Karlsruher Institut für Technologie

Bachelor Thesis

On the spectra of Schrödinger operator with periodic delta potential

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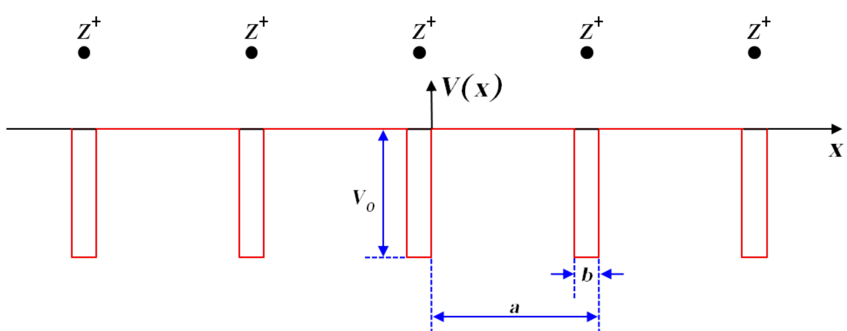
Chapter 1

Introduction

The problem considered in this thesis arises from the Kronig-Penney model which describes an idealised quantum-mechanical system, that demonstrates a particle behaving as a matter wave moving in one-dimension trough 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. They create an electromagnetic field around themselves and hence any particle moving through such a crystal would be subject to a periodic 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 a, the potential function $V(x)$ in the lattice can be approximated by a rectangular potential like this:



where b is the "support" and ρ the magnitude of the potential.

This thesis will examine the spectrum of an operator describing a special case of the Kronig-Penney model, namely by taking the limit $b \to 0$ with a finite modulus of the potential which represents the ion creating a finite singular potential.

Mathematical Basics

For the upcoming analysis we need some basic concepts from functional analysis and spectral theory I want to briefly recapitulate

Topics I don't know if I'm supposed to introduce them:

- Introducing: weak formulation

I will introduce

- Defining: symmetric and self-Adjoint operators
- Introducing weak derivates

Let C_c^∞ denote the linear space containing all smooth function $f\colon \mathbb{R} \to \mathbb{R}$ with compact support, i.e. for $f \in C_c^\infty$ there exists a compact interval $I \subseteq \mathbb{R}$ such that $f(x) = 0$ for all $x \notin I$. Together with the supremums norm $\|\cdot\|_\infty$ is C_c^∞ a normed vector space.

Hilbert and Sobolev spaces

A normed vector space $(X, \|\cdot\|)$ is called a pre-Hilbert space, if there exists a scalar product $\langle \cdot, \cdot, \rangle$ on $X \times X$ such that

$$\|x\| = \langle x, x \rangle^{\frac{1}{2}}$$

Any pre-Hilbert space that is additionally also a complete space is called a Hilbert space.

For $\Omega \subseteq \mathbb{R}$ the Sobolev space $H^k(\Omega)$ is defined to be the subset of functions f in $L^2(\Omega)$ such that the function f and its weak derivatives up to some order k have a finite $L^2(\Omega)$ norm. Furthermore, the space $H^k(\Omega)$ admits an inner product, which is defined in terms of the $L^2(\Omega)$ inner product:

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

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

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 $D(\mathbb{R})$ the space C_0^∞ equipped with this topology. As the space of distribution, $D'(\mathbb{R})$ we now denote all linear functionals on C_0^∞ that are continuous with respect to this topology.

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 be

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

Which implies the definition

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

Moreover, is easily seen that $\delta_{x_0}(f) = \lim_{\epsilon \to 0} \delta_\epsilon(f) = f(x_0)$.

Proof: We have

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

The substitution $z := \frac{x-x_0}{\sqrt{2}\epsilon}$ implies

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

Using the taylor series of f in x_0 we obtain

$$f(x) = f(x_0) + \mathcal{O}(\epsilon),$$

Hence:

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

where we used the fact that $\int_{-\infty}^{\infty} e^{-z^2}$ is a Gaussian integral and equal to $\sqrt{\pi}$. We can see that through :

$$\left(\int_{-\infty}^{\infty} e^{-x^2}dx\right)\left(\int_{-\infty}^{\infty} e^{-y^2}dy\right) = \int_{\mathbb{R}^2} e^{(x^2+y^2)}d(x,y).$$

