Karlsruher Institut für Technologie

Bachelor Thesis

On the spectra of the Schrödinger operator with periodic delta potential

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Chapter 1

Introduction

The problem considered in this thesis arises from the Kronig-Penney model, see for example [Hee02, chapter 3], which describes 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 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.

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.

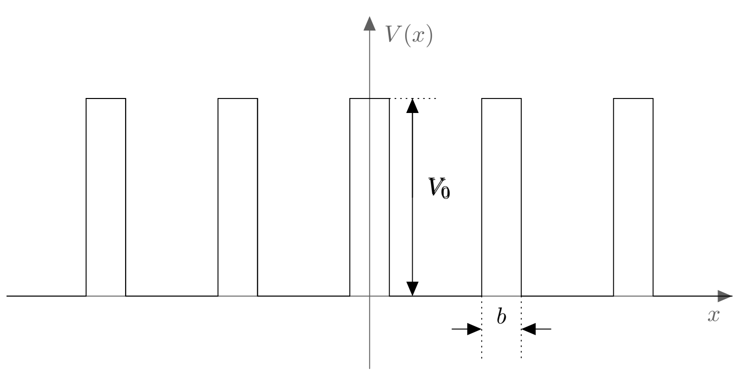

Figure 1.1: Potential $V(x)$ of the Kronig-Penney model

In 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 this means taking the limit $b \to 0$ while V_0 remains of order ρb^{-1}. Therefore, we will extend the research in [DLP$^+$11] where the spectrum of periodic differential operators with smooth coefficients was 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, the spectral bands represent energy levels. Only electron with a energy level within the spectral band can exists inside the crystal. Hence, the possible areas between the intervals, if they exist, represent forbidden energy levels. A result of Bragg's law, standing waves form n the boundary between the spectral band and the forbidden energy levels, see for a detailed explanation [Hee02, section 3.2]. The closer now the electrons accumulate to the nucleus of the relative ion the energetically more favourable are the standing waves which is a desired state by the electrons. Therefore, the Bragg's law can be considered as cause of the forbidden energy levels. Because of this causality, for the knowing possible energetically levels within periodic crystal lattices we need knowledge about the corresponding spectral properties.

The remainder of this thesis is structured as follows. We begin with some preliminaries in Chapter 2 to review some concepts from functional analyses and spectral theory. In Chapter 3, we will examine the operator and show that its self-adjointness, which is our first step in analysing its spectrum. The main mathematical tool for analysing the spectrum of such an operator is the so-called Floquet–Bloch theory. We will transfer the spectral problem the 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. There we are able to analyse the spectrum of the restricted operator by showing the compactness of its resolvent while varying semi-periodic boundary conditions. In Chapter 5 we introduce two concepts to transfer the results from the restricted case into the unrestricted, namely the above mentioned Floquet transformation and the Bloch waves. Based on this methods, in Chapter 6 we are able to show the main result for the one-dimensional case, i.e. 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. We close this thesis in Chapter 8, where we discuss possible gaps between the compact intervals and list current researches.

Chapter 2

Preliminaries

For the upcoming analysis some basic concepts from functional analysis and spectral theory are here briefly reviewed:

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

Definition (Weak derivative)**:** *Let $\Omega \subseteq \mathbb{R}$ be open, and $f \in L^1_{loc}(\Omega)$. 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 $\varphi \in C_0^\infty(\Omega)$.

Let $\alpha \in \mathbb{N}$. 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.5. A central point in this study will be a special Hilbert space the Sobolev space $H^k(\Omega)$.

Definition: *Let $\Omega \subseteq \mathbb{R}$ be open. The sobolev space $H^k(\Omega)$ is defined as*

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

and we equipped it with the norm $\|\cdot\|_{H^k(\Omega)} \coloneqq \left(\sum_{0\leq\alpha\leq k} \|D^\alpha \cdot\|^2_{L^2(\Omega)}\right)^{\frac{1}{2}}$.

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

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

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

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

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

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

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

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

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

Of special interest in this thesis will be one distribution, the Delta-Distribution δ_{x_0} where $x_0 \in \mathbb{R}$. 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

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

see also [Wei16, section 1.4]. However, for our analysis there is another, equivalent definition of the Delta-Distribution handy. 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, we can show that

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

for proof see Theorem A.3.

