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 [6, Chap. 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 like this:

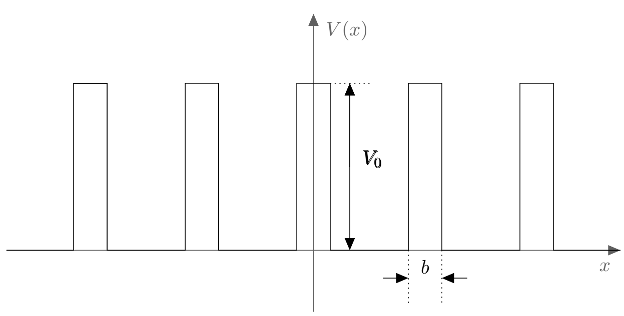

Figure 1.1: Potential $V(x)$ of the Kronig-Penney model

where b is the "support" and ρ the magnitude of the potential. We are interested in the spectrum of the operator describing the situation of 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}.

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 $x \notin I$. 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*

$$-\int_\Omega f\varphi' = \int_\Omega g\varphi$$

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. A central point in this study will be a special Hilbert space the Sobolev space $H^k(\Omega)$.

Definition: *Let us define the space*

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

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

By admitting the inner product in terms of the $L^2(\Omega)$ inner product for all derivatives up to order k:

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

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.

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

for all $i \in \mathbb{N}_0$. One can proof that this concept of convergence generates a topology on C_0^∞ and one usually denoted 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.

An important example for a distribution is the Dirac delta function δ_{x_0} where $x_0 \in \mathbb{R}$. It is defined as the weak limit of a weakly converging sequence of functionals over normed symmetric around x_0 cumulative distribution functions δ_ϵ, where the support of those cumulative distributions converges to zero. It holds $\delta_{x_0} = \lim_{\epsilon\to 0} \delta_\epsilon$ in $\mathfrak{D}'(\mathbb{R})$. An example for such a sequence is

$$\delta_\epsilon(x) = \frac{1}{\sqrt{2\pi}\epsilon} e^{-\frac{x^2}{2\epsilon^2}}. \tag{2.1}$$

Which implies the definition

$$\delta_{x_0}(f) := \int_{\mathbb{R}} \delta_{x_0} f(x)dx := \lim_{\epsilon\to 0} \int_{\mathbb{R}} \delta_\epsilon(x - x_0) f(x)dx.$$

Moreover, we can check that $\delta_{x_0}(f) = \lim_{\epsilon\to 0} \delta_\epsilon(f) = f(x_0)$, for a proof see [10, Chap. 1.4].

Definition: *Let X, Y be Banach spaces and let $A\colon \mathcal{D}(A) \to Y$ be a linear operator with domain $\mathcal{D}(A) \subseteq X$.*

a) 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.

b) The operator $A^* : \mathcal{D}(A^*) \to H$ is called the adjoint of A and is defined by

$$\mathcal{D}(A^*) := \{u \in H : \exists u^* \in H \ \forall v \in \mathcal{D}(A) \langle u, Av\rangle = \langle u^*, v\rangle\}$$

and $A^*u := u^*$ for $u \in \mathcal{D}(A^*)$. Note that for $u \in \mathcal{D}(A^*)$, u^* is uniquely determined.

Definition: *Let X be a Hilbert space, $\langle\cdot,\cdot\rangle$ denotes the scalar product on X and A a bounded operator. We call*

a) A symmetric, if $\langle Tx, y\rangle = \langle x, Ty\rangle$ for all $x, y \in \mathcal{D}(A)$, and *b) A self-adjoint, if A is densely defined on X and coincides with its adjoint.*

Definition: *Furthermore, let I denote the identity operator on X and A be a linear, bounded and closed operator.*

a) $\lambda \in \mathbb{C}$ belongs in the resolvent set of A, $\lambda \in \rho(A)$, if

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

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

c) $\lambda \in \rho(A) \to R(\lambda, A) = (A - \lambda I)^{-1}$ is the resolvent function of A.

Finally, in chapters 4 and 7 we will examine so called compact operators and some of their properties.

