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 $i \in \mathbb{Z}$.[1]

Henceforth, consider for a $\mu \in \mathbb{R}^2$ 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.

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

[2]removed here 'small enough', its at this point just too far fetched. Have to implement it at a later point

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

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

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 $u \in H^1$ 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. *For the bilinear form $B[u, v]$ as left-hand of* (1.2)

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

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

Proof:

i) The boundedness of $B[u, v]$ one see through

$$|B(u, \varphi)|^2 \leq \|u'\| \cdot \|v'\| + 2\rho \sum_{i \in \mathbb{Z}} |u(x_i)|^2 |v(x_i)|^2 - \mu \|u\| \cdot \|v\|$$

$$\leq \|u'\| \cdot \|v'\| + 8\rho \cdot \|u\|^2_{H^1(\mathbb{R})} \|v\|^2_{H^1(\mathbb{R})} - \mu \|u\| \cdot \|v\|$$

$$= (8\rho - \mu) \|u\| \cdot \|v\| + 8\rho (\|u\| \cdot \|v'\| + \|u'\| \cdot \|v\|) + (8\rho + 1) \|u'\| \cdot \|v'\|$$

$$\leq \alpha \cdot \|u\|_{H^1} \cdot \|\varphi\|_{H^1}$$

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

$$B(u, u) = \langle u', u' \rangle + \rho \sum_{i \in \mathbb{Z}} u(x_i)^2 - \mu \langle u, u \rangle$$

$$\geq \langle u', u' \rangle - \mu \langle u, u \rangle \geq \langle u', u' \rangle + \langle u, u \rangle$$

$$= \|u\|^2_{H^1}.$$

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

$$B(u, u) = \langle u', u' \rangle + \rho \sum_{i \in \mathbb{Z}} |u(x_i)|^2 - \mu \langle u, u \rangle$$

$$= \langle u', u' \rangle + \rho \sum_{i \in \mathbb{Z}} \left| u(\tilde{x}_i) + \int_{\tilde{x}_i}^{x_i} u(x) dx \right|^2 - \mu \langle u, u \rangle$$

$$\geq \langle u', u' \rangle + 2\rho \left(\int_{\mathbb{R}} |u(x)|^2 dx + \int_{\mathbb{R}} |u'(\tau)|^2 d\tau \right) - \mu \langle u, u \rangle$$

$$= (2\rho + 1) \|u'\|^2 + (2\rho - \mu) \|u\|^2$$

$$\geq \beta \|u\|^2_{H^1},$$

$\square$

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

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

As H^1 is dense in L^2 this means 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 $\mathcal{D}(A) = \mathcal{R}(R_\mu)$ follows.

Chapter 3

The Domain

[1] 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

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

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[1] Here, is also going to be some introduction text, at least it is missing for me...

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

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

The opposite inclusion is shown, as $\mathcal{R}(R_\mu) = \mathcal{D}(A)$, by proving for a $u \in B$ 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 v having 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 important later.[2]

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[2]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 for all $v \in H^1$:

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

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. $\qquad\square$

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 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 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

$$
\begin{aligned}
H_k^1 := \Big\{ H^1(\Omega) : \psi(-\tfrac{1}{2}) &= e^{ik}\psi(-\tfrac{1}{2}), \psi'(-\tfrac{1}{2}) = e^{ik}\psi'(-\tfrac{1}{2}) \\
&\text{and } \psi'(x_0 - 0) - \psi'(x_0 + 0) + \rho\psi'(x_0) = 0 \Big\}.
\end{aligned}
\tag{4.1}
$$

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 analogously

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

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 $H_{loc}^2(\mathbb{R})$ 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 4.1. *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

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

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

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

Now, choosing here $v = u_j$ 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 is

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

From (4.3) follows for a $f \in B_{H^1} := \{f \in H_k^1(\Omega) : \|f\| \leq 1\}$ that

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

and with that we can approximate f by simple functions through partitioning Ω into n_ϵ^3 equidistant intervals. As our simple functions are 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. [4] $\qquad \square$

Now, we want to transform the eigenvalue problem (4.2) such that the boundary

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[3]epsilon finite...