Since our focus will be on the Schrödinger operator, we will require 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 $graph(A) := \{(x, Ax) : x \in \mathcal{D}(A)\} \subseteq X \times Y$ is a closed set with respect to the product topology.*

Moreover, we will study a certain class of operators, the self-adjoint operators. For this we define:

Definition: *Let X be a Hilbert space and $\langle \cdot, \cdot \rangle_X$ denote the scalar product on X. Le $A\colon \mathcal{D}(A) \to X$ 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 $\mathcal{D}(A^*) := \{u \in X\colon\ \exists u^* \in X\ \forall v \in \mathcal{D}(A)\ \langle u, Av\rangle = \langle u^*, v\rangle\}$ and $A^*u := u^*$ 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 and $\mathcal{D}(A) \supseteq \mathcal{D}(A^*)$, for proof refer to [RS08, page 256]. Since our main result is to characterise the spectrum of the Schrödinger operator, we still 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 $A - \lambda I\colon \mathcal{D}(A) \to Y$ bijective,*

then due to the Closed Graph Theorem is $(A - \lambda I)^{-1}\colon X \to \mathcal{D}(A)$ a bounded linear operator,

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

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

Eventually, in Chapters 4 and 7 we will examine so-called compact operators and some of their properties.

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

Throughout this thesis we will need some theorems and lemmata from functional analysis and spectral theory, which are listed in the appendix.

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. 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 function 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 the Delta-Distribution. If we suppose for a moment that the problem is smooth, more specifically, that the potential 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 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

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

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

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

Remark: *Since $C_0^\infty(\mathbb{R})$ is dense in $L^2(\mathbb{R})$, (3.3) holds also for all $v \in H^1(\mathbb{R})$.*

3.1 The resolvent-mapping of the one-dimensional Schrödinger operator

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 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

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

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

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

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

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

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

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

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

b) Let $u \in H^1(\mathbb{R})$. For the coercivity, we note first that for the given sesquilinear form $B[u,u] \in \mathbb{R}$ holds. Assuming $\rho \geq 0$ yields for $\mu < -1$ 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 $\beta = \min\left\{2\rho h + 1u, 2\rho\frac{1}{h} - \mu\right\}$. $\square$

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 yields for the boundedness

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

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

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

Now, using (3.3), (3.5) with a small enough $\mu \in \mathbb{R}$ yields with Cauchy–Schwarz's inequality

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

which shows the boundedness of the mapping R_μ. Taking 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

$$0 = B_\mu[u_1, v] - B_\mu[u_2, v] = \int_{\mathbb{R}} (f_1(x) - f_2(x))\overline{v(x)} dx \quad \forall v \in C_0^\infty(\mathbb{R}). \tag{3.7}$$

As $C_0^\infty(\mathbb{R})$ is dense in $L^2(\mathbb{R})$, we know from the equation (3.7) 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. $\square$

3.2 The domain of the one-dimensional Schrödinger operator

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*

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

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: *Note, R_μ is the resolvent 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

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

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

$$\int_{x_k}^{x_{k+1}} u'(x)\overline{v'(x)}dx = \int_{x_k}^{x_{k+1}} (Au)(x)\overline{v(x)}dx \iff \int_{x_k}^{x_{k+1}} -u(x)\overline{v''(x)}dx = \int_{x_k}^{x_{k+1}} (Au)(x)\overline{v(x)}dx, \tag{3.8}$$

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 $v \in C^\infty(\mathbb{R})$ 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

$$u'(x_k-0) - u'(x_k+0) + \rho u(x_k) = 0, \tag{3.9}$$

and therefore

$$\mathcal{D}(A) \subseteq \Big\{u \in H^1(\mathbb{R})\colon u\big|_{(x_i,x_{i+1})} \in H^2(x_i,x_{i+1}), u'(x_j-0)-u'(x_j+0)+\rho u(x_j) = 0\ \forall i,j \in \mathbb{Z}\Big\} \tag{3.10}$$

Finally, choosing a function $v \in C_0^\infty(\mathbb{R})$ with $\operatorname{supp} v = (x_{-n}, x_n)$ in (3.3) for some arbitrary $n \in \mathbb{N}$ yields with partial integration on every interval (x_i, x_{i+1}) by using (3.9) that

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

$$\iff \sum_{i=-n}^{n-1} \int_{x_i}^{x_{i+1}} u''(x)\overline{v(x)}dx = -\int_{x_{-n}}^{x_n} f(x)\overline{v(x)}dx - \mu \int_{x_{-n}}^{x_n} u(x)\overline{v(x)}dx. \tag{3.11}$$

