l_m) *and* (r_m). *Then* $\operatorname{Lim}_l(SA) = \{SL\}$ *and* $\operatorname{Lim}_r(SA) = SR$. *Therefore,*

$$\mathcal{I}^{per}_{stab}(SA) = \{SA, B\} \quad with \quad B = \begin{pmatrix} \ddots & & & & & \\ & M_2 & & & & \\ & & M_2 & & & \\ & & & M_1 & & \\ & & & & M_1 & \\ & & & & & \ddots \end{pmatrix}.$$

Both stability indicators are invertible, and thus the PFSM is applicable to SA *despite not being applicable to* A. *If the invariance of the applicability under shifts applied from the left is desired, the LPFSM is a better choice, see Proposition 3.37. However, this comes to the price of losing shift-invariance from the right.*

3.6 References

Almost all results of Section 3.2, 3.3 and 3.4 are based on joint work Fabian Gabel, Dennis Gallaun, Julian Großmann and Marko Lindner and published in [41]. An exception is Theorem 3.11 which is due to the author and not published, and Proposition 3.12 which is an adaptation of [71, Theorem 8]. Section 3.5 and 3.5.2 contain well known results about approximation methods and the FSM that can be found in [62]. The results of Section 3.5.3, in particular Theorems 3.32 and 3.34, are due to the author and seem to be new.

Chapter 4

Discrete Schrödinger Operators

In the 1920s W. Heisenberg and his co-workers [12] as well as E. Schrödinger [89] proposed a model of quantum physics for which von Neumann [105] then gave the mathematical foundation. He used operators on Hilbert spaces to describe physical quantities, so-called observables. A key property of quantum physics is that observables exists which cannot be measured simultaneously. Putting this in mathematical terms, this means that the observables do not commute. In contrast to classical physics, this phenomenon could no longer be described with the real numbers. This lead to the development of quantum theory in Hilbert spaces which revolves around the Schrödinger equation

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\Psi(t) = H\Psi(t), \tag{4.1}$$

where $\hbar$ is the Planck constant and $\Psi(t)$ is a normalized element of a Hilbert space X, called the wave function, that describes the quantum state of a particle at time $t \geq 0$. The self-adjoint but usually unbounded operator H with domain inside X is called Hamiltonian. As an analogue of the total energy of a system, the Hamiltonian is given by the sum of kinetic and potential energy. Omitting constants, the kinetic energy is described by the negative Laplacian $-\Delta := -\sum\limits_{k=1}^{d} \dfrac{\partial^2}{\partial x_k^2}$ in the continuous case $X = L^2(\mathbb{R}^d)$. In that case, the potential energy is given by a multiplication operator V by a function in $L^2(\mathbb{R}^d)$, called the potential. Therefore, a possible form of the Hamiltonian

$$H = -\Delta + V. \tag{4.2}$$

Solving the differential equation (4.1) with initial value $\psi(0)$ yields the time-independent Schrödinger equation

$$\Psi(t) = e^{iHt/\hbar}\Psi(0). \tag{4.3}$$

Note that $e^{iHt/\hbar}$ is a unitary operator. An analytic solution of (4.3) is only known for very few and relatively simple model Hamiltonians, such as the hydrogen atom in three dimensions that has a potential $V(x) = \frac{1}{\|x\|}$.

Throughout this work we focus on discrete Schrödinger operators in one dimension. They are defined by

$$(Hx)_n \;=\; x_{n-1} + v(n)x_n + x_{n+1}, \quad n \in \mathbb{Z}. \tag{4.4}$$

The function $v : \mathbb{Z} \to \mathbb{R}$ is referred to as the potential of H. Considering that the discrete Laplacian on $\ell^2(\mathbb{Z})$ is given by

$$\Delta_{\text{disc}} := S^{-1} - 2I + S, \qquad (\Delta_{\text{disc}}x)_n = x_{n-1} - 2x_n + x_{n+1}, \tag{4.5}$$

it is not hard to see that (4.4) is indeed a discretized version of (4.2). The summand $2I$ from the discrete Laplacian is omitted in (4.4) since it corresponds only to a shift in the potential.

The operator H from (4.4), also called Hamiltonian, acts via matrix-vector multiplication by a two-sided infinite matrix $(H_{ij})_{i,j\in\mathbb{Z}}$ with main diagonal $H_{ii} = v(i)$, super- and subdiagonal $H_{i,i\pm1} = 1$ and all other entries equal to zero:

$$H = \begin{pmatrix} \ddots & \ddots & & & \\ \ddots & v(0) & 1 & & \\ & 1 & v(1) & 1 & \\ & & 1 & v(2) & \ddots \\ & & & \ddots & \ddots \end{pmatrix}.$$

Sometimes we make the dependence of H on the potential v explicit and write $H(v)$ instead of H. We also write $H(w)$ with a finite word w and mean the periodic Schrödinger operator on $\ell^2(\mathbb{Z})$ with the potential that is the periodic continuation of w such that $(H(w))_{1,1} = w(1)$. Analogously, we define $H(\lambda)$ for a real number λ to be the discrete Schrödinger operator with potential that is constant and equal to λ. Apart from the motivation above, we will no longer consider the continuous case $X = L^2(\mathbb{R}^d)$, and whenever we write Schrödinger operator we mean a discrete Schrödinger operator in the sense of (4.4).

Classes of potentials The methods involved in the study of Schrödinger operators depend on the properties of the potential. In this work we only study bounded potentials, which leads to bounded and self-adjoint operators H. We start with integer-valued potentials in Section 4.1. Then we continue with periodic potentials in Section 4.2. In Section 4.3 and 4.4 we consider aperiodic, more precisely Sturmian potentials. Note that for all classes mentioned above the potential can take only finitely many values.

The spectrum of discrete Schrödinger operators

The spectral values of H have a physical interpretation as energy levels that the described quantum system can attain. We follow the convention to denote the spectral variable by E instead of λ throughout this chapter.

By the spectral theorem for bounded self-adjoint operators [103, Chapter 3], the spectrum of H has three parts: the pure point spectrum, the absolutely continuous spectrum and the singular continuous spectrum. The so-called RAGE theorem [103, Section 5.2], named after Ruelle, Amrein, Georgescu and Enß provides a link between the three spectral types and the localization or delocalization of states $\psi(t)$ in (4.3). For instance, pure point spectrum of H corresponds to the system staying in a compact region. In contrast, the absolutely continuous spectrum of H corresponds to the system leaving every fixed region in time average. This happens for periodic Schrödinger operators since they have only absolutely continuous spectrum.

Compressions, essential spectra and Dirichlet eigenvalues Throughout this chapter we will study the relation between the spectrum of H and the spectrum of its half line compression

$$(H^+x)_n \;=\; x_{n-1} + v(n)x_n + x_{n+1}, \quad n \in \mathbb{N}, \qquad \text{where} \quad x_0 := 0, \tag{4.6}$$

on $\ell^2(\mathbb{N})$.

Recall from Lemma 2.39 that if H is right-self-similar, meaning that H is a limit operator of H^+, then $\sigma(H^+) \supset \sigma(H) = \sigma_{\text{ess}}(H^+)$. For discrete Schrödinger operators being right-self-similar means that every finite subword of the potential v of H (understood as an infinite string) occurs infinitely often (at least up to arbitrary precision) in the right half of v. In this case, the spectrum of H^+ arises from $\sigma(H) = \sigma_{\text{ess}}(H^+)$ by including eigenvalues of H^+, the so-called Dirichlet-eigenvalues. Their name addresses their cause: the truncation, i.e. introduction of a homogeneous Dirichlet boundary condition $x_0 = 0$.

We have seen in Section 3.5 that trying to compute $\sigma(H)$ via a truncation technique like the FSM then such Dirichlet eigenvalues typically lead to spectral pollution, being, erroneously, caused by the method rather than by the physical model behind the operator H.

Transfer matrices. In order to examine the kernel of H or H^+, it is useful to reformulate the scalar three-term recurrence

$$0 \;=\; (Hx)_n \;=\; x_{n-1} + v(n)x_n + x_{n+1}, \quad n \in \mathbb{Z} \tag{4.7}$$

as a vector-valued two-term recursion

$$\begin{pmatrix} x_{n+1} \\ x_n \end{pmatrix} = \begin{pmatrix} -v(n) & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x_n \\ x_{n-1} \end{pmatrix}. \tag{4.8}$$

The matrix $T(n) := \begin{pmatrix} -v(n) & -1 \\ 1 & 0 \end{pmatrix}$ from (4.8) is the transfer matrix. We include the spectral variable E into (4.7) and get

$$0 \;=\; ((H-E)x)_n \;=\; x_{n-1} + (v(n)-E)x_n + x_{n+1}, \quad n \in \mathbb{Z},$$

which leads to the transfer matrices

$$T(n,E) := \begin{pmatrix} E - v(n) & -1 \\ 1 & 0 \end{pmatrix}. \tag{4.9}$$

Note that transfer matrices always have a determinant equal to 1 and are therefore invertible. Transfer matrices are an efficient and popular tool in the study of discrete Schrödinger operators, see e.g. [102]. For instance, they can be used to prove the following useful lemma.

Lemma 4.1. *(a) Let $x, y \in \ker(H)$. If $x_i = y_i$ and $x_{i+1} = y_{i+1}$ for any $i \in \mathbb{Z}$ then $x = y$. In particular, if $x \in \ker(H)$ with $x \neq 0$ then no two consecutive elements of x can be* 0.

(b) Let $x, y \in \ker(H^+)$. If $x_i = y_i$ and $x_{i+1} = y_{i+1}$ for any $i \in \mathbb{N}$ then $x = y$. Moreover, if $x \in \ker(H)$ with $x \neq 0$ then $x_1 \neq 0$.

Proof. For the first part let $j > i + 1$. Then

$$\begin{aligned} \begin{pmatrix} x_{j+1} \\ x_j \end{pmatrix} &= T(j)\dots T(i+1) \begin{pmatrix} x_{i+1} \\ x_i \end{pmatrix} \\ &= T(j)\dots T(i+1) \begin{pmatrix} y_{i+1} \\ y_i \end{pmatrix} = \begin{pmatrix} y_{j+1} \\ y_j \end{pmatrix}. \end{aligned}$$

Similarly, for $j < i$ we compute

$$\begin{aligned} \begin{pmatrix} x_{j+1} \\ x_j \end{pmatrix} &= T(j+1)^{-1}\dots T(i)^{-1} \begin{pmatrix} x_{i+1} \\ x_i \end{pmatrix} \\ &= T(j+1)^{-1}\dots T(i)^{-1} \begin{pmatrix} y_{i+1} \\ y_i \end{pmatrix} = \begin{pmatrix} y_{j+1} \\ y_j \end{pmatrix}. \end{aligned}$$

Thus, we get $x = y$. The second part can be shown analogously using the Dirichlet boundary condition $x_0 = 0$.

□

As a direct consequence of Lemma 4.1 we find that the dimension of the kernel of H in the space of sequences over $\mathbb{Z}$ is always 2. The solutions of (4.7) in that space are called generalized eigenvectors. Estimating the decay or growth of generalized eigenvectors yields results on the spectrum of the operator. For instance, if a bounded generalized eigenvector exists for $H - E$ then $E \in \sigma(H)$ and, by definition, if a generalized eigenvector is square-summable then it is a proper eigenvector (in $\ell^2(\mathbb{Z})$) for the eigenvalue E of H.

We end this introduction by taking a look at the simplest Schrödinger operator possible, the discrete Laplacian.

Example 4.2. *We consider the free Laplacian* $H_\Delta := H(-2) = \Delta_{\text{disc}}$ *from* (4.5)

H_Δ *and* H_Δ^+ *are a Laurent operator and a Toeplitz operator, respectively. Thus, the methods of Section 2.5.1 apply. According to* (2.10) *and* (2.11) *we compute*

$$\sigma(H_\Delta) = \sigma(H_\Delta^+) = [-4, 0],$$

using that the symbol of H *is* $-2 + 2\cos$.
More generally, for $\lambda \in \mathbb{R}$ *we have* $\sigma(H(\lambda)) = [-2 + \lambda, 2 + \lambda]$.

4.1 Integer-valued potentials

Our study of discrete Schrödinger operators starts with potentials that are integer-valued. In 2017 Lindner and Söding proved the applicability of the FSM for the integer-valued Fibonacci Hamiltonian [72], which is an aperiodic Schrödinger operator. As part of the proof they observed that the invertibility of the two-sided operator already implied the invertibility of its compressions. In this section we will show that this implication is not necessarily due to the special aperiodic structure of the Fibonacci Hamiltonian, but rather a feature of the integer-valued potential. This section is based on joint work with Marko Lindner [73].

Proposition 4.3. *([73, Proposition 3.1]) Let* H^+ *be a discrete Schrödinger operator on the half-line,* $\ell^2(\mathbb{N})$*, as in* (4.6)*, with an integer-valued potential* $v : \mathbb{N} \to \mathbb{Z}$*. Then* H^+ *is injective.*

Proof. In order to show that H^+ is injective, take a vector $x \in \ell^2(\mathbb{N})$ with $H^+ x = 0$. We further assume that $x \neq 0$, which will lead to a contradiction. Recall from Lemma 4.1 that we can assume that $x_1 \neq 0$. By scaling we can put $x_1 = 1$. By (4.8) and the definition of the transfer matrices $T(k)$, the other entries of x satisfy the condition

$$\begin{pmatrix} x_{n+1} \\ x_n \end{pmatrix} = T(n) \dots T(1) \begin{pmatrix} x_1 \\ x_0 \end{pmatrix} = T(n) \dots T(1) \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad n \in \mathbb{N}. \tag{4.10}$$

Since, by assumption, $v(k) \in \mathbb{Z}$ for all $k \in \mathbb{N}$, we find that $T(k) = \begin{pmatrix} -v(k) & -1 \\ 1 & 0 \end{pmatrix} \in \mathbb{Z}^{2\times 2}$. Thus (4.10) implies that $x_n \in \mathbb{Z}$ for all $n \in \mathbb{N}$. As an integer sequence in $\ell^2(\mathbb{N})$, x can only have finitely many non-zero entries. Therefore, there exists an $n \in \mathbb{N}$ such that $x_n = x_{n+1} = 0$. Using Lemma 4.1, we get that $x = 0$, contradicting our assumption. We thus have shown that H^+ is injective since it cannot have any nontrivial vectors x with $H^+ x = 0$. □

So, after this proposition, we have that the invertibility of the self-adjoint operator $H^+ : \ell^2(\mathbb{N}) \to \ell^2(\mathbb{N})$ with integer-valued potential is equivalent to the closedness of its range. The latter is for discrete Schrödinger operators not only a necessary but also a sufficient condition for Fredholmness.

Lemma 4.4. *([73, Lemma 3.2]) Let H be a discrete Schrödinger operator,* (4.4)*, and H^+ its half-line compression,* (4.6)*. Then the following implications hold,*

$$(i) \iff (ii) \implies (iii) \iff (iv),$$

where

(i)	*H is a Fredholm operator,*	(iii)	*H^+ is a Fredholm operator,*
(ii)	*H has a closed range,*	(iv)	*H^+ has a closed range.*

If H is right-self-similar then all four statements are equivalent.

Proof. The implications $(i) \Rightarrow (ii)$ and $(iii) \Rightarrow (iv)$ are standard. Their reverse directions follow from the observations $\dim\ker(H) \leq 2$ and $\dim\ker(H^+) \leq 1$, which are direct consequences of Lemma 4.1.

The implication $(i) \Rightarrow (iii)$ can be readily seen with limit operators. By Theorem 2.32 and $\mathrm{Lim}(H) \supset \mathrm{Lim}_+(H) = \mathrm{Lim}(H^+)$.

The equivalence of the Fredholmness of H and the Fredholmness of H^+ for right-self-similar operators is a direct consequence of Lemma 2.39(c). ☐

Observe that Lemma 4.4 holds for any discrete Schrödinger operator, not only for the ones with integer potential. Combining the previous two results we arrive at the following theorem.

Theorem 4.5. *([73, Theorem 1.2]) For a discrete Schrödinger operator H on $\ell^2(\mathbb{Z})$, as in* (4.4)*, with an integer-valued potential $v : \mathbb{Z} \to \mathbb{Z}$, and its half-line compression H^+, as in* (4.6)*, the following implication holds:*

$$H \text{ is a Fredholm operator on } \ell^2(\mathbb{Z}) \qquad \implies \qquad H^+ \text{ is invertible on } \ell^2(\mathbb{N}).$$

In particular, H^+ is invertible if H is invertible.

Proof. Let H be Fredholm. Since H^+ is self-adjoint, it suffices to show that it is injective and has a closed range. Injectivity follows by Proposition 4.3 and the assumption that $v(n)$ takes values in the integers. From Lemma 4.4 it follows that H^+ has closed range.

☐

Recall from Section 3.5.2, more precisely from Theorem 3.24, that the invertibility of compressions is directly linked to the applicability of the FSM. Namely, the stability indicators for the FSM applied to H are given by

$$\mathcal{I}_{\text{stab}}(H) = \{H\} \cup \bigcup_{L\in\mathrm{Lim}_l(H)} \{L^+\} \cup \bigcup_{R\in\mathrm{Lim}_r(H)} \{R^-\}.$$

With that in mind, Theorem 4.5 can be used to guarantee the applicability of the FSM. Recall that we call H FSM-simple if the FSM is applicable to H is and only if H is invertible.

Theorem 4.6. *([73, Theorem 1.2]) Let H be a discrete Schrödinger operator* (4.4) *on $\ell^2(\mathbb{Z})$ with an integer-valued potential $v : \mathbb{Z} \to \mathbb{Z}$. Then both H and H^+ are FSM-simple.*

Proof. We start with the two-sided case, H on $\ell^2(\mathbb{Z})$. Let H be invertible. Then H is in particular Fredholm. By Theorem 2.32, all $L \in \mathrm{Lim}_-(H)$ and $R \in \mathrm{Lim}_+(H)$ are also invertible. Because the convergence of the matrix entries is by being eventually constant, L and R are again discrete Schrödinger operators with integer potential.

Let Φ be the flip operator on $\ell^2(\mathbb{Z})$ defined by $(\Phi x)_i = x_{-i+1}$ for $i \in \mathbb{Z}$. It is clear that Φ is an isometric isomorphism. For $R \in \mathrm{Lim}_+(H)$ also $\Phi R \Phi$ is invertible and a discrete Schrödinger operator with integer potential.

We apply Theorem 4.5 to $L \in \mathrm{Lim}_-(H)$ in place of H and also to$\Phi R \Phi$ in place of H, where $R \in \mathrm{Lim}_+(H)$. Then L^+ and $(\Phi R \Phi)^+$ are invertible on $\ell^2(\mathbb{N})$. With the help of the invertible flip operator from $\ell^2(\mathbb{N})$ to $\ell^2(\mathbb{Z}_-)$ that is given by the respective restriction of Φ we can see that the invertibility of $(\Phi R \Phi)^+$ implies the invertibility of R^-.

Because this is true for all $L \in \mathrm{Lim}_-(H)$ and $R \in \mathrm{Lim}_+(H)$, we get, by Theorem 3.24, that the full FSM is applicable to H.

In the one-sided case, H^+ on $\ell^2(\mathbb{N})$, assume that H^+ is invertible. We then use Corollary 3.25 to see that the FSM is applicable to H^+. □

Corollary 4.7. *([73, Corollary 3.3]) For a discrete Schrödinger operator H on $\ell^2(\mathbb{Z})$, as in* (4.4)*, with an integer-valued potential $v : \mathbb{Z} \to \mathbb{Z}$, and its half-line compression H^+, as in* (4.6)*, the following holds:*

If H has a closed range then the FSM is applicable to H^+.

Proof. Let the range of H be closed. By Lemma 4.4, H is a Fredholm operator, and by Theorem 4.5, H^+ is invertible. Since H^+ is FSM-simple, by Theorem 4.6, it follows that the FSM is applicable to H^+. □

For the rest of this section we investigate possible directions of extension of the previous results, as well as its limitations. Clearly, the results of this section also hold for H_- in place of H^+. However, we cannot replace “integer-valued” by “rational-valued” in Theorems 4.5 and 4.6 and in Proposition 4.3. We refer to Example 4.31 where it is shown for a 3-periodic Schrödinger operator that H is invertible while H_+ is not. In particular, the claims of Proposition 4.3 and Theorem 4.5, do obviously not apply in this situation.

Unlike H^+, the full-space operator H is not always injective if it has an integer-valued potential. See the following example:

Example 4.8. *We construct a potential $v \in \{-3, 0, 3\}^{\mathbb{Z}}$ such that there is a solution x of* (4.7) *that decays exponentially at both $+\infty$ and $-\infty$. We set $v(n) := \begin{cases} -3 & \text{if } n < 0 \\ 0 & \text{if } n = 0 \\ 3 & \text{if } n > 0 \end{cases}$. Then for $n \in \mathbb{N}$ the transfer matrices are identical and given by*

$$T(n) = \begin{pmatrix} -3 & -1 \\ 1 & 0 \end{pmatrix},$$

with eigenvalues $\lambda_{1,2} = \frac{-3\pm\sqrt{5}}{2}$. We focus on $\lambda_1 = \frac{-3+\sqrt{5}}{2}$ since $|\lambda_1| < 1$. A corresponding eigenvector is $\begin{pmatrix} 1 \\ \frac{-3-\sqrt{5}}{2} \end{pmatrix} =: \begin{pmatrix} x_1 \\ x_0 \end{pmatrix}$. Then, for positive n, $|x_n| \le |\lambda|^n \left| \begin{pmatrix} x_1 \\ x_0 \end{pmatrix} \right|$ decays exponentially as $n \to \infty$.

Having fixed x_0 and x_1 we need to show that x decays exponentially also at $-\infty$. This can be done by checking that

$$\begin{pmatrix} x_0 \\ x_{-1} \end{pmatrix} = T(0)^{-1} \begin{pmatrix} x_1 \\ x_0 \end{pmatrix} = \begin{pmatrix} \frac{-3-\sqrt{5}}{2} \\ -1 \end{pmatrix}$$

is an eigenvector of the transfer matrices in the backwards direction, given by

$$T(n)^{-1} = \begin{pmatrix} 0 & 1 \\ -1 & 3 \end{pmatrix}$$

for negative n*. Indeed,*

$$T(n)^{-1}\begin{pmatrix} x_0 \\ x_{-1} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 3 \end{pmatrix}\begin{pmatrix} \frac{-3-\sqrt{5}}{2} \\ -1 \end{pmatrix} = \begin{pmatrix} -1 \\ \frac{-3+\sqrt{5}}{2} \end{pmatrix} = -\lambda_1 \begin{pmatrix} \frac{-3-\sqrt{5}}{2} \\ -1 \end{pmatrix}$$

with the same λ_1 *as above. In particular,* $|\lambda_1| < 1$ *ensures that the norm of* $\begin{pmatrix} x_j \\ x_{j-1} \end{pmatrix} = T(-1)^j \begin{pmatrix} x_0 \\ x_{-1} \end{pmatrix}$ *decays exponentially as* $j \to -\infty$*. The exponential decay on both sides ensures that the generalized eigenvector* x *lies in* $\ell^2(\mathbb{Z})$ *and therefore is indeed a proper eigenvector of* H*.*

The applicability of the FSM for invertible Schrödinger operators with integer potential is guaranteed by Theorem 4.6. The next example shows that a similar statement does not hold for the periodic finite section method. In other words, Schrödinger operators with integer potential are always FSM-simple but not necessarily PFSM-simple.

Example 4.9. *We start with the discrete Schrödinger operator* H *with potential*

$$v = \begin{cases} -3 & \textit{if } n \le 0 \\ 3 & \textit{if } n > 0 \end{cases}.$$

Compared to the potential from Example 4.8 we only replaced the $v(0) = 0$ *by* $v(0) = -3$*. This change is crucial: in the previous example* $T(0)^{-1}$ *was responsible for the alignment of the eigenspaces of the transfer matrices in both forward and backward direction. Now this is no longer the case. For any choice of* x_0, x_1 *the vector* x *that arises from the recursion* (4.7) *will grow exponentially in at least one direction,* $+\infty$ *of* $-\infty$*. Therefore* H *is injective.*

The limit operators of H *are just* $H(3)$ *and* $H(-3)$*. They are invertible, see Example 4.2, and therefore* H *is also Fredholm. Altogether this means that* H *is invertible. The stability indicators of the PFSM,* $\mathcal{I}^{per}_{stab}(H)$ *are just* H *and shifts of* $-H$*, compare Theorem 3.32 and* (3.30)*. Hence, it is easy to see that the PFSM is applicable to* H*.*

So let us perform some surgeries on H *that keep the invertibility alive but remove the applicability of the PFSM. Consider the potential* $\widehat{v}$ *that is identical to* v*, except that* $\widehat{v}(n) = 0$ *for* $n = 10^k$ *and* $n = 10^k + 1$ *for every* $k \in \mathbb{N}$*. Let* $\widehat{H}$ *denote the discrete Schrödinger operator with potential* $\widehat{v}$*. We implanted two consecutive zeros infinitely many times. The corresponding transfer matrices multiply to the negative identity:*

$$T(10^k+1)T(10^k) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

for $k \in \mathbb{N}$*. This means that the behavior of a generalized eigenvector* x *is only shifted by two indices. Since the perturbations are sparse, any generalized eigenvector of* $\widehat{H}$ *still grows exponentially in at least one direction. In particular,* $\widehat{H}$ *is injective. Applying the same arguments to the limit operators of* $\widehat{H}$ *and using Favard's condition (see Proposition 2.33) we find that* $\widehat{H}$ *is invertible.*

Let us take a look at the other elements in $\mathcal{I}^{per}_{stab}(H)$. $\operatorname{Lim}_-(H)$ is a singleton, containing only $L := H(-3)$. $\operatorname{Lim}_+(H)$ contains $H(3)$ as well as shifts of

$$H = \begin{pmatrix} \ddots & \ddots & & & & \\ \ddots & 3 & b & & & \\ & a & 0 & b & & \\ & & a & 0 & b & \\ & & & a & 3 & \ddots \\ & & & & \ddots & \ddots \end{pmatrix}.$$

Now take the sequence r defined by $r_k = 10^k$ for $k \in \mathbb{N}$ and set $R := \widehat{H}_r \in \operatorname{Lim}_+(\widehat{H})$. Then we find the stability indicator

$$P_{-\mathbb{Z}}R + P_{\mathbb{N}}L = \begin{pmatrix} \ddots & \ddots & & & & & \\ \ddots & 3 & b & & & & \\ & a & 3 & b & & & \\ & & a & 0 & b & & \\ & & & a & -3 & b & \\ & & & & a & -3 & \ddots \\ & & & & & \ddots & \ddots \end{pmatrix},$$

that is just a flipped version of the operator H in Example 4.8, which is not invertible. Therefore, the PFSM is not applicable to $\widehat{H}$.

The idea of a transfer matrix can easily be generalized to any tridiagonal matrix with constant sub- and superdiagonal, such as the non-self-adjoint Anderson model, see Section 3.3. We consider the matrix representation

$$H = \begin{pmatrix} \ddots & \ddots & & & \\ \ddots & v(0) & b & & \\ & a & v(1) & b & \\ & & a & v(2) & \ddots \\ & & & \ddots & \ddots \end{pmatrix},$$

with $a, b \in \mathbb{C}$. The difference equation

$$(Hx)_n \;=\; ax_{n-1} + v(n)x_n + bx_{n+1}, \quad n \in \mathbb{Z}, \tag{4.11}$$

then yields the transfer matrix $T(n) = \begin{pmatrix} -\frac{v(n)}{b} & -\frac{a}{b} \\ 1 & 0 \end{pmatrix}$.

Theorem 4.5 only relies on Proposition 4.3 and integer transfer matrices $T(n) \in \mathbb{Z}^{2\times 2}$. Hence, it also holds if a and all $v(n)$ are integer multiples of b.

However, for Theorem 4.6, we need, besides injectivity and a closed range of the half-line compression, also injectivity of its adjoint. Arguing via Proposition 4.3 again, in order to guarantee integer transfer matrices, also $\frac{b}{a}$ and all $\frac{v(n)}{a}$ have to be integer. So in total, all $v(n)$ have to be integer multiples of $a = \pm b \neq 0$. Despite the restrictions this covers a non-normal case. We summarize our observations in the following proposition.

Proposition 4.10. *Let H be given by* (4.11). *If $a = \pm b \neq 0$ and $v(n)$ is an integer multiple of a then H^+ and $(H^+)^*$ are injective. If, in addition, H is Fredholm then H^+ is invertible. Moreover, both H and H^+ are FSM simple.*

We return to the case $a, b = 1$, but now look at complex potentials. The ideas of this section generalize to values in a set $\mathcal{R} \subset \mathbb{C}$ with

(i) $-1, 0, 1 \in \mathcal{R}$, (iii) $(\mathcal{R}, +, \cdot)$ is a ring,
(ii) $v(n) \in \mathcal{R}$ for all $n \in \mathbb{Z}$, (iv) 0 is an isolated point of $\mathcal{R}$.

From $(i), (ii), (iii)$ it follows that $T(n) \in \mathcal{R}^{2\times 2}$ and hence $x_n \in \mathcal{R}$ in (4.10) for all $n \in \mathbb{N}$. From (iv) it follows that, just as two lines below (4.10), $x \in \ell^2(\mathbb{N})$ implies $x \in c_{00}(\mathbb{N})$.

By (i) and (iii), $s - t = s + (-1) \cdot t \in \mathcal{R}$ for all $s, t \in \mathcal{R}$. By (iii), with every $r \in \mathcal{R}$, also $r^2, r^3, \ldots \in \mathcal{R}$, so that, by (iv), the only $r \in \mathcal{R}$ with $|r| < 1$ is $r = 0$. As a consequence of these observations, $\mathcal{R}$ is discrete with $|s - t| \geq 1$ for all $s, t \in \mathcal{R}$ with $s \neq t$.

Examples of such a set $\mathcal{R}$ are grids $\mathcal{R} = r^1\mathbb{Z} + r^2\mathbb{Z} + \cdots + r^n\mathbb{Z}$ with $n \in \mathbb{N}$ and a fixed $r \in \mathcal{C}$ with $r^n = 1$. In particular, this leads to $\mathcal{R} = \mathbb{Z}$ for $n \in \{1, 2\}$, $\mathcal{R} = \mathbb{Z} + i\mathbb{Z}$ for $n = 4$, while $n \in \{3, 6\}$ lead to the same honeycomb grid $\mathcal{R}$, since 3 is odd and $\mathbb{Z} = -\mathbb{Z}$. Note that $n > 6$ is impossible as it leads to the existence of different $s, t \in \mathcal{R}$ with $|s - t| < 1$ and $n = 5$ has the same problem as its grid coincides with the one for $n = 10 > 6$.

In these special cases, Theorem 4.5 and Theorem 4.6 also hold for complex valued potentials. For a general theory on Dirichlet eigenvalues for complex valued potentials see [51] and [57].