Definition: *Let X be a normed space and Y a Banach space. A linear operator $A \colon X \to Y$ is called compact, if $T(U_X)$ is relativ compact in Y.*

Additionally, throughout this thesis we will need some theorems and lemmata from functional analysis and spectral theory, which will be 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 its self-adjointness. Later, in chapters 4 and 6, we will need these results to deduce 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 Dirac 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 $i \in \mathbb{Z}$.

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 Dirac delta function. If we suppose for a moment that the problem is smooth, more specifically, that the potential is instead given by (2.1), 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

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

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

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

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: *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*

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

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

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

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

$$B_\mu[u,v] = l_f(v) \quad \forall v \in H^1(\mathbb{R}). \tag{3.6}$$

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 (3.5) as for an arbitrary $\rho \in \mathbb{R}$ there exists $\alpha \in \mathbb{R}$ such that

$$\begin{aligned}
|B(u,\varphi)|^2 &\leq \|u'\|_{L^2(\mathbb{R})}\|v'\|_{L^2(\mathbb{R})} + 2|\rho| \sum_{i\in\mathbb{Z}} |u(x_i)|^2 |v(x_i)|^2 + |\mu|\, \|u\|_{L^2(\mathbb{R})}\|v\|_{L^2(\mathbb{R})} \\
&\leq \|u'\|_{L^2(\mathbb{R})}\|v'\|_{L^2(\mathbb{R})} + 8|\rho| \|u\|^2_{H^1(\mathbb{R})}\|v\|^2_{H^1(\mathbb{R})} + |\mu|\, \|u\|_{L^2(\mathbb{R})}\|v\|_{L^2(\mathbb{R})} \\
&= (8|\rho| + |\mu|)\|u\|_{L^2(\mathbb{R})}\|v\|_{L^2(\mathbb{R})} + 8|\rho| \|u\|_{L^2(\mathbb{R})}\|v'\|_{L^2(\mathbb{R})} \\
&\quad + 8|\rho| \|u'\|_{L^2(\mathbb{R})}\|v\|_{L^2(\mathbb{R})} + (8|\rho| + 1)\|u'\|_{L^2(\mathbb{R})}\|v'\|_{L^2(\mathbb{R})} \\
&\leq \alpha \|u\|_{H^1(\mathbb{R})}\|\varphi\|_{H^1(\mathbb{R})}
\end{aligned}$$

where $\alpha = \max\{8|\rho| + |\mu|\,, 8|\rho| + 1\}$.

b) For the coercivity, we note first that for the given sesquilinear form $B[u,u] \in \mathbb{R}$ holds for all $u \in H^1(\mathbb{R})$. Assuming first $\rho \geq 0$ 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 $h < \frac{1}{2|\rho|}$ and with that if $\mu < -\frac{2|\rho|}{h}$ there exists $\beta \in \mathbb{R}$ such that

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

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: It is easily seen that l_f is linear, for the boundedness the Cauchy–Schwarz inequality yields

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

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).

Due to the linearity of the integral and the uniqueness of the solution, R_μ is a linear operator. Hence, 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

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

This 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 $R_\mu f_1 = R_\mu f_2$ holds (3.6) yields

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

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

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

hence $f_1 = f_2$ 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*

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

Note that this definition is consistent with the formal definition in (3.1) and as we will show is independent of μ, still assuming $\mu < \min\{-1, -\frac{2|\rho|}{h}\}$.

Remark: *Note that 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 u or rather $\mathcal{D}(A)$. However, we already know by Lax-Milram's Theorem that $u \in H^1(\mathbb{R})$. First, let us 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

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

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 obtain

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

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

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

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

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

$$\mathcal{D}(A) \subseteq \Big\{u \in \bigcap_{i\in\mathbb{Z}} H^2(x_i, x_{i+1}) : u'(x_i - 0) - u'(x_i + 0) + \rho u(x_i) = 0 \ \forall i \in \mathbb{Z}\Big\}. \tag{3.10}$$

