

# 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

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

on the whole of  $\mathbb{R}$  where  $f$  is a function modelling an external force and  $x_i$  are periodically distributed.  $\Omega_k$  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

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

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

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

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

Now, as we can interpret the lefthand 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

$$(i) \quad |B[u, v]| \leq \alpha \|u\| \|v\| \quad (u, v \in H^1(\mathbb{R}))$$

and

$$(ii) \quad \beta \|u\|^2 \leq B[u, u] \quad (u \in H^1(\mathbb{R}))$$

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.*

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

□

**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  $R_\mu: L^2(\mathbb{R}) \rightarrow H^1(\mathbb{R}), f \mapsto u$  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

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



# Chapter 2

## The Domain

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

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

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<sup>1</sup>Here HAS to be some more text but I don't know what

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

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

Now as  $\mathcal{D}(R_\mu) = L^2(\mathbb{R})$  and  $\mathcal{R}(R_\mu) = \mathcal{D}(R_\mu^{-1})$ , we want to show that for each  $f, g \in L^2(\mathbb{R})$

$$\gamma := \langle R_\mu f, g \rangle - \langle f, R_\mu g \rangle = 0$$

Now, choose  $u, v \in \mathcal{D}(A)$  such that  $R_\mu f = u, R_\mu g = v$ . Using this fact in combination with (1.2) for those two  $u, v$  one gets for all  $\varphi, \psi \in H^1$

$$\begin{aligned}
\int u' \varphi' + \rho \sum_{i \in \mathbb{Z}} u(i) \varphi(i) - \mu \int u \varphi &= \int f \varphi \\
\int v' \psi' + \rho \sum_{i \in \mathbb{Z}} v(i) \psi(i) - \mu \int v \psi &= \int g \psi
\end{aligned}$$

As it has to hold for all  $\varphi, \psi \in H_k^1$  the special choice of  $\varphi = v$  and  $\psi = u$  yields  $\gamma = 0$  and  $R_\mu$  is therefore symmetric. All in all we can use this to show that  $R_\mu$  is self-adjoint, as we get for an arbitrary  $v^* \in \mathcal{D}(R_\mu^{-1})$  there exists a  $v \in \mathcal{R}(R_\mu^{-1}) = \mathcal{D}(R_\mu)$ :

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

So  $v^* \in \mathcal{R}(R_\mu)$  which means that  $R_\mu^{-1}$  is self-adjoint. As  $A$  is simply  $R_\mu^{-1}$  shifted

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<sup>2</sup>I haven't understood this proof yet. As  $R$  is symmetric  $\mathcal{D}(R^*) \supseteq \mathcal{D}(R)$  we therefore have to show  $\mathcal{D}(R^*) \subseteq \mathcal{D}(R)$  to show the self-adjointness...

by the real constant  $\mu$ ,  $A$  is self-adjoint as well.

□



# Chapter 3

## Fundamental domain of periodicity and the Brillouin zone

Let  $\Omega$  be the fundamental domain of periodicity associated with (1.1), e.g.  $\Omega = \Omega_0$ . 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  $k \in \overline{B}$ , we now consider now the operator <sup>1</sup>

$$A_k: H_k^1 \rightarrow L^2(\mathbb{R}), \quad \psi \mapsto -\Delta\psi + \rho \cdot \delta_{x_0}\psi \quad (3.1)$$

where

$$H_k^1 := \left\{ H^1(\mathbb{R}) : \psi\left(-\frac{1}{2}\right) = e^{ik}\psi\left(\frac{1}{2}\right) \right\} \quad (3.2)$$

As  $H_k^1$  is a Hilbert space we can use the same arguments as in 1.1 and 1.2 to show that the resolvent  $R_{\mu,k}$  for  $A_k$  is well defined and therefore again

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

and we consider the eigenvalue problem

$$A_k\psi = \lambda\psi \text{ on } \Omega, \quad (3.3)$$

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<sup>1</sup>Where does Lax-Milgram reappear?

