Chapter 1

The Operator

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 and x_i are periodically distributed. Ω_k will denote the periodicity cell containing delta point x_k and let w.o.l.g. $x_0 = 0$ and $|\Omega_i| = 1$ $\forall i \in \mathbb{Z}$. 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 $u \in H^1(\mathbb{R})$.

This expression actually converges as for arbitrary $\tilde{x}_i \in \Omega_i$

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

Now, 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 $\alpha, \beta >$ 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 1.1. *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 1.2. *$B[u, u]$ is coercive.*

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

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

and for $\rho < 0$:

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

□

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

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

Chapter 2

The Domain

For every fixed $k \in \mathbb{Z}$ choosing a $v \in C^\infty(\mathbb{R})$ with $\operatorname{supp} v = \Omega_k$ as test function 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 $\mathcal{D}(A) \subset \left\{u \in \bigcap_{i \in \mathbb{Z}} (H^2(x_i - 1/2, x_i) \cap H^2(x_i, x_i + 1/2))\right\}$.

Next, again for an arbitrary $k \in \mathbb{Z}$ choosing a $v \in C^\infty(\mathbb{R})$ such that $\operatorname{supp} v = \Omega_k$ and integrating in (1.2) on both sides of x_k by parts 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 for a v with $\operatorname{supp} v = (x_k - 1/2, x_k + 1/2)$ 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

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

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

Theorem 2.1. *A is a self-adjoint operator*

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

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 aswell. $\square$

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 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 precicely, define A_k as follows: let us consider the problem to find for $f \in L^2(\Omega)$ a $u \in H_k^1$ 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

$$\begin{aligned} H_k^1 := \Big\{ H^1(\Omega) : \psi(-\frac{1}{2}) = e^{ik}\psi(-\frac{1}{2}), \psi'(-\frac{1}{2}) = e^{ik}\psi'(-\frac{1}{2}) \\ \text{and } \psi'(x_0 - 0) - \psi'(x_0 + 0) + \rho\psi'(x_0) = 0 \Big\} \end{aligned} \tag{3.1}$$

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

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

Subsequently, we will now mainly consider the eigenvalue problem

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

In writing the boundary condition in the form (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. Furthermore we know that (3.2), (3.1) is a symmetric eigenvalue problem[2] in $L^2(\Omega)$ and ψ from (3.2) extended to the whole of $\mathbb{R}$ by (3.1) solves also the eigenvalue problem of A with the same eigenvalue.

Since Ω is bounded, the subsequently shown compactness can be used to prove that (3.2), (3.1) 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

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

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

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

[1] I think I will explain this also in more detail

[2] explain this in more detail

Though such u_j has to satisfy

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

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 this u_j is bounded in $H^1(\Omega)$. As $H^1(\Omega) \subset C(\Omega)$:

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

From (3.3) for a $f \in B_{H^1} := \{f \in H_k^1(\Omega) : \|f\| \leq 1\}$ $\exists g \in \{g_1, \dots, g_{n_\epsilon}\} : \quad \|f-g\| \leq \epsilon$ 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 $\forall f \in B_{H_k^1}$. 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. □

Now, we want to transform the eigenvalue problem (3.2) such that the boundary condition is independent from k. Define therefore

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

Then,

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

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

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

Furthermore, using (3.2) and (3.1),

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

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

$$\tilde{A}_k\varphi = \lambda\varphi \text{ on } \Omega, \tag{3.4}$$

$$\varphi(x-\frac{1}{2}) = \varphi(x+\tfrac{1}{2}) \tag{3.5}$$

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

$$(Uf)(x,k) := \frac{1}{\sqrt{|B|}}\sum_{n\in\mathbb{Z}} f(x-n)e^{ikn} \quad (x\in\Omega, k\in B) \tag{3.6}$$

Theorem 3.2. *$U\colon L^2(\mathbb{R}) \to L^2(\Omega \times B)$ is an isometric isomorphism, with inverse*

$$(U^{-1}g)(x-n) = \frac{1}{\sqrt{|B|}} \int_B g(x,k) e^{-ikn} dk \quad (x \in \Omega, n \in \mathbb{Z}) \tag{3.7}$$

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

$$U^{-1}g = \frac{1}{\sqrt{|B|}} \int_B g(\cdot,k) dk. \tag{3.8}$$

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

$$\int_{\mathbb{R}} |f(x)|^2 dx = \sum_{n\in\mathbb{Z}} \int_\Omega |f(x-n)|^2 dx. \tag{3.9}$$

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 (3.6) (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 (3.9), 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 (3.7) or (3.8). Let $g \in L^2(\Omega \times B)$, and define

$$f(x-n) \coloneqq \frac{1}{\sqrt{|B|}} \int_B g(x,k) e^{-ikn} dk \quad (x \in \Omega, n \in \mathbb{Z}). \tag{3.10}$$

