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Chapter 1

Introduction

An important problem in mathematical physics is the solution of the one-dimensional Schrödinger equation with distributional potential, which is formally defined by the operation

$$-\frac{d^2}{dx^2}+\rho\sum_{i\in\mathbb{Z}}\delta_{x_i} \tag{1.1}$$

on the whole of $\mathbb{R}$, where δ denotes the Dirac delta distribution 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 $|\Omega_i| = 1$ for all $i \in \mathbb{Z}$.

Henceforth, consider for $\mu \in \mathbb{R}$ the problem

$$\int u'\overline{v'}+\rho\sum_{i\in\mathbb{Z}}u(x_i)\overline{v(x_i)}-\mu\int u\overline{v}=\int f\overline{v}\quad \forall v\in H^1(\mathbb{R}), \tag{1.2}$$

where $u \in H^1(\mathbb{R})$ and $f \in L^2(\mathbb{R})$ is a function modelling an external force.
The left-hand side of problem (1.2) is actually convergent as for arbitrary $\tilde{x}_i \in \Omega_i$

$$\begin{aligned}\sum_{i\in\mathbb{Z}}|u(x_i)|^2 &\leq \sum_{i\in\mathbb{Z}}\left(\left|u(\tilde{x}_i)+\int_{\tilde{x}_i}^{x_i}u'(\tau)d\tau\right|\right)^2\\ &\leq 2\sum_{i\in\mathbb{Z}}\left(\int_{\Omega_i}|u(x)|^2dx+\int_{\Omega_i}\left|u'(\tau)\right|^2d\tau\right)\\ &\leq 2\cdot\|u\|^2_{H^1(\mathbb{R})}.\end{aligned} \tag{1.3}$$

Chapter 2

The Operator

As we can interpret the left-hand side of (1.2) as a bounded bilinear mapping $B\colon H^1(\mathbb{R}) \times H^1(\mathbb{R}) \to \mathbb{R}$, Lax Milgram's Theorem asserts the existence of a unique element $u \in H^1(\mathbb{R})$ satisfying

$$B[u, v] = \langle f, v \rangle$$

if there exist constants $\alpha, \beta > 0$ such that

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

and

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

Taking these two condition under examination, (1.3) yields for the norm of $B[u, v]$ both.

Theorem 2.1. *The bilinear form $B[u, v]$ as left-hand of* (1.2) *has for all $u, v \in H^1(\mathbb{R})$ the properties*

i) $B[u, v]$ *is bounded.*

ii) $B[u, u]$ *is coercive.*

Proof:

i) The boundedness follows from

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

ii) For the coercivity assume first $\rho \ge 0$. For $\mu < -1$:

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

For $\rho < 0$ there exists a $\mu \in (-\infty, 2\rho)$ such that

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

$\square$

where $u \in H^1(\mathbb{R})$ is the unique solution to the problem (1.2). Thus, 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 the mapping is one-to-one since for $u_1 = u_2$

$$
0 = B[u_1,v] - B[u_2,v] = \int (f_1 - f_2)\overline{v} \quad \forall v \in H^1(\mathbb{R}). \tag{2.1}
$$

As $H^1(\mathbb{R})$ is dense in $L^2(\mathbb{R})$ this yields that the equation (2.1) holds also for all $v \in L^2(\mathbb{R})$

and therefore $f_1 = f_2$ almost everywhere. Accordingly R_μ is bijective and we can define the Schrödinger operator as follows

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

from which follows that R_μ is the resolvent of A.

2.1 The Domain

For every fixed $k \in \mathbb{Z}$ choosing a test function $v \in C^\infty(\mathbb{R})$ with $\operatorname{supp} v = \Omega_k$ in (1.2) yields

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

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

Next, again for an arbitrary $k \in \mathbb{Z}$ a test function $v \in C^\infty(\mathbb{R})$ with $\operatorname{supp} v = \Omega_k$ and integration by parts on both sides of x_k in (1.2) yields

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

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

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

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

such that

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

The action of the operator is defined by

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

The opposite inclusion is shown, as $\mathcal{R}(R_\mu) = \mathcal{D}(A)$, by proving for $u \in B$ that 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

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

Theorem 2.2. *R_μ is a 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. $\square$

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 show 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. $\square$

Chapter 3

Fundamental domain of periodicity and the Brillouin zone

Let Ω be the fundamental domain of periodicity associated with (1.1), 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 defined by the operation