As we integrate over the whole $\mathbb{R}^2$ substituting in polar coordinates with the substition $z := \rho^2$ yields

$$\int_0^{2\pi}\int_0^{\infty} e^{-\rho^2}\rho d\rho d\varphi = 2\pi\int_0^{\infty} e^{-\rho^2}\rho d\rho = \pi\int_0^{\infty} e^{-z^2}dz = \pi\left[-e^{-z}\right]_0^{\infty} = \pi$$

□

Spectrum and resolvent of an operator

Let X be a Banach space and let $A\colon \mathcal{D}\to X$ be a linear operator with domain $D(A)\supset X$. Let I denote the identity operator on X. Then we define for any $\lambda\in\mathbb{C}$

a) λ belongs in the resolvent set of A, $\lambda\in\rho(A)$, if and only if

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

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

c) $\lambda \in \rho(A) \to R(\lambda, A) = (\lambda - A)^{-1}$ 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: First, we note that the resolvent set is bounded as for $|\lambda| > \|A\|$ then $\|\lambda^{-1}A\| < 1$ and the operator $A - \lambda I = -\lambda(I - \lambda^{-1}A)$ has by the Neumann series the inverse

$$R(\lambda, A) = (A - \lambda I)^{-1} = -\sum_{k=0}^{\infty} \lambda^{-k-1} A^k.$$

Now, to show that $\rho(A)$ is open we have proceed by showing that for any $\lambda \in \rho(A)$ there exist $\epsilon > 0$ such that all μ with $|\lambda - \mu| < \epsilon$ are also in $\rho(A)$. For that consider

$$\begin{aligned} A - \mu I &= A - \lambda I + (\lambda - \mu) I \\ &= (A - \lambda I)\left(I + (\lambda - \mu)(A - \lambda I)^{-1}\right). \end{aligned}$$

The last expression is an invertible operator because $T - \lambda I$ is invertible by the assumption and $I + (\lambda - \mu)(T - \lambda I)^{-1}$ is invertible again by the Neumann series, since $\|(\lambda - \mu)(A - \lambda I)^{-1}\| < 1$ if $\epsilon < \|(A - \lambda I)^{-1}\|$. $\square$

Chapter 2

The 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. 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.o.l.g. let $x_0 = 0$ and $|\Omega_i| = 1$ for all $i \in \mathbb{Z}$.

In general, one cannot say given a right-hand side $f \in L^2(\mathbb{R})$ in which sense a solution exists to the problem $Au = f$, as the potential is given by a singular distribution. Hence, we consider for $\mu \in \mathbb{R}$ the problem

$$\int_{\mathbb{R}} u'\overline{v'} + \rho \sum_{i \in \mathbb{Z}} u(x_i)\overline{v(x_i)} - \mu \int u\overline{v} = \int f\overline{v} \quad \forall v \in H^1(\mathbb{R}), \tag{2.2}$$

where $u \in H^1(\mathbb{R})$ and $f \in L^2(\mathbb{R})$.

We should first note that left-hand side of problem (2.2) is actually well-defined and finite, as for any $h \in (0,1]$ we find for every $i \in \mathbb{Z}$ a point $\tilde{x}_i \in \Omega_i$ such that

$$
\begin{aligned}
\sum_{i\in\mathbb{Z}} |u(x_i)|^2 &\le \sum_{i\in\mathbb{Z}} \left(\left| u(\tilde{x}_i) - \int_{x_i}^{\tilde{x}_i} u'(\tau) d\tau \right| \right)^2 \\
&\le \sum_{i\in\mathbb{Z}} \left(2|u(\tilde{x}_i)|^2 + 2h \int_{x_i}^{x_i+h} \left| u'(\tau) \right|^2 d\tau \right) \\
&\le 2 \sum_{i\in\mathbb{Z}} \left(\frac{1}{h} \int_{\Omega_i} |u(x)|^2 dx + h \int_{\Omega_i} \left| u'(\tau) \right|^2 d\tau \right). \qquad (2.3)
\end{aligned}
$$

The particularly choice of $h = 1$ yields hence

$$\sum_{i\in\mathbb{Z}} |u(x_i)|^2 \le 2\|u\|^2_{H^1(\mathbb{R})}. \qquad (2.4)$$