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,

$$\begin{aligned} \int_{\Omega \times B} |g(x,k)|^2 dx dk &= \textstyle\int_\Omega \sum_{n \in \mathbb{Z}} |f(x-n)|^2 dx && (3.11) \\ &= \textstyle\sum_{n \in \mathbb{Z}} \int_\Omega |f(x-n)|^2 dx && (3.12) \\ &= \textstyle\int_{\mathbb{R}} |f(x)|^2 dx, && (3.13) \end{aligned}$$

i.e. $f \in L^2(\mathbb{R})$. Now (3.6) 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 (3.10) implies $Uf = g$ and (3.7). Now (3.8) follows from (3.7) using $g(x+n,k) = e^{ikn} g(x,k)$. $\square$

Chapter 4

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

$$f_l(x) := \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \langle (Uf)(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)} \psi_s(x, K) dk \quad (x \in \mathbb{R}). \tag{4.1}$$

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

$$g_l(x, k) := \sum_{s=1}^{l} \langle (Uf)(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)} \psi_s(x, k). \tag{4.2}$$

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 3.2. Altogether, Lebesgue's Dominated Convergence theorem implies

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

i.e.,

$$\|Uf - g_l\|_{L^2(\Omega\times B)} \to 0 \text{ as } l \to \infty \tag{4.3}$$

Using (4.1), (4.2) and (3.8), we find that $f_l = U^{-1}g_l$, whence (4.3) 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 (3.2).

$\square$

Chapter 5

The spectrum of A

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

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

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 (3.4), (3.5) depend continuously on k. Thus, since B is compact and connected,

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

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 (3.2) 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 (5.2) implies that

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

The first part of the statement (5.1) is

Theorem 5.1. $\sigma(A) \supset \bigcup_{s\in\mathbb{N}} I_s$.

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

$$A\psi_s(\cdot,k) = \lambda\psi_s(\cdot,k) \tag{5.4}$$

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, (5.4) 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,

$$\begin{aligned}
(A-\lambda I)u_l &= \sum_{j\in\mathbb{N}}\left[(-\frac{d^2}{dx^2}-\lambda)u_l|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right] \qquad (5.5)\\
&= \sum_{j\in\mathbb{N}}\left[\left(-\frac{d^2}{dx^2}-\lambda\right)\left(\eta\left(\frac{|\cdot|}{l}\right)\psi_s(\cdot,k)\right)\Big|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right]\\
&\quad -\frac{2}{l}\sum_{j\in\mathbb{N}}\left[\left(\eta'\left(\frac{|\cdot|}{l}\right)\psi_s'(\cdot,k)\right)|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right]\\
&\quad -\frac{1}{l^2}\sum_{j\in\mathbb{N}}\left[\left(\eta''\left(\frac{|\cdot|}{l}\right)\psi_s(\cdot,k)\right)|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right]\\
&= \sum_{j\in\mathbb{N}}\left[\eta\left(\frac{|\cdot|}{l}\right)\left(-\frac{d^2}{dx^2}-\lambda\right)\psi_s(\cdot,k)|_{(x_j,x_{j+1})}\cdot \mathbb{1}_{(x_j,x_{j+1})}\right]+R
\end{aligned}$$

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

$$\|R\| \leq \frac{c}{l}\|\psi_s(\cdot, k)\|_{H^1(K_l)} \leq c\frac{1}{\sqrt{l}}, \tag{5.6}$$

with K_l denoting the ball in $\mathbb{R}$ with radius l, centered at x_0. Together with (5.4), (5.5) and (5.6), 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, $\lambda \in \sigma(A)$. $\square$

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

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

$$u_l := \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \frac{1}{\lambda_s(k) - \lambda} \langle (Uf)(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)} \psi_s(x, k) dk \tag{5.7}$$

Here, note that, due to 5.3, some $\delta > 0$ exists such that

$$|\lambda_s(k) - \lambda| \geq \delta \text{ for all } s \in \mathbb{N}, k \in B \tag{5.8}$$

In particular, the boundary value problem

$$\begin{aligned} (A - \lambda I)v(\cdot, k) &= (Uf)(\cdot, k) \text{ on } \Omega, \\ v(\frac{1}{2}) &= e^{ik} v(-\frac{1}{2}) \end{aligned} \tag{5.9}$$

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 (3.2) and (5.8) 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, (5.9) gives

$$a$$

[1] whats that?

whence (5.7) 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 4.1 gives

$$u_l \to u, \quad f_l \to f \quad \text{ in } L^2(\mathbb{R}). \tag{5.10}$$

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 4.2 implies $u_l \in D(A)$, and

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

Since A is closed, (5.10) 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

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

Consequently $\|Au\| \le \alpha \|u\|$ 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

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

Hence $\beta \|u\| \le \|Au\|$. 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 $\beta\|u - \tilde{u}\|^2 \leq B[u - \tilde{u}, u - \tilde{u}] = 0$. $\square$

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