4.2 Periodic potentials

We return to the setting of real-valued potentials. Now consider the case that v is K-periodic, meaning that $v(j + K) = v(j)$ for all $j \in \mathbb{Z}$ and some $K \in \mathbb{N}$, called the period of v. The resulting Schrödinger operator defined by (4.4) is then K-periodic in the sense of Section 2.5. Therefore, we can regard H as a block Laurent operator and use results for its spectrum such as Theorem 2.47 and 2.49. Additionally, we use methods from the theory of Schrödinger operators such as transfer matrices. The spectral theory of periodic Schrödinger operators is usually referred to as Floquet–Bloch theory, an overview is given in [102, Chapter 7] and [87, Chapter XIII.16].

Throughout this section assume v and H to be K-periodic. The spectral theory of such periodic Schrödinger operators is well-developed, see, e.g., [34, 81, 102]. Nevertheless, we give the reader an introduction such that this section mainly focuses on to the spectral theory of periodic Schrödinger operators with a new interpretation of these facts in the framework of limit operator theory. This section is based on joint work with Fabian Gabel, Dennis Gallaun, Julian Großmann and Marko Lindner [40].

4.2.1 Two-Sided periodic Schrödinger operators

We use the transfer matrices from (4.9):

$$T(n, E) := \begin{pmatrix} E - v(n) & -1 \\ 1 & 0 \end{pmatrix}.$$

We directly see that for each n and E the determinant of the transfer matrix is 1. Especially, this means that eigenvalues of a transfer matrix always come in pairs $\{\lambda_i, \lambda_i^{-1}\}$. For a periodic potential with period K, we define the monodromy matrix

$$M(E) := T(K, E) \cdots T(2, E)\, T(1, E)\,. \tag{4.12}$$

When it is clear from the context that we only consider the energy $E = 0$, we will write $T(n) := T(n, 0)$ and $M := M(0)$. Obviously, $M(E)$ brings us from $\binom{x_1}{x_0}$ to $\binom{x_{K+1}}{x_K}$, and then again from $\binom{x_{K+1}}{x_K}$ to $\binom{x_{2K+1}}{x_{2K}}$, and so on.

For the reader's convenience we restate parts of Proposition 2.45 applied to the Schrödinger operator H.

Lemma 4.11. *(a) Every limit operator of H is again a K-periodic Schrödinger operator and*

$$\mathrm{Lim}(H) = \{S^{-k}HS^k : k = 0, \dots, K-1\} = \mathrm{Lim}_+(H) = \mathrm{Lim}_-(H)\,.$$

(b) $\sigma(B) = \sigma(H) = \sigma_{\mathrm{ess}}(H)$ for all $B \in \mathrm{Lim}(H)$.

(c) H is invertible on $\ell^2(\mathbb{Z})$ if and only if H is injective on $\ell^\infty(\mathbb{Z})$.

We see that the restriction of the potential of a limit operator to $1..K$ is just a cyclic permutation of the restriction of v, the potential of H, to $1..K$. It is well known that the trace of a matrix product is invariant under cyclic permutations, which leads to the following result.

Corollary 4.12. *For $B \in \mathrm{Lim}(H)$ let $M_B(E)$ denote the monodromy matrix of B. Then we have the identity* $\mathrm{tr}(M_B(E)) = \mathrm{tr}(M(E))$ *for all $E \in \mathbb{R}$.*

Proof. From Lemma 4.11 it follows that the monodromy matrix for B is given by

$$M_B(E) = T(\tau(K-1), E) \cdots T(\tau(1), E)\, T(\tau(0), E)\,,$$

where $(\tau(K-1), \dots, \tau(1), \tau(0))$ is just a cyclic permutation of $(0, 1, \dots, K-1)$. Consequently, $\mathrm{tr}(M_B(E)) = \mathrm{tr}(M(E))$. □

We point out the equivalence given in Lemma 4.11(c): H is invertible if and only if there is no bounded sequence $x \neq 0$, such that $Hx = 0$. Therefore, the question of invertibility boils down to the existence of a bounded sequence, which can be characterized by the monodromy matrix.

Lemma 4.13. *There exists $x \in \ell^\infty(\mathbb{Z})$ with $x \neq 0$ and $Hx = 0$ if and only if there are some $\alpha, \beta \in \mathbb{R}$ such that*

(a) $(\alpha, \beta) \neq (0, 0)$ and

(b) the two-sided sequence $\left(M^n \begin{pmatrix}\alpha \\ \beta\end{pmatrix}\right)_{n\in\mathbb{Z}}$ is bounded.

Proof. Let $x \neq 0$ be a bounded solution of $Hx = 0$. By Lemma 4.1, at least one of x_0, x_1 has to be non-zero. Choose $\alpha = x_1$ and $\beta = x_0$. Then

$$\begin{pmatrix} x_{nK+1} \\ x_{nK} \end{pmatrix} = M^n \begin{pmatrix} x_1 \\ x_0 \end{pmatrix} \tag{4.13}$$

is clearly bounded as a sequence in $n \in \mathbb{Z}$.

For the other implication let x be the sequence generated by the three-term recursion (4.8) with initial values $x_1 = \alpha$ and $x_0 = \beta$, with α and β from (b). Then $x \neq 0$. To see that x is bounded, we again use (4.13) and obtain that the subsequence $\binom{x_{Kn+1}}{x_{Kn}}$ is bounded for $n \in \mathbb{Z}$. Now for any $j \in \mathbb{Z}$ $\binom{x_{j+1}}{x_j}$ can be obtained from $\binom{x_{Kn+1}}{x_{Kn}}$ by multiplication with at most $K-1$ transfer matrices for some $n \in \mathbb{Z}$. Hence, the entire sequence x is bounded. □

The following proposition resembles a well-known result about the spectrum of periodic Schrödinger operators, which can be described by a trace condition of the monodromy matrix, see, e.g., [81].

Proposition 4.14. *([40, Proposition 3.4]) Let* E *be real. Then* $E \in \sigma(H)$ *if and only if the so-called trace condition,* $|\mathrm{tr}(M(E))| \leq 2$*, holds.*

Proof. By Lemma 4.11(c), a real number E lies in the resolvent set if and only if $H - E$ is injective on $\ell^\infty(\mathbb{Z})$. Using Lemma 4.13, this is equivalent to the claim that for all $(\alpha, \beta) \neq (0, 0)$, the two-sided sequence

$$\left(M(E)^n \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \right)_{n \in \mathbb{Z}}$$

is unbounded. This is satisfied if and only if both eigenvalues λ_1, λ_2 of $M(E)$ fulfill $|\lambda_i| \neq 1$. Since $M(E)$ has determinant $\det(M(E)) = 1$ and its eigenvalues are reciprocal, this is equivalent to the characteristic polynomial $p(\lambda) = \lambda^2 - \mathrm{tr}(M(E))\lambda + 1$ having two distinct real solutions. Note here that two identical solutions would be ± 1 and two proper complex solutions would be λ_1, $\overline{\lambda_1}$ with product 1, hence $|\lambda_i| = 1$. However, having two distinct real solutions is equivalent to the discriminant of p being positive, which yields the condition $\mathrm{tr}(M(E))^2 > 4$. □

In the following examples, we illustrate the use of the trace condition from Proposition 4.14 for determining the spectrum of periodic Schrödinger operators.

Example 4.15. *([40, Example 3.5])*

(a) If the potential v *is constant with* $v(1) \in \mathbb{R}$*, which means* $K = 1$*, then* $\mathrm{tr}(M(E)) = E - v(1)$ *and* $\sigma(H) = [-2 + v(1), 2 + v(1)]$.

(b) If the potential v *has period* 2*, with* $v(1) = -1$ *and* $v(2) = 1$*, we get* $\mathrm{tr}(M(E)) = E^2 - 3$ *and* $\sigma(H) = [-\sqrt{5}, -1] \cup [1, \sqrt{5}]$.

(c) More generally, for a 2*-periodic potential, we have*

$$\mathrm{tr}(M(E)) = -2 + (E - v(1))(E - v(2))\,.$$

This shows that for $v(1) \neq v(2)$ *the spectrum consists of two intervals, namely*

$$\sigma(H) = \Big[\frac{1}{2}(v(1) + v(2) - \delta),\, \min\{v(1), v(2)\}\Big] \\ \cup \Big[\max\{v(1), v(2)\},\, \frac{1}{2}(v(1) + v(2) + \delta)\Big]\,,$$

where $\delta = \sqrt{16 + v(1)^2 - 2v(1)v(2) + v(2)^2}$ *denotes the discriminant of the polynomial* $\mathrm{tr}(M(E))$.

(d) For a potential v *with period* 3 *given by* $v(1) = 0$*,* $v(2) = 1$ *and* $v(3) = 0$*, we get* $\mathrm{tr}(M(E)) = E^3 - E^2 - 3E + 1$*. Therefore, the spectrum is given by* $\sigma(H) = [-\sqrt{3}, -1] \cup [1 - \sqrt{2}, 1] \cup [1 + \sqrt{2}, \sqrt{3}]$.

The previous example suggests that the spectrum of a K-periodic Schrödinger operator consists of K closed intervals. While this is not always exactly the case, we can say that the spectrum is a union of closed intervals, called bands. The following corollary shows that K is an upper bound on the number of bands.

Corollary 4.16. *([40, Corollary 3.6]) If H ist K-periodic then the spectrum consists of at most K bands. More precisely, there are numbers $a_1 \le b_1 \le a_2 \le \cdots \le a_K \le b_K$ with*

$$\sigma(H) = \bigcup_{i=1}^{K} [a_i, b_i] \, .$$

Proof. The trace of $M(E)$ gives us a polynomial p_K in the variable E with degree K. A real number E lies in $\sigma(H)$ if and only if $-2 \le p_K(E) \le 2$, by Proposition 4.14. The real zeros of the polynomials $p_K \pm 2$ give us the numbers $\{a_i, b_i\}_{i=1,\dots,K}$. □

In addition to the trace condition we can compute the spectrum of H with the Fourier transform as for any periodic band-dominated operator, see Theorem 2.49. To this end, we decompose H into a block Laurent operator with three blocks:

$$h_0 = H_{1..K}, \quad h_{-1} = \begin{pmatrix} & & \\ & & \\ 1 & & \end{pmatrix} \quad \text{and} \quad h_1 = \begin{pmatrix} & & 1 \\ & & \\ & & \end{pmatrix} .$$

Then the symbol h of H is given by

$$h(\varphi) := H_{1..K} + \begin{pmatrix} & & \mathrm{e}^{\mathrm{i}\varphi} \\ & & \\ \mathrm{e}^{-\mathrm{i}\varphi} & & \end{pmatrix} = \begin{pmatrix} v_1 & 1 & & & & \mathrm{e}^{-\mathrm{i}\varphi} \\ 1 & v_2 & 1 & & & \\ & 1 & v_3 & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & v_{K-1} & 1 \\ \mathrm{e}^{\mathrm{i}\varphi} & & & & 1 & v_K \end{pmatrix} \tag{4.14}$$

for any $\varphi \in [0, 2\pi]$. Now Theorem 2.49 yields that

$$\sigma(H) = \bigcup_{\varphi \in [0,2\pi]} \sigma(h(\varphi)). \tag{4.15}$$

In the analysis of Schrödinger operators this is referred to as Floquet-Bloch theory. For more details see, e.g., [31, Thm 4.4.9], [81] and [102, Chapter 7]. The assertion of Corollary 4.16 can also be drawn from (4.15) since $h(\varphi)$ has at most K real eigenvalues that depend continuously on φ.

One can show that $\operatorname{tr} M(E)$ attains the values ± 2 exactly at the eigenvalues of $h(\varphi)$ for $\varphi = 0$ and $\varphi = \pi$, see [102, Section 7.2].

Lemma 4.17. *[102, p. 121] Let $E_1^+ \le E_2^+ \le \cdots \le E_K^+$ be the eigenvalues of $h(0)$ and let $E_1^- \le E_2^- \le \cdots \le E_K^-$ be the eigenvalues of $h(\pi)$. Then*

$$\sigma(H) = [E_1^+, E_1^-] \cup [E_2^-, E_2^+] \cup \cdots \cup [E_K^\pm, E_K^\mp]$$

or

$$\sigma(H) = [E_1^-, E_1^+] \cup [E_2^+, E_2^-] \cup \cdots \cup [E_K^\mp, E_K^\pm],$$

where $\pm$ is the sign of $(-1)^{K+1}$ and $\mp$ is the sign of $(-1)^K$. Moreover, $E_j^+ = E_{j+1}^+$ if and only if $M(E_j^+) = I$ and $E_j^- = E_{j+1}^-$ if and only if $M(E_j^-) = -I$.

We see that the gaps of the spectrum of H are given by (E_j^+, E_{j+1}^+) or (E_j^-, E_{j+1}^-).

Definition 4.18. We call the interval $[E_j^+, E_{j+1}^+] \cap [E_j^-, E_{j+1}^-]$ the j-th gap of the spectrum of H. If the interior of a gap is non-empty we say the gap is open, otherwise we say that it is a closed gap.

It is clear from the above discussion that the boundary of a gap is part of the spectrum while the interior of a gap is in the resolvent set. In fact, every bounded component of $\mathbb{R} \cap \rho(H)$ corresponds to a gap as defined above. This correspondence is one-to-one if all gaps are open. Including the boundary points in the definition of a spectral gap might seem counterintuitive, but it turns out to be useful when analyzing the location of Dirichlet eigenvalues.

4.2.2 One-Sided Periodic Schrödinger operators

In this section, we consider the compressions H^+ and H^- of H on the spaces $\ell^2(\mathbb{N})$ and $\ell^2(\mathbb{Z}_-)$, respectively. The following lemma allows us to restrict ourselves to one of the two compressions, H^+ or H^-.

Lemma 4.19. *([40, Lemma 3.7]) Let H^{R} denote the Schrödinger operator with the reversed potential $v^{\mathrm{R}}(n) := v(-n+1)$, $n \in \mathbb{Z}$. Then*

(a) $\sigma(H) = \sigma(H^{\mathrm{R}})$,

(b) $\sigma(H^-) = \sigma((H^{\mathrm{R}})^+)$ *and*

(c) $\mathrm{tr}(M_H) = \mathrm{tr}(M_{H^{\mathrm{R}}})$.

Proof. Consider the flip operators

$$\Phi\colon \ell^p(\mathbb{Z}) \to \ell^p(\mathbb{Z}), \quad (x_n)_{n\in\mathbb{Z}} \mapsto (x_{-n+1})_{n\in\mathbb{Z}}$$

and

$$\Phi_-\colon \ell^p(\mathbb{N}) \to \ell^p(\mathbb{Z}_-), \quad (x_n)_{n\in\mathbb{N}} \mapsto (x_{-n+1})_{n\in\mathbb{Z}_-}\,.$$

Clearly, Φ and Φ_- are isomorphisms. The claims (a) and (b) follow from the identities $H = \Phi H^{\mathrm{R}} \Phi^{-1}$ and

$$H^- = \Phi_-(H^{\mathrm{R}})^+\Phi_-^{-1}\,,$$

which is a straightforward calculation.

To prove trace identity (c), we use that a transfer matrix $T = T(n, E)$ always has the property:

$$T^{-1} = FTF \quad \text{with} \quad F = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\,.$$

Hence, we also have $FM_HF = T(K-1)^{-1}\cdots T(0)^{-1} = M_{H^{\mathrm{R}}}^{-1}$. Taking the trace yields:

$$\mathrm{tr}(M_H) = \mathrm{tr}(FM_HF) = \mathrm{tr}\left(M_{H^{\mathrm{R}}}^{-1}\right) = \mathrm{tr}\left(M_{H^{\mathrm{R}}}\right)\,,$$

where the last equality holds for every real matrix with determinant 1. $\square$

Since H is right-self-similar, i.e. $H \in \operatorname{Lim}(H^+)$, the spectrum of H^+ contains that of H and maybe some additional eigenvalues. The latter clearly have something to do with the entries of H^+ near the cut-off. Indeed, the following proposition due to Hagger gives a characterization of the Dirichlet eigenvalues in terms of finite cut-off matrices as well as the monodromy matrix. It follows directly from [47, Section 4.2.3], where it is even stated for non-self-adjoint operators with three periodic diagonals.

Proposition 4.20. *([40, Proposition 3.8]) Assume for the period $K \geq 2$. Then*

$$\sigma(H^+) = \sigma(H) \cup \big\{E \in \mathbb{R} : M(E)_{2,1} = 0 \text{ and } |M(E)_{1,1}| < 1\big\}. \tag{4.16}$$

For the monodromy matrix we have the formula

$$M(E) = (-1)^{K+1} \begin{pmatrix} -\det(H_{1..K} - E) & -\det(H_{2..K} - E) \\ \det(H_{1..K-1} - E) & \det(H_{2..K-1} - E) \end{pmatrix}. \tag{4.17}$$

Proof. With the help of limit operators we quickly find that $\sigma(H) = \sigma_{\text{ess}}(H^+)$. Since the spectrum of H is real $\mathbb{C} \setminus \sigma_{\text{ess}}(H^+)$ is connected and thus unbounded. With this, identity (4.16) is a direct consequence of Theorem 2.50 as the tridiagonal matrix representation of H^+ has constant upper and lower diagonals.

The formula (4.17) is from [47, Section 4.2.3]. In a nutshell, the proof of Hagger is by induction, using that the entries of $M(E)$ and the determinants of the matrices both follow a recursion formula with the same coefficients:

$$\begin{aligned} (M_K(E)_{1,1} &= (E - v(K))(M_{K-1}(E))_{1,1} - (M_{K-1}(E))_{2,1} \\ &= (E - v(K))(M_{K-1}(E))_{1,1} - (M_{K-2}(E))_{1,1}, \\ \det(H_{1..K} - E) &= (E - v(K)) \det(H_{1..K-1} - E) - \det(H_{1..K-2} - E). \end{aligned}$$

Here $M_n(E) = T_n(E) \dots T_1(E)$. The second identity is an application of Laplace's expansion formula. For a more detailed proof in the self-adjoint case see also [36, Proposition 2.3.13].

Additionally, we provide an alternative proof for the identity

$$M(E)_{1,1} = (-1)^K \det(H_{1..K} - E), \tag{4.18}$$

following the ideas of [25, Proposition 2.2.5]. The determinant of $H_{1..K} - E$ is a monic polynomial with roots given by the eigenvalues of $H_{1..K}$. With Lemma 4.1 we see that these roots are simple. Hence, it remains to show that $\det(M(E))_{1,1})$ is also a monic polynomial of degree K with the same roots. The property that $(M(E))_{1,1}$ is a monic polynomial of degree K is a consequence of (4.12) and the structure of the transfer matrices. For an eigenvalue E_0 of $H_{1..K}$ with eigenvector $x \in \mathbb{C}^K$ we know that $x_1 \neq 0$, see Lemma 4.1. Then the Dirichlet boundary conditions at 0 and $K + 1$ mean that

$$\begin{pmatrix} 0 \\ x_n \end{pmatrix} = M(E_0) \begin{pmatrix} x_1 \\ 0 \end{pmatrix}.$$

In particular, $(M(E_0))_{1,1} = 0$. This means that the roots of $(M(E))_{1,1}$ are the eigenvalues of $H_{1..K}$ which are the roots of $\det(H_{1..K} - E)$. Thus, we have proven that $M(E)_{1,1} = \pm \det(H_{1..K} - E)$. From here, it can be seen that the sign of in (4.18) is given by $(-1)^K$. The identities for the other entries can be proven similarly. □

Note that our access to the essential spectrum $\sigma_{\text{ess}}(H^+)$ is always via limit operators, since it is often rather straightforward once the framework is understood. However, also other proofs for the essential spectrum are known, see, e.g., [98, Theorem 7.2.1].

As a consequence of Proposition 4.20 we see that a Dirichlet eigenvalue E of H is subject to two conditions:

(a) E is an eigenvalue of $H_{1..K-1}$ and

(b) $|\det(H_{1..K} - E)| < 1$.

Finding the Dirichlet eigenvalues can therefore be done in two steps. First, compute the eigenvalues of $H_{1..K-1}$ which we call the candidates for Dirichlet eigenvalues. Then check for each candidate whether condition (b) is fulfilled.

Definition 4.21. We call $E \in \mathbb{R}$ a (Dirichlet) candidate of H^+ if E is an eigenvalue of $H_{1..K-1}$ holds. The set of all candidates of H^+ is denoted by $\Omega(H^+)$.

Next, we present an application of Cauchy's interlacing property to K-periodic Schrödinger operator H. For $\varphi \in [0, 2\pi)$ let $H^{\varphi}_{1..K-1}$ denote $h(\varphi)$, the symbol of H from (4.14). We compare $H_{1..K-1}$ and $H^{\varphi}_{1..K}$. Both correspond to finite-dimensional restrictions of the operator equation with Dirichlet and periodic boundary conditions, respectively. Recall from above that $\sigma(H_{1..K-1})$ is a superset of the Dirichlet eigenvalues while $H^{\varphi}_{1..K}$ captures the spectrum of H when taking the union over $\varphi \in [0, 2\pi)$, see (4.15). Observe that $H_{1..K-1}$ is just a restriction of $H^{\varphi}_{1..K}$ to the subspace spanned by the first $K-1$ elements of the canonical basis. As a consequence, one finds the following classical interlacing result, cf. [102, Theorem 4.5].

Proposition 4.22. *The eigenvalues of $H_{0..K-2}$ and $H^{\varphi}_{0..K-1}$ are interlacing for every $\varphi \in [0, 2\pi]$, that is*

$$\widetilde{E}^{\varphi}_1 \leq E_1 \leq \widetilde{E}^{\varphi}_2 \leq E_2 \leq \cdots \leq E_{K-1} \leq \widetilde{E}^{\varphi}_K$$

where $E_1 \leq \cdots \leq E_{K-1}$ and $\widetilde{E}_{1,\varphi} \leq \cdots \leq \widetilde{E}_{K,\varphi}$ denote the eigenvalues of $H_{0..K-2}$ and $H^{\varphi}_{0..K-1}$, respectively.

Proof. The proof can be done analogously to [97, Proposition 2.2] by using the min-max principle, see Lemma 2.6. Accordingly, the eigenvalues of $H_{1..K-1}$ are given by:

$$E_k = \max_{D \in \mathcal{F}^{K-1}_{k-1}} \min \Big\{ \langle y, H_{1..K-1} y \rangle : y \in \mathbb{C}^{K-1}\,,\ y \perp D\,,\ \|y\| = 1 \Big\} \tag{4.19}$$

$$E_k = \min_{D \in \mathcal{F}^{K-1}_{K-1-k}} \max \Big\{ \langle y, H_{1..K-1} y \rangle : y \in \mathbb{C}^{K-1}\,,\ y \perp D\,,\ \|y\| = 1 \Big\}. \tag{4.20}$$

Here, $\mathcal{F}^N_m$ stands for the set of m-dimensional subspaces of $\mathbb{C}^N$ for $m \in \mathbb{N}$. We start by using (4.19): Since $H_{1..K-1}$ can be identified with $H^{\varphi}_{1..K}$ restricted to the subspace $\mathbb{C}^{K-1} \oplus 0$, we get the following inequality for a subspace $D \in \mathcal{F}^K_{k-1}$ and $k = 1, \ldots, K-1$ by

$$\begin{aligned}
&\min \Big\{ \langle y, H^{\varphi}_{1..K} y \rangle : y \in \mathbb{C}^K\,,\ y \perp D\,,\ \|y\| = 1 \Big\} \\
&\quad \leq \min \Big\{ \langle y, H^{\varphi}_{1..K} y \rangle : y = z \oplus 0 \in \mathbb{C}^{K-1} \oplus \mathbb{C}\,,\ y \perp D\,,\ \|y\| = 1 \Big\} \\
&\quad = \min \Big\{ \langle z, H_{1..K-1} z \rangle : z \in \mathbb{C}^{K-1}\,,\ z \perp P_{K-1}(D)\,,\ \|z\| = 1 \Big\},
\end{aligned}$$

where $P_{K-1}(D)$ is the orthogonal projection of D to $\mathbb{C}^{K-1}$. Taking the maximum over all subspaces $D \in \mathcal{F}^K_{k-1}$ on both sides, we get:

$$E^\varphi_k \leq E_k \quad \text{for } k = 1, \dots, K-1$$

Now with an analogue argument, we show the interlacing property by using (4.20). For a subspace $D \in \mathcal{F}^K_{K-k}$, we get:

$$\max\Big\{\langle y, H^\varphi_{1..K} y\rangle : y \in \mathbb{C}^K\,,\ y \perp D\,,\ \|y\| = 1\Big\}$$
$$\geq \max\Big\{\langle z, H_{1..K-1} z\rangle : z \in \mathbb{C}^{K-1}\,,\ z \perp P_{K-1}(D)\,,\ \|z\| = 1\Big\}.$$

Then taking the minimum on both sides, we obtain

$$E_{k-1} \leq E^\varphi_k \quad \text{for } k = 2, \dots, K$$

and the wanted result. ☐

Proposition 4.22 yields that the candidates for Dirichlet eigenvalues lie in the gaps of $\sigma(H)$.

Example 4.23. *Recall from Example 4.15(d) that the 3-periodic Schrödinger operator with potential* $v(1) = 0$, $v(2) = 1$, $v(3) = 0$ *has spectrum* $[-\sqrt{3}, -1] \cup [1-\sqrt{2}, 1] \cup [\sqrt{3}, 1+\sqrt{2}]$. *Solving* $\det(H_{1..2} - E) = E^2 - E - 1 = 0$ *yields the candidates* $E_{1,2} = \frac{1\pm\sqrt{5}}{2}$. *Checking whether* $|\det(H_{1..3} - E)| < 1$ *holds, we find that one of them is indeed a Dirichlet eigenvalue. We plot the spectrum*

$$\sigma(H^+) = \sigma(H) \cup \Big\{\frac{1-\sqrt{5}}{2}\Big\}.$$

in Figure 4.1.

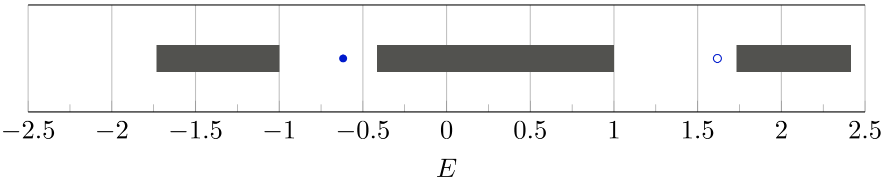

Figure 4.1: The spectrum of the 3-periodic operator H from Example 4.23 is plotted in gray. The Dirichlet eigenvalue is the blue dot, while the candidate $E = (1+\sqrt{5})/2$ that is not an eigenvalue is displayed as green circle.

Example 4.24. *Consider a 2-periodic Schrödinger operator H as in Example 4.15(c). For the spectrum of H^+, we calculate, according to Proposition 4.20,*

$$\sigma(H_{1..2-1}) = \sigma\big(v(1)\big) = \{v(1)\}$$

and

$$\det(H_{1..2} - v(1)) = \det\left(\begin{pmatrix} v(1) - v(1) & 1 \\ 1 & v(2) - v(1)\end{pmatrix}\right) = -1.$$

The first identity means that the only candidate is located at $v(1)$, which is also part of the spectrum. Together with the second identity this implies $\sigma(H^+) = \sigma(H)$, meaning that no 2-periodic Schrödinger operator has Dirichlet eigenvalues.

In Example 4.24 we encountered a candidate for a Dirichlet eigenvalue which also lies in the spectrum of H. This is peculiar since by Lemma 4.22 the candidates always lie in the gaps. This means that in this case the candidate lies on the edge of a spectral band. It turns out that this setting prohibits the candidate from becoming a Dirichlet eigenvalue.

Corollary 4.25. *Let $E \in \Omega(H_+)$. E is also in the spectrum of H if and only if $|\det(H_{1..K} - E)| = 1$. In particular, if $|\operatorname{tr}(M(E))| \leq 2$ then E is not a Dirichlet eigenvalue.*

Proof. Since E is a candidate, it is an eigenvalue of $H_{1..K-1}$. Using Proposition 4.20 together with the condition $E \in \sigma(H_{1..K-1})$ we find that $M(E)$ is of the form

$$M(E) = (-1)^{K+1} \begin{pmatrix} -\det(H_{1..K} - E) & -\det(H_{2..K} - E) \\ 0 & \det(H_{2..K-1} - E) \end{pmatrix} .$$

As a consequence, the eigenvalues of $M(E)$ are $-\det(H_{1..K} - E)$ and $\det(H_{2..K-1} - E)$. The proof of Proposition 4.14 shows that if $E \in \sigma(H)$ then both these eigenvalues of $M(E)$ lie on the unit circle. We thus find that $|\det(H_{1..K} - E)| = 1$ which, together with Proposition 4.20 concludes the proof. □

In the light of the previous corollary we move focus of our analysis of the Dirichlet eigenvalues away from the spectrum of H, i.e. where $|\operatorname{tr}(M(E))| < 2$ holds. Note that we can always restrict to the case $E = 0$ by adding or subtracting constants from the potential. Also recall that $M \coloneqq M(0)$ abbreviates the monodromy matrix for energy $E = 0$.

Proposition 4.26. *([40, Proposition 3.11]) If H is invertible, that is, $|\operatorname{tr}(M)| > 2$, the following are equivalent:*

(i) *the compression H^+ is not injective on $\ell^\infty(\mathbb{N})$,*

(ii) *the compression H^+ is not invertible on $\ell^2(\mathbb{N})$,*

(iii) $M_{2,1} = 0$ *and* $|M_{1,1}| < 1$,

(iv) $\binom{1}{0}$ *is an eigenvector of M w.r.t. eigenvalue λ with $|\lambda| < 1$.*

Proof. Recall from Proposition 2.20 that the invertibility of H^+ on $\ell^p(\mathbb{N})$ is independent of $p \in [1, \infty]$. With that in mind, (i)⇒(ii) follows directly. For (ii)⇒(i) we use that the invertibility of H implies that H_+ is a Fredholm operator on $\ell^\infty(\mathbb{N})$. Hence, H_+ has closed range but is not invertible. As a self-adjoint operator, H_+ can therefore not be injective.

The equivalence of (ii) and (iii) can be seen directly by Proposition 4.20.

Lastly, (iii)⇔(iv) is obvious: the 2×2-matrix M has the eigenvector $\binom{1}{0}$ if and only if $M_{2,1} = 0$. The corresponding eigenvalue is then $M_{1,1}$.

□

Note that $|M_{1,1}| = 1$ is impossible in Proposition 4.26(iii) if $M_{2,1} = 0$ because, by $\det(M) = 1$, then both eigenvalues of M would have to have modulus one, contradicting $|\operatorname{tr}(M)| > 2$.

In the following we will study periodic potentials that take on only two different values. A main ingredient will be the equivalence of the negations of Proposition 4.26(ii) and (iii):

$$H^+ \text{ is invertible on } \ell^2(\mathbb{N}) \quad \Longleftrightarrow \quad M_{2,1} \neq 0 \text{ or } |M_{1,1}| > 1 . \tag{4.21}$$

4.2.3 The FSM for periodic Schrödinger operators with binary potentials

We examine the properties of Dirichlet eigenvalues and the applicability of the FSM for periodic Schrödinger operators with $\{0,1\}$-valued potentials and their relatives. Such operators can be used for the approximation of aperiodic Schrödinger operators, see Section 4.3. To balance between the Laplace interaction term and the pointwise multiplication by the potential, one often introduces a so-called coupling constant $\lambda > 0$ as a weight for the $\{0,1\}$-valued potential v. The result is a discrete Schrödinger operator with a $\{0,\lambda\}$-valued potential which we call a binary potential.