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

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

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

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 (3.11) by

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

for some $c \in \mathbb{R}$. Since c is independent of n, from (3.12) follows that

$$\sum_{i\in\mathbb{Z}} \|u''\|^2_{L^2(x_i,x_{i+1})} < \infty.$$

This yields

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

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

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

We are furthermore able to show in (3.13) the reverse inclusion by using the operator 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 $\mathcal{D}(R_\mu) = L^2(\mathbb{R})$ define $f \coloneqq -u''$ on (x_k, x_{k+1}) for all $i \in \mathbb{Z}$; as we know that $u \in H^2\Big(\mathbb{R} \setminus \bigcup_{i\in\mathbb{Z}} x_i\Big)$ we can therefore ensure $f \in L^2$. Hence, we have to show that $u = R_\mu(f - \mu u)$ or equivalently

$$\int_{\mathbb{R}} u'\overline{v'} + \rho \sum_{i\in\mathbb{Z}} u(x_i)\overline{v(x_i)} - \mu \int_{\mathbb{R}} u\overline{v} = \int_{\mathbb{R}} (f - \mu u)\overline{v}$$

$$\iff \sum_{i\in\mathbb{Z}} \int_{\Omega_i} u'\overline{v'} + \rho \sum_{i\in\mathbb{Z}} u(x_i)\overline{v(x_i)} = - \sum_{i\in\mathbb{Z}} \int_{x_i}^{x_{i+1}} u''\overline{v}.$$

For each $k \in \mathbb{Z}$ partial integration with a function $v \in C_0^\infty(\mathbb{R})$ having $\operatorname{supp} v = \Omega_k$ yields

$$\int_{\Omega_k} u'\overline{v'} + \rho u(x_k)\overline{v(x_k)} = \left(\int_{x_k-\frac{1}{2}}^{x_k} + \int_{x_k}^{x_k+\frac{1}{2}}\right) u'\overline{v'} + u'(x_k-0)\overline{v(x_k)} - u'(x_k+0)\overline{v(x_k)}$$

$$\iff u'(x_k-0) - u'(x_k+0) - \rho u(x_k) = 0.$$

Consequently, we conclude that

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

Remark: *The definition of A is independent of μ.*

Proof: Since as seen above the domain is independent of μ and μ-dependent terms cancel each other out. □

3.3 The self-adjointness of the Schrödinger operator

In chapter 6, we will use the fact that the operator A is self-adjoint, from which follows that A is a closed and symmetric operator. For this we first need 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):

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

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 additionally our first result about the spectrum of A.

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} are 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

$$\langle R_\mu^{-1} u, v \rangle = \langle u, v^* \rangle \quad \forall u \in \mathcal{D}(R_\mu^{-1}), \tag{3.14}$$

then $v \in \mathcal{D}(R_\mu^{-1})$ and $R_\mu^{-1} v = v^*$. In (3.14) 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 $R_\mu^{-1} v = v^*$, 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 can be used, with the help of tools we introduce in chapter 5, to determine the eigenvalues of the unrestricted problem, which is exactly the approach we will use 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. For fixed $k \in B$, in this chapter we consider the operator A_k on Ω formally defined by the operation

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

For brevity let us introduce the following:

Definition: *We define for every k the set of quasi-periodic functions*

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

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

Proof: Due to the fact that convergence in H^1 implies the convergence on the boundary of Ω. □

We will hereafter refer to the boundary conditions in (4.1) as quasi-periodic boundary conditions. Analogously to section 3.1, we now define A_k by considering the problem of finding for $f \in L^2(\Omega)$ a function $u \in H_k^1$ such that the equation

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

holds for all $v \in H_k^1$. One can apply the same arguments as above to prove that

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

is well-defined and injective. Consequently, we define

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

In the remainder of this chapter we will further investigate the operator A_k. For this purpose, we shall 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.

4.1 The compactness of the restricted resolvent

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

Proof: Let $(f_j)_j \in L^2(\Omega)$ 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

$$\int_\Omega u_j'\overline{v'} + \rho u_j(x_0)\overline{v(x_0)} - \mu \int_\Omega u_j\overline{v} = \int_\Omega f_j\overline{v} \quad \forall v \in H_k^1. \tag{4.2}$$

Now, the particular choice of $v = u_j$ in (4.2) 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 now from the compact embedding theorem for Sobolev spaces. $\square$

4.2 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 [9, page 74 - 76]. We will from now consider the eigenvalue problem to find $\psi \in H_k^1$ such that

$$A_k\psi = \lambda\psi \text{ on } \Omega. \tag{4.3}$$

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 $\lambda_w(k)$ we can see that

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

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

$$\tilde{\lambda}_w(k) = \frac{1}{\lambda_w(k)} - \mu$$

is an eigenvalue for the same eigenfunction w except that now for the operator A_k. Using all of this we see that A_k has a purely discrete spectrum satisfying

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

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).

