

# 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

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

on the whole of  $\mathbb{R}$ , where  $f$  is a function modelling an external force,  $\delta$  denotes the Dirac delta distribution and  $x_i$  are periodically distributed points on  $\mathbb{R}$ .  $\Omega_k$  will hereafter identify the periodicity cell containing delta point  $x_k$  and let w.o.l.g.  $x_0 = 0$  and  $|\Omega_i| = 1 \ \forall i \in \mathbb{Z}$ .<sup>1</sup>

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

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

where  $f \in L^2(\mathbb{R})$  and  $u \in H^1(\mathbb{R})$ .

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<sup>1</sup>Obviously, here is going to be much more but for starters this should suffice

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

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

# Chapter 2

## The Operator

As we can interpret the left-hand side of (1.2) as a bounded bilinear mapping  $B: H^1(\mathbb{R}) \times H^1(\mathbb{R}) \rightarrow \mathbb{R}$ , 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.*

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

□

and

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

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

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

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  $R_\mu: L^2(\mathbb{R}) \rightarrow H^1(\mathbb{R}), f \mapsto u$  is well-defined; obviously the mapping is one-to-one since for  $u_1 = u_2$

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

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  $R_\mu$  is bijective and in turn we can define the Schrödinger operator as follows

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

# Chapter 3

## The Domain

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

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

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

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

$$\begin{aligned} & - \left( \int_{x_k-1/2}^{x_k} + \int_{x_k}^{x_k+1/2} \right) u'' \cdot \bar{v} + \left( u'(x_k - 0) \overline{v(x_k)} - u'(x_k + 0) \overline{v(x_k)} \right) \\ & + \rho u(x_k) \overline{v(x_k)} = - \int_{x_k-1/2}^{x_k} u'' \bar{v} - \int_{x_k}^{x_k+1/2} u'' \bar{v} \end{aligned}$$

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  $R_\mu$ . More specifically, as  $\mathcal{D}(R_\mu) = L^2(\mathbb{R})$  define  $f := Au$  and show that  $u = R_\mu(f - \mu u)$ :

$$\begin{aligned} \int_{\mathbb{R}} u' \bar{v}' + \rho \sum_{i \in \mathbb{Z}} u(x_i) \overline{v(x_i)} - \mu \int_{\mathbb{R}} u \bar{v} &= \int_{\mathbb{R}} (f - \mu u) \bar{v} \\ \iff \sum_{i \in \mathbb{Z}} \int_{\Omega_i} u' \bar{v}' + \rho u(x_i) \overline{v(x_i)} &= - \sum_{i \in \mathbb{Z}} \int_{x_i - 1/2}^{x_i} u'' \bar{v} + \int_{x_i}^{x_i + 1/2} u'' \bar{v} \end{aligned}$$

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

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

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.<sup>1</sup>

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<sup>1</sup>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  $\forall v \in H^1$ :

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

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  $R_\mu$  is symmetric. Both can be used to show that  $R_\mu$  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  $R_\mu^{-1}$  self-adjoint. As  $A$  is simply  $R_\mu^{-1}$  shifted by the real constant  $\mu$ ,  $A$  is self-adjoint as well.  $\square$



# Chapter 4

## Fundamental domain of periodicity and the Brillouin zone

Let  $\Omega$  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  $\Omega$ . As commonly used by literature the reciprocal lattice for  $\Omega$  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  $\Omega$  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

$$\begin{aligned} H_k^1 := \left\{ H^1(\Omega) : \psi\left(-\frac{1}{2}\right) = e^{ik}\psi\left(-\frac{1}{2}\right), \psi'\left(-\frac{1}{2}\right) = e^{ik}\psi'\left(-\frac{1}{2}\right) \right. \\ \left. \text{and } \psi'(x_0 - 0) - \psi'(x_0 + 0) + \rho\psi'(x_0) = 0 \right\} \end{aligned} \quad (4.1)$$

Using the fact that  $H_k^1$  is a closed subspace<sup>1</sup> 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

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

Subsequently, we will now mainly consider the eigenvalue problem

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

In writing the boundary condition in the form (4.1), we understand  $\psi$  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<sup>2</sup> in  $L^2(\Omega)$  and  $\psi$  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  $\Omega$  is bounded, the subsequently shown compactness can be used to prove 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

$$\lambda_1(k) \leq \lambda_2(k) \leq \dots \leq \lambda_s(k) \rightarrow \infty \text{ as } s \rightarrow \infty$$

