Bachelorthesis

On the spectra of Schrödinger operator with periodic delta potential

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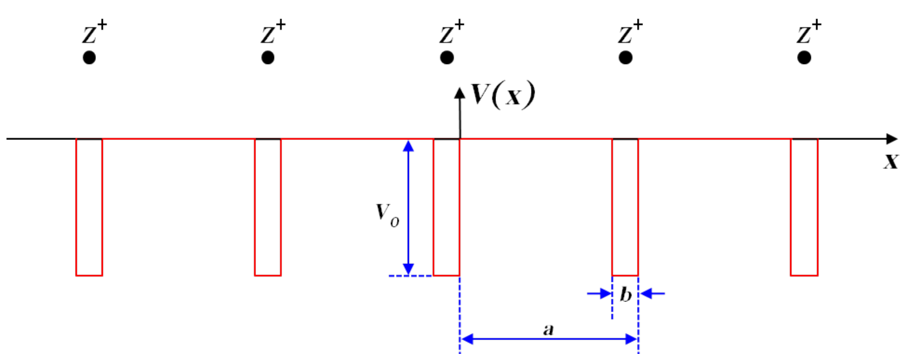
Chapter 1

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 takes local maximum. Such an array occurs commonly 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 a quantum particle, as it behaves like a wave, penetrates the barrier and continues its movement beyond[1]. 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:



[1]The likelihood that the particle will pass through the barrier is given by the transmission coefficient, whereas the likelihood that it is reflected is given by the reflection coefficient. Schrödinger's wave-equation allows these coefficients to be calculated.

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

Fourier series

do I have to do this?

Weak derivate and weak formulation

do I have to do this?
Let C_c^∞ denote the linear space containing all smooth function 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 $x \notin I$. Togerther 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 apre-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.
The Sobolev space H^k is defined to be the subset of functions f in $L^2(\mathbb{R})$ such that the function f and its weak derivatives up to some order k have a $finite L^2$ norm. A
Furthermore, the space H^k admits an inner product, which is defined in terms of the L^2 inner product:

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

The space H^k becomes a Hilbert space with this inner product.
... and using the fact that $C_c^\infty(\mathbb{R})$ is dense in $H^1(\mathbb{R})$

Distributons

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.

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

and on this interval f_n converges uniformally against f, i.e.

$$\|(f_n^{(i)} - f^{(i)}) \cdot \mathbb{1}_I\|_\infty \to 0 \quad \forall n \to \infty$$

forall all $i \in \mathbb{N}_0$. One can proof that 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 denote now all linear functionals on C_0^∞ that are continuous under this topology.

An important example for a distribution is the delta distribution 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 cumulative distribution functions δ_ϵ, whereas the support of those cumulative distributions converges to zero. 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 $\delta_{x_0}(f) = f(x_0)$.

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

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

where $\mathcal{O}(\epsilon)$ is at least of order ϵ. 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 :

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

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

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

$\square$

Spektrum 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

$\lambda I - A\colon D(A)\to X$ bijektiv, 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 above introduced problem can be modelled by a one-dimensional Schrödinger operator where the potential is given by a delta-distribution. Thereby the operator A is formally defined through the operation

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

on the whole of $\mathbb{R}$, where δ_{x_i} denotes the Dirac delta distribution in x_i and x_i are periodically distributed points on $\mathbb{R}$. Ω_k will hereafter identify the periodicity cell containing delta point x_k and let w.o.l.g. $x_0 = 0$ and $a \coloneqq |\Omega_i| = 1$ for all $i \in \mathbb{Z}$.

In general, one cannot expect that (2.1) has a classical solution. For the existence of a classical solution, all the problem has to be sufficiently regular, which for a distributional potential is never the case. Nevertheless, for $\mu \in \mathbb{R}$ the problem

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

where $u \in H^1(\mathbb{R})$ and $f \in L^2$ requires much less regularity, as it is the weak-formulation of our operator A shifted by the constant μ.