At the end of this chapter, we transform the eigenvalue problem (4.3) such that the boundary condition is independent of k. This allows us to show the following.

Theorem 4.2: *The eigenvalues of A_k as function $k \mapsto \lambda_s(k)$ of k are continuous in $k \in \overline{B}$.*

Proof: For this, we first define

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

Then,

$$\begin{aligned}
A_k\psi_s(x,k) &= \frac{d^2}{dx^2}\psi_s(x,k)\big|_{(x_0-\frac{1}{2},x_0)} \cdot \mathbb{1}_{(x_0-\frac{1}{2},x_0)} + \frac{d^2}{dx^2}\psi_s(x,k)\big|_{(x_0,x_0+\frac{1}{2})} \cdot \mathbb{1}_{(x_0,x_0+\frac{1}{2})} \\
&= e^{ikx}\left(\frac{d}{dx} + ik\right)^2 \varphi_s(x,k)\big|_{(x_0-\frac{1}{2},x_0)} \cdot \mathbb{1}_{(x_0-\frac{1}{2},x_0)} \\
&\quad + e^{ikx}\left(\frac{d}{dx} + ik\right)^2 \varphi_s(x,k)\big|_{(x_0,x_0+\frac{1}{2})} \cdot \mathbb{1}_{(x_0,x_0+\frac{1}{2})}.
\end{aligned} \tag{4.4}$$

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

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

and using (4.3) 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 and from theorem 4.1 follows that $(\varphi_s(\cdot,k))_{s\in\mathbb{N}}$ is an orthonormal and complete system of eigenfunctions to the periodic eigenvalue problem

$$\tilde{A}_k\varphi=\lambda_s(k)\varphi \text{ on } \Omega, \tag{4.5}$$

$$\varphi(x-\frac{1}{2})=\varphi(x+\frac{1}{2}). \tag{4.6}$$

with the identical eigenvalue sequence $(\lambda_s(s))_{s\in\mathbb{N}}$ as in (4.3) by (4.4). □

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 the Floquet transformation 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 [3, Chap. 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 $f \in L^2(\mathbb{R})$,

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

where we used Beppo Levi's Theorem to exchange summation and integration. This 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 $x \in \Omega$, 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 we have $\|Uf\|_{L^2(\Omega\times B)} = \|f\|_{L^2(\mathbb{R})}$. It is for us still to show that the mapping U is surjective, and that U^{-1} is given by (5.2) or (5.3). Let $g \in L^2(\Omega \times B)$, then define

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

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 then yields

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

which means $f \in L^2(\mathbb{R})$. For almost every $x \in \Omega$ (5.1) gives

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

whence (5.5) implies $Uf = g$ and (5.2). 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 $l \in \mathbb{N}$, 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 last 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

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

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

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

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 Lebesgue's 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

$$\|Uf - g_l\|_{L^2(\Omega\times B)} \to 0 \text{ as } l \to \infty \tag{5.8}$$

Using (5.6), (5.7) and (5.3), we find that $f_l = U^{-1} g_l$, whence (5.8) gives

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

and the assertion follows since $U\colon L^2(\mathbb{R}) \to L^2(\Omega \times B)$ is isometric by theorem 5.1. $\square$

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 characterise the dependence of I_s of k, more specifically that $\lambda_s(k)$ is continuous in k and hence I_s being for each k a compact interval.