By defining $w_n := \sum_{i=-n}^{n-1} u''\mathbb{1}_{[x_i,x_{i+1}]}$ we can estimate the left-hand side of (3.11) by

$$\begin{aligned}
|\langle w_n, v\rangle| &\le \left|\int_{x_{-n}}^{x_n} f(x)\overline{v(x)}dx\right| + \left|\mu \int_{x_{-n}}^{x_n} u(x)\overline{v(x)}dx\right| \\
&\le \|f\|_{L^2(x_{-n},x_n)}\|v\|_{L^2(x_{-n},x_n)} + |\mu|\|u\|_{L^2(x_{-n},x_n)}\|v\|_{L^2(x_{-n},x_n)} \\
&\le c\|v\|_{L^2(x_{-n},x_n)}, \qquad (3.12)
\end{aligned}$$

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 (3.12), follows that $\sum_{i\in\mathbb{Z}} \|u''\|^2_{L^2(x_i,x_{i+1})} < \infty$. This yields the inclusion

$$\mathcal{D}(A) \subseteq \left\{u \in H^1(\mathbb{R}) : u \in H^2\Big(\mathbb{R} \setminus \bigcup_{i\in\mathbb{Z}} x_i\Big), u'(x_j - 0) - u'(x_j + 0) + \rho u(x_j) = 0 \ \forall j \in \mathbb{Z}\right\}. \tag{3.13}$$

Hence, for an arbitrary $u \in \mathcal{D}(A)$ we know from (3.8) and (3.13) that

$$Au = \begin{cases} -u'' & \text{on } (x_k - \frac{1}{2}, x_k) \\ -u'' & \text{on } (x_k, x_k + \frac{1}{2}), \end{cases} \quad \forall k \in \mathbb{Z}. \tag{3.14}$$

We are furthermore able to show in (3.13) the reverse inclusion by using the resolvent R_μ. But first let us, again for brevity, denote with B the right-hand side of (3.13). 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 $f := -u''$ 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 $f \in L^2(\mathbb{R}) = \mathcal{D}(R_\mu)$. We want to show that $u = R_\mu(f - \mu u)$ or equivalently

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

For each $k \in \mathbb{Z}$ partial integration on both side 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

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

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

$$\mathcal{D}(A)=\Big\{u\in H^1(\mathbb{R}):u\in H^2\Big(\mathbb{R}\setminus\bigcup_{i\in\mathbb{Z}}x_i\Big),u'(x_j-0)-u'(x_j+0)+\rho u(x_j)=0\ \forall j\in\mathbb{Z}\Big\}. \quad (3.15)$$

Remark: *From* (3.14) *and* (3.15) *follows that the definition of A is independent of μ.*

3.3 The self-adjointness of the Schrödinger operator

In Chapter 6 we will need the fact that the operator A is self-adjoint. For 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 symmetric operator has an entirely real spectrum, this theorem yields further our first result about the spectrum of A, for a proof see Theorem A.7.

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

Proof: We proceed by proving first 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 that if $v\in\mathcal{D}({R_\mu^{-1}}^*)$ and $v^*\in L^2(\mathbb{R})$ are such that

$$\langle R_\mu^{-1}u,v\rangle=\langle u,v^*\rangle\quad\forall u\in\mathcal{D}(R_\mu^{-1}), \quad (3.16)$$

then $v \in \mathcal{D}(R_\mu^{-1})$ and $R_\mu^{-1} v = v^*$. In (3.16) for any $u \in \mathcal{D}(R_\mu^{-1})$ exists $f \in L^2(\mathbb{R})$ such that $u = R_\mu f$; using use 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. $\square$

Chapter 4

Fundamental domain of periodicity and the Brillouin zone

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

Let Ω be the fundamental domain of periodicity associated with (3.1), for simplicity let $\Omega \coloneqq \Omega_0$ 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 $k \in B$ the set*

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

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

In this chapter, we will 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 $k \in B$.

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

Proof: See Theorem A.2. □

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 and injective. Consequently, we are able to define

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

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

4.1 The domain of the restricted Schrödinger operator

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

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

In the remainder of this chapter we will further investigate the operator A_k. For this purpose, we need to show that $R_{\mu,k}$ is compact from which we deduce that the eigenfunctions of A_k form a complete and orthonormal system in H_k^1.