For $K \in \mathbb{N}$ and $w \in \{0,1\}^K$, let $v \in \{0,\lambda\}^{\mathbb{Z}}$ be the periodic extension of λw. We consider the discrete Schrödinger operator H with potential v. Note that we do not specify λ yet but keep it as a variable during most of the following computations.

Let us consider projection methods for H. Since H is periodic, we directly find that the periodic finite section method is applicable to H if the dimensions of the finite operators are multiples of the period of the potential, see Corollary 3.36. Regarding the finite section method the situation is different. Recall from Theorem 3.24 that the stability indicators for the FSM, $\mathcal{I}_{\text{stab}}(H)$, are given by

(S1) H,

(S2) all L^+ with $L \in \operatorname{Lim}_-(H)$,

(S3) all R^- with $R \in \operatorname{Lim}_+(H)$.

So for the applicability of the FSM we need to look at the union of spectra

$$\sigma(H) \quad \cup \bigcup_{B\in\operatorname{Lim}(H)} \left(\sigma(B^+) \cup \sigma(B^-)\right). \tag{4.22}$$

In order to apply the results of Section 4.2.2 for the invertibility of one-sided periodic Schrödinger operators recall from Lemma 4.19 that we can replace the operator B^- with $\widetilde{B}^+$ in (4.22), where $\widetilde{B} = B^{\mathrm{R}}$ is the Schrödinger operator with the reversed potential. Additionally, consider the matrices

$$M^{(j)} = \begin{pmatrix} -v(j+K) & -1 \\ 1 & 0 \end{pmatrix} \cdots \begin{pmatrix} -v(j+2) & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} -v(j+1) & -1 \\ 1 & 0 \end{pmatrix} \tag{4.23}$$

$$\widetilde{M}^{(j)} = \begin{pmatrix} -v(j+1) & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} -v(j+2) & -1 \\ 1 & 0 \end{pmatrix} \cdots \begin{pmatrix} -v(j+K) & -1 \\ 1 & 0 \end{pmatrix} \tag{4.24}$$

for $j \in \mathbb{Z}$. Recall from Proposition 4.20 that the Dirichlet eigenvalues are captured by the condition

$$M_{2,1} \neq 0 \qquad \text{or} \qquad |M_{1,1}| > 1\,. \tag{4.25}$$

Theorem 4.27. *([40, Theorem 1.3]) Let H be a K-periodic discrete Schrödinger operator on $\ell^2(\mathbb{Z})$. In addition, let $M^{(j)}$ and $\widetilde{M}^{(j)}$ be given by* (4.23) *and* (4.24)*. Then the following holds:*

(a) The FSM is applicable to H if and only if $|\operatorname{tr}(M^{(0)})| > 2$ and

$$M^{(0)}, \ldots, M^{(K-1)} \text{ and } \widetilde{M}^{(0)}, \ldots, \widetilde{M}^{(K-1)} \text{are subject to (4.25).}$$

(b) The FSM is applicable to H^+ if and only if $|\operatorname{tr}(M^{(0)})| > 2$ *and*

$$M^{(0)} \textit{ and } \widetilde{M}^{(0)}, \dots, \widetilde{M}^{(K-1)} \textit{are subject to } (4.25)\,.$$

Proof. We start with statement (a). Recall that invertibility of H is characterized by the trace formula thanks to Proposition 4.14. Consequently, we assume H to be invertible for the rest of the proof.

In order to complete the proof of (a), we want to use Proposition 4.26 in order to conclude that the invertibility of the one-sided compressions L^+ and $\widetilde{R}^+$ is characterized by the condition (4.25) for their respective monodromy matrices.

Indeed, the limit operators are again periodic Schrödinger operators. Moreover, they are invertible by Theorem 2.32. As a result, Proposition 4.26 applies and all compressions L^+ and $\widetilde{R}^+$ are invertible if and only if their monodromy matrices M_L and $M_{\widetilde{R}}$ are subject to condition (4.25). It is not hard to see that for each $L \in \operatorname{Lim}_-(H)$ the corresponding monodromy matrix M_L is one of the matrices $M^{(j)}$ in (4.23) with $j = 1 \dots K$ and vice versa. The same holds for the matrices $M_{\widetilde{R}}$ and those in (4.24). More precisely, $L = S_{-j} H S_j$ for some $j \in \{0, \dots, K-1\}$ which yields $M_L = M^{(j)}$. Analogously, $\widetilde{M}^{(j)} = M_{\widetilde{R}}$ with limit operator $R = S^{j-1} H S^{-j+1} \in \operatorname{Lim}_+(H)$. For statement (b), we employ Corollary 3.25 which characterizes applicability of the FSM to H^+ by invertibility of H^+ and of its limit operators $\widetilde{R}^+$ for $R \in \operatorname{Lim}_+(H)$. As in the proof of part (a), the invertibility of H^+ and the limit operators $\widetilde{R}^+$ is characterized by the condition (4.25) through Proposition 4.26.

□

We have seen in Example 4.24 that the compressions of 2-periodic Schrödinger operators do not have any Dirichlet eigenvalues. As a consequence, we get the following result.

Proposition 4.28. *([40, Theorem 1.1(c)]) Let H be a discrete Schrödinger operator with 2-periodic potential v. Then H is FSM-simple.*

Proof. This follows from the fact that the limit operators of H are again 2-periodic Schrödinger operators that are invertible assuming H is invertible. Then also the invertibility of their compressions follows due to the computations in Example 4.24. Since these compressions, together with H itself, make up the stability indicators of the FSM for H, see Theorem 3.24, we find that the FSM is applicable to H if H is invertible. □

Note that H is right-self-similar and therefore Corollary 3.26 holds: if H is FSM-simple then H^+ is also FSM simple. If the potential has some invariance under reflection such that the matrices in (4.23) and (4.24) are the same then the converse implication also holds. In order to make this more precise, we need the following definition.

Definition 4.29. For $K \in \mathbb{N}$ we call $w \in \mathbb{R}^K$ a palindrome if

$$w = (w_1, w_2, \dots, w_K) = (w_K, \dots, w_2, w_1) =: w^{\mathrm{R}}.$$

Corollary 4.30. *If $v \in \mathbb{R}^{\mathbb{Z}}$ is the periodic extension of a palindrome, meaning that the finite word $v_j \dots v_{j+K}$ is a palindrome for some $j \in \mathbb{Z}$, then the FSM is applicable to H if and only if it is applicable to H^+.*

4.2.4 Examples

Theorem 4.27 shows how the quantities $\sigma(H)$, $\sigma(B_+)$ and $\sigma(B_-)$ of (4.22) can be computed. We know from Section 4.2.2 that $\sigma(H)$ consists of at most K closed spectral bands. Further, for each $B \in \mathrm{Lim}(H)$, the spectra $\sigma(B_+)$ and $\sigma(B_-)$ are supersets of $\sigma(B) = \sigma(H)$, only larger by at most one Dirichlet eigenvalue per spectral gap. In this section we will do these computations for four periodic Schrödinger operators.

The first example was announced in Section 4.1, where we claimed that when passing from integer-valued to rational-valued potentials the operator H is no longer necessarily FSM-simple.

Example 4.31. *([40, Example 4.2]) The* 3*-periodic Schrödinger operator* H *with continuously repeated potential* $v(1) = 2$, $v(2) = \frac{1}{2}$, *and* $v(3) = \frac{1}{2}$ *has monodromy matrices*

$$M^{(0)} = \begin{pmatrix} 2 & \frac{3}{4} \\ 0 & \frac{1}{2} \end{pmatrix}, \quad M^{(1)} = \begin{pmatrix} 2 & 0 \\ -\frac{3}{4} & \frac{1}{2} \end{pmatrix}, \quad M^{(2)} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 2 \end{pmatrix}.$$

The trace of $M^{(0)}$ *is* $2 + \frac{1}{2} = \frac{5}{2} > 2$, *whence* H *is invertible. The traces of* $M^{(1)}$ *and* $M^{(2)}$ *are, of course, also* $\frac{5}{2}$. *However, for the Dirichlet eigenvalues we compute*

$$M^{(2)}_{2,1} = 0 \qquad \textit{and} \qquad |M^{(2)}_{1,1}| = \frac{1}{2} < 1$$

so that $M^{(2)}$ *fails the test* (4.25), *whence one particular* L^+ *with* $L \in \mathrm{Lim}_-(H)$ *is not invertible, by Proposition 4.20. More precisely,* $L^+ = (S^{-2}HS^2)^+ = (H_l)^+$ *with* $l = (l_n) = (-3n + 2)$.

The word $v(2)v(3)v(4)$ *is a palindrome and therefore the FSM is also applicable to* H^+. *Indeed, it is easy to check that* $\widetilde{M}^{(2)} = M^{(2)}$ *so that also* $\widetilde{M}^{(2)}$ *fails* (4.25). *This means that* $R^- = H^- = (H_r)^-$ *with* $r = (r_n) = (3n + 2)$ *is not invertible.*

By Theorem 4.27(a), the full FSM is not applicable to H *– although* H *is invertible. Hence,* H *is not FSM-simple.*

One further checks that the matrices $\widetilde{M}^{(0)} = M^{(1)}$ *and* $\widetilde{M}^{(1)} = M^{(0)}$ *pass the test* (4.25) *which allows to conclude that the applicability of the FSM only fails because of the two "bad" compressions of the limit operators* H_l *and* H_r *identified above. However, with the detailed knowledge about the underlying "bad" sequences* $(l_n) = (-3n + 2)$ *and* $(r_n) = (3n + 2)$ *corresponding to these limit operators, we can choose cut-off sequences* (l'_n) *and* (r'_n) *that asymptotically the remainders of* $l'_n/3$ *and* $l'_n/3$ *is not* 2. *Then the FSM with cut-off sequences* (l'_n) *and* (r'_n) *is applicable to* H.

We continue with three examples that have binary potentials, i.e. they only take values in $\{0, \lambda\}$. In the first one, λ is irrational.

Example 4.32. *([40, Example 4.4]) The* 5*-periodic Schrödinger operator* H *with* $(v(1), v(2), v(3), v(4), v(5)) = \frac{1}{\sqrt{2}}(1, 1, 0, 1, 0)$ *has five monodromy matrices* $M^{(0)}$ *to* $M^{(4)}$ *and five reversed order monodromy matrices* $\widetilde{M}^{(0)}$ *to* $\widetilde{M}^{(4)}$. *All ten matrices have the trace* $-\frac{3}{\sqrt{2}} \notin [-2, 2]$, *implying that* H *is invertible. But the first monodromy matrix*

$$M^{(0)} = \begin{pmatrix} -\frac{1}{\sqrt{2}} & -1 \\ 0 & -\sqrt{2} \end{pmatrix} = \widetilde{M}^{(3)}$$

fulfills $M^{(0)}_{2,1} = 0$ *and* $|M^{(0)}_{1,1}| < 1$*. We conclude that the FSM is not applicable. Here one* L^+ *and one* R^- *are not invertible. One can check that the other matrices* $M^{(j)}$ *and* $\widetilde{M}^{(j)}$ *pass the test* (4.25)*, though. Again we find that this operator* H *is not FSM-simple. We plot the set* (4.22) *with varying* λ *for this operator in Figure 4.2.*

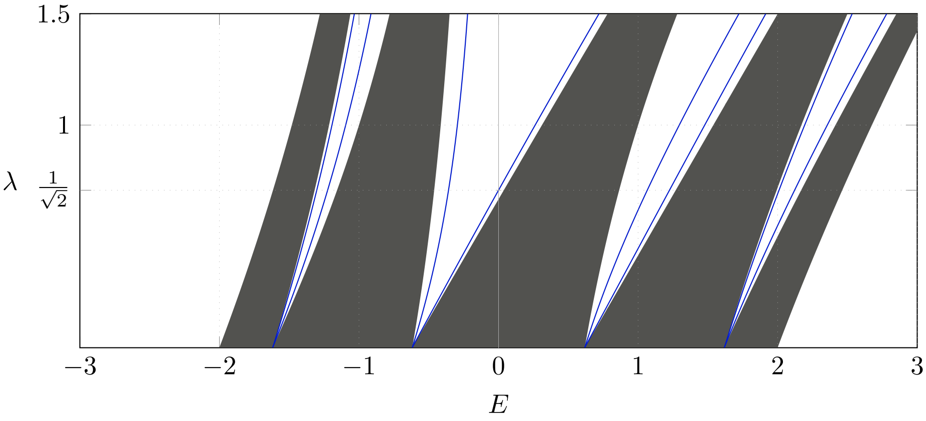

Figure 4.2: ([40, Figure 2]) Union (4.22) of spectra for H with potential $v = \lambda \cdot (1, 1, 0, 1, 0)$, periodically extended, while λ changes along the vertical axis. The spectral bands are shown in gray and the Dirichlet eigenvalues in blue. This time we see that one Dirichlet eigenvalue crosses the vertical line at energy $E = 0$ and height $\lambda = \frac{1}{\sqrt{2}}$. Since the plot at that point is blue but not gray, we find that the FSM is not applicable despite H being invertible, see Example 4.32. In Section 4.2.5, we detect this value of λ algebraically.

Next, let us move to rational λ. We will show in the next section that this guarantees that H is FSM simple for $K \leq 8$. However, for $K = 9$ we present a counterexample.

Example 4.33. *([40, Example 4.5]) Consider the* 9*-periodic potential* v *with* $(v(1), \dots, v(9)) = \frac{1}{2}(1, 1, 0, 1, 0, 1, 0, 1, 1)$*. For the corresponding Schrödinger operator* H *the monodromy matrix has trace equal to* $-\frac{5}{2} \notin [-2, 2]$*, whence* H *is invertible. Since* v *is the periodic extension of a palindrome we get* $M^{(j)} = \widetilde{M}^{(-j)}$ *for all* j*. The* $(2, 1)$*-entry of* $M^{(j)}$ *is zero for* $j = 0$ *and for* $j = 1$*:*

$$M^{(0)} = \begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & -2 \end{pmatrix} = \widetilde{M}^{(0)}, \qquad M^{(1)} = \begin{pmatrix} -2 & -\frac{3}{4} \\ 0 & -\frac{1}{2} \end{pmatrix} = \widetilde{M}^{(1)}.$$

Furthermore, the $(1, 1)$*-entry of* $M^{(0)}$ *is less than one in modulus. Consequently, the FSM does not apply to* H*, so that* H *is not FSM-simple. The same holds for* H^+*, see Corollary 4.30. We plot the set* (4.22) *for* H *in Figure 4.3. At* $E = 3$ *and* $\lambda = 2$*, two spectral bands merge into one before breaking up again.*

Lastly, we consider a potential that leads to a Schrödinger operator H that is not FSM-simple while its compression H^+ is FSM-simple.

Example 4.34. *([40, Example 4.6]) Consider the* 9*-periodic potential with* $(v(1), \dots, v(9)) = \frac{1}{\sqrt{2}}(1, 1, 1, 0, 1, 1, 0, 1, 0)$*. For the corresponding Schrödinger operator* H *we readily check that*

$$M^{(1)} = \begin{pmatrix} -\frac{1}{\sqrt{2}} & 2 \\ 0 & -\sqrt{2} \end{pmatrix}$$

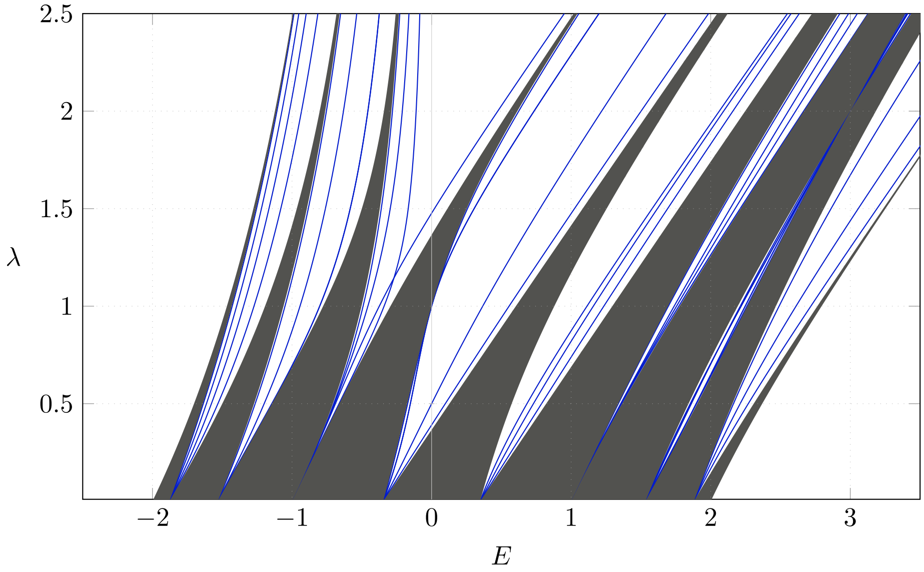

Figure 4.3: ([40, Figure 3]) Union (4.22) of spectra for H with the periodic extension of $\lambda \cdot (1, 1, 0, 1, 0, 1, 0, 1, 1)$, while λ changes along the vertical axis. The spectral bands are shown in gray and the Dirichlet eigenvalues in blue. This time we see that one Dirichlet eigenvalue crosses the vertical line at energy $E = 0$ and height $\lambda = \frac{1}{2}$. So, for $\lambda = \frac{1}{2}$, H is invertible (not gray) but the FSM is not applicable (blue). Unlike for periods $K < 9$, this crossing happens at a rational value of λ. In Section 4.2.5, we show how to detect these examples algebraically, and in Example 4.33 it is proven that this operator with $\lambda = \frac{1}{2}$ is indeed not FSM-simple.

and therefore, as in Example 4.32, the FSM is not applicable to H. *However, in contrast to Example 4.32, there is no* $j \in \{0, \dots, K-1\}$ *such that* $\widetilde{M}^{(j)} = M^{(1)}$. *In fact, one can check that the conditions of Theorem 4.27(b) are satisfied, i.e. that the FSM is applicable to* H^+. *For an extensive list of all matrices* $M^{(j)}$ *and* $\widetilde{M}^{(j)}$ *see [37].*

In this computation, we assume that the finite vector $\frac{1}{\sqrt{2}}(1, 1, 1, 0, 1, 1, 0, 1, 0)$ *forms entries* $v(1), \dots, v(9)$ *of the potential. If we place it at* $v(0), \dots, v(8)$ *then the corresponding* $M^{(0)}$, *instead of* $M^{(1)}$, *fails the test* (4.25), *so that* H^+ *is not invertible, whence the FSM is not applicable to it.*

The periodic Schrödinger operators presented in this section were a result of an algorithmic analysis of binary, more precisely $\{0, \lambda\}$-valued potentials. We present this approach together with its results in the next section.

4.2.5 Systematic studies of binary potentials

In this section, we show an algorithm to find examples like Examples 4.32 and 4.33 that are not FSM-simple. For a fixed K the algorithm checks every possible K-periodic binary potential, it can even be used to prove a positive result by not finding such examples.

Schrödinger operators with constant potential are just the free Laplacian from Example 4.2 for some energy E. In this case the applicability of the FSM is straightforward: H is FSM-simple and invertible if the diagonal entry is outside $[-2, 2]$. Thus, we assume for the period that $K \geq 2$.

Taking $E = 0$ and computing the monodromy matrix M according to (4.12) we obtain a 2×2 matrix with entries that are polynomials in λ. Due to (4.21), we are particularly interested in values λ where $M_{2,1} = 0$. Computing roots of a polynomial is in general a hard task, so let us take a closer look at the polynomial $M_{2,1}(\lambda)$. We say a polynomial p is even if $p(x) = p(-x)$ for all $x \in \mathbb{R}$. If $p(x) = -(p(-x))$ for all x in $\mathbb{R}$ then we say that p is odd.

Lemma 4.35. *The degree of* $M_{2,1}$ *is at most* $K - 1$ *and* $M_{2,1}$ *is an even or an odd polynomial.*

Proof. For $j \in \mathbb{N}$ we write

$$M^{(j)} = T(j) \cdots T(2)\,T(1)$$

Recall from the definition of the monodromy matrix that

$$M = M^{(K)} = T(K)\,T(K-1) \cdots T(2)\,T(1) = \begin{pmatrix} -v(K) & -1 \\ 1 & 0 \end{pmatrix} M^{(K-1)}\,. \tag{4.26}$$

This means that $M_{2,1} = M_{1,1}^{(K-1)}$. Thus, the statement about the degree of $M_{2,1}$ will follow once $\deg(M_{1,1}^{(j)}) \leq j$ is established for all $j \in \mathbb{N}$. This can be done by induction. The base case is clear since $M_{1,1}^{(1)}$ is either 0 or λ. For the induction step assume that $\deg(M_{1,1}^{(k)}) \leq k$ for all $1 \leq k \leq j$. We can argue as above to get that $\deg(M_{2,1}^{(k)}) \leq k - 1$, the case $k = 1$ follows directly from the definition of the transfer matrix. Now, by (4.26), $M_{1,1}^{(j+1)}(\lambda) = -\lambda M_{1,1}^{(j)}(\lambda) - M_{2,1}^{(j)}(\lambda)$ and therefore $\deg((M)_{1,1}^{(j+1)}) \leq j + 1$. This concludes the proof for the bound on the degree of $M_{2,1}$.

It remains to show that $M_{2,1}$ is even or odd. The procedure is similar as above. We also show that $M_{1,1}$ is odd when $M_{2,1}$ is even and even when $M_{2,1}$ is odd. The proof is again for all $M^{(j)}$ by induction over j. For the base case the structure of the transfer matrix, $M_{2,1}^{(1)} = 1$ is even and $M_{1,1}^{(1)} = v(1)$ is λ or 0. For the induction step assume we need to cover two cases: either

(a) $M_{1,1}^{(j)}$ is even and $M_{2,1}^{(j)}$ is odd or

(b) $M_{1,1}^{(j)}$ is odd and $M_{2,1}^{(j)}$ is even.

In the first case the formula $M_{1,1}^{(j+1)} = -v(j+1)M_{1,1}^{(j)} - M_{2,1}^{(j)}$ yields that $M_{1,1}^{(j)}$ is odd. Since $M_{2,1}^{(j+1)} = M_{1,1}^{(j)}$ is even the first case is covered. The second case can be checked analogously. □

As a consequence of Lemma 4.35 the roots of $M_{2,1}$ can be computed even if the degree exceeds 4. For even polynomials the substitution $\mu = \lambda^2$ can be used to reduce the degree from 6 or 8 to 3 or 4. The same can be done for odd polynomials after factoring out the trivial root $\lambda = 0$. Therefore, the roots of $M_{2,1}$ can be computed up to a degree of 9, which corresponds to period $K = 10$.

Due to the exponential growth of the set of K-periodic potentials in K we demonstrate the procedure for period $K = 3$ in Table 4.1. Whenever the value of K is clear from context we abbreviate $w := (v(1), \ldots, v(3))$.

We conclude that, for all 3-periodic binary potentials

$$M_{2,1} = 0 \qquad \overset{\text{Table 4.1}}{\Longrightarrow} \qquad |\operatorname{tr}(M)| = 2 \tag{4.27}$$

holds. Together with Corollary 4.25 this excludes the existence of any Dirichlet eigenvalue.

Recall that all $L \in \operatorname{Lim}_-(H)$ and all $\widetilde{R} \in \operatorname{Lim}_-(H^{\mathrm{R}})$ are again 3-periodic Schrödinger operators with $\{0, \lambda\}$-valued potential. Hence, they can also be found in Table 4.1. Moreover, they are invertible if H is invertible by Theorem 2.32. With the same arguments we can derive that

w	M	zeros of $M_{2,1}$	$\mathrm{tr}(M)$	at candidates
$(0,0,0)$	$\left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$	$\varnothing$	0	
$(0,0,1)$	$\left(\begin{smallmatrix} \lambda & 1 \\ -1 & 0 \end{smallmatrix}\right)$	$\varnothing$	λ	
$(0,1,0)$	$\left(\begin{smallmatrix} 0 & 1 \\ -1 & \lambda \end{smallmatrix}\right)$	$\varnothing$	λ	
$(0,1,1)$	$\left(\begin{smallmatrix} \lambda & -\lambda^2+1 \\ -1 & \lambda \end{smallmatrix}\right)$	$\varnothing$	2λ	
$(1,0,0)$	$\left(\begin{smallmatrix} \lambda & 1 \\ -1 & 0 \end{smallmatrix}\right)$	$\varnothing$	0	
$(1,0,1)$	$\left(\begin{smallmatrix} 2\lambda & 1 \\ -1 & 0 \end{smallmatrix}\right)$	$\varnothing$	2λ	
$(1,1,0)$	$\left(\begin{smallmatrix} \lambda & 1 \\ \lambda^2-1 & \lambda \end{smallmatrix}\right)$	$\{-1,1\}$	2λ	$\{-2,2\}$
$(1,1,1)$	$\left(\begin{smallmatrix} -\lambda^3+2\lambda & -\lambda^2+1 \\ \lambda^2-1 & \lambda \end{smallmatrix}\right)$	$\{-1,1\}$	$-\lambda^3+3\lambda$	$\{-2,2\}$

Table 4.1: Procedure to find Dirichlet eigenvalues for 3-periodic potentials. The third column shows the candidates for each potential. Since at each candidate the trace condition is fulfilled there is no Dirichlet eigenvalue, see Corollary 4.25.

all corresponding compressions $L_{\pm}$ and $\widetilde{R}_{+}$ are invertible if H is invertible. With Theorem 3.24 and the identification of R_{-} with $\widetilde{R}_{+}$ as in the proof of Theorem 4.27 we can conclude that H is FSM-simple whenever $K = 3$.

For $K = 4$, the corresponding table is easily computed and shows the same implications. As an illustration, Figure 4.4 shows the 4-periodic example given by $w = (1,1,0,1)$. In this case, we get

$$M = \begin{pmatrix} -2\lambda^2 + 1 & -2\lambda \\ \lambda & 1 \end{pmatrix},$$

so that $\lambda = 0$ is the only zero of $M_{2,1}$. In this case, however $\mathrm{tr}(M) = 2$. After checking the other 15 cases of $w \in \{0,1\}^4$ in the same manner, we get the same implication (4.27). With the same arguments as in the 3-periodic case, we find that H is also FSM-simple if $K = 4$.

The number of cases for period K is obviously 2^K. In order to draw conclusion for larger K we implemented the algorithm described above in the computer algebra system *SageMath*, cf. [33]. Recall from Lemma 4.35 and the discussion thereafter that all computations can be made purely symbolic. A complete study of up to 9-periodic potentials together with the code are published in [37]. It proves the following result:

Theorem 4.36. *([40, Theorem 1.1]) Let H be a periodic discrete Schrödinger operator on with potential v that only takes values in $\{0, \lambda\}$.*

(a) If $K \leq 4$ then H is FSM simple for any $\lambda \in \mathbb{R}$.

(b) If $K \leq 8$ then H is FSM simple for any $\lambda \in \mathbb{Q}$.

Remark 4.37. Recall from Theorem 4.6 that H is FSM simple for any integer valued potential. Now Theorem 2.49 shows that if the potential is binary and periodic with period less than nine then we can move away from integers to rationals. For periods less than five we can even include irrational λ. The bounds $K = 4$ and $K = 8$ are sharp, however, as Examples 4.32 and 4.33 show.

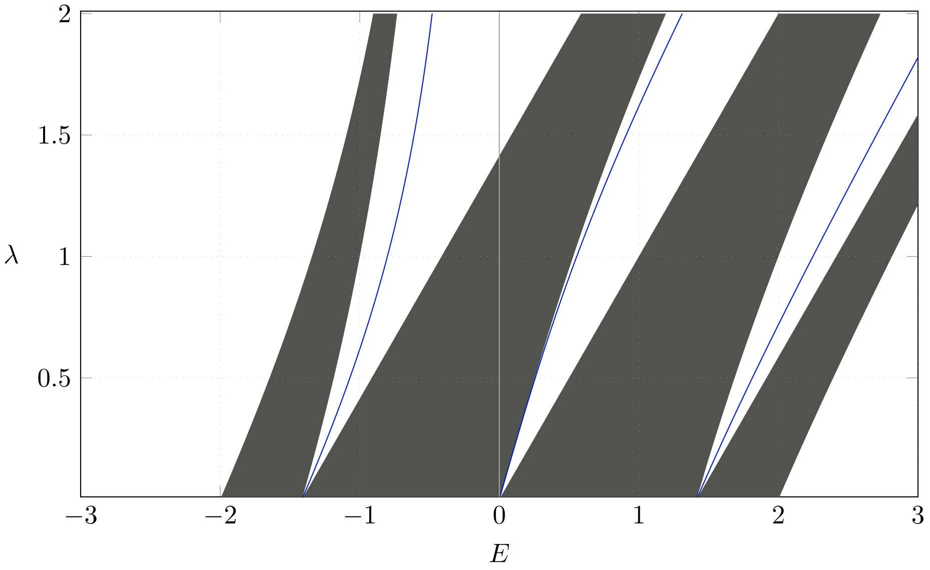

Figure 4.4: ([40, Figure 1]) Union (4.22) of spectra for H with potential $v = \lambda \cdot (1, 1, 0, 1)$, periodically extended, while λ changes along the vertical axis. The spectral bands are shown in gray and the Dirichlet eigenvalues in blue. If we look at the vertical line at energy $E = 0$ we see no blue line crossing outside the gray area. Thus, the plot suggests that, whenever H is invertible, then also all the B_+ and B_- are invertible. We conclude that H is FSM-simple.

4.3 Aperiodic potentials

In contrast to periodic potentials, cf. Section 4.2, and pseudoergodic potentials, cf. Section 3.3, the definition of aperiodicity is much less straightforward. Usually, the term is used when referring to something that is deterministic and not periodic. In many works some additional structure is required. For a broad overview see [53].

We will start by introducing Sturmian potentials, an important class of aperiodic potentials. The most famous member of this class is the Fibonacci Hamiltonian that possesses even more structure than most Sturmian words since it lies in the intersection with another class of aperiodic potentials, so-called substitution potentials.

A common theme among both classes of potentials is that they permit a natural approximation by periodic operators without spectral pollution. By proving this we recover results of Sütő [100], Bellissard [10], Beckus [8] and Kellendonk [54] on the spectral approximation on the axis as well as on the half-axis by different means. We will use limit operator techniques introduced in Section 2.4.3 and the approximation of spectral quantities via the approximation of submatrices that was discussed in Section 3.1. Lastly, we will study the location of the Dirichlet eigenvalues extensively, find a new interlacing property and connect the results to the applicability of the FSM.

Schrödinger operators with aperiodic potentials can be used to model quasicrystals. The most famous example of an aperidodic structure for such a two-dimensional quasicrystal is the so-called Penrose tiling, cf. [99]. The standard one-dimensional quasicrystal model on $\ell^2(\mathbb{Z})$ is a discrete Schrödinger operator with Sturmian potential, where the Fibonacci Hamiltonian, cf. [56, 79], serves as one well-understood example, see, e.g., [27] and [25]. The results of this section are based on joint work with Fabien Gabel, Dennis Gallaun, Julian Großmann and Marko Lindner [39].

