Bachelor Thesis

On the spectra of the Schrödinger operator with periodic delta potential

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Chapter 1

Introduction

In this thesis, we are interested in an idealised quantum-mechanical system that models a quantum particle behaving as a matter wave moving in one dimension through an infinite periodic array of rectangular potential barriers, i.e. through a space area in which a potential attains a local maximum. Such an array commonly occurs in models of periodic crystal lattices where the potential is caused by ions in the crystal structure. Those charged atoms or molecules create an electromagnetic field around themselves. Hence, any particle moving through such a crystal would be subject to a recurrent electromagnetic potential. Although a solid particle, simplified as a point mass, would be reflected at such a barrier there is a possibility that the quantum particle, as it behaves like a wave, penetrates the barrier and continues its movement beyond. This problem is considered in the Kronig-Penney model, see for example [Hee02, Chapter 3].

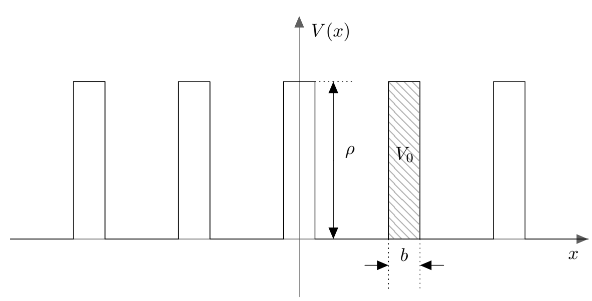

Figure 1.1: Potential $V(x)$ of the Kronig-Penney model

Assuming the spacing between all ions is equidistant, the potential function $V(x)$ in the lattice can be approximated by a rectangular potential as depicted in Figure 1.1, where b is the width of the support and ρ the magnitude of the potentials.

As the main focus of this thesis, we are interested in the spectrum of the operator describing the situation in the Kronig-Penney model when the particle moves through periodically distributed, singular potentials. With respect to the above assumptions this means taking the limit $b \to 0$ while V_0 remains of order ρb^{-1}. On this account, we will build on the research presented in [DLP$^+$11] where the spectrum of periodic differential operators with smooth coefficients has been analysed. We will show that an operator modelling the aforementioned situation has, as in the case of smooth coefficients, a spectrum that consists of a union of compact intervals in $\mathbb{R}$ which form a so-called spectral band.

In a physical sense, spectral bands represent energy levels. Only an electron with an energy level within the spectral band can exist inside the crystal. In other words, any gaps between the spectral bands, if they exist, represent a forbidden energy range. According to Bragg's law, standing waves form at the boundary between the spectral bands and the forbidden energy levels. The closer the electrons orbit the nucleus of their atom the more energetically favourable are the standing waves which is a preferable state by the electrons, for a detailed explanation see [Hee02, Section 3.2]. Therefore, Bragg's law provides an explanation for the forbidden energy levels. Because of this principle, in order to determine possible energy levels within periodic crystal lattices knowledge about the corresponding spectral properties is needed.

The remainder of this thesis is structured as follows. We begin with a few preliminaries in Chapter 2 to recall some key concepts in functional analysis and spectral theory. In Chapter 3, we introduce the Schrödinger operator with a periodic Delta-Potential, describing the motion of an electron under study, and, as the first step into the analysis of its spectrum, we show that the operator is self-adjoint. As principal mathematical tool for analysing the spectrum of the operator we use the Floquet-Bloch theory. We then transfer the spectral problem of the periodic operator on the whole of $\mathbb{R}$ to a family of eigenvalue problems on the periodicity cell. Hence, we proceed in Chapter 4 by restricting the problem to its fundamental domain of periodicity. We analyse the spectrum of the restricted operator by showing the compactness of its resolvent function while varying quasi-periodic boundary conditions.

In order to be able to extend the restricted-case results to the more general periodic case, in Chapter 5 we introduce two more concepts, the Floquet transformation and the Bloch waves. Based on these methods, in Chapter 6 we show our main result for the one-dimensional case, i.e. that such an operator has a spectrum consisting of a union of compact intervals in $\mathbb{R}$, and extrapolate this result to the multi-dimensional case in Chapter 7. Finally, we conclude this thesis in Chapter 8 with a brief discussion of possible gaps between the compact intervals and with an overview of some recent research.

Chapter 2

Preliminaries

To lay the groundwork for the upcoming analysis, this chapter briefly reviews some key concepts in functional analysis and spectral theory.

Let $\Omega \subseteq \mathbb{R}$ be open and let $C_0^\infty(\Omega)$ denote the linear space containing all smooth functions $f : \Omega \to \mathbb{R}$ with compact support, i.e. for $f \in C_0^\infty(\Omega)$ there exists $I \subseteq \Omega$ such that $f(x) = 0$ for all $x \notin I$. Furthermore, let I denote the identity operator on the respective space, i.e. $Ix = x$ for all x, and hereafter $\langle x, x \rangle$ will denote the scalar product in $L^2(\mathbb{R})$.

Definition (Weak derivative)**:** *For $f \in L^1_{loc}(\Omega)$, the function f is said to have the weak derivative $g \in L^1_{loc}(\Omega)$ in Ω if*

$$-\int_\Omega f(x)\varphi'(x)dx = \int_\Omega g(x)\varphi(x)dx$$

holds for all $\varphi \in C_0^\infty(\Omega)$.

For $\alpha \in \mathbb{N}$, we denote with $D^\alpha u$ the α-th weak derivate of u, therewith, if two functions are weak derivatives of the same function they are equal except on a set with Lebesgue measure zero, i.e. they are equal almost everywhere, for a proof see Theorem A.1.23. As a basic tool in this study we use a Hilbert space that combines the concepts of weak differentiability and Lebesgue norms, the Sobolev space $H^k(\Omega)$.

Definition: *The Sobolev space $H^k(\Omega)$ is defined as*

$$H^k(\Omega) := \left\{u \in L^2(\Omega) : D^\alpha u \text{ exists and } D^\alpha u \in L^2(\Omega) \text{ for } 0 \leq \alpha \leq k\right\}$$

The space is equipped with the norm $\|\cdot\|_{H^k(\Omega)} := \left(\sum_{0\le\alpha\le k}\|D^\alpha\cdot\|^2_{L^2(\Omega)}\right)^{\frac{1}{2}}$.

The space $H^k(\Omega)$ admits an inner product which is defined in terms of the $L^2(\Omega)$ inner product:

$$\langle u,v\rangle_{H^k(\Omega)} = \sum_{\alpha=0}^{k}\langle D^\alpha u, D^\alpha v\rangle_{L^2}.$$

Moreover, $H^k(\Omega)$ becomes a Hilbert space with this inner product.

Definition (Distributions)**:** *On $C_0^\infty(\Omega)$ a sequence (f_n) converges to $f\in C_0^\infty(\Omega)$ if the support of all members of the sequence is in a compact interval $I\subset\mathbb{R}$, i.e.*

$$\mathrm{supp}(f_n)\subseteq I \quad \forall n\in\mathbb{N},$$

and on this interval f_n and all its derivatives converge uniformly to f, i.e.

$$\|f_n^{(i)} - f^{(i)}\|_\infty \to 0 \quad \text{for } n\to\infty$$

for all $i\in\mathbb{N}_0$. This concept of convergence induces a topology on $C_0^\infty(\Omega)$, and henceforth, we denote with $\mathfrak{D}(\Omega)$ the space $C_0^\infty(\Omega)$ equipped with this topology.

In the remainder of this thesis, we denote with $\mathfrak{D}'(\Omega)$ the space of all linear functionals on $C_0^\infty(\Omega)$ that are continuous with respect to this topology and call those functionals distributions.

The Delta-Distribution δ_{x_0} where $x_0\in\mathbb{R}$, will be of special interest in this thesis. For a given $x_0\in\mathbb{R}$ we define the Delta-Distribution $\delta_{x_0}\in\mathfrak{D}'(\mathbb{R})$ for $f\in\mathfrak{D}(\mathbb{R})$ through

$$\delta_{x_0}(f) := f(x_0),$$

furthermore by density of $C_0^\infty(\Omega)$ in $L^p(\Omega)$ (Theorem A.1.2) we extend this definition to $H^k(\Omega)$, for a more detailed explanation see [Wer06, p. 429]. For our analysis, however, another, equivalent definition of the Delta-Distribution is more convenient. Let us define the sequence of functionals δ_ϵ for $\epsilon>0$ and $f\in\mathfrak{D}(\mathbb{R})$ through

$$\delta_\epsilon(f) := \frac{1}{\sqrt{2\pi}\epsilon}\int_{\mathbb{R}} e^{-\frac{(x-x_0)^2}{2\epsilon^2}} f(x)dx. \tag{2.1}$$

Each functional is symmetric around x_0 and its support "converges" to the point x_0 as ϵ

tends to 0. Furthermore, it can be shown that

$$\delta_{x_0}(f) = \lim_{\epsilon \to 0} \delta_\epsilon(f),$$

for proof see Theorem A.1.1.

Since our focus will be on the Schrödinger operator, we will need the following definitions and properties of operators between Banach spaces.

Definition: *Let X, Y be Banach spaces and let $A\colon \mathcal{D}(A) \to Y$ be a linear operator with domain $\mathcal{D}(A) \subseteq X$. We call A closed if graph$(A) \coloneqq \{(x, Ax) : x \in \mathcal{D}(A)\} \subseteq X \times Y$ is a closed set with respect to the product topology.*

Moreover, we are concerned with the self-adjoint operators. Thus, we define:

Definition: *Let X be a Hilbert space and $\langle \cdot, \cdot \rangle_X$ denote the scalar product on X. Let $A\colon \mathcal{D}(A) \to X$ be a linear operator where $\mathcal{D}(A) \subseteq X$.*

a) If A is densely defined, the adjoint $A^*\colon \mathcal{D}(A^*) \to X$ of A is defined by

$$\mathcal{D}(A^*) \coloneqq \{u \in X\colon\ \exists u^* \in X\ \forall v \in \mathcal{D}(A)\ \langle u, Av \rangle = \langle u^*, v \rangle\} \text{ and } A^*u \coloneqq u^*$$

for $u \in \mathcal{D}(A^*)$; note that, for $u \in \mathcal{D}(A^*)$, u^* is unique.

b) We call A symmetric, if $\langle Ax, y \rangle_X = \langle x, Ay \rangle_X$ for all $x, y \in \mathcal{D}(A)$, and

c) We call A self-adjoint, if A is densely defined on X and coincides with its adjoint.

Since every symmetric operator A has the property $\mathcal{D}(A) \subseteq \mathcal{D}(A^*)$ it follows that A is self-adjoint if A is a symmetric operator, the adjoint is well-defined and $\mathcal{D}(A) \supseteq \mathcal{D}(A^*)$, for proof refer to [RS08, p. 256]. Our main objective is to characterise the spectrum of the Schrödinger operator, hence we also need the following definitions.

Definition: *Let I denote the identity operator on X and $A\colon X \supseteq \mathcal{D}(A) \to Y$ be a linear, closed operator.*

a) $\lambda \in \mathbb{C}$ belongs in the resolvent set of A, $\lambda \in \rho(A)$, if $(A - \lambda I)\colon \mathcal{D}(A) \to Y$ is bijective, note that due to the Closed Graph Theorem (Theorem A.1.5)

$$(A - \lambda I)^{-1}\colon X \to \mathcal{D}(A) \text{ is a bounded operator.}$$

b) $\sigma(A) = \mathbb{C} \setminus \rho(A)$ *is called the spectrum of* A.

c) $\rho(A) \ni \lambda \mapsto R(\lambda, A) := (A - \lambda I)^{-1}$ *is the resolvent function of* A.

In Chapters 4 and 7 we examine the so-called compact operators and some of their properties.

Definition: *Let* X, Y *be Banach spaces and* $U_X := \{x \in X : |x| < 1\}$. *A linear operator* $A\colon X \to Y$ *is called compact, if* $T(U_X)$ *is relatively compact in* Y.

In the Appendix, further theorems and lemmata of functional analysis and spectral theory used in this thesis are listed.

Chapter 3

The one-dimensional Schrödinger operator

The mathematical representation of the problem stated above can be done by introducing a one-dimensional Schrödinger operator A where the potential is given by a periodic Delta-Distribution. In this chapter we will examine properties of A such as its domain and show its self-adjointness. Later, in Chapters 4 and 6, we will need these results to deduce our main result, i.e. characteristics of the spectrum of A.

Formally the operation of A is defined by

$$-\frac{d^2}{dx^2} + \rho \sum_{i \in \mathbb{Z}} \delta_{x_i} \tag{3.1}$$

on the whole of $\mathbb{R}$, where δ_{x_i} denotes the Delta-Distribution supported at the point x_i, cf. also Section 3.2. Ω_k will hereafter identify the periodicity cell containing point x_k and w.l.o.g. let $x_0 = 0$ and $|\Omega_i| = 1$ for all $i \in \mathbb{Z}$. By this assumption, we then can rearrange all other points where the Delta-Distribution is supported $(x_i)_{i \in \mathbb{Z} \setminus \{0\}}$ such that $x_i = x_0 + i$ for all $i \in \mathbb{Z} \setminus \{0\}$.