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

Proof: Let us define

$$H^1_{per} \coloneqq \left\{ v \in H^1(\Omega) : v\left(x - \frac{1}{2}\right) = v\left(x + \frac{1}{2}\right)\right\}.$$

In the transformed eigenvalue problem (4.5) the boundary conditions (4.6) are periodic and independent of k. By Poincare's min-max principle for eigenvalues we have

$$\lambda_s(k) = \min_{\substack{U\subseteq H^1_{per}(\Omega)\\ \dim U = s}} \max_{v\in U\setminus\{0\}} \frac{\langle A_k v, v\rangle_{L^2(\Omega)}}{\langle v, v\rangle_{L^2(\Omega)}}.$$

Now, let $k \in B$ be fixed. For all $\tilde{k} \in B$ and all $v \in H^1_{per}(\Omega)$ using triangular inequality we can estimate for $J \in \left\{(x_0 - \frac{1}{2}, x_0), (x_0, x_0 + \frac{1}{2})\right\}$:

$$\frac{\langle\left(\frac{d}{dx} + i\tilde{k}\right) v, \left(\frac{d}{dx} + i\tilde{k}\right) v\rangle_{L^2(J)}}{\langle v, v\rangle_{L^2(J)}} \begin{Bmatrix} \leq \\ \geq \end{Bmatrix} \frac{\langle\left(\frac{d}{dx} + ik\right) v, \left(\frac{d}{dx} + ik\right) v\rangle_{L^2(J)}}{\langle v, v\rangle_{L^2(J)}}$$
$$\begin{Bmatrix} + \\ - \end{Bmatrix} \frac{2|k-\tilde{k}|\|v'\|_{L^2(J)}\|v\|_{L^2(J)}}{\|v\|^2_{L^2(J)}} \begin{Bmatrix} + \\ - \end{Bmatrix} \left||k|^2 - |\tilde{k}|^2\right| \tag{6.2}$$

Moreover, we can estimate

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

Hence (6.2) 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

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

Now, thew eigenvalue $\lambda_s(k)$ is also an eigenvalue of the problem (4.3), where the operator is dependent on k rather than on the boundary conditions. However, all eigenvalues of (4.3) are by the min-max-principle dominated by eigenvalues of the eigenvalue problem of A_k with Dirichlet boundary conditions and, as the eigenvalues for the Dirichlet boundary condition are independent of k, $\lambda_s(k)$ is uniformly bounded and hence continuous. □

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

$$I_s \textit{ is a compact real interval for each } s \in \mathbb{N}. \tag{6.3}$$

From (6.3) 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 (4.3) with Neumann boundary conditions. Since $\mu_s \to \infty$ as $s \to \infty$, we obtain $\min I_s \to \infty$ as $s \to \infty$, which together with (6.3) implies that

$$\bigcup_{s\in\mathbb{N}} I_s \text{ is closed.} \tag{6.4}$$

Now, we start proving (6.1) by proving the following theorem.

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

$$A_k \psi_s(\cdot, k) = \lambda \psi_s(\cdot, k) \tag{6.5}$$

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.

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

thus $\psi_s \in \mathcal{D}(A)$ 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

$$\eta(x) = 1 \text{ for } |x| \leq \frac{1}{4}, \quad \eta(x) = 0 \text{ for } |x| \geq \frac{1}{2}, \tag{6.6}$$

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

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

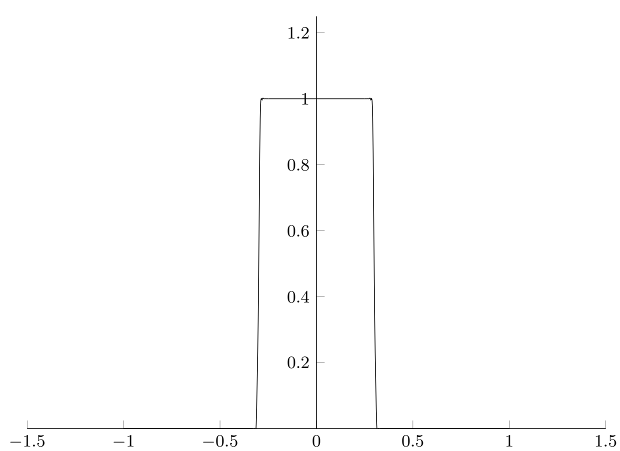

Figure 6.1: Example for a function η

Then

$$
\begin{aligned}
(A-\lambda I)u_l &= \sum_{i\in\mathbb{N}} \left[(-\frac{d^2}{dx^2} - \lambda) u_l|_{(x_i,x_{i+1})} \cdot \mathbb{1}_{(x_i,x_{i+1})} \right] \\
&= \sum_{i\in\mathbb{N}} \left[\eta\left(\frac{|\cdot|}{l}\right) \left(-\frac{d^2}{dx^2} - \lambda\right) \psi_s(\cdot,k)|_{(x_i,x_{i+1})} \cdot \mathbb{1}_{(x_i,x_{i+1})} \right] + R
\end{aligned} \tag{6.7}
$$

