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:

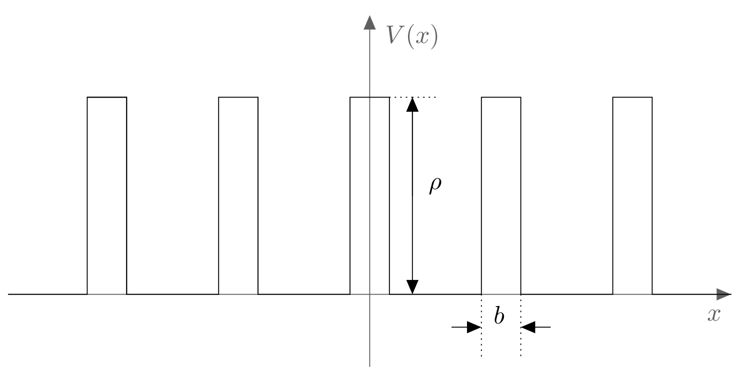

Figure 1.1: Kronig-Penney model

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.

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

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

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

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 [9].

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 $graph(A) := \{(x, Ax) : x \in \mathcal{D}(A)\} \subseteq X \times Y$ 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

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

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.*

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 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

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

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

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

We will now show that for each $f \in L^2(\mathbb{R})$ the equation (2.3) has a unique solution.

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

$$l(v) \coloneqq \int_{\mathbb{R}} fv$$

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

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

Then (2.3) is equivalent to finding $u \in H^1(\mathbb{R})$ such that

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

The existence of a unique $u \in H^1(\mathbb{R})$ satisfying (2.6) follows from Lax-Milgram's Theorem if the sesquilinear form B is bounded and coercive, which we will prove in the next theorem.

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

Thus, there exists a unique solution $u \in H^1(\mathbb{R})$ to the problem (2.6) for fixed $f \in L^2(\mathbb{R})$, and the operator $R_\mu \colon L^2(\mathbb{R}) \to L^2(\mathbb{R}), f \mapsto u$ is well-defined for $\mu \in \mathbb{R}$ small enough, taking in mind that $\mathcal{R}(R_\mu) \subseteq H^1(\mathbb{R})$. This mapping is injective since for $u_1 = u_2$

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

Since further $H^1(\mathbb{R})$ is dense in $L^2(\mathbb{R})$ this yields that the equality (2.7) holds also for all $v \in L^2(\mathbb{R})$ and therefore $f_1 = f_2$ almost everywhere. Consequently R_μ is invertible and as a result we can now define the Schrödinger operator as follows

$$A \coloneqq R_\mu^{-1} + \mu I$$

from which additionally follows that R_μ is the resolvent of A.

2.1 The domain of A

First, we define

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

If we now consider 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 furthermore

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

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

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

Next, a test function $v \in C^\infty(\mathbb{R})$ sucht that $\operatorname{supp} v = \Omega_k$ will yield for an arbitrary $k \in \mathbb{Z}$ from (2.3) through integration by parts on both sides of x_k that

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

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

But as $v \in C^\infty(\mathbb{R})$ was arbitrary, choosing one that is non-zero in x_k yields

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

and therefore

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

Using both these properties, choosing a function $v \in C_0^\infty(x_{-n}, x_{n+1})$ in (2.3) yields with partial integration on every interval (x_i, x_{i+1}) with for every $i \in \mathbb{Z}$ that

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

$$\iff \sum_{i=-n}^{n-1}\int_{x_i}^{x_{i+1}} u''\overline{v} = -\int_{x_{-n}}^{x_n} f\overline{v} - \mu\int_{x_{-n}}^{x_n} u\overline{v} \tag{2.9}$$

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 (2.9) by

$$\begin{aligned} |\langle w_n, v\rangle| &\le \left|\mu\int_{x_{-n}}^{x_n} u\overline{v}\right| + \left|\int_{x_{-n}}^{x_n} fv\right| \\ &\le |\mu|\|u\|_{L^2(x_{-n},x_n)}\|v\|_{L^2(x_{-n},x_n)} + \|f\|_{L^2(x_{-n},x_n)}\|v\|_{L^2(x_{-n},x_n)} \\ &\le c\|v\|_{L^2(x_{-n},x_n)}, \end{aligned} \tag{2.10}$$

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

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

Since $u \in H^1(\mathbb{R})$ this yields

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

Hence, for an arbitrary $u \in \mathcal{D}(A)$ it follows

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

We can further prove the opposite inclusion for (2.1). 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 also know that $f \in L^2$ and 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 having $\operatorname{supp} v = (x_k - \frac{1}{2}, x_k + \frac{1}{2})$ 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

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

2.2 The operator A is self-adjoint

In chapter 5, we will further utilise the fact that the operator A is self-adjoint. A self-adjoint operator is always closed, symmetric and has a completely real spectrum which narrows the analysis of its spectrum down.