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

More precisely, define A_k by considering the problem to find for $f \in L^2(\Omega)$ a function $u \in H_k^1$ such that

$$\int_\Omega u'\overline{v'} + \rho u(x_0)\overline{v(x_0)} - \mu \int_\Omega u\overline{v} = \int_\Omega f\overline{v} \quad \forall v \in H_k^1,$$

where

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

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 apply the same arguments as above to show that now the operator $R_{\mu,k}$ is well-defined and define again

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

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

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 $(u_j)_{j\geq 1} \in H^1_k$ such that

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

and each u_j for $j \geq 1$ has to satisfy

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

Now, choosing in (3.2) $v = u_j$ yields with (1.3) 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 shows that $(u_j)_{j\geq 1}$ is bounded in $H^1(\Omega)$. As $H^1(\Omega) \subset C(\Omega)$ it holds

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

From (3.3) follows for $f \in B_{H^1} := \{f \in H^1_k(\Omega) : \|f\| \leq 1\}$ that

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

Now, given an $\epsilon > 0$ we partition Ω into n_ϵ equidistant intervals I_k, i.e. $\Omega = \bigcup_{j=1}^{n_\epsilon} I_j$. As all $f \in B_{H^1_k}$ are by (1.3) uniformly bounded on Ω, there exist for each subinterval I_k a finite number of constants $c_1(I_k), \ldots, c_{\nu_\epsilon}(I_k)$ such that

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

Hence, a simple function $g \in L^2(\Omega)$ with function value c_k on interval I_k would yield

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

This means for all $\epsilon > 0$ there exists a finite set of simple functions $\{g_1, \ldots, g_N\}$ such that for all $f \in B_{H_k^1}$ there exists a $\nu \in \{1, \ldots, N\}$ such that $\|f - g_\nu\| \leq \epsilon$. Together with the closure of H_k^1 this yields the compact embedding of H_k^1 in $L^2(\Omega)$ and thus $R_{\mu,k}$ is compact. □

3.1 The Spectrum of A_k

As from now, consider the periodic 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.

Since Ω is bounded, and $R_{\mu,k}$, as resolvent of A_k, is a compact and symmetric operator, A_k has a purely discrete spectrum satisfying

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

and the corresponding eigenfunction can be chosen such that they depend on k in a measurable way[1] and that they form a $\langle\cdot,\cdot\rangle$-orthonormal and complete system $(\psi_s(\cdot,k))_{s\in\mathbb{N}}$ of eigenfunctions for (3.1).

Now, we want to transform the eigenvalue problem (3.4) such that the boundary condition is independent from k. Define therefore

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

[1] see [M. Reed and B. Simon. Methods of modern mathematical physics I–IV]

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), gives

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

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

$$
\begin{aligned}
\tilde{A}_k\varphi =&\quad \lambda\varphi \text{ on } \Omega, &(3.5)\\
\varphi(x-\frac{1}{2}) =&\quad \varphi(x+\tfrac{1}{2}). &(3.6)
\end{aligned}
$$

with the same eigenvalue sequence $(\lambda_s(s))_{s\in\mathbb{N}}$ as in (3.4). We shall see that the spectrum of the operator A can be constructed from the eigenvalue sequences $(\lambda_s(s))_{s\in\mathbb{N}}$ by varying k over the Brillouin zone B.

3.2 The Floquet transormation

An important step towards this aim is the Floquet transformation

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

Theorem 3.2. *$U\colon L^2(\mathbb{R}) \to L^2(\Omega \times B)$ 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)*, we have*

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

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

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

Here, we can exchange summation and integration by Beppo Levi's Theorem. Therefore,

$$\sum_{n\in\mathbb{Z}} |f(x-n)|^2 < \infty \text{ for a.e. } x \in \Omega.$$

Thus, $(Uf)(x,k)$ is well-defined by (3.7) (as a Fourier series with variable k) for a.e. $x \in \Omega$, and Parseval's equality gives, for these x,

$$\int_B |(Uf)(x,k)|^2 dk = \sum_{n\in\mathbb{Z}} |f(x-n)|^2.$$

By (3.10), this expression is in $L^2(\Omega)$, and

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

We are left to show that U is onto, and that U^{-1} is given by (3.8) or (3.9). Let $g \in L^2(\Omega\times B)$, and define

