Bachelor Thesis

On the spectra of 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 [7, 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:
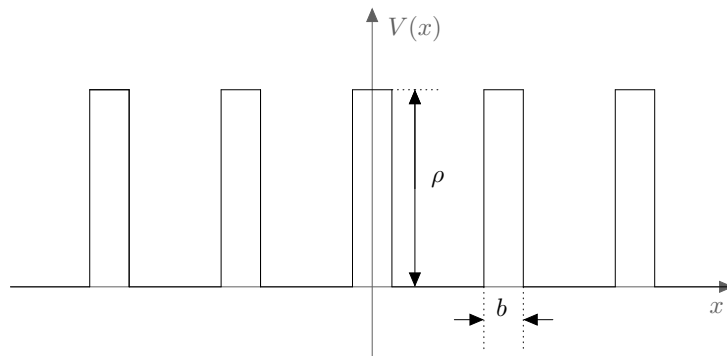

Figure 1.1: Potential $V(x)$ of the Kronig-Penney model

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}.

Mathematical Basics

For the upcoming analysis we need some basic concepts from functional analysis and spectral theory I wish to briefly review:

Let C_c^∞ 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 will hereafter $\langle x, x \rangle$ denote the scalar product in $L^2(\mathbb{R})$.

Definition (Weak derivative)**:** *Let $\Omega \subseteq \mathbb{R}$ be an open set and let u be a function in the Lebesgue space $L^1(\Omega)$. Then v in $L^1(\Omega)$ is a weak derivative of u if,*

$$\int_\Omega u(t)\varphi'(t)dt = -\int_\Omega v(t)\varphi(t)dt$$

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

Now, an important example for a Hilbert space is the Sobolev space $H^k(\Omega)$, which is defined to be the set of functions f in $L^2(\Omega)$ such that the function f and its weak derivatives up to the order k have a finite $L^2(\Omega)$ norm, by admitting the inner product in terms of the $L^2(\Omega)$ inner product for all derivatives up to order k:

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

Definition (Distributions)**:** *On C_0^∞ a sequence (f_n) converges against $f \in C_0^\infty$ 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 against f, i.e.

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

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 $\mathcal{D}(\mathbb{R})$ the space C_0^∞ equipped with this topology. From now on, we denote with $D'(\mathbb{R})$ 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 limit of a weakly converging sequence of functionals over normed symmetric around x_0 cumulative distribution functions δ_ϵ, whereas the support of those cumulative distributions converges to zero. It holds $\delta_{x_0} = \lim_{\epsilon \to 0} \delta_\epsilon$ in $D'(\mathbb{R})$. An example for such a sequence is

$$\delta_\epsilon(x) = \frac{1}{\sqrt{2\pi\epsilon}} e^{-\frac{x^2}{2\epsilon^2}}. \tag{1.1}$$

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, is easily seen that $\delta_{x_0}(f) = \lim_{\epsilon \to 0} \delta_\epsilon(f) = f(x_0)$, for a proof see [10].

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

    a) We call A closed if $\mathrm{graph}(A) := \{(x, Ax) : x \in \mathcal{D}(A)\} \subseteq X \times Y$ is a closed set.

Are X, Y Hilbert spaces and A a bounded operator we call

    b) A symmetric, if $\langle Tx, y \rangle = \langle x, Ty \rangle$ for all $x, y \in \mathcal{D}(A)$, and

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

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

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

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

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

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

Theorem 1.1: *The resolvent set $\rho(A) \subseteq \mathbb{C}$ of a bounded linear operator A is an open set.*

Proof: See [4, Chap. 6]   □

Chapter 2

The one-dimensional Schrödinger operator A

The mathematical representation of the above introduced problem 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 are going to examine properties of A such as its domain and show that A is self-adjoint. Later, in chapters 3 and 5, we will need these results to deduce characteristics about the spectrum of A.

Formally the operation of A is defined by

$$-\frac{d^2}{dx^2} + \rho \sum_{i \in \mathbb{Z}} \delta_{x_i} \tag{2.1}$$

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, given $f \in L^2(\mathbb{R})$, in which sense a solution to the formal problem

$$Au = f \tag{2.2}$$

exists since the potential in A is consists of a singular distribution. If we suppose for a moment that the problem is smooth, more specifically if the potential is given by (1.1), then formally multiplying it by a test function and integrating by parts yields the so called weak-formulation to the problem for whose solution less regularity is needed. 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

$$\int_{\mathbb{R}} u'\overline{v'} + \rho \sum_{i \in \mathbb{Z}} u(x_i)\overline{v(x_i)} - \mu \int_{\mathbb{R}} u\overline{v} = \int_{\mathbb{R}} f\overline{v} \quad \forall v \in C_0^\infty(\mathbb{R}), \tag{2.3}$$

holds and call it the weak-formulation of (2.2).