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 $\frac{l}{2}$. Thus, note that $\psi_s(\cdot,k) \in H^2_{loc}(\mathbb{R})$, the semi-periodic structure of $\psi_s(\cdot,k)$ implies

$$
\|R\|_{L^2(\mathbb{R})} \leq \frac{c}{l} \|\psi_s(\cdot,k)\|_{H^1(B_l)} \leq c\frac{1}{\sqrt{l}}. \tag{6.8}
$$

Now, the semi-periodic structure allows us find additionally an upper boundary for u_l:

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

Together with (6.4), (6.5) and (6.7), this gives

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

As moreover $u_l \in \mathcal{D}(A)$, this results in

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

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 arbitrary m-th order linear differential operator with periodic coefficients. Again, for the sake of completeness, we include the proof here, as given in [3, Chap. 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 (6.4), there exists some $\delta > 0$ such that

$$
|\lambda_s(k) - \lambda| \geq \delta \quad \text{ for all } s \in \mathbb{N}, k \in B \tag{6.9}
$$

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

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

and

$$u_l \coloneqq \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \frac{1}{\lambda_s(k)-\lambda} \langle (Uf)(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)} \psi_s(x,k) dk \tag{6.10}$$

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 $v \in \mathcal{D}(A_k)$

$$(A_k - \lambda I)v(\cdot,k) = (Uf)(\cdot,k) \quad \text{ on } \Omega. \tag{6.11}$$

Due to (6.11), both $v(\cdot,k)$ and $\psi_s(\cdot,k)$ satisfy semi-periodic boundary conditions. Hence, (4.3), (6.9) 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 $u \coloneqq U^{-1}v \in L^2(\mathbb{R})$. Thus, (6.11) 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 (6.10) 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

$$u_l \to u, \quad f_l \to f \quad \text{ in } L^2(\mathbb{R}) \text{ as } l \to \infty. \tag{6.12}$$

We will now prove that

$$\langle u_l, (A - \lambda I)v\rangle = \langle f_l, v\rangle \text{ for all } l \in \mathbb{N}, v \in \mathcal{D}(A); \tag{6.13}$$

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, (6.12) 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 (6.13). 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 (6.9), $(A_k - \lambda I)\varphi \in L^\infty(K)$ 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 (6.10), the fact that φ has compact support in the interior of K and (4.3) 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. (6.13). □

Chapter 7

The spectrum for the multi-dimensional case

In this last chapter, we will examine a more complex situation. We now 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 merely 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 a periodicity cell in $\mathbb{R}^n$ 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 with the conditions $\dim S = n-1$ and $S \subseteq \overset{\circ}{Y}$. Furthermore, let $B \subseteq Y$ denote the set enclosed by S, such that $S = \partial B$. We will denote for any $j \in \mathbb{Z}^n$ with $Y_j = Y + j$ the jth copy of Y, 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 S_i^+ and S_i^- the opposing edges of Y for $i = 1, 2$.

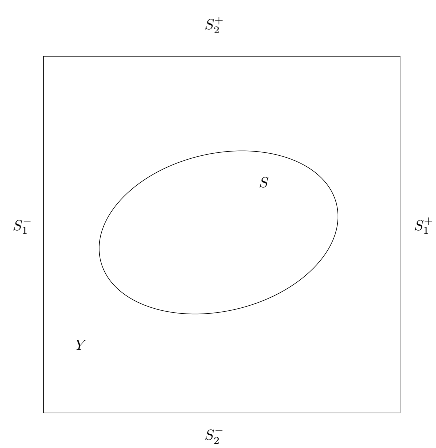

Figure 7.1: Periodicity cell for the multi-dimensional potential

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 Dirac delta distribution on hypersurface S_i. Let us recall that on a hypersurface S the Dirac delta acts on $u \in C_0^\infty(\mathbb{R}^n)$ by

$$\int_{\mathbb{R}^n} \delta_S u := \int_S u ds.$$

where s is the hypersurface measure associated to S_j, for a more detailed explanation see [5].

