Essential spectra of difference operators on $\mathbb{Z}^n$-periodic graphs

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Abstract

Let $(\mathcal{X}, \rho)$ be a discrete metric space. We suppose that the group $\mathbb{Z}^n$ acts freely on X and that the number of orbits of X with respect to this action is finite. Then we call X a $\mathbb{Z}^n$-periodic discrete metric space. We examine the Fredholm property and essential spectra of band-dominated operators on $l^p(X)$ where X is a $\mathbb{Z}^n$-periodic discrete metric space. Our approach is based on the theory of band-dominated operators on $\mathbb{Z}^n$ and their limit operators.

In case X is the set of vertices of a combinatorial graph, the graph structure defines a Schrödinger operator on $l^p(X)$ in a natural way. We illustrate our approach by determining the essential spectra of Schrödinger operators with slowly oscillating potential both on zig-zag and on hexagonal graphs, the latter being related to nano-structures.

1 Introduction

In the last years, spectral properties of Schrödinger operators on quantum graphs have attracted a lot of attention due to their interesting mathematical properties and due to existing and expected applications in nano-structures as well (see, for instance, [4, 9, 38]). Quantum graph models also occur in chemistry [26, 37] and physics [4, 15] (see also the references therein). The spectral properties of Schrödinger operators on quantum graphs considered by P. Kuchment and collaborators in a series of papers [14, 15, 16, 17, 18, 19]. Direct and inverse spectral problems for Schrödinger operators on graphs connected with zig-zag carbon nano-tubes was considered in [12, 13].

It was shown in [16, 17] that the spectral analysis of quantum Hamiltonian on periodic graphs splits into two parts: the spectral analysis of a Hamiltonian on a single edge, and the spectral analysis on a combinatorial graph. This observation makes difference operators on combinatorial graphs to an essential tool in the theory of differential operators on quantum graphs.

The main theme of this paper is the essential spectrum of difference operators (with the Schrödinger operators as a prominent example) acting on the spaces $l^p(X)$ where X is the set of the vertices of a combinatorial graph Γ. We exclusively consider discrete graphs Γ on which the group $\mathbb{Z}^n$ acts freely and which have a finite fundamental domain with respect to this action.

We introduce a Banach algebra $\mathcal{A}_p(X)$ of so-called band-dominated difference operators $l^p(X)$ for $1 < p < \infty$. Following [31, 32] and [33], we introduce for each operator $A \in \mathcal{A}_p(X)$ a family $\mathrm{op}_p(A)$ of *limit operators* of A, and we show that an operator $A \in \mathcal{A}_p(X)$ is *Fredholm* on $l^p(X)$ if and only if all operators in $\mathrm{op}_p(A)$ are invertible and if the norms of their inverses are uniformly bounded. In general, the limit operators of an operator A are simpler objects than the operator A itself. Thus, the limit operators method often provides an effective tool to study the Fredholmness of operators in $\mathcal{A}_p(X)$.

For operators in the so-called Wiener algebra $\mathcal{W}(X)$ (which is a non-closed subalgebra of every algebra $\mathcal{A}_p(X)$, the uniform boundedness of norms of inverse operators to limit operators follows already from their invertibility. This basic fact implies the useful identity

$$\mathrm{sp}_{ess}\, A = \bigcup_{A_h \in \mathrm{op}\, A} \mathrm{sp}\, A_h \tag{1}$$

where the set of the limit operators of A, the spectra $\mathrm{sp}\, A_h$ of the limit operators of A and, hence, also the essential spectrum $\mathrm{sp}_{ess}\, A$ of A are independent of p.

In case $X = \mathbb{Z}^n$, formula (1) was obtained in [31], see also [33]. In [29], we applied this formula to study electromagnetic Schrödinger operators on the lattice $\mathbb{Z}^n$. In particular, we determined the essential spectra of the Hamiltonian of the 3-particle problem on $\mathbb{Z}^n$.

In [27], one of the authors obtained an identity similar to (1) for perturbed pseudodifferential operators on $\mathbb{R}^n$. He applied this result to study the location of the essential spectra of electromagnetic Schrödinger operators, square-root Klein-Gordon, and Dirac operators under general assumptions with respect to the behavior of magnetic and electric potentials at infinity. By means of this method, also a very simple and transparent proof of the well known Hunziker, van Winter, Zjislin theorem (HWZ-Theorem) on the location of essential spectra of multi-particle Hamiltonians was obtained.

It should be noted that formulas similar to (1) have been obtained independently (but later) in [21] by means of admissible geometric methods. We also mention the papers [8, 7, 23, 3] and the references therein where C^*-algebra techniques have been applied to study essential spectra of Schrödinger operators.

The present paper is organized as follows. In Section 2 we collect some auxiliary material from [33] on matrix band-dominated operators on the lattice $\mathbb{Z}^n$. In Section 3 we introduce the Banach algebra $\mathcal{A}_p(X)$ of band-dominated operators acting on $l^p(X)$ where X is a periodic discrete metric space on which the group $\mathbb{Z}^n$ acts freely. We construct an isomorphism between the Banach algebra $\mathcal{A}_p(X)$ and the Banach algebra $\mathcal{A}_p(\mathbb{Z}^n, \mathbb{C}^N)$ of all (block) band-dominated operators on $l^p(\mathbb{Z}^n, \mathbb{C}^N)$ where N is the number of points in the fundamental domain of X with respect to the action of $\mathbb{Z}^n$. Applying this isomorphism and the results of Section 2, we derive necessary and sufficient conditions for $A \in \mathcal{A}_p(X)$ to be a Fredholm operator. We also introduce a Wiener algebra $\mathcal{W}(X)$ and derive formula (1) for operators in $\mathcal{W}(X)$.

In Section 4 we introduce the class of periodic band-dominated operators. We say that $A \in \mathcal{A}_p(X)$ is a periodic operator if it commutes with each operator L_h of left shift by $h \in \mathbb{Z}^n$ on $l^p(X)$. Note that, for periodic operators, $\operatorname{sp}_{ess} A = \operatorname{sp} A$. With each periodic operator $A \in \mathcal{W}(X)$, we associate a continuous function $\sigma_A : \mathbb{T}^n \to \mathbb{C}^{N\times N}$, called the symbol of A. In the terminology of [15, 16], $\sigma_A(t)$ is just the Floquet transform of A. We prefer to follow the theory of discrete convolutions and use the discrete Fourier transform to define σ_A.

Let $\lambda_j(t)$, $j = 1, \ldots, N$ be the eigenvalues of $\sigma_A(t)$. Then

$$\operatorname{sp} A = \bigcup_{j=1}^{N} \mathcal{C}_j(A)$$

where $\mathcal{C}_j(A) := \{\lambda \in \mathbb{C} : \lambda = \lambda_j(t),\ t \in \mathbb{T}^n\}$. If A is a self-adjoint operator on $l^2(X)$, then the $\mathcal{C}_j(A)$ can be identified with segments.

In Section 5 we consider operators in the Wiener algebra $\mathcal{W}(X)$ with slowly oscillating coefficients. These operators are distinguished by two remarkable properties: their limit operators are periodic operators, and all limit operators belong to the Wiener algebra again. Via formula (1) we thus obtain a complete description of the essential spectra of operators with slowly oscillating coefficients.

In Section 6 we apply these results to Schrödinger operators with slowly oscillating electrical potentials. As already mentioned, every $\mathbb{Z}^n$-periodic graph induces a related Schrödinger operator in a natural way (it is only this place where the graph structure becomes important). As illustrations we calculate the essential spectra of Schrödinger operators with slowly oscillating potentials on the *zig-zag* graph and on the *hexagonal* graph. Some other spectral problems on such graphs which are connected with carbon nano-structures were considered in [12, 13, 18].

In Section 7 we examine the essential spectrum of the Hamiltonian of the motion of two particles on a periodic graph Γ around a heavy nucleus. For the lattice $\Gamma = \mathbb{Z}^n$ we considered this problem in [29]. See also the papers [2, 1, 20, 24, 25] and the references therein which are devoted to discrete multi-particle problems.

The limit operators approach does also apply to study the essential spectrum of pseudodifferential operators on periodic quantum graphs. We plan to develop these ideas in a forthcoming paper.

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2 Band-dominated operators on $\mathbb{Z}^n$

In this section we fix some notations and recall some facts concerning the Fredholm property of band-dominated operators on $l^p(\mathbb{Z}^n)$. The Fredholm properties of these operators are fairly well understood. All details can be found in [31]; see also the monograph [33] for a comprehensive account.

We will use the following notations. Given a Banach space X, let $\mathcal{L}(X)$ refer to the Banach algebra of all bounded linear operators on X and $\mathcal{K}(X)$ to the closed ideal of the compact operators. An operator $A \in \mathcal{L}(X)$ is called a *Fredholm operator* if its kernel $\ker A := \{x \in X : Ax = 0\}$ and its cokernel $\operatorname{coker} A := X/A(X)$ are finite dimensional linear spaces. Equivalently, A is Fredholm if the coset $A + \mathcal{K}(X)$ is invertible in the Calkin algebra $\mathcal{L}(X)/\mathcal{K}(X)$. The *essential spectrum* of A is the set of all complex numbers λ for which the operator $A - \lambda I$ is not Fredholm on X, whereas the discrete spectrum of A consists of all isolated eigenvalues of finite multiplicity. We denote the essential spectrum of A by $\mathrm{sp}_{ess}\, A$, the discrete spectrum by $\mathrm{sp}_{dis}\, A$, and the usual spectrum by $\mathrm{sp}\, A$. Sometimes we also write $\mathrm{sp}\,(A : X \to X)$ instead of $\mathrm{sp}\, A$ in order to emphasize the underlying space X (with obvious modifications for the essential and the discrete spectrum). Clearly,

$$\mathrm{sp}_{dis}\,(A) \subseteq \mathrm{sp}\,(A) \setminus \mathrm{sp}_{ess}\,(A)$$

for every operator $A \in \mathcal{L}(X)$. If A is a self-adjoint operator, then equality holds in this inclusion.