Remark: *Since $C_0^\infty(\mathbb{R})$ is dense in $H^1(\mathbb{R})$ with respect to the norm in $H^1(\mathbb{R})$, (2.3) holds also for all $v \in H^1(\mathbb{R})$.*

We should first note that the left-hand side of problem (2.3) is actually well-defined and finite, as for any $h \in (0,1]$ we can estimate

$$\sum_{i \in \mathbb{Z}} |u(x_i)|^2 \leq \sum_{i \in \mathbb{Z}} \left(2|u(x_i + h)|^2 + 2h \int_{x_i}^{x_i+h} \left| u'(\tau) \right|^2 d\tau \right)$$

$$\leq 2 \sum_{i \in \mathbb{Z}} \left(\frac{1}{h} \int_{\Omega_i} |u(x)|^2 dx + h \int_{\Omega_i} \left| u'(\tau) \right|^2 d\tau \right). \tag{2.4}$$

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

$$\sum_{i \in \mathbb{Z}} |u(x_i)|^2 \leq 2\|u\|_{H^1(\mathbb{R})}^2. \tag{2.5}$$

2.1 The resolvent-mapping of A

To explicitly define our operator A we will first show that for each $f \in L^2(\mathbb{R})$ the equation (2.3) 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*

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

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

$$B_\mu[u,v] = l_f(v) \quad \forall v \in H^1(\mathbb{R}). \tag{2.6}$$

The existence of a unique $u \in H^1(\mathbb{R})$ satisfying (2.6) 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, but above all note that $B[u, u] \in \mathbb{R}$.

Theorem 2.1: *The sesquilinear form B_μ is (for small enough $\mu \in \mathbb{R}$)*

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

$$|B_\mu[u, v]| \leq \alpha \|u\| \|v\|$$

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

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

$$\beta \|u\|^2 \leq B_\mu[u, u]$$

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

Proof:

i) The boundedness follows from (2.5) as for an arbitrary $\rho \in \mathbb{R}$ there exists $\alpha \in \mathbb{R}$ such that

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

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

ii) For the coercivity, we first assume $\rho \geq 0$. Now, if $\mu < -1$ we get

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

Analogously for $\rho < 0$, using (2.4) 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

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

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

Theorem 2.2: *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

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

$\qquad\qquad\square$

Therefore, as in theorem 2.1 used we will subsequent assume that $\mu \in \mathbb{R}$ is small enough. In return Lax-Migram's Theorem shows that for any fixed $f \in L^2(\mathbb{R})$ a unique solution $u \in H^1(\mathbb{R})$ to the problem (2.6) 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 (2.6).*

Taking in account that R_μ is a linear operator, which is easy to see, there are two more properties of R_μ for us left to show.

Theorem 2.3: *The mapping R_μ is bounded and injective.*

Proof: For $f \in L^2(\mathbb{R})$ there exists $u \in \mathcal{D}(A)$ such that

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

Now, using (2.5) with a small enough $\mu \in \mathbb{R}$ yields with Cauchy–Schwarz's inequality

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

Taking in mind that $\mathcal{R}(R_\mu) \subseteq H^1(\mathbb{R})$, we know that for $u_1 = u_2$

$$0 = B_\mu[u_1, v] - B_\mu[u_2, v] = \int_\mathbb{R} (f_1 - f_2)\overline{v} \quad \forall v \in H^1(\mathbb{R}). \tag{2.7}$$

As $H^1(\mathbb{R})$ is dense in $L^2(\mathbb{R})$ this yields that the equality (2.7) holds also for all $v \in L^2(\mathbb{R})$, hence $f_1 = f_2$ almost everywhere. $\qquad\square$

2.2   The domain of A

Resulting from theorem 2.3, 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 makes sense regarding formal definition in (2.1) and as show below is independent of μ.