In general, one cannot say in which sense a solution to the formal problem

$$Au = f \quad \text{for } f \in L^2(\mathbb{R}) \tag{3.2}$$

exists since the potential in A consists of Delta-Distributions. If we suppose for a moment that this periodic differential expression is smooth, more specifically, that the potential in every point x_k is instead given by (2.1) for some $\epsilon > 0$, then formally multiplying it by a test function and integrating by parts yields the so-called weak formulation to the smooth problem whose solution requires less regularity. Motivated by this, by taking the limit of the potential in the weak formulation, we henceforth consider the problem to find for $\mu \in \mathbb{R}$ a function $u \in H^1(\mathbb{R})$ such that

$$\int_{\mathbb{R}} u'(x)\overline{v'(x)}dx + \rho \sum_{i\in\mathbb{Z}} u(x_i)\overline{v(x_i)} - \mu \int_{\mathbb{R}} u(x)\overline{v(x)}dx = \int_{\mathbb{R}} f(x)\overline{v(x)}dx \quad \forall v \in C_0^\infty(\mathbb{R}), \tag{3.3}$$

holds and call (3.3) the weak formulation of (3.2). We should note that the left-hand side of problem (3.3) is actually well-defined and finite, as for any $h \in (0,1]$ we can estimate the norm with the help of some integration methods via

$$\begin{aligned}\sum_{i\in\mathbb{Z}} |u(x_i)|^2 &\leq \sum_{i\in\mathbb{Z}} \left(2|u(x_i+h)|^2 + 2h\int_{x_i}^{x_i+h} |u'(\tau)|^2 \, d\tau \right) \\ &\leq 2\sum_{i\in\mathbb{Z}} \left(\frac{1}{h}\int_{\Omega_i} |u(x)|^2 dx + h\int_{\Omega_i} |u'(\tau)|^2 \, d\tau \right).\end{aligned} \tag{3.4}$$

The choice of $h = 1$ yields hence the estimation

$$\sum_{i\in\mathbb{Z}} |u(x_i)|^2 \leq 2\|u\|^2_{H^1(\mathbb{R})}. \tag{3.5}$$

Remark: *The problem* (3.3) *holds also for all* $v \in H^1(\mathbb{R})$ *since* $C_0^\infty(\mathbb{R})$ *is dense in* $L^2(\mathbb{R})$, *for proof see Theorem A.1.2.*

3.1 The resolvent-mapping

As a first step, in order to define the operator A explicitly, we will show that for each $f \in L^2(\mathbb{R})$ the equation (3.3) has a unique solution $u \in H^1(\mathbb{R})$.

Definition: *Given* $f \in L^2(\mathbb{R})$, *we define a functional* $l_f \colon H^1(\mathbb{R}) \to \mathbb{C}$ *by*

$$l_f(v) := \int_{\mathbb{R}} f(x)\overline{v(x)}dx$$

and a sesquilinear form $B_\mu\colon H^1(\mathbb{R})\times H^1(\mathbb{R})\to\mathbb{C}$ for $\mu\in\mathbb{R}$ by

$$B_\mu[u,v] := \int_{\mathbb{R}} u'(x)\overline{v'(x)}dx + \rho\sum_{i\in\mathbb{Z}} u(x_i)\overline{v(x_i)} - \mu\int_{\mathbb{R}} u(x)\overline{v(x)}dx.$$

As a result, (3.3) is equivalent to finding for $\mu\in\mathbb{R}$ a function $u\in H^1(\mathbb{R})$ such that

$$B_\mu[u,v] = l_f(v) \tag{3.6}$$

holds for all $v\in H^1(\mathbb{R})$. The existence of a unique $u\in H^1(\mathbb{R})$ satisfying (3.6) now follows from Lax-Milgram's Theorem (Theorem A.1.13) if the sesquilinear form B_μ is bounded and coercive and if l_f is a bounded linear functional on $H^1(\mathbb{R})$, which we will prove in the next two theorems.

Theorem 3.1: *The sesquilinear form B_μ is for sufficiently small $\mu\in\mathbb{R}$*

a) bounded, i.e. there exists a constant $\alpha>0$ such that

$$|B_\mu[u,v]| \le \alpha\|u\|_{H^1(\mathbb{R})}\|v\|_{H^1(\mathbb{R})}$$

holds for all $u,v\in H^1(\mathbb{R})$.

b) coercive, i.e. there exists a constant $\beta>0$ such that

$$\beta\|u\|^2_{H^1(\mathbb{R})} \le Re(B_\mu[u,u])$$

holds for all $u\in H^1(\mathbb{R})$.

Proof:

a) The boundedness follows from the Cauchy–Schwarz inequality (Theorem A.1.4) and (3.5) as for an arbitrary $\rho\in\mathbb{R}$

$$\begin{aligned}|B(u,v)|^2 &\le 3\|u'\|^2_{L^2(\mathbb{R})}\|v'\|^2_{L^2(\mathbb{R})} + 3\rho^2\left(\sum_{i\in\mathbb{Z}}|u(x_i)|^2\right)\left(\sum_{i\in\mathbb{Z}}|v(x_i)|^2\right) + 3\mu^2\|u\|^2_{L^2(\mathbb{R})}\|v\|^2_{L^2(\mathbb{R})}\\ &\le 3\|u'\|^2_{L^2(\mathbb{R})}\|v'\|^2_{L^2(\mathbb{R})} + 12\rho^2\|u\|^2_{H^1(\mathbb{R})}\|v\|^2_{H^1(\mathbb{R})} + 3\mu^2\|u\|^2_{L^2(\mathbb{R})}\|v\|^2_{L^2(\mathbb{R})}\\ &\le \alpha\|u\|^2_{H^1(\mathbb{R})}\|v\|^2_{H^1(\mathbb{R})},\end{aligned}$$

holds for all $u,v\in H^1(\mathbb{R})$ where $\alpha=\max\left\{12\rho^2+3\mu^2, 12\rho^2+3\right\}$.

b) Let $u \in H^1(\mathbb{R})$. Regarding the coercivity, we note first that for the given sesquilinear form by definition $B[u,u] \in \mathbb{R}$ holds. Assuming $\rho \geq 0$ yields for $\mu \leq -1$ that

$$\begin{aligned}
B[u,u] &= \langle u', u' \rangle + \rho \sum_{i\in\mathbb{Z}} |u(x_i)|^2 - \mu \langle u, u \rangle \\
&\geq \langle u', u' \rangle + \langle u, u \rangle \\
&= \|u\|^2_{H^1(\mathbb{R})}.
\end{aligned}$$

Analogously, for $\rho < 0$, using (3.4) we can choose $0 < h < \frac{1}{2|\rho|}$ and with that if $\mu < -\frac{2|\rho|}{h}$

$$\begin{aligned}
B[u,u] &= \langle u', u' \rangle + \rho \sum_{i\in\mathbb{Z}} |u(x_i)|^2 - \mu \langle u, u \rangle \\
&\geq \langle u', u' \rangle + 2\rho \sum_{i\in\mathbb{Z}} \left(\frac{1}{h} \int_{\Omega_i} |u(x)|^2 dx + h \int_{\Omega_i} |u'(\tau)|^2 \, d\tau \right) - \mu \langle u, u \rangle \\
&= (2\rho h + 1)\|u'\|^2_{L^2(\mathbb{R})} + (2\rho \frac{1}{h} - \mu)\|u\|^2_{L^2(\mathbb{R})} \\
&\geq \beta \|u\|^2_{H^1(\mathbb{R})},
\end{aligned}$$

where $\beta = \min\left\{2\rho h + 1, 2\rho\frac{1}{h} - \mu\right\}$. □

Theorem 3.2: *Given $f \in L^2(\mathbb{R})$ the functional l_f is a bounded linear functional on $H^1(\mathbb{R})$.*

Proof: That l_f is linear follows from the linearity of the integral. The Cauchy–Schwarz inequality (Theorem A.1.4) yields for the boundedness

$$|l_f(v)| \leq \|f\|_{L^2(\mathbb{R})}\|v\|_{L^2(\mathbb{R})} \leq \|f\|_{L^2(\mathbb{R})}\|v\|_{H^1(\mathbb{R})}$$ □

Therefore, as used in Theorem 3.1, we will subsequently assume that $\mu \in \mathbb{R}$ is small enough. In return, Lax-Migram's Theorem proves that for any fixed $f \in L^2(\mathbb{R})$ a unique solution $u \in H^1(\mathbb{R})$ to the problem (3.6) exists. This on the other hand allows us to proceed as follows.

Definition: *Let us define $R_\mu \colon L^2(\mathbb{R}) \to L^2(\mathbb{R}), f \mapsto u$ with u being the solution of* (3.6).

Again, due to the linearity of the integral and the uniqueness of the solution, R_μ is a linear operator. There are two more properties of R_μ for us left to show to explicitly define the operator A.

Theorem 3.3: *The mapping R_μ is bounded and injective.*

Proof: By Theorem 3.1 there exists for $f \in L^2(\mathbb{R})$ a function $u \in \mathcal{D}(A)$ as a solution of (3.6) and hence

$$\|R_\mu f\|^2_{L^2(\mathbb{R})} = \|u\|^2_{L^2(\mathbb{R})} \le \|u\|^2_{H^1(\mathbb{R})}. \tag{3.7}$$

Now, using (3.3), (3.5) and (3.7) with a small enough $\mu \in \mathbb{R}$ yields with the Cauchy–Schwarz inequality (Theorem A.1.4)

$$\|R_\mu f\|^2_{L^2(\mathbb{R})} \le \int_{\mathbb{R}} |u'(x)|^2 dx + \rho \sum_{i\in\mathbb{Z}} |u(x_i)|^2 - \mu \int_{\mathbb{R}} |u(x)|^2 dx \le \|f\|_{L^2(\mathbb{R})} \|u\|_{L^2(\mathbb{R})},$$

which shows the boundedness of the mapping R_μ. Bearing in mind that the range $\mathcal{R}(R_\mu) \subseteq H^1(\mathbb{R})$, we know that for $f_1, f_2 \in L^2(\mathbb{R})$ there exist $u_1, u_2 \in \mathcal{R}(R_\mu)$ with $u_i = R_\mu f_i$ for $i = 1, 2$. If now furthermore $R_\mu f_1 = R_\mu f_2$ holds, (3.6) yields

$$0 = B_\mu[u_1, v] - B_\mu[u_2, v] = \int_{\mathbb{R}} (f_1(x) - f_2(x))\overline{v(x)} dx \quad \forall v \in C_0^\infty(\mathbb{R}). \tag{3.8}$$

Since $C_0^\infty(\mathbb{R})$ is dense in $L^2(\mathbb{R})$ (Theorem A.1.2) we know from the equation (3.8) that

$$0 = \int_{\mathbb{R}} (f_1(x) - f_2(x))\, \overline{v(x)} dx \quad \forall v \in L^2(\mathbb{R}),$$

i.e. $f_1 = f_2$ almost everywhere. □

3.2 The domain

Resulting from Theorem 3.3, we know that R_μ is invertible. This allows us to define the aforementioned operator A explicitly.

Definition: *Let $A\colon \mathcal{D}(A) \subseteq L^2(\mathbb{R}) \to L^2(\mathbb{R})$ be the linear operator defined by*

$$A := R_\mu^{-1} + \mu I, \quad \mathcal{D}(A) = \mathcal{R}(R_\mu).$$

Note that this definition is consistent with the formal definition in (3.1) and we will show that it is independent of the choice of $\mu \in \mathbb{R}$, still assuming μ is small enough as chosen in Theorem 3.1.

Remark: *R_μ is thus the resolvent function of A.*

We will now use the fact that every element $u \in \mathcal{D}(A) = \mathcal{R}(R_\mu)$ is a solution of (3.6) to find additional necessary characteristics of $\mathcal{D}(A)$. However, we already know by Lax-Milram's Theorem that $u \in H^1(\mathbb{R})$. Let us first for the sake of brevity define

$$H^2\Big(\mathbb{R}\backslash\bigcup_{i\in\mathbb{Z}} x_i\Big) := \Big\{u \in L^2(\mathbb{R}) : u\big|_{(x_i,x_{i+1})} \in H^2(x_i, x_{i+1})\ \forall i \in \mathbb{Z}, \sum_{i\in\mathbb{Z}} \|u\|^2_{H^2(x_i,x_{i+1})} < \infty\Big\}.$$

Then, considering in (3.3) any fixed $k \in \mathbb{Z}$ and an arbitrary test function $v \in C_0^\infty(\mathbb{R})$ with $\operatorname{supp} v \subseteq [x_k, x_{k+1}]$ we get

$$\int_{x_k}^{x_{k+1}} u'(x)\overline{v'(x)}dx = \int_{x_k}^{x_{k+1}} (Au)(x)\overline{v(x)}dx$$

$$\Longleftrightarrow \int_{x_k}^{x_{k+1}} -u(x)\overline{v''(x)}dx = \int_{x_k}^{x_{k+1}} (Au)(x)\overline{v(x)}dx, \tag{3.9}$$

whence $u'' \in L^2(x_k, x_{k+1})$ and $Au = -u''$ on (x_k, x_{k+1}). Since we chose an arbitrary $k \in \mathbb{Z}$, we can note

$$\mathcal{D}(A) \subseteq \Big\{u \in H^1(\mathbb{R}) \colon u\big|_{(x_i,x_{i+1})} \in H^2(x_i, x_{i+1})\ \forall i \in \mathbb{Z}\Big\}.$$

Using this, a test function $v \in C_0^\infty(\mathbb{R})$ with the property $\operatorname{supp} v = \Omega_k$ yields in (3.3) for any $k \in \mathbb{Z}$ through integration by parts on both sides of x_k that

$$-\int_{x_k-\frac{1}{2}}^{x_k} u''(x)\overline{v(x)}dx - \int_{x_k}^{x_k+\frac{1}{2}} u''(x)\overline{v(x)}dx + \Big(u'(x_k-0)\overline{v(x_k)} - u'(x_k+0)\overline{v(x_k)}\Big)$$

$$+\rho u(x_k)\overline{v(x_k)} = -\int_{x_k-\frac{1}{2}}^{x_k} u''(x)\overline{v(x)}dx - \int_{x_k}^{x_k+\frac{1}{2}} u''(x)\overline{v(x)}dx.$$

Now, choosing in addition v to be non-zero in x_k yields

$$u'(x_k-0) - u'(x_k+0) + \rho u(x_k) = 0, \tag{3.10}$$

and therefore

$$\mathcal{D}(A) \subseteq \Big\{u \in H^1(\mathbb{R}) \colon u\big|_{(x_i,x_{i+1})} \in H^2(x_i, x_{i+1}), u'(x_j-0)-u'(x_j+0)+\rho u(x_j) = 0\ \forall i,j \in \mathbb{Z}\Big\} \tag{3.11}$$

Finally, choosing a function $v \in C_0^\infty(\mathbb{R})$ with $\operatorname{supp} v = (x_{-n}, x_n)$ in (3.3) for an arbitrary

$n \in \mathbb{N}$ yields with partial integration on every interval (x_i, x_{i+1}) by using (3.10):

$$\sum_{i=-n}^{n-1} -\int_{x_i}^{x_{i+1}} u''(x)\overline{v(x)}dx + \sum_{i=-n}^{n-1} u'\overline{v}\Big|_{x_i}^{x_{i+1}} + \rho \sum_{i=-n}^{n-1} u(x_i)\overline{v(x_j)} - \mu \int_{x_{-n}}^{x_n} u(x)\overline{v(x)}dx$$

$$= \int_{x_{-n}}^{x_n} f(x)\overline{v(x)}dx$$

$$\iff \sum_{i=-n}^{n-1} \int_{x_i}^{x_{i+1}} u''(x)\overline{v(x)}dx = -\int_{x_{-n}}^{x_n} f(x)\overline{v(x)}dx - \mu \int_{x_{-n}}^{x_n} u(x)\overline{v(x)}dx. \tag{3.12}$$