Let $p \geq 1$ be a real number and n a positive integer. As usual, we write $l^p(\mathbb{Z}^n)$ for the Banach space of all functions $u : \mathbb{Z}^n \to \mathbb{C}$ for which

$$\|u\|^p_{l^p(\mathbb{Z}^n)} := \sum_{x \in \mathbb{Z}^n} |u(x)|^p < \infty$$

and $l^\infty(\mathbb{Z}^N)$ for the Banach space of all bounded functions $u : \mathbb{Z}^n \to \mathbb{C}$ with norm

$$\|u\|_{l^\infty(\mathbb{Z}^n)} := \sup_{x \in \mathbb{Z}^n} |u(x)|.$$

For every positive integer N, let $l^p(\mathbb{Z}^n)^N$ stand for the Banach space of all vectors $u = (u_1, \ldots, u_N)$ of functions $u_i \in l^p(\mathbb{Z}^n)$ with norm

$$\|u\|^p_{l^p(\mathbb{Z}^n)^N} := \sum_{i=1}^N \|u_i\|^p_{l^p(\mathbb{Z}^n)}$$

Likewise, one can identify $l^p(\mathbb{Z})^N$ with the Banach space $l^p(\mathbb{Z}^n, \mathbb{C}^N)$ of all functions $u : \mathbb{Z}^n \to \mathbb{C}^N$ for which

$$\|u\|^p_{l^p(\mathbb{Z}^n,\, \mathbb{C}^N)} := \sum_{x \in \mathbb{Z}^n} \sum_{i=1}^N |u_j(x)|^p < \infty.$$

Clearly, the Banach spaces $l^p(\mathbb{Z}^n)^N$ and $l^p(\mathbb{Z}^n, \mathbb{C}^N)$ are isometric to each other. We also consider the Banach spaces $l^\infty(\mathbb{Z}^n)^N$ and $l^\infty(\mathbb{Z}^n, \mathbb{C}^N)$ with norms

$$\|u\|_{l^\infty(\mathbb{Z}^n)^N} := \sup_{1\le i\le N} \|u_i\|_{l^\infty(\mathbb{Z}^n)}$$

and

$$\|u\|_{l^\infty(\mathbb{Z}^n, \mathbb{C}^N)} := \sup_{x\in\mathbb{Z}^n} \sup_{1\le i\le N} |u_i(x)|.$$

Again, these spaces are isometric to each other in a natural way. Note also that $l^\infty(\mathbb{Z}^n, \mathbb{C}^{N\times N})$ can be made to a C^*-algebra by providing the matrix algebra $\mathbb{C}^{N\times N}$ with a C^*-norm.

We consider operators on $l^p(\mathbb{Z}^n, \mathbb{C}^N)$ which are constituted by shift operators and by operators of multiplication by bounded functions. The latter are defined as follows: For $\alpha \in \mathbb{Z}^n$, the shift operator V_α is the isometry acting on $l^p(\mathbb{Z}^n, \mathbb{C}^N)$ by $(V_\alpha u)(x) := u(x-\alpha)$. Further, each function a in $l^\infty(\mathbb{Z}^n, \mathbb{C}^{N\times N})$ induces a multiplication operator aI on $l^p(\mathbb{Z}^n, \mathbb{C}^N)$ via $(au)(x) := a(x)u(x)$. Clearly,

$$\|aI\|_{\mathcal{L}(l^p(\mathbb{Z}^n, \mathbb{C}^N))} = \|a\|_{l^\infty(\mathbb{Z}^n, \mathbb{C}^{N\times N})}.$$

A *band operator* on $l^p(\mathbb{Z}^n, \mathbb{C}^N)$ is an operator of the form

$$A = \sum_{|\alpha|\le m} a_\alpha V_\alpha \tag{2}$$

with coefficients $a_\alpha \in l^\infty(\mathbb{Z}^n, \mathbb{C}^{N\times N})$. The closure in $\mathcal{L}(l^p(\mathbb{Z}^n, \mathbb{C}^N))$ of the set of all band operators is a subalgebra of $\mathcal{L}(l^p(\mathbb{Z}^n, \mathbb{C}^N))$. We denote this algebra by $\mathcal{A}(l^p(\mathbb{Z}^n, \mathbb{C}^N))$ and call its elements *band-dominated operators* (BDO for short). In a completely analogous way, band-dominated operators on $l^\infty(\mathbb{Z}^n, \mathbb{C}^N)$ are defined.

Our main tool to study Fredholm properties of band-dominated operators are the associated limit operators.

Definition 1 *Let $A \in \mathcal{L}(l^p(\mathbb{Z}^n, \mathbb{C}^N))$, and let $h : \mathbb{N} \to \mathbb{Z}^n$ be a sequence tending to infinity. A linear operator A_h is called the limit operator of A with respect to the sequence h if*

$$V_{-h(m)} A V_{h(m)} \to A_h \quad \textit{and} \quad V_{-h(m)} A^* V_{h(m)} \to A_h^*$$

strongly as $m \to \infty$. We let $\mathrm{op}_p\, A$ denote the set of all limit operators of A.

Here and in what follows, convergence of a sequence in $\mathbb{Z}^n$ to infinity means convergence of this sequence to infinity in the one-point compactification of $\mathbb{Z}^n$ (which makes sense since $\mathbb{Z}^n$ is a locally compact metric space).

There are operators on $l^p(\mathbb{Z}^n, \mathbb{C}^N)$ which do not possess limit operators at all. But if A is a band-dominated operator then one can show via a Cantor diagonal argument that *every* sequence h tending to infinity has a subsequence g for which the limit operator A_g exists. Moreover, the operator spectrum of

A stores the complete information on the Fredholmness of A, as the following theorem states. (In case $n = 1$ there is also a sufficiently nice formula for the Fredholm index of A which expresses this index in terms of local indices of the limit operators of A, see [30].)

Theorem 2 *An operator $A \in \mathcal{A}(l^p(\mathbb{Z}^n, \mathbb{C}^N))$ is Fredholm if and only if all limit operators of A are invertible and if*

$$\sup_{A_h \in \mathrm{op}_p(A)} \|A_h^{-1}\| < \infty. \tag{3}$$

The uniform boundedness condition (3) is often difficult to check: It is one thing to verify the invertibility of an operator and another one to provide a good estimate for the norm of its inverse. It is therefore of vital importance to single out classes of band-dominated operators for which this condition is automatically satisfied. One of these classes is defined by imposing conditions of the decay of the norms of the coefficients. More precisely, we consider band-dominated operators of the form

$$A := \sum_{\alpha \in \mathbb{Z}^n} a_\alpha V_\alpha$$

where

$$\sum_{\alpha \in \mathbb{Z}^n} \|a_\alpha\|_{l^\infty(\mathbb{Z}^n, \mathbb{C}^{N \times N})} < \infty. \tag{4}$$

One can show that the set $W(\mathbb{Z}^n, \mathbb{C}^N)$ of all operators with property (4) forms an algebra and that the term on the left-hand side of (4) defines a norm which makes $W(\mathbb{Z}^n, \mathbb{C}^N)$ to a Banach algebra. We refer to this algebra as the *Wiener algebra* and write $\|A\|_{W(\mathbb{Z}^n, \mathbb{C}^N)}$ for the norm of an operator in $W(\mathbb{Z}^n, \mathbb{C}^N)$. Clearly, operators in the Wiener algebra act boundedly on each of the spaces $l^p(\mathbb{Z}^n, \mathbb{C}^N)$ (including $p = \infty$) and

$$\|A\|_{\mathcal{L}(l^p(\mathbb{Z}^n, \mathbb{C}^N))} \leq \|A\|_{W(\mathbb{Z}^n, \mathbb{C}^N)}.$$

Hence, $W(\mathbb{Z}^n, \mathbb{C}^N) \subseteq \mathcal{A}(l^p(\mathbb{Z}^n, \mathbb{C}^N))$ for every p.

One important property of the Wiener algebra is its inverse closedness in each of the algebras $\mathcal{L}(l^p(\mathbb{Z}^n, \mathbb{C}^N))$, i.e., if $A \in W(\mathbb{Z}^n, \mathbb{C}^N)$ has an inverse in $\mathcal{L}(l^p(\mathbb{Z}^n, \mathbb{C}^N))$, then A^{-1} belongs to $W(\mathbb{Z}^n, \mathbb{C}^N)$ again. This fact implies that the spectrum of an operator $A \in W(\mathbb{Z}^n, \mathbb{C}^N)$ considered as acting on $l^p(\mathbb{Z}^n, \mathbb{C}^N)$ does not depend on $p \in (1, \infty)$. Also the operator spectrum $\mathrm{op}_p(A)$ proves to be independent of p, which justifies to write $\mathrm{op}\, A$ instead. Note finally that all limit operators of operators in the Wiener algebra belong to the Wiener algebra again.