4.2 The compactness of the restricted resolvent

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 as well. 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

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

Thus, $\|u_j\|_{H^1(\Omega)} \leq C$ for all j. The assertion follows from the Compact Embedding Theorem for Sobolev spaces, see Theorem A.13. $\square$

4.3 The spectrum of the restricted Schrödinger operator

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 [Wei15, page 74 - 76]. We will from 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. We understand ψ extended by the boundary condition on $\partial\Omega$ in (4.1) 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

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

is an eigenvalue for the eigenfunction w except that now 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 [Eva98, page 643 - 645].

At the end 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 define first

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

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 the operator $\tilde{A}_k\colon \mathcal{D}(A_k)\to L^2(\mathbb{R})$ through

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

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 $(\lambda_s(s))_{s\in\mathbb{N}}$ 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 above by varying k over the Brillouin zone B. For this purpose we will need two results involving to be able to move the problem from $L^2(\mathbb{R})$ to $L^2(\Omega \times B)$ whereas $\Omega \times B$ is compact by assumption. For the sake of completeness, we include here the proofs of both theorems, as given in [DLP$^+$11, section 3.4, 3.5].

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 semi-periodicity condition* (4.1)*, the inverse formular 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

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

We can apply Beppo Levi's Theorem which 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 the fact that

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

forms an orthonormal basis of $L^2(B)$ and Parseval's equality gives for these x

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

This expression is in $L^2(\Omega)$ by (5.4) and Tonelli's theorem, and we conclude $\|Uf\|_{L^2(\Omega\times B)} = \|f\|_{L^2(\mathbb{R})}$. It is for us still left 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 we know that for almost every $x \in \Omega$ we have $g(x,k) \in L^2(B)$, and with this, Parseval's theorem 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 and using Tonelli's theorem and the Monotone Convergence Theorem 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

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

whence (5.5) implies $Uf = g$ and (5.2), the desired result. Now (5.3) follows from (5.2) and exploiting $g(x+n,k) = e^{ikn} g(x,k)$. □

5.2 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: The previous theorem 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. 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

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

where

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

Moreover, we get by Bessel's inequality

$$\|(Uf)(\cdot, k) - g_l(\cdot, k)\|^2_{L^2(\Omega)} \leq \|(Uf)(\cdot, k)\|^2_{L^2(\Omega)}$$

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

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

All in all, this means by Tonelli's Theorem

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

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

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

which is the desired result. $\square$

Chapter 6

The spectrum of the one-dimensional Schrödinger operator

Finally, we are able 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 $I_s \coloneqq \{\lambda_s(k) : k \in \overline{B}\}$ $(s \in \mathbb{N})$. We will prove that each I_s is a compact interval, this 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 $s \in \mathbb{N}$ is the function $k \mapsto \lambda_s(k)$ 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 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 $k \in B$ be fixed. For all $\tilde{k} \in B$ and all $v \in \mathcal{D}(\tilde{A}_k)$ using triangular inequality we can estimate 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 can estimate

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

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

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

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 on the boundary conditions. However, all eigenvalues of (4.4) are by the min-max-principle 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 semi-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. □

Remark: *As B is compact and connected and $\lambda_s(k)$ is a continuous function of $k \in B$ 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 semi-periodic boundary conditions. Since $\mu_s \to \infty$ 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

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

We regard $\psi_s(\cdot, k)$ as extended to the whole of $\mathbb{R}$ by the boundary condition (4.1), whence, due to the periodic structure of A, ψ_s satisfies

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

"locally", i.e.

$$\psi_s \in \Big\{\psi \in H^1_{loc}(\mathbb{R}) : \psi \in H^2\Big(\mathbb{R} \setminus \bigcup_{i\in\mathbb{Z}} x_i\Big), \psi'(x_j - 0) - \psi'(x_j + 0) + \rho\psi(x_j) = 0 \ \forall j \in \mathbb{Z}\Big\},$$

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

$$\eta(x) = 1 \text{ for } |x| \leq \frac{1}{4}, \quad \eta(x) = 0 \text{ for } |x| \geq \frac{1}{2}, \tag{6.8}$$

and define, for each $l \in \mathbb{N}$,

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

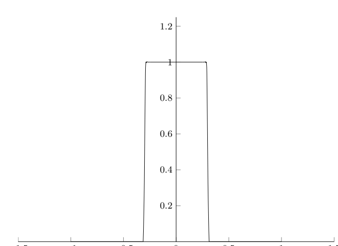

Figure 6.1: Example for a function η

As $\psi_s \in \mathcal{D}(A)$ we know $u_l \in \mathcal{D}(A)$, hence, we see that