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

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

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<sup>1</sup>I think I will explain this also in more detail

<sup>2</sup>explain this in more detail

Though such  $u_j$  has to satisfy

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

Now, choosing here  $v = u_j$  and (1.3) yields for  $\mu$  small enough

$$\|u_j\|_{H^1(\Omega)} \leq \|f_j\|_{L^2(\Omega)} \|u_j\|_{L^2(\Omega)} \leq c \sqrt{\text{vol}(\Omega)}$$

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

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

From (4.3) for a  $f \in B_{H^1} := \{f \in H_k^1(\Omega) : \|f\| \leq 1\} \exists g \in \{g_1, \dots, g_{n_\epsilon}\} : \|f - g\| \leq \epsilon$  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  $\Omega$  into  $n_\epsilon$  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.  $\square$

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

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

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  $\tilde{A}_k: D(A_k) \rightarrow L^2(\mathbb{R})$  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),

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

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

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

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

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

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

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

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

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

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

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

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

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  $\Omega$ ,

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

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

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

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*

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

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

*Proof.* Since  $Uf \in L^2(\Omega \times B)$ , 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

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

where

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

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

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

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

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

i.e.,

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

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

$$\|U(f - f_l)\|_{L^2(\Omega \times B)} \rightarrow 0 \text{ as } l \rightarrow \infty,$$

and the assertion follows since  $U: L^2(\mathbb{R}) \rightarrow L^2(\Omega \times B)$  is isometric by Lemma (4.2). □



# 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, Poincaré'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  $\mu_s \rightarrow \infty$  as  $s \rightarrow \infty$ , we obtain

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

which together with (6.2) implies that

$$\bigcup_{s \in \mathbb{N}} I_s \text{ is close.} \quad (6.3)$$

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

$$A\psi_s(\cdot, k) = \lambda\psi_s(\cdot, k) \quad (6.4)$$

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  $\psi_s \in H_{loc}^2(\mathbb{R})$

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,

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

where  $R$  is a sum of products of derivatives (of order  $\geq 1$ ) of  $\eta(\frac{|\cdot|}{l})$ , and derivatives (of order  $\leq 1$ ) of  $\psi_s(\cdot, k)$ . Thus (note that  $\psi_s(\cdot, k) \in H_{loc}^2(\mathbb{R})$ ), and the semi-periodic structure of  $\psi_s(\cdot, k)$  implies

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

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

$$\frac{1}{\|u_l\|} \|(A - \lambda I)u_l\| \rightarrow 0 \text{ as } l \rightarrow \infty$$

Thus, either  $\lambda$  is an eigenvalue of  $A$ , or  $(A - \lambda I)^{-1}$  exists but is unbounded. In both cases,  $\lambda \in \sigma(A)$ .  $\square$

**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  $l \in \mathbb{N}$ ,

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

and

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

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

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

In particular, the boundary value problem

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

unique solution for every  $k \in B$ . Bloch wave expansion<sup>1</sup> gives

$$\begin{aligned} \|(Uf)(\cdot, k)\|_{L^2(\Omega)}^2 &= \sum_{s=1}^{\infty} |\langle (Uf)(\cdot, k), \psi_s(\cdot, k) \rangle|^2 \\ &= \sum_{s=1}^{\infty} |\langle (A - \lambda)v(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)}|^2 \end{aligned}$$

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

$$\begin{aligned} \|(Uf)(\cdot, k)\|_{L^2(\Omega)}^2 &= \sum_{s=1}^{\infty} |\lambda_s(k) - \lambda|^2 |\langle v(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)}|^2 \\ &\geq \delta^2 \|v(\cdot, k)\|_{L^2(\Omega)}^2 \end{aligned}$$

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*

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<sup>1</sup>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

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

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. □

# 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*

$$B: H \times H \rightarrow \mathbb{R}$$

*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  $f: H \rightarrow \mathbb{R}$  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

$$B[u, v] = \langle w, v \rangle \quad (\text{A.1})$$

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  $A: H \rightarrow H$  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

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

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

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

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

**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:

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



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