Definition 4.38. For $\lambda \in \mathbb{R}$, $\alpha \in [0, 1] \setminus \mathbb{Q}$ and $\theta \in [0, 1)$ we define $H_{\lambda,\alpha,\theta}$ to be the discrete

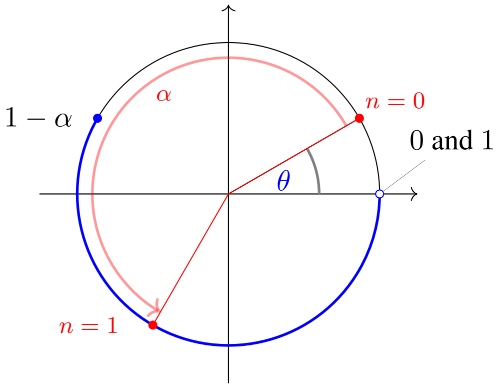

Figure 4.5: Visualization of (4.28) as rotation around a circle with the choice $\alpha = \frac{1}{2}(\sqrt{5}-1)$.

Schrödinger operator on $\ell^2(\mathbb{Z})$ with potential $\lambda v_{\alpha,\theta}$, where

$$v_{\alpha,\theta}(n) = \chi_{[1-\alpha,1)}(n\alpha + \theta \bmod 1)\,. \tag{4.28}$$

In the same way, we define $\widetilde{H}_{\lambda,\alpha,\theta}$ to be the discrete Schrödinger operator with potential $\lambda\widetilde{v}_{\alpha,\theta}$, where

$$\widetilde{v}_{\alpha,\theta}(n) = \chi_{(1-\alpha,1]\cup\{0\}}(n\alpha + \theta \bmod 1)\,. \tag{4.29}$$

We call $H_{\lambda,\alpha,\theta}$ and $\widetilde{H}_{\lambda,\alpha,\theta}$ Schrödinger operators with Sturmian potential, $\lambda \in \mathbb{R}$ is called the coupling constant, α the slope and θ the offset, cf. [75, 93]. The compressions $H^+_{\lambda,\alpha,\theta}$ and $\widetilde{H}^+_{\lambda,\alpha,\theta}$ on $\ell^2(\mathbb{N})$ are defined accordingly.

Since α is irrational, this potential is not periodic. The already mentioned Fibonacci Hamiltonian arises when setting $\alpha = \frac{1}{2}(\sqrt{5}-1)$ while leaving λ and θ as variables.

In the definition of the potential (4.28) the term $\chi_{[1-\alpha,1)}(n\alpha + \theta \bmod 1)$ can be illustrated as a rotation around a circle, where α describes the step size and θ the starting point. We visualize this in Figure 4.5.

When comparing $\widetilde{v}_{\alpha,\theta}$ to $v_{\alpha,\theta}$, only the interval boundaries have changed from $[\cdot,\cdot)$ to $(\cdot,\cdot]$. In the definition (4.29) we also take a union with $\{0\}$ since the term $n\alpha + \theta \bmod 1$ can be 0. In the spirit of Figure 4.5 we identify 0 and 1 here, and will always omit mentioning the union with $\{0\}$ from now on.

4.3.1 Rational approximation of Sturmian words

In this section we prove basic combinatorial properties for Sturmian potentials that will be the base of spectral results for the Schrödinger operators in the following sections. In a combinatorial context, we refer to elements of $\{0,1\}^{\mathbb{Z}}$ as (infinite) words.

For $\alpha \in [0,1]$ irrational and $\theta \in [0,1)$, we consider the Sturmian words $v_{\alpha,\theta}$ and $\widetilde{v}_{\alpha,\theta}$ defined by (4.28) and (4.29). Observe that these two words satisfy a symmetry property, namely, for all $k \in \mathbb{Z}$, we have

$$\begin{aligned} v_{\alpha,\theta}(k) &= \chi_{[1-\alpha,1)}(k\alpha + \theta \bmod 1) \\ &= \chi_{(1-\alpha,1]}(-k\alpha - \alpha - \theta \bmod 1) \end{aligned} \tag{4.30}$$

$$= \widetilde{v}_{\alpha,(-\alpha-\theta \bmod 1)}(-k)\,.$$

If $\theta = 0$, we use the shorthand notation $v_\alpha := v_{\alpha,0}$ and $\widetilde{v}_\alpha := \widetilde{v}_{\alpha,0}$. Then $v_\alpha(k) = \widetilde{v}_{\alpha,1-\alpha}(-k)$.

The properties of Sturmian words are closely linked to the continued fraction expansion of the slope,

$$\alpha = \cfrac{1}{a_1 + \frac{1}{a_2 + \frac{1}{a_3 + \dots}}} =: [a_1, a_2, a_3, \dots] \quad \text{with} \quad a_1, a_2, \dots \in \mathbb{N}.$$

Terminating the continued fraction expansion for a given $m \in \mathbb{N}$, i.e. removing the terms $+\frac{1}{a_{m+1}+\dots}$, we get a rational number $\alpha_m := \frac{p_m}{q_m}$.

Definition 4.39. For $\alpha \in [0,1] \setminus \mathbb{Q}$ and $m \in \mathbb{N}$ we call the rational number α_m, derived from terminating the continued fraction expansion as above, the m-th rational approximant of α. In the following we let p_m and q_m denote the nominator and denominator of the irreducible integer fraction representation of α_m.

It is not hard to show that the numbers p_m and q_m satisfy the following recursion

$$p_{-1} := 1\,,\ p_0 := 0\,,\ p_m := a_m p_{m-1} + p_{m-2}\,, \tag{4.31}$$

$$q_{-1} := 0\,,\ q_0 := 1\,,\ q_m := a_m q_{m-1} + q_{m-2}\,. \tag{4.32}$$

The following estimates for the approximation of α_m to α hold, see [59, Theorem 5] or [55, Theorem 9, Theorem 13],

$$\frac{1}{q_m(q_{m+1}+q_m)} < \left|\alpha - \frac{p_m}{q_m}\right| < \frac{1}{q_m q_{m+1}} \leq \frac{1}{m(m+1)} \tag{4.33}$$

and also

$$\frac{p_0}{q_0} < \frac{p_2}{q_2} < \dots < \alpha < \dots < \frac{p_3}{q_3} < \frac{p_1}{q_1}\,.$$

Additionally, the rational approximant $\alpha_m := \frac{p_m}{q_m}$ is the best approximation, in the sense that

$$\|q\alpha\| > \|q_m\alpha\| \text{ for all } q \text{ with } 1 \leq q < q_m \quad \text{and} \quad \|q_m\alpha\| = |q_m\alpha - p_m|\,,$$

where we use the notation $\|x\| := \operatorname{dist}(x, \mathbb{Z})$ for the distance of a real number x to $\mathbb{Z}$, also for the rest of this section.

Example 4.40. *For the golden ratio $\alpha = \frac{\sqrt{5}-1}{2}$ it is well-known that the continued fraction expansion only consists of ones, i.e. $\alpha = [1,1,1,\dots]$ for $m \in \mathbb{N}$. The corresponding sequence of rational approximants yields*

$$0 < \frac{1}{2} < \frac{3}{5} < \frac{8}{13} < \frac{21}{34} < \dots < \alpha < \dots < \frac{34}{55} < \frac{13}{21} < \frac{5}{8} < \frac{2}{3} < 1\,.$$

Both p_m and q_m are Fibonacci numbers, which is not surprising when considering the recursions (4.31) *and* (4.32).

We aim to approximate the aperiodic words $v_{\alpha,\theta}$ by periodic words that stem from the rational approximations $\alpha_m = \frac{p_m}{q_m}$, as this will lead to an approximation of $H_{\lambda,\alpha,\theta}$ by periodic Schrödinger operators. This is a fruitful approach since the spectral theory of periodic Schrödinger operators is well understood, see Section 4.2.

Given an irrational $\alpha \in [0,1]$ with corresponding continued fraction expansion $[a_1, a_2, a_3, \dots]$, we define words s_m of finite length over the alphabet $\Sigma = \{0,1\}$ by the recursion:

$$s_{-1} := 1,\ s_0 := 0,\ s_1 := s_0^{a_1-1} s_{-1},\ s_m := s_{m-1}^{a_m} s_{m-2}, \quad m \geq 2. \tag{4.34}$$

Comparing (4.34) with (4.32) we find that the length of the word s_m is equal to q_m. For $m \geq 2$, the word s_{m-1} is a prefix of s_m. Therefore, the pointwise limit $v_+ \in \{0,1\}^{\mathbb{N}}$ exists:

$$v_+(n) = \lim_{m\to\infty} s_m(n), \qquad \text{for all } n \in \mathbb{N}.$$

The words s_m also possess a nice symmetry property, as it contains a palindrome.

Lemma 4.41 ([11, Proposition 4.5]). *Let $\alpha \in [0,1]$ be irrational and consider the words s_m defined by* (4.34). *Then there exist palindromes π_m, $m \geq 2$, such that*

$$s_m = \begin{cases} \pi_m 10\,, & m \text{ even,} \\ \pi_m 01\,, & m \text{ odd.} \end{cases}$$

So far it looks like the finite words s_m have nothing to do with our infinite aperiodic word $v_{\alpha,\theta}$. But this is far from true, the words s_m are the building blocks of $v_{\alpha,\theta}$. For instance, with $\theta = 0$ we find that the Sturmian word $v_{\alpha,0}$, restricted to $\{1,2,3,\dots\}$, coincides with the one-sided infinite word v_+, see [10]. The following lemma by Bellissard et al. in [10] shows that Sturmian words have a periodic structure locally:

Lemma 4.42. *Let $\alpha \in [0,1]$ be irrational, $m \geq 3$. Then, for $v \in \{v_\alpha, \widetilde{v}_\alpha\}$, the following holds:*

(a) For all $1 \leq k \leq q_m - 2$, we have $v(q_{m-1} + k) = v(k)$.

(b) For all $k \geq 2$, we have $v(-k) = v(k-1)$.

Note that the original result is only formulated for v_α but the proof for $\widetilde{v}_\alpha$ is analogous. So far v_+ gives us an understanding of the behavior of v_α on $\mathbb{N}$. Now the symmetry property of (b) in Lemma 4.42 allows us to also look at v_α on the negative half-axis.

It follows that the Sturmian word $v_{\alpha,0}$, restricted to $\mathbb{Z}_-$, is equal to the one-sided infinite word v_- given by the following limit

$$v_-(n) := \lim_{\substack{q_m \geq |n|+1 \\ m\to\infty}} s_{2m}(q_m - n) \qquad \text{for all } n \in \mathbb{Z}_-.$$

Due to the recursion (4.34) we find that s_{2m-2} is a suffix of s_{2m} and therefore the limit exists.

From now on we will define $v_{\beta,\theta}$ and $\widetilde{v}_{\beta,\theta}$ exactly as in (4.28) and (4.29) for all values of $\beta \in [0,1]$. Rational values of β lead to periodic words instead of Sturmian words. In the following we will use α for irrational slopes only and β for slopes that can be both rational and irrational. Let us continue with a technical lemma that is needed for later results. Recall that $\|x\| = \operatorname{dist}(x,\mathbb{Z})$.

Lemma 4.43. *([39, Lemma 3.5]) Let $\beta \in [0,1]$, $k \in \mathbb{Z}$, and $|\theta| < \frac{1}{2}$. We have*

$$v_{\beta,0}(k) = v_{\beta,\pm\theta \bmod 1}(k) \quad \text{and} \quad \widetilde{v}_{\beta,0}(k) = \widetilde{v}_{\beta,\pm\theta \bmod 1}(k)$$

if one of the following conditions is fulfilled:

(a) $\|k\beta\| > |\theta|$ *and* $\|(k+1)\beta\| > |\theta|$.

(b) $\|k\beta\| \geq |\theta|$, $\|(k+1)\beta\| > |\theta|$, *and* $k\beta \pm \theta \notin \mathbb{Z}$.

(c) $\|k\beta\| > |\theta|$, $\|(k+1)\beta\| \geq |\theta|$, *and* $(k+1)\beta \pm \theta \notin \mathbb{Z}$.

Proof. We only show the result for $v_{\beta,\theta}$ because, for $\widetilde{v}_{\beta,\theta}$, the proof works completely analogously. For the first part, let $|\theta| < \frac{1}{2}$ and $k \in \mathbb{Z}$ be such that $\|k\beta\| > |\theta|$ and $\|(k+1)\beta\| > |\theta|$. Then the following holds:

$$\begin{aligned} & k\beta \bmod 1 \in [1-\beta, 1) \\ \iff & \exists m \in \mathbb{Z} \text{ with } 1-\beta \leq k\beta - m < 1 \\ \iff & \exists m \in \mathbb{Z} \text{ with } k\beta < m+1 \leq (k+1)\beta \\ \iff & \exists m \in \mathbb{Z} \text{ with } k\beta \pm \theta < m+1 \leq (k+1)\beta \pm \theta \\ \iff & k\beta \pm \theta \bmod 1 \in [1-\beta, 1)\,. \end{aligned}$$

For the remaining part we use that $k\beta \pm \theta \notin \mathbb{Z}$ implies $\|k\beta\| \neq |\theta|$ and $(k+1)\beta \pm \theta \notin \mathbb{Z}$ implies $\|(k+1)\beta\| \neq |\theta|$. This means that both of condition (b) and (c) imply (a), which proves the statement. □

For given irrational α recall that we can obtain rational approximations α_m by cutting off the continued fraction expansion after m steps. The next lemma shows that this translates to an approximation of the aperiodic word $v_{\alpha,0}$ by $v_{\alpha_m,0}$.

Lemma 4.44. *([39, Lemma 3.6]) Let* $\alpha \in [0,1] \setminus \mathbb{Q}$, $m \geq 2$, *and* $\alpha_m = \frac{p_m}{q_m}$ *the* m*-th rational approximant to* α. *Then*

$$v_{\alpha_m}(k) = v_\alpha(k) \quad \textit{for all} \begin{cases} -q_m + 1 \leq k \leq q_{m+1}\,, & m \textit{ even,} \\ -q_{m+1} - 1 \leq k \leq q_m - 2\,, & m \textit{ odd,} \end{cases}$$

and

$$\widetilde{v}_{\alpha_m}(k) = \widetilde{v}_\alpha(k) \quad \textit{for all} \begin{cases} -q_{m+1} - 1 \leq k \leq q_m - 2\,, & m \textit{ even,} \\ -q_m + 1 \leq k \leq q_{m+1}\,, & m \textit{ odd.} \end{cases}$$

Proof. First, we find that

$$v_\alpha(-1) = 1 = v_{\alpha_m}(-1) = v_{\alpha_m}(q_m - 1) \qquad \text{and} \qquad v_\alpha(0) = 0 = v_{\alpha_m}(0) = v_{\alpha_m}(q_m) \tag{4.35}$$

Next, we show that $v_{\alpha_m}(k) = v_\alpha(k)$ for $1 \leq k \leq q_m - 2$. To this end, let us fix $1 \leq k \leq q_m - 2$ and set $\theta_k := k(\alpha - \alpha_m)$. Using the estimates (4.33), yields

$$|\theta_k| < \frac{1}{2} \quad \text{and} \quad \min\left\{\|k\alpha_m\|, \|(k+1)\alpha_m\|\right\} \geq \frac{1}{q_m} > |\theta_k|\,.$$

With Lemma 4.43(a) and (4.35) we get the identity

$$v_{\alpha_m,0}(k) = v_{\alpha_m,\theta_k \bmod 1}(k) = v_{\alpha,0}(k) \quad \text{for all } 1 \leq k \leq q_m - 2\,. \tag{4.36}$$

Recall that, by Lemma 4.41, there is a palindrome π_m such that $s_m = \pi_m 10$ if m is even and $s_m = \pi_m 01$ if m is odd. Hence, (4.36) yields that the period of v_{α_m} is equal to $\pi_m 10$. Now, using the local periodicity and the symmetry properties from Lemma 4.42 for v_α, we get the following diagram for even m:

k	$-q_m - 1 \ldots$	-1	0	$1 \ldots q_m$	$\ldots$	$\ldots a_{m+1}q_m$	$\ldots q_{m+1}$
$v_\alpha(k)$	s_m^{R}	1	0	s_m	$\ldots$	s_m	s_{m-1}
$v_\alpha(k)$	$0\,\mathbf{1}\ \pi_m$	1	0	$\pi_m\ 1\,0$	$\ldots$	$\pi_m\ 1\,0$	$\pi_{m-1}\ 0\,1$
$v_{\alpha_m}(k)$	$1\,\mathbf{0}\ \pi_m$	1	0	$\pi_m\ 1\,0$	$\ldots$	$\pi_m\ 1\,0$	$\pi_{m-1}\ 0\,1$

Here, s_m^{R} denotes the reversed word of s_m. The bold numbers mark the first positions where v_α does not coincide with the periodic word v_{α_m}. This shows that the interval for k in the statement of the lemma is maximal. For m odd, we have $s_m = \pi_m 01$ and therefore get the following diagram:

k	$-q_{m+1} - 1 \ldots$	$-a_{m+1}q_m - 1 \ldots$	$\ldots$	$-q_m - 1 \ldots$	-1	0	$1 \ldots q_m$
$v_\alpha(k)$	s_{m-1}^{R}	s_m^{R}	$\ldots$	s_m^{R}	1	0	s_m
$v_\alpha(k)$	$0\,1\ \pi_{m-1}$	$1\,0\ \pi_m$	$\ldots$	$1\,0\ \pi_m$	1	0	$\pi_m\ 0\,1$
$v_{\alpha_m}(k)$	$0\,1\ \pi_{m-1}$	$1\,0\ \pi_m$	$\ldots$	$1\,0\ \pi_m$	1	0	$\pi_m\ \mathbf{1}\,0$

Hence, $v_{\alpha_m}(k) = v_\alpha(k)$ for $-q_{m+1} - 1 \leq k \leq q_m - 2$. This proves the first part of the lemma. The identity of $\widetilde{v}_{\alpha_m}(k)$ and $\widetilde{v}_\alpha(k)$ for the stated values of k now follows from the observation that $\widetilde{v}_\alpha(k)$ and $v_\alpha(k)$ only differ for $k \in \{-1, 0\}$ while $\widetilde{v}_{\alpha_m}$ and v_{α_m} differ on $\{q_m k - 1, q_m k : k \in \mathbb{Z}\}$. □

The tables in the proof of Lemma 4.44 show that one of the bounds for k in the statement of the lemma, namely the one that involves $\pm q_m$ is sharp. The other bound that involves $\pm q_{m+1}$ is not sharp and the two potentials coincide on a slightly larger interval. We omit the cumbersome computations for the exact interval around 0 on which v_α and v_{α_m} coincide since we are only interested in the fact that each $k \in \mathbb{Z}$ is eventually contained in that interval.

Example 4.45. *For the important Fibonacci case* $\alpha = \frac{\sqrt{5}-1}{2}$ *we take a closer look at the words* s_m*,* π_m *and* v_{α_m}*. Recall that all coefficients* a_j *of the continued fraction expansion are* 1*. By definition,* $s_0 = 0$ *and* $s_1 = 1$*. For* $m \geq 2$ *the words* s_m *are given by the recursion* $s_m = s_{m-1}s_{m-2}$*:*

$$\begin{aligned}
&s_0 = 0, \quad s_1 = 1, \quad s_2 = 10, \quad s_3 = 101, \quad s_4 = 10110,\\
&s_5 = 10110101, \quad s_6 = 1011010110110,\\
&s_7 = 101101011011010110101.
\end{aligned}$$

With the periodic approximation from Example 4.40 we find that the words $\tilde{s}_m := v_{\alpha_m}(1)..v_{\alpha_m}(q_m)$ *are*

$$\begin{aligned}
&\tilde{s}_0 = 0, \quad \tilde{s}_1 = 1, \quad \tilde{s}_2 = 10, \quad \tilde{s}_3 = 1\mathbf{10}, \quad \tilde{s}_4 = 10110\\
&\tilde{s}_5 = 101101\mathbf{10}, \quad \tilde{s}_6 = 1011010110110,\\
&\tilde{s}_7 = 1011010110110101101\mathbf{10}.
\end{aligned}$$

We clearly see that s_m *and* $\tilde{s}_m$ *coincide for even* m *but differ in the last two elements for odd* m*. This is of course in accordance with Lemma 4.44. Also note how omitting the last two elements of* s_m *or* $\tilde{s}_m$ *yields a palindrome.*

So far, we have only seen that the Sturmian word $v_{\alpha,\theta}$ coincides with its periodic approximation $v_{\alpha_m,\theta}$ for $\theta = 0$. The following lemma covers the other values of θ.

Lemma 4.46. *([39, Lemma 3.8]) Let $\alpha \in [0,1] \setminus \mathbb{Q}$, $m \geq 2$, and $\alpha_m = \frac{p_m}{q_m}$ the m-th rational approximant to α.*

(a) If $\theta = k_0\alpha \bmod 1$ for some $k_0 \in \mathbb{Z}$ choose m sufficiently large such that $|k_0| \leq q_{m-1}$. Then for $-q_m + 1 \leq k \leq q_m - 2$, the following holds:

$$v_{\alpha_m,\theta}(k) = \begin{cases} \widetilde{v}_{\alpha,\theta}(k) & \text{if } m \text{ is even,} \\ v_{\alpha,\theta}(k) & \text{if } m \text{ is odd.} \end{cases}$$

(b) If $\theta \notin \{k_0\alpha \bmod 1 : k_0 \in \mathbb{Z}\}$ then for each $D \in \mathbb{N}$ there is an m_0 such that for all $m \geq m_0$ and for all $k = -D, \dots, D$

$$v_{\alpha_m,\theta}(k) = v_{\alpha,\theta}(k).$$

Proof. Let $k_0 \in \mathbb{Z}$ with $q_{m-1} \geq |k_0|$, and set $\theta_m := k_0\alpha_m \bmod 1$. Then, for all $k \in \mathbb{Z}$,

$$v_{\alpha,\theta}(k) = v_{\alpha,0}(k+k_0) \quad \text{and} \quad v_{\alpha_m,\theta_m}(k) = v_{\alpha_m,0}(k+k_0)\,,$$

and, by Lemma 4.44, we conclude

$$v_{\alpha,0}(k+k_0) = v_{\alpha_m,0}(k+k_0) \quad \text{for} -q_m + 1 \leq k + k_0 \leq q_m - 2\,. \tag{4.37}$$

As $q_m \geq n \geq 2$ by assumption, identity (4.37) implies that the q_m-periodic word $v_{\alpha_m,0}$ coincides with $v_{\alpha,0}$ for at least one full period. Combining this with Lemma 4.42 allows us to extend the region of indices specified in (4.37) to the left and right by one more period. Thus, the assumption $q_{m-1} \geq |k_0|$ implies

$$v_{\alpha,\theta}(k) = v_{\alpha_m,\theta_m}(k) \quad \text{for} -q_m + 1 \leq k \leq q_m - 2\,.$$

Similar to the proof of Lemma 4.44, we use a perturbation argument to pass from v_{α_m,θ_m} to $v_{\alpha_m,\theta}$. We consider two cases.

Case 1: assume that $(k+k_0)\alpha_m \notin \mathbb{Z}$ and $(k+k_0+1)\alpha_m \notin \mathbb{Z}$. We define $x := k_0(\alpha - \alpha_m)$. Then the approximation rate estimates (4.33) give that

$$|x| < \frac{1}{q_m} \leq \min\big\{\|(k_0+k)\alpha_m\|, \|(k_0+k+1)\alpha_m\|\big\}.$$

Now, Lemma 4.43(a) yields

$$v_{\alpha_m,\theta_m}(k) = v_{\alpha_m,0}(k+k_0) = v_{\alpha_m,x \bmod 1}(k+k_0) = v_{\alpha_m,\theta}(k).$$

This shows

$$v_{\alpha,\theta}(k) = v_{\alpha_m,\theta}(k) \quad \text{for} -q_m + 1 \leq k \leq q_m - 2\,.$$

Note that, for this range of k, we also have $v_{\alpha,\theta}(k) = \widetilde{v}_{\alpha,\theta}(k)$.

Case 2: assume that $(k+k_0)\alpha_m \in \mathbb{Z}$ or $(k+k_0+1)\alpha_m \in \mathbb{Z}$. We first check the case $k + k_0 = jq_m$ for $j \in \mathbb{Z}$. Then $v_{\alpha_m,\theta_m} = 0$ and $\widetilde{v}_{\alpha_m,\theta_m} = 1$. We get that

$$v_{\alpha_m,\theta}(k) = \chi_{[1-\alpha_m,1)}((jq_m - k_0)\alpha_m + k_0\alpha \bmod 1)$$

$$\begin{aligned}
&= \chi_{[1-\alpha_m,1)}(k_0(\alpha-\alpha_m) \bmod 1)\\
&= \begin{cases} \chi_{[-\alpha_m,0)}(k_0(\alpha-\alpha_m)) & = 1 = \widetilde{v}_{\alpha_m,\theta_m}(k) \quad m \text{ even},\\ \chi_{[-\alpha_m,0)\cup[1-\alpha_m,1)}(k_0(\alpha-\alpha_m)) & = 0 = v_{\alpha_m,\theta_m}(k) \quad m \text{ odd},\end{cases}
\end{aligned}$$

holds. For $k+k_0+1 = jq_m$ for $j \in \mathbb{Z}$, we compute

$$\begin{aligned}
v_{\alpha_m,\theta}(k) &= \chi_{[1-\alpha_m,1)}((jq_m-k_0-1)\alpha_m + k_0\alpha \bmod 1)\\
&= \chi_{[1-\alpha_m,1)}(k_0(\alpha-\alpha_m) - \alpha_m \bmod 1)\\
&= \begin{cases} \chi_{[-\alpha_m,0)}(k_0(\alpha-\alpha_m)-\alpha_m) & = 0 = \widetilde{v}_{\alpha_m,\theta_m}(k) \quad m \text{ even},\\ \chi_{[-\alpha_m,0)\cup[1-\alpha_m,1)}(k_0(\alpha-\alpha_m)-\alpha_m) & = 1 = v_{\alpha_m,\theta_m}(k) \quad m \text{ odd}.\end{cases}
\end{aligned}$$

This proves the case (a).

Finally, we prove (b), i.e. the case that $\theta \notin \{k_0\alpha \bmod 1 : k_0 \in \mathbb{Z}\}$. Let $D \in \mathbb{N}$ and set $\varepsilon := \min_{k\in -D..D} \|k\alpha+\theta\| > 0$. Choose m_0 sufficiently large such that $|(D+1)(\alpha-\alpha_{m_0})| < \varepsilon$. Then, for $m \geq m_0$ and $-D \leq k \leq D$,

$$\begin{aligned}
v_{\alpha,\theta}(k) &= \chi_{[1-\alpha,1)}(k\alpha+\theta \bmod 1)\\
&= \chi_{[1-\alpha,1)}(k\alpha+\theta-(k+1)(\alpha-\alpha_m) \bmod 1)\\
&= \chi_{[1-\alpha,1)}(k\alpha_m+\theta-\alpha+\alpha_m \bmod 1)\\
&= v_{\alpha_m,\theta}(k).
\end{aligned}$$

□

Let us put the previous result in an operator theoretic context. The entrywise convergence of the potentials $v_{\alpha_m,0}$ to $v_{\alpha,0}$ implies that the corresponding operators converge strongly, $H_{\lambda,\alpha_m,0} \to H_{\lambda,\alpha,0}$ as $m \to \infty$. This result originally appeared in [100]. Lemma 4.46 tells us how to generalize this for other values of θ.

Corollary 4.47 ([100, Proposition 4]). *Let* $\alpha \in [0,1] \setminus \mathbb{Q}$.

(a) If $\theta = 0$ *or* $\theta \notin \{k_0\alpha \bmod 1 : k_0 \in \mathbb{Z}\}$ *then*

$$H_{\lambda,\alpha,\theta} = \lim_{m\to\infty} H_{\lambda,\alpha_m,\theta} \qquad \text{and} \qquad \widetilde{H}_{\lambda,\alpha,\theta} = \lim_{m\to\infty} \widetilde{H}_{\lambda,\alpha_m,\theta}.$$

(b) If $\theta \in \{k_0\alpha \bmod 1 : k_0 \in \mathbb{Z}\}$ *then*

$$H_{\lambda,\alpha,\theta} = \lim_{m\to\infty} H_{\lambda,\alpha_{2m+1},\theta} \qquad \text{and} \qquad \widetilde{H}_{\lambda,\alpha,\theta} = \lim_{m\to\infty} H_{\lambda,\alpha_{2m},\theta}.$$

Strong convergence alone is of course not sufficient for the convergence of the spectra. We have seen in Section 3.3, more precisely in Theorem 3.9, that the set of column submatrices, $\mathcal{C}_N$ is a useful tool to establish convergence of spectra. For a discrete Schrödinger operator the set of column submatrices is determined by the potential v. Indeed, there is an obvious one-to-one correspondence between N consecutive columns of $H_{\lambda,\alpha,\theta}$ and N consecutive entries of $v_{\alpha,\theta}$. The latter are called finite subwords of $v_{\alpha,\theta}$.

We further aim to characterize the essential spectrum of $H_{\lambda,\alpha,\theta}$ with the help of limit operators. Also here, the limit operators of the Schrödinger operator are completely determined by the potential. To be more precise, the limit operators of $H_{\lambda,\alpha,\theta}$ are again discrete Schrödinger operators with a potential that is given by certain limits of $v_{\alpha,\theta}$, called the limit words. Before diving into the spectral analysis of $H_{\lambda,\alpha,\theta}$ we therefore first have to understand the subwords and limit words of $v_{\alpha,\theta}$.

4.3.2 Subwords and limit words

We abbreviate $v := (v_{\alpha,\theta}(n))_{n\in\mathbb{Z}}$. Then we can write

$$H_{\lambda,\alpha,\theta} = S^{-1} + S + \lambda\, M_v\,, \quad x \in \ell^2(\mathbb{Z})\,.$$

Let $h = (h_1, h_2, \dots)$ be a sequence in $\mathbb{Z}$ with $h_k \to \pm\infty$, so that the limit operator $(H_{\lambda,\alpha,\theta})_h$ of $H_{\lambda,\alpha,\theta}$ exists. Then

$$(H_{\lambda,\alpha,\theta})_h = S^{-1} + S + \lambda\, M_{v_h}$$

with a new potential

$$v_h := \lim_{k\to\infty} S^{-h_k} v$$

where the limit is taken w.r.t. pointwise convergence. The set

$$\mathcal{F}_v := \Big\{ \lim_{k\to\infty} S^{-h_k} v : h_k \to \pm\infty \text{ such that the limit exists} \Big\}$$

of all such potentials v_h is the so-called subshift generated by the sequence v. The same can be done for periodic words $v = v_{\alpha_m,\theta}$. In that case, the subshift generated by v is finite.

For Sturmian potentials, the subshift is explicitly known, see, e.g., [23, Theorem 2.14] and the appendix of [28].

Proposition 4.48. *Let $\alpha \in [0,1] \setminus \mathbb{Q}$ and $\theta \in [0,1)$. Then the following holds:*

(i) The subshift of $v_{\alpha,\theta}$ is given by

$$\mathcal{F}_{v_{\alpha,\theta}} = \big\{ v_{\alpha,\psi}, \widetilde{v}_{\alpha,\psi} : \psi \in [0,1) \big\}\,. \tag{4.38}$$

In particular, $\mathcal{F}_{v_{\alpha,\theta}} = \mathcal{F}_{v_{\alpha,0}} = \mathcal{F}_{\widetilde{v}_{\alpha,\theta}}$.

