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 f is a function modelling an external force, 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 $|\Omega_i| = 1 \ \forall i \in \mathbb{Z}$.[1]

Henceforth, consider for a $\mu \in \mathbb{R}$ small enough 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 $f \in L^2(\mathbb{R})$ and $u \in H^1(\mathbb{R})$.

[1] Obviously, here is going to be much more but for starters this should suffice

The expression (1.2) actually converges as for arbitrary $\tilde{x}_i \in \Omega_i$

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

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 $u \in H^1$ 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 $B[u, v]$ is bounded.*

Proof.

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

□

and

Theorem 2.2. *$B[u, u]$ is coercive.*

Proof. Lets first assume $\rho \geq 0$ then for $\mu < -1$:

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

and for $\rho < 0$:

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

□

such that that the problem (1.2) has the unique element $u \in H$ and with that the resolvent mapping $R_\mu\colon L^2(\mathbb{R}) \to H^1(\mathbb{R}), f \mapsto u$ is well-defined; obviously the mapping is one-to-one since for $u_1 = u_2$

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

and as H^1 is dense in L^2 this means that this equation 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 turn we can define the Schrödinger operator as follows

$$A \coloneqq R_\mu^{-1} + \mu I \text{ and with that } \mathcal{D}(A) = \mathcal{R}(R_\mu)$$

Chapter 3

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 analogously 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

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

and the action of the operator is defined by

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

The opposite inclusion is shown, as $\mathcal{R}(R_\mu) = \mathcal{D}(A)$, by proving that a $u \in B$ is also in the range of R_μ. More specifically, as $\mathcal{D}(R_\mu) = L^2(\mathbb{R})$ define $f := Au$ and show that $u = R_\mu(f - \mu u)$:

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

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

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

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

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

such that

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

Furthermore, A is self-adjoint which will be later important.[1]

[1] Here HAS to be some more text but I don't know what

Theorem 3.1. *A is a self-adjoint operator*

Proof. First, focus on $R_\mu(A)^{-1} = (A - \mu I)$ which is a symmetric operator as $\forall v \in H^1$:

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

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 also R_μ is symmetric. Both can be used to show that R_μ is even self-adjoint, as for an arbitrary $v^* \in \mathcal{D}(R_\mu^{-1})$ there exists a $v \in \mathcal{R}(R_\mu^{-1}) = \mathcal{D}(R_\mu)$:

$$
\langle u, v^*\rangle = \langle R_\mu^{-1} R_\mu u, v^*\rangle = \langle R_\mu u, v\rangle = \langle u, R_\mu v\rangle
$$

Which means $v^* \in \mathcal{R}(R_\mu)$ and therefore is R_μ^{-1} self-adjoint. As A is simply R_μ^{-1} shifted by the real constant μ, A is self-adjoint as well. □

Chapter 4

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 with that $x_0 = 0$ being the delta-point contained in Ω. As commonly used by literature the reciprocal lattice for Ω is equal to $[-\pi, \pi]$, this set is 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 as follows: let us consider the problem to find for $f \in L^2(\Omega)$ a $u \in H^1_k$ such that

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

where

$$H^1_k := \Big\{H^1(\Omega) : \psi(-\frac{1}{2}) = e^{ik}\psi(-\frac{1}{2}), \psi'(-\frac{1}{2}) = e^{ik}\psi'(-\frac{1}{2}) \\ \text{and } \psi'(x_0 - 0) - \psi'(x_0 + 0) + \rho\psi'(x_0) = 0\Big\} \tag{4.1}$$

Using the fact that H_k^1 is a closed subspace[1] of $H^1(\mathbb{R})$ one can apply the same arguments as above for A to show that the resolvent $R_{\mu,k}$ of A_k is well defined and analogous to before define

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

As from now, consider the eigenvalue problem

$$A_k\psi = \lambda\psi \text{ on } \Omega, \tag{4.2}$$

In writing the boundary condition in (4.1), we understand ψ extended to the whole of $\mathbb{R}$. In fact, (4.1) forms boundary conditions on $\partial\Omega$, so-called semi-periodic boundary conditions. Furthermore we know that (4.2), (4.1) is a symmetric eigenvalue problem[2] in $L^2(\Omega)$ and ψ from (4.2) extended to the whole of $\mathbb{R}$ by (4.1) solves also the eigenvalue problem of A with the same eigenvalue.

Since Ω is bounded, the subsequently shown compactness can be used to verify that (4.2), (4.1) has a $\langle\cdot,\cdot\rangle$-orthonormal and complete system $(\psi_s(\cdot,k))_{s\in\mathbb{N}}$ of eigenfunctions in $H^2_{loc}(\mathbb{R})$, with corresponding eigenvalues satisfying

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

The eigenfunctions $\psi_s(\cdot,k)$ are called Bloch waves. They can be chosen such that they depend on k in a measurable way (see [M. Reed and B. Simon. Methods of modern mathematical physics I–IV]).