For operators in the Wiener algebra, the Fredholm criterion in Theorem 2 reduces to the following much simpler assertion.

Theorem 3 *Let $A \in W(\mathbb{Z}^n, \mathbb{C}^N)$. The operator A is Fredholm on $l^p(\mathbb{Z}^n, \mathbb{C}^N)$ if and only if there exists a $p_0 \in [1, \infty]$ such that all limit operators of A are invertible on $l^{p_0}(\mathbb{Z}^n, \mathbb{C}^N)$.*

Theorem 3 has the following useful consequence.

Theorem 4 *For $A \in W(\mathbb{Z}^n, \mathbb{C}^N)$, the essential spectra of $A : l^p(\mathbb{Z}^n, \mathbb{C}^N) \to l^p(\mathbb{Z}^n, \mathbb{C}^N)$ do not depend on $p \in (1, \infty)$, and*

$$\mathrm{sp}_{ess}\, A = \bigcup_{A_h \in \mathrm{op}\, A} \mathrm{sp}\, A_h. \tag{5}$$

3 BDO on periodic discrete metric spaces

3.1 Periodic discrete metric spaces

By a *discrete metric space* we mean a countable set X together with a metric ρ such that every ball

$$B_r(x_0) := \{x \in X : \rho(x, x_0) \leq r\}$$

is a finite set. For each discrete metric space X, we introduce some standard Banach spaces over X. For $p \in (1, \infty)$, let $l^p(X)$ denote the Banach space of all complex-valued functions u on X with norm

$$\|u\|^p_{l^p(X)} := \sum_{x \in X} |u(x)|^p,$$

and write $l^\infty(X)$ for the Banach space of all bounded functions u of X with norm

$$\|u\|_{l^\infty(X)} := \sup_{x \in X} |u(x)|$$

A *periodic discrete metric space* is a discrete metric space provided with the free action of the group $\mathbb{Z}^n$. More precisely, let X be a discrete metric space, and let there be a mapping

$$\mathbb{Z}^n \times X \to X, \quad (\alpha, x) \to \alpha \cdot x$$

satisfying

$$0 \cdot x = x \quad \text{and} \quad (\alpha + \beta) \cdot x = \alpha \cdot (\beta \cdot x)$$

for arbitrary elements $\alpha, \beta \in \mathbb{Z}^n$ and $x \in X$, which leaves the metric invariant,

$$\rho(\alpha \cdot x, \alpha \cdot y) = \rho(x, y) \tag{6}$$

for all elements $\alpha \in \mathbb{Z}^n$ and $x, y \in X$. Recall also that the group $\mathbb{Z}^n$ acts *freely* on X if whenever the equality $x = \alpha \cdot x$ holds for elements $x \in X$ and $\alpha \in \mathbb{Z}^n$ then, necessarily, $\alpha = 0$.

For each element $x \in X$, consider its orbit $\{\alpha \cdot x \in X : \alpha \in \mathbb{Z}^n\}$ with respect to the action of $\mathbb{Z}^n$. Any two orbits are either disjoint or identical. Hence, there is a binary equivalence relation on X, by calling two points equivalent if they belong to the same orbit. The set of all orbits of X with respect to the action of

$\mathbb{Z}^n$ is denoted by $X/\mathbb{Z}^n$. A basic assumption throughout what follows is that the orbit space $X/\mathbb{Z}^n$ is *finite*. Thus, there is a finite subset $\mathcal{M} := \{x_1, x_2, \ldots, x_N\}$ of X such that the orbits

$$X_j := \{\alpha \cdot x_j \in X : \alpha \in \mathbb{Z}^n\}$$

satisfy $X_i \cap X_j = \emptyset$ if $x_i \neq x_j$ and $\cup_{i=1}^N X_i = X$. If all these conditions are satisfied then we call X is a *periodic discrete metric space* with respect to $\mathbb{Z}^n$ or simply $\mathbb{Z}^n$-periodic.

The free action of $\mathbb{Z}^n$ on X guarantees that the mapping

$$U_j : \mathbb{Z}^n \to X_j, \quad \alpha \mapsto \alpha \cdot x_j$$

is a bijection for every $j = 1, \ldots, N$. For each complex-valued function f on X, let $Uf : \mathbb{Z}^n \to \mathbb{C}^N$ be the function

$$(Uf)(\alpha) := ((U_1 f)(\alpha), \ldots, (U_N f)(\alpha)).$$

Clearly, the mapping U is a linear isometry from $l^p(X)$ onto $l^p(\mathbb{Z}^n, \mathbb{C}^N)$, and the mapping $A \mapsto UAU^{-1}$ is an isometric isomorphism from $\mathcal{L}(l^p(X))$ onto $\mathcal{L}(l^p(\mathbb{Z}^n, \mathbb{C}^N))$ for every $p \in [1, \infty]$.

Another consequence of our assumptions is that

$$\lim_{\mathbb{Z}^n \ni \alpha \to \infty} \rho(\alpha \cdot x, y) = \infty. \tag{7}$$

for all points $x, y \in X$. Indeed, suppose that (7) is wrong. Then there are points $x, y \in X$, a positive constant M, and a sequence α of pairwise different points in $\mathbb{Z}^n$ such that

$$\rho(\alpha(n) \cdot x, y) \leq M \quad \text{for all } n \in \mathbb{N}. \tag{8}$$

The free action of $\mathbb{Z}^n$ on X implies that $(\alpha(n) \cdot x)_{n \in \mathbb{N}}$ is a sequence of pairwise different points in X. Hence, (8) implies that the ball with center y and radius M contains infinitely many points, a contradiction. ∎

3.2 Band-dominated operators on X

Let X be a periodic discrete metric space and $p \in [1, \infty)$. We consider linear operators A on $l^p(X)$ for which there exists a function $k_A \in l^\infty(X \times X)$ such that

$$(Au)(x) = \sum_{y \in X} k_A(x, y) u(y) \quad \text{for all } x \in X \tag{9}$$

and for all finitely supported functions u on X (note that the latter form a dense subspace of $l^p(X)$). The function k_A is called the *generating function* of the operator A. It is easily seen that every bounded operator A on $l^p(X)$ is of this form and is, thus, generated by a bounded function. The converse is certainly not true. It is also clear that every operator A determines its generating function uniquely, since

$$(A\delta_y)(x) = k_A(x,\, y)$$

where δ_y is the function on X which is 1 at y and 0 at all other points.

An operator A of the form (9) is called a *band operator* if there exists an $R > 0$ such that $k_A(x,\, y) = 0$ whenever $\rho(x,\, y) > R$.

Example 5 Every operator aI of multiplication by a function $a \in l^\infty(X)$ is a band operator. ∎

Example 6 For $\alpha \in \mathbb{Z}^n$, let T_α be the operator of shift by α on $l^p(X)$, i.e., $(T_\alpha u)(x) := u((-\alpha)\cdot x)$. Clearly, T_α is a band operator which acts as an isometry on $l^p(X)$. Hence, every operator of the form

$$\sum_{|\alpha|\le m} a_\alpha T_\alpha \tag{10}$$

with $a_\alpha \in l^\infty(X)$ is a band operator (but there are band operators which can not be represented of this form). ∎

Proposition 7 *If A is a band operator on $l^p(X)$, then UAU^{-1} is a band operator on $l^p(\mathbb{Z}^n,\, \mathbb{C}^N)$.*

Proof. The operator UAU^{-1} has the matrix representation

$$(UAU^{-1}f)_i(\alpha) = \sum_{j=1}^{N} \sum_{\beta\in\mathbb{Z}^n} r_A^{ij}(\alpha,\, \beta) f_j(\beta) \tag{11}$$

where $\alpha \in \mathbb{Z}^n$, $i = 1,\, \ldots,\, N$ and

$$r_A^{ij}(\alpha,\, \beta) := k_A(\alpha\cdot x_i,\, \beta\cdot x_j). \tag{12}$$

From (7) we conclude that

$$\rho(\alpha\cdot x_i,\, \beta\cdot x_j) = \rho(x_i,\, (\beta-\alpha)\cdot x_j) \to \infty$$

as $|\alpha-\beta| \to \infty$. Thus, there is an $R_1 > 0$ such that $r_A^{ij}(\alpha,\, \beta) = 0$ if $|\alpha-\beta| > R_1$. In other words, every r_A^{ij} is the generating function of a band operator on $l^p(\mathbb{Z}^n)$, implying that UAU^{-1} is a band operator on $l^p(\mathbb{Z}^n,\, \mathbb{C}^N)$. ∎

The preceding proposition implies in particular that every band operator is bounded on $l^p(X)$ for $p \in [1,\, \infty]$.

For $p \in [1,\, \infty]$, let $\mathcal{A}_p(X)$ stand for the closure in $\mathcal{L}(l^p(X))$ of the set of all band operators. The operators in $\mathcal{A}_p(X)$ are called *band-dominated operators on X*. Note that the class $\mathcal{A}_p(X)$ depends heavily on p (whereas the class of the band operators is independent of p). One can show easily (for example, by employing the preceding proposition and the well properties of band-dominated operators on $\mathbb{Z}^n$) that $\mathcal{A}_p(X)$ is a Banach algebra and even a C^*-algebra if $p = 2$.