Theorem 2.2: *R_μ and R_μ^{-1} are symmetric operator.*

Now, using both symmetries we can show that A is self-adjoint:

Theorem 2.3: *A is a self-adjoint operator.*

Chapter 3

Fundamental domain of periodicity and the Brillouin zone

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

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

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 $v \in H_k^1$. 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 now

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

This chapter is going to provide additional information about the operator $R_{\mu,k}$. We will see that the eigenfunctions of A_k form a complete and orthonormal system in H_k^1. Using this fact we can then deduce additional properties about the spectrum of A_k and A in chapter 5.

Theorem 3.1: *The operator $R_{\mu,k}$ is compact.*

3.1 The spectrum of the operator A_k

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

$$A_k\psi = \lambda\psi \text{ on } \Omega. \tag{3.2}$$

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 [8]. 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 (3.2) 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 (3.2) and (3.1), hence yields

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

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

$$\tilde{A}_k\varphi = \lambda_s(k)\varphi \text{ on } \Omega, \tag{3.3}$$

$$\varphi(x-\frac{1}{2}) = \varphi(x+\frac{1}{2}). \tag{3.4}$$

with the identical eigenvalue sequence $(\lambda_s(s))_{s\in\mathbb{N}}$ as in (3.2).

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 eigenvalue sequences $(\lambda_s(k))_{s\in\mathbb{N}}$ by varying k over the Brillouin zone B. For that we need two results involving the Floquet transformation, which transfers 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*

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

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*

$$f_l(x) \coloneqq \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \langle (Uf)(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)} \psi_s(x, k) dk \quad (x \in \mathbb{R}). \tag{4.4}$$

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

Chapter 5

The spectrum of A

We will now prove the principal result, stating that for the operator A it holds

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

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

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

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

$$I_s \textit{ is a compact real interval for each } s \in \mathbb{N}. \tag{5.2}$$

Through (5.2) 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 (3.2) 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 (5.2) implies that

$$\bigcup_{s\in\mathbb{N}} I_s \text{ is closed.} \tag{5.3}$$

The first part of the statement (5.1) is

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

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

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 $i = 1, 2$.

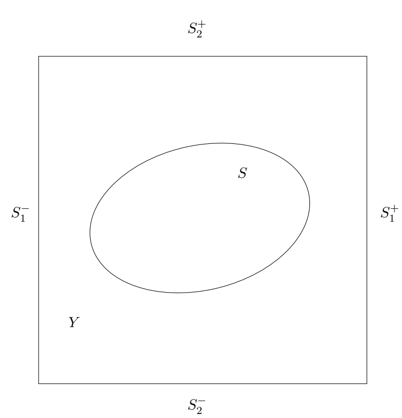

Figure 6.1: Periodicity cell for the multi-dimensional potential

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

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

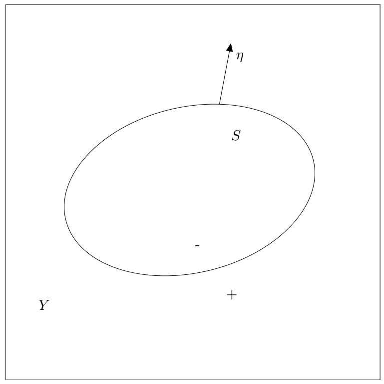

Figure 6.2: Periodicity cell with normal η on S

Now, restricting again this problem to a fundamental domain of periodicity, for example Y, We consider, analogous to before, the problem to find

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

such that

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

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

$$A_k^n \coloneqq R_{\mu,k}^n + \mu I.$$

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* $R_{\mu,k}^n$ *is compact.*

By similar transformations of the problem (6.3) as in (3.3) and (3.4) we are able to show that the eigenvalues of A_k^n 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 (**??**), 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