We will now show that for each $f \in L^2(\mathbb{R})$ the equation (2.2) has a unique solution. Given $f \in L^2(\mathbb{R})$, we define a functional $l\colon H^1(\mathbb{R}) \to \mathbb{R}$ through

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

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

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

Then (2.2) is equivalent to finding $u \in H^1(\mathbb{R})$ such that

$$B_\mu[u,v] = l(v) \quad \forall v \in H^1(\mathbb{R}). \qquad (2.5)$$

The existence of a unique $u \in H^1(\mathbb{R})$ satisfying (2.5) 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 $\mu \in \mathbb{R}$ small enough*

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

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

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

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

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

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

Analogously for $\rho < 0$, using (2.3) 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

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

Resulting in B_μ being coercive for μ small enough. □

Thus, there exists a unique solution $u \in H^1(\mathbb{R})$ to the problem (2.5) 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 one-to-one since for $u_1 = u_2$

$$0 = B_\mu[u_1, v] - B_\mu[u_2, v] = \int (f_1 - f_2)\overline{v} \quad \forall v \in H^1(\mathbb{R}). \tag{2.6}$$

Since further $H^1(\mathbb{R})$ is dense in $L^2(\mathbb{R})$ this yields that the equality (2.6) holds also for all $v \in L^2(\mathbb{R})$ and therefore $f_1 = f_2$ almost everywhere. Accordingly R_μ is invertible and in return 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

If for every fixed $k \in \mathbb{Z}$ we consider in (2.2) a test function $v \in C^\infty(\mathbb{R})$ such that $\operatorname{supp} v = \Omega_k$ we get furthermore

$$\int_{x_k-\frac{1}{2}}^{x_k} u'(x)\overline{v'(x)}dx = \int_{x_k-\frac{1}{2}}^{x_k} Au\overline{v} \iff \int_{x_k-\frac{1}{2}}^{x_k} -u(x)\overline{v''(x)}dx = \int_{x_k-\frac{1}{2}}^{x_k} Au\overline{v},$$

whence $Au = -u'' \in L^2(x_k - \frac{1}{2}, x_k)$. Analogous arguments yield that $Au = -u'' \in L^2(x_k, x_k + \frac{1}{2})$. As $k \in \mathbb{Z}$ was arbitrary we obtain

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

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 (2.2) 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

$$\mathcal{D}(A) \subseteq \Big\{ u \in \bigcap_{i \in \mathbb{Z}} H^2(x_i, x_{i+1}) : u'(x_i - 0) - u'(x_i + 0) + \rho u(x_i) = 0, \ \forall i \in \mathbb{Z} \Big\} =: B \quad (2.7)$$

Hence, for an arbitrary $u \in D(A)$ 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 (2.7). 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 $i \in \mathbb{Z}$. We have to show $u = R_\mu(f - \mu u)$ or equivalently

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

$$\iff \sum_{i \in \mathbb{Z}} \int_{\Omega_i} u'\overline{v'} + \rho u(x_i)\overline{v(x_i)} = - \sum_{i \in \mathbb{Z}} \int_{x_i - \frac{1}{2}}^{x_i} u''\overline{v} + \int_{x_i}^{x_i + \frac{1}{2}} u''\overline{v}.$$

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

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

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

such that we conclude

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

2.2 A being self-adjoint

In chapter 4, 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 our analysis its spectrum down.

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

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

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

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

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

such that R_μ is also symmetric. □

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

Theorem 2.3. *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

$$\langle R_\mu^{-1} u, v\rangle = \langle u, v^*\rangle, \quad \forall u \in \mathcal{D}(R_\mu^{-1}) \tag{2.8}$$

then $v \in \mathcal{D}(R_\mu^{-1})$ and $R_\mu^{-1} v = v^*$. In (2.8) 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. □

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

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

As before, we want to define A_k by considering the weak formulation to the corresponding problem, i.e. for $f \in L^2(\Omega)$ finding $u \in H_k^1$ 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 $v \in H_k^1$ where

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

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 $H^1(\mathbb{R})$, and one can apply analogous 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. Hence we define similarly

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

and see therefore that $R_{\mu,k}$ is the resolvent of A_k.

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^1_k. Using this fact we can then deduce additional properties about the spectrum of A_k and A in chapter 4.