By defining $w_n \coloneqq \sum_{i=-n}^{n-1} u''\mathbb{1}_{[x_i,x_{i+1}]}$ we can estimate the left-hand side of (3.12) through

$$\begin{aligned} |\langle w_n, v\rangle| &\leq \left|\int_{x_{-n}}^{x_n} f(x)\overline{v(x)}dx\right| + \left|\mu \int_{x_{-n}}^{x_n} u(x)\overline{v(x)}dx\right| \\ &\leq \|f\|_{L^2(x_{-n},x_n)}\|v\|_{L^2(x_{-n},x_n)} + |\mu|\|u\|_{L^2(x_{-n},x_n)}\|v\|_{L^2(x_{-n},x_n)} \\ &\leq c\|v\|_{L^2(x_{-n},x_n)}, \end{aligned} \tag{3.13}$$

for some $c \in \mathbb{R}$, since $f \in L^2(\mathbb{R})$ and $u \in H^1(\mathbb{R})$. This constant is independent of n, from which, with (3.13), follows that $\sum_{i\in\mathbb{Z}} \|u''\|^2_{L^2(x_i,x_{i+1})} < \infty$. This yields the inclusion

$$\mathcal{D}(A) \subseteq \left\{u \in H^1(\mathbb{R}) : u \in H^2\Big(\mathbb{R} \setminus \bigcup_{i\in\mathbb{Z}} x_i\Big), u'(x_j - 0) - u'(x_j + 0) + \rho u(x_j) = 0 \ \forall j \in \mathbb{Z}\right\}. \tag{3.14}$$

Hence, for an arbitrary $u \in \mathcal{D}(A)$ we know from (3.9) and (3.14) that

$$Au = \begin{cases} -u'' & \text{on } (x_k - \frac{1}{2}, x_k) \\ -u'' & \text{on } (x_k, x_k + \frac{1}{2}), \end{cases} \quad \forall k \in \mathbb{Z}. \tag{3.15}$$

We are furthermore able to show in (3.14) the reverse inclusion by using the resolvent function R_μ. But first let us, again for brevity, denote with B the right-hand side of (3.14). Now, since $\mathcal{R}(R_\mu) = \mathcal{D}(A)$, we proceed by proving that each $u \in B$ is also in the range of R_μ. More specifically, as $\mathcal{D}(R_\mu) = L^2(\mathbb{R})$ let us define $f \coloneqq -u''$ on (x_k, x_{k+1}) for all $i \in \mathbb{Z}$; as we already know that $u \in H^2\Big(\mathbb{R} \setminus \bigcup_{i\in\mathbb{Z}} x_i\Big)$, we can therefore ensure $f \in L^2(\mathbb{R}) = \mathcal{D}(R_\mu)$. For the reverse inclusion we want to show that $u = R_\mu(f - \mu u)$ or equivalently

$$\begin{aligned}\int_{\mathbb{R}} u'(x)\overline{v'(x)}dx + \rho\sum_{i\in\mathbb{Z}} u(x_i)\overline{v(x_i)} - \mu\int_{\mathbb{R}} u(x)\overline{v(x)}dx &= \int_{\mathbb{R}} (f(x)-\mu u(x))\overline{v(x)}dx \\ \iff \sum_{i\in\mathbb{Z}}\int_{\Omega_i} u'(x)\overline{v'(x)} + \rho\sum_{i\in\mathbb{Z}} u(x_i)\overline{v(x_i)} &= -\sum_{i\in\mathbb{Z}}\int_{x_i}^{x_{i+1}} u''(x)\overline{v(x)}dx.\end{aligned}$$

For each $k \in \mathbb{Z}$ partial integration on both sides of x_k with a function $v \in C_0^\infty(\mathbb{R})$ having $\operatorname{supp} v = \Omega_k$ and $v(x_k) \neq 0$ yields

$$\begin{aligned}\int_{\Omega_k} u'(x)\overline{v'(x)}dx + \rho u(x_k)\overline{v(x_k)} &= \int_{x_k-\frac{1}{2}}^{x_k} u'(x)\overline{v'(x)}dx + \int_{x_k}^{x_k+\frac{1}{2}} u'(x)\overline{v'(x)}dx \\ &\quad - u'(x_k-0)\overline{v(x_k)} + u'(x_k+0)\overline{v(x_k)},\end{aligned}$$

which is equivalent to

$$u'(x_k-0)\overline{v(x_k)} - u'(x_k+0)\overline{v(x_k)} + \rho u(x_k)\overline{v(x_k)} = 0.$$

Consequently, we conclude that

$$\mathcal{D}(A) = \Big\{u \in H^1(\mathbb{R}) : u \in H^2\Big(\mathbb{R}\setminus\bigcup_{i\in\mathbb{Z}} x_i\Big), u'(x_j-0) - u'(x_j+0) + \rho u(x_j) = 0 \ \forall j \in \mathbb{Z}\Big\}. \tag{3.16}$$

Remark: *From* (3.15) *and* (3.16) *follows that the definition of A is independent of μ.*

3.3 The self-adjointness

In Chapter 6 we will need the fact that the operator A is self-adjoint. To prove this we first have to show that R_μ and R_μ^{-1} are symmetric operators.

Theorem 3.4: *R_μ and R_μ^{-1} are symmetric operators.*

Proof: We start with $R_\mu^{-1} = (A - \mu I)$. As for all $v \in \mathcal{D}(A)$ with (3.3) follows:

$$\begin{aligned}\langle R_\mu^{-1}u, v\rangle &= \langle (A-\mu I)u, v\rangle \\ &= \int_{\mathbb{R}} u'(x)\overline{v'(x)}dx - \mu\int_{\mathbb{R}} u(x)\overline{v(x)}dx + \rho\sum_{i\in\mathbb{Z}} u(x_i)\overline{v(x_i)} \\ &= \langle u, (A-\mu I)v\rangle = \langle u, R_\mu^{-1}v\rangle,\end{aligned}$$

thus, R_μ^{-1} is symmetric. Now, as $\mathcal{D}(R_\mu) = L^2(\mathbb{R})$ and $\mathcal{R}(R_\mu) = \mathcal{D}(R_\mu^{-1})$ for each $f, g \in L^2(\mathbb{R})$ it follows

$$\langle R_\mu f, g\rangle = \langle R_\mu f, R_\mu^{-1} R_\mu g\rangle = \langle f, R_\mu g\rangle,$$

thus, R_μ is also symmetric. □

Using the fact that R_μ and R_μ^{-1} are symmetric operators we can now prove the main statement of this section. Since every self-adjoint operator has an entirely real spectrum, this theorem yields furthermore our first result about the spectrum of A, for a proof see Theorem A.1.21.

Theorem 3.5: *A is a self-adjoint operator.*

Proof: We begin the proof of this theorem by proving that R_μ^{-1} is self-adjoint. As we already know that R_μ^{-1} is symmetric, showing that R_μ^{-1} is self-adjoint is equivalent to showing for $u \in \mathcal{D}(R_\mu^{-1})$ that if $v \in \mathcal{D}(R_\mu^{-1^*})$ and $v^* \in L^2(\mathbb{R})$ are such that

$$\langle R_\mu^{-1} u, v\rangle = \langle u, v^*\rangle \quad \forall u \in \mathcal{D}(R_\mu^{-1}), \tag{3.17}$$

then $v \in \mathcal{D}(R_\mu^{-1})$ and $R_\mu^{-1} v = v^*$. By Theorem 3.3, in (3.17) exists $f \in L^2(\mathbb{R})$ such that $u = R_\mu f$; using the fact that R_μ is symmetric and defined on the whole of $L^2(\mathbb{R})$ yields

$$\langle f, v\rangle = \langle R_\mu f, v^*\rangle = \langle f, R_\mu v^*\rangle,$$

which means that $v \in \mathcal{R}(R_\mu) = \mathcal{D}(R_\mu^{-1})$ and $R_\mu v^* = v$, i.e. R_μ^{-1} is self-adjoint. As the operator A is simply R_μ^{-1} shifted by $\mu \in \mathbb{R}$, A is hence self-adjoint as well. □

Chapter 4

The restricted operator on the fundamental domain of periodicity

In this chapter we will restrict the Kronig-Penney model to one periodicity cell and examine the spectrum of the resulting operator. With the help of tools we will introduce in Chapter 5, solving the eigenvalue problem on the period cell while varying specific boundary conditions for the solution functions can be used to determine the eigenvalues of the unrestricted problem, which is the approach we will adopt in Chapter 6.

Let Ω be a fundamental domain of periodicity associated with (3.1), for simplicity let $\Omega := \Omega_0$ and thus $x_0 = 0$ being contained in Ω. As commonly used in literature, the reciprocal lattice for Ω is $[-\pi, \pi)$, the so-called one-dimensional Brillouin zone B, see for example [DLP$^+$11, Chapter 3]. For brevity let us introduce the following:

Definition: *We define for every $k \in \overline{B}$ the set*

$$H^1_k := \left\{ \psi \in H^1(\Omega) : \ \psi\left(\frac{1}{2}\right) = e^{ik}\psi\left(-\frac{1}{2}\right) \right\}. \tag{4.1}$$

Hereafter, we will refer to the boundary conditions in (4.1) *as quasi-periodic boundary conditions.*

Henceforth, we consider the operator A_k on Ω formally defined by the operation

$$-\frac{d^2}{dx^2} + \rho\delta_{x_0},$$

subject to the space H_k^1 for fixed $k \in \overline{B}$.

Remark: H_k^1 *is a closed subspace of* $H^1(\Omega)$ *and hence a Hilbert space.*

Proof: See Theorem A.1.6. □

Analogously to Section 3.1, we now define A_k by considering the problem to find for $f \in L^2(\Omega)$ a function $u \in H_k^1$ such that the equation

$$\int_\Omega u'(x)\overline{v'(x)}dx + \rho u(x_0)\overline{v(x_0)} - \mu \int_\Omega u(x)\overline{v(x)}dx = \int_\Omega f(x)\overline{v(x)}dx \tag{4.2}$$

holds for all $v \in H_k^1$. Using the last remark, i.e. that H_k^1 is a Hilbert space, we can use similar arguments as in Section 3.1 to prove that

$$R_{\mu,k} \colon L^2(\Omega) \to H_k^1, f \mapsto u$$

is well-defined, bounded and injective. Consequently, we are able to define A_k by means of $R_{\mu,k}$:

$$A_k \coloneqq R_{\mu,k}^{-1} + \mu I, \quad \mathcal{D}(A_k) = \mathcal{R}(R_{\mu,k}^{-1}).$$

Remark: $R_{\mu,k}$ *is thus the resolvent function of* A_k*.*

4.1 The domain

We already know that $\mathcal{D}(A_k) \subseteq H_k^1$. Therefore, proceeding as in Section 3.2, by choosing the similar test functions $v \in H_k^1$ in (4.2), we are able to show that

$$\mathcal{D}(A_k) = \Big\{\psi \in H^1(\Omega) \colon \; \psi\left(\frac{1}{2}\right) = e^{ik}\psi\left(-\frac{1}{2}\right), \; \psi'\left(\frac{1}{2}\right) = e^{ik}\psi'\left(-\frac{1}{2}\right), \; u\big|_{(-\frac{1}{2},0)} \in H^2\left(\left(-\frac{1}{2},0\right)\right)$$
$$u\big|_{(0,\frac{1}{2})} \in H^2\left(\left(0,\frac{1}{2}\right)\right), \; u'(x_0-0) - u(x_0+0) + \rho u(x_0) = 0\Big\}.$$

The last three properties can be obtained by following the same approach as in Section 3.2. The quasi-periodic condition on ψ results from the boundary condition on H_k^1. To establish the quasi-periodic condition on ψ' we proceed as follows. Choosing in (4.2) a function $v \in \mathcal{D}(A_k)$ with $\operatorname{supp} v = \Omega$, $v\,(x_0) = 0$ and $v\left(\frac{1}{2}\right) \neq 0$ and partial integration yields

$$-\int_\Omega u''(x)\overline{v(x)}dx + u'(x)\overline{v(x)}\big|_{-\frac{1}{2}}^{\frac{1}{2}} + -\mu \int_\Omega u(x)\overline{v(x)}dx = \int_\Omega f(x)\overline{v(x)}dx$$

$$\Longleftrightarrow \; u'\left(\frac{1}{2}\right)e^{-ik} = u'\left(-\frac{1}{2}\right),$$

whereas in the last step we used the fact that $A_k u = f$ and that $v \in H_k^1$. In the remainder of this chapter we will further investigate the operator A_k. We will show that the eigenfunctions of A_k form a complete and orthonormal system in $L^2(\mathbb{R})$. For this purpose, we first need to prove that $R_{\mu,k}$ is compact.