Proposition 8 *Let X be a periodic discrete metric space and $p \in [1, \infty]$. The mapping $A \mapsto UAU^{-1}$ is an isomorphism between the Banach algebras $\mathcal{A}_p(X)$ and $\mathcal{A}_p(\mathbb{Z}^n, \mathbb{C}^N)$.*

Proof. Note that an operator A is a band operator on $l^p(X)$ if and only if UAU^{-1} is a band operator on $l^p(\mathbb{Z}^n, \mathbb{C}^N)$. The assertion follows since the mapping $A \mapsto UAU^{-1}$ is a continuous isomorphism between the Banach algebras $\mathcal{L}(l^p(X))$ and $\mathcal{L}(l^p(\mathbb{Z}^n, \mathbb{C}^N))$. ■

3.3 Limit operators and Fredholmness

Let X be a $\mathbb{Z}^n$-periodic discrete metric space. The goal of this section is a criterion for the Fredholmness of band-dominated operators on $l^p(X)$. This criterion makes use of the limit operators of A which, in a sense, reflect the behaviour of A at infinity. Here is the definition.

Definition 9 *Let $1 < p < \infty$, and $h : \mathbb{N} \to \mathbb{Z}^n$ be a sequence tending to infinity. We say that A_h is a* limit operator *of $A \in \mathcal{L}(l^p(X))$ defined by the sequence h if*

$$T_{h(m)}^{-1} A T_{h(m)} \to A_h \quad \text{and} \quad T_{h(m)}^{-1} A^* T_{h(m)} \to A_h^* \quad \text{as } m \to \infty$$

strongly on $l^p(X)$ and $l^p(X)^* = l^q(X)$ with $1/p + 1/q = 1$, respectively. We denote the set of all limit operators of $A \in \mathcal{L}(l^p(X))$ by $\mathrm{op}_p(A)$ and call this set the operator spectrum *of A.*

Note that the generating function of the shifted operator $T_\alpha^{-1} A T_\alpha$ is related with that of A by

$$k_{T_\alpha^{-1} A T_\alpha}(x, y) = k_A((-\alpha) \cdot x, (-\alpha) \cdot y) \tag{13}$$

and that the generating functions of $T_{h(m)}^{-1} A T_{h(m)}$ converge point-wise on $X \times X$ to the generating function of the limit operator A_h if the latter exists.

It is an important property of band-dominated operators that their operator spectrum is not empty. More general, one has the following result which can be proved by an obvious Cantor diagonal argument (see [31, 32, 33]).

Proposition 10 *Let $p \in (1, \infty)$ and $A \in \mathcal{A}_p(X)$. Then every sequence $h : \mathbb{N} \to G$ which tends to infinity possesses a subsequence g such that the limit operator A_g of A with respect to g exists.*

The following theorem settles the basic relation between the Fredholmness of a band-dominated operator A and the invertibility of its limit operators. It follows easily from Theorem 2 if one takes into account that the mapping

$$\mathcal{A}_p(X) \to \mathcal{A}_p(\mathbb{Z}^n, \mathbb{C}^N), \quad A \mapsto UAU^{-1}$$

is an isomorphism of Banach algebras and that the relation

$$(UAU^{-1})_h = UA_hU^{-1}$$

between the limit operators of A and UAU^{-1} holds.

Theorem 11 *Let $p \in (1, \infty)$ and $A \in \mathcal{A}_p(X)$. Then A is a Fredholm operator on $l^p(X)$ if and only if all limit operators of A are invertible and if the norms of their inverses are uniformly bounded,*

$$\sup_{A_h \in op(A)} \|A_h^{-1}\| < \infty. \tag{14}$$

3.4 The Wiener algebra of X

The goal of this section is to single out a class of band-dominated operators for which the uniform boundedness condition (14) is redundant.

Definition 12 *Let X be a $\mathbb{Z}^n$-periodic discrete metric space. The set $\mathcal{W}(X)$ consists of all linear operators A for which there is a function h_A in $l^1(\mathbb{Z}^n)$ such that*

$$\max_{j \in \{1, \ldots, N\}} \sum_{i=1}^{N} |r_A^{ij}(\alpha, \beta)| \leq h_A(\alpha - \beta) \tag{15}$$

for all $\alpha, \beta \in \mathbb{Z}^n$.

We introduce a norm in $\mathcal{W}(X)$ by

$$\|A\|_{\mathcal{W}(X)} := \inf \|h\|_{l^1(\mathbb{Z}^n)} \tag{16}$$

where the infimum is taken over all sequences $h \in l^1(\mathbb{Z}^n)$ for which inequality (15) holds in place of h_A.

Proposition 13 *The set $\mathcal{W}(X)$ with the norm (16) is a Banach algebra, and the mapping $A \mapsto UAU^{-1}$ is an isometrical isomorphism between the Banach algebras $\mathcal{W}(X)$ and $\mathcal{W}(\mathbb{Z}^n, \mathbb{C}^N)$.*

The proof is straightforward. We refer to the algebra $\mathcal{W}(X)$ as the *Wiener algebra*.

Proposition 14 *Let $p \in [1, \infty]$.*

(i) Every operator $A \in \mathcal{W}(X)$ is bounded on each of the spaces $l^p(X)$.

(ii) The algebra $\mathcal{W}(X)$ is inverse closed in each of the algebras $\mathcal{L}(l^p(X))$.

Proposition 14 follows from Proposition 13 and the related results for the special case $X = \mathbb{Z}^n$ presented in [31, 32] and [33]. ■

The following result highlights the importance of the Wiener algebra in our context.

Theorem 15 *Let $A \in \mathcal{W}(X)$. Then A is a Fredholm operator on $l^p(X)$ with $p \in (1, \infty)$ if and only if there is a $p_0 \in [1, \infty]$ such that all limit operators of A are invertible on $l^{p_0}(X)$. Moreover $\mathrm{sp}_{ess}\, A$ does not depend on $p \in (1, \infty)$, and*

$$\mathrm{sp}_{ess}\, A = \bigcup_{A_h \in \mathrm{op}\,(A)} \mathrm{sp}\, A_h. \tag{17}$$

Theorem 15 follows immediately from Proposition 13 and Theorems 3 and 4.

The following result states a sufficient condition for the absence of the discrete spectrum of an operator $A \in \mathcal{A}_p(X)$.

Proposition 16 *Let $A \in \mathcal{A}_p(X)$ and suppose there is a sequence $h : \mathbb{N} \to \mathbb{Z}^n$ for which the limit operator A_h exists in the sense of norm convergence,*

$$\lim_{m\to\infty} \|T_{h_m}^{-1} A T_{h_m} - A_h\| = 0. \tag{18}$$

Then $\mathrm{sp}_{ess}\, A = \mathrm{sp}\, A$.

Proof. Let $\lambda \notin \mathrm{sp}_{ess}\, A$. Then, by Theorem 11, $\lambda \notin \mathrm{sp}\, A_h$. It follows from (18) that $\lambda \notin \mathrm{sp}\, A$. Hence, $\mathrm{sp}\, A \subseteq \mathrm{sp}_{ess}\, A$, which implies the assertion. ■

4 Periodic operators on periodic metric spaces

Let X be a $\mathbb{Z}^n$-periodic discrete metric space. An operator $A \in \mathcal{L}(l^p(X))$ is said to be $\mathbb{Z}^n$*-periodic* if it is invariant with respect to left shifts by elements of $\mathbb{Z}^n$, that is if

$$T_\alpha A = A T_\alpha \qquad \text{for every } \alpha \in \mathbb{Z}^n.$$

The following is a straightforward consequence of Proposition 16.

Proposition 17 *Let $A \in \mathcal{A}_p(X)$ be a $\mathbb{Z}^n$-periodic operator. Then*

$$\mathrm{sp}_{ess}\, A = \mathrm{sp}\, A.$$

The explicit description of the spectrum (= the essential spectrum) of $\mathbb{Z}^n$-periodic operators is possible by means of the Fourier transform. One easily checks that $A \in \mathcal{W}(X)$ is $\mathbb{Z}^n$-periodic on X if and only if the generating function k_A of A satisfies the following periodicity condition: For all group elements $\gamma \in \mathbb{Z}^n$ and all points $x, y \in X$,

$$k_A(\gamma \cdot x,\, \gamma \cdot y) = k_A(x,\, y).$$

This equality implies that the functions $r_A^{ij}(\alpha,\, \beta) := k_A(\alpha \cdot x_i,\, \beta \cdot x_j)$ satisfy

$$r_A^{ij}(\alpha,\, \beta) = k_A((\alpha - \gamma) \cdot x_i,\, (\beta - \gamma) \cdot x_j)$$

for all $\gamma \in \mathbb{Z}^n$, whence $r_A^{ij}(\alpha,\, \beta) = r_A^{ij}(\alpha - \beta,\, 0)$. Hence, for $i = 1, \ldots, N$,

$$\begin{aligned}
(UAU^{-1}f)_i(\alpha) &= \sum_{j=1}^{N} \sum_{\beta\in\mathbb{Z}^n} r_A^{ij}(\alpha,\, \beta)\, (U_j f)(\beta) \\
&= \sum_{j=1}^{N} \sum_{\beta\in\mathbb{Z}^n} r_A^{ij}(\alpha - \beta,\, 0)\, (U_j f)(\beta) \\
&= \sum_{j=1}^{N} \sum_{\beta\in\mathbb{Z}^n} r_A^{ij}(\beta,\, 0)\, (V_\beta U_j f)(\alpha)
\end{aligned}$$

where

$$|r_A^{ij}(\beta,\,0)| \le h(\beta)$$

for a some non-negative function $h \in l^1(\mathbb{Z}^n)$. Thus, we arrived at the following proposition.