Remark: *This allows us to draw the conclusions 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 (2.6) 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

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

Then, considering in (2.3) 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

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

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

$$\mathcal{D}(A) \subseteq \left\{ u \in \bigcap_{i\in\mathbb{Z}} H^2(x_i, x_{i+1}) \right\}.$$

Next, a test function $v \in C^\infty(\mathbb{R})$ with the property $\operatorname{supp} v = \Omega_k$ yields in (2.3) for any $k \in \mathbb{Z}$ through integration by parts on both sides of x_k that

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

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

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

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

and therefore

$$\mathcal{D}(A) \subseteq \left\{ u \in \bigcap_{i\in\mathbb{Z}} H^2(x_i, x_{i+1}) : u'(x_i-0) - u'(x_i+0) + \rho u(x_i) = 0 \ \forall i \in \mathbb{Z} \right\}. \qquad (2.8)$$

Last but not least we need one properties. Choosing a function $v \in C_0^\infty(\mathbb{R})$ with $\operatorname{supp} v = (x_{-n}, x_{n+1})$ in (2.3) yields with partial integration on every interval (x_i, x_{i+1}) with that

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

$$\Longleftrightarrow \sum_{i=-n}^{n-1} \int_{x_i}^{x_{i+1}} u''\overline{v} = -\int_{x_{-n}}^{x_n} f\overline{v} - \mu \int_{x_{-n}}^{x_n} u\overline{v} \qquad (2.9)$$

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 (2.9) by

$$|\langle w_n, v\rangle| \leq \left|\mu \int_{x_{-n}}^{x_n} u\overline{v}\right| + \left|\int_{x_{-n}}^{x_n} fv\right|$$

$$\leq |\mu| \|u\|_{L^2(x_{-n},x_n)} \|v\|_{L^2(x_{-n},x_n)} + \|f\|_{L^2(x_{-n},x_n)} \|v\|_{L^2(x_{-n},x_n)}$$

$$\leq c\|v\|_{L^2(x_{-n},x_n)}, \qquad (2.10)$$

for some $c \in \mathbb{R}$. Since c is independent of n we hence know by (2.10) that

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

This yields

$$\mathcal{D}(A) \subseteq \left\{ u \in H^1(\mathbb{R}) : u \in H^2\Big(\mathbb{R} \setminus \bigcup_{i \in \mathbb{Z}} x_i\Big), u'(x_j - 0) - u'(x_j + 0) - \rho u(x_j) = 0 \ \forall j \right\}. \quad (2.11)$$

For an arbitrary $u \in \mathcal{D}(A)$ we know hence from (2.11) that

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

For the reverse inclusion of (2.11) we use the operator R_μ but first let us, again for brevity, denote with B the right-hand side of (2.11). Now, since $\mathcal{R}(R_\mu) = \mathcal{D}(A)$, we proceed by proving each $u \in B$ is also in the range of R_μ. More specifically, as $\mathcal{D}(R_\mu) = L^2(\mathbb{R})$ define $f := -u''$ 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 ensure $f \in L^2$. Hence, we have to show $u = R_\mu(f - \mu u)$ or equivalently

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

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

For each $k \in \mathbb{Z}$ partial integration with a function $v \in C_c^\infty(\mathbb{R})$ having $\operatorname{supp} v = (x_k - \tfrac{1}{2}, x_k + \tfrac{1}{2})$ yields

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

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

Such that we conclude

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

Remark: *The definition of A is independent of μ since as seen above the domain is independent of μ and μ-dependent terms cancel each other out.*

2.3 The operator A is self-adjoint

In chapter 5, we will use the fact that the operator A self-adjoint, from with follows that A is a closed and symmetric operator. For this purpose we start by showing that R_μ and R_μ^{-1} are symmetric operators.

Theorem 2.4: R_μ and R_μ^{-1} are symmetric operator.

Proof: First, focus on $R_\mu^{-1} = (A - \mu I)$. As for all $v \in \mathcal{D}(A)$:

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

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

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

such that R_μ is also symmetric. $\square$

Now, using the fact that R_μ and R_μ^{-1} are both symmetric we can prove that A is self-adjoint.

Theorem 2.5: A is a self-adjoint operator.

Proof: As we already know that R_μ and 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

$$\langle R_\mu^{-1} u, v \rangle = \langle u, v^* \rangle, \quad \forall u \in \mathcal{D}(R_\mu^{-1}) \tag{2.12}$$

then $v \in \mathcal{D}(R_\mu^{-1})$ and $R_\mu^{-1} v = v^*$. In (2.12) we define $u \coloneqq R_\mu f$ for any $f \in L^2(\mathbb{R})$ and use the fact that R_μ is symmetric and defined on the whole of $L^2(\mathbb{R})$:

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

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 self-adjoint as well. $\square$

Every symmetric operator has an entirely real spectrum, hence theorem 2.5 yields our first result about the spectrum of A.

Chapter 3

Fundamental domain of periodicity and the Brillouin zone

In this chapter we will restrict the Kronig-Penney to one periodicity cell and examine the spectrum of the resulting operator. Solving the eigenvalue problem on the period cell while varying boundary conditions can be used to determine the eigenvalues of the unrestricted problem, which is exactly the approach we will use in chapter 5.

