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

The left-hand side of problem (1.2) is actually convergent as for arbitrary $\tilde{x}_i \in \Omega_i$

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

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

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

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

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

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

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

□

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

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

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

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

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 $u \coloneqq R_\mu f$ 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 $R_{\mu,k} \colon L^2(\Omega) \to H_k^1, f \mapsto u$ 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 $(u_j)_{j\geq 1} \in H_k^1$ 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

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

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

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

Now, for $\epsilon > 0$ we partition Ω into n_ϵ equidistant intervals I_k, i.e. $\Omega = \bigcup_{j=1}^{n_\epsilon} I_j$. As all $f \in B_{H_k^1}$ 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

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

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 $\{g_1, \dots, g_N\}$ such that for all $f \in B_{H_k^1}$ there exists a $\nu \in \{1, \dots, N\}$ 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. $\square$

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

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

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,

$$\begin{aligned}\int_{\Omega\times B}|g(x,k)|^2dxdk &= \textstyle\int_\Omega \sum_{n\in\mathbb{Z}}|f(x-n)|^2dx &(3.12)\\ &= \textstyle\sum_{n\in\mathbb{Z}}\int_\Omega |f(x-n)|^2dx &(3.13)\\ &= \textstyle\int_{\mathbb{R}}|f(x)|^2dx, &(3.14)\end{aligned}$$

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

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

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,

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

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, $\lambda \in \sigma(A)$. $\square$

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),

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

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

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

i.e. (4.12). □

Bibliography

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Erklärung

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

Ort, den Datum