Proposition 18 *Every $\mathbb{Z}^n$-periodic operator $A \in \mathcal{W}(X)$ is isometrically equivalent to the shift invariant matrix operator $UAU^{-1} \in W(\mathbb{Z}^n,\,\mathbb{C}^N)$.*

Under the conditions of the previous proposition, we associate with A a function $\sigma_A : \mathbb{T}^n \to \mathbb{C}^{N\times N}$ via

$$\sigma_A(t) := \sum_{\beta\in\mathbb{Z}^n} r_A(\beta)\, t^\beta$$

where $\mathbb{T}$ is the torus $\{z \in \mathbb{C} : |z| = 1\}$, $r_A(\beta)$ is the matrix $(r_A^{ij}(\beta,\,0))_{i,\,j=1}^N$, and $t^\beta := t_1^{\beta_1} \dots t_n^{\beta_n}$ for $t = (t_1,\,\dots,\,t_n) \in \mathbb{T}^n$ and $\beta = (\beta_1,\,\dots,\,\beta_n) \in \mathbb{Z}^n$. The function σ_A is referred to as the *symbol* of A. It is well known that the operator

$$(\tilde{A}u)(\alpha) := \sum_{\beta\in\mathbb{Z}^n} r_A(\alpha-\beta,\,0)u(\beta)$$

is invertible on $l^p(\mathbb{Z}^n,\,\mathbb{C}^N)$ with $p \in [1,\,\infty]$ if and only if $\det \sigma_A \neq 0$ on $\mathbb{T}^n$.

For $t \in \mathbb{T}^n$, let $\lambda_A^j(t)$ with $j = 1,\,\dots,\,N$ denote the eigenvalues of the matrix $\sigma_A(t)$. The enumeration of the eigenvalues can be chosen in such a way that $\lambda_A^j(t)$ depends continuously on t for every j. Thus, the sets

$$\mathcal{C}_j(A) := \{\lambda \in \mathbb{C} : \lambda = \lambda_A^j(t),\, t \in \mathbb{T}^n\}, \quad j = 1,\,\dots,\,N \tag{19}$$

are compact and connected curves in the complex plane, called the *spectral* or *dispersion curves* of A.

Proposition 19 *Let $A \in \mathcal{W}(X)$ be a $\mathbb{Z}^n$-periodic operator. Then*

$$\operatorname{sp} A = \operatorname{sp}_{ess} A = \bigcup_{j=1}^N \mathcal{C}_j(A). \tag{20}$$

If, moreover, $A \in \mathcal{W}(X)$ is a self-adjoint $\mathbb{Z}^n$-periodic operator on $l^2(X)$, then σ_A is a Hermitian matrix-valued function. Hence, the λ_A^j are continuous real-valued functions, and

$$\mathcal{C}_j(A) = [\alpha_j(A),\,\beta_j(A)] \quad \text{for } j = 1,\,\dots,\,N$$

where $\alpha_j(A) := \min_{t\in\mathbb{T}^n} \lambda_A^j(t)$ and $\beta_j(A) := \max_{t\in\mathbb{T}^n} \lambda_A^j(t)$. Thus, the spectrum of a self-adjoint $\mathbb{Z}^n$-periodic operator on a periodic metric space is the union of at most N compact intervals (with N the number of orbits of X under the action of $\mathbb{Z}^n$).

5 Operators with slowly oscillating coefficients on periodic metric spaces

Let again X be a $\mathbb{Z}^n$-periodic discrete metric space. A function $a \in l^\infty(X)$ is called *slowly oscillating* if, for every two points $x, y \in X$,

$$\lim_{\alpha \to \infty} (a(\alpha \cdot x) - a(\alpha \cdot y)) = 0. \tag{21}$$

The set of all slowly oscillating functions on X forms a C^*-subalgebra of $l^\infty(X)$ which we denote by $SO(X)$. Note that the class $SO(X)$ does not only depend on X but also on the action of $\mathbb{Z}^n$ on X.

Let $a \in SO(X)$ and $h : \mathbb{N} \to G$ be a sequence tending to infinity. The Bolzano-Weierstrass Theorem and a Cantor diagonal argument imply that there is a subsequence g of h such that the functions $x \mapsto a(g(m) \cdot x)$ converge point-wise to a function $a_g \in l^\infty(X)$ as $m \to \infty$. The condition (21) ensures that the limit function a_g is $\mathbb{Z}^n$-periodic on X. Indeed, for every $\alpha \in \mathbb{Z}^n$,

$$a_g(x) - a_g(\alpha \cdot x) = \lim_{m \to \infty} (a(g(m) \cdot x) - (a(g(m) \cdot (\alpha \cdot x))) = 0.$$

We consider the operators of the form

$$A = \sum_{k,\, l=1}^{\infty} b_k \, A_{kl} \, c_l I \tag{22}$$

where the A_{kl} are $\mathbb{Z}^n$-periodic operators in $\mathcal{W}(X)$ and the b_k and c_l are slowly oscillating functions satisfying

$$\sum_{k,\, l=1}^{\infty} \|b_k\|_{l^\infty(X)} \, \|A_{kl}\|_{\mathcal{W}(X)} \, \|c_l\|_{l^\infty(X)} < \infty.$$

Let $h : \mathbb{N} \to \mathbb{Z}^n$ be a sequence tending to infinity. Then

$$T_{h(m)}^{-1} A T_{h(m)} = \sum_{k,\, l=1}^{\infty} (T_{h(m)}^{-1} b_k) \, A_{kl} \, (T_{h(m)}^{-1} c_l) I.$$

One can assume without loss that the point-wise limits

$$\lim_{m \to \infty} (T_{h(m)}^{-1} b_k)(x) =: b_k^h, \qquad \lim_{m \to \infty} (T_{h(m)}^{-1} c_l)(x) =: c_l^h$$

exist (otherwise we pass to a suitable subsequence of h). As we have seen above, the limit functions b_k^h and c_l^h are $\mathbb{Z}^n$-periodic on X. Consequently, the limit operators A_h of A are $\mathbb{Z}^n$-periodic operators of the form

$$A_h = \sum_{k,\, l=1}^{\infty} b_k^h \, A_{kl} \, c_l^h I.$$

Now, the following is an immediate consequence of Theorem 15.

Theorem 20 *Let A be an operator with slowly oscillating coefficients of the form* (22)*. Then A is a Fredholm operator on $l^p(X)$ if and only if, for every operator $A_h \in \operatorname{op} A$,*

$$\det \sigma_{A_h}(t) \neq 0 \quad \textit{for every}\, t \in \mathbb{T}^n.$$

Moreover,

$$\operatorname{sp}_{ess} A = \bigcup_{A_h \in \operatorname{op}(A)} \operatorname{sp} A_h = \bigcup_{A_h \in \operatorname{op}(A)} \bigcup_{j=1}^{N} \mathcal{C}_j(A_h).$$

6 Schrödinger operators on periodic graphs

By a *discrete infinite graph* we mean a countable set X together with a binary relation $\sim$ which is anti-reflexive (i.e., there is no $x \in X$ such that $x \sim x$) and symmetric and which has the property that for each $x \in X$ there are only finitely many $y \in X$ such that $x \sim y$. The points of X are called the *vertices* and the pairs (x, y) with $x \sim y$ the *edges* of the graph. Due to anti-reflexivity, the graphs under consideration do not possess loops. We write $m(x)$ for the number of edges starting (or ending) at the vertex x of X. If $x \sim y$, we say that the vertices x, y are *adjacent*.

For technical reasons it will be convenient to assume that the graph $(X, \sim)$ is connected, i.e., given distinct points $x, y \in X$, there are finitely many points $x_0, x_1, \ldots, x_n \in X$ such that $x_0 = x$, $x_n = y$ and $x_i \sim x_{i+1}$ for $i = 0, \ldots, n$. The smallest number n with this property defines the *graph distance* $\rho(x, y)$ of x and y. Together with $\rho(x, x) := 0$, this defines a metric ρ on X which makes X to discrete metric space.

We call $(X, \sim)$ a *$\mathbb{Z}^n$-periodic discrete graph* if it is a connected discrete infinite graph, if the group $\mathbb{Z}^n$ operates freely from the left on X, and if the group action respects the graph structure, i.e.,

$$x \sim y \qquad \text{if and only if} \qquad \alpha \cdot x \sim \alpha \cdot y$$

for arbitrary vertices $x, y \in X$ and group elements $\alpha \in \mathbb{Z}^n$. Clearly, every group with these properties leaves the graph distance invariant, that is, X becomes a $\mathbb{Z}^n$-periodic discrete metric space. If $(X, \sim)$ is a $\mathbb{Z}^n$-periodic graph, then the function m is $\mathbb{Z}^n$-periodic, too, that is, $m(\alpha \cdot x) = m(x)$ for every $x \in X$ and $\alpha \in \mathbb{Z}^n$.