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

where R is a sum of products of derivatives of order ≥ 1 of $\eta\left(\frac{|\cdot|}{l}\right)$, and derivatives of order ≤ 1 of $\psi_s(\cdot,k)$. Let use denote with B_l the ball around 0 with radius $\frac{l}{2}$ and let, for simplicity, $c \in \mathbb{R}$ be a generic constant. Thus, note that $\psi_s(\cdot,k) \in H^1_{loc}(\mathbb{R})$, the semi-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 semi-periodic structure allows us find additionally an upper boundary for u_l:

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

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

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

This results eventually in the property

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

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

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 an 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

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

and

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

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 $k \in B$ 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 semi-periodic boundary conditions. Hence, (4.4), (6.12) and Parseval's identity 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

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

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, (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 interval containing $\operatorname{supp}(\varphi)$ 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

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

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 last 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 Y denote the periodicity cell in $\mathbb{R}^n$ relating to the problem introduced above and B^n the corresponding Brillouin zone, for simplicity assume Y being the unit cube $Y = [0,1]^n$. Contained in Y let S be a smooth surface without a boundary subject to the conditions $\dim S = n-1$ and $S \subseteq \mathring{Y}$. Furthermore, let $B \subseteq Y$ denote the set enclosed by S, such that $S = \partial B$. We will denote with $Y_j = Y + j$ the jth copy of Y 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 $B_j = B + j$. Finally, we denote with Y_i^+ and Y_i^- the opposing edges of Y for $i = 1, 2$. For an illustration see 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 $C_0^\infty(\mathbb{R}^n)$ is dense in $H^1(\mathbb{R}^n)$ 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 since*

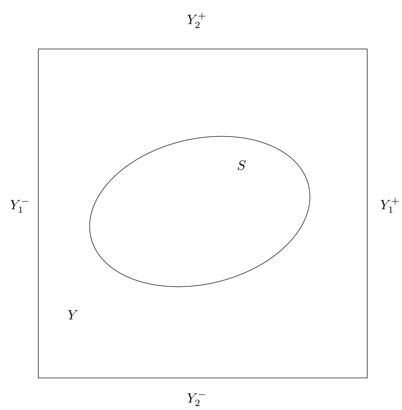

Figure 7.1: Periodicity cell for the multi-dimensional potential

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 they are in $L^2(\mathbb{R})$ by [Eva98, page 251, Theorem 5.1] and [AF03, page 164], and thus, the second term on the left-hand side in (7.2) is well defined by the next remark.

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

Proof: First, the Cauchy–Schwarz inequality yields

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

Both terms on the right-hand side can then be finitely estimated by the Trace Theorem [Eva98, page 258] and Poincare's inequality for some $h > 0$ through

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

for some $c \in \mathbb{R}$. $\square$

Given $f \in L^2(\mathbb{R}^n)$, following the proves 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

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

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

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

is a bounded, linear functional. Hence, Lax-Migram's Theorem proves the existence of a unique solution $u \in H^1(\mathbb{R}^n)$ in (7.2) for any $f \in L^2(\mathbb{R}^n)$, and 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 equally Theorem 3.3. □

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

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

such that we can again characterise $\mathcal{D}(A^n)$ explicitly by transferring the methods used in Section 3.2.

Theorem 7.2 (Characterisation of $\mathcal{D}(A^n)$)**:** *Let $\Omega \coloneqq \mathbb{R}^n \setminus \overline{\bigcup_{j\in\mathbb{Z}^n} B_j}$. We can further characterise the solution $u \in \mathcal{D}(A^n)$ from* (7.2)*, namely for all $j \in \mathbb{Z}^n$ it holds:*

1. $\Delta u \in L^2(B_j)$, $\Delta u \in L^2(\Omega)$ *and* $\sum_{j\in\mathbb{Z}^n} \|\Delta u\|^2_{L^2(B_j)} < \infty$
2. $u\big|_{S_j-0} = u\big|_{S_j+0}$
3. $\frac{\partial u}{\partial \eta_j}\big|_{S_j-0} - \frac{\partial u}{\partial \eta_j}\big|_{S_j+0} - \rho u\big|_{S_j} = 0$ *where η_j denotes the normal on S_j*

Proof: In Section 3.2 we used particular functions $v \in C^\infty(\mathbb{R})$ to prove equivalent properties of $\mathcal{D}(A)$. By using the same approach with equivalent functions for the multi-dimensional case ing in (7.2) asserted follows. □

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 transform to a family of eigenvalue problems on the periodicity cell. First, we need the self-adjointness of the operator A^n.