4.2 The compactness of the resolvent function

Theorem 4.1: *The operator $R_{\mu,k}$ is compact.*

Proof: Let $(f_j)_{j\in\mathbb{N}} \in L^2(\Omega)$ be a bounded sequence. We will show that

$$u_j := R_{\mu,k} f_j \quad \text{for all } j \geq 1$$

is a bounded sequence with respect to the H^1-Norm. Each such u_j is by definition in H_k^1 and has to satisfy

$$\int_\Omega u_j'(x)\overline{v'(x)}dx + \rho u_j(x_0)\overline{v(x_0)} - \mu \int_\Omega u_j(x)\overline{v(x)}dx = \int_\Omega f_j(x)\overline{v(x)}dx \quad \forall v \in H_k^1. \tag{4.3}$$

Now, the particular choice of $v = u_j$ in (4.3) yields with (3.5) for small enough μ

$$\|u_j\|^2_{H^1(\Omega)} \leq \|f_j\|_{L^2(\Omega)} \|u_j\|_{L^2(\Omega)} \leq c\sqrt{|\Omega|}).$$

Thus, $\|u_j\|_{H^1(\Omega)} \leq C$ for all j and the assertion follows from the Compact Embedding Theorem for Sobolev spaces, see Theorem A.1.7. □

4.3 The spectrum

Using the compactness of $R_{\mu,k}$, we know on the one hand that every non-zero $\lambda \in \sigma(R_{\mu,k})$ is an eigenvalue of $R_{\mu,k}$ and on the other hand that the at most countable sequence of eigenvalues can only accumulate at 0, for proofs see [Wer06, p. 271]. We will now consider the eigenvalue problem to find $\psi \in \mathcal{D}(A_k) \subseteq H_k^1$ such that

$$A_k \psi = \lambda \psi \text{ on } \Omega. \tag{4.4}$$

The eigenvalue λ depends on the boundary condition we set on the domain, more specifically, it is a function of k. In writing the boundary condition in the form (4.1), we understand ψ extended to the whole of $\mathbb{R}$ and call them Bloch waves. By considering any eigenfunction w of $R_{\mu,k}$ with the corresponding eigenvalue $\lambda(k)$ we can see that

$$A_k w = R_{\mu,k}^{-1} w + \mu w = \left(\frac{1}{\lambda(k)} + \mu \right) w,$$

i.e. A_k has the same sequence of eigenfunctions as $R_{\mu,k}$, and then respectively

$$\tilde{\lambda}(k) \coloneqq \frac{1}{\lambda(k)} - \mu \tag{4.5}$$

is an eigenvalue for the eigenfunction w of the operator A_k. Using the compactness of $R_{\mu,k}$ and (4.5), we see that A_k has a purely discrete spectrum satisfying

$$\lambda_1(k) \leq \lambda_2(k) \leq \ldots \leq \lambda_s(k) \to \infty \text{ as } s \to \infty. \tag{4.6}$$

and the corresponding eigenfunctions form a $\langle \cdot, \cdot \rangle$-orthonormal and complete system $(\psi_s(\cdot, k))_{s \in \mathbb{N}}$ of eigenfunctions for (4.1), for proof see Theorem A.1.9.

Finally, in the last part of this chapter, we transform the eigenvalue problem (4.4) such that the boundary condition is independent of k. This step is needed in Chapter 6 to show that the eigenvalues in (4.4) depend continuously on k. For this, we first define

$$\varphi_s(x, k) \coloneqq e^{-ikx} \psi_s(x, k).$$

This yields

$$
\begin{aligned}
A_k\psi_s(x,k) &= \frac{d^2}{dx^2}\psi_s(x,k)\big|_{(x_0-\frac{1}{2},x_0)}\cdot \mathbb{1}_{(x_0-\frac{1}{2},x_0)} + \frac{d^2}{dx^2}\psi_s(x,k)\big|_{(x_0,x_0+\frac{1}{2})}\cdot \mathbb{1}_{(x_0,x_0+\frac{1}{2})} \\
&= e^{ikx}\left(\frac{d}{dx}+ik\right)^2 \varphi_s(x,k)\big|_{(x_0-\frac{1}{2},x_0)}\cdot \mathbb{1}_{(x_0-\frac{1}{2},x_0)} \\
&\quad + e^{ikx}\left(\frac{d}{dx}+ik\right)^2 \varphi_s(x,k)\big|_{(x_0,x_0+\frac{1}{2})}\cdot \mathbb{1}_{(x_0,x_0+\frac{1}{2})}.
\end{aligned} \tag{4.7}
$$

Therefore, we define an operator $\tilde{A}_k \colon \mathcal{D}(A_k) \to L^2(\mathbb{R})$ through

$$
\tilde{A}_k\varphi_s(x,k) \coloneqq \begin{cases} \left(\frac{d}{dx}+ik\right)^2 \varphi_s(x,k)|_{(x_0-\frac{1}{2},x_0)} & \text{for } x \in (x_0-\frac{1}{2},x_0) \\ \left(\frac{d}{dx}+ik\right)^2 \varphi_s(x,k)|_{(x_0,x_0+\frac{1}{2})} & \text{for } x \in (x_0,x_0+\frac{1}{2}). \end{cases}
$$

Note that we defined the operator $\tilde{A}_k$ to determine eigenvalues and eigenfunctions of A_k, hence we require $\mathcal{D}(\tilde{A}_k) = \mathcal{D}(A_k)$. Using (4.4) and (4.1), yields

$$
\varphi_s\left(x-\frac{1}{2},k\right) = e^{-ik(x-\frac{1}{2})}\psi_s\left(x-\frac{1}{2},k\right) = e^{-ik(x+\frac{1}{2})}\psi_s\left(x+\frac{1}{2},k\right) = \varphi_s\left(x+\frac{1}{2},k\right).
$$

From this, (4.6) and from Theorem 4.1 follows that $(\varphi_s(\cdot,k))_{s\in\mathbb{N}}$ is an orthonormal and complete system of eigenfunctions in $L^2(\mathbb{R})$ to the periodic eigenvalue problem

$$
\tilde{A}_k\varphi = \lambda_s(k)\varphi \text{ on } \Omega, \tag{4.8}
$$

$$
\varphi\left(x-\frac{1}{2}\right) = \varphi\left(x+\frac{1}{2}\right), \tag{4.9}
$$

with the identical eigenvalue sequence $(\lambda_s(k))_{s\in\mathbb{N}}$ as in (4.4) by (4.7).

Chapter 5

The Floquet transformation and the Bloch waves

In Chapter 6 we will show that the spectrum of the operator A can be constructed from the eigenvalue sequences $(\lambda_s(k))_{s\in\mathbb{N}}$ introduced in (4.8) by varying k over the Brillouin zone B. For this purpose we will need two results involving the Floquet transformation and the Bloch waves, to be able to relate the problem from $L^2(\mathbb{R})$ to $L^2(\Omega \times B)$. For the sake of completeness, we include here the proofs of both theorems, as given in [DLP$^+$11, Section 3.4, 3.5]. However, as we intend to use these results in both the one-dimensional and the multi-dimensional case, we will not simplify expressions such as $|B|$ and $|\Omega|$, in order to keep them applicable in both settings.

5.1 Properties of the Floquet transformation

Theorem 5.1: *The Floquet transformation* $U\colon L^2(\mathbb{R}) \to L^2(\Omega \times B)$

$$(Uf)(x,k) := \frac{1}{\sqrt{|B|}} \sum_{n\in\mathbb{Z}} f(x-n)e^{ikn} \quad (x \in \Omega, k \in B) \tag{5.1}$$

is an isometric isomorphism, with inverse given by

$$(U^{-1}g)(x-n) = \frac{1}{\sqrt{|B|}} \int_B g(x,k)e^{-ikn}dk \quad (x \in \Omega, n \in \mathbb{Z}). \tag{5.2}$$

If $g(\cdot, k)$ is extended to the whole of $\mathbb{R}$ by the quasi-periodicity condition (4.1)*, the inverse formula simplifies to*

$$U^{-1}g = \frac{1}{\sqrt{|B|}} \int_B g(\cdot, k)dk. \tag{5.3}$$

Proof: For $f \in L^2(\mathbb{R})$ we have

$$\|f\|^2_{L^2(\mathbb{R})} = \int_{\mathbb{R}} |f(x)|^2 dx = \sum_{n\in\mathbb{Z}} \int_\Omega |f(x-n)|^2 dx. \tag{5.4}$$

Applying the Monotone Convergence Theorem (Theorem A.1.14) shows that

$$\sum_{n\in\mathbb{Z}} |f(x-n)|^2 < \infty \text{ for almost every } x \in \Omega.$$

Thus, $(Uf)(x, k)$ is well-defined by (5.1) (as a Fourier series with variable k) for almost every $x \in \Omega$. Using Parseval's identity (Theorem A.1.16), the fact that

$$\vartheta_n(k) := \frac{1}{\sqrt{|B|}} e^{ikn}$$

forms an orthonormal basis of $L^2(B)$, for proof see Theorem A.1.12, yields

$$\int_B |(Uf)(x,k)|^2 dk = \sum_{n\in\mathbb{Z}} |f(x-n)|^2.$$

This expression is in $L^2(\Omega)$ by (5.4) and Fubini's Theorem (Theorem A.1.12), and we conclude $\|Uf\|_{L^2(\Omega\times B)} = \|f\|_{L^2(\mathbb{R})}$. It remains to show that the mapping U is surjective, and that U^{-1} is given by (5.2) or (5.3). For $g \in L^2(\Omega \times B)$, let us define

$$f(x-n) := \frac{1}{\sqrt{|B|}} \int_B g(x,k) e^{-ikn} dk \quad (x \in \Omega, n \in \mathbb{Z}). \tag{5.5}$$

Using Fubini's Theorem (Theorem A.1.12) we know that for almost every $x \in \Omega$ we have $g(x, k) \in L^2(B)$, and with this, Parseval's identity (Theorem A.1.16) states for fixed $x \in \Omega$ that $\sum_{n\in\mathbb{Z}} |f(x-n)|^2 = \int_B |g(x,k)|^2 dk$. Integrating this equality over Ω, using Fubini's Theorem (Theorem A.1.12) and the Monotone Convergence Theorem (Theorem A.1.14) then yields

$$\int_{\Omega\times B} |g(x,k)|^2 dx dk = \int_\Omega \sum_{n\in\mathbb{Z}} |f(x-n)|^2 dx = \sum_{n\in\mathbb{Z}} \int_\Omega |f(x-n)|^2 dx = \int_{\mathbb{R}} |f(x)|^2 dx,$$

i.e. $f \in L^2(\mathbb{R})$. Therefore, for almost every $x \in \Omega$ follows from (5.1) that

$$f(x-n) = \frac{1}{\sqrt{|B|}} \int_B (Uf)(x,k) e^{-ikn} dk$$

for $n \in \mathbb{Z}$, whence (5.5) implies $Uf = g$ and (5.2), the desired result. The equality

$$g(x+n,k) = e^{ikn} g(x,k)$$

and (5.2) yield (5.3). $\square$

5.2 The completeness of the Bloch waves

Using the Floquet transformation U, we can now prove the property of completeness of the Bloch waves $\psi_s(\cdot,k)$ in $L^2(\Omega)$ when we vary k over the Brillouin zone B.

Theorem 5.2: *For each $f \in L^2(\mathbb{R})$ and $l \in \mathbb{N}$, we define*

$$f_l(x) := \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \langle (Uf)(\cdot,k), \psi_s(\cdot,k) \rangle_{L^2(\Omega)} \psi_s(x,k) dk \quad (x \in \mathbb{R}). \tag{5.6}$$

Then, $f_l \to f$ in $L^2(\mathbb{R})$ as $l \to \infty$.

Proof: Theorem 5.1 tells us that $(Uf) \in L^2(\Omega \times B)$, which in return means that

$$(Uf)(\cdot,k) \in L^2(\Omega)$$

for almost all $k \in B$ by Fubini's Theorem (Theorem A.1.12). Since $(\psi_s(\cdot,k))_{s\in\mathbb{N}}$ is an orthonormal and complete system of eigenfunctions in $L^2(\Omega)$ for each $k \in B$, we derive with the help of the Dominated Convergence Theorem (Theorem A.1.8)

$$\lim_{l\to\infty} \|(Uf)(\cdot,k) - g_l(\cdot,k)\|_{L^2(\Omega)} = 0 \text{ for almost every } k \in B$$

where

$$g_l(x,k) := \sum_{s=1}^{l} \langle (Uf)(\cdot,k), \psi_s(\cdot,k) \rangle_{L^2(\Omega)} \psi_s(x,k). \tag{5.7}$$

Moreover, we get by Bessel's inequality (Theorem A.1.3) $\|(Uf)(\cdot,k) - g_l(\cdot,k)\|^2_{L^2(\Omega)} \leq \|(Uf)(\cdot,k)\|^2_{L^2(\Omega)}$ for all $l \in \mathbb{N}$ and almost every $k \in B$. Next, $\|(Uf)(\cdot,k)\|^2_{L^2(\Omega)} \in L^1(B)$

as a function of k by Theorem 5.1, thus by the Dominated Convergence Theorem (Theorem A.1.8)

$$\lim_{l\to\infty}\int_B \|(Uf)(\cdot,k)-g_l(\cdot,k)\|^2_{L^2(\Omega)}dk = \int_B \lim_{l\to\infty}\|(Uf)(\cdot,k)-g_l(\cdot,k)\|^2_{L^2(\Omega)}dk = 0.$$

All in all, this means by Fubini's Theorem (Theorem A.1.12)

$$\|Uf-g_l\|_{L^2(\Omega\times B)} = \int_B\int_\Omega |(Uf)(x,k)-g_l(d,k)|^2\,dxdk \to 0 \text{ as } l\to\infty \tag{5.8}$$

Using (5.6), (5.7) and (5.3), we find that $f_l = U^{-1}g_l$. Whence (5.8) and since $U\colon L^2(\mathbb{R})\to L^2(\Omega\times B)$ is isometric by Theorem 5.1 it follows that

$$\|Uf-g_l\|_{L^2(\Omega\times B)} = \|U(f-f_l)\|_{L^2(\Omega\times B)} = \|f-f_l\|_{L^2(\Omega\times B)} \to 0 \text{ as } l\to\infty,$$

which is the desired result. $\square$

Chapter 6

The spectrum of the one-dimensional Schrödinger operator

Finally, we are ready to prove the main result for the one-dimensional case stating that for the operator A it holds that

$$\sigma(A) = \bigcup_{s \in \mathbb{N}} I_s, \tag{6.1}$$

where $I_s \coloneqq \{\lambda_s(k) : k \in \overline{B}\}$ for all $s \in \mathbb{N}$. We will prove that each I_s is a compact interval, which means that the spectrum shows a "band-gap" structure.

To prove this equality we first need to show that $\lambda_s(k)$ is continuous in k, and hence, I_s is for each k a compact interval in $\mathbb{R}$.