[4]I somehow skipped the finite coveer?!

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 (4.2) and (4.1), gives

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

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

$$
\begin{aligned}
\tilde{A}_k \varphi &= \lambda \varphi \text{ on } \Omega, & (4.4) \\
\varphi\left(x - \frac{1}{2}\right) &= \varphi\left(x + \frac{1}{2}\right). & (4.5)
\end{aligned}
$$

with the same eigenvalue sequence $(\lambda_s(s))_{s \in \mathbb{N}}$ as in (4.2). 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

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

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

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

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

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 $g(x + n, k) = e^{ikn} g(x, k)$. $\quad\square$

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

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

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

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

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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

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

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

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

Then,

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

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

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 $l \in \mathbb{N}$,

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

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and

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

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

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

In particular, the boundary value problem

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

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 $u := U^{-1}v \in L^2(\mathbb{R})$.

---

[1] whats that?

Thus, (6.9) gives

$$\langle (Uf)(\cdot, k), \psi_s(\cdot, k)\rangle_{L^2(\Omega)} = \langle (A - \lambda I)(Uu)(\cdot, k), \psi_s(\cdot, k)\rangle_{L^2(\Omega)}$$

$$= \langle (Uu)(\cdot, k), (A - \lambda I)\psi_s(\cdot, k)\rangle_{L^2(\Omega)}$$

$$= (\lambda_s(k) - \lambda)\langle Uu(\cdot, k), \psi_s(\cdot, k)\rangle_{L^2(\Omega)}$$

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

$$(A - \lambda I)u_l = f_l \text{ for all } l \in \mathbb{N} \tag{6.11}$$

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

Left to prove is (6.11), i.e. that

$$\langle u_l, (A - \lambda I)\varphi\rangle_{L^2(\mathbb{R})} \quad \forall \varphi \in C_0^\infty(\mathbb{R}). \tag{6.12}$$

Let $\varphi \in C_0^\infty(\mathbb{R})$ be fixed, and let $K \subseteq \mathbb{R}$ denote an open interval containing $\text{supp}(\varphi)$

in its interior. Both the functions

$$r_s(x,k) := \frac{1}{\lambda_s(k) - \lambda} \langle (Uf)(\cdot,k), \psi_s(\cdot,k) \rangle_{L^2(\Omega)} \psi_s(x,k) \overline{(A - \lambda I)\varphi(x)},$$

$$t_s(x,k) := \langle (Uf)(\cdot,k), \psi_s(\cdot,k) \rangle_{L^2(\Omega)} \psi_s(x,k) \overline{\varphi(x)}$$

are easily seen to be in $L^2(K \times B)$ by Fubini's Theorem, since (6.8), and the fact that $(A - \lambda I)\varphi \in L^\infty(K)$ and $\varphi \in L^\infty(K)$, imply both

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

are bounded by $C\|(Uf)(\cdot,k)\|_{L^2(\Omega)}^2 \|\psi_s(\cdot,k)\|_{L^2(K)}^2$ the latter factor is bounded as a function of k because K is covered by a finite number of copies of Ω, and the former is in $L^1(B)$ by Theorem 4.2.

Since $K \times B$ is bounded, r and t are also $L^1(K \times B)$. 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 (6.7),

$$\int_K u_l(x) \overline{(A - \lambda I)\varphi} dx = \frac{1}{\sqrt{|B|}} \sum_{s=1}^l \int_K \left(\int_B r_s(x,k) dk \right) dx$$

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

$$\langle \psi_s(\cdot,k), (A - \lambda I)\varphi \rangle_{L^2(K)} dk.$$

Since φ has compact support in the interior of K, $(A - \lambda I)$ may be moved to $\psi_s(\cdot,k)$,

and hence (4.2) gives

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

$$= \frac{1}{\sqrt{|B|}}\sum_{s=1}^{l}\int_B \left(\int_K t_s(x, k)dx\right)dk$$

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

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

$$= \int_K f_l(x)\overline{\varphi(x)},$$

i.e. (6.12). □