(ii) The subshift of $v_{\alpha_m,\theta}$ is given by the finite set

$$\mathcal{F}_{v_{\alpha_m,\theta}} = \big\{ v_{\alpha_m,\psi}, \widetilde{v}_{\alpha_m,\psi} : \psi \in [0,1) \big\}\,.$$

In particular, $\mathcal{F}_{v_{\alpha_m,\theta}} = \mathcal{F}_{v_{\alpha_m,0}} = \mathcal{F}_{\widetilde{v}_{\alpha_m,\theta}}$.

As equation (4.38) shows, the subshift $\mathcal{F}_{v_{\alpha,\theta}}$ does not depend on θ and also does not change when switching to the potential $\widetilde{v}_{\alpha,\theta}$. Therefore, the shorthand notation $\mathcal{F}_\alpha = \mathcal{F}_{v_{\alpha,\theta}}$ is well-defined. The same is true for $\mathcal{F}_{\alpha_m} = \mathcal{F}_{v_{\alpha_m,\theta}}$.

Next, we examine the finite subwords of words in the subshifts $\mathcal{F}_\alpha$ and $\mathcal{F}_{\alpha_m}$.

Definition 4.49. We call w a finite word over $\{0,1\}$ if $w \in \{0,1\}^N$ for some $N \in \mathbb{N}$. For a finite word w and a finite or infinite word v we call w a subword of v if

$$w = v(j) \dots v(j+N-1) \tag{4.39}$$

for some $N, j \in \mathbb{N}$. We write $w \prec v$ when w is a subword of v. Sometimes we specify that w is a subword of length N. The set of all subwords of v of length N is denoted by $\mathcal{W}_N(v)$.

For a word $v : \mathbb{Z} \to \{0,1\}$, we define v_+ to be the restriction of v onto $\mathbb{N}$ and v_- to be the restriction onto $\mathbb{Z}_-$.

Lemma 4.50. *([39, Lemma 3.10]) Let $\mathcal{F}$ be either $\mathcal{F}_\alpha$ or $\mathcal{F}_{\alpha_m}$. Then for $v \in \mathcal{F}$ and $w \prec v$ we have that*

- *(a) $w \prec u$ for all $u \in \mathcal{F}$ and w occurs infinitely many times in u,*
- *(b) $w \prec v_+$ and w occurs infinitely many times in v_+,*
- *(c) $w \prec v_-$ and w occurs infinitely many times in v_-.*

Proof. Part (a) follows from [74, Proposition 2.1.18]. For part (b), take $w \prec v_{\alpha,\theta}$. Hence, we find $N, j \in \mathbb{Z}$ such that (4.39) holds. Choose $(k_n)_{n\in\mathbb{N}} \subset \mathbb{N}$ such that $k_n\alpha + \psi \bmod 1$ converges to $j\alpha + \theta \bmod 1$ from above. Since $\chi_{[1-\alpha,1)}$ is right-continuous, there is an $n_0 \in \mathbb{N}$ such that for all $n \geq n_0, l \in 0..N-1$ we have that

$$\begin{aligned} v_{\alpha,\psi}(k_n + j) &= \chi_{[1-\alpha,1)}((k_n + j)\alpha + \psi \bmod 1) \\ &= \chi_{[1-\alpha,1)}((j + l)\alpha + \theta \bmod 1) = v_{\alpha,\theta}(j + l). \end{aligned}$$

Hence, $w \prec (v_{\alpha,\psi})_+$. The proof for (c) is analogous. □

For a K periodic word v it is clear that $|\mathcal{W}_N(v)| \leq K$ whenever $N > K$. Hence, the number $|\mathcal{W}_N(v)|$, sometimes called the subword complexity of v, stays bounded as $N \to \infty$. In contrast, for pseudoergodic words over $\{0, 1\}$ the subword complexity is, by definition, $|\mathcal{W}_N(v)| = 2^N$ and therefore grows exponentially, cf. Section 3.3. In fact, both periodicity and pseudoergodicity can be characterized by the subword complexity function $N \mapsto |\mathcal{W}_N(v)|$, see [22]. Sturmian words have the slowest growth of subword complexity out of all non-periodic words, namely $|\mathcal{W}_N(v)| = N+1$ for v Sturmian. For one-sided words v, one even has that $|\mathcal{W}_N(v)| = N + 1$ is a characterization of Sturmian words, see [11].

Lemma 4.51. *([39, Lemma 3.11]) Let $v \in \mathcal{F}_\alpha$ and $v_m \in \mathcal{F}_{\alpha_m}$. Then v has precisely $N + 1$ different subwords of length N. Moreover, for each $N \in \mathbb{N}$, there exists $m_0 \in \mathbb{N}$, such that, for all $m \geq m_0$, we have $\mathcal{W}_N(v) = \mathcal{W}_N(v_m)$.*

Proof. For the first statement see [11]. It remains to show that $\mathcal{W}_N(v) = \mathcal{W}_N(v_m)$ for sufficiently large m. Due to Lemma 4.50 it suffices to only prove the case $v = v_{\alpha,0}$. Let $N \in \mathbb{N}$ and choose $m \in \mathbb{N}$ such that $q_m \geq 2N$ is large enough such that all elements of $\mathcal{W}_N(v)$ occur in $0..q_m - 2$. By Lemma 4.44, $\mathcal{W}_N(v) \subset \mathcal{W}_N(v_m)$.

Now let $w \in \mathcal{W}_N(v_m)$. Since v_m is q_m-periodic, we may assume that

$$w \prec (v_m(-q_m + 1), \ldots, v_m(q_m - 2)) \; .$$

Now the claim follows from Lemma 4.44. □

4.3.3 Spectrum of $H_{\lambda,\alpha,\theta}$

Throughout this section we assume without further notice that $\lambda \in \mathbb{R} \setminus \{0\}$, $\alpha \in [0, 1] \setminus \mathbb{Q}$ and $\theta \in [0, 1)$. The results of Section 4.3.2 can be directly elevated to the level of operators, as the following result shows. As a consequence of Proposition 4.48, we get a characterization for the limit operators of $H_{\lambda,\alpha,\theta}$.

Corollary 4.52. *Then*

$$L_{\lambda,\alpha} := \{H_{\lambda,\alpha,\psi}, \widetilde{H}_{\lambda,\alpha,\psi} : \psi \in [0,1)\} = \operatorname{Lim}(H_{\lambda,\alpha,\theta}) = \operatorname{Lim}(\widetilde{H}_{\lambda,\alpha,\theta})$$

In particular, $L_{\lambda,\alpha} = \operatorname{Lim}(H)$ *for all* $H \in L_{\lambda,\alpha}$*, i.e. all elements of* $L_{\lambda,\alpha}$ *are self-similar and recurrent.*

The property that $H_{\lambda,\alpha,\theta}$ is self similar and recurrent has immediate consequences for the spectrum of the operator, see Section 2.4.4.

Theorem 4.53. *([39, Proposition 4.4 and 4.6]) Define* $L_{\lambda,\alpha}$ *as in Corollary 4.52. Then the following hold:*

(a) *All elements of* $L_{\lambda,\alpha}$ *have the same norm, lower norm and spectrum.*

(b) $\operatorname{Lim}(H) = \operatorname{Lim}_+(H) = \operatorname{Lim}_-(H)$ *for all* $H \in L_{\lambda,\alpha}$.

(c) *Each* $H \in L_{\lambda,\alpha}$ *is left- and right-self-similar.*

(d) $\sigma_{\text{ess}}(H^+) = \sigma_{\text{ess}}(H) = \sigma(H)$ *for all* $H \in L_{\lambda,\alpha}$.

(e) $\sigma(H^+) \supset \sigma(H)$ *for all* $H \in L_{\lambda,\alpha}$.

Proof. Part (a) and (b) follow directly from Lemma 2.43. Combining part (b) with self-similarity we find that for $H \in L_{\lambda,\alpha}$ also $H \in \operatorname{Lim}(H) = \operatorname{Lim}_+(H)$ holds, which proves (c). Lastly, part (d) and (e) are a consequence of Lemma 2.39 for right-self-similar operators. □

The results of Theorem 4.53 also hold for the finite set $L_{\lambda,\alpha_m} := \{H_{\lambda,\alpha_m,\psi}, \widetilde{H}_{\lambda,\alpha_m,\psi} : \psi \in [0,1)\}$, which are the limit operators of a periodic approximant $H_{\lambda,\alpha_m,\theta}$. This is due to the fact that periodic Schrödinger operators are self-similar and recurrent as well, see Section 4.2, in particular Lemma 4.11 and Theorem 2.50.

Note also that the fact that all elements of $L_{\lambda,\alpha}$ have the same spectrum, which is only essential spectrum, is well known, see e.g. [10].

Remark 4.54. For periodic Schrödinger operators we have seen that the inclusion $\sigma(H) \subset \sigma(H^+)$ can be strict, i.e. Dirichlet eigenvalues can exist. We will see in Example 4.71 with the Fibonacci Hamiltonian that the same can happen in the aperiodic case.

We continue with a famous trace condition due to [100] that can be used to obtain upper bounds on the spectrum of $H_{\lambda,\alpha,\theta}$. Recall from the spectral theory of periodic Schrödinger operators in Section 4.2 that the monodromy matrix was the product of the transfer matrices $M(E)$ over one period, see (4.12). By Proposition 4.14, the spectrum of a periodic Schrödinger operator is then given by $\{E \in \mathbb{R} : |\operatorname{tr}(M(E))| \leq 2\}$.

For a Schrödinger operator with Sturmian potential $H_{\lambda,\alpha,\theta}$ define

$$M_{\lambda,\alpha,\theta}(n,E) := T_{\lambda,\alpha,\theta}(n,E) \cdots T_{\lambda,\alpha,\theta}(1,E). \tag{4.40}$$

For the Fibonacci Hamiltonian Sütő [100] used a recursion formula for $\operatorname{tr} M_{\lambda,\alpha,\theta}(q_{m+1},E)$ in terms of $\operatorname{tr} M_{\lambda,\alpha,\theta}(q_m,E)$ and $\operatorname{tr} M_{\lambda,\alpha,\theta}(q_{m-1},E)$ in order to prove an approximation result for $\sigma(H_{\lambda,\alpha,\theta})$. Later Bellissard [10] generalized this result to Schrödinger operators with Sturmian potential. It is stated in the following proposition.

Proposition 4.55 ([10, Proposition 4])**.** *Let $\lambda > 0$. Then $E \in \mathbb{R}$ is in the resolvent set of $H_{\lambda,\alpha,\theta}$ if and only if*

$$\exists m \in \mathbb{N}: \left|\operatorname{tr}\left(M_{\lambda,\alpha,0}(q_m, E)\right)\right| > 2 \textit{ and } \left|\operatorname{tr}\left(M_{\lambda,\alpha,0}(q_{m+1}, E)\right)\right| > 2 \tag{4.41}$$

holds, where q_m is given by (4.32)*. In this case,*

$$\left|\operatorname{tr}\left(M_{\lambda,\alpha,0}(q_k, E)\right)\right| > 2$$

for all $k \geq m$.

Let us consider the converse of Proposition 4.55. The set

$$\Sigma_m := \{E \in \mathbb{R} : \left|\operatorname{tr}\left(M_{\lambda,\alpha,0}(q_m, E)\right)\right| \leq 2\} \cup \{E \in \mathbb{R} : \left|\operatorname{tr}\left(M_{\lambda,\alpha,0}(q_{m+1}, E)\right)\right| \leq 2\}$$

is a decreasing upper bound on the spectrum of $H_{\lambda,\alpha,\theta}$, i.e. $\Sigma_{m+1} \subset \Sigma_m$ and $\sigma(H_{\lambda,\alpha,\theta}) \subset \Sigma_m$ for all $m \in \mathbb{N}$. In terms of convergence of spectra, we only have $\sigma(H_{\lambda,\alpha,\theta}) = \bigcap_{m=m_0}^{\infty} \Sigma_m$ for each $m_0 \in \mathbb{N}$, see also [100, Proposition 5], which is not equivalent to Hausdorff convergence.

Remark 4.56. The monodromy matrices used (4.41) in Proposition 4.55 are not exactly the monodromy matrices of the periodic approximants $H_{\lambda,\alpha,\theta}$. However, Lemma 4.44 implies that at most two factors in (4.40) are swapped. Indeed, we can also use the monodromy matrices of the periodic Schrödinger operators $H_{\lambda,\alpha_m,0}$ and $H_{\lambda,\alpha_{m+1},0}$ in (4.41) because of the relation

$$\operatorname{tr}(M_{\lambda,\alpha,0}(q_m, E)) = \operatorname{tr}(M_{\lambda,\alpha_m,0}(q_m, E))\,. \tag{4.42}$$

Let us verify (4.42) for m even and m odd separately.

For $m = 2$ this follows directly from Lemma 4.44. For $m \geq 4$ even, $T_{\lambda,\alpha_m,0}(k, E) = T_{\lambda,\alpha,0}(k, E)$ for all $k \in \{1, \ldots, q_m\}$ as a consequence of Lemma 4.44. The equality of the transfer matrices then directly implies relation (4.42). Therefore, only the case for m odd remains to be shown. We use the local periodicity of the potential given in Lemma 4.42 with $k = q_m - q_{m-1}$ and obtain

$$\begin{aligned} M_{\lambda,\alpha,0}(q_m, E) &= T_{\lambda,\alpha,0}(q_m, E) \cdots T_{\lambda,\alpha,0}(1, E) \\ &= T_{\lambda,\alpha,0}(q_m - q_{m-1}, E) \cdots T_{\lambda,\alpha,0}(1 - q_{m-1}, E) \\ &= T_{\lambda,\alpha_m,0}(q_m - q_{m-1}, E) \cdots T_{\lambda,\alpha_m,0}(1 - q_{m-1}, E)\,. \end{aligned}$$

The last equality holds again by Lemma 4.44. We wow, take the trace on both sides and use the periodicity of v_{α_m}. Since the trace is invariant under cyclic permutations we arrive also in this case at the claimed relation (4.42). Accordingly, we can write

$$\Sigma_m = \sigma(H_{\lambda,\alpha_m,\theta}) \cup \sigma(H_{\lambda,\alpha_{m+1},\theta}).$$

In their works, Sütő and Bellissard use the trace condition (4.41) to show the following result.

Proposition 4.57. *([100, 10]) For all $\lambda > 0$, $\alpha \in [0, 1] \setminus \mathbb{Q}$ and $\theta \in [0, 1)$ the spectrum of $H_{\lambda,\alpha,\theta}$ is a Cantor set of zero Lebesgue measure and $H_{\lambda,\alpha,\theta}$ has no eigenvalues.*

The property that the spectrum is a Cantor set means that it contains neither an interval not isolated points while of course being non-empty. The absence of isolated points is due to the absence of eigenvalues which in turn can be proven by a so-called Gordon-type argument, see [96, 100]. As a consequence, Sütő and Bellissard found that the spectral type of Schrödinger operators with Sturmian potentials is purely singular continuous.

In order to establish the convergence of $\sigma(H_{\lambda,\alpha_m,\theta})$ to $\sigma(H_{\lambda,\alpha,\theta})$ in Hausdorff distance we want to employ Proposition 3.9. This requires that the column submatrices $\mathcal{C}_N$ of both operators eventually coincide for each $N \in \mathbb{N}$. As mentioned before, the column submatrices of the Schrödinger operator are determined by the finite subwords of the potential. We summarize this finding in the following lemma, which follows immediately from the definition of $\mathcal{C}_N$ and $\mathcal{W}_N$.

Lemma 4.58. *Let H and $\widehat{H}$ be Schrödinger operators with potential v and $\widehat{v}$, respectively. Then $\mathcal{C}_N(H) = \mathcal{C}_N(\widehat{H})$ if and only if $\mathcal{W}_N(v) = \mathcal{W}_N(\widehat{v})$.*

Finally, we are in the position to prove the following result, that has also been found by Beckus and his co-authors [8] independently.

Theorem 4.59. *([39, Proposition 4.16]) Set $A = H_{\lambda,\alpha,\theta}$ and $A_m = H_{\lambda,\alpha_m,\theta}$, and let $E \in \mathbb{R}$. Then,*

(a) $\nu(A - E) = \lim_{m\to\infty} \nu(A_m - E)$,

(b) $(A_m - E)_{m\in\mathbb{N}}$ is stable if and only if $A - E$ is invertible. In which case, $\lim_{n\to\infty} \|(A_m - E)^{-1}\| = \|(A - E)^{-1}\|$.

(c) $\sigma(A_m) \to \sigma(A)$ as $m \to \infty$ in the Hausdorff metric.

Proof. Lemma 4.51 and Lemma 4.58 imply that for each $N \in \mathbb{N}$ we have $\mathcal{C}_N(A) = \mathcal{C}_N(A_m)$ for sufficiently large m. Then we apply Theorem 3.9 and obtain part (a). Part (b) and (c) follow from self-adjointness. □

Remark 4.60. In [10], Proposition 4.55 was only shown for positive coupling constant λ. With the help of the previous proposition we can extend the result to negative λ. Let $\lambda < 0$, and observe that $T_{-\lambda,\alpha,\theta}(k, -E) = \begin{pmatrix} -E+\lambda & -1 \\ 1 & 0 \end{pmatrix} = -T_{\lambda,\alpha,\theta}(k, E)^T$. Using that the trace is invariant under reversing the potential, see Lemma 4.19, we get

$$\left|\operatorname{tr}\left(M_{-\lambda,\alpha,0}(q_m, -E)\right)\right| = \left|\operatorname{tr}\left(M_{\lambda,\alpha,0}(q_m, E)\right)\right| .$$

Due to Remark 4.56 and Proposition 4.14, we have $\sigma(H_{\lambda,\alpha_m,\theta}) = -\sigma(H_{-\lambda,\alpha_m,\theta})$. With Theorem 4.59, the identity of spectra carries over to the aperiodic operators. Thus, we also have

$$-\sigma(H_{\lambda,\alpha,\theta}) = \sigma(H_{-\lambda,\alpha,\theta}) ,$$

i.e. the spectrum for $H_{-\lambda,\alpha,\theta}$ is already determined by $\sigma(H_{\lambda,\alpha,\theta})$ which in turn is characterized by Proposition 4.55.

4.4 Dirichlet eigenvalues for aperiodic potentials

The results of Section 4.4.1 and 4.4.2 are based on joint work with Fabien Gabel, Dennis Gallaun, Julian Großmann and Marko Lindner [39].

4.4.1 Spectral convergence for one-sided operators

Throughout this section let $\lambda \in \mathbb{R} \setminus \{0\}$, $\alpha \in [0,1] \setminus \mathbb{Q}$ and $\theta \in [0,1)$. We define the discrete Schrödinger operator with Sturmian potential $H_{\lambda,\alpha,\theta}$ as in Definition 4.38. We set $\alpha_m = \frac{p_m}{q_m}$ to be the m-th rational approximation of α according to Definition 4.39. Then $H_{\lambda,\alpha_m,\theta}$ defines a periodic Schrödinger operator for each $m \in \mathbb{N}$ with

$$H_{\lambda,\alpha_m,0} \to H_{\lambda,\alpha,0} \qquad \text{and} \qquad \sigma(H_{\lambda,\alpha_m,0}) \to \sigma(H_{\lambda,\alpha,0}) \qquad \text{as } m \to \infty.$$

see Corollary 4.47 and Theorem 4.59. Also, by Theorem 4.53 $\sigma(H_{\lambda,\alpha,\theta})$ is independent of $\theta \in [0,1)$.

We now turn our attention to the Dirichlet eigenvalues of the compressions $H^+_{\lambda,\alpha,\theta}$. So far we have only established that

$$\sigma(H^+_{\lambda,\alpha,\theta}) \supset \sigma(H_{\lambda,\alpha,\theta}),$$

where the right-hand side does not depend on θ while the left-hand side may.

An additional obstacle is that the strong convergence $H_{\lambda,\alpha_m,\theta} \to H_{\lambda,\alpha,\theta}$ does not hold for all $\theta \in [0,1)$. In contrast to the two-sided case, strong convergence is necessary to obtain convergence of the respective spectra, compare Proposition 3.14 and Theorem 3.9.

This requires a careful choice of sequences A_m depending on θ. Fortunately, for a Schrödinger operator A with Sturmian potential Lemma 4.46 yields the following sequences (A_m) such that $A_m \to A$ holds:

	$A = H_{\lambda,\alpha,\theta}$	$A = \widetilde{H}_{\lambda,\alpha,\theta}$
$\theta = 0$	$H_{\lambda,\alpha_m,0}$	$\widetilde{H}_{\lambda,\alpha_m,0}$
$\theta = -k_0\alpha \bmod 1$ with $k_0 \in \mathbb{N}$	$H_{\lambda,\alpha_{2m+1},\theta}$	$H_{\lambda,\alpha_{2m},\theta}$
$\theta \neq -k_0\alpha \bmod 1$ for all $k_0 \in \mathbb{N}$	$H_{\lambda,\alpha_m,\theta}$	$H_{\lambda,\alpha_m,\theta}$

Table 4.2: Given a periodic Schrödinger operator A and a condition on the offset θ, the corresponding table entry gives sequence (A_m) used for approximation.

Theorem 4.61. *([39, Proposition 4.18]) Let A and A_m be defined as in Table 4.2 and $E \in \mathbb{R}$. Then*

(a) $\nu(A^+) = \lim_{m\to\infty} \nu(A^+_m)$,

(b) $((A_m - E)^+)_{m\in\mathbb{N}}$ *is stable if and only if* $(A - E)^+$ *is invertible,*

(c) $\sigma(A^+_m) \to \sigma(A^+)$ *as* $m \to \infty$ *in the Hausdorff metric.*

Moreover, if $E \notin \sigma(A)$ then

$$\left\|((A - E)^+)^{-1}\right\| = \lim_{m\to\infty} \left\|((A_m - E)^+)^{-1}\right\| .$$

Proof. For part (a) we aim to apply Proposition 3.14. It has already been established in the previous section that for each N we can find a sufficiently large m such that $\mathcal{C}_N(A_m) = \mathcal{C}_N(A)$ holds, see Lemma 4.51 and Lemma 4.58. Hence, only the strong convergence $A^+_m \to A^+$ remains to be shown. However, the choice of A_m is done exactly in a way that the convergence is guaranteed by Lemma 4.44 and Lemma 4.46. Note that the pointwise convergence of the potentials is only needed on $\mathbb{N}$ and that $H_{\lambda,\alpha,k\alpha} = \widetilde{H}_{\lambda,\alpha,k\alpha}$ for $k \in \mathbb{N}$.

Lastly, part (b) and (c) follow from the self-adjointness, exactly as in Theorem 4.59. □

We illustrate the spectral approximation of the Fibonacci Hamilton with the matrices A_m from Theorem 4.61 in Figure 4.6.

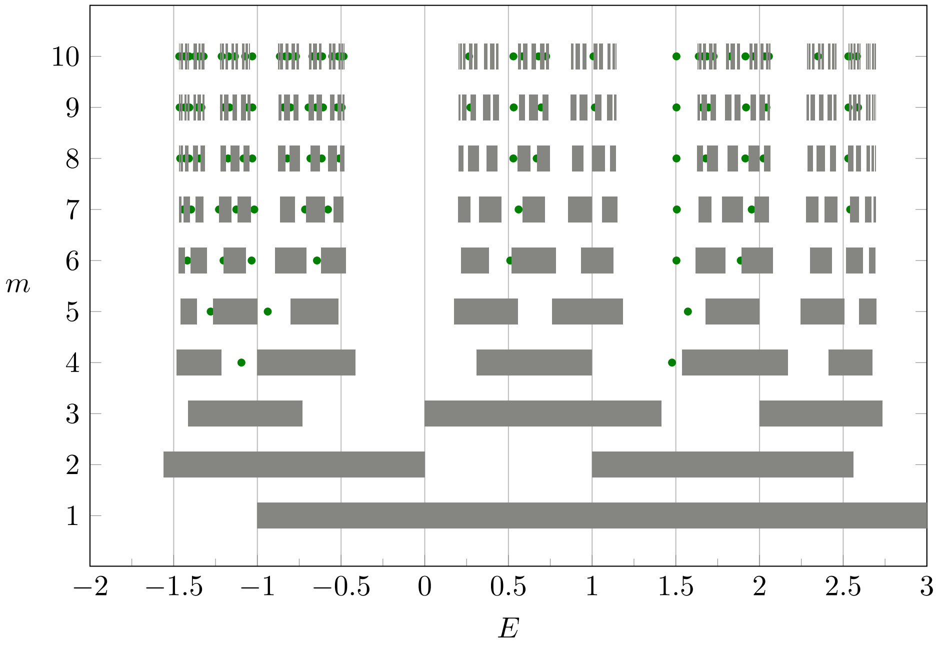

Figure 4.6: Spectra of A_m^+ for $m \in 2..10$ and $\lambda = 1$, $\alpha = (\sqrt{5}-1)/2$ and $\theta = 0$. The spectral bands of the two-sided operators A_m are plotted in gray and the Dirichlet eigenvalues are plotted in blue. By Theorem 4.61 we have $\sigma(A_m^+) \to \sigma(H^+_{\lambda,\alpha,\theta})$ as $m \to \infty$.

Recall that the spectrum of each A_m^+ consist of essential spectrum, that is given by $\sigma(A_m)$ and possibly Dirichlet eigenvalues. For the latter we get the following consequence.

Proposition 4.62. *Let A and A_m be defined as in Table 4.2. For $m_0 \in \mathbb{N}$ let $U \subsetneq \operatorname{int}(\rho(A_{m_0}) \cap \rho(A_{m_0+1}))$ be a closed interval. Then, either*

(a) $\sigma(A_m^+) \cap U = \emptyset$ for infinitely many m, in which case also $\sigma(A^+) \cap \operatorname{int}(U) = \emptyset$, or

(b) $\sigma(A_m^+) \cap U$ consists of a single eigenvalue for all m sufficiently large. As $m \to \infty$, these eigenvalues converge to an eigenvalue of A^+, which is the only element in $\sigma(A^+) \cap U$.

Proof. If $\sigma(A_m^+) \cap U = \emptyset$ for infinitely many m we use the Hausdorff convergence of spectra from Theorem 4.61 and obtain that $\sigma(A^+) \cap \operatorname{int}(U) = \emptyset$.

Let us now consider the remaining case that $\sigma(A_m^+) \cap U = \emptyset$ for only finitely many m. By Proposition 4.55 U is a subset of the resolvent set of A_m for all $m \geq m_0$ and of A, and therefore $\sigma(A_m^+) \cap U$ can only consist of eigenvalues for $m \geq m_0$. Moreover, by Proposition 4.22, there can be at most one eigenvalue of A_m^+ in U. The assumption $\sigma(A_m^+) \cap U \neq \emptyset$ implies that there is exactly one eigenvalue of A_m^+ in U. Again, due to the Hausdorff convergence of the spectra we find that there is also exactly one eigenvalue of A^+ in U. □

The results of Theorem 4.61 allow us to check the invertibility of all operators $(H_{\lambda,\alpha,\theta})^+$ for $\theta \in [0,1)$. In the following we show that it is sufficient to only check this for $\theta \in \{k_0\alpha \bmod 1 : k_0 \in \mathbb{Z}\}$ if a uniform boundedness condition is satisfied. The Schrödinger operators with Sturmian potential that have an offset in $\{k_0\alpha \bmod 1 : k_0 \in \mathbb{Z}\}$ are exactly those of the form $S^k H_{\lambda,\alpha,0} S^{-k}$.

Recall from Section 4.3 that $\mathcal{F}_\alpha = \big\{v_{\alpha,\psi}, \widetilde{v}_{\alpha,\psi} : \psi \in [0,1)\big\}$ and $L_{\lambda,\alpha} = \{H_{\lambda,\alpha,\psi}, \widetilde{H}_{\lambda,\alpha,\psi} : \psi \in [0,1)\} = \operatorname{Lim}(H_{\lambda,\alpha,\theta})$. We start with a lemma on the structure of $\mathcal{F}_\alpha$.

Lemma 4.63. *For $n \in \mathbb{N}$, let $v_n \in \mathcal{F}_\alpha$. Let further θ_n denote the offset of v_n.*

(a) Then there is a subsequence (v_{n_j}) that converges pointwise, i.e. $v_{n_k}(i)$ converges for every $i \in \mathbb{Z}$.

(b) If $\{\theta_n : n \in \mathbb{N}\}$ is dense in $[0,1]$, then, for each $v \in \mathcal{F}_\alpha$, there is a subsequence (v_{n_j}) that converges pointwise to v.

Proof. Part (a) follows from the fact that $L_{\lambda,\alpha}$ is sequentially compact, see Proposition 2.37.

For part (b), let $\psi \in [0,1)$ be the offset of v. If $v = v_{\alpha,\psi}$, we choose a subsequence (θ_{n_j}) that converges to ψ from the right and argue as in the proof of part (a) that $v_{n_j} \to v$ pointwise. For the case that $v = \widetilde{v}_{\alpha,\psi}$, we do the same with convergence from the left. If $\psi = 0$, then we take a subsequence (θ_{n_j}) that converges to 1. ☐

Proposition 4.64. *([39, Proposition 4.19]) It holds that*

$$\inf_{B\in L_{\lambda,\alpha}} \nu(B^+) = \min_{B\in L_{\lambda,\alpha}} \nu(B^+) = \inf_{k\in\mathbb{Z}} \nu(H^+_{\lambda,\alpha,\theta_k}) \,. \tag{4.43}$$

In particular, all operators B^+ for $B \in L_{\lambda,\alpha}$ are invertible if and only if for all $k \in \mathbb{Z}$ the operators $(H_{\lambda,\alpha,\theta_k})^+$ with $\theta_k := k\alpha \bmod 1$ are invertible and their inverses are uniformly bounded in k. In that case,

$$\sup_{B\in L_{\lambda,\alpha}} \|(B^+)^{-1}\| = \max_{B\in L_{\lambda,\alpha}} \|(B^+)^{-1}\| = \sup_{k\in\mathbb{Z}} \|(H^+_{\lambda,\alpha,\theta_k})^{-1}\|$$

Proof. We only show (4.43), as the rest follows from self-adjointness. For the first identity, take a sequence $(A_n) \subset L_{\lambda,\alpha}$ such that $\lim_{n\to\infty} \nu(A_n^+) = \inf_{B\in L_{\lambda,\alpha}} \nu(B^+)$. By Lemma 4.63(a), there exists $C \in L_{\lambda,\alpha}$ such that $A_n^+ \to C^+$ as $n \to \infty$. Together with Lemma 4.50, we find that the conditions of Proposition 3.14 are satisfied and therefore $\nu(C^+) = \inf_{B\in L_{\lambda,\alpha}} \nu(B^+)$. Hence, the infimum in (4.43) is indeed a minimum.