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

Proof: todo. □

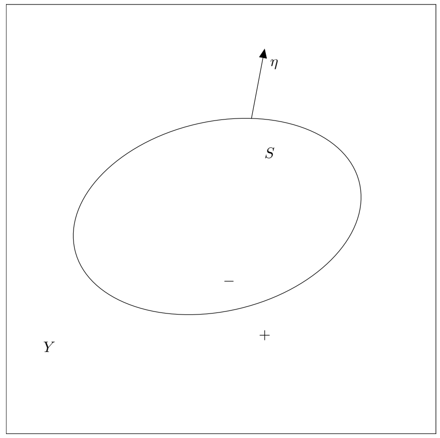

Figure 7.2: Normal η on the hypersurface S in a periodicity cell

We restrict this multi-dimensional problem to a corresponding fundamental domain of periodicity, let this for simplicity be Y. Let us consider the problem to find

$$u \in H^1_{k,n} := \left\{ w \in H^1(Y) \colon w\big|_{Y_j^+} = w\big|_{Y_j^-} e^{ik_j} \text{ for } k \in [-\pi,\pi]^2, j = 1,2 \right\}$$

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 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 the definition

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

as the operator considering multi-dimensional case of our problem on the fundamental cell of periodicity. The semi-periodic boundary conditions on $H^1_{k,n}$ require a solution $u \in H^1_{k,n}$ of (7.3) to satisfy furthermore

$$\frac{\partial u}{\partial x_j}\Big|_{Y_j^+} = e^{ik_j} \frac{\partial u}{\partial x_j}\Big|_{Y_j^-} \quad \text{for } j = 1,2.$$

Theorem 7.3: *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. Using the Compact Embedding Theorem for Sobolev spaces yields the claim, for proof see Theorem A.13 . □

Now, we will consider the eigenvalue problem to find $\psi \in \mathcal{D}(A_k^n)$ such that

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

We understand ψ_s extended by the boundary condition on Y in $H_{k,n}^1$ to the whole of $\mathbb{R}^n$ and call them Bloch waves. Using the compactness of $R_{\mu,k}^n$, we know on the one hand that every non-zero $\lambda \in \sigma(A_k^n)$ is an eigenvalue of A_k^n and that the purely discrete spectrum satisfies

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

By [Eva98, page 643 - 645] we know that the to (7.5) corresponding eigenfunctions 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), similar to the one in (4.8) and (4.9), we are then able to show that the eigenvalues of A_k^n are continuous functions of $k \in \overline{B}$, and thus $I_s^n = \{\lambda_s^n(k) : k \in \overline{B}\}$ is again a compact real interval for each $s \in \mathbb{N}$.

Ultimately, the main result for this multi-dimensional case follows from using the same arguments as in Chapter 6.3 based on Bloch waves, Floquet transform and a similar cut-off function η as in (6.8). We are namely able to show 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

Outlook and conclusion

Auf jeden Fall zunächst verbale summary of the main findings of this thesis.

We have to notice that we haven't determined the nature of the spectrum that is if there are possible gaps in the spectrum. However,...
Floquet–Bloch theory does not give an answer to the question if there are really gaps in the spectrum or if the bands actually overlap. An asymptotic answer (for sufficiently "high contrast" in the coefficients) has been given in 'A. Figotin and P. Kuchment. Band gap structure of spectra of periodic dielectric and acoustic media. II. Two-dimensional photonic crystals. SIAM J. Appl. Math., 56:1561–1620, 1996'.
In a more concrete case, existence of a gap has been proved by computer-assisted means in 'V. Hoang, M. Plum, and C. Wieners. A computer-assisted proof for photonic band gaps. Zeitschrift für Angewandte Mathematik und Physik, 60:1–18, 2009'.
'S. Albeverio, F. Gesztesy, R. Hoegh-Krohn, H. Holden *Solvable Models in Quantum Mechanics*. Second edition, with an appendix by P. Exner xvi+488 p.; AMS Chelsea Publishing, volume 350, Providence, R.I., 2005'

Hier auf Literatur verwiesen, die aktuell daran ansetzt.