Theorem 6.1: *For all $s \in \mathbb{N}$, the function $k \mapsto \lambda_s(k)$ is continuous in $k \in \overline{B}$.*

Proof: In the transformed eigenvalue problem (4.8) the boundary conditions (4.9) are periodic and independent of k. By Poincare's min-max principle (Theorem A.1.18) for eigenvalues we have

$$\lambda_s(k) = \min_{\substack{U \subseteq \mathcal{D}(\tilde{A}_k) \\ \dim U = s}} \max_{v \in U \setminus \{0\}} \frac{\langle \tilde{A}_k v, v \rangle_{L^2(\Omega)}}{\langle v, v \rangle_{L^2(\Omega)}}. \tag{6.2}$$

Now, let $k \in \overline{B}$ be fixed. For all $\tilde{k} \in \overline{B}$ and all $v \in \mathcal{D}(\tilde{A}_k)$ using triangular inequality yields for $J \in \left\{(x_0 - \frac{1}{2}, x_0), (x_0, x_0 + \frac{1}{2})\right\}$:

$$\frac{\langle \left(\frac{d}{dx} + i\tilde{k}\right) v, \left(\frac{d}{dx} + i\tilde{k}\right) v\rangle_{L^2(J)}}{\langle v, v\rangle_{L^2(J)}} \begin{Bmatrix} \leq \\ \geq \end{Bmatrix} \frac{\langle \left(\frac{d}{dx} + ik\right) v, \left(\frac{d}{dx} + ik\right) v\rangle_{L^2(J)}}{\langle v, v\rangle_{L^2(J)}} \\ \begin{Bmatrix} + \\ - \end{Bmatrix} \frac{2|k - \tilde{k}| \|v'\|_{L^2(J)} \|v\|_{L^2(J)}}{\|v\|^2_{L^2(J)}} \begin{Bmatrix} + \\ - \end{Bmatrix} \left| |k|^2 - |\tilde{k}|^2 \right|. \tag{6.3}$$

Moreover, we find

$$\begin{aligned} 2\|v'\|_{L^2(J)} \|v\|_{L^2(J)} &\leq 2\| \left(\frac{d}{dx} + ik\right) v\|_{L^2(J)} \|v\|_{L^2(J)} + 2|k| \|v\|^2_{L^2(J)} \\ &\leq \| \left(\frac{d}{dx} + ik\right) v\|^2_{L^2(J)} + \|v\|^2_{L^2(J)} + 2|k| \|v\|^2_{L^2(J)} \\ &\leq \langle \left(\frac{d}{dx} + ik\right) v, \left(\frac{d}{dx} + ik\right) v\rangle_{L^2(J)} + (1 + 2|k|) \|v\|^2_{L^2(J)}. \end{aligned}$$

Hence, (6.3) yields

$$\frac{\langle \left(\frac{d}{dx} + i\tilde{k}\right) v, \left(\frac{d}{dx} + i\tilde{k}\right) v\rangle_{L^2(J)}}{\langle v, v\rangle_{L^2(J)}} \begin{Bmatrix} \leq \\ \geq \end{Bmatrix} (1 \begin{Bmatrix} + \\ - \end{Bmatrix} |k - \tilde{k}|) \frac{\langle \left(\frac{d}{dx} + ik\right) v, \left(\frac{d}{dx} + ik\right) v\rangle_{L^2(J)}}{\langle v, v\rangle_{L^2(J)}} \\ \begin{Bmatrix} + \\ - \end{Bmatrix} \left(|k - \tilde{k}|(1 + 2|k|) + \left| |k|^2 - |\tilde{k}|^2 \right| \right).$$

Thus the min-max-principle gives for $|k - \tilde{k}| < 1$

$$\lambda_s(\tilde{k}) \leq \left(1 + |k - \tilde{k}|\right) \lambda_s(k) + \left(|k - \tilde{k}|(1 + 2|k|) + \left| |k|^2 - |\tilde{k}|^2 \right| \right)$$

and

$$\lambda_s(\tilde{k}) \geq \left(1 - |k - \tilde{k}|\right) \lambda_s(k) - \left(|k - \tilde{k}|(1 + 2|k|) + \left| |k|^2 - |\tilde{k}|^2 \right| \right),$$

which, eventually, yields

$$|\lambda_s(\tilde{k}) - \lambda_s(k)| \leq |k - \tilde{k}| \left(\lambda_s(k) + 1 + 2|k| + |k| + |\tilde{k}| \right), \tag{6.4}$$

for $|k - \tilde{k}| < 1$. Now, the eigenvalue $\lambda_s(k)$ is by construction also an eigenvalue of the problem (4.4), where the operator is dependent on k rather than the boundary conditions.

However, all eigenvalues of (4.4) are by Poincare's min-max-principle (Theorem A.1.18) dominated by eigenvalues of the eigenvalue problem of A_k with Dirichlet boundary conditions, since the domain with Dirichlet conditions is a superset of the domain with the quasi-periodic boundary conditions. Since the eigenvalues for the Dirichlet boundary condition are independent of k, $\lambda_s(k)$ is uniformly bounded, and hence by (6.4), $\lambda_s(k)$ is continuous in k. $\square$

Remark: *As $\overline{B}$ is a compact and connected set and $\lambda_s(k)$ is a continuous function of $k \in \overline{B}$ we derive for* (6.1)

$$I_s \textit{ is a compact real interval for each } s \in \mathbb{N}. \tag{6.5}$$

From (6.2) and (6.5) also follows that $\mu_s \leq \lambda_s(k)$ for all $s \in \mathbb{N}$, $k \in \overline{B}$ with $(\mu_s)_{s\in\mathbb{N}}$ denoting the sequence of eigenvalues of problem (4.4) with Neumann boundary conditions, since the domain with Neumann conditions is a subset of the domain with the quasi-periodic boundary conditions. By analogous calculations as in Section 4.3, but now with Neumann boundary conditions on $\mathcal{D}(A_k)$, we see that $\mu_s \to \infty$ as $s \to \infty$, hence, we obtain $\min I_s \to \infty$ as $s \to \infty$, which together with (6.5) implies that

$$\bigcup_{s\in\mathbb{N}} I_s \text{ is closed.} \tag{6.6}$$

Using this property we are now able to prove the first inclusion of the main statement (6.1).

Theorem 6.2: $\sigma(A) \supseteq \bigcup_{s\in\mathbb{N}} I_s$.

Proof: Let $\lambda \in \bigcup_{s\in\mathbb{N}} I_s$, i.e. $\lambda = \lambda_s(k)$ for some $s \in \mathbb{N}$ and some $k \in \overline{B}$, and

$$A_k\psi_s(\cdot, k) = \lambda\psi_s(\cdot, k) \tag{6.7}$$

As introduced in Chapter 4, we regard $\psi_s(\cdot, k)$ extended to the whole of $\mathbb{R}$, whence, due to the periodic structure of A, ψ_s satisfies

$$A\psi_s = \lambda\psi_s$$

"locally", i.e. $\psi_s \in \left\{\psi \in H^1_{loc}(\mathbb{R}) : \psi \in H^2_{loc}\left(\mathbb{R}\setminus\bigcup_{i\in\mathbb{Z}} x_i\right), \psi'(x_j-0)-\psi'(x_j+0)+\rho\psi(x_j) = 0\ \forall j \in \mathbb{Z}\right\}$, and $-\psi_s'' = \lambda\psi_s$ on $\mathbb{R} \setminus \bigcup_{i\in\mathbb{Z}} x_i$. Now, if we choose a function $\eta \in H^2(\mathbb{R})$ such that

$$\eta(x) = 1 \text{ for } |x| \leq \frac{1}{2}, \quad \eta(x) = 0 \text{ for } |x| \geq 1, \tag{6.8}$$

we are able to define, for each $l \in \mathbb{N}$,

$$\kappa_l(x) := \eta\left(\frac{|x|}{l}\right)\psi_s(x,k)$$

for all $x \in \mathbb{R}$; for an illustration see Figures 6.1, 6.2 and 6.3 where a schematic of the real part is depicted; the analogous complex part is not depicted here. As $\psi_s \in \mathcal{D}(A)$ we know $\kappa_l \in \mathcal{D}(A)$, hence, we see that

$$\begin{aligned}(A-\lambda I)\kappa_l &= \sum_{i\in\mathbb{N}}\left[(-\frac{d^2}{dx^2}-\lambda)\kappa_l|_{(x_i,x_{i+1})}\cdot \mathbb{1}_{(x_i,x_{i+1})}\right] \qquad (6.9)\\ &= \sum_{i\in\mathbb{N}}\left[\eta\left(\frac{|\cdot|}{l}\right)\left(-\frac{d^2}{dx^2}-\lambda\right)\psi_s(\cdot,k)|_{(x_i,x_{i+1})}\cdot \mathbb{1}_{(x_i,x_{i+1})}\right] + R\end{aligned}$$

where R is a sum of products of derivatives of order ≥ 1 of $\eta\left(\frac{|\cdot|}{l}\right)$ and of order ≤ 1 of $\psi_s(\cdot,k)$. Let use denote with B_l the ball around 0 with radius l and let, for simplicity, $c \in \mathbb{R}$ be a generic constant. Thus, since $\psi_s(\cdot,k) \in H^1_{loc}(\mathbb{R})$, the quasi-periodic structure of $\psi_s(\cdot,k)$ implies

$$\|R\|_{L^2(\mathbb{R})} \leq \frac{c}{l}\|\psi_s(\cdot,k)\|_{H^1(B_l)} \leq c\frac{1}{\sqrt{l}}. \tag{6.10}$$

Now, the quasi-periodic structure allows us additionally to find an upper boundary for κ_l:

$$\|\kappa_l\|_{L^2(\mathbb{R})} \geq c\|\psi_s(\cdot,k)\|_{L^2(K_l)} \geq c\sqrt{l}. \tag{6.11}$$

Together with (6.6), (6.7) and (6.9), (6.11) yields

$$\frac{1}{\|\kappa_l\|_{L^2(\mathbb{R})}}\|(A-\lambda I)\kappa_l\|_{L^2(\mathbb{R})} \leq \frac{c}{l},$$

which eventually results in the property

$$\frac{1}{\|\kappa_l\|_{L^2(\mathbb{R})}}\|(A-\lambda I)\kappa_l\|_{L^2(\mathbb{R})} \to 0 \text{ as } l \to \infty.$$

Thus, either λ is an eigenvalue of A, or $(A-\lambda I)^{-1}$ exists but is unbounded. In both cases, $\lambda \in \sigma(A)$. $\square$

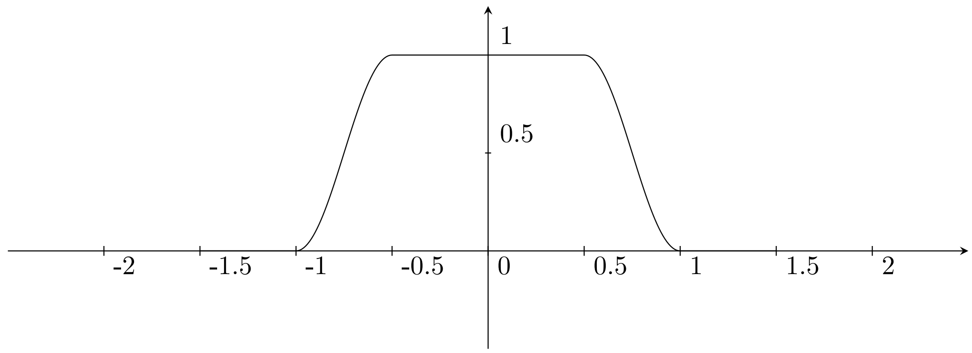

Figure 6.1: Example for the function η

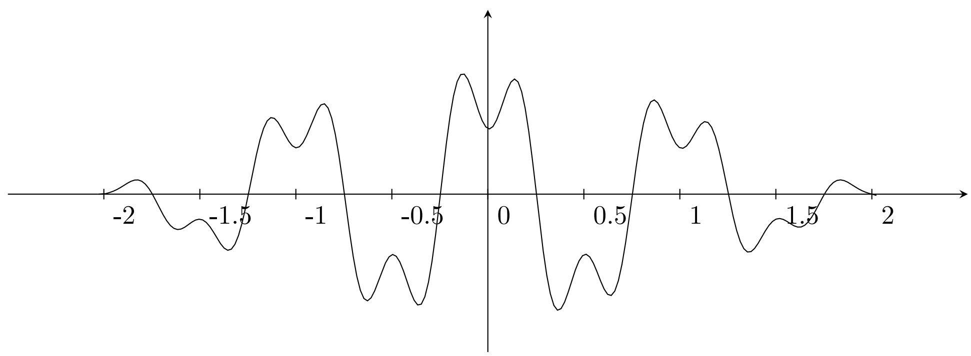

Figure 6.2: A schematic of the real part of a Bloch wave in one dimension

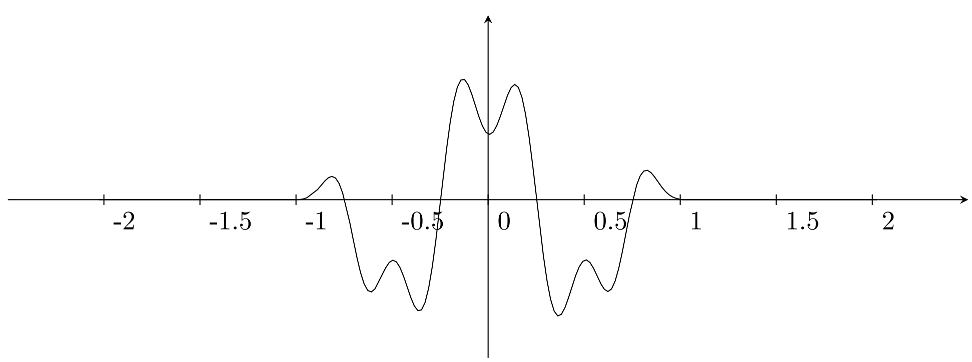

Figure 6.3: Resulting real part of the function u_l

The other inclusion can be established by using the properties of the Floquet transformation shown above and the completeness of the Bloch waves. Hence, this proof follows that for a general m-th order linear differential operator with periodic coefficients. Again, for the sake of completeness, we include the proof here, as given in [DLP$^+$11, Section 3.6].

Theorem 6.3: $\sigma(A) \subseteq \bigcup_{s\in\mathbb{N}} I_s$.