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

For fixed $x \in \Omega$, Parseval's Theorem gives

$$\sum_{n\in\mathbb{Z}} |f(x-n)|^2 = \int_B |g(x,k)|^2 dk,$$

whence, by integration over Ω,

$$\int_{\Omega\times B} |g(x,k)|^2 dxdk = \int_\Omega \sum_{n\in\mathbb{Z}} |f(x-n)|^2 dx \tag{3.12}$$

$$= \sum_{n\in\mathbb{Z}} \int_\Omega |f(x-n)|^2 dx \tag{3.13}$$

$$= \int_\mathbb{R} |f(x)|^2 dx, \tag{3.14}$$

i.e. $f \in L^2(\mathbb{R})$. Now (3.7) gives, for a.e. $x \in \Omega$,

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

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 are now able to prove a completeness property 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*

$$f_l(x) := \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \langle (Uf)(\cdot,k), \psi_s(\cdot,k) \rangle_{L^2(\Omega)} \psi_s(x,K) dk \quad (x \in \mathbb{R}). \tag{3.15}$$

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

Proof: Sine $Uf \in L^2(\Omega \times B)$, we have $(Uf)(\cdot,k) \in L^2(\Omega)$ for a.e. $k \in B$ by Fubini's Theorem. Since $(\psi_s(\cdot,k))_{s\in\mathbb{N}}$ is orthonormal and complete in $L^2(\Omega)$ for each $k \in B$, we obtain

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

where

$$g_l(x,k) := \sum_{s=1}^{l} \langle (Uf)(\cdot,k), \psi_s(\cdot,k) \rangle_{L^2(\Omega)} \psi_s(x,k). \tag{3.16}$$

Thus, for $\chi(k) := \|(Uf)(\cdot,k) - g_l(\cdot,k)\|^2_{L^2(\Omega)}$, we get

$$\chi_l(k) \to 0 \text{ as } l \to \infty \text{ for a.e. } k \in B,$$

and moreover, by Bessel's inequality,

$$\chi_l(k) \leq \|(Uf)(\cdot,k)\|^2_{L^2(\Omega)} \text{ for all } l \in \mathbb{N} \text{ and a.e. } k \in B$$

and $\|(Uf)(\cdot,k)\|^2_{L^2(\Omega)}$ is in $L^1(B)$ as a function of k by Theorem 3.2. Altogether, Lebesgue's Dominated Convergence theorem implies

$$\int_B \chi_l(k)dk \to 0 \text{ as } l \to \infty,$$

i.e.,

$$\|Uf - g_l\|_{L^2(\Omega\times B)} \to 0 \text{ as } l \to \infty \tag{3.17}$$

Using (3.15), (3.16) and (3.9), we find that $f_l = U^{-1}g_l$, whence (3.17) 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 section, we will prove the main result stating that

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

where

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

For each $s \in \mathbb{N}, \lambda_s$ is a continuous function of $k \in \overline{B}$, which follows by standard arguments from the fact that the coefficients in the eigenvalue problem (3.5), (3.6) depend continuously on k. Thus, since B is compact and connected,

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

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

$$\mu_s \leq \lambda_s(k) \text{ for all } s \in \mathbb{N}, k \in \overline{B}$$

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

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

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

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

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

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

Then,

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

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

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

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

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

Again, by the semiperiodicity of $\psi_s(\cdot, k)$,

$$\|u_l\| \geq c\|\psi_s(\cdot, k)\| \geq c\sqrt{l}$$

with $c > 0$. We obtain therefore

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

Because 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 $u := U^{-1}v \in L^2(\mathbb{R})$. 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 3.16 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 easily seen to be in $L^2(K \times B)$ by Fubini's Theorem, since (4.8) and the fact that $(A-\lambda I)\varphi \in L^\infty(K)$ and $\varphi \in L^\infty(K)$, imply both

$$\int_K |r_s(x,k)|^2 dx \quad \text{and} \quad \int_K |t_s(x,k)|^2 dx$$

are bounded by $C\|(Uf)(\cdot,k)\|^2_{L^2(\Omega)}\|\psi_s(\cdot,k)\|^2_{L^2(K)}$ 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 $L^2(B)$ by Theorem 3.2.

Since $K \times B$ is bounded, r and t are also $L^2(K \times B)$. Therefore, Fubini's Theorem implies that the order of integration with respect to x and k may be exchanged for r and t.

Thus, by (4.7),

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

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). $\square$