Theorem 4.1. *The operator $R_{\mu,k}$ is compact.*

Proof. For each bounded sequence $(f_j)_{j\ge1} \in L^2(\Omega)$ there exist $(u_j)_{j\ge1} \in H_k^1$, such that

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

[1] I think I will explain this also in more detail
[2] explain this in more detail and/or why do we need this

and this u_j has to satisfy

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

Now, choosing here $v = u_j$ and (1.3) yields 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 is bounded in $H^1(\Omega)$. As $H^1(\Omega) \subset C(\Omega)$:

$$|f(x) - f(y)| \leq c|x-y|^{1/2} \text{ for some } c > 0 \tag{4.3}$$

From (4.3) for a $f \in B_{H^1} \coloneqq \{f \in H_k^1(\Omega)$ it follows that

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

And with that we can approximate f by simple functions through partitioning Ω into n_ϵ equidistant intervals. As our simple function is constant on each subinterval, we chose this constant c_k such that $|f(\frac{k}{n}) - c_{k+1}| < \frac{1}{n}$ which leads to

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

Which means $\forall f \in B_{H_k^1}$: $\|f - g\| \leq \epsilon$. Together with the closure of H_k^1 this yields the compact embedding of H_k^1 in $L^2(\Omega)$, such that $R_{\mu,k}$ is compact. $\square$

Now, we want to transform the eigenvalue problem (4.2) such that the boundary condition is independent from k. Define therefore

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

Then,

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

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

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

Furthermore, using (4.2) and (4.1),

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

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

$$\tilde{A}_k\varphi = \lambda\varphi \text{ on } \Omega, \tag{4.4}$$

$$\varphi(x-\frac{1}{2}) = \varphi(x+\tfrac{1}{2}) \tag{4.5}$$

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

An important step towards this aim is the Floquet transformation

$$(Uf)(x,k) := \frac{1}{\sqrt{|B|}} \sum_{n\in\mathbb{Z}} f(x-n)e^{ikn} \quad (x \in \Omega, k \in B) \tag{4.6}$$

Theorem 4.2. $U\colon L^2(\mathbb{R}) \to L^2(\Omega \times B)$ *is an isometric isomorphism, with inverse*

$$(U^{-1}g)(x-n) = \frac{1}{\sqrt{|B|}} \int_B g(x,k)e^{-ikn}dk \quad (x \in \Omega, n \in \mathbb{Z}) \tag{4.7}$$

If $g(\cdot,k)$ *is extended to the whole of* $\mathbb{R}$ *by the semi-periodicity condition* (4.1)*, we have*

$$U^{-1}g = \frac{1}{\sqrt{|B|}} \int_B g(\cdot,k)dk. \tag{4.8}$$

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

$$\int_{\mathbb{R}} |f(x)|^2 dx = \sum_{n\in\mathbb{Z}} \int_{\Omega} |f(x-n)|^2 dx. \tag{4.9}$$

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 (4.6) (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 (4.9), 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 (4.7) or (4.8). Let

$g \in L^2(\Omega \times B)$, and define

$$f(x-n) := \frac{1}{\sqrt{|B|}} \int_B g(x,k) e^{-ikn} dk \quad (x \in \Omega, n \in \mathbb{Z}). \tag{4.10}$$

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,

$$\int_{\Omega \times B} |g(x,k)|^2 dx dk = \int_\Omega \sum_{n \in \mathbb{Z}} |f(x-n)|^2 dx \tag{4.11}$$

$$= \sum_{n \in \mathbb{Z}} \int_\Omega |f(x-n)|^2 dx \tag{4.12}$$

$$= \int_{\mathbb{R}} |f(x)|^2 dx, \tag{4.13}$$

i.e. $f \in L^2(\mathbb{R})$. Now (4.6) 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 (4.10) implies $Uf = g$ and (4.7). Now (4.8) follows from (4.7) using $g(x+n,k) = e^{ikn} g(x,k)$. $\square$

Chapter 5

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

$$f_l(x) := \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \langle (Uf)(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)} \psi_s(x, K) dk \quad (x \in \mathbb{R}). \tag{5.1}$$

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

$$g_l(x, k) := \sum_{s=1}^{l} \langle (Uf)(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)} \psi_s(x, k). \tag{5.2}$$

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 4.2. Altogether, Lebesgue's Dominated Convergence theorem implies

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

i.e.,

$$\|Uf - g_l\|_{L^2(\Omega\times B)} \to 0 \text{ as } l \to \infty \tag{5.3}$$

Using (5.1), (5.2) and (4.8), we find that $f_l = U^{-1}g_l$, whence (5.3) 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 (4.2).