We should note that left-hand side of problem (2.2) is actually convergent, as for arbitrary $\tilde{x}_i \in \Omega_i$

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

We will now examine 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 $l\colon H^1 \to \mathbb{R}$ through Riesz' Representation Theorem with

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

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

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

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

$$B_\mu[u,v] = l(v) \quad \forall v \in H^1(\mathbb{R}). \qquad (2.4)$$

The existence of an unique $u \in H^1(\mathbb{R})$ satisfying (2.4) follows from Lax Milgram's Theorem asserts if the bilinear form B is bounded and coercive, which we will prove in the next theorem.

Theorem 2.1. *The bilinear form $B_\mu[u,v]$ as left-hand of (2.2) has for all $u,v \in H^1(\mathbb{R})$ the properties*

i) $B_\mu[u,v]$ is bounded, i.e. there exists a constant $\alpha > 0$ such that

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

ii) $B_\mu[u,u]$ is coercive, i.e. there exists a constant $\beta > 0$ such that

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

Proof:

i) The boundedness follows from

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

ii) For the coercivity assume first $\rho \geq 0$, in order that for $\mu < -1$:

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

Same for $\rho < 0$, where $\mu < 2\rho$:

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

$\square$

Thus, there is a function $u \in H^1(\mathbb{R})$ as the unique solution to the problem (2.4) for fixed $f \in L^2(\mathbb{R}$ and the operator $R_\mu \colon L^2(\mathbb{R}) \to H^1(\mathbb{R}), f \mapsto u$ is for $\mu \in \mathbb{R}$ small enough well-defined; obviously this mapping is one-to-one since for $u_1 = u_2$

$$
0 = B_\mu[u_1, v] - B_\mu[u_2, v] = \int (f_1 - f_2)\overline{v} \quad \forall v \in H^1(\mathbb{R}). \tag{2.5}
$$

As further $H^1(\mathbb{R})$ is dense in $L^2(\mathbb{R})$ this yields that the equation (2.5) holds also for all $v \in L^2(\mathbb{R})$ and therefore $f_1 = f_2$ almost everywhere. Accordingly R_μ is bijective 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

Lax Milgram's Theorem guarantees a solution $u \in H^1(\mathbb{R})$ of (2.2), nevertheless the operator A yields additional properties about such a solution, more specifically about the domain of A. For every fixed $k \in \mathbb{Z}$ we therefore consider in (2.2) a test function $v \in C^\infty(\mathbb{R})$ such that $\operatorname{supp} v = \Omega_k$, then

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

such that $Au = -u'' \in L^2$ on $(x_k - 1/2, x_k)$ and analogous on $(x_k, x_k + 1/2)$. As $k \in \mathbb{Z}$ was arbitrary this means

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

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

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

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

But as we chose $v \in C^\infty(\mathbb{R})$ this is equivalent to

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

such that

$$\mathcal{D}(A) \subset \left\{ u \in \bigcap_{i\in\mathbb{Z}} H^2(x_i, x_{i+1}) : u'(x_i - 0) - u'(x_i + 0) + \rho u(x_i) = 0,\ \forall i \in \mathbb{Z} \right\} =: B \quad (2.6)$$

The operator is hence well-defined by the action

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

We can further prove the opposite inclusion for (2.6). As $\mathcal{R}(R_\mu) = \mathcal{D}(A)$, 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 $f := Au$. To show $u = R_\mu(f - \mu u)$ consider

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

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

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

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

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

such that we conclude

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

2.2 The self-adjointness

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 $v \in D(A)$:

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

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

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

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

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

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 the delta-point contained in Ω. As commonly used by literature the reciprocal lattice for Ω is equal to $[-\pi, \pi]$, the so called one-dimensional Brillouin zone B. For fixed $k \in \overline{B}$, consider now the operator A_k on Ω formally denoted by the operation

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

Again, define A_k by considering the weak formulation to this problem, i.e. for $f \in L^2(\Omega)$ find 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 $v \in H_k^1$ 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 trace of Ω, H_k^1 is a closed subspace of $H^1(\mathbb{R})$, and one can therefore apply the same arguments as above to show that $R_{\mu,k}\colon L^2(\Omega) \to H_k^1, f \mapsto u$ is well-defined and define in return

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

such that $R_{\mu,k}$ is the resolvent of A_k.