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

Proof: For each bounded sequence $(f_j)_j \in L^2(\Omega)$ we can define

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

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, choosing in (3.2) $v = u_j$ yields with (2.4) for μ small enough

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

Which means that $(u_j)_j$ is bounded in $H^1(\Omega)$. 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 $f \in B_{H^1_k}$ are uniformly bounded on Ω by (2.4), there exist for each subinterval I_k a finite number of constants $c_{1,k}, \ldots, c_{\nu_\epsilon,k}$ such that

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

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 $k \in \{1, \dots, n_\epsilon\}$, such that

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

This means in conclusion that $B_{H^1_k}$ is totally bounded in $L^2(\Omega)$. Furthermore, H^1_k is a closed subset of $H^1(\Omega)$ as convergence in $H^1(\mathbb{R})$ implies convergence on the boundary, and this yields the compact embedding of H^1_k in $L^2(\Omega)$. Thus, the operator $R_{\mu,k}$ is compact. $\square$

3.1 The spectrum of the restricted operator A_k

As from now, consider the eigenvalue problem to find $\psi \in H^1_k$ 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 so is

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

an eigenvalue for the same eigenfunction ψ for the operator A. Since Ω is bounded, and $R_{\mu,k}$ is a compact and symmetric operator, A_k has also 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). Therefore, we transform the eigenvalue problem (3.4) such that the boundary condition is independent from k, define

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

Then,

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

Defining the operator $\tilde{A}_k \colon D(A_k) \to L^2(\mathbb{R})$ 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 (3.4) and (3.1), 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

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

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

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

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 carries the 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 REF, I still want to list them here for completeness.

3.2 The Floquet transformation

Theorem 3.2. *The Floquet transformation* $U\colon L^2(\mathbb{R}) \to L^2(\Omega \times B)$

$$(Uf)(x,k) := \frac{1}{\sqrt{|B|}} \sum_{n\in\mathbb{Z}} f(x-n)e^{ikn} \quad (x \in \Omega, k \in B). \tag{3.7}$$

is an isometric isomorphism, with inverse given by

$$(U^{-1}g)(x-n) = \frac{1}{\sqrt{|B|}} \int_B g(x,k)e^{-ikn}dk \quad (x \in \Omega, n \in \mathbb{Z}). \tag{3.8}$$

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

$$U^{-1}g = \frac{1}{\sqrt{|B|}} \int_B g(\cdot,k)dk. \tag{3.9}$$

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

$$\int_{\mathbb{R}} |f(x)|^2 dx = \sum_{n\in\mathbb{Z}} \int_\Omega |f(x-n)|^2 dx, \tag{3.10}$$

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 (3.7) (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 (3.10), 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 (3.8) or (3.9). Let $g \in$

$L^2(\Omega \times B)$, then define

$$f(x-n) := \frac{1}{\sqrt{|B|}} \int_B g(x,k) e^{-ikn} dk \quad (x \in \Omega, n \in \mathbb{Z}). \tag{3.11}$$

Parseval's Theorem gives for fixed $x \in \Omega$ that $\sum_{n\in\mathbb{Z}} |f(x-n)|^2 = \int_B |g(x,k)|^2 dk$. Integrating 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 $x \in \Omega$ (3.7) gives

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

whence (3.11) implies $Uf = g$ and (3.8). Now (3.9) follows from (3.8) and exploiting $g(x+n,k) = e^{ikn} g(x,k)$. □

3.3 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 3.3. *For each $f \in L^2(\mathbb{R})$ and $l \in \mathbb{N}$, define*

$$f_l(x) := \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \langle (Uf)(\cdot,k), \psi_s(\cdot,k) \rangle_{L^2(\Omega)} \psi_s(x,k) dk \quad (x \in \mathbb{R}). \tag{3.12}$$

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

$$g_l(x,k) := \sum_{s=1}^{l} \langle (Uf)(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)} \psi_s(x,k). \tag{3.13}$$

Moreover, we get by Bessel's inequality

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

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 3.2, 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

$$\|Uf - g_l\|_{L^2(\Omega\times B)} \to 0 \text{ as } l \to \infty \tag{3.14}$$

If $g(\cdot,k)$ is extended to the whole of $\mathbb{R}$ by the semi-periodicity condition (3.1), using (3.12), (3.13) and (3.9), we find that $f_l = U^{-1} g_l$, whence (3.14) gives