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

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

holds for all $v \in H^1(\mathbb{R}^n)$. Note that in the second term we denote by uv the traces. They are well defined as $u, v \in H^1(\mathbb{R})$ and hence the trace in $L^2(\mathbb{R})$. For a detailed explanation see [1, page 164].

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

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

Both terms on the right-hand side can be finitely estimated by the trace theorem [4, page 258] since

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

for some $h > 0$.

We can once again exert Lax-Migram's Theorem to prove the existence of a unique solution $u \in H^1(\mathbb{R}^n)$ in (7.2) for any $f \in L^2(\mathbb{R}^n)$ if $\mu \in \mathbb{R}$ is small enough. Hence, we can define the operator $R^n_\mu \colon f \mapsto u$ where $u \in H^1(\mathbb{R}^n)$ is the solution of (7.2). Same as in theorem 3.3 we can proof that R^n_μ is a bounded and injective operator. This on the other hand enables us to define A^n by means of R^n_μ:

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

Using similar methods as in chapter 3 we can prove the following two results.

Theorem 7.1 (Characterisation of $\mathcal{D}(A^n)$)**:** *Let* $\Omega := \mathbb{R}^n \setminus \overline{\bigcup_{j \in \mathbb{Z}^n} B_j}$. *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 the the equivalent properties of $\mathcal{D}(A)$. Hence, choosing in (7.2) similar functions to those above will yield the asserted. □

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

Proof: □

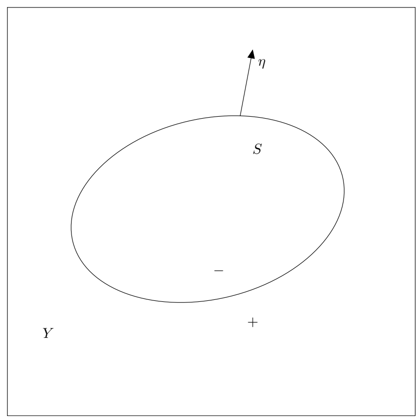

Figure 7.2: Normal η on the hypersurface S in a periodicity cell

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

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

such that

$$\int_Y \nabla u \overline{\nabla v} + \rho \int_S u\overline{v} ds - \mu \int_Y u\overline{v} = \int_Y f\overline{v} \tag{7.3}$$

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 injective. This allows us to define

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

as the operator considering our problem only on one periodicity cell. 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

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

Theorem 7.2: *The operator $R^n_{\mu,k}$ is compact.*

Proof: As in chapter 4, using the compact embedding theorem for Sobolev spaces yields the desired. □

By similar transformations of the problem (7.3) as in (4.5) and (4.6) we are then able to show that the eigenvalues of A^n_k are continuous functions of $k \in \overline{B}$, and thus $I_s = \{\lambda_s(k) : k \in \overline{B}\}$ is 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 4 based on Bloch waves, Floquet transform and a similar cut-off function η as in (6.6). 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, i.e.

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

Chapter 8

Outlook and Conclusion

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,...

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 [11, page 259]. $\square$

Theorem A.2: *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.3 (Approximation by test functions)**:** *$C_0^\infty(\mathbb{R})$ is dense in $L^p(\mathbb{R})$, if $1 \leq p < \infty$.*

Proof: See [11, page 82]. $\square$

Theorem A.4 (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. $\square$

Theorem A.5: *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 $\square$

Theorem A.6 (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 [4, page 645] $\square$

Theorem A.7: *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. $\square$

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

Theorem A.8 (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 [4, page 272]. $\square$

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 $(u_n)_n$ 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 [4, page 274]. $\square$

Theorem A.9 (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 [8, Amd to prob. 51]. $\square$

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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, 30th September 2016