Proof: Let $\lambda \in \mathbb{R} \setminus \bigcup_{s\in\mathbb{N}} I_s$. Hence, due to (6.6), there exists some $\delta > 0$ such that

$$|\lambda_s(k) - \lambda| \geq \delta \quad \text{ for all } s \in \mathbb{N}, k \in B \tag{6.12}$$

We are going to prove that $\lambda \in \rho(A)$, i.e. for each $f \in L^2(\mathbb{R})$ there exists some $u \in \mathcal{D}(A)$ satisfying $(A - \lambda I)u = f$. For an arbitrary $f \in L^2(\mathbb{R})$ and $l \in \mathbb{N}$, we define at first

$$f_l(x) \coloneqq \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \langle (Uf)(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)} \psi_s(x,k) dk$$

and

$$u_l \coloneqq \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \frac{1}{\lambda_s(k) - \lambda} \langle (Uf)(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)} \psi_s(x,k) dk \tag{6.13}$$

Since λ is chosen to be outside of the spectrum, the operator $(A_k - \lambda I)$ is invertible, and therefore the following equation has for every $f \in L^2(\mathbb{R})$ and $k \in \overline{B}$ a unique solution $v \in \mathcal{D}(A_k)$

$$(A_k - \lambda I)v(\cdot,k) = (Uf)(\cdot,k) \quad \text{ on } \Omega. \tag{6.14}$$

Due to (6.14), both $v(\cdot,k)$ and $\psi_s(\cdot,k)$ satisfy quasi-periodic boundary conditions. Hence, (4.4), (6.12) and Parseval's identity (Theorem A.1.16) yield

$$\begin{aligned}
\|(Uf)(\cdot,k)\|^2_{L^2(\Omega)} &= \sum_{s=1}^{\infty} |\langle (Uf)(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)}|^2 \\
&= \sum_{s=1}^{\infty} |\langle (A_k - \lambda)v(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)}|^2 \\
&= \sum_{s=1}^{\infty} |\lambda_s(k) - \lambda|^2 |\langle v(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)}|^2 \\
&\geq \delta^2 \|v(\cdot,k)\|^2_{L^2(\Omega)}.
\end{aligned}$$

By Theorem 5.1 we know that $f \in L^2(\Omega \times B)$. This implies $v \in L^2(\Omega \times B)$, and we can define $u := U^{-1}v \in L^2(\mathbb{R})$. Thus, (6.14) gives

$$\begin{aligned}\langle (Uf)(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)} &= \langle (A_k - \lambda I)(Uu)(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)} \\ &= \langle (Uu)(\cdot,k), (A_k - \lambda I)\psi_s(\cdot,k)\rangle_{L^2(\Omega)} \\ &= (\lambda_s(k) - \lambda)\langle Uu(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)}.\end{aligned}$$

Now, we are able to apply Theorem 5.2 which yields for (6.13) that

$$u_l(x) = \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \langle (Uu)(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)} \psi_s(x,k) dk,$$

and whence Theorem 5.2 gives

$$u_l \to u, \quad f_l \to f \quad \text{in } L^2(\mathbb{R}) \text{ as } l \to \infty. \tag{6.15}$$

We will now prove that, in a distributional sense,

$$(A - \lambda I)u_l = f_l,$$

for all $l \in \mathbb{N}$, which implies that

$$\langle u_l, (A - \lambda I)v\rangle = \langle f_l, v\rangle \text{ for all } l \in \mathbb{N}, v \in \mathcal{D}(A); \tag{6.16}$$

As A is self-adjoint, by Theorem 3.5, this implies $u_l \in \mathcal{D}(A)$, and $(A - \lambda I)u_l = f_l$ for all $l \in \mathbb{N}$. As furthermore every self-adjoint operator is also closed (Theorem (A.1.19)), (6.15) now implies

$$u \in \mathcal{D}(A) \text{ and } (A - \lambda I)u = f,$$

which is the desired result.

Eventually, we are left to prove (6.16). So, let $\varphi \in C_0^\infty(\mathbb{R})$ be fixed, and let $K \subseteq \mathbb{R}$ denote an open ball containing $\text{supp}(\varphi)$ in its interior. By Fubini's Theorem we know that

$$r_s(x,k) := \frac{1}{\lambda_s(k) - \lambda} \langle (Uf)(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)} \psi_s(x,k) \overline{(A - \lambda I)\varphi(x)},$$

and

$$t_s(x,k) \coloneqq \langle (Uf)(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)} \psi_s(x,k)\overline{\varphi(x)}$$

are in $L^2(K \times B)$, since (6.12), $(A_k - \lambda I)\varphi \in L^\infty(K)$ and $\varphi \in L^\infty(K)$ imply

$$\|r_s\|_{L^2(K\times B)} \leq c\|(Uf)(\cdot,k)\|^2_{L^2(\Omega)}\|\psi_s(\cdot,k)\|^2_{L^2(K)}$$

and analogously for t_s. As K is bounded there exists a finite number of copies of Ω such that they cover K, hence $\psi_s(\cdot,k)$ is in $L^2(K)$ as a function of k, and $(Uf)(\cdot,k)$ is in $L^1(B)$ by Theorem 5.1. Since B is equally bounded, r and t are also in $L^1(K \times B)$. Therefore, Fubini's Theorem implies that the order of integration with respect to x and l may be exchanged for r and t. Thus, by (6.13), the fact that φ has compact support in the interior of K and (4.4) we conclude

$$\begin{aligned}
\int_K u_l(x)\overline{(A-\lambda I)\varphi(x)}dx &= \frac{1}{\sqrt{|B|}}\sum_{s=1}^{l}\int_K\left(\int_B r_s(x,k)dk\right)dx \\
&= \frac{1}{\sqrt{|B|}}\sum_{s=1}^{l}\int_B \langle (Uf)(\cdot,k),\psi_s(\cdot,k)\rangle_{L^2(\Omega)}\langle \psi_s(\cdot,k),\varphi\rangle_{L^2(K)}dk \\
&= \int_K\left[\frac{1}{\sqrt{|B|}}\sum_{s=1}^{l}\int_B \langle (Uf)(\cdot,k),\psi_s(\cdot,k)\rangle_{L^2(\Omega)}\psi_s(x,k)dk\right]\overline{\varphi(x)}dx \\
&= \int_K f_l(x)\overline{\varphi(x)}dx,
\end{aligned}$$

i.e. (6.16). □

Chapter 7

The spectrum of the multi-dimensional Schrödinger operator

In this chapter, we want to model the movement of a particle in $\mathbb{R}^n$ with periodically distributed, smooth, $(n-1)$-dimensional surfaces supporting a potential. To show that the basic concepts presented in the previous chapters hold also in the new setting, we will give a formal justification of applicability of the one-dimensional proofs to the multi-dimensional case in a series of theorems.

To start with, let Ω denote a periodicity cell in $\mathbb{R}^n$ relating to the problem introduced above and B^n the corresponding Brillouin zone, for simplicity assume Ω being the unit cube $[0,1]^n$. Contained in Ω let S be a smooth surface without a boundary subject to the conditions $\dim S = n-1$ and $S \subseteq \mathring{\Omega}$. Furthermore, let $D \subseteq Y$ denote the set enclosed by S, such that $S = \partial D$. We will denote with $\Omega_j = Y + j$ the jth copy of Ω for any $j \in \mathbb{Z}^n$, which results through translation of the periodicity cell by j, and analogously for $S_j = S + j$ and $D_j = D + j$. Finally, we denote with Ω_i^+ and Ω_i^- the opposing edges of Ω for $i = 1, \ldots, n$, as illustrated in Figure 7.1.

The mathematical representation of the above is a multi-dimensional Schrödinger operator

A^n whose operation is formally defined by

$$-\Delta + \rho \sum_{i\in\mathbb{Z}} \delta_{S_i} \tag{7.1}$$

on the whole of $\mathbb{R}^n$, where δ_{S_i} denotes the Delta-Distribution on hypersurface S_i. Let us recall that on a hypersurface S the Delta-Distribution acts on $\varphi \in C_0^\infty(\mathbb{R}^n)$ by

$$\delta_S(\varphi) := \int_S \varphi(s) ds.$$

where s is the hypersurface measure associated to S_j; for a more detailed explanation see [For12, Chapter 14]. Since every function in $H^1(\mathbb{R}^n)$ can be approximated by a sequence in $C_0^\infty(\mathbb{R}^n)$ (Theorem A.1.2), we find for every $u \in H^1(\mathbb{R}^n)$ a sequence $(u_n)_{n\in\mathbb{N}} \in C_0^\infty(\mathbb{R}^n)$ such that $\lim_{n\to\infty} u_n = u$, and hence we define

$$\delta_S(u) := \lim_{n\to\infty} \delta_S(u_n).$$

Remark: *This definition is independent of the chosen sequence in $C_0^\infty(\mathbb{R}^n)$.*

Proof: For $u \in H^1(\mathbb{R}^n)$ let $(u_n)_{n\in\mathbb{N}}, (v_n)_{n\in\mathbb{N}} \in C_0^\infty(\mathbb{R}^n)$ such that

$$\lim_{n\to\infty} \|u_n - u\|_{H^1(\mathbb{R}^n)} = 0 \quad \text{and} \quad \lim_{n\to\infty} \|v_n - u\|_{H^1(\mathbb{R}^n)} = 0.$$

As $(u_n - v_n) \in C_0^\infty(\mathbb{R}^n)$, we then get with the help of Cauchy Schwarz inequality (Theorem A.1.4) and the Trace Theorem (Theorem A.1.22)

$$\lim_{n\to\infty} \int_S |u_n(s) - v_n(s)|\, ds \leq c|D| \lim_{n\to\infty} \|u_n - v_n\|_{H^1(\Omega)} = 0.$$

□

Again motivated by the weak formulation, given a right-hand side $f \in L^2(\mathbb{R}^n)$ we consider for some $\mu \in \mathbb{R}$ the problem to find $u \in H^1(\mathbb{R}^n)$ such that

$$\int_{\mathbb{R}^n} \nabla u(x)\overline{\nabla v(x)} dx + \rho \sum_{i\in\mathbb{Z}^n} \int_{S_j} u(s)\overline{v(s)} ds - \mu \int_{\mathbb{R}^n} u(x)\overline{v(x)} dx = \int_{\mathbb{R}^n} f(x)\overline{v(x)} dx \tag{7.2}$$

holds for all $v \in H^1(\mathbb{R}^n)$. Note that in the second term we denote by u, v the traces. As $u, v \in H^1(\mathbb{R})$, the traces are in $L^2(\mathbb{R}^n)$ by [Eva98, p. 251, Theorem 5.1] and [AF03, p.

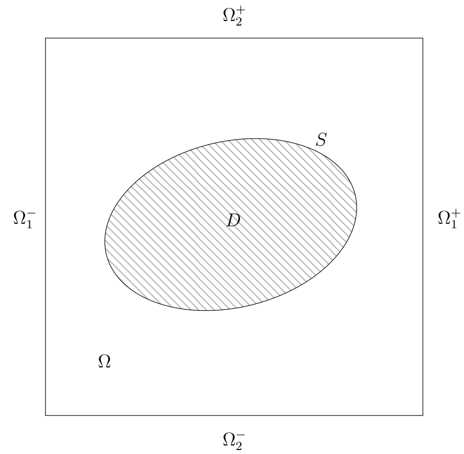

Figure 7.1: Periodicity cell for the multi-dimensional potential

164], and thus, in view of the following remark, the second term on the left-hand side of (7.2) is well-defined.

Remark: *The term in* (7.2) *originating from the potential is finite.*

Proof: First, the Cauchy–Schwarz inequality yields

$$\left| \sum_{j \in \mathbb{Z}^n} \int_{S_j} u(s)\overline{v(s)} ds \right|^2 \leq \left(\sum_{j \in \mathbb{Z}^n} \|u\|^2_{L^2(S_j)} \right) \left(\sum_{j \in \mathbb{Z}^n} \|v\|^2_{L^2(S_j)} \right).$$

For both terms on the right-hand side we need an upper bound, similar to the estimation we found in Chapter 3. Through the Trace Theorem (Theorem A.1.22) and Poincaré inequality (Theorem A.1.17) we can find a constant $c \in \mathbb{R}$ such that

$$\|u\|^2_{L^2(S_j)} \leq c \left(\frac{1}{h} \|u\|^2_{L^2(\Omega)} + h \|\nabla u\|^2_{L^2(\Omega)} \right).$$

□

Given $f \in L^2(\mathbb{R}^n)$, following the proofs in Section 3.1 we can show that for a $\mu \in \mathbb{R}$ small enough the sesquilinear form $B_\mu \colon H^1(\mathbb{R}^n) \times H^1(\mathbb{R}^n) \to \mathbb{C}$, defined by

$$B_\mu[u, v] := \int_{\mathbb{R}^n} \nabla u(x) \overline{\nabla v(x)} dx + \rho \sum_{i \in \mathbb{Z}^n} \int_{S_j} u(s)\overline{v(s)} ds - \mu \int_{\mathbb{R}^n} u(x)\overline{v(x)} dx,$$

is bounded and coercive. Furthermore, the functional $l_f\colon H^1(\mathbb{R}) \to \mathbb{C}$ defined by

$$l_f(v) := \int_{\mathbb{R}^n} f(x)\overline{v}(x)dx$$

is a bounded, linear functional. Hence, Lax-Migram's Theorem (Theorem A.1.13) ensures the existence of a unique solution $u \in H^1(\mathbb{R}^n)$ in (7.2) for any $f \in L^2(\mathbb{R}^n)$. In return, the operator $R^n_\mu\colon L^2(\mathbb{R}^n) \to H^1(\mathbb{R}^n), f \mapsto u$, where $u \in H^1(\mathbb{R}^n)$ is the solution of (7.2), is well-defined.

Theorem 7.1: *R^n_μ is an injective, bounded linear operator.*

Proof: The proof follows that of Theorem 3.3. □

This, on the other hand, enables us to explicitly define A^n by means of R^n_μ:

$$A^n := \left(R^n_\mu\right)^{-1} + \mu I, \quad \mathcal{D}(A^n) = \mathcal{R}(R^n_\mu),$$

such that R^n_μ is the resolvent function of A^n. Therefore, we can characterise $\mathcal{D}(A^n)$ by employing the same methods as used in Section 3.2.