$\square$

Chapter 6

The spectrum of A

In this section, we will prove the main result stating that

$$\sigma(A) = \bigcup_{s \in \mathbb{N}} I_s \tag{6.1}$$

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 (4.4), (4.5) depend continuously on k. Thus, since B is compact and connected,

$$I_s \text{ is a compact real interval, for each } s \in \mathbb{N}. \tag{6.2}$$

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 (4.2) 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 (6.2) implies that

$$\bigcup_{s\in\mathbb{N}} I_s \text{ is close.} \tag{6.3}$$

The first part of the statement (6.1) is

Theorem 6.1. $\sigma(A) \supset \bigcup_{s\in\mathbb{N}} I_s$.

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

$$A\psi_s(\cdot,k) = \lambda\psi_s(\cdot,k) \tag{6.4}$$

We regard $\psi_s(\cdot,k)$ as extended to the whole of $\mathbb{R}$ by the boundary condition (4.1), whence, due to the periodicity of A, (6.4) 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 $l \in \mathbb{N}$,

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

Then,

$$\begin{aligned}
(A-\lambda I)u_l &= \sum_{j\in\mathbb{N}} \left[(-\frac{d^2}{dx^2}-\lambda)u_l|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right] \qquad (6.5)\\
&= \sum_{j\in\mathbb{N}} \left[\left(-\frac{d^2}{dx^2}-\lambda\right)\left(\eta\left(\frac{|\cdot|}{l}\right)\psi_s(\cdot,k)\right)\Big|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right]\\
&\quad -\frac{2}{l}\sum_{j\in\mathbb{N}}\left[\left(\eta'\left(\frac{|\cdot|}{l}\right)\psi_s'(\cdot,k)\right)\Big|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right]\\
&\quad -\frac{1}{l^2}\sum_{j\in\mathbb{N}}\left[\left(\eta''\left(\frac{|\cdot|}{l}\right)\psi_s(\cdot,k)\right)\Big|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right]\\
&= \sum_{j\in\mathbb{N}}\left[\eta\left(\frac{|\cdot|}{l}\right)\left(-\frac{d^2}{dx^2}-\lambda\right)\psi_s(\cdot,k)|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right] + R
\end{aligned}$$

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

$$\|R\| \leq \frac{c}{l}\|\psi_s(\cdot,k)\|_{H^1(K_l)} \leq c\frac{1}{\sqrt{l}}, \tag{6.6}$$

with K_l denoting the ball in $\mathbb{R}$ with radius l, centered at x_0. Together with (6.4), (6.5) and (6.6), 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 6.2. $\sigma(A) \subset \bigcup_{s\in\mathbb{N}} I_s$.

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

$$u_l := \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \frac{1}{\lambda_s(k) - \lambda} \langle (Uf)(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)} \psi_s(x, k) dk \tag{6.7}$$

Here, note that, due to 6.3, some $\delta > 0$ exists such that

$$|\lambda_s(k) - \lambda| \geq \delta \text{ for all } s \in \mathbb{N}, k \in B \tag{6.8}$$

In particular, the boundary value problem

$$\begin{aligned} (A - \lambda I) v(\cdot, k) &= (Uf)(\cdot, k) \text{ on } \Omega, \\ v(\frac{1}{2}) &= e^{ik} v(-\frac{1}{2}) \end{aligned} \tag{6.9}$$

unique solution for every $k \in B$. Bloch wave expansion[1] 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 (4.2) and (6.8) 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 4.2, this implies $v \in L^2(\Omega \times B)$, and we can define $u := U^{-1} v \in L^2(\mathbb{R})$. Thus, (6.9) gives

$$a$$

[1] whats that?

whence (6.7) 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 5.1 gives

$$u_l \to u, \quad f_l \to f \quad \text{ in } L^2(\mathbb{R}). \tag{6.10}$$

We will now prove that in the distributional sense

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

which implies that $\langle u_l, (A - \lambda I)v \rangle = \langle f_l, v \rangle$ for all $v \in D(A)$, whence Theorem 5.2 implies $u_l \in D(A)$, and

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

Since A is closed, (6.10) now implies

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

which is the desired result. $\square$

Appendix A

Appendix

Theorem A.1 (Lax-Milgram)**.** *Let H be a real Hilbert space, with norm $\|\cdot\|$ and inner product $\langle\cdot,\cdot\rangle$ as well as the pairing of H with its dual space. Assume that*

$$B\colon H \times H \to R$$

is a bilinear mapping, for which there exist constant $\alpha, \beta > 0$ such that

$$|B[u,v]| \leq \alpha\|u\|\|v\| \quad (u, v \in H)$$

and

$$\beta\|u\|^2 \leq B[u,u] \quad (u \in H)$$

Finally, let $f\colon H \to \mathbb{R}$ be a bounded linear functional on H.