Appendix

Theorem A.1 (The open set of resolvent values)**:** *The resolvent set $\rho(A) \subseteq \mathbb{C}$ of a bounded linear operator A is an open set.*

Proof: See [Wer06, page 259]. $\square$

Theorem A.2: *H^1_k is a closed subspace of $H^1(\Omega)$ and hence a Hilbert space.*

Proof: todo $\square$

Theorem A.3: *Proof:* This limit exists and it holds that $\delta_{x_0} \in \mathfrak{D}'(\mathbb{R})$ and $\delta_{x_0}(f) = \lim_{\epsilon \to 0} \delta_\epsilon(f) = f(x_0)$, for a proof see

Remark: *The Delta-Distribution can also be defined equivalently either as a distribution or as a measure.*

$\square$

Theorem A.4: *For A beeing 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 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. $\square$

Theorem A.5 (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

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

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

$$\int_\Omega (g - \tilde{g})\, \varphi = 0$$

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

Theorem A.6 (Approximation by test functions)**:** *$C_0^\infty(\mathbb{R})$ is dense in $L^p(\mathbb{R})$, if $1 \leq p < \infty$.*

Proof: See [Wer06, page 82]. ☐

Theorem A.7 (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.8: *H_k^1 is a closed subspace of $H^1(\Omega)$, and therefore a Hilbert space with respect to the norm of $H^1(\Omega)$.*

Proof: coming ☐

Theorem A.9 (Riesz' representation theorem)**:** *Let H be a Hilbert space, and let H^* denote its dual space, consisting of all continuous linear functionals from H into $\mathbb{R}$ or $\mathbb{C}$. If x is an element of H, then the function φ_x, for all y in H defined by*

$$\varphi_x(y) = \langle y, x\rangle_H ,$$

where $\langle \cdot, \cdot\rangle_H$ denotes the inner product of the Hilbert space, is an element of H^*. Hence, every element of H^* can be written uniquely in this form.

Proof: See [Wei15, page 88] ☐

Theorem A.10 (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 [Wei15, page 66] ☐

Theorem A.11 (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, page 645] ☐

Theorem A.12: *Let $[a, b]$ be a compact interval in $\mathbb{R}$. Then, $H^1([a, b])$ is embedded in $C([a, b])$*

Proof: Let f be a smooth function and $x, y \in [a, b]$ such that $x \leq y$, then:

Thus, the supremum norm is dominated by the H^1-norm, which implies that, which means that this estimation holds for the completion H1([a, b]) as well. ☐

We need the next theorem in two versions, once in Chapter 4 and once in 7. This is also why I will separate the proofs:

Theorem A.13 (Compact Embedding Theorem for Sobolev spaces)**:** *Assume U is a bounded open subset of $\mathbb{R}^n$, and ∂U is C^1. Define $p^* := \frac{2n}{n-2}$.*

a) *Suppose $n > 2$. Then $H^1(U) \subset\subset L^q(U)$ for each $1 \leq q \leq p^*$.*

Proof: Follows from Rellich-Kondrachov Compactness Theorem, see for example [Eva98, page 272]. □

b) *Suppose $n \in \{1, 2\}$. Then $H^1(U) \subset\subset L^2(U)$.*

Proof: To proof the embedding for $p = 2$ note that from Rellich-Kondrachov Compactness Theorem it follows that $p^* \to \infty$ if $p \to n$. It is easily seen that if $(u_n)_{n\in\mathbb{N}}$ is a $H^1(U)$-bounded sequence, then so it is bounded in $W^{1,n-\epsilon}(U)$ for some $\epsilon > 0$. Choosing ϵ such that $(n-\epsilon)^* > n$ hence allows using again via part a) the Rellich-Kondrachov Compactness Theorem and this provides he existence of a $L^2(U)$ convergent subsequence.
For $n = 1$ this follows from Morrey's inequality and the Arzela Ascoli compactness criterion, see for example [Eva98, page 274]. □

Theorem A.14 (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*

- $|B[u,v]| \leq \alpha\|u\|\|v\| \quad (u, v \in H)$ *and*
- $Re(B[u,u]) \geq \beta\|u\|^2 \quad (u \in H)$,

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]. □

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Decleration

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 the statute of the Karlsruhe Institute of Technology for good scientific practice in their currently valid version.

Karlsruhe, 30 September 2016