Theorem 7.2 (Characterisation of $\mathcal{D}(A^n)$)**:** *Let $Y := \mathbb{R}^n \setminus \overline{\bigcup_{j\in\mathbb{Z}^n} D_j}$. We can further characterise the solution $u \in \mathcal{D}(A^n)$ from (7.2), on the fundamental domain of periodicity as depicted in Figure 7.2, namely for all $j \in \mathbb{Z}^n$ it holds:*

a) $\Delta u \in L^2(D_j)$, $\Delta u \in L^2(Y)$ *and* $\sum_{j\in\mathbb{Z}^n} \|\Delta u\|^2_{L^2(D_j)} < \infty$

b) $u\big|_{S_j-0} = u\big|_{S_j+0}$

c) $\frac{\partial u}{\partial \eta_j}\big|_{S_j-0} - \frac{\partial u}{\partial \eta_j}\big|_{S_j+0} + \rho u\big|_{S_j} = 0$ *where η_j denotes the normal on S_j*

Proof: Comparing these properties to those in $\mathcal{D}(A)$ in Section 3.2 we can see that by analogously choosing particular functions $v \in C^\infty_0(\mathbb{R}^n)$ in (7.2) the three asserted properties follow. The first is the equivalent to (3.15), the second is a consequence of $u \in H^1(\mathbb{R}^n)$ and the third follows from partial integration in (7.2) with a $v \in C^\infty_0(\mathbb{R}^n)$ such that $\operatorname{supp} v = \Omega$. □

We are interested in the periodic spectral problem of the operator A^n. Therefore, we will again relate the spectrum of the operator A^n on the whole of $\mathbb{R}^n$ via the Floquet transformation to a family of eigenvalue problems on the periodicity cell. However, first we need to show the self-adjointness of the operator A^n.

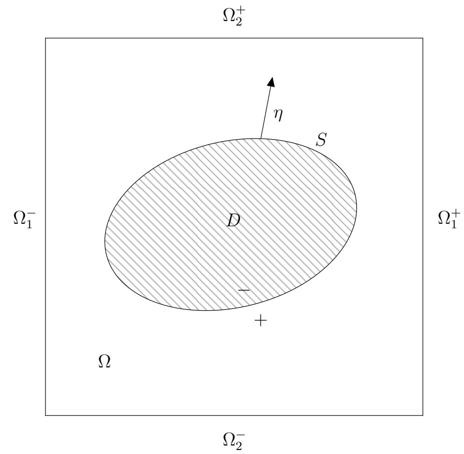

Figure 7.2: Normal η on the hypersurface S in a periodicity cell

Remark: *The operator A^n is self-adjoint.*

Proof: The operators R_μ^n and $\left(R_\mu^n\right)^{-1}$ are symmetric. The fact that for any $u \in \mathcal{D}\left(\left(R_\mu^n\right)^{-1}\right)$ there exists $f \in L^2(\mathbb{R}^n)$ such that $u = R_\mu^n f$ and that R_μ^n is defined on the whole of $L^2(\mathbb{R}^n)$ then yields the self-adjointness of A^n similarly to the proof given in Section 3.3. $\square$

The periodicity cell we will now focus on can be chosen arbitrarily, let this for simplicity be Y. For brevity, let us define for $k \in \overline{B^n}$

$$H^1_{k,n} := \left\{ w \in H^1(Y) \colon w\big|_{\Omega_j^+} = w\big|_{\Omega_j^-} e^{ik_j} \text{ for } k \in \overline{B^n}, j = 1, \dots, n \right\},$$

and consider the problem to find $u \in H^1_{k,n}$ such that

$$\int_Y \nabla u(x) \overline{\nabla v(x)} dx + \rho \int_S u(s) \overline{v(s)} ds - \mu \int_Y u(x) \overline{v(x)} dx = \int_Y f(x) \overline{v(x)} dx \tag{7.3}$$

holds for all $v \in H^1_{k,n}$.

Again, Lax-Milgram's Theorem (Theorem A.1.13) ensures the existence of a unique solution $u \in H^1_{k,n}$ if $\mu \in \mathbb{R}$ is small enough, and the operator $R_{\mu,k} \colon f \mapsto u$ is in return well-defined, and we can show that $R_{\mu,k}$ is injective. This allows us to define

$$A_k^n := \left(R^n_{\mu,k}\right)^{-1} + \mu I, \quad \mathcal{D}(A_k^n) = \mathcal{R}(R^n_{\mu,k}),$$

as the operator for the multi-dimensional case of our problem on the fundamental domain of periodicity.

Theorem 7.3 (Characterisation of $\mathcal{D}(A_k^n)$)**:** *Let* $Y := \mathbb{R}^n \setminus \overline{\bigcup_{j\in\mathbb{Z}^n} D_j}$. *We can characterise the solution* $u \in \mathcal{D}(A_k^n) \subseteq H^1_{k,n}$ *from* (7.2)*, such that for all* $j \in \mathbb{Z}^n$ *it holds:*

a) $\Delta u \in L^2(D_j)$, $\Delta u \in L^2(Y)$ *and* $\sum_{j\in\mathbb{Z}^n} \|\Delta u\|^2_{L^2(B_j)} < \infty$

b) $u\big|_{S_j-0} = u\big|_{S_j+0}$

c) $\frac{\partial u}{\partial \eta_j}\big|_{S_j-0} - \frac{\partial u}{\partial \eta_j}\big|_{S_j+0} + \rho u\big|_{S_j} = 0$ *where* η_j *denotes the normal on* S_j

d) $u\big|_{\Omega_j^+} = u\big|_{\Omega_j^-} e^{ik_j}$, $\frac{\partial u}{\partial x_j}\big|_{\Omega_j^+} = e^{ik_j}\frac{\partial u}{\partial x_j}\big|_{\Omega_j^-}$ *for* $j = 1, \ldots, n$

Proof: The first three properties can be proven as in Theorem 7.2. The quasi-periodic condition on the function $u \in \mathcal{D}(A_k^n)$ follows from the boundary condition in $H^1_{k,n}$. The quasi-periodic boundary conditions on $H^1_{k,n}$ require a solution $u \in H^1_{k,n}$ to satisfy additionally quasi-periodic conditions for their weak derivative

$$\frac{\partial u}{\partial x_1}\big|_{\Omega_1^+} = e^{ik_1}\frac{\partial u}{\partial x_1}\big|_{\Omega_1^-}.$$

We can see this by partial integration in (7.3) with a function $v \in C_0^\infty(\mathbb{R}^n)$ such that $U_j^+, U_j^- \not\subset \operatorname{supp} v$ where $U_j^+ \supset \Omega_j^+$ and $U_j^- \supset \Omega_j^-$ are neighbourhoods of the opposing edges for $j = 2, \ldots, n$, and analogously for the other coordinates. $\square$

Theorem 7.4: *The operator* $R^n_{\mu,k}$ *is compact.*

Proof: As in Chapter 4, we can show that $R^n_{\mu,k}$ is a bounded operator. The claim follows from the Compact Embedding Theorem for Sobolev spaces, for proof see Theorem A.1.7. $\square$

For our ultimate goal, we then consider the eigenvalue problem to find $\psi \in \mathcal{D}(A_k^n)$ such that

$$A_k^n \psi_s = \lambda_s^n(k)\psi_s \text{ on } \Omega. \tag{7.4}$$

As before, in writing the boundary condition in the form in $H^1_{k,n}$, we regard $\psi_s(\cdot, k)$ extended to the whole of $\mathbb{R}^n$ and call the eigenfunctions Bloch waves. Using the compactness of $R^n_{\mu,k}$, we know furthermore that every non-zero $\lambda \in \sigma(A_k^n)$ is an eigenvalue of A_k^n and that the purely discrete spectrum satisfies

$$\lambda_1^n(k) \le \lambda_2^n(k) \le \ldots \le \lambda_s^n(k) \to \infty \text{ as } s \to \infty. \tag{7.5}$$

Taking into account Theorem A.1.9 we know that the eigenfunctions corresponding to (7.4) form a $\langle\cdot,\cdot\rangle$-orthonormal and complete system $(\psi_s(\cdot,k))_{s\in\mathbb{N}}$ of eigenfunctions in $L^2(\mathbb{R}^n)$. By transformations of the problem (7.4) such that the boundary condition is independent of k, similar to those in (4.8) and (4.9), we are then able to show that the eigenvalues of A_k^n are continuous functions of $k \in \overline{B^n}$, and thus $I_s^n = \{\lambda_s^n(k) : k \in \overline{B^n}\}$ is again a compact real interval for each $s \in \mathbb{N}$.

Finally, our main result for the multi-dimensional case follows from using the same arguments as in Chapter 6.3 based on a similar cut-off function η as in (6.8), Bloch waves and the Floquet transformation, now for the multi-dimensional situation, to relate the spectrum of the operator on the whole of $\mathbb{R}^n$ to a family of eigenvalue problems on the periodicity cell while varying the boundary condition. We claim that the spectrum of a self-adjoint Schrödinger operator with periodic delta-potential on a hypersurface is the union of the compact intervals I_s^n, i.e.

$$\sigma(A^n) = \bigcup_{s\in\mathbb{N}} I_s^n.$$

Chapter 8

Summary and conclusions

This thesis examined the spectrum of an operator describing the situation in the Kronig-Penney model when a particle moves through periodically distributed, singular potentials. The main result obtained from solving the problem with the help of the Floquet-Bloch theory is that such an operator has a real, band-gap structured spectrum.

First, we examined the periodic, one-dimensional Schrödinger operator where the delta potentials are periodically aligned along one axis and showed that the operator is self-adjoint. With the help of the Floquet transformation, we related the spectrum of this periodic operator on the whole of $\mathbb{R}$ to a family of eigenvalue problems on the corresponding periodicity cell. On the periodicity cell, we chose the eigenfunctions, the so-called Bloch waves, to be subject to semi-periodic boundary conditions depending on a parameter which varied over the Brillouin zone. We then proved the band-gap structure of the spectrum of the operator under consideration in $\mathbb{R}$. Finally, we gave a formal justification of applicability of the approach in $\mathbb{R}$ also to the case when the particle moves in $\mathbb{R}^n$ with periodically distributed, smooth, $(n-1)$-dimensional surfaces supporting a potential, such that the result in $\mathbb{R}$ also holds in $\mathbb{R}^n$.

However, it is still not straightforward to conclude that there really are any *gaps* in the band-gap structure since the Floquet–Bloch theory allows for gaps of any width, i.e. it also admits bands of zero width. A systematic analysis of such a quantum mechanical problem has been provided in [AGHKH12]. Furthermore, in a more concrete context of polarised waves in two dimensions, the existence of band gaps has been computer-assisted analysed in [HPW09].

Two recent papers offer further insight into the analysis of elliptic operators, a generalisation of the Laplace operators. In [Kuc16] an overview of periodic elliptic operators is provided and the main techniques and results of the theory are surveyed. The suggested approach is applicable not only to the standard model example of Schrödinger operator with periodic potential but also to a wide variety of periodic elliptic equations and systems. In [KP16] methods of homogenisation theory are used to study asymptotic behaviour of the spectrum of the elliptic operator $A_\epsilon = -\frac{1}{b^\epsilon}\operatorname{div}(e^\epsilon \nabla)$ for $\epsilon \to 0$ in a bounded domain subject to Dirichlet conditions on the boundary. For ϵ tending to 0 both coefficients a and b become high contrast in a small neighbourhood of a hyperplane intersecting the domain. The same problem is examined under the assumption that the domain consists of an infinite straight strip (waveguide) and a hyperplane intersecting the domain is parallel to its boundary. It is shown that the spectrum in this case, given that the coefficients become high contrast in a small neighbourhood of a hyperplane, has at least one gap.

Appendix

Theorem A.1.1 (Alternative definition of the Delta-Distribution)**:** *For the sequence of functionals δ_ϵ for $\epsilon > 0$, $x_0 \in \mathbb{R}$ and $f \in \mathfrak{D}(\mathbb{R})$ defined through $\delta_\epsilon(f) \coloneqq \frac{1}{\sqrt{2\pi}\epsilon}\int_{\mathbb{R}} f(x)e^{-\frac{(x-x_0)^2}{2\epsilon^2}}dx$ it holds that*

$$\delta_{x_0}(f) = \lim_{\epsilon\to 0} \delta_\epsilon(f).$$

Proof: By definition we have

$$\delta_\epsilon(f) = \frac{1}{\sqrt{2\pi}\epsilon}\int_{-\infty}^{\infty} f(x)e^{-\frac{(x-x_0)^2}{2\epsilon^2}}dx.$$

Substituting $z \coloneqq \frac{x-x_0}{\sqrt{2}\epsilon}$ yields

$$\frac{1}{\sqrt{2\pi}\epsilon}\int_{-\infty}^{\infty} f(x)e^{-\frac{(x-x_0)^2}{2\epsilon^2}}dx = \frac{1}{\sqrt{2\pi}\epsilon}\int_{-\infty}^{\infty} f(\sqrt{2}\epsilon z + x_0)e^{-z^2}dz.$$

Now, using the Taylor series of f around x_0 and a formula for the Gaussian integral we then get

$$\lim_{\epsilon\to 0}\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-z^2}\left(f(x_0) + \mathcal{O}(\epsilon)\right)dz = f(x_0)\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-z^2}dz = f(x_0).$$

□

Theorem A.1.2 (L^p-Approximation by test functions)**:** *For $U \subseteq \mathbb{R}^n$ open, $C_0^\infty(U)$ is dense in $L^p(U)$, if $1 \le p < \infty$.*

Proof: See [AF03, p. 31]. □

Theorem A.1.3 (Bessel's inequality)**:** *Let H be a Hilbert space, and suppose that $e_1, e_2, ...$*

is an orthonormal sequence in H. Then, for any $x \in H$ one has

$$\sum_{k=1}^{\infty} |\langle x, e_k \rangle_H|^2 \leq \|x\|^2$$

where $\langle \cdot, \cdot \rangle_H$ denotes the inner product in the Hilbert space H.

Proof: See [Wer06, p. 233]. □

Theorem A.1.4 (Cauchy–Schwarz inequality)**:** *For all vectors u and v of an inner product space it is true that*

$$|\langle u, v \rangle|^2 \leq \langle u, u \rangle \cdot \langle v, v \rangle,$$

where $\langle \cdot, \cdot \rangle$ is the inner product.