Let Ω be the fundamental domain of periodicity associated with (2.1), for simplicity let $\Omega := \Omega_0$ and thus $x_0 = 0$ being contained in Ω. As commonly used in literature the reciprocal lattice for Ω is $[-\pi, \pi]$, the so called one-dimensional Brillouin zone B. For fixed $k \in \overline{B}$, in this chapter we consider the operator A_k on Ω formally defined by the operation

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

Definition: *For every k we define for brevity the set of quasi-periodic functions*

$$H_k^1 := \left\{ \psi \in H^1(\Omega) : \ \psi(\frac{1}{2}) = e^{ik} \psi(-\frac{1}{2}) \right\}. \tag{3.1}$$

Remark: *Due to the fact that convergence in H_k^1 implies the convergence on the boundary of Ω, H_k^1 is a closed subspace of $H^1(\mathbb{R})$.*

Analogous to before, we 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 $v \in H^1_k$. One can apply the same arguments as above to prove that

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

is well-defined and injective. Consequently, we define now

$$A_k := R^{-1}_{\mu,k} + \mu I.$$

This chapter is now going to provide additional information about the operator $R_{\mu,k}$. We shall see that $R_{\mu,k}$ and that the eigenfunctions of A_k form a complete and orthonormal system in H^1_k.

3.1   The compactness of $R_{\mu,k}$

Theorem 3.1: *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 bounded a bounded sequence as well. Each such u_j is by definition in H^1_k and has to satisfies

$$\int_\Omega u'_j \overline{v'} + \rho u_j(x_0)\overline{v(x_0)} - \mu \int_\Omega u_j \overline{v} = \int f_j \overline{v} \quad \forall v \in H^1_k. \tag{3.2}$$

Now, the particular choice of $v = u_j$ in (3.2) yields with (2.5) for μ small enough

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

The compact embedding follows from the subsequently show estimation. As $H^1(\Omega) \subseteq C^{\frac{1}{2}}(\overline{\Omega})$ we can further estimate

$$|f(x) - f(y)| \leq c|x - y|^{\frac{1}{2}} \text{ for some } c > 0, \tag{3.3}$$

from which for $f \in B_{H^1_k} := \{f \in H^1_k(\Omega) : \|f\|_{H^1(\Omega)} \leq 1\}$ it follows that

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

For an arbitrary $\epsilon > 0$ we now partition Ω into n_ϵ equidistant, disjoint intervals I_k, i.e.

$\Omega = \bigcup_{j=1}^{n_\epsilon} I_j$. As all $f \in B_{H_k^1}$ are uniformly bounded on Ω by (2.5), there exist for each subinterval I_k a finite number of constants $c_{1,k}, \ldots, c_{\nu_\epsilon,k}$ such that

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

Hence, there are finitely many step functions such that for any $f \in L^2(\Omega)$ one of those step functions, let's call it $g \in L^2(\Omega)$ with function value c_k on sub interval I_k for each $k \in \{1, \ldots, n_\epsilon\}$, such that

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

This means in conclusion that $B_{H_k^1}$ is totally bounded in $L^2(\Omega)$ and in return H_k^1 can be compactly embedded in $L^2(\Omega)$. Thus, the operator $R_{\mu,k}$ is compact. $\qquad \square$

3.2 The spectrum of the operator A_k

As from now, consider the eigenvalue problem to find $\psi \in H_k^1$ such that

$$A_k \psi = \lambda \psi \text{ on } \Omega. \tag{3.4}$$

In writing the boundary condition in (3.1), we understand ψ extended to the whole of $\mathbb{R}$. In fact, (3.1) forms boundary conditions on $\partial\Omega$, so-called semi-periodic boundary conditions. Obviously, A_k has the same sequence of eigenfunctions as $R_{\mu,k}$, and if $\tilde{\lambda}$ is an eigenvalue for the eigenfunction ψ of $R_{\mu,k}$ then respectively is

$$\lambda = \frac{1}{\tilde{\lambda}} - \mu$$

an eigenvalue for the same eigenfunction ψ for the operator A, for proof see [9]. Since Ω is bounded, and $R_{\mu,k}$ is a compact and symmetric operator, A_k has moreover 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 eigenfunction form a $\langle \cdot, \cdot \rangle$-orthonormal and complete system $(\psi_s(\cdot, k))_{s \in \mathbb{N}}$ of eigenfunctions for (3.1). We transform the eigenvalue problem (3.4) such that the boundary condition is independent from k, define

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

Then,

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

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

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

and using (3.4) and (3.1), hence yields

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

Which shows that $(\varphi_s(\cdot, k))_{s \in \mathbb{N}}$ is an orthonormal and complete system of eigenfunctions of the periodic eigenvalue problem

$$\tilde{A}_k \varphi = \lambda_s(k) \varphi \text{ on } \Omega, \tag{3.5}$$

$$\varphi\left(x - \frac{1}{2}\right) = \varphi\left(x + \frac{1}{2}\right). \tag{3.6}$$

with the identical eigenvalue sequence $(\lambda_s(s))_{s \in \mathbb{N}}$ as in (3.4).