Since $\{H_{\lambda,\alpha,\theta_k} : k \in \mathbb{Z}\}$ is a subset of $L_{\lambda,\alpha}$, we immediately get

$$\min_{B\in L_{\lambda,\alpha}} \nu(B^+) \le \inf_{k\in\mathbb{Z}} \nu(H^+_{\lambda,\alpha,\theta_k}) \,.$$

For the other inequality, take $C \in L_{\lambda,\alpha}$ with $\nu(C^+) = \min_{B\in L_{\lambda,\alpha}} \nu(B^+)$. By Lemma 4.63(b), we find a subsequence (θ_{k_j}) such that $C^+ = \lim_{j\to\infty} H^+_{\lambda,\alpha,\theta_{k_j}}$. Again, Proposition 3.14 yields $\nu(H^+_{\lambda,\alpha,\theta_{k_j}}) \to \nu(C^+)$ which proves that

$$\min_{B\in L_{\lambda,\alpha}} \nu(B^+) \ge \inf_{k\in\mathbb{Z}} \nu(H^+_{\lambda,\alpha,\theta_k}) \,.$$ ☐

Remark 4.65. With the same method as in the proof of Proposition 4.64, one can also check that $H^+_{\lambda,\alpha,\theta}$ and $\widetilde{H}^+_{\lambda,\alpha,\theta}$ are invertible for every $\theta \in [0,1)$ if and only if, for all $k \in \mathbb{Z}$, the operators $\widetilde{H}^+_{\lambda,\alpha,\theta_k}$ are invertible and their inverses are uniformly bounded in k.

In particular, we have that the operators $H^+_{\lambda,\alpha,\theta_k}$, $k \in \mathbb{Z}$, are all invertible and their inverses are uniformly bounded in k if and only if the same holds for $\widetilde{H}^+_{\lambda,\alpha,\theta_k}$.

4.4.2 The finite section method for $H_{\lambda,\alpha,\theta}$

In the previous section, we have used an approximation method with periodic operators that has been properly tailored for the aperiodic Schrödinger operators. By using the periodic approximations, we are able to approximate spectra and lower norms of $H_{\lambda,\alpha,\theta}$. However, these approximants are still operators of infinite rank. Therefore, when it comes to solving a linear system $H_{\lambda,\alpha,\theta}x = b$ for $x, b \in \ell^2(\mathbb{Z})$, the FSM is better suited since it lets us pass to finite-dimensional systems, which are usually easier to solve.

Additionally, finite sections of $H_{\lambda,\alpha,\theta}$ appear in the integrated density of states (IDS). The IDS N is a function from $\mathbb{R}$ to $\mathbb{R}$ associated to the family $L_{\lambda,\alpha}$ that is defined via the functional calculus. We do not go into detail here, but mention that for almost every $\theta \in [0, 1)$ the IDS $N(E)$ can be computed for $E \in \mathbb{R}$ by

$$\lim_{n\to\infty} \frac{|\{\sigma((H_{\lambda,\alpha,\theta})_{1..n}) \cap (-\infty, E]\}|}{n},$$

compare [4, 26]. Thus, the IDS is given by the ratio between eigenvalues of the finite section that are smaller than E and the size of the finite sections.

We start by giving conditions for the applicability of the FSM based on the results of the previous section. All results of this chapter still hold for the FSM applied to $H_{\lambda,\alpha,\theta} - E$. Accordingly, we have to replace all operators $H_{\lambda,\alpha_m,\theta}$ by $H_{\lambda,\alpha_m,\theta} - E$ and so on.

Theorem 4.66. *([39, Theorem 5.2]) For $k \in \mathbb{Z}$, we set $\theta_k := k\alpha \bmod 1$. Then the following are equivalent:*

(i) The finite section method for $H_{\lambda,\alpha,\theta}$ is applicable.

(ii) The operators $H^+_{\lambda,\alpha,\psi}$ and $\widetilde{H}^+_{\lambda,\alpha,\psi}$ are invertible for every $\psi \in [0, 1)$.

(iii) The operators $H^+_{\lambda,\alpha,\theta_k}$ are invertible for all $k \in \mathbb{Z}$ and their inverses are uniformly bounded.

(iv) The operators $\widetilde{H}^+_{\lambda,\alpha,\theta_k}$ are invertible for all $k \in \mathbb{Z}$ and their inverses are uniformly bounded.

(v) For all $k \in \mathbb{Z}$, the sequence $(H^+_{\lambda,\alpha_m,\theta_k})_{m\in\mathbb{N}}$ is stable and

$$\sup_{k\in\mathbb{Z}} \big(\limsup_{m\to\infty} \|(H^+_{\lambda,\alpha_m,\theta_k})^{-1}\| \big) = \limsup_{m\to\infty} \big(\max_{k\in\mathbb{Z}} \|(H^+_{\lambda,\alpha_m,\theta_k})^{-1}\| \big) < \infty. \tag{4.44}$$

Here, we use the convention that $\|A^{-1}\| := \infty$ in the case that an operator A is not invertible. Moreover, we have that

$$\|A_n^{-1}\| \le \sup_{k\in\mathbb{Z}} \big(\limsup_{m\to\infty} \|(H^+_{\lambda,\alpha_m,\theta_k})^{-1}\| \big)$$

where A_n denote the finite submatrices that are obtained by applying the FSM to $H_{\lambda,\alpha,\theta}$.

Proof. For the equivalence (i) $\Leftrightarrow$(ii) we want to apply Theorem 3.24. We find that the stability indicators are given by

$$\mathcal{I}_{\text{stab}}(H_{\lambda,\alpha,\theta}) = \{H_{\lambda,\alpha,\theta}\} \cup \{B^+, B^- : B \in L_{\lambda,\alpha}\},$$

where $L_{\lambda,\alpha} = \{H_{\lambda,\alpha,\psi}, \widetilde{H}_{\lambda,\alpha,\psi} : \psi \in [0, 1)\}$. We know from Theorem 4.53, that the invertibility of any B^+ with $B \in L_{\lambda,\alpha}$ implies the invertibility of $H_{\lambda,\alpha,\theta}$. Moreover, the symmetry property (4.30) reveals that for each $B \in L_{\lambda,\alpha}$ the compression B^- is just a flip of C^+ for some other $C \in L_{\lambda,\alpha}$. Consequently, if all compressions B^+ for $B \in L_{\lambda,\alpha}$ are invertible, then also all compressions B^- are invertible. We thus find that all stability indicators are invertible if and only if condition (ii) holds. This settles the equivalence (i) ⇔(ii).

From Proposition 4.64 and the subsequent Remark 4.65, we know that the invertibility of all $H^+_{\lambda,\alpha,\psi}$ and $\widetilde{H}^+_{\lambda,\alpha,\psi}$ for $\psi \in [0,1)$ is equivalent the uniform boundedness of $\|H^{-1}_{\lambda,\alpha,\theta_k}\|$ for $k \in \mathbb{Z}$. Therefore, we have (ii)⇔(iii) ⇔(iv). Recall that for the operators $H^+_{\lambda,\alpha,\theta_k}$ and $\widetilde{H}^+_{\lambda,\alpha,\theta_k}$, $k \in \mathbb{Z}$ we have the approximation result Theorem 4.61. It states that (iii) and (iv) together are equivalent to

$$\sup_{k\in\mathbb{Z}} \big(\limsup_{m\to\infty} \|(H^+_{\lambda,\alpha_m,\theta_k})^{-1}\| \big) < \infty.$$

Therefore, it only remains to show that

$$\sup_{k\in\mathbb{Z}} \big(\limsup_{m\to\infty} \|(H^+_{\lambda,\alpha_m,\theta_k})^{-1}\| \big) = \limsup_{m\to\infty} \big(\max_{k\in\mathbb{Z}} \|(H^+_{\lambda,\alpha_m,\theta_k})^{-1}\| \big) .$$

In order to prove this, note that $H_{\lambda,\alpha_m,\theta_k}$ is a q_m-periodic Schrödinger operator and hence $\{H_{\lambda,\alpha_m,\theta_k} : k \in \mathbb{Z}\}$ is a finite set. Thus,

$$\sup_{k\in\mathbb{Z}} \|(H^+_{\lambda,\alpha_m,\theta_k})^{-1}\| = \max_{k\in\mathbb{Z}} \|(H^+_{\lambda,\alpha_m,\theta_k})^{-1}\| .$$

Moreover,

$$\sup_{k\in\mathbb{Z}} \big(\limsup_{m\to\infty} \|(H^+_{\lambda,\alpha_m,\theta_k})^{-1}\| \big) \le \limsup_{m\to\infty} \big(\sup_{k\in\mathbb{Z}} \|(H^+_{\lambda,\alpha_m,\theta_k})^{-1}\| \big)$$

is standard. For the other inequality, we use that the inverse of the lower norm is the norm of the inverse operator. Therefore, we want to show

$$\inf_{k\in\mathbb{Z}} \big(\liminf_{m\to\infty} \nu(H^+_{\lambda,\alpha_m,\theta_k}) \big) \le \liminf_{m\to\infty} (\inf_{k\in\mathbb{Z}} \nu(H^+_{\lambda,\alpha_m,\theta_k})) . \tag{4.45}$$

Let δ denote the right-hand side of (4.45). Then for all $N \in \mathbb{N}$ there are integers $k(N)$ and $m(N)$ such that $q_{m(N)-1} > k(N)$ and

$$\nu\big((H_{\lambda,\alpha_{m(N)},\theta_{k(N)}})_+\big) \le \delta + \frac{1}{N} .$$

Lemma 4.46 yields $v_{\alpha_{m(N)},\theta_{k(N)}}(l) = v_{\alpha,\theta_{k(N)}}(l)$ for $-q_{m(N)} + 1 \le l \le q_{m(N)} - 2$.

Using Lemma 4.63, we can find a sequence $(N_j)_{j\in\mathbb{N}}$ tending to infinity such that $v_{\alpha_{m(N)},\theta_{k(N)}}(l)$ converges pointwise to some Sturmian word v with slope α, that is $v = v_{\alpha,\psi}$ or $v = \widetilde{v}_{\alpha_\psi}$ for some $\psi \in [0,1)$. Let $B \in L_{\lambda,\alpha}$ denote the Schrödinger operator with potential v.

$$\delta + \frac{1}{N_j} \ge \nu\big(\big(H_{\lambda,\alpha_{m(N_j)},\theta_{k(N_j)}}\big)_+\big) \xrightarrow{j\to\infty} \nu(B_+) .$$

Hence, $\nu(B_+) \le \delta$. Now Theorem 4.61 and Proposition 4.64 give

$$\inf_{k\in\mathbb{Z}} \big(\liminf_{m\to\infty} \nu((H_{\lambda,\alpha_m,\theta_k})_+) \big) \le \delta ,$$

which proves (4.45). □

Remark 4.67. The applicability of the FSM for $\widetilde{H}_{\lambda,\alpha,\theta}$ is equivalent to the applicability of the FSM for $H_{\lambda,\alpha,\theta}$, and therefore to any of the conditions (i)–(v). Furthermore, in part (v), the operators $(H_{\lambda,\alpha,\theta_k})_+$ can be replaced by $(\widetilde{H}_{\lambda,\alpha,\theta_k})_+$.

Now we can check the applicability of the FSM with the help of the one-sided periodic Schrödinger operators $H^+_{\lambda,\alpha_m,\theta}$ for which the spectrum can be computed explicitly.

Corollary 4.68. *([39, Corollary 5.5]) The finite section method for $H_{\lambda,\alpha,\theta}$ is applicable if and only if there exists $m_0 \geq 0$ such that*

$$\left|\operatorname{tr}\left(M_{\lambda,\alpha,0}(q_{m_0})\right)\right| > 2 \quad \textit{and} \quad \left|\operatorname{tr}\left(M_{\lambda,\alpha,0}(q_{m_0+1})\right)\right| > 2 \tag{4.46}$$

and

$$\liminf_{m\to\infty} \operatorname{dist}(0, G_m) \neq 0 \tag{4.47}$$

with

$$G_m := \bigcup_{k=1}^{q_m} \left\{E \in \sigma\Big(\big(H_{\lambda,\alpha_m,0}\big)_{k..q_m+k-2}\Big) : \left|\det\Big(\big(H_{\lambda,\alpha_m,0} - E\big)_{k..q_m+k-1}\Big)\right| < 1\,.\right\}.$$

Proof. By the equivalence (i) $\Leftrightarrow$ (v) in Theorem 4.66, the finite section method for $H_{\lambda,\alpha,\theta}$ is applicable if and only if for all $k \in \mathbb{Z}$ the sequence $(H^+_{\lambda,\alpha_m,\theta_k})_{m\in\mathbb{N}}$ is stable and (4.44) holds.

Due to Proposition 4.55 we have that (4.46) implies that

$$\left|\operatorname{tr}\left(M_{\lambda,\alpha,0}(q_m)\right)\right| > 2 \tag{4.48}$$

holds for all $m \geq m_0$. With Proposition 4.14 and Remark 4.56 we have that (4.48) is equivalent to $\operatorname{dist}(0, \sigma(H_{\lambda,\alpha_m,0})) > \varepsilon$ for $m \geq m_0$ and some $\varepsilon > 0$. Since the spectra of the two-sided periodic Schrödinger operators are independent of the offset, we have

$$0 \notin \limsup_{m\in\mathbb{N}} \bigcup_{k\in\mathbb{Z}} \sigma(H_{\lambda,\alpha_m,\theta_k})\,.$$

So far, we have established the stability of the sequence of two-sided operators $((H_{\lambda,\alpha_m,\theta_k})_{m\in\mathbb{N}})$. Now we have to show that also the Dirichlet eigenvalues stay away from 0.

Further, by Proposition 4.20, E is a Dirichlet eigenvalue of $H^+_{\lambda,\alpha_m,\theta_k}$ if and only if $E \in \sigma((H_{\lambda,\alpha_m,\theta_k})_{0..q_m-2})$ and $|\det((H_{\lambda,\alpha_m,\theta_k} - E)_{0..q_m-1})| < 1$. Now let the set G'_m be defined by

$$\bigcup_{k\in\mathbb{N}} \left\{E \in \sigma((H_{\lambda,\alpha_m,\theta_k})_{0..q_m-2}) : |\det((H_{\lambda,\alpha_m,\theta_k} - E)_{0..q_m-1})| < 1\right\}.$$

Observe that, for all $k \in \mathbb{Z}$, the operators $H_{\lambda,\alpha_m,\theta_k}$ are q_m-periodic Schrödinger operators over the same alphabet. Even more is true: their corresponding Sturmian words v_{α,θ_k} only differ by a circular shift. Hence $G'_m = G_m$. Consequently, (4.46) and (4.47) together are equivalent to

$$0 \notin \limsup_{m\in\mathbb{N}} \bigcup_{k\in\mathbb{Z}} \sigma(H^*_{\lambda,\alpha_m,\theta_k}). \tag{4.49}$$

Now, we use that $\|A^{-1}\|^{-1} = \operatorname{dist}(0, \sigma(A))$ for an invertible self-adjoint operator A and obtain that (4.49) is equivalent to (v) in Theorem 4.66. □

Checking the Applicability of the FSM Numerically

In order to examine the applicability of the FSM for aperiodic Schrödinger operators, we have to check the invertibility of all one-sided Schrödinger operators with the same slope α, see Theorem 4.66 above. In this section, we describe a method to verify the invertibility of all these operators, see Algorithm 1 below and the code in [37] for an implementation. Again, we investigate the invertibility via the lower norm. Recall from (3.23) that the approximate lower norm of a one-sided Schrödinger operator A_+ is attained either with a vector that has finite support containing 1 or it is also attained by the two-sided operator A. We will see that, for the applicability of the FSM, we only need to look at elements with support at 1. For $N \in \mathbb{N}$, we write $[A]_N \colon \mathbb{C}^N \to \mathbb{C}^{N+1}$ for the restriction $A_+\chi_{[1,N]}I$ with the natural embeddings. As before, we set $\theta_k := k\alpha \bmod 1$ for $k \in \mathbb{Z}$.

As the following results will show, a key tool to investigate the applicability of the FSM for $H_{\lambda,\alpha,\theta}$ is the set $\Gamma_N := \{[H_{\lambda,\alpha,\theta_k}]_N : k \in \mathbb{Z}\} \subset \mathbb{C}^{(N+1)\times N}$. Since $v_{\alpha,\theta}$ has only $N+1$ different subwords of length N, see Lemma 4.51, we find that $|\Gamma| = N+1$. For an efficient algorithm to generate these subwords see [80].

We use the error bounds for the approximation of the lower norm given in Lemma 3.3.

Lemma 4.69. *([39, Lemma 5.7]) Let $\lambda \in \mathbb{R}$, $\alpha \in [0,1] \setminus \mathbb{Q}$ and $\theta \in [0,1)$. For $N \in \mathbb{N}$ and $\varepsilon_N > 0$ satisfying*

$$\varepsilon_N > 4 \sin \frac{\pi}{2N+2}, \tag{4.50}$$

we have that

$$\inf_{k\in\mathbb{Z}} \nu((H_{\lambda,\alpha,\theta_k})_+) \geq \min_{B\in\Gamma_N} \nu(B) - \varepsilon_N.$$

Proof. For $k \in \mathbb{Z}$, let us write $A_k := H_{\lambda,\alpha,\theta_k}$. Instead of using Lemma 3.3 for an approximation error estimate, we use a sharper bound that holds for $p = 2$, see [16, 17, 20]. This estimate is exactly $\nu((A_k)_+) \geq \nu_N((A_k)_+) - \varepsilon_N$. Now we take the infimum over $k \in \mathbb{Z}$ and apply Proposition 3.14:

$$\inf_{k\in\mathbb{Z}} \nu((A_k)_+) \geq \inf_{k\in\mathbb{Z}} \min \{\nu([A_k]_N), \nu_N(A_k)\} - \varepsilon_N\,.$$

It is easy to verify that, for all $j \in \mathbb{Z}$,

$$\nu_N(A_j) \geq \inf_{k\in\mathbb{Z}} \nu([A_k]_N) = \min_{B\in\Gamma_N} \nu(B)$$

holds. □

Let us put the previous result into the context of the FSM.

Theorem 4.70. *([39, Theorem 5.8]) Let $\lambda \in \mathbb{R}$, $\alpha \in [0,1] \setminus \mathbb{Q}$ and $\theta \in [0,1)$. Then the FSM is applicable to $H_{\lambda,\alpha,\theta}$ if and only if there are $N \in \mathbb{N}$ and ε_N satisfying* (4.50) *such that*

$$\min_{B\in\Gamma_N} \nu(B) > \varepsilon_N\,. \tag{4.51}$$

In that case, we have that

$$\limsup_{n\to\infty} \left\| \left((H_{\lambda,\alpha,\theta})_{i,j=1}^n \right)^{-1} \right\| \leq \frac{1}{\min\limits_{B\in\Gamma_N} \nu(B) - \varepsilon_N}\,. \tag{4.52}$$

Proof. We use Theorem 4.66, namely the equivalence (i)$\Leftrightarrow$(iii). Hence, the FSM is applicable to $H_{\lambda,\alpha,\theta}$ if and only if $\inf_{k\in\mathbb{Z}} \nu((H_{\lambda,\alpha,\theta_k})_+) > 0$. Again, we pass from the lower norm to the norms of the inverses by taking the reciprocal. Now we can apply Lemma 4.69 and obtain

$$\inf_{k\in\mathbb{Z}} \nu([H_{\lambda,\alpha,\theta_k}]_N) - \varepsilon_N \le \inf_{k\in\mathbb{Z}} \nu((H_{\lambda,\alpha,\theta_k})_+) \le \inf_{k\in\mathbb{Z}} \nu([H_{\lambda,\alpha,\theta_k}]_N) .$$

On the one hand, this shows that the FSM is applicable if $\nu([H_{\lambda,\alpha,\theta_k}]_N) > \varepsilon_N$. On the other hand, if the FSM is applicable, then $\inf_{k\in\mathbb{Z}} \nu([H_{\lambda,\alpha,\theta_k}]_N)$ is bounded from below by $\inf_{k\in\mathbb{Z}} \nu((H_{\lambda,\alpha,\theta_k})_+)$. Then, for sufficiently large N, the corresponding ε_N becomes smaller than this bound. Hence, $\nu([H_{\lambda,\alpha,\theta_k}]_N) > \varepsilon_N$. This concludes the proof of the first statement.

The identity (4.52) follows from Proposition 3.29. ☐

As a consequence of the above, Algorithm 1 below, that is from [39], can be used to check the applicability of the FSM. Due to the nature of Theorem 4.70 the algorithm can only be used to confirm the applicability of the FSM. If the return value is `false` then this only means that the applicability test has failed for the given value of N. In order to rule out the applicability one would have to perform the test for all $n \in \mathbb{N}$ which is of course not feasible.

Algorithm 1 Algorithm to check the applicability of the FSM for $H_{\lambda,\alpha,\theta}$ based on Theorem 4.70. The output of `generate_subwords` is the set $\mathcal{W}_N(v_\alpha)$, see Definition 4.49. For an efficient implementation see [80]. The function `construct_matrix` returns the $(N+1)\times N$ matrix with w on its main diagonal and 1 on the first sub- and superdiagonal. During the loop, `construct_matrix(`w`)` generates exactly the set Γ_N. The function `min_SVD` returns the smallest singular value of a matrix. Therefore, the `if`-statement in line 8 checks (4.51). A return value `false` does not necessarily mean that the FSM is not applicable.

```
 1: procedure CHECK_APPLICABILITY($\lambda$, $\alpha$, $N$)
 2:     $\varepsilon_N = 4\sin\frac{\pi}{2(N+2)}$
 3:     $\mathcal{W}_N$ = generate_subwords($\alpha$, $N$)        ▷ generates all subwords of length $N$
 4:     $M = \emptyset$
 5:     for $w \in$ words do
 6:         $H$ = construct_matrix($w$)
 7:         $M$ =$M\cup$ min_SVD($H$)
 8:     if $\min(M) > \varepsilon_N$ then
 9:         return true
10:     else
11:         return false
```

We close this subsection by applying Algorithm 1 to recover and extend the results of [72] where a different approach was used. In particular, we show that the FSM for the Fibonacci Hamiltonian is applicable.

Example 4.71. *We consider the case* $\lambda = 1$ *and set* $N = 100$ *and* $\alpha = \frac{\sqrt{5}-1}{2}$. *From* (4.50) *we get the error bound*

$$\varepsilon_N := 4\sin\frac{\pi}{202} \approx 0.062.$$

Computing $\nu_N(B)$ *for all* 101 *matrices* $B \in \Gamma_{100}(H)$, *corresponding to the* 101 *subwords of* $v_{\alpha,0}$ *of length* 100, *we find that*

$$\min_{B\in\Gamma_N} \nu(B) \ge 0.126 > \varepsilon_N .$$

Therefore, (4.51) *holds. With Lemma 4.69 we conclude that*

$$\inf_{k\in\mathbb{Z}} \nu((H_{\lambda,\alpha,\theta_k})_+) \geq 0.126 - \varepsilon_N \geq 0.063 > 0.$$

By Theorem 4.66 we find that $(H_{\lambda,\alpha,\theta})_+$ *is invertible for every* $\theta \in [0,1)$. *Now Theorem 4.70 implies that the FSM is applicable to* $H_{\lambda,\alpha,\theta}$ *for all* $\theta \in [0,1)$. *Moreover, due to* (4.52)*,*

$$\limsup_{n\to\infty} \left\| ((H_{\lambda,\alpha,\theta})_{i,j=1}^n)^{-1} \right\| \leq \frac{1}{0.063} \approx 15.87\,.$$

The above computations also reveal that there is a $k \in \mathbb{Z}$ *such that* $\nu([H_{\lambda,\alpha,\theta_k}]_N) \approx 0.127$. *However, it is clear from Proposition 4.55 and Figure 4.6 that dist*$(0, \sigma_{\mathrm{ess}}((H_{\lambda,\alpha,\theta_k}))_+) \geq 0.2$. *Since*

$$\nu((H_{\lambda,\alpha,\theta_k})_+) \leq \nu([H_{\lambda,\alpha,\theta_k}]_N) < \mathit{dist}(0, \sigma_{\mathrm{ess}}((H_{\lambda,\alpha,\theta_k})_+)),$$

we find that $(H_{\lambda,\alpha,\theta_k})_+$ *has an eigenvalue* E_0 *in the gap around* 0 *with* $0.126 - \varepsilon_N < |E_0| < 0.127$.

Figure 4.7 compares $\min_{B\in\Gamma_N} \nu(B)$ *and* ε_N *for* $N = 1,\ldots,100$. *We can see that the crucial condition* (4.51)*, i.e.* $\min_{B\in\Gamma_N} \nu(B) > \varepsilon_N$ *holds for* $N \geq 49$.

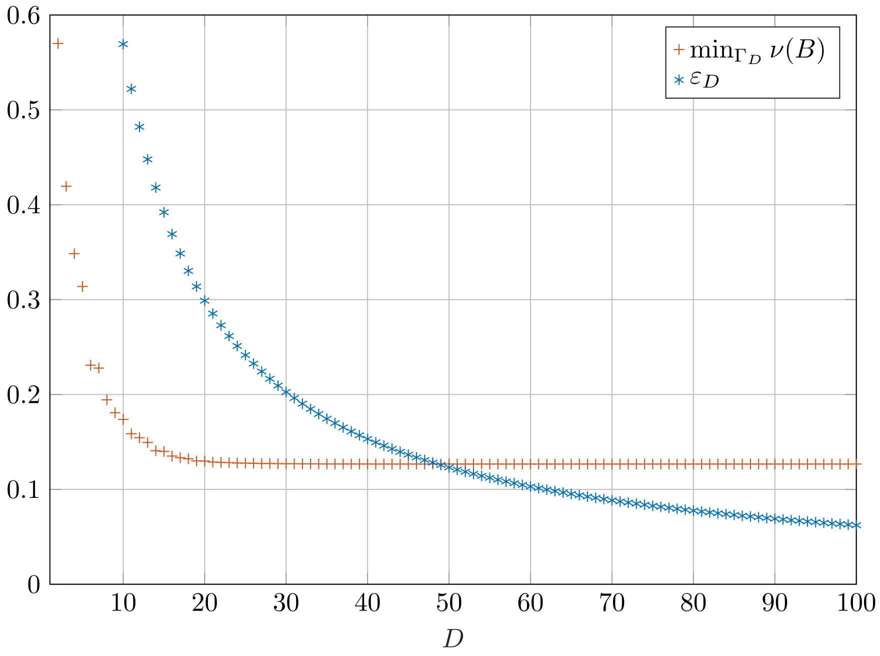

Figure 4.7: ([39, Figure 3]) Comparison of the quantities involved in condition (4.51) with α and λ from Example 4.71 and $N \in \{1,\ldots,100\}$. It can be seen that the conditions of Theorem 4.70 hold for $N \geq 49$.

4.4.3 Eigenvalues and candidates for decomposable words

In the following we give a result that links the structure of words to the location of the eigenvalue candidates for the corresponding periodic Schrödinger operators. For now, the potentials do not necessarily have to come from the periodic approximation of Sturmian words. We rather consider the following property.

Definition 4.72. For finite words s, v, w we say that s can be decomposed into v and w if $s = u_1 \dots u_n$ with $u_i \in \{v, w\}$ for $i = 1, \dots, n$. If $u_i = v$ and $u_j = w$ for some $i, j \in \{1, \dots, n\}$ then we say s can be decomposed into v and w non-trivially. If further $\mathcal{D}$ is a set of tuples of finite words and M is a set of finite words, then we say M is decomposable with $\mathcal{D}$ if every $s \in M$ can be decomposed into v and w, where $(v, w) \in \mathcal{D}$.

For $a, b \in \mathbb{R}$, we use the notation $[\![a, b]\!] := [\min(a, b), \max(a, b)]$.

Definition 4.73. We say that two finite real sets $A = \{a_1, \dots, a_{n+1}\}$ and $B = \{b_1, \dots, b_n\}$, $n \in \mathbb{N}$, are interlacing if

$$a_1 \leq b_1 \leq a_2 \leq \cdots \leq a_n \leq b_n \leq a_{n+1}. \tag{4.53}$$

Furthermore, we say that a finite real set A separates two finite real sets B and C if for every $b \in B$ and $c \in C$ there exists an $a \in A$ such that $a \in [\![b, c]\!]$. In particular, if A is interlacing with $B \cup C$ then A separates B and C.

Also recall that for a finite word v the periodic Schrödinger operator with the potential that is the periodic continuation of v is denoted by $H(v)$, with the convention that $(H(v))_{1,1} = v(1)$.

Proposition 4.74. *Let v, w be finite real words.*

(a) If $s = vw$ then $\Omega(H(s)^+)$ is interlacing with $\Omega(H(v)^+) \cup \Omega(H(w)^+)$.

(b) If s can be decomposed non-trivially into v and w then $\Omega(H(s)^+)$ separates $\Omega(H(v)^+)$ and $\Omega(H(w)^+)$.

Proof. (a) Note that $\Omega(H(v)^+) \cup \Omega(H(w)^+)$ is given by the eigenvalues of

$$B := \begin{pmatrix} H(w)_{1..|w|-1} & \\ & H(v)_{1..|v|-1} \end{pmatrix}.$$

Define $Q \in \mathbb{C}^{l \times l}$ with $l = |w| + |v| - 1$ by

$$Q := \begin{pmatrix} 0 & \mathbf{1}_{|w|} \\ \mathbf{1}_{|v|-1} & 0 \end{pmatrix}$$

and set $C := Q^T H(s)_{1..|s|-1} Q$. Recalling the definition of eigenvalue candidates, Definition 4.21, $\Omega(H(s)^+) = \sigma(H(s)_{1..|s|-1}) = \sigma(C)$. Hence it remains to show that the eigenvalues of B and C are interlacing. Since

$$H(s)_{1..|s|-1} = \left(\begin{array}{cc|c} H(v)_{1..|v|-1} & 1 & \\ 1 & v(|v|) & 1 \\ \hline & 1 & H(w)_{1..|w|-1} \end{array}\right)$$

we get

$$C = \left(\begin{array}{c|cc} H(w)_{1..|w|-1} & & 1 \\ \hline & H(v)_{1..|v|-1} & 1 \\ 1 & 1 & v(|v|) \end{array}\right).$$

Now we are in the same position as in Proposition 4.22 and the statement follows analogously.

(b) We decompose $s = u_1 \dots u_n$ with $u_i \in \{v, w\}$ for $i = 1 \dots n$ for some $n \in \mathbb{N}$. We prove the statement by induction over n. For $n = 2$ we have $s = vw$ or $s = wv$, hence the assertion follows directly from part (a).

To prove the statement for $n + 1$ we can decompose s as follows

$$s = u_1 \dots u_n u_{n+1} ,$$

where $u_i = v$ and $u_j = w$ for some $i, j \in \{1 \dots n + 1\}$.

Let $a \in \Omega(H(v)^+)$ and $b \in \Omega(H(w)^+)$. If $u_1 = u_{n+1}$ then we can apply the induction hypothesis on the word $\hat{s} := u_1 \dots u_n$ to obtain a $c \in \Omega(H(u_1 \dots u_n)_+) \cap [\![a, b]\!]$. Together with part (a) applied to $s = \hat{s}u_{n+1}$ we arrive at the statement.