Every $\mathbb{Z}^n$-periodic discrete graph $\Gamma := (X, \sim)$ induces a canonical difference operator Δ_Γ on $l^p(X)$, called the (discrete) *Laplace operator* or *Laplacian* of Γ, via

$$(\Delta_\Gamma u)(x) := \frac{1}{m(x)} \sum_{y \sim x} u(y), \quad x \in X. \tag{23}$$

Evidently, Δ_Γ is a $\mathbb{Z}^n$-periodic band operator.

Let $v \in l^\infty(X)$. The operator $\mathcal{H}_\Gamma := \Delta_\Gamma + vI$ is referred to as the (discrete) *Schrödinger operator with electric potential* v on the graph X. Given a sequence

$h : \mathbb{N} \to \mathbb{Z}^n$ tending to infinity, there exist a subsequence g of h and a function $v^g \in l^\infty(X)$ such that $v(g(m) \cdot x) \to v^g(x)$ as $m \to \infty$ for every $x \in X$. It turns out that the operator

$$\mathcal{H}_\Gamma^g := \Delta_\Gamma + v^g I$$

is the limit operator of $\mathcal{H}_\Gamma$ defined by the sequence g and that every limit operator of $\mathcal{H}_\Gamma$ is of this form. Thus, Theorem 15 implies the following.

Theorem 21 *The Schrödinger operator $\mathcal{H}_\Gamma = \Delta_\Gamma + vI$ with bounded potential v is a Fredholm operator on $l^p(X)$ with $p \in (1, \infty)$ if and only if there is a $p_0 \in [1, \infty]$ such that all limit operators of $\mathcal{H}_\Gamma$ are invertible on $l^{p_0}(X)$. The essential spectrum of $\mathcal{H}_\Gamma$ does not depend on $p \in (1, \infty)$, and*

$$\operatorname{sp}_{ess} \mathcal{H}_\Gamma = \bigcup_{\mathcal{H}_\Gamma^h \in \operatorname{op}(\mathcal{H}_\Gamma)} \operatorname{sp} \mathcal{H}_\Gamma^h. \tag{24}$$

For an explicit description of the essential spectrum of the Schrödinger operator $\mathcal{H}_\Gamma$ we first assume that v is a periodic potential. Then the operator UvU^{-1} is the operator of multiplication by the diagonal matrix $\operatorname{diag}(v(x_1), \ldots, v(x_N))$. Hence,

$$U\mathcal{H}_\Gamma U^{-1} = \sum_{\alpha \in \{-1, 0, 1\}^n} a_\alpha V_\alpha + \operatorname{diag}(v(x_1), \ldots, v(x_N)),$$

where the a_α are certain constant $N \times N$ matrices which depend on the structure of the graph Γ. Consequently,

$$\sigma_{\mathcal{H}_\Gamma}(t) = \sum_{\alpha \in \{-1, 0, 1\}^n} a_\alpha t^\alpha + \operatorname{diag}(v(x_1), \ldots, v(x_N)), \quad t \in \mathbb{T}^n.$$

If the potential v is real-valued, then $\mathcal{H}_\Gamma$ acts as a self-adjoint operator on $l^2(X)$, and $\sigma_{\mathcal{H}_\Gamma}$ is a Hermitian matrix-valued function on $\mathbb{T}^n$. From Proposition 19 we conclude that

$$\operatorname{sp} \mathcal{H}_\Gamma = \bigcup_{j=1}^N \mathcal{C}_j(\mathcal{H}_\Gamma)$$

where $\mathcal{C}_j(\mathcal{H}_\Gamma)$ is the real interval $[a_j, b_j]$ with $a_j := \min_{t \in \mathbb{T}^n} \lambda^j_{\mathcal{H}_\Gamma}(t)$ and $b_j := \max_{t \in \mathbb{T}^n} \lambda^j_{\mathcal{H}_\Gamma}(t)$.

Next we consider Schrödinger operators $\mathcal{H}_\Gamma = \Delta_\Gamma + vI$ with slowly oscillating potential v. As we have seen in the previous section, all limit operators of $\mathcal{H}_\Gamma$ are of the form

$$\mathcal{H}_\Gamma^g = \Delta_\Gamma + v^g I$$

with periodic potentials v^g. Theorem 21 together with Theorem 15 yield the following.

Theorem 22 *Let $\mathcal{H}_\Gamma = \Delta_\Gamma + vI$ with $v \in SO(X)$. Then*

$$\operatorname{sp}_{ess} \mathcal{H}_\Gamma = \bigcup_{\mathcal{H}_\Gamma^g \in \operatorname{op}(\mathcal{H}_\Gamma)} \bigcup_{j=1}^N \mathcal{C}_j(\mathcal{H}_\Gamma^g)$$

with the spectral curves $\mathcal{C}_j(\mathcal{H}_\Gamma^g)$ *defined as in* (19).

If the slowly oscillating potential v is real-valued, then the spectral curves $\mathcal{C}_j(\mathcal{H}_\Gamma^g)$ are (possibly overlapping) intervals on the real line.

The following examples clarify the structure of the essential spectrum of Schrödinger operators on some special periodic graphs. The graphs under consideration are embedded into $\mathbb{R}^n$ for some n. This embedding allows one to consider the vertices of the graph as vectors and to use the linear structure of $\mathbb{R}^n$ in order to describe the group action.

Example 23 (The Cayley graph of $\mathbb{Z}^n$) As every finitely generated group, the group $\mathbb{Z}^n$ induces a graph (called the Cayley graph of the group) the vertices of which are the points in $\mathbb{Z}^n$ and with edges $(\alpha,\ \alpha \pm e_i)$ where $\alpha \in \mathbb{Z}^n$ and where $e_i := (0,\ \ldots,\ 0,\ 1, 0,\ \ldots,\ 0)$ with the 1 at the ith position and $i = 1,\ \ldots,\ n$. The Laplace operator $\Delta_{\mathbb{Z}^n}$ is of the form

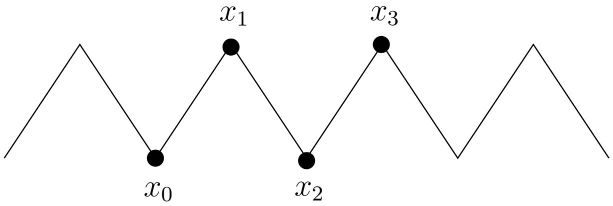
$$(\Delta_{\mathbb{Z}^n} u)(x) = \frac{1}{2n} \sum_{i=1}^{n} (u(x+e_i) + u(x-e_i)),$$

which leads to the symbol

$$\sigma_{\Delta_{\mathbb{Z}^n}}(t) := \frac{1}{2n} \sum_{i=1}^{n} (t_i + t_i^{-1}), \quad t \in \mathbb{T}^n.$$

Hence, $\operatorname{sp} \Delta_{\mathbb{Z}^n} = [-1,\ 1]$. ■

Example 24 (The zigzag graph) Let $\Gamma = (X, \sim)$ be the zigzag graph in the plane $\mathbb{R}^2$ as shown in Figure 24. The graph Γ is periodic with respect to the action $g \cdot x_n := x_{n+2g}$ of the group $\mathbb{Z}$, and the set $\mathcal{M} = \{x_1,\ x_2\}$ of vertices represents the fundamental domain.



One should mention that, as a graph, the zigzag graph is isomorphic to the Cayley graph of the group $\mathbb{Z}$ and, in both cases, it is the same group $\mathbb{Z}$ which acts on the graph. The difference lies in the way in which $\mathbb{Z}$ acts. For the Cayley graph, the group element α maps the vertex x to $\alpha + x$, whereas α maps x to $2\alpha + x$ for the zigzag graph. The latter action is visualized by the zigzag form.

The operator $U \Delta_\Gamma U^{-1}$ has the matrix representation

$$U \Delta_\Gamma U^{-1} = \frac{1}{2} \begin{pmatrix} 0 & I + V_{(1,\,0)} \\ I + V_{(-1,\,0)} & 0 \end{pmatrix}$$

in the basis induced by $\mathcal{M}$. Hence,

$$\sigma_{\Delta_\Gamma}(t) = \frac{1}{2}\begin{pmatrix} 0 & 1+t \\ 1+t^{-1} & 0 \end{pmatrix}, \quad t \in \mathbb{T},$$

and a straightforward calculation shows that the spectral curves of Δ_Γ are

$$\{\lambda \in \mathbb{C} : \lambda = \pm\cos^2\varphi/2,\ \varphi \in [0,\, 2\pi]\}.$$

Hence, the spectrum of the Laplacian Δ_Γ of the zigzag graph is the interval $[-1,\, 1]$.