Chapter 4

The Floquet transformation

In the next chapter we are going to show that the spectrum of the operator A can be constructed through the above introduced eigenvalue sequences $(\lambda_s(k))_{s \in \mathbb{N}}$ by varying k over the Brillouin zone B. For this transfer we will need two results involving the Floquet transformation. With those we are able to move the problem from $L^2(\mathbb{R})$ to $L^2(\Omega \times B)$ whereas $\Omega \times B$ is by assumption compact. Even though the following two results do not differ in both the statement or the proof from standard theory, as in [1, Chap. 3], I still want to list them here for completeness.

Theorem 4.1: *The Floquet transformation* $U \colon L^2(\mathbb{R}) \to L^2(\Omega \times B)$

$$(Uf)(x,k) := \frac{1}{\sqrt{|B|}} \sum_{n \in \mathbb{Z}} f(x-n)e^{ikn} \quad (x \in \Omega, k \in B). \tag{4.1}$$

is an isometric isomorphism, with inverse given by

$$(U^{-1}g)(x-n) = \frac{1}{\sqrt{|B|}} \int_B g(x,k)e^{-ikn}dk \quad (x \in \Omega, n \in \mathbb{Z}). \tag{4.2}$$

If $g(\cdot,k)$ *is extended to the whole of* $\mathbb{R}$ *by the semi-periodicity condition* (3.1)*, the inverse simplifies to*

$$U^{-1}g = \frac{1}{\sqrt{|B|}} \int_B g(\cdot,k)dk. \tag{4.3}$$

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

$$\int_\mathbb{R} |f(x)|^2 dx = \sum_{n \in \mathbb{Z}} \int_\Omega |f(x-n)|^2 dx, \tag{4.4}$$

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 (4.1) (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 (4.4), and

$$\|Uf\|_{L^2(\Omega\times B)} = \|f\|_{L^2(\mathbb{R})}.$$

We still haven't shown that U is onto, and that U^{-1} is given by (4.2) or (4.3). Let $g \in L^2(\Omega \times B)$, then define

$$f(x-n) := \frac{1}{\sqrt{|B|}}\int_B g(x,k)e^{-ikn}dk \quad (x \in \Omega, n \in \mathbb{Z}). \tag{4.5}$$

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

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

which means $f \in L^2(\mathbb{R})$. For almost every $x \in \Omega$ (4.1) gives

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

whence (4.5) implies $Uf = g$ and (4.2). Now (4.3) follows from (4.2) and exploiting $g(x+n,k) = e^{ikn}g(x,k)$. $\qquad\square$

4.1 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 4.2: *For each $f \in L^2(\mathbb{R})$ and $l \in \mathbb{N}$, define*

$$f_l(x) := \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \langle (Uf)(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)} \psi_s(x, k) dk \quad (x \in \mathbb{R}). \tag{4.6}$$

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. As $(\psi_s(\cdot, k))_{s \in \mathbb{N}}$ 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

$$g_l(x, k) := \sum_{s=1}^{l} \langle (Uf)(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)} \psi_s(x, k). \tag{4.7}$$

Moreover, we get by Bessel's inequality

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

for all $l \in \mathbb{N}$ and almost every $k \in B$. Next, $\|(Uf)(\cdot, k)\|_{L^2(\Omega)}^2 \in L^1(B)$ as a function of k by Theorem 4.1, thus by Lebesgue's Dominated Convergence theorem

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

All in all, this means

$$\|Uf - g_l\|_{L^2(\Omega \times B)} \to 0 \text{ as } l \to \infty \tag{4.8}$$

If $g(\cdot, k)$ is extended to the whole of $\mathbb{R}$ by the semi-periodicity condition (3.1), using (4.6), (4.7) and (4.3), we find that $f_l = U^{-1}g_l$, whence (4.8) gives

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

$\square$

Chapter 5

The spectrum of A

Now, in the 5th chapter will now prove the main result for the one-dimensional case stating that for the operator A it holds that

$$\sigma(A) = \bigcup_{s \in \mathbb{N}} I_s, \tag{5.1}$$

where $I_s := \{\lambda_s(k) : k \in \overline{B}\}$ $(s \in \mathbb{N})$.