In chapter is going to provide additional information about the operator $R_{\mu,k}$. We shall see that the eigenfunctions of A form a complete and orthonormal system in H_k^1 and use this fact to deduce additional properties about the spectrum of A_k and also A in chapter 4.

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

Proof: For each bounded sequence $(f_j)_{j\geq 1} \in L^2(\Omega)$ there exist $(u_j)_{j\geq 1} \in H_k^1$ by

$$u_j = R_{\mu,k} f_j \quad \forall j \geq 1.$$

Each such u_j has to satisfy

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

Now, choosing in (3.2) $v = u_j$ yields with (2.3) 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 $(u_j)_{j\geq 1}$ is bounded in $H^1(\Omega)$. As $H^1(\Omega) \subset C(\Omega)$ we can further estimate

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

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

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

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 by (2.3) uniformly bounded on Ω, there exist for each subinterval I_k a finite number of constants $c_{1,k}, \ldots, c_{\nu_\epsilon,k}$ such that

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

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

sucht that

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

In conclusion this means that $B_{H_k^1}$ is totally bounded in $L^2(\Omega)$ and with the closure of H_k^1 this yields the compact embedding of H_k^1 in $L^2(\Omega)$. Thus, $R_{\mu,k}$ is compact. □

3.1 The Spectrum of the restricted operator A_k

As from now, consider the eigenvalue problem

$$A_k\psi = \lambda\psi \text{ on } \Omega \text{ for } \psi \in H_k^1. \tag{3.4}$$

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 same the 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:

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

Then,

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

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

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

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

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

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

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

In the next chapter we shall see 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

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

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 by (3.10) in $L^2(\Omega)$, 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 yields then

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

which means $f \in L^2(\mathbb{R})$. For almost every $x \in \Omega$ (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) using $g(x+n,k) = e^{ikn}g(x,k)$. □

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 eigenfunction 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

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

By Bessel's inequality, we get moreover

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

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

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

and the assertion follows since $U\colon L^2(\mathbb{R}) \to L^2(\Omega \times B)$ is isometric by Lemma 3.2. $\square$

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 $I_s := \{\lambda_s(k) : k \in \overline{B}\}$ $(s \in \mathbb{N})$. As B is compact and connected, for each of those sets I_s holds that

$$I_s \text{ is a compact real interval for each } s \in \mathbb{N}, \tag{4.2}$$

as λ_s is a continuous function of $k \in \overline{B}$ for all $s \in \mathbb{N}$, which follows by standard arguments from the fact that the coefficients in the transformed eigenvalue problem (3.5), (3.6) depend continuously on k.

Todo: Proof Plum

Moreover, Poincare's min-max principle for eigenvalues implies 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

$$\min I_s \to \infty \text{ as } s \to \infty,$$

which together with (4.2) implies that

$$\bigcup_{s\in\mathbb{N}} I_s \text{ is close.} \tag{4.3}$$

The first part of the statement (4.1) is

Theorem 4.1. $\sigma(A) \supset \bigcup_{s\in\mathbb{N}} I_s$.

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

$$A_k\psi_s(\cdot,k) = \lambda\psi_s(\cdot,k) \tag{4.4}$$

We regard $\psi_s(\cdot,k)$ as extended to the whole of $\mathbb{R}$ by the boundary condition (3.1), whence, due to the periodicity of A, (4.4) holds for all $x \in \mathbb{R}$ and $\psi_s \in H^2_{loc}(\mathbb{R})$
We choose a function $\eta \in H^2(\mathbb{R})$ such that