Next consider the Schrödinger operator $\mathcal{H}_\Gamma := \Delta_\Gamma + vI$ with $\mathbb{Z}$-periodic potential v. Thus, v is completely determined by its values on $\mathcal{M}$, and we write $v_1 := v(x_1)$ and $v_2 := v(x_2)$. Then

$$\sigma_{\mathcal{H}_\Gamma - \lambda I}(t) = \begin{pmatrix} v_1 - \lambda & (1+t)/2 \\ (1+t^{-1})/2 & v_2 - \lambda \end{pmatrix}, \quad t \in \mathbb{T},$$

which implies that the spectral curves of $\mathcal{H}_\Gamma$ are

$$\left\{\lambda \in \mathbb{C} : \lambda = \frac{1}{2} \pm \frac{\sqrt{(v_1 - v_2)^2 + 4\cos^2\varphi/2}}{2(v_1+v_2)},\ \varphi \in [0,\, 2\pi]\right\}.$$

If, for example, v_1 and v_2 are real numbers with $v_1 < v_2$, then $\mathrm{sp}_{ess}\,\mathcal{H}_\Gamma = \mathrm{sp}\,\mathcal{H}_\Gamma$ is the union of the disjoint intervals

$$\left[\frac{1}{2} - \frac{\sqrt{(v_1 - v_2)^2 + 4}}{2(v_1+v_2)},\ \frac{v_1}{v_1+v_2}\right] \bigcup \left[\frac{v_2}{v_1+v_2},\ \frac{1}{2} + \frac{\sqrt{(v_1 - v_2)^2 + 4}}{2(v_1+v_2)}\right], \tag{25}$$

that is, one observes a gap $(\frac{v_1}{v_1+v_2},\, \frac{v_2}{v_1+v_2})$ in the spectrum.

Finally, let the potential v be slowly oscillating. Then the essential spectrum of $\mathcal{H}_\Gamma$ is the union

$$\begin{aligned} &\bigcup_h \left[\frac{1}{2} - \frac{\sqrt{(v_1^h - v_2^h)^2 + 4}}{2(v_1^h+v_2^h)},\ \frac{\min\{v_1^h,\, v_2^h\}}{v_1^h+v_2^h}\right] \\ &\quad \bigcup_h \left[\frac{\max\{v_1^h,\, v_2^h\}}{v_1^h+v_2^h},\ \frac{1}{2} + \frac{\sqrt{(v_1^h - v_2^h)^2 + 4}}{2(v_1^h+v_2^h)}\right] \end{aligned} \tag{26}$$

where the unions are taken with respect to all sequences h for which the limits

$$v_j^h := \lim_{m\to\infty} v(h(m)\cdot x_j), \quad j = 1,\, 2, \tag{27}$$

exist. Set

$$a_{\mathcal{H}_\Gamma} := \limsup_{\mathbb{Z}\ni\alpha\to\infty} \frac{v(\alpha\cdot x_1)}{v(\alpha\cdot x_1) + v(\alpha\cdot x_2)},$$

$$b_{\mathcal{H}_\Gamma} := \liminf_{\mathbb{Z}\ni\alpha\to\infty} \frac{v(\alpha\cdot x_2)}{v(\alpha\cdot x_1) + v(\alpha\cdot x_2)}.$$

Thus, if the inequality

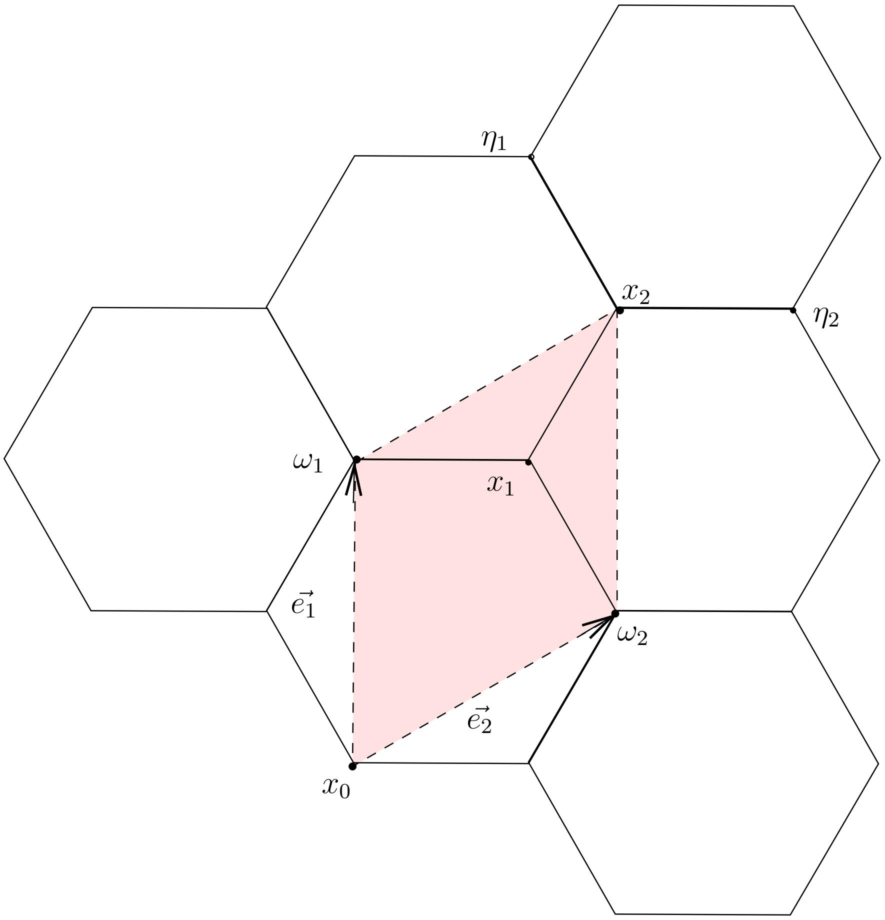
$$a_{\mathcal{H}_\Gamma} < b_{\mathcal{H}_\Gamma} \tag{28}$$

holds, then the operator $\mathcal{H}_\Gamma$ has the gap $(a_{\mathcal{H}_\Gamma},\, b_{\mathcal{H}_\Gamma})$ in its essential spectrum. Of course, this interval can contain points of the discrete spectrum of $\mathcal{H}_\Gamma$. ■

Example 25 (The honeycomb graph) Let $\Gamma = (X, \sim)$ be the hexagonal graph shown in Figure 25. We consider this graph as embedded into $\mathbb{R}^2$ and let e_1 and e_2 be the vectors indicated in the figure. The group $\mathbb{Z}^2$ operates on Γ via

$$(\alpha_1, \alpha_2) \cdot x := x + \alpha_1 e_1 + \alpha_2 e_2$$

(where $\alpha_1,\, \alpha_2 \in \mathbb{Z}$ and $x \in X$). A fundamental domain $\mathcal{M}$ for this action is provided by any two vertices $x_1,\, x_2$ as marked in the figure.



Hence, we have to identify $l^p(X)$ with $l^p(\mathbb{Z}^2,\, \mathbb{C}^2)$, and the Laplacian Δ_Γ has the following matrix representation with respect to $\mathcal{M}$

$$U\Delta_\Gamma U^{-1} = \frac{1}{3}\begin{pmatrix} 0 & I + V_{e_1} + V_{e_2} \\ I + V_{e_1}^{-1} + V_{e_2}^{-1} & 0 \end{pmatrix}.$$

Consequently,

$$\sigma_{\Delta_\Gamma}(t) = \frac{1}{3}\begin{pmatrix} 0 & 1 + t_1 + t_2 \\ 1 + t_1^{-1} + t_2^{-1} & 0 \end{pmatrix}, \quad t = (t_1, t_2) \in \mathbb{T}^2,$$

and the spectral curves of the Laplacian Δ_Γ are

$$\mathcal{C}_\pm := \{\lambda \in \mathbb{C} : \lambda = \pm|1 + e^{i\varphi_1} + e^{i\varphi_2}|/3, \ \varphi_1, \varphi_2 \in [0, 2\pi]\}.$$

The curves $\mathcal{C}_\pm$ coincide with the intervals $[0, 1]$ and $[-1, 0]$, respectively, whence $\operatorname{sp}\Delta_\Gamma = [-1, 1]$.

Let now v be a $\mathbb{Z}^2$-periodic potential and set $v_j := v(x_j)$ for $j = 1, 2$. A calculation similar to Example 24 yields that the spectral curves of the Schrödinger operator $\mathcal{H}_\Gamma := \Delta_\Gamma + vI$ are

$$\left\{\lambda \in \mathbb{C} : \lambda = \frac{1}{2} \pm \frac{\sqrt{(v_1 - v_2)^2 + 4\mu(\varphi_1, \varphi_2)}}{2(v_1 + v_2)}\right\},$$

where

$$\mu(\varphi_1, \varphi_2) := |1 + e^{i\varphi_1} + e^{i\varphi_2}|^2/9, \quad \varphi_1, \varphi_2 \in [0, 2\pi].$$

Hence, as in Example 24, $\operatorname{sp}_{ess}\mathcal{H}_\Gamma = \operatorname{sp}\mathcal{H}_\Gamma$ is given by the union (25). Let finally v be a slowly oscillating potential on X. Since the image of the function μ is the interval $[0, 1]$, the essential spectrum of the Schrödinger operator on the honeycomb graph Γ is given by formulas (26) and (27). If the condition (28) holds, then a gap $(a_{\mathcal{H}_\Gamma}, b_{\mathcal{H}_\Gamma})$ occurs in the essential spectrum of $\mathcal{H}_\Gamma$. ■