To show this equality we first need to characterise the dependence of I_s from k, more specifically that $\lambda_s(k)$ is continuous in k and hence I_s a compact interval.

Theorem 5.1: *For all $s \in \mathbb{N}$ the function $\lambda_s(k)$ is continuous in $k \in \overline{B}$.*

Proof: By assumption our potential is bounded and we define

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

In the transformed eigenvalue problem (3.5) the boundary conditions (3.6) are periodic and independent from 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 $J \in \{(x_0 - \frac{1}{2}, x_0), (x_0, x_0 + \frac{1}{2})\}$:

$$\frac{\langle \left(\frac{d}{dx} + i\tilde{k}\right) v, \left(\frac{d}{dx} + i\tilde{k}\right) v \rangle_{L^2(J)}}{\langle v, v \rangle_{L^2(J)}} \left\{{\leq \atop \geq}\right\} \frac{\langle \left(\frac{d}{dx} + ik\right) v, \left(\frac{d}{dx} + ik\right) v \rangle_{L^2(J)}}{\langle v, v \rangle_{L^2(J)}}$$

$$\left\{{+ \atop -}\right\} \frac{2|k - \tilde{k}| \|v'\|_{L^2(J)} \|v\|_{L^2(J)}}{\|v\|_{L^2(J)}^2} \left\{{+ \atop -}\right\} \left||k|^2 - |\tilde{k}|^2\right| \quad (5.2)$$

Moreover, we can estimate

$$2\|v'\|_{L^2(J)} \|v\|_{L^2(J)} \leq 2\| \left(\frac{d}{dx} + ik\right) v\|_{L^2(J)} \|v\| + 2|k| \|v\|_{L^2(J)}^2$$

$$\leq \| \left(\frac{d}{dx} + ik\right) v\|_{L^2(J)}^2 + \|v\|_{L^2(J)}^2 + 2|k| \|v\|_{L^2(J)}^2$$

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

Hence (5.2) yields

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

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

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

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

Which means ultimately

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

Now, the eigenvalue $\lambda_s(k)$ is also an eigenvalue of the problem (3.4), where the operator is dependent on k and not the boundary conditions. However, all eigenvalues of (3.4) 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 from k, $\lambda_s(k)$ is uniformly bounded and hence continuous. $\qquad \square$

Remark: *As B is compact, connected and $\lambda_s(k)$ is a continuous function of $k \in B$ we derive for (5.1)*

$$I_s \text{ is a compact real interval for each } s \in \mathbb{N}. \qquad (5.3)$$

Through (5.3) we get moreover 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 (3.4) 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 (5.3) implies that

$$\bigcup_{s \in \mathbb{N}} I_s \text{ is closed.} \tag{5.4}$$

The first part of the statement (5.1) is

Theorem 5.2: $\sigma(A) \supset \bigcup_{s \in \mathbb{N}} I_s$.

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

$$A_k \psi_s(\cdot, k) = \lambda \psi_s(\cdot, k) \tag{5.5}$$

We regard $\psi_s(\cdot, k)$ as extended to the whole of $\mathbb{R}$ by the boundary condition (3.1), whence, due to the periodic structure of A, ψ_s satisfies

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

"locally", i.e.

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

thus $\psi_s \in \mathcal{D}(A)$ and $-\psi_s'' = \lambda \psi_s$ on each $\Omega_j \setminus \{x_j\}$. Now, if we choose a function $\eta \in H^2(\mathbb{R})$ such that

$$\eta(x) = 1 \text{ for } |x| \leq \frac{1}{4}, \quad \eta(x) = 0 \text{ for } |x| \geq \frac{1}{2}, \tag{5.6}$$

and define, for each $l \in \mathbb{N}$,
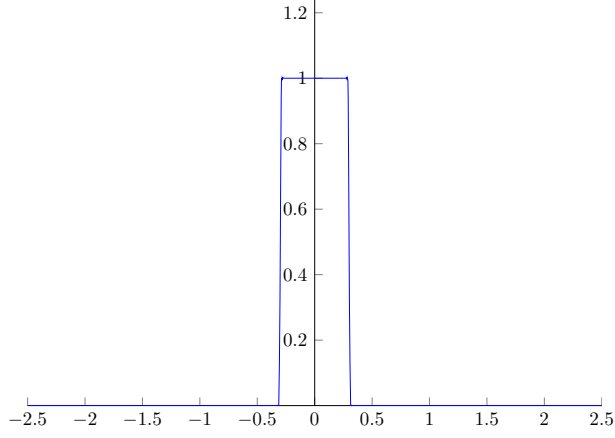
$$u_l(x) := \eta\left(\frac{|x|}{l}\right) \psi_s(x, k).$$