If $u_1 \neq u_{n+1}$ then at least one of $u_1 \dots u_n$ and $u_2 \dots u_{n+1}$ can be decomposed non-trivially into v and w. Again, we apply the induction hypothesis and part (a) to prove the assertion. □

Observe that the interlacing of candidates described in Proposition 4.74 is not necessarily strict, meaning that (4.53) does not always hold with "<" instead of "≤". For instance, when doubling a word v the previous result yields that when treating $H(v) = H(vv)$ as a $2|v|$-periodic operator, $\Omega(H(vv))$ is a superset of $\Omega(H(v))$. However, we can characterize the exceptions with the following results.

Lemma 4.75. *Let v, w be finite words. If at least two of the sets $\Omega(H(vw))$, $\Omega(H(w))$, $\Omega(H(v))$ contain $E \in \mathbb{R}$ then all of them contain E.*

Proof. We abbreviate $D^u_{a..b} := \det(H(u)_{a..b} - E)$. Hence, $E \in \Omega(H(u)) \Leftrightarrow D^u_{1..|u|-1} = 0$ for $u \in \{v, w, vw\}$. We abbreviate $s = vw$. Then Laplace's formula for the determinant of $H(s)_{1..|s|-1} - E$ applied to row number $|v|$ yields

$$\begin{aligned} D^s_{1..|s|-1} =& (s(|v|) - E) D^v_{1..|v|-1} D^w_{1..|w|-1} \\ & - D^v_{1..|v|-2} D^w_{1..|w|-1} \\ & - D^w_{2..|w|-1} D^v_{1..|v|-1} . \end{aligned} \tag{4.54}$$

Laplace's formula for $D^v_{1..|v|-1}$ yields that $D^v_{1..|v|-1} = 0 \Rightarrow D^v_{1..|v|-2} \neq 0$ and analogously $D^w_{1..|w|-1} = 0 \Rightarrow D^w_{2..|w|-1} \neq 0$. Now the statement follows from (4.54). □

We denote the j-th gap of the spectrum of $H(u)$ by G^j_u, see Definition 4.18. The resulting "labels" of the gaps are not to be confused with the gap labels for aperiodic Schrödinger operators as in [9] or [25, Chapter 4.10], for example.

Lemma 4.76. *Let v, w be finite words and $j, k \in \mathbb{N}$. If for $s = vw$ we have $G^j_v \cap G^k_w \subset \rho(H(s))$ then $G^j_v \cap G^k_w \subset G^{j+k}_s$, i.e. the intersection of the j-th gap of $H(v)$ and the k-th gap of $H(w)$ lies in the $j + k$-th gap of $H(s)$.*

Proof. For a word u and $\theta \in \mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$ we write

$$H^u_\theta := \begin{pmatrix} u(1) & 1 & & \theta \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ \overline{\theta} & & 1 & u(|u|) \end{pmatrix} .$$

Due to Theorem 2.49, the spectrum of $H(u)$ is given by $\bigcup_{\theta\in\mathbb{T}}\sigma(H^u_\theta)$.

For $\theta,\varphi,\psi\in\mathbb{T}$ consider the matrices $C_{\varphi,\psi} := \begin{pmatrix} H^v_\varphi & \\ & H^w_\psi \end{pmatrix}$ and $H^s_\theta - C_{\varphi,\psi}$. Omitting zero entries, we get

$$H^s_\theta - C_{\varphi,\psi} \cong \left(\begin{array}{cc|cc} & -\varphi & & \theta \\ -\overline{\varphi} & & 1 & \\ \hline & 1 & & -\psi \\ \overline{\theta} & & -\overline{\psi} & \end{array}\right).$$

For any choice of φ and ψ choose θ such that $\varphi\psi = \theta$. Then $H^s_\theta - C_{\varphi,\psi}$ is self-adjoint, has rank 2 and trace 0, therefore it has exactly one positive and one negative non-zero eigenvalue. With $n = |s|$ let $E^\theta_1 \le \cdots \le E^\theta_n$ be the eigenvalues of H^s_θ and $\widetilde{E}^{\varphi,\psi}_1 \le \cdots \le \widetilde{E}^{\varphi,\psi}_n$ be the eigenvalues of $C_{\varphi,\psi}$.

Now Weyl's inequality for eigenvalues yields for all $i\in\{2,\dots,n-1\}$ that

$$E^\theta_{i-1} \le \widetilde{E}^{\varphi,\psi}_i \le E^\theta_{i+1} \quad\text{and}\quad \widetilde{E}^{\varphi,\psi}_{i-1} \le E^\theta_i \le \widetilde{E}^{\varphi,\psi}_{i+1}, \tag{4.55}$$

see Lemma 2.7. Let $E \in G^j_v \cap G^k_w$. It is clear that $\widetilde{E}^{\varphi,\psi}_{k+j} \le E \le \widetilde{E}^{\varphi,\psi}_{k+j+1}$. From (4.55) we get that $E^\theta_{k+j-1} \le E \le E^\theta_{k+j+2}$, but we need to show that $E^\theta_{k+j} \le E \le E^\theta_{k+j+1}$ holds.

Assume the contrary, i.e. $E < E^\theta_{k+j}$ or $E^\theta_{k+j+1} < E$ for some $E \in G^v_k \cap G^k_w$. We will only consider the first case since the latter can be proven analogously. Then let E_{right} be the smallest element of $\sigma(H(v)) \cup \sigma(H(w))$ that is larger than E. By assumption, we have that $[E, E_{\text{right}})$ cannot contain any element of $\sigma(H(s))$. Thus,

$$E_{\text{right}} \le E^\theta_{k+j} \text{ for all } \theta\in\mathbb{T}. \tag{4.56}$$

Depending on which of the two sets, $\sigma(H^v_\varphi)$ or $\sigma(H^w_\psi)$, contains E_{right} either for some fix $\varphi\in\mathbb{T}$ and all $\psi\in\mathbb{T}$ we have $E_{\text{right}} = \widetilde{E}^{\varphi,\psi}_{j+k+1}$ or the same holds for all φ and some fix ψ. Again, we only consider the first case, since the latter can be checked similarly.

Together with (4.55) and (4.56) we obtain $E^\theta_{k+j} \le \widetilde{E}^{\varphi,\psi}_{j+k+1} = E_{\text{right}} \le E^\theta_{k+j}$ for some $\varphi\in\mathbb{T}$ and all $\psi,\theta\in\mathbb{T}$ with $\varphi\psi = \theta$. This leads to a contradiction since varying ψ and θ will leave $\widetilde{E}^{\varphi,\psi}_{j+k+1}$ unchanged, but E^θ_{k+j} is non-constant in θ. □

The reader might recognize condition $G^j_v \cap G^k_w \subset \rho(H(s))$ from the trace condition in Proposition 4.55 for Sturmian words which roughly says that if $E\in\mathbb{R}$ is in the resolvent set for two consecutive periodic approximants then it will also be in the resolvent set for all subsequent approximants. Indeed, combining Proposition 4.55 with (4.34) we can immediately apply Lemma 4.76 to the Fibonacci Hamiltonian.

Corollary 4.77. *Let $\alpha = \frac{1-\sqrt{5}}{2}$. If E is in the j-th gap of $\sigma(H_m)$ and in the k-the gap of $\sigma(H_{m+1})$ then E is in the $j+k$-th gap of $\sigma(H_{m+2})$.*

Let us now turn our focus from the candidates back to the eigenvalues.

Lemma 4.78. *Let v, w be finite words and $s = vw$. If $E_v \in \sigma_p(H(v)^+)$ and $E_w \in \sigma_p(H(w)^+)$ then $\sigma(H(s)^+) \cap [\![E_v, E_w]\!] \neq \emptyset$.*

Proof. Set $E = \frac{E_v+E_w}{2}$ and $E_{\text{mean}} = \frac{E_v-E_w}{2}$. For $k \in \{0,\dots,|s|-1\}$ define $g(k) := \begin{cases} E_{\text{mean}} & \text{if } k < |v| \\ -E_{\text{mean}} & \text{else} \end{cases}$. We extend g periodically to $\mathbb{Z}$. Now define the periodic Schrödinger operator $G_s := H(s) + gI$. Then the monodromy matrix of G_s at E is given by

$$M_{G_s}(E) = M_{H(w)}(E_w) M_{H(v)}(E_v)\,.$$

Due to Proposition 4.20, both $M_{H(w)}(E_w)$ and $M_{H(v)}(E_v)$ are upper triangular matrices with a top left entry that is smaller than 1 in modulus. As a consequence,

$$M_{G_s}(E) = \begin{pmatrix} m_{11} & * \\ 0 & * \end{pmatrix},$$

with $|m_{11}| < 1$. Again by Proposition 4.20, this means that E is an eigenvalue of G_s^+. Therefore,

$$\nu(H(s)^+ - E) \le \|H(s)^+ - G_s^+\| + \nu(G_s^+ - E) = \|gI\| + 0 = E_{\text{mean}}\,.$$

Consequently, $\operatorname{dist}(E, \sigma(H(s)^+)) \le E_{\text{mean}}$.

□

In the following, let s^{R} denote the reversed word of a finite word s, that is $s^{\mathrm{R}}(k) = s(|s|-k+1)$ for $k \in 1..|s|$.

Lemma 4.79. *Let v, w, w' be finite words with $|w| = |w'| = 1$. Then for $s = vw$ and $s' = v^{\mathrm{R}}w'$ we have*

$$\Omega(H(s)^+) = \Omega(H(s')^+) = \sigma_p(H(s)^+) \uplus \sigma_p(H(s')^+) \uplus \mathcal{E}, \tag{4.57}$$

with $\mathcal{E} \subset \sigma_{\text{ess}}(H(s)^+) = \sigma_{\text{ess}}(H(s')^+)$ and $\uplus$ denoting the disjoint union.

Proof. Let K denote the length of s. By assumption, the restrictions of both words s and s' onto $1..K-1$ are reversions of each other. Therefore, the matrices $H(s)_{1..K-1}$ and $H(s')_{1..K-1}$ are similar, and we immediately get $\Omega(H(s)^+) = \Omega(H(s')^+)$.

In order to prove the remaining part, take $E \in \Omega(H(s)^+) = \Omega(H(s')^+)$ and let M_s and $M_{s'}$ be the monodromy matrices at energy E associated to the words s and s', respectively. Then $(M_s)_{2,1} = (M_{s'})_{2,1} = 0$, see Proposition 4.20. We further denote by $T_s(k)$ and $T_{s'}(k)$ the respective transfer matrices associated to $s(k)$ and $s'(k)$ with energy E. Since the inverse of a transfer matrix $\begin{pmatrix} * & -1 \\ 1 & 0 \end{pmatrix}$ is of the form $\begin{pmatrix} 0 & 1 \\ -1 & * \end{pmatrix}$ we find that

$$(M_v)_{1,1} = (T_s(K)^{-1} M_s)_{1,1} = 0,$$

where M_v denotes the monodromy matrix associated to v at energy E. We therefore set $M_v =: \begin{pmatrix} 0 & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$, where $a_{12}a_{21} = -1$. Then

$$M_s = T_s(K) M_v = \begin{pmatrix} -a_{21} & * \\ 0 & a_{12} \end{pmatrix}. \tag{4.58}$$

Now we can use that

$$F M_v^{-1} F = M_{v^{\mathrm{R}}} \quad \text{with} \quad F = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

cf. the proof of Lemma 4.19. Then

$$M_{s'} = T_{s'}(K) M_{v^{\mathrm{R}}} = T_{s'}(K) F (M_v)^{-1} F\,. \tag{4.59}$$

By the standard formula for inverses of 2×2-matrices with determinant 1, (4.59) yields

$$\begin{aligned} M_{s'} &= T_{s'}(K) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & a_{12} \\ a_{21} & a_{22} \end{pmatrix}^{-1} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ &= T_{s'}(K) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a_{22} & -a_{12} \\ -a_{21} & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} * & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -a_{21} \\ -a_{12} & a_{22} \end{pmatrix} \\ &= \begin{pmatrix} a_{12} & * \\ 0 & -a_{21} \end{pmatrix}. \end{aligned} \tag{4.60}$$

Comparing (4.58) and (4.60) we find that M_s and $M_{s'}$ both are upper triangular matrices, and their diagonal entries are swapped. Using Proposition 4.14, we find that

$$E \in \sigma_{\mathrm{ess}}(H(s)^+) \Leftrightarrow |a_{12}| = |a_{21}| = 1 \Leftrightarrow E \in \sigma_{\mathrm{ess}}(H(s')^+).$$

Moreover, if $|a_{12}| \neq 1$ then Proposition 4.20 yields

$$E \in \sigma_p(H(s)^+) \Leftrightarrow |a_{12}| < 1 \Leftrightarrow |a_{21}| > 1 \Leftrightarrow E \notin \sigma_p(H(s')^+).$$

□

The symmetry property from the previous lemma has an interesting consequence for words that consist of a palindrome and an extra letter.

Corollary 4.80. *If $v = ux$, where u is a palindrome, i.e. $u = u^{\mathrm{R}}$, and $|x| = 1$. Then $\sigma_p(H(v)^+) = \emptyset$ and $\Omega(H(v)^+) \subset \sigma_{\mathrm{ess}}(H(v)^+)$.*

Proof. We apply Lemma 4.79 to $s = s' = u$ and $w = x$. Since the union in (4.57) is disjoint we see that $\sigma_p(H(v)^+) = \sigma_p(H(v)^+) \cap \sigma_p(H(u^{\mathrm{R}}x)^+) = \emptyset$. □

4.4.4 Interlacing of candidates for Sturmian potentials

Throughout this section let us abbreviate $H := H_{\lambda,\alpha,0}$ and $H_m := H_{\lambda,\alpha_m,0}$ or $H := \widetilde{H}_{\lambda,\alpha,0}$ and $H_m := \widetilde{H}_{\lambda,\alpha_m,0}$ for $\lambda > 0$ and $\alpha \in [0,1] \setminus \mathbb{Q}$ and $\alpha_m = \frac{p_m}{q_m}$ arising from the continued fraction expansion of α see Section 4.3.1. We can use this shorthand notation since the results of this section, except for the examples, are independent of α and λ and the choice between $H_{\lambda,\alpha,0}$ and $\widetilde{H}_{\lambda,\alpha,0}$. Additionally, set $S := \sigma(H)$, $S_m := \sigma(H_m)$, $S^+ := \sigma(H^+)$ and $S_m^+ := \sigma(H_m^+)$. We have seen in Theorem 4.59 and Theorem 4.61 that

$$S_m \to S \qquad \text{and} \qquad S_m^+ \to S^+ \tag{4.61}$$

in Hausdorff distance, and we even have an upper bound on the convergence rate. In the previous section we used these results for a numerical method to prove whether the FSM is applicable.

However, these results can also be combined with a new observation on the behavior of the Dirichlet candidates of H_m^+ to say even more about the spectrum S^+. Recall from Definition 4.21 that a (Dirichlet) candidate E of H_m^+ satisfies $E \in \sigma((H_m^+)_{1..q_m-1})$. Let Ω_m denote the set of candidates of H_m^+. By Proposition 4.20, the eigenvalues of H_m^+ are given by candidates of H_m^+ that additionally satisfy $|\det((H_m^+)_{1..q_m})| < 1$. We write $\Pi := \sigma_p(H^+)$ and $\Pi_m := \sigma_p(H_m^+)$.

Sturmian potentials with $\theta = 0$

Due to the recursive composed nature of Sturmian words (4.34) with offset 0 it seems natural to investigate their periodic approximations. The finite words $s_m$from (4.34) have the same length q_m as one period of the periodic infinite word v_{α_m}. Let us recall how they correlate.

Definition 4.81. For $m \geq 2$ let $\tilde{s}_m$ be the restriction of v_{α_m} to $1..q_m$. We call $\tilde{s}_m$ the stem of v_{α_m}.

By Lemma 4.44, $s_m = \tilde{s}_m$ for even m. If m is odd then $s_m(k) = \tilde{s}_m(k)$ holds only for $k = 1, \dots, q_m - 2$. More precisely, we have that

$$s_m = \begin{cases} \pi_m 10 & \text{if } m \text{ is even,} \\ \pi_m 01 & \text{if } m \text{ is odd,} \end{cases} \qquad \text{and} \qquad \tilde{s}_m = \pi_m 10, \tag{4.62}$$

where π_m is a palindrome, see Lemma 4.41.

It is easy to see that $H(s_m)^+ \to H^+$ and also that the finite subwords of their potentials coincide eventually as $m \to \infty$. Therefore, with Proposition 3.14 we have in addition to (4.61) that

$$\sigma(H(s_m)) \to \sigma(H) \qquad \text{and} \qquad \sigma(H(s_m)^+) \to \sigma(H^+)$$

as $m \to \infty$.

Example 4.82. *Let us begin with this investigation with the Fibonacci-Hamiltonian, i.e. fix* $\alpha = \frac{\sqrt{5}-1}{2}$ *and* $\theta = 0$*. We have the recursion* (4.34)*,* $s_{m+1} = s_m s_{m-1}$ *for all* $m \in \mathbb{N}$*. Thus, the candidates of* $H(s_m)^+$ *and* $H(s_{m-1})^+$ *together are interlacing with the candidates of* $H(s_{m+1})^+$ *by Proposition 4.74(a). However, for the candidates of* $H_m^+ = H(\tilde{s}_m)^+$ *a recursive composition of* $\tilde{s}_m$ *analogue to* (4.34) *is needed.*

The plot of the spectra S_m *and the candidates* Ω_m *for* $m = 1, \dots, 10$ *in Figure 4.8 suggests that the candidates of eigenvalues,* Ω_m*, show the same interlacing behavior nonetheless.*

We provide an analogue of the recursion (4.34) for the words $\tilde{s}_m$. Recall that $a_1, a_2, \dots$ are the coefficients from the continued fraction of α and that for the case of the Fibonacci word, that is $\alpha = \frac{\sqrt{5}}{2}$, we have $a_m = 1$ for all $m \in \mathbb{N}$.

Lemma 4.83. *Let* $m \in \mathbb{N}$*. Then*

$$\tilde{s}_{m+2} = \begin{cases} \tilde{s}_m \tilde{s}_{m+1}^{a_{m+2}} & m \text{ even,} \\ \tilde{s}_{m+1}^{a_{m+2}} \tilde{s}_m & m \text{ odd.} \end{cases} \tag{4.63}$$

Furthermore, if $a_{m+2} = 1$ *then* Ω_{m+2} *is interlacing with* $\Omega_{m+1} \cup \Omega_m$*. If* $a_{m+2} \geq 1$ *then* Ω_{m+2} *separates* Ω_{m+1} *and* Ω_m*.*

Proof. Let us first prove

$$s_{m+1}\tilde{s}_m = s_m \tilde{s}_{m+1}. \tag{4.64}$$

We use (4.62). With the appropriate choice of $a, b \in \{0, 1\}, a \neq b$,

$$\begin{aligned} s_{m+1}\tilde{s}_m &= \underbrace{s_m^{a_{m+1}} \pi_{m-1}}_{\pi_{m+1}} ab\pi_m 01 \\ &= \underbrace{\pi_{m-1} (s_m^{\mathrm{R}})^{a_{m+1}} ab\pi_m}_{\pi_{m+1}} 01 \end{aligned}$$

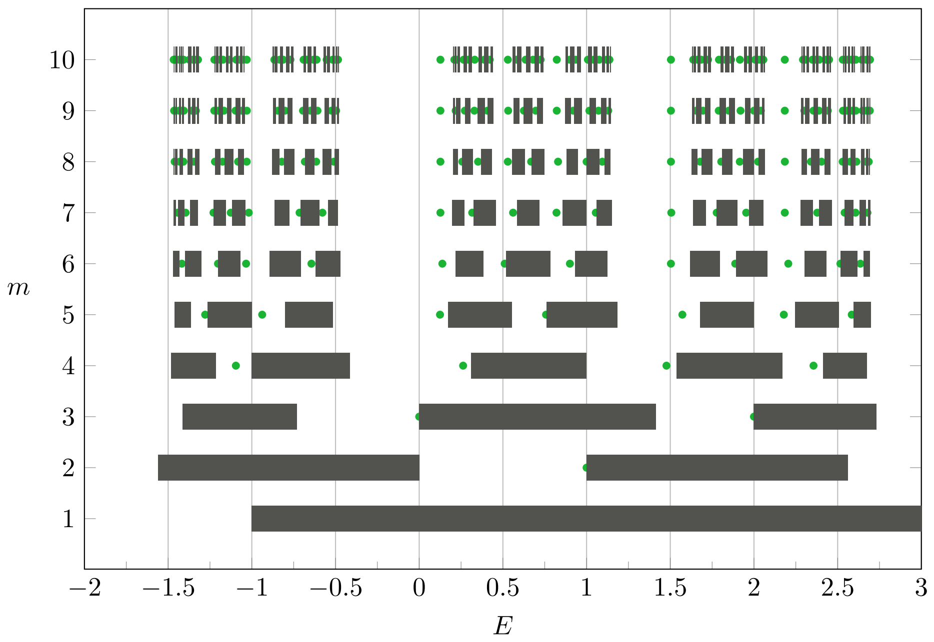

Figure 4.8: For $\alpha = \frac{\sqrt{5}-1}{2}$ the spectra S_m of the approximants are displayed in gray and the candidates of eigenvalues Ω_m are displayed as green dots.

$$= \pi_m ba(s_m)^{a_{m+1}}\pi_{m-1}01$$
$$= s_m(s_m)^{a_{m+1}}\tilde{s}_{m-1} = s_m\tilde{s}_{m+1}.$$

Next we prove (4.63). For even m we use (4.64) together with $s_m = \tilde{s}_m$ multiple times and obtain $\tilde{s}_{m+2} = s_{m+1}^{a_{m+2}}\tilde{s}_m = s_{m+1}^{a_{m+2}-1}\tilde{s}_m\tilde{s}_{m+1} = \cdots = \tilde{s}_m\tilde{s}_{m+1}^{a_{m+2}}$. For odd m we have $s_{m+1} = \tilde{s}_{m+1}$. Therefore, we immediately get $\tilde{s}_{m+2} = s_{m+1}^{a_{m+2}}\tilde{s}_m = \tilde{s}_{m+1}^{a_{m+2}}\tilde{s}_m$. Hence, we have proven the recursion formula (4.63). The assertions about the candidates now directly follow from Proposition 4.74. □

Recall from Proposition 4.55 that

$$S_{m+2} \subset S_m \cup S_{m+1}. \tag{4.65}$$

Hence, if $E \in \mathbb{R}$ is in a gap of S_{m_0} and of S_{m_0+1} then it will be in a gap for all S_m, $m \geq m_0$. Let us consider an interval G that lies in two consecutive gaps, meaning that the previous condition is satisfied for all $E \in G$. Assume that we find that a candidate E_{m_0} of $H_{m_0}^+$ and a candidate E_{m_0+1} of $H_{m_0+1}^+$, both lying in G. Then we know from Lemma 4.83 that there is a candidate E_{m_0+2} of $H_{m_0+2}^+$ between them, i.e. $E_{m_0+2} \in [\![E_{m_0}, E_{m_0+1}]\!]$. We can iterate this argument to find that H_m^+ has a candidate in $[\![E_{m_0}, E_{m_0+1}]\!]$ for all $m \geq m_0$. Since there is exactly one candidate per gap we find that all candidates of H_m^+ that are in G are always in $[\![E_{m_0}, E_{m_0+1}]\!]$. This means that we can rule out Dirichlet eigenvalues for the rest of G.

Corollary 4.84. *Let G be a component of $G_m \cap G_{m+1}$. If G contains a candidate E_m of H_m^+ and a candidate E_{m+1} of H_{m+1}^+ then*

(a) for $j \geq m+1$ there exists an $E \in \Omega_j \cap [\![E_m, E_{m+1}]\!]$,

(b) *for* $j \geq m+1$ *we have* $G \setminus [\![E_m, E_{m+1}]\!] \subset \rho(H_j^+)$*,*

(c) $G \setminus [\![E_m, E_{m+1}]\!] \subset \rho(H^+)$*.*

Observe in Figure 4.8 how the candidates of H_m^+ for $m \geq 5$ that lie in the gap around $E = 1.5$ are "trapped" in $[\![E_5, E_6]\!] \approx [1.5, 1.6]$. With Corollary 4.84 we find that the remaining gap cannot contain Dirichlet eigenvalues for larger m and also for the aperiodic operator H.

In many cases the condition in Corollary 4.84 is too strict: if we have a non-empty component G of $G_m \cap G_{m+1}$, it may happen that $\{E_m, E_{m+1}\} \not\subset G$. Indeed, this happens for the Fibonacci Hamiltonian in the gap around 0 for $m = 3$. We take a closer look at the situation in Figure 4.9. In this case, there is still always a Π_k-candidate in $[\![E_m, E_{m+1}]\!]$ for $k > m+1$. However, it is not guaranteed that it also lies in G or even in the same gap.

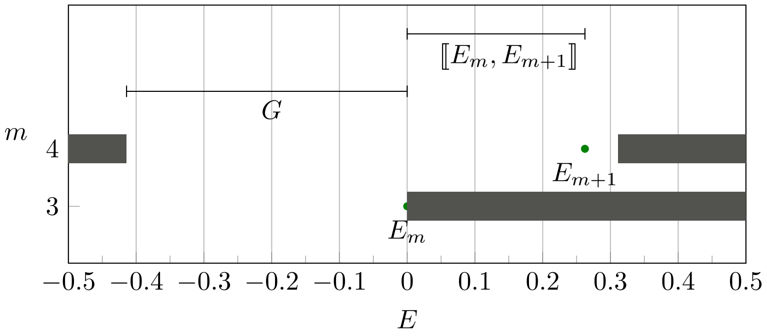

Figure 4.9: Section of spectra of H_3 and H_4 for the Fibonacci-Hamiltonian, cf. Figure 4.8. For $m = 3$ we observe that $[\![E_m, E_{m+1}]\!]$, G as described in Corollary 4.84 are disjoint, in particular $E_m, E_{m+1} \notin G$.

Before we can prove a result similar to Corollary 4.84 without the restriction that both candidates lie in G, we need to label the candidates in Ω_m.

Definition 4.85. For $m \in \mathbb{N}$ we label the elements of Ω_m from smallest to largest, such that the smallest element is called the first candidate of H_m^+ and the largest element is called the q_m-th candidate of H_m^+.

Lemma 4.86. *For* $m \in \mathbb{N}$*,* $k \in 1..q_m$ *and* $j \in 1..q_{m+1}$ *the following hold:*

(a) *The* k*-th candidate of* H_m^+ *is in the* k*-th gap of* $\sigma(H_m)$*.*

(b) *The* $k + a_{m+2}j$*-th candidate of* H_{m+2}^+ *lies in* $[\![E_m, E_{m+1}]\!]$*, where* E_m *is the* k*-th candidate of* H_m^+ *and* E_{m+1} *is the* j*-th candidate of* H_{m+1}^+*.*

Proof. Part (a) follows directly from the interlacing of spectral bands and candidates, see Proposition 4.22. For part (b) we use the decomposition of $\tilde{s}_{m+2}$ into $\tilde{s}_{m+1}$ and $\tilde{s}_m$ from Lemma 4.83. In the case of $a_{m+2} = 1$ the interlacing of candidates, see Proposition 4.74(a). For larger $a_{m+2} = 1$ we apply the same result multiple times. □

Proposition 4.87. *For* $k \in \{m, m+1\}$ *let* G'_k *be a component of* G_k *and* $E_k \in \Omega_k \cap G'_k$*. Then the following hold for* $G = G'_m \cap G'_{m+1}$*:*

(a) $\exists E \in \Omega_j \cap [\![E_m, E_{m+1}]\!]$ *for* $j \geq m+1$*,*

(b) $G \setminus \llbracket E_m, E_{m+1} \rrbracket \subset \rho(H_j^+)$ *for* $j \geq m+1$,

(c) $G \setminus \llbracket E_m, E_{m+1} \rrbracket \subset \rho(H^+)$.

Proof. We abbreviate $I := \llbracket E_m, E_{m+1} \rrbracket$. The assertion (a) still follows directly from Proposition 4.74. For the proof of (b) we denote the unique candidate of H_j^+ in I by E_j.

In order to avoid the trivial case, we assume that $G \neq \emptyset$. Observe that $G \subset \rho(H_j)$ and that there can be at most one $E_j \in \Omega_j \cap G$. It remains to show that E_j belongs to the same component of $\rho(H_j)$ as G, thereby not allowing any other candidates in G, in particular there are none in $G \setminus I$. If $I \subset G$ the assertion follows directly, see Corollary 4.84.

So let us explore the case $I \not\subset G$. At first glance, it might happen for $j = m+2$ that there is a gap $\widetilde{G}$ of $\sigma(H_{m+2})$ such that $\widetilde{G} \cap G = \emptyset$ and $\widetilde{G} \cap I \neq \emptyset$. Then $E_{m+2} \in \widetilde{G}$ and there is another, uncontrolled eigenvalue E_G in the gap containing G, possibly in $G \setminus I$. We sketch such a situation in Figure 4.10.

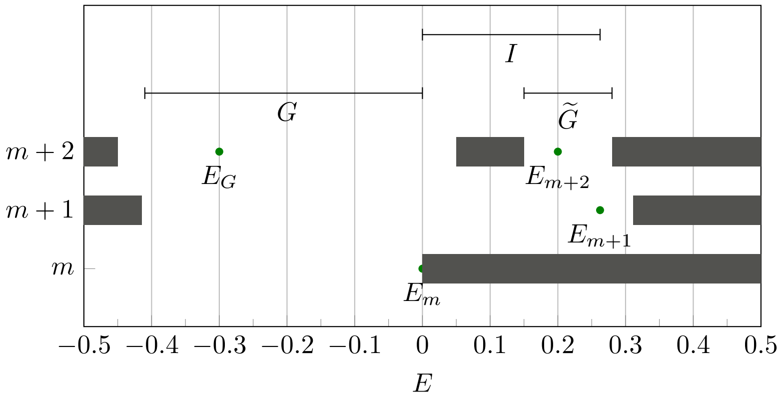

Figure 4.10: Sections of spectra of the fictitious operators H_m, H_{m+1} and H_{m+2} with corresponding candidates as described in the proof of Proposition 4.87. Grey bars are the spectrum of the two-sided operators, green dots are candidates of eigenvalues for the corresponding one-sided operator. I, G and $\widetilde{G}$ are as described in the proof, where we will show that such a situation cannot arise. Note that the spectra and the candidates obey (4.65), the interlacing of candidates (Proposition 4.74) and the interlacing of bands and candidates (Proposition 4.22).

We show that this cannot happen by proving that E_{m+2} is in the same component of $\rho(H_{m+2})$ as G. Let G_m be the k_m-th gap of $\sigma(H_m)$ and G_{m+1} be the k_{m+1}-th gap of $\sigma(H_{m+1})$. The recursion $s_{m+2} = s_{m+1}^{a_{m+1}} s_m$ together with Lemma 4.76 yields that G is in the $a_{m+2}k_{m+1} + k_m$-th gap of $\sigma(H_{m+2})$.

With Lemma 4.86 (a) and the observations above we find that G contains the $k_m + k_{m+1}$-th candidate of H_{m+2}^+.

However, since E_m is the k_m-th candidate of H_m^+ and E_{m+1} is the k_{m+1}-th candidate of H_{m+1}^+, part (b) of Lemma 4.86 yields that E_{m+2} has to be the $a_{m+2}k_{m+1} + k_m$-th candidate of H_{m+2}^+. Hence, we get that E_{m+2} is in the same gap as G.