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

□

Chapter 4

The spectrum of A

In this chapter, we will prove the main result stating that for the Schrödinger operator A with periodic delta potential

$$\sigma(A) = \bigcup_{s\in\mathbb{N}} I_s \tag{4.1}$$

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

Theorem 4.1. *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

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

In the transformed eigenvalue problem (3.5), (3.6) are our boundary conditions 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 $k \in B$ fixed. Then for all $\tilde{k} \in B$ and all $v \in H^1_{per}(\Omega)$ using triangular inequality we can estimate for $J \in \{(x_0 - \frac{1}{2}, x_0), (x_0, x_0 + \frac{1}{2})\}$:

$$\frac{\langle \left(\frac{d}{dx} + i\tilde{k}\right) v, \left(\frac{d}{dx} + i\tilde{k}\right) v\rangle_{L^2(J)}}{\langle v, v\rangle_{L^2(J)}} \begin{Bmatrix} \le \\ \ge \end{Bmatrix} \frac{\langle \left(\frac{d}{dx} + ik\right) v, \left(\frac{d}{dx} + ik\right) v\rangle_{L^2(J)}}{\langle v, v\rangle_{L^2(J)}}$$
$$\begin{Bmatrix} + \\ - \end{Bmatrix} \frac{2|k - \tilde{k}|\|v'\|_{L^2(J)}\|v\|_{L^2(J)}}{\|v\|^2_{L^2(J)}} \begin{Bmatrix} + \\ - \end{Bmatrix} \left| |k|^2 - |\tilde{k}|^2 \right| \tag{4.2}$$

Moreover,

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

Hence (4.2) yields

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

Thus the min-max-principle gives

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

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. □

As B is compact and connected and $\lambda_s(k)$ is a continuous function of $k \in B$ we derive for (4.1)

$$I_s \text{ is a compact real interval for each } s \in \mathbb{N}. \tag{4.3}$$

This implies 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 ("free") 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 (4.3) implies that

$$\bigcup_{s \in \mathbb{N}} I_s \text{ is closed.} \tag{4.4}$$

The first part of the statement (4.1) is

Theorem 4.2. $\sigma(A) \supset \bigcup_{s \in \mathbb{N}} I_s$.

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

$$A_k \psi_s(\cdot, k) = \lambda \psi_s(\cdot, k) \tag{4.5}$$

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.

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

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

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

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

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

Then

$$
\begin{aligned}
(A-\lambda I)u_l &= \sum_{j\in\mathbb{N}}\left[(-\frac{d^2}{dx^2}-\lambda)u_l|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right] \qquad (4.6)\\
&= \sum_{j\in\mathbb{N}}\left[\left(-\frac{d^2}{dx^2}-\lambda\right)\left(\eta\left(\frac{|\cdot|}{l}\right)\psi_s(\cdot,k)\right)\Big|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right]\\
&\quad -\frac{2}{l}\sum_{j\in\mathbb{N}}\left[\left(\eta'\left(\frac{|\cdot|}{l}\right)\psi_s'(\cdot,k)\right)\Big|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right]\\
&\quad -\frac{1}{l^2}\sum_{j\in\mathbb{N}}\left[\left(\eta''\left(\frac{|\cdot|}{l}\right)\psi_s(\cdot,k)\right)\Big|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right]\\
&= \sum_{j\in\mathbb{N}}\left[\eta\left(\frac{|\cdot|}{l}\right)\left(-\frac{d^2}{dx^2}-\lambda\right)\psi_s(\cdot,k)|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right]+R
\end{aligned}
$$

where R is a sum of products of derivatives of order ≥ 1 of $\eta\left(\frac{|\cdot|}{l}\right)$, and 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

$$
\|R\| \leq \frac{c}{l}\|\psi_s(\cdot,k)\|_{H^1((x_0-\frac{l}{2},x_0+\frac{l}{2}))} \leq c\frac{1}{\sqrt{l}}. \qquad (4.7)
$$

Together with (4.4), (4.5) and (4.6), this gives

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

Now, as moreover $u_l\in D(A)$ 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, $\lambda\in\sigma(A)$. □