Figure 5.1: Example for a "cut-off" function η

Then

$$(A - \lambda I)u_l = \sum_{i \in \mathbb{N}} \left[(-\frac{d^2}{dx^2} - \lambda)u_l|_{(x_i, x_{i+1})} \cdot \mathbb{1}_{(x_i, x_{i+1})} \right] \tag{5.7}$$

$$= \sum_{i \in \mathbb{N}} \left[\left(-\frac{d^2}{dx^2} - \lambda \right) \left(\eta\left(\frac{|\cdot|}{l} \right) \psi_s(\cdot, k) \right) \Big|_{(x_i, x_{i+1})} \cdot \mathbb{1}_{(x_i, x_{i+1})} \right]$$

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

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

$$\|R\|_{L^2(\mathbb{R})} \leq \frac{c}{l} \|\psi_s(\cdot, k)\|_{H^1((\frac{l}{2}, \frac{l}{2}))} \leq c\frac{1}{\sqrt{l}}. \tag{5.8}$$

Together with (5.4), (5.5) and (5.7), this gives

$$\frac{1}{\|u_l\|} \|(A - \lambda I)u_l\| \leq \frac{c}{l}$$

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

$$\frac{1}{\|u_l\|} \|(A - \lambda I)u_l\| \to 0 \text{ as } l \to \infty$$

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

The other inclusion can be shown by using the previous shown properties of the Floquet

transformation and the completeness of the Bloch waves. Hence, this prove doesn't differ from the one for an arbitrary m-th order linear differential operator with periodic coefficients. Again, due to completeness I still want to list the proof here, even though one can find it for example in [1, Chap. 3]

Theorem 5.3: $\sigma(A) \subset \bigcup_{s \in \mathbb{N}} I_s$.

Proof: Let $\lambda \in \mathbb{R} \setminus \bigcup_{s \in \mathbb{N}} I_s$. Hence, due to (5.4), there exists some $\delta > 0$ such that

$$|\lambda_s(k) - \lambda| \geq \delta \quad \text{for all } s \in \mathbb{N}, k \in B \tag{5.9}$$

We have 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

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

and

$$u_l := \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \frac{1}{\lambda_s(k) - \lambda} \langle (Uf)(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)} \psi_s(x, k) dk \tag{5.10}$$

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

$$(A_k - \lambda I)v(\cdot, k) = (Uf)(\cdot, k) \quad \text{on } \Omega. \tag{5.11}$$

Due to (5.11), both $v(\cdot, k)$ and $\psi_s(\cdot, k)$ satisfy semi-periodic boundary conditions. Hence, (3.4), (5.9) and Parseval's identity yield

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

By Theorem 4.1 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, (5.11) gives

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

Now, we are able to apply Theorem 4.2 this yields for (5.10) 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 4.2 gives

$$u_l \to u, \quad f_l \to f \quad \text{in } L^2(\mathbb{R}) \text{ as } l \to \infty. \tag{5.12}$$

We will now prove that

$$\langle u_l, (A - \lambda I)v\rangle = \langle f_l, v\rangle \text{ for all } l \in \mathbb{N}, v \in \mathcal{D}(A); \tag{5.13}$$

As A is self-adjoint, by Theorem 2.5, 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, (5.12) 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 (5.13). So, let $\varphi \in C_0^\infty(\mathbb{R})$ be fixed, and let $K \subseteq \mathbb{R}$ denote an open interval containing $\text{supp}(\varphi)$ in its interior. By Fubini's Theorem we know that

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

and

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

are in $L^2(K \times B)$, since (5.9), $(A_k - \lambda I)\varphi \in L^\infty(K)$ 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. Now , 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 4.1. 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 (5.10), the fact that φ has compact support in the interior of K and (3.4) we conclude

$$\int_K u_l(x)\overline{(A - \lambda I)\varphi(x)}dx = \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_K \left(\int_B r_s(x, k)dk \right) dx$$

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

$$= \int_K \left[\frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \langle (Uf)(\cdot, k), \psi_s(\cdot, k)\rangle_{L^2(\Omega)} \psi_s(x, k)dk \right] \overline{\varphi(x)}dx$$

$$= \int_K f_l(x)\overline{\varphi(x)}dx,$$

i.e. (5.13). $\qquad\square$

Chapter 6

The multi-dimensional case

In this last chapter, we are going to 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, as below.