Proof: See [Wer06, p. 20]. □

Theorem A.1.5 (Closed graph theorem)**:** *Let X be a Banach space. Is A a closed operator and $\mathcal{D}(A) = X$, then A is continuous on X.*

Proof: See [Eva98, p. 638]. □

Theorem A.1.6 (Closeness of H^1_k in $H^1(\Omega)$)**:** *H^1_k is a closed subset1 of $H^1(\Omega)$, and therefore a Hilbert space with respect to the norm of $H^1(\Omega)$.*

Proof: Let $(f_n)_{n\in\mathbb{N}}$ be a sequence in H^1_k converging to $f \in H^1(\Omega)$. We already know that convergence with respect to the H^1-Norm implies convergence of the function and its derivative almost everywhere. Let us therefore define $g \coloneqq f - f_n$ then

$$\begin{aligned}
\left| g\left(-\frac{1}{2}\right) \right|^2 &\leq 2|g(x)|^2 + 2\left(\int_{-\frac{1}{2}}^{x} |g'(\tau)| d\tau\right)^2 \\
&\leq 2|g(x)|^2 + 2\int_{-\frac{1}{2}}^{\frac{1}{2}} |g'(\tau)|^2 d\tau \\
&\leq 2\int_{-\frac{1}{2}}^{\frac{1}{2}} |g(\tau)|^2 d\tau + 2\int_{-\frac{1}{2}}^{\frac{1}{2}} |g'(\tau)|^2 d\tau \\
&= 2\|g\|^2_{H^1(-\frac{1}{2},\frac{1}{2})} \longrightarrow 0
\end{aligned}$$

for $j \to \infty$, and analogously on the other boundary. □

Theorem A.1.7 (Compact Embedding Theorem for Sobolev spaces)**:**

a) *Let $U \subseteq \mathbb{R}^n$ be a bounded open set of class C^1. Then the following compact embeddings hold:*

- $H^1(U) \subseteq L^q(U)$ *for every* $q \in [1, p^*)$*, where* $n \geq 3$ *and* $p^* = \frac{2n}{n-2}$.
- $H^1(U) \subseteq L^q(U)$ *for every* $q \in [1, \infty)$*, if* $n = 2$.

Proof: Follows from Rellich-Kondrachov Compact Embedding Theorem, see [Pre13, p. 163] and [Eva98, p. 272]. $\square$

b) *Let $U \subseteq \mathbb{R}$ be a bounded, connected and open set. Then the embedding $H^1(U) \subseteq L^2(U)$ is compact.*

Proof: By Theorem A.1.10 $H^1(U) \subseteq C^{\frac{1}{2}}(U)$, hence we can estimate

$$|f(x) - f(y)| \leq c|x - y|^{\frac{1}{2}} \tag{$*$}$$

for some $c > 0$ and for all $x, y \in U$. Let $B_{H^1_k} := \{f \in H^1_k(U) : \|f\|_{H^1(U)} \leq 1\}$, then for $f \in B_{H^1_k}$ it holds that

$$|f(x)|^2 \leq 2\|f\|^2_{L^2(U)} + 2 \leq 4 \quad \forall x \in U. \tag{$**$}$$

For an arbitrary $\epsilon > 0$ we now partition U into n_ϵ equidistant, disjoint intervals I_k, i.e. $U = \bigcup_{k=1}^{n_\epsilon} I_k$. Since all $f \in B_{H^1_k}$ are uniformly bounded on U by $(**)$, there exist for each subinterval I_k a finite number of constants $c_{1,k}, \ldots, c_{\nu_\epsilon,k}$ such that

$$\forall f \in B_{H^1_k}\ \exists j \in \{1, \ldots, \nu_\epsilon\} : \left| f\left(\frac{k}{n_\epsilon}\right) - c_{j,k} \right| < \frac{1}{n_\epsilon}\ \forall k \in \{1, \ldots, n_\epsilon\}.$$

Therefore, there are finitely many step functions such that for any $f \in L^2(U)$ there exists one of those step functions $g \in L^2(U)$, with function value c_k on subinterval I_k for each $k \in \{1, \ldots, n_\epsilon\}$, such that by $(*)$

$$\begin{aligned}
\|f - g\|^2_{L^2(U)} &= \sum_{k=0}^{n_\epsilon - 1} \int_{\frac{k}{n_\epsilon}}^{\frac{k+1}{n_\epsilon}} |f(x) - c_{k+1}|^2 dx \\
&\leq 2 \sum_{k=0}^{n_\epsilon - 1} \int_{\frac{k}{n_\epsilon}}^{\frac{k+1}{n_\epsilon}} \left| f(x) - f\left(\frac{k}{n_\epsilon}\right) \right|^2 dx + 2 \sum_{k=0}^{n_\epsilon - 1} \int_{\frac{k}{n_\epsilon}}^{\frac{k+1}{n_\epsilon}} \left| f\left(\frac{k}{n_\epsilon}\right) - c_{k+1} \right|^2 dx \\
&\leq 2 \sum_{k=0}^{n_\epsilon - 1} \frac{c}{n_\epsilon^2} + 2 \sum_{k=0}^{n_\epsilon - 1} \frac{1}{n_\epsilon^3} = \frac{2}{n_\epsilon}\left(c + \frac{1}{n_\epsilon}\right) < \epsilon
\end{aligned}$$

for n_ϵ large enough. This means, in conclusion, that $B_{H^1_k}$ is totally bounded in $L^2(U)$ and in return, since H^1_k is closed, it can be compactly embedded in $L^2(U)$. $\square$

Theorem A.1.8 (Dominated Convergence Theorem)**:** *Let f_n be a sequence of real-valued measurable functions on a measure space (S, Σ, μ). Suppose that the sequence converges pointwise to a function f and is dominated by some integrable function g in the sense that*

$$|f_n(x)| \leq g(x)$$

for all numbers n in the index set of the sequence and all points $x \in S$. Then f is integrable and

$$\lim_{n\to\infty} \int_S |f_n - f| \, d\mu = 0$$

which also implies $\lim_{n\to\infty} \int_S f_n \, d\mu = \int_S f \, d\mu$.

Proof: See [Wer06, p. 516]. $\square$

Theorem A.1.9 (Eigenvectors of a compact, symmetric operator)**:** *Let H be a separable Hilbert space, and suppose $S\colon H \to H$ is a compact and symmetric operator. Then there exists a countable orthonormal basis of H consisting of eigenvectors of S.*

Proof: See [Eva98, p. 645]. $\square$

Theorem A.1.10 (Embedding of H^1 in $C^{\frac{1}{2}}$)**:** *Let $[a, b]$ be a compact interval in $\mathbb{R}$. Then, $H^1([a, b])$ is embedded in $C^{\frac{1}{2}}([a, b])$*

Proof: See [Eva98, p. 269]. $\square$

Theorem A.1.11 (Equivalent definitions of closed operators)**:** *Let X, Y be two Banach spaces. A linear operator $A\colon X \supset \mathcal{D}(A) \to Y$ is closed if for every sequence $(x_n)_{n\in\mathbb{N}}$ in $\mathcal{D}(A)$ from*

$$x_n \to x \in X \text{ and } Tx_n \to y \in Y$$

follows that $x \in D$ and $Tx = y$.

Proof: See [Wer06, p. 156]. $\square$

Theorem A.1.12 (Fubini's Theorem for integrable functions)**:** *Suppose X and Y are σ-finite measure spaces, and suppose that $X \times Y$ is given the product measure (which* *is unique as X and Y are σ-finite). Fubini's Theorem states that if $f(x,y)$ is $X \times Y$ integrable, meaning that it is measurable and*

$$\int_{X\times Y} |f(x,y)|\, d(x,y) < \infty,$$

then

$$\int_X \left(\int_Y f(x,y)\, dy \right) dx = \int_Y \left(\int_X f(x,y)\, dx \right) dy = \int_{X\times Y} f(x,y)\, d(x,y).$$

The first two integrals are iterated integrals with respect to two measures, respectively, and the third is an integral with respect to the product measure

Proof: See [Wer06, p. 514]. □

Theorem A.1.13 (Lax-Milgram)**:** *Let H be a Hilbert space where $\|\cdot\|$ denotes the norm on H, and let $B\colon H \times H \to \mathbb{C}$ be a sesquilinear form. If there exist constants $\alpha, \beta > 0$ such that*

a) $|B[u,v]| \leq \alpha\|u\|\|v\| \quad (u, v \in H)$ *and*

b) $Re(B[u,u]) \geq \beta\|u\|^2 \quad (u \in H)$,

then there exists to each $l \in H^*$ a unique $w \in H$ such that

$$B[v,w] = l(v)$$

hold for all $v \in H$.

Proof: See [Plu15, Amd to problem 51]. □

Theorem A.1.14 (Monotone Convergence Theorem)**:** *Let (X, Σ, μ) be a measure space. Let $f_1, f_2, \ldots$ be a pointwise non-decreasing sequence of $[0,\infty]$-valued Σ–measurable functions, i.e. for every $k \geq 1$ and every x in X,*

$$0 \leq f_k(x) \leq f_{k+1}(x).$$

Next, set the pointwise limit of the sequence (f_n) to be f. That is, for every x in X,

$$f(x) := \lim_{k\to\infty} f_k(x).$$

Then f is Σ–measurable and

$$\lim_{k\to\infty}\int f_k \,\mathrm{d}\mu = \int f \,\mathrm{d}\mu.$$

Proof: See [Wer06, p. 516]. □

Theorem A.1.15 (Orthonormality of ϑ)**:** *The sequence*

$$\vartheta_n(k) := \frac{1}{\sqrt{|B|}} e^{ikn}$$

forms an orthonormal basis of $L^2(B)$.

Proof: For $m, n \in \mathbb{N}$ we see that

$$\langle \vartheta_n, \vartheta_m \rangle_{L^2(B)} = \frac{1}{|B|}\int_B e^{ikn}\overline{e^{ikm}} dk = \frac{1}{|B|}\int_B e^{ik(n-m)} dk = \begin{cases} 0 & \text{for } n \neq m \\ 1 & \text{for } n = m, \end{cases}$$

hence the asserted follows. □

Theorem A.1.16 (Parseval's identity)**:** *Suppose that H is a Hilbert space with inner product $\langle\cdot,\cdot\rangle$. Let (e_n) be an orthonormal basis of H; i.e., the linear span of the e_n is dense in H, and the e_n are mutually orthonormal:*

$$\langle e_m, e_n \rangle = \begin{cases} 1 & \text{if } m = n \\ 0 & \text{if } m \neq n. \end{cases}$$

Then Parseval's identity asserts that for every $x \in H$,

$$\sum_n |\langle x, e_n \rangle|^2 = \|x\|^2.$$

Proof: See [Wer06, p. 236]. □

Theorem A.1.17 (Poincare's inequality)**:** *If a domain $\Omega \subset \mathbb{R}^n$ has finite width, then there exists a constant $c = c(p)$ such that for all $\varphi \in C_0^\infty(\Omega)$*

$$\|\varphi\|_{L^p(\Omega)} \leq c\|\nabla\varphi\|_{L^p(\Omega)}$$

With Theorem A.1.2 this can be extended to every function $u \in L^p(\Omega)$.

Proof: See [AF03, p. 183]. □

Theorem A.1.18 (Poincare's min-max principle for eigenvalues)**:** *Let X be a seperable Hilbert space and $\langle \cdot, \cdot \rangle_X$ denote the scalar product on X. Let $A\colon \mathcal{D}(A) \to X$ be a self-adjoint operator where $\mathcal{D}(A) \subseteq X$. If the set of eigenvalues λ_s is at most countable, then*

$$\lambda_s = \min_{\substack{U \subseteq \mathcal{D}(A) \\ \dim U = s}} \max_{v \in U \setminus \{0\}} \frac{\langle Av, v \rangle_X}{\langle v, v \rangle_X}.$$

Proof: See [Tes14, p. 119]. □

Theorem A.1.19 (Properties of self-adjoint operators)**:**

a) Every self-adjoint is symmetric and closed.

Proof: Follows directly from the definitions for self-adjoint and closed operators. □

b) For A being a self-adjoint operator, $\lambda \in \rho(A)$, $(A - \lambda I)^{-1}$ is bounded.

Proof: Since every self-adjoint is closed, $(A - \lambda I)$ is as the shift with $\lambda \in \mathbb{R}$ also closed. Furthermore, the graph of $(A - \lambda I)^{-1}$ is simply the graph of $(A - \lambda I)$ rotated and hence $(A - \lambda I)^{-1}$ is closed as well. The closed Graph Theorem now yields the desired result. □

Theorem A.1.20 (Properties of the resolvent set)**:** *The resolvent set $\rho(A) \subseteq \mathbb{C}$ of a bounded linear operator A is an open set.*

Proof: See [Wer06, p. 259]. □

Theorem A.1.21 (The spectrum of self-adjoint operators)**:** *The spectrum of a self-adjoint operator A is real.*

Proof: Let λ be an eigenvalue of A, i.e. there exists $x \in X$ such that $Ax = \lambda x$. From this it follows that $\langle Ax, x \rangle = \langle \lambda x, x \rangle$. Using then the fact that A is self-adjoint we can further deduce

$$\lambda \langle x, x \rangle = \langle \lambda x, x \rangle = \langle Ax, x \rangle = \langle x, Ax \rangle = \langle x, \lambda x \rangle = \overline{\lambda} \langle x, x \rangle$$

Hence, $\lambda = \overline{\lambda}$, which shows the desired result. □

Theorem A.1.22 (Trace Theorem)**:** *Assume U is bounded and ∂U is C^1. Then there exists a bounded linear operator*

$$T\colon H^1(U) \to L^2(\partial U)$$

such that

a) $Tu = u\big|_{\partial U}$ *if* $u \in H^1(U) \cap C(\overline{U})$

b) $\|Tu\|_{L^2(\partial U)} \leq C\|u\|_{H^1(U)}$

for each $u \in H^1(U)$, with the constant C depending only on U.

Proof: See [Eva98, p. 258]. $\square$

Theorem A.1.23 (Uniqueness of weak derivatives)**:** *Let $\Omega \subseteq \mathbb{R}$ be open, if it exists, the α-th weak derivative of u is uniquely determined up to a set of measure zero.*

Proof: Assume that $g, \tilde{g} \in L^1_{loc}(\Omega)$ satisfy for all $\varphi \in C_0^\infty(\Omega)$

$$(-1)^\alpha \int_\Omega f\varphi' = \int_\Omega g\varphi = \int_\Omega \tilde{g}\varphi.$$

Then $\int_\Omega (g - \tilde{g})\,\varphi = 0$ for all $\varphi \in C_0^\infty(\Omega)$, whence $g - \tilde{g} = 0$ almost everywhere. $\square$

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Declaration

I declare that I have developed and written the enclosed thesis completely by myself, have not used sources or means without declaration in the text and designated the included passage from other works, whether in substance or in principle, as such and that I adhered to the statute of the Karlsruhe Institute of Technology for good scientific practice in their currently valid version.

Karlsruhe, September 30, 2016