Then there exists a unique element $u \in H$ such that

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

for all $v \in H$.

Proof. For each fixed element $u \in H$, the mapping $v \mapsto B[u,v]$ is a bounded linear functional on H; whence the Riesz' Representation Theorem asserts the existence of a unique element $w \in H$ satisfying

$$B[u,v] = \langle w, v\rangle \tag{A.1}$$

Let us write $Au = w$ whenever (A.1) holds; so that

$$B[u,v] = \langle Au, v\rangle \quad (u, v \in H)$$

We first claim $A\colon H \to H$ is a bounded linear operator. Indeed if $\lambda_1, \lambda_2 \in \mathbb{R}$ and $u_1, u_2 \in H$, we see for each $v \in H$ that

$$\begin{aligned}
\langle A(\lambda_1 u_1 + \lambda_2 u_2), v\rangle &= B[\lambda_1 u_1 + \lambda_2 u_2, v],\ \text{(by (A.1))}\\
&= \lambda_1 B[u_1, v] + \lambda_2 B u_2, v]\\
&= \lambda_1 \langle Au_1, v\rangle + \lambda_2 \langle Au_2, v\rangle,\ \text{(by (A.1) again)}\\
&= \langle \lambda_1 Au_1 + \langle_2 Au_2, v\rangle.
\end{aligned}$$

This equality obtains for each $v \in H$, and so A is linear. Furthermore

$$\|Au\|^2 = \langle Au, Au\rangle = B[u, Au] \leq \alpha \|u\| \|Au\|.$$

Consequently $\|Au\| \leq \alpha \|u\|$ for all $u \in H$, and so A is bounded.

Next we assert

$$\begin{cases} A \text{ is one-to-one, and} \\ R(A),\ \text{the range of } A,\ \text{is close in } H. \end{cases} \tag{A.2}$$

To prove this, let us compute

$$\beta \|u\|^2 \leq B[u,u] = \langle Au, u\rangle \leq \|Au\| \|u\|$$

Hence $\beta \|u\| \leq \|Au\|$. This inequality easily implies (A.2).

We demonstrate now

$$R(A) = H \tag{A.3}$$

For if not, then, since $R(A)$ is closed, there would exist a nonzero element $w \in H$ with $w \in R(A)^{\perp}$. But this fact in turn implies the contradiction $\beta\|w\|^2 \leq B[w,w] = \langle Aw, w\rangle = 0$.
Next, we observe once more from the Riesz' Representation Theorem that

$$\langle f, v\rangle = \langle w, v\rangle \text{ for all } v \in H$$

for some element $w \in H$. We then utilise (A.2) and (A.3) to find $u \in H$ satisfying $Au = w$. Then

$$B[u,v] = \langle Au, v\rangle = \langle w, v\rangle = \langle f, v\rangle (v \in H)$$

and this is the claim.

Finally, we show there is at most one element $u \in H$ verifying the claim. For if both $B[u,v] = \langle f, v\rangle$ and $B[\tilde{u}, v] = \langle f, v\rangle$, then $B[u - \tilde{u}, v] = 0$ $(v \in H)$. We set $v = u - \tilde{u}$ to find $\beta\|u - \tilde{u}\|^2 \leq B[u - \tilde{u}, u - \tilde{u}] = 0$. □

Theorem A.2 (Sobolev Embedding)**.**

$$H^1[0,1] \subset C[0,1].$$

Proof. Prove that the H^1 norm dominates the C norm, namely, sup-norm, on $C_c^\infty[0,1]$. First, for $0 \leq x \leq y \leq 1$, the difference between maximum and minimum values of $f \in C_c^\infty[0,1]$ is constrained:

$$|f(y) - f(x)| = |\int_x^y f'(t)dt| \leq \left(\int_0^1 |f'(t)|^2 dt\right)^{1/2} \cdot |x - y|^{\frac{1}{2}} = \|f'\|_{L^2} \cdot |x - y|^{\frac{1}{2}}$$

Let $y \in [0,1]$ be such that $|f(y) = \min_x |f(x)|$. Then, using this inequality,

$$\begin{aligned}
|f(x)| &\leq |f(y)| + |f(x) - f(y)| \\
&\leq \int_0^1 |f(t)dt + |f(x) - f(y)| \\
&\leq \|f\| + \|f'\| \ll 2\left(\|f\|^2 + \|f'\|^2\right)^{1/2} = 2\|f\|_{H^1}
\end{aligned}$$

Thus, on $C_c^\infty[0,1]$ the H^1 norm dominates the sup-norm and therefore this comparison holds on the H^1 completion $H^1[0,1]$, and $H^1[0,1] \subset C[0,1]$. $\square$