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 $Y = [0,1]^n$ and hence $B = [-\pi, \pi]^n$. 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 $B_j = B + j$. Furthermore, we denote with S_i^+ and S_i^- the opposing edges of Y for $i = 1, 2$.
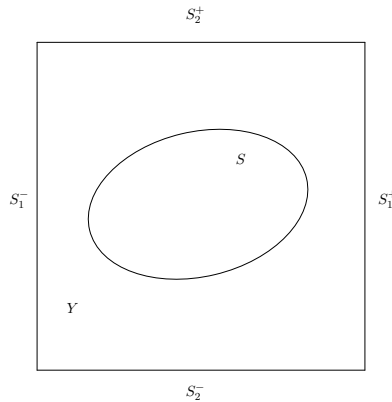

Figure 6.1: Periodicity cell for the multi-dimensional potential

The mathematical representation of the above is a multi-dimensional Schrödinger operator A^n whose operation is formally defined by

$$-\Delta + \rho \sum_{i \in \mathbb{Z}} \delta_{S_i} \tag{6.1}$$

on the whole of $\mathbb{R}^n$, where δ_{S_i} denotes the Dirac delta distribution on hypersurface S_i. that integrates any function $u \in L^2(\mathbb{R})$ over the compact set S_i.

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

$$\int_{\mathbb{R}^n} \nabla u \overline{\nabla v} + \rho \sum_{i \in \mathbb{Z}^n} \int_{S_j} u \overline{v} ds - \mu \int_{\mathbb{R}^n} u \overline{v} = \int_{\mathbb{R}^n} f \overline{v} \tag{6.2}$$

holds for all $v \in H^1(\mathbb{R}^n)$, where s is the hypersurface measure associated to all S_j.

Remark: *The term originating from the potential is finite as*

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

Both terms on the right-hand side can be finitely estimated by the Trace theorem [3, Chap. 5] as

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

for some $h > 0$.

We can once again exert Lax-Migram's Theorem to prove in (6.2) the existence of a unique solution $u \in H^1(\mathbb{R}^n)$ in (6.2) for any $f \in L^2(\mathbb{R}^n)$ if μ is small enough, define the operator injective $R^n_\mu \colon f \mapsto u$ and define A^n by means of R^n_μ.

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

Theorem 6.1 (Characterisation of $\mathcal{D}(A^n)$)**:** *Let $\Omega := \mathbb{R}^n \setminus \overline{\bigcup_{j \in \mathbb{Z}^n} B_j}$. By choosing similar to above different functions $v \in C^\infty(\mathbb{R}^n)$ in (6.2) we can further characterise such $u \in \mathcal{D}(A^n)$, 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. $u|_{S_j - 0} = u|_{S_j + 0}$

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
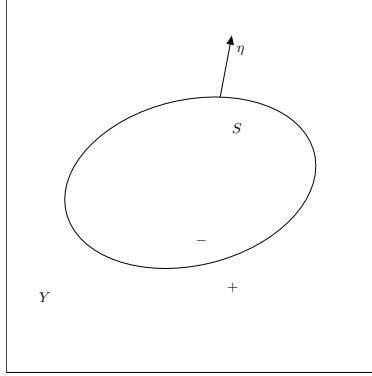

Figure 6.2: Normal η on the hypersurface S in a periodicity cell

Now, restricting again this problem to a fundamental domain of periodicity, for example Y, We 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

$$\int_Y \nabla u \overline{\nabla v} + \rho \int_S u\overline{v} ds - \mu \int_Y u\overline{v} = \int_Y f\overline{v} \qquad (6.3)$$

for all $v \in H^1_{k,n}$. Again exerting Lax-Milgram's Theorem the existence of a unique solution $u \in H^1_{k,n}$ is ensured if μ 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

$$A^n_k := R^n_{\mu,k} + \mu I.$$

The semi-periodic boundary conditions on $H^1_{k,n}$ require a solution $u \in H^1_{k,n}$ to (6.3) 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 6.2: *The operator* $R^n_{\mu,k}$ *is compact.*

Proof: As in chapter 3 used, the compact embedding yields the desired result, for a multi-dimensional proof see [6, Chap. 4]. □

By similar transformations of the problem (6.3) as in (3.5) and (3.6) we are 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, using the same arguments as in Chapter 4 based on Bloch waves, Floquet transform and a similar cut-off function η as in (5.6), we are then able to prove the main result even for this multi-dimensional case, namely that the spectrum of a self-adjoint Schrödinger operator with periodic delta-potential on a hypersurface is the union of compact intervals, i.e.

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

6.1 Outlook

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,...

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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, den 13. September 2016