Theorem 4.3. *$\sigma(A)\subset\bigcup_{s\in\mathbb{N}} I_s$.*

Proof: Let $\lambda\in\mathbb{R}\setminus\bigcup_{s\in\mathbb{N}} I_s$. We have to prove that $\lambda\in\rho(A)$, i.e. for each $f\in L^2(\mathbb{R})$ there exists some $u\in D(A)$ satisfying $(A-\lambda I)u=f$. For given $f\in L^2(\mathbb{R})$, we define, for $l\in\mathbb{N}$,

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

and

$$u_l := \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \frac{1}{\lambda_s(k) - \lambda} \langle (Uf)(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)} \psi_s(x, k) dk \tag{4.8}$$

Here, due to (4.4) there exists some $\delta > 0$ such that

$$|\lambda_s(k) - \lambda| \geq \delta \quad \text{ for all } s \in \mathbb{N}, k \in B \tag{4.9}$$

In particular, consider for fixed $k \in B$ and $v \in \mathcal{D}(A_k)$:

$$(A_k - \lambda I)v(\cdot, k) = (Uf)(\cdot, k) \quad \text{ on } \Omega, \tag{4.10}$$

which has a unique solution as $\lambda \in \mathbb{R} \setminus \bigcup_{s \in \mathbb{N}} I_s$. Parseval yields

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

Since both $v(\cdot, k)$ and $\psi_s(\cdot, k)$ satisfy semi-periodic boundary conditions, $A - \lambda I$ can be moved to $\psi_s(\cdot, k)$ in the inner product, and hence (3.4) and (4.9) give

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

By Theorem 3.2, this implies $v \in L^2(\Omega \times B)$, and we can define $u := U^{-1} v \in L^2(\mathbb{R})$. Thus, (4.10) gives

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

whence (4.8) implies

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

and Theorem 3.3 gives

$$u_l \to u, \quad f_l \to f \quad \text{ in } L^2(\mathbb{R}). \tag{4.11}$$

We will now prove that

$$(A - \lambda I)u_l = f_l \text{ for all } l \in \mathbb{N} \tag{4.12}$$

which implies that $\langle u_l, (A - \lambda I)v\rangle = \langle f_l, v\rangle$ for all $v \in D(A)$, whence Theorem 3.13 implies $u_l \in D(A)$, and

$$(A - \lambda I)u_l = f_l \quad \text{ for all } l \in \mathbb{N}$$

Since A is closed, (4.11) now implies

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

which is the desired result.

We are left to prove is (4.12), i.e. that

$$\langle u_l, (A - \lambda I)\varphi\rangle_{L^2(\mathbb{R})} = \langle f_l, \varphi\rangle_{L^2(\mathbb{R})} \quad \forall \varphi \in C_0^\infty(\mathbb{R}). \tag{4.13}$$

So, let $\varphi \in C_0^\infty(\mathbb{R})$ be fixed, and let $K \subseteq \mathbb{R}$ denote an open interval containing $\mathrm{supp}(\varphi)$ in its interior. Both the functions

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

are in $L^2(K \times B)$ by Fubini's Theorem, since (4.9) and the fact that $(A_k - \lambda I)\varphi \in L^\infty(K)$ and $\varphi \in L^\infty(K)$, imply both

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

and

$$\|t_s\|_{L^2(K\times B)} \le \tilde{c}\|(Uf)(\cdot,k)\|^2_{L^2(\Omega)}\|\psi_s(\cdot,k)\|^2_{L^2(K)},.$$

the latter factor is bounded as a function of k because K is covered by a finite number of copies of Ω, and the former is in $L^1(B)$ by Theorem 3.2.

Since $K \times B$ is 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 (4.8),

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

Since φ has compact support in the interior of K, $(A-\lambda I)$ may be moved to $\psi_s(\cdot,k)$, and hence (3.4) gives

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

i.e. (4.13). $\square$

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Erklärung

Hiermit versichere ich, dass ich diese Arbeit selbständig verfasst und keine anderen, als die angegebenen Quellen und Hilfsmittel benutzt, die wörtlich oder inhaltlich übernommenen Stellen als solche kenntlich gemacht und die Satzung des Karlsruher Instituts für Technologie zur Sicherung guter wissenschaftlicher Praxis in der jeweils gültigen Fassung beachtet habe.

Karlsruhe, den 13. September 2016