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

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

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

Then,

$$\begin{aligned}
(A-\lambda I)u_l &= \sum_{j\in\mathbb{N}}\left[(-\frac{d^2}{dx^2}-\lambda)u_l|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right] \qquad (4.5)\\
&= \sum_{j\in\mathbb{N}}\left[\left(-\frac{d^2}{dx^2}-\lambda\right)\left(\eta\left(\frac{|\cdot|}{l}\right)\psi_s(\cdot,k)\right)\Big|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right]\\
&\quad -\frac{2}{l}\sum_{j\in\mathbb{N}}\left[\left(\eta'\left(\frac{|\cdot|}{l}\right)\psi_s'(\cdot,k)\right)\Big|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right]\\
&\quad -\frac{1}{l^2}\sum_{j\in\mathbb{N}}\left[\left(\eta''\left(\frac{|\cdot|}{l}\right)\psi_s(\cdot,k)\right)\Big|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right]\\
&= \sum_{j\in\mathbb{N}}\left[\eta\left(\frac{|\cdot|}{l}\right)\left(-\frac{d^2}{dx^2}-\lambda\right)\psi_s(\cdot,k)|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right]+R
\end{aligned}$$

where R is a sum of products of derivatives (of order ≥ 1) of $\eta(\frac{|\cdot|}{l})$, and derivatives (of order ≤ 1) of $\psi_s(\cdot,k)$. Thus (note that $\psi_s(\cdot,k) \in H^2_{loc}(\mathbb{R})$), and the semi-periodic structure of $\psi_s(\cdot,k)$ implies

$$\|R\| \le \frac{c}{l}\|\psi_s(\cdot,k)\|_{H^1(K_l)} \le c\frac{1}{\sqrt{l}}, \tag{4.6}$$

with K_l denoting the ball in $\mathbb{R}$ with radius l centered at x_0. Together with (4.4), (4.5) and (4.6), this gives

$$\|(A-\lambda I)u_l\| \le \frac{c}{\sqrt{l}}$$

Again, by the semiperiodicity of $\psi_s(\cdot,k)$, which gives us that $\|u_l\| \geq c\|\psi_s(\cdot,k)\| \geq c\sqrt{l}$ for $c > 0$, we obtain

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

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

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. that for each $f \in L^2(\mathbb{R})$ some $u \in D(A)$ exists 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

$$u_l := \frac{1}{\sqrt{|B|}}\sum_{s=1}^{l}\int_B \frac{1}{\lambda_s(k)-\lambda}\langle (Uf)(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)}\psi_s(x,k)dk \tag{4.7}$$

Here, note that, due to (4.3) some $\delta > 0$ exists such that

$$|\lambda_s(k)-\lambda| \geq \delta \text{ for all } s \in \mathbb{N}, k \in B \tag{4.8}$$

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

$$(A_k - \lambda I)v(\cdot,k) = (Uf)(\cdot,k) \text{ on } \Omega, \tag{4.9}$$

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

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

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 (4.8) 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 $u \coloneqq U^{-1}v \in L^2(\mathbb{R})$. Thus, (4.9) 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 (4.7) 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

$$u_l \to u, \quad f_l \to f \quad \text{ in } L^2(\mathbb{R}). \tag{4.10}$$

We will now prove that in the distributional sense

$$(A - \lambda I)u_l = f_l \text{ for all } l \in \mathbb{N} \tag{4.11}$$

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

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

Since A is closed, (4.10) now implies

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

which is the desired result.

Left to prove is (4.11), i.e. that

$$\langle u_l, (A-\lambda I)\varphi\rangle_{L^2(\mathbb{R})} = \langle f_l, \varphi\rangle_{L^2(\mathbb{R})} \quad \forall \varphi \in C_0^\infty(\mathbb{R}). \tag{4.12}$$

Let $\varphi \in C_0^\infty(\mathbb{R})$ be fixed, and let $K \subseteq \mathbb{R}$ denote an open interval containing $\operatorname{supp}(\varphi)$ in its interior. 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 (4.8) and the fact that $(A_k-\lambda I)\varphi \in L^\infty(K)$ and $\varphi \in L^\infty(K)$, imply both

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

and

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

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 (4.7),

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

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. (4.12). □