By induction, we get the same result for all $j \geq m+2$. Thus, we arrive at (b). With the spectral convergence (4.61) we have that (b)$\Rightarrow$ (c). $\square$

Looking back at Figure 4.9, Proposition 4.87 (unlike Corollary 4.84) now allows us to conclude that the Fibonacci Hamiltonian with $\lambda = 1$ and $\theta = 0$ does not have a Dirichlet eigenvalue in the interval $[-0.4, 0]$. Note that the approximations necessary for this conclusion are of relatively low order, namely $q_3 = 3$ and $q_4 = 5$.

Let us consider the following partition of the set of candidates:

$$\Omega_m \;=\; \Omega_m^+ \;\dot\cup\; \Omega_m^- \;\dot\cup\; \Omega_m^0,$$

where $\Omega_m^+ := \{E \in \Omega_m : |\det(H_{1..q_m} - E)| < 1\}$, $\Omega_m^- := \{E \in \Omega_m : |\det(H_{1..q_m} - E)| > 1\}$ and $\Omega_m^0 := \{E \in \Omega_m : |\det(H_{1..q_m} - E)| = 1\}$. This partition reveals a symmetry property of the set of candidates.

Proposition 4.88. *With the notation from above we have the following:*

- *(a)* $\Omega_m^+ = \sigma_p(H_m^+) = \Pi_m$,
- *(b)* $\Omega_m^- = \sigma_p(P_{-\mathbb{N}} H_m P_{-\mathbb{N}})$,
- *(c)* $\Omega_m^0 \subseteq \sigma_{\text{ess}}(H_m^+) = \sigma_{\text{ess}}(P_{-\mathbb{N}} H_m P_{-\mathbb{N}}) = \sigma(H_m) = S_m$.

Proof. Part (a) is by Proposition 4.20. Part (c) follows from Corollary 4.25, in this case the candidate lies on the edge of a spectral band. For part (b) let us use the flip operators, i.e. canonical isomorphisms Φ from $\ell^2(\mathbb{N})$ to $\ell^2(-\mathbb{N})$. If we understand the operator $\Phi^{-1} P_{-\mathbb{N}} H_m P_{-\mathbb{N}} \Phi$ on $\ell^2(\mathbb{N})$ as matrix we denote the first q_m diagonal entries of that matrix, understood as a word, by s'. Then, using periodicity,

$$s' = v_{\alpha_m}(-1) \dots v_{\alpha_m}(-q_m) = v_{\alpha_m}(q_m - 1) \dots v_{\alpha_m}(0).$$

Compare this to the corresponding word of H_m^+:

$$s = \tilde{s}_m = v_{\alpha_m}(1) \dots v_{\alpha_m}(q_m).$$

If we set $v = v_{\alpha_m}(1) \dots v_{\alpha_m}(q_m - 1)$ then $s = v v_{\alpha_m}(q_m)$ and $s' = v^{\mathrm{R}} v_{\alpha_m}(0)$. Thus, we can use Lemma 4.79 to obtain the trichotomy (4.57). □

In short, Proposition 4.88 states that a candidate in Ω_m is either a Dirichlet eigenvalue of H_m^+ or one of $P_{-\mathbb{N}} H_m P_{-\mathbb{N}}$ or part of the essential spectrum $\sigma_{\text{ess}}(H_m^+) = \sigma_{\text{ess}}(P_{-\mathbb{N}} H_m P_{-\mathbb{N}}) = \sigma(H_m)$. Sending m to ∞ the set Ω_m recovers not only the Dirichlet eigenvalues of H^+ and $P_{-\mathbb{N}} H_m P_{-\mathbb{N}}$ but much more.

Proposition 4.89. *For the set of candidates we have* $\Omega_m \to S^+ \cup S^-$ *as* $m \to \infty$ *in Hausdorff distance, where* $S^- = \sigma(P_{-\mathbb{N}} H P_{-\mathbb{N}})$.

Proof. Due to Lemma 4.44 $H_m^- \to H^-$. Together with Lemma 4.50, Lemma 4.51 and Theorem 3.9 we get that $S_m^- \to S^-$, where $S_m^- := \sigma(H_m^-)$. Since $\Omega_m \subset S_m^+ \cup S_m^-$ we get

$$\limsup_{m\to\infty} \Omega_m \subset \limsup_{m\to\infty} (S_m^+ \cup \limsup_{m\to\infty} S_m^-) = \limsup_{m\to\infty} S_m^+ \cup \limsup_{m\to\infty} S_m^- = S^+ \cup S^-.$$

We therefore still need to show that

$$S^+ \cup S^- \subset \liminf_{m\to\infty} \Omega_m, \tag{4.66}$$

i.e. for all $E \in S^+ \cup S^-$ there is a sequence (E_m) such that $E_m \in \Omega_m$ for all $m \in \mathbb{N}$ and $E_m \to E$ as $m \to \infty$. We will do this for the three parts of $(S^+ \setminus S) \cup (S^- \setminus S) \cup S = S^+ \cup S^-$ separately.

For $E \in S^+ \setminus S$ the spectral convergence $S_m^+ \to S^+$ yields that there is a sequence (E_m) with $E_m \in S_m^+$ such that $E_m \to E$. Since $\operatorname{dist}(E, S) > 0$ and $S_m \to S$ as $m \to \infty$ only finitely many E_m can be from S_m. Therefore, $E_m \in S_m^+ \setminus S_m \subset \Omega_m$ for m sufficiently large. This means that $S^+ \setminus S \subset \liminf_{m\to\infty} \Omega_m$. Similarly, using Proposition 4.88 we can show that $S^- \setminus S \subset \liminf_{m\to\infty} \Omega_m$.

In order to arrive at (4.66) and thereby finishing the proof it only remains to show that $S \subset \liminf_{m\to\infty} \Omega_m$. Let $\varepsilon > 0$ and $E \in S$ be given. Since S is a Cantor set, see Proposition 4.57, every neighborhood of E contains infinitely many elements of the spectrum S and the resolvent set alike. By Proposition 4.55 we find a gap G_m with $\emptyset \neq G_m \subset U_{\frac{\varepsilon}{2}}(E)$ for all sufficiently large m. Since G_m contains a candidate, i.e. $\Omega_m \cap G_m \neq \emptyset$, we arrive at the statement. ☐

The proof of Proposition 4.89 mainly uses the convergence of the spectra and the property that S is a Cantor set. Let us sketch another proof that instead uses a tool that might come as a surprise to the reader – stability indicators for the FSM.

Alternative proof of Proposition 4.89. The elements of Ω_m are eigenvalues of $(H_m)_{1..q_m-1}$ which is just a finite section of H_m^+. The problem is that at this point we do not have a sequence of finite sections of the same operator, as H_m^+ varies with m. However, we can avoid this problem by only focussing on even m for now, since

$$H_{1..q_m-1} = (H_m)_{1..q_m-1}$$

for even m, see Lemma 4.44.

We recall the stability indicators $\mathcal{I}_{\text{stab}}(H^+)$ for the cut-off sequence $r = (r_m) = (q_{2m} - 1)$ from Corollary 3.25:

$$\mathcal{I}_{\text{stab}}(H^+) = \{H^+\} \cup \{R^- : R \in \operatorname{Lim}_r(H^+)\}.$$

Again by Lemma 4.44, the potentials of H and H_m coincide on the interval $-q_m+1..q_{m+1}$ for even m. Thus, the potentials of $S_{-r_m} H S_{r_m}$ and $S_{-r_m} H_m S_{r_m} = S H_m S^{-1}$ coincide on the interval $-q_{2m}+1-r_m..q_{2m+1}-r_m \supset -q_{2m}..q_{2m-1}$. This interval covers any integer for sufficiently large m. Hence, $\lim_{m\to\infty} S_{-r_m} H S_{r_m} = \lim_{m\to\infty} S H_m S^{-1} = SHS^{-1}$. We conclude that $\operatorname{Lim}_r(H^+)$ is a singleton containing SHS^{-1} and that $\mathcal{I}_{\text{stab}}(H^+) = \{H^+, (SHS^{-1})^-\}$. Note that the latter of the two operators is invertible if and only if $P_{-\mathbb{N}} H P_{-\mathbb{N}}$ is invertible.

Since the stability indicators stay the same when passing to subsequences of r Proposition 3.29 yields that $\lim \|(H_m)_{1..r_m}^{-1}\|$ exists and is equal to $\max\left(\|(H^+)^{-1}\|, \|(P_{-\mathbb{N}} H P_{-\mathbb{N}})^{-1}\|\right)$. By self-adjointness, this already implies the convergence of spectra, i.e.

$$\Omega_{2m} = \sigma((H_m)_{1..r_m}) \to \sigma(H^+) \cup \sigma(P_{-\mathbb{N}} H P_{-\mathbb{N}}) \quad \text{as } m \to \infty.$$

For more details on how the convergence of (pseudo)spectra of finite sections and related sequences can be characterized by the stability indicators see [69].

In order to get the same convergence for Ω_{2m+1} we use that

$$(H_m)_{1..q_m-1} = (H_m)_{1-q_m..-1} = H_{-q_m+1..-1} = (SHS^{-1})_{-q_m+2..0}$$

holds for odd m. Therefore, we consider the FSM for the compression $(SHS^{-1})^-$ on $\ell^2(-\mathbb{N})$ with cut-off sequence $l_m = -q_{2m+1} + 2$. Similar to the case for even m, the stability indicators turn out to be only the operator $(SHS^{-1})^-$ itself and H^+, since $\operatorname{Lim}_l((SHS^{-1})^-) = \{H^+\}$. Then the convergence of spectra follows exactly as above. ☐

Next, we apply Lemma 4.78 to the Sturmian setting.

Corollary 4.90. *Let $m_0 \in \mathbb{N}$ such that there is a non-empty interval $G \subset G_m \cap G_{m+1}$. If both $H^+_{m_0}$ and $H^+_{m_0+1}$ have eigenvalues E_1 and E_2 in G then for all $m \geq m_0$ the compressions H^+_m and H^+ have an eigenvalue in $[\![E_1, E_2]\!]$.*

Sturmian potentials with $\theta \in [0, 1)$

For a Sturmian word v_α with offset 0 Lemma 4.83 yields a decomposition of the stem $\tilde{s}_m$ of the approximant v_{α_m} into the stems $\tilde{s}_{m-1}$ and $\tilde{s}_{m-2}$ of the predecessors $v_{\alpha_{m-1}}$ and $v_{\alpha_{m-2}}$. This idea can be iterated, such that for any fixed $n \in \mathbb{N}$ and any $m > n+1$ the word $\tilde{s}_m$ can be decomposed non-trivially into $\tilde{s}_{n+1}$ and $\tilde{s}_n$. This decomposition was the key ingredient for the application of the interlacing of candidates from Proposition 4.74 throughout this section.

Can we achieve something similar for $v_{\alpha,\theta}$ with $\theta \neq 0$? For $\theta = \alpha$, which corresponds to a single shift of $v_{\alpha,0}$ to the left, we can shift the approximants also to the left and maintain $\sigma(H^+_{\alpha_m,\alpha_m}) \to \sigma(H_{\alpha,\alpha})$ as $m \to \infty$.

Definition 4.91. Let V denote the circular left shift of a finite word, for $w = w_1 w_2 \dots w_n$ that is $V(w) = w_2 \dots w_n w_1$.

Then, for $m \geq 2$ the stems of the approximants v_{α_m,α_m} are given by $V(\tilde{s}_m)$, meaning that

$$v_{\alpha_m,\alpha_m}(k) = V(\tilde{s}_m)(k) \qquad \text{for } k \in 1..q_m.$$

Since for all m the word $\tilde{s}_m$ starts with the same letter (namely 1), we find that for $n \in \mathbb{N}$ and $m > n+1$ the decomposability of $\tilde{s}_m$ into $\tilde{s}_n$ and $\tilde{s}_{n+1}$ also implies $V(\tilde{s}_m)$ can be decomposed non-trivially into $V(\tilde{s}_{n+1})$ and $V(\tilde{s}_n)$. Therefore, we can also apply Proposition 4.74, and the results of Section 4.4.4, e.g. Proposition 4.87 hold also if we use $v_{\alpha,\alpha}$ instead of $v_{\alpha,0}$ and v_{α_m,α_m} instead of $v_{\alpha_m,0}$.

For $\theta = k\alpha$, $k \in \mathbb{N}$, iterating this idea will inevitably fail since eventually the first letters of $V^k(\tilde{s}_{n+1})$ and $V^k(\tilde{s}_n)$ do not coincide. In the following we present a different approach to obtain decompositions of $V^k(s_m)$ for $k \in \mathbb{Z}$ and $m \in \mathbb{N}$ into appropriate shifts of approximants.

We abbreviate $s_{m,k} := V^k(s_m)$ and $\tilde{s}_{m,k} := V^k(\tilde{s}_m)$. Our goal is to find for $n \geq 0$ a set Γ_n of pairs of words, such that all $\tilde{s}_{m,k}$ for $m > n$, $k \in \mathbb{Z}$ can be decomposed non-trivially into the two words of an element of Γ_n. An obvious choice for such a Γ_n for all n is $\Gamma^0 = \{(0,1)\}$, since every Sturmian word can be decomposed into the words 0 and 1. Alternatively, one could just use all possible pairs of finite words $\Gamma^* = \{(u,v) : u, v \in \{0,1\}^*\}$.

We aim to apply the interlacing of candidates from Proposition 4.74 in order to localize Dirichlet eigenvalues. In particular, we want to have gaps that stay open as $m \to \infty$ and follow the candidates inside them, as in Proposition 4.87. On the one hand, it is useful to have long words in Γ_n in order to have many gaps and candidates, which allows a precise localization of the candidates of all v_{α_m,θ_k}. Thus, the set $\Gamma^0 = \{(0,1)\}$ cannot be used to locate any candidates, since H^1_+ and H^0_+ have no gaps and candidates. On the other hand, $|\Gamma_n|$ should be as small as possible, since every pair enlarges the set of possible locations for Dirichlet eigenvalues. Thus, the set Γ^*_n cannot be used to locate any candidates.

We suggest a better choice for Γ_n below. In the light of Lemma 4.83 one might suggest that Γ_n should consist of pairs $(\tilde{s}_{n,j_1}, \tilde{s}_{n+1,j_2})$ with (j_1, j_2) from some appropriate index set. However, we replace the words $\tilde{s}_{n+1,j_2}$ by similar words w_{n+1,j_2} which leads to a simpler and more useful set Γ_n.

Definition 4.92. For that we define $w_m := s_{m-1}\tilde{s}_{m-2}$ and $w_{m,k} := V^k(w_m)$.

In case $a_m = 1$ for all $m \in \mathbb{N}$, that is the Fibonacci word, we therefore have $w_m = \tilde{s}_m$. Using the trace recursion formula from, e.g. [100], we also get

$$\rho(H_{m-1}) \cap \rho(H(w_m)) \subset \rho(H_m).$$

Thus, one can think of w_{m+1} as an intermediate step between $\tilde{s}_{m-1}$ and $\tilde{s}_m$.

For $n \in \mathbb{N}$ we set

$$\Gamma_n = \{(\tilde{s}_{n,j_1}, w_{n+1,j_2}) : (j_1, j_2) \in \mathcal{I}_n\}, \tag{4.67}$$

with the set of index pairs

$$\begin{aligned} \mathcal{I}_n = \{&(j,j) : j \in 0..q_n - 1\} \\ &\cup \{(-q_{n-1} + j, q_n + j) : j \in 0, ..q_{n-1} - 1\} \end{aligned} \tag{4.68}$$

for n even and

$$\begin{aligned} \mathcal{I}_n = \{&(j,j) : j \in 0..q_n - 2\} \\ &\cup \{(-q_{n-1} + j, q_n + j) : j \in -1..q_{n-1} - 1\} \end{aligned}$$

for n odd.

Whenever m is clear from context, set $\theta_k := k\alpha_m \mod 1$. Then $\tilde{s}_{m,k}$ are the stems of $v_{\alpha_m,\theta_k} : k \in \mathbb{Z}$. The decomposability of $\tilde{s}_{m,k}$ that is proven in the following lemma will therefore be useful to localize Dirichlet eigenvalues of the operators $H_{\lambda,\alpha,\theta_k}$.

Lemma 4.93. *Let $n \in \mathbb{Z}$ with $n \geq 2$. Then for $m > n+1$ and all $k \in \mathbb{Z}$ there is a $(u_1, u_2) \in \Gamma_n$, with Γ_n from* (4.67)*, such that $\tilde{s}_{m,k}$ can be decomposed non-trivially into u_1 and u_2.*

Proof. For the convenience of the reader we first gather some equalities that have either been checked before, see Lemma 4.83 and (4.64), or can be checked via similar computations:

(I) $s_{m+1}\tilde{s}_m = s_m\tilde{s}_{m+1}$,

(II) $s_{m+1} = s_m^{a_{m+1}} s_{m-1}$, whence $\tilde{s}_{m+1} = s_m^{a_{m+1}} \tilde{s}_{m-1}$,

(III) for m even: $\tilde{s}_m = s_m$,

(IV) $\tilde{s}_{m+2} = \begin{cases} \tilde{s}_m \tilde{s}_{m+1}^{a_{m+2}} & m \text{ even}, \\ \tilde{s}_{m+1}^{a_{m+2}} \tilde{s}_m & m \text{ odd} \end{cases}$,

(V) for m even: $V^{q_m}(w_{m+1}) = \tilde{s}_{m-1}s_m = V^{-q_{m-1}}(\tilde{s}_m)\tilde{s}_{m-1}$,

(VI) for m odd: $V^{q_m}(w_{m+1}) = \tilde{s}_{m-1}s_m = \tilde{s}_{m-1}\, V^{-q_{m-1}}\,(\tilde{s}_m)$.

We now proceed to prove the statement of the lemma for even n, divided into four steps for different values of k.

Step 1: We first check the decomposition for $k = 0$. With (II), $\tilde{s}_{n+1}$ can be decomposed non-trivially into $\tilde{s}_{n,0}$ and $w_{n+1,0}$. Then use (IV) for induction to obtain a decomposition for larger m. Hence, we can write

$$\tilde{s}_m = u_1u_2u_3 \ldots u_N \qquad \text{with} \quad u_i \in \{w_{n+1}, \tilde{s}_n\} \text{and some } N \in \mathbb{N}.$$

We now only have to find a decomposition of $\tilde{s}_{m,k}$ for $k = 1, \dots, q_n + q_{n-1} - 1$ since for all other $k \in \mathbb{Z}$ we can return to the case $0 \leq k \leq q_n + q_{n-1} - 1$ by relabelling the subwords u_i. In fact, the cases $k = q_n, \dots, q_n + q_{n-1} - 1$ need only to be checked for $u_1 = w_{n+1}$.

Step 2: If $k \in 1..q_n - 1$ then we can decompose

$$\tilde{s}_{m,k} = V^k(\tilde{s}_m) = V^k(u_1)\, V^k\,(u_2)\, V^k\,(u_3) \cdots V^k\,(u_N)\,,$$

since the first q_n letters of all words u_i coincide. This is due to $w_{n+1} = s_n \tilde{s}_{n-1} = \tilde{s}_n \tilde{s}_{n-1}$ for even n. Hence, $\tilde{s}_{m,k}$ can be decomposed into $w_{n+1,k}$ and $\tilde{s}_{n,k}$.

Step 3: It remains to find a decomposition for the case $u_1 = w_{n+1}$ and $q_n \leq k < q_n + q_{n-1}$. We start with $k = q_n$ and find that $V^{q_n}(\tilde{s}_m) = \tilde{s}_{n-1} u_2 \dots u_N s_n$. Using (V), we apply the following equalities to $V^{q_n}(\tilde{s}_m)$ from left to right, i.e. for $j \in \mathbb{N}$ starting at 2 and increasing to N:

$$\begin{aligned} \tilde{s}_{n-1} u_j \dots &= V^{q_n}(w_{n+1}) \tilde{s}_{n-1} \dots && \text{if } u_j = w_{n+1}, \\ \tilde{s}_{n-1} u_j \dots &= V^{-q_{n-1}}(\tilde{s}_n) \tilde{s}_{n-1} \dots && \text{if } u_j = s_n. \end{aligned}$$

We arrive at

$$V^{q_n}(\tilde{s}_m) = \hat{u}_1 \dots \hat{u}_{N-1} \tilde{s}_{n-1} s_n, \quad \hat{u}_i \in \{w_{n+1,q_n}, \tilde{s}_{n,-q_{n-1}}\}.$$

Applying (V) again, more specifically $\tilde{s}_{n-1} s_n = w_{n+1,q_n}$, we obtain a decomposition of $\tilde{s}_{m,q_n}$ into w_{n+1,q_n} and $\tilde{s}_{n,-q_{n-1}}$:

$$V^{q_n}(\tilde{s}_m) = \hat{u}_1 \hat{u}_2 \hat{u}_3 \dots \hat{u}_N\,, \qquad \hat{u}_i \in \{w_{n+1,q_n}, \tilde{s}_{n,-q_{n-1}}\}\,. \tag{4.69}$$

Step 4: Now for $u_1 = w_{n+1}$ and $k \in \{q_n+1, \dots, q_n+q_{n-1}-1\}$ set $k' := k - q_n \in 1..q_{n-1}-1$. With (V) it is easily seen that $\tilde{s}_{n,-q_{n-1}}$ coincides with the first q_n elements of w_{n+1,q_n}. Hence,

$$V^{k'}(\hat{u}_1 \hat{u}_2) = V^{k'}(\hat{u}_1) V^{k'}(\hat{u}_2) \tag{4.70}$$

for $\hat{u}_1, \hat{u}_2 \in \{\tilde{s}_{n,-q_{n-1}}, w_{n+1,q_n}\}$. We combine (4.69) and (4.70) and obtain

$$\tilde{s}_{m,k} = V^{k'}(V^{q_n}(\tilde{s}_m)) = V^{k'}(\hat{u}_1)\, V^{k'}\,(\hat{u}_2)\, V^{k'}\,(\hat{u}_3) \cdots V^{k'}\,(\hat{u}_N)\,. \tag{4.71}$$

Therefore, for $k \in q_n..q_n + q_{n-1} - 1$ the word $\tilde{s}_{m,k}$ can be decomposed into $\tilde{s}_{n,-q_{n-1}+k'}$ and $w_{n+1,q_n+k'}$, which correspond exactly to the pairs of indices given in the second part of the union in (4.68). Hence, we have proven the statement of the lemma for even n.

The proof for n odd is almost the same, except that Step 2 only works for $k \in \{0, \dots, q_{n-2}\}$. In step 3 we apply (VI) right-to-left instead of (V) left-to-right and still obtain (4.71).

For $k = q_n - 1$ we observe that all $\hat{u}_i$ in (4.71) have the same ending, and therefore, applying a right shift, we obtain a decomposition of $\tilde{s}_{m,q_n-1}$ into $\tilde{s}_{n,-q_{n-1}-1}$ and w_{n+1,q_n-1}. □

For a word u and an interval $G \subset \rho(H(u))$ let $E_G(u)$ denote the candidate of $H(u)^+$ that lies in the same gap of $\sigma(H(u))$ as G.

Theorem 4.94. *Let $n \in \mathbb{N}$ and $G \subset \rho(H_n) \cap \rho(H_{n+1})$ be an interval. Then for the set*

$$D := \bigcup_{(u,w) \in \Gamma_n} [\![E_G(u), E_G(w)]\!]$$

the following hold:

(a) $G \setminus D \subset \rho(H^+_{\lambda,\alpha_m,\theta_k})$ *for* $m \geq n$ *and* $k \in \mathbb{Z}$*,*

(b) $G \setminus D \subset \rho(H^+_{\lambda,\alpha,\theta})$ *for all* $\theta \in [0,1)$*.*

(c) The FSM is applicable to $H - E$ *for all* $E \in G \setminus D$*.*

Proof. We start with part (a). Recall from Proposition 4.55 that the condition $G \subset \rho(H_n) \cap \rho(H_{n+1})$ implies that G is part of a gap that remains open, meaning that G is a gap of Π_m for all $m \geq n$. By Lemma 4.93 $\tilde{s}_{m,k}$ can be decomposed non-trivially into u and w for some $(u,w) \in \Gamma_n$. Then Proposition 4.74 yields that $\Omega(H(\tilde{s}_{m,k}))$ separates $\Omega(u)$ and $\Omega(w)$. In particular, there is a candidate of $H(\tilde{s}_{m,k})$ in $[\![E_G(u), E_G(w)]\!]$ and therefore

$$E_G(\tilde{s}_{m,k}) \in D \qquad \text{for } m \geq n \text{ and } k \in \mathbb{Z}. \tag{4.72}$$

Since there can be only one candidate of $H(\tilde{s}_{m,k})$ in the same gap as G, condition (4.72) already implies that no candidates and therefore no Dirichlet eigenvalues lie in $G \setminus D$. Using that $H(\tilde{s}_{m,k}) = H_{\lambda,\alpha_m,\theta_k}$ we get (a).

By Theorem 4.61 the spectra of $H_{\lambda,\alpha_m,\theta_k}$ converge to the spectrum of $H_{\lambda,\alpha,\theta_k}$ for $k \geq 0$. For $k < 0$ we get the same result by passing to a subsequence of odd m. Therefore, property (a) carries over to $H_{\lambda,\alpha,\theta_k}$. Then part (b) follows from Proposition 4.64. Finally, part (c) follows from Theorem 4.66. ☐

Example 4.95. *We consider the case* $\alpha = \frac{\sqrt{5}-1}{2}$*, the Fibonacci Hamiltonian with coupling constant* $\lambda = 1$*. Choose* $n = 4$*. Then* $q_{n-1} = 3$*,* $q_n = 5$ *and* $q_{n+1} = |w_{n+1}| = 8$*.*

We restrict our investigation to the spectral gap around 0*. Set* $G := [-0.414, 0.174] \subset \rho(H_4) \cap \rho(H_5)$ *and we abbreviate* $E(v) = E_G(v)$*. The candidates of* Γ_4 *in* G *are given in Table 4.3, rounded to three digits. Note that the numbers that appear in multiple rows are precisely the same, since they are eigenvalues of similar matrices. The values from Table 4.3 are sketched in Figure 4.11.*

(j,k)	$E(\tilde{s}_{4,j})$	$E(w_{5,k})$
$(0,0)$	0.262	0.124
$(1,1)$	-0.414	-0.516
$(2,2)$	0.262	0.124
$(3,3)$	-0.295	-0.334
$(4,4)$	-0.295	-0.477
$(2,5)$	0.262	0.174
$(3,6)$	-0.295	-0.477
$(4,7)$	-0.295	-0.334

Table 4.3: Candidates of each pair of words contained in Γ_4 from Example 4.95.

With Theorem 4.94 we find that for all $m > 4$ *and* $\theta \in [0,1)$ *the candidate of* $H^+_{\alpha_m,\theta}$ *that lies in* G *has to lie in* $D = \bigcup_{u,w \in \Gamma_4} [\![E(u), E(w)]\!] \approx [-0.414, -0.295] \cup [0.124, 0.174]$*. In particular, no candidate, and therefore no eigenvalue of* $H^+_{\lambda,\alpha_m,\theta}$ *or* $H^+_{\lambda,\alpha,\theta}$ *lies in* $U := G \setminus D \approx [-0.295, 0.124]$*. Moreover, the FSM is applicable to* $H_{\lambda,\alpha,\theta} - E$ *for all* $E \in U$ *and all* $\theta \in [0,1)$*.*

Applying this method for larger n *reveals more intervals in* G *that stay free of eigenvalues, see Figure 4.12.*

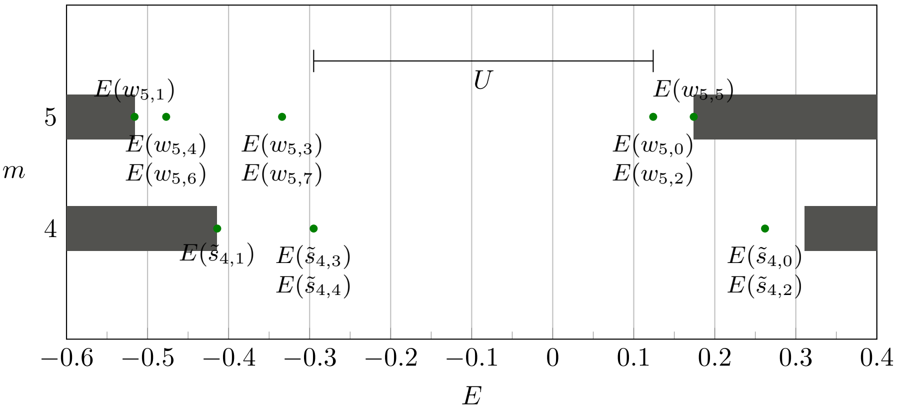

Figure 4.11: The spectral gap at 0 of the 4-th approximation of the Fibonacci Hamilton. The candidates of $H^+(\tilde{s}_{4,j})$ and $H^+(w_{5,k})$ are displayed for all j, k, see Table 4.3. Note that for all pairs $(\tilde{s}_{4,j}, w_{5,k}) \in \Gamma_4$ the respective candidates are either both left or both right of the interval U, meaning that U stays free of Dirichlet eigenvalues for all higher approximations and all shifts of the potential.

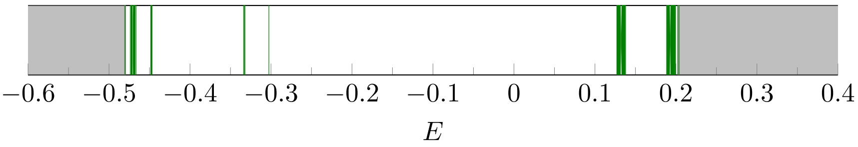

Figure 4.12: The spectral gap at 0 of the 8-th approximation of the Fibonacci Hamilton with $\lambda = 1$. The set $\sigma(H_8) \cup \sigma(H_9)$ is displayed in gray. the set D from Theorem 4.94 with $n = 8$ and G containing 0 is displayed in green. All other values are guaranteed to be in the resolvent set of $H^+_{1,\alpha,\theta}$ for all $\theta \in [0, 1)$.

4.5 References

Section 4.1 is based on joint work with Marko Lindner and is published in [73]. Section 4.2.1 and 4.2.2 contain known results for periodic Schrödinger operators. Great sources are [87] and [102]. Proposition 4.20 can be found in [47]. The remaining parts of Section 4.2 are published by Fabian Gabel, Dennis Gallaun, Julian Großmann, Marko Lindner and the author in [36, 40]. They can also be found in the PhD thesis of Fabian Gabel [36].

Section 4.3 mostly covers known results about Schrödinger operators with Sturmian potential. For an up-to-date overview we recommend the book of Damanik and Filman [25]. Lemmas 4.46 and Theorem 4.53 are published by Fabian Gabel, Dennis Gallaun, Julian Großmann, Marko Lindner and the author in [39]. Theorem 4.53 can also be found in [8]. Sections 4.4.1 and 4.4.2 are also based on joint work with Fabian Gabel, Dennis Gallaun, Julian Großmann and Marko Lindner and published in [39]. The results in Sections 4.4.3 and 4.4.4 are due to the author and seem to be new.

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