7 A three-particle problem

Let $\Gamma := (X, \sim)$ be a $\mathbb{Z}^n$-periodic discrete graph. We consider the Schrödinger operator

$$\begin{aligned}\mathcal{H}u \ := \ & \Delta_\Gamma \otimes I_X + I_X \otimes \Delta_\Gamma + \\ & +(W_1 I_X) \otimes I_X + I_X \otimes (W_2 I_X) + W_{12} I\end{aligned} \tag{29}$$

on $l^2(X \times X)$. This operator describes the motion of two particles with coordinates $x^1, x^2 \in X$ with masses 1 on the graph Γ around a heavy nuclei located at the point $x_0 \in X$. Therefore, $\mathcal{H}$ is also called a 3-particle Schrödinger operator. In (29), Δ_Γ is again the Laplacian on the graph Γ, I_X is the identity operator on $l^2(X)$, $I = I_X \otimes I_X$ is the identity operator on $l^2(X \times X)$, W_1 and W_2 are real-valued functions on X defined by

$$W_j(x^j) = w_j(\rho(x^j, x_0)), \quad j = 1, 2,$$

and W_{12} is a real-valued function on $X \times X$ given by

$$W_{12}(x^1,\, x^2) = w_{12}(\rho(x^1,\, x^2)).$$

Here ρ denotes the given metric on X, and w_1, w_2 and w_{12} are functions on the real interval $[0,\, \infty)$ which satisfy

$$\lim_{z \to \infty} w_1(z) = \lim_{z \to \infty} w_2(z) = \lim_{z \to \infty} w_{12}(z) = 0.$$

Clearly, $\mathcal{H}$ is a band operator on $l^2(X \times X)$. We are going to describe its essential spectrum via formula (24), for which we need the limit operators of $\mathcal{H}$ and their spectra. Note that the spectrum of the Laplacian Δ_Γ depends on the structure of the graph Γ and that this spectrum has a band structure (= is the union of closed intervals). In Examples 23 – 25 we had $\operatorname{sp} \Delta_\Gamma = [-1,\, 1]$.

We agree upon the following notation. For non-empty subsets E, F of $\mathbb{R}$, we let

$$E + F := \{z \in \mathbb{R} : z = x + y,\, x \in E,\, y \in F\}$$

denote their algebraic sum, and we set $2E := E + E$.

Let $g = (g^1,\, g^2) : \mathbb{N} \to \mathbb{Z}^n \times \mathbb{Z}^n$ be a sequence tending to infinity. We have to distinguish the following cases (all other possible cases can be reduced to these cases by passing to suitable subsequences of g):

Case 1. The sequence g^1 tends to infinity, whereas g^2 is constant. Then the limit operator $\mathcal{H}_g$ of $\mathcal{H}$ is unitarily equivalent to the operator

$$\mathcal{H}_2 := \Delta_\Gamma \otimes I_X + I_X \otimes (\Delta_\Gamma + W_2 I_X). \tag{30}$$

Case 2. Here g^2 tends to infinity and g^1 is constant. Then the limit operator $\mathcal{H}_g$ of $\mathcal{H}$ is unitarily equivalent to the operator

$$\mathcal{H}_1 := (\Delta_\Gamma + W_1 I_X) \otimes I_X + I_X \otimes \Delta_\Gamma. \tag{31}$$

Case 3. Both g^1 and g^2 tend to infinity. There are two subcases:

Case 3a. The sequence $g^1 - g^2$ tends to infinity. In this case the limit operator is the free discrete Hamiltonian

$$\Delta_\Gamma \otimes I_X + I_X \otimes \Delta_\Gamma$$

the spectrum of which is equal to $2 \operatorname{sp} \Delta_\Gamma$.

Case 3b. The sequence $g^1 - g^2$ is constant. Then the limit operator $\mathcal{H}_g$ of $\mathcal{H}$ is unitarily equivalent to the operator of interaction

$$\mathcal{H}_{12} := \Delta_\Gamma \otimes I_X + I_X \otimes \Delta_\Gamma + W_{12} I. \tag{32}$$

Note that the operators $\mathcal{H}_1$, $\mathcal{H}_2$ and $\mathcal{H}_{12}$ are invariant with respect to shifts by elements of the form $(0,\, g)$, $(g,\, 0)$ and $(g,\, g)$ of $\mathbb{Z}^n \times \mathbb{Z}^n$, respectively. It follows from Proposition 16 that these operators do not possess discrete spectra. From formula (24) we further conclude

$$\mathrm{sp}_{ess}\,\mathcal{H} = \mathrm{sp}\,\mathcal{H}_1 \cup \mathrm{sp}\,\mathcal{H}_2 \cup \mathrm{sp}\,\mathcal{H}_{12}. \tag{33}$$

The following proposition is well known. For a proof see [34], Theorem VIII.33 and its corollary.

Proposition 26 *Let $A \in \mathcal{L}(H)$ and $B \in \mathcal{L}(K)$ be bounded self-adjoint operators on Hilbert spaces H, K. Then*

$$\mathrm{sp}\,(A \otimes I_K + I_H \otimes B) = \mathrm{sp}\,A + \mathrm{sp}\,B.$$

This proposition implies in our setting that

$$\mathrm{sp}\,\mathcal{H}_2 = \mathrm{sp}\,\Delta_\Gamma + \mathrm{sp}\,(\Delta_\Gamma + W_2 I_X).$$

Since the Schrödinger operator $\Delta_\Gamma + W_2 I_X$ is a compact perturbation of the Laplacian Δ_Γ, one has

$$\mathrm{sp}_{ess}\,(\Delta_\Gamma + W_2 I_X) = \mathrm{sp}\,\Delta_\Gamma \cup \{\lambda_k^{(2)}\}_{k=1}^\infty$$

where $\{\lambda_k^{(2)}\}_{k=1}^\infty$ is the sequence of the eigenvalues of $\Delta_\Gamma + W_2 I_X$ which are located outside the spectrum of Δ_Γ. Thus,

$$\mathrm{sp}\,\mathcal{H}_2 = 2\,\mathrm{sp}\,\Delta_\Gamma + \cup_{k=1}^\infty (\lambda_k^{(2)} + \mathrm{sp}\,\Delta_\Gamma).$$

In the same way one finds

$$\mathrm{sp}\,\mathcal{H}_1 = 2\,\mathrm{sp}\,\Delta_\Gamma + \cup_{k=1}^\infty (\lambda_k^{(1)} + \mathrm{sp}\,\Delta_\Gamma)$$

where the $\lambda_k^{(1)}$ run through the points of the discrete spectrum of $\Delta_\Gamma + W_1 I_X$ which are located outside the spectrum of Δ_Γ.

Recall that in Examples 23 – 25, $\mathrm{sp}\,\Delta_\Gamma = [-1,\, 1]$. Hence, in the context of these examples,

$$\mathrm{sp}\,\mathcal{H}_j = [-2,\, 2] \bigcup_{k=1}^\infty [\lambda_k^{(j)} - 1,\, \lambda_k^{(j)} + 1].$$

One can also give a simple estimate for the location of the spectrum of $\mathcal{H}_{12}$ by means of the following well-known result (see, e.g., [22], p. 357).

Proposition 27 *Let A be a bounded self-adjoint operator on the Hilbert space H. Then $\{a,\, b\} \subseteq \mathrm{sp}\,A \subseteq [a,\, b]$ where*

$$a := \inf_{\|h\|=1} \langle Ah,\, h\rangle, \quad b := \sup_{\|h\|=1} \langle Ah,\, h\rangle.$$

This observation implies the following inclusions for the spectra of the operators $\mathcal{H}_1$, $\mathcal{H}_2$ and $\mathcal{H}_{12}$. For $j = 1, 2$ one has

$$2 \operatorname{sp} \Delta_\Gamma \subseteq \operatorname{sp} \mathcal{H}_j \subseteq 2 \operatorname{sp} \Delta_\Gamma + \left[\inf_{x \in X} W_j(x),\ \sup_{x \in X} W_j(x) \right],$$

whereas

$$2 \operatorname{sp} \Delta_\Gamma \subseteq \operatorname{sp} \mathcal{H}_{12} \subseteq 2 \operatorname{sp} \Delta_\Gamma + \left[\inf_{y \in X \times X} W_{12}(y),\ \sup_{y \in X \times X} W_{12}(y) \right].$$

In the context of Examples 23 – 25, these inclusions specify to

$$[-2,\, 2] \subseteq \operatorname{sp} \mathcal{H}_j \subseteq \left[-2 + \inf_{x \in X} W_j(x),\ 2 + \sup_{x \in X} W_j(x) \right],$$

$$[-2,\, 2] \subseteq \operatorname{sp} \mathcal{H}_{12} \subseteq \left[-2 + \inf_{x \in X \times X} W_{12}(x),\ 2 + \sup_{x \in X \times X} W_{12}(x) \right].$$

Thus, Theorem 21 yields for these examples

$$\operatorname{sp}_{ess} \mathcal{H} \subseteq [m - 2,\, M + 2]$$

where

$$m := \min \left\{ \inf_{x \in X} W_1(x),\ \inf_{x \in X} W_2(x),\ \inf_{x \in X \times X} W_{12}(x) \right\},$$

$$M := \max \left\{ \sup_{x \in X} W_1(x),\ \sup_{x \in X} W_2(x),\ \sup_{x \in X \times X} W_{12}(x) \right\}.$$

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