In writing the boundary condition in the form, we understand  $\psi$  extended to the whole of  $\mathbb{R}$ . In fact, (3.2) forms boundary conditions on  $\partial\Omega$ , so-called semi-periodic boundary conditions. Furthermore we know that (3.3), (3.2) is a symmetric eigenvalue problem in  $L^2(\Omega)$  and  $\psi$  from 3.3 extended to the whole of  $\mathbb{R}$  by (3.2) 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 (3.3), (3.2) 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. Academic Press (Harcourt Brace Jovanovich, Publishers), New York, 1975–1980., XIII.16, Theorem XIII.98]).<sup>2</sup>

**Theorem 3.1.** *The operator  $R_{\mu,k}$  is compact.*

*Proof.*  $R_{\mu,k}$  is compact since for  $(f_j)_{j \geq 1} \in L^2(\Omega) : \|f_j\|_{L^2(\Omega)} \leq c \ \forall j \geq 1$  there exists for all  $j \in \mathbb{N}$   $u_j \in H_k^1$  with

$$R_{\mu,k} f_j = u_j$$

now we show  $\|u_j\|_{H^1} \leq \tilde{c}$  but has such a  $u_j$  has to satisfy

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

choosing  $v = u$  and using (1.3) it follows for  $\mu$  small enough

$$c \|u_j\|_{H^1(\Omega)} \leq \left| \int_{\Omega} f_j v \right| \leq \underbrace{\|f_j\|_{L^2(\Omega)}}_{\leq c} \underbrace{\|u_j\|_{L^2(\Omega)}}_{\leq D \sqrt{\text{vol}(\Omega)}}$$

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<sup>2</sup>todo some expl

and  $H^1$  can be compactly embedding into  $L^2$ , since for  $B_{H_k^1} := \{f \in H_k^1(\Omega) : \|f\| \leq 1\}$ .

We want to show that  $\forall \epsilon > 0 \exists g_1, \dots, g_{n_\epsilon}$ :

$$\forall f \in B \exists g \in \{g_1, \dots, g_{n_\epsilon}\} : \|f - g\| \leq \epsilon$$

Together with the closure of  $H_k^1$  this yields the compact embedding. Now, as  $H^1(\Omega) \subset C(\Omega)$ :

$$|f(x) - f(y)| \leq c|x - y|^{1/2} \text{ for some } c > 0 \quad (3.4)$$

Now, for a  $f \in B_{H^1}$  follows from (3.4) that

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

And with that we can approximate a  $f \in B$  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

$$|f(\frac{k}{n}) - c_{k+1}| < \frac{1}{n}$$

such that

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

□

Now define

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

Then,

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

We therefore define the operator  $\tilde{A}_k: D(A_k) \rightarrow L^2(\mathbb{R})$ ,

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

Furthermore, using (3.3) and (3.2),

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

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

$$\tilde{A}_k \varphi = \lambda \varphi \text{ on } \Omega, \tag{3.5}$$

$$\varphi(x - \frac{1}{2}) = \varphi(x + \frac{1}{2}) \tag{3.6}$$

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

$$(Uf)(x, k) := \frac{1}{\sqrt{|B|}} \sum_{n \in \mathbb{Z}} f(x - n) e^{ikn} \quad (x \in \Omega, k \in B) \tag{3.7}$$

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

$$(U^{-1}g)(x - n) = \frac{1}{\sqrt{|B|}} \int_B g(x, k) e^{-ikn} dk \quad (x \in \Omega, n \in \mathbb{Z}) \quad (3.8)$$

If  $g(\cdot, k)$  is extended to the whole of  $\mathbb{R}$  by the semi-periodicity condition (3.2), we have

$$U^{-1}g = \frac{1}{\sqrt{|B|}} \int_B g(\cdot, k) dk. \quad (3.9)$$

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

$$\int_{\mathbb{R}} |f(x)|^2 dx = \sum_{n \in \mathbb{Z}} \int_{\Omega} |f(x - n)|^2 dx. \quad (3.10)$$

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

$$f(x - n) := \frac{1}{\sqrt{|B|}} \int_B g(x, k) e^{-ikn} dk \quad (x \in \Omega, n \in \mathbb{Z}). \quad (3.11)$$

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  $\Omega$ ,

$$\int_{\Omega \times B} |g(x, k)|^2 dx dk = \int_{\Omega} \sum_{n \in \mathbb{Z}} |f(x - n)|^2 dx \quad (3.12)$$

$$= \sum_{n \in \mathbb{Z}} \int_{\Omega} |f(x - n)|^2 dx \quad (3.13)$$

$$= \int_{\mathbb{R}} |f(x)|^2 dx, \quad (3.14)$$

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

# 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*

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

*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

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

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 3.2. Altogether, Lebesgue's Dominated Convergence theorem implies

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

i.e.,

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

Using (4.1), (4.2) and (3.9), we find that  $f_l = U^{-1}g_l$ , whence (4.3) 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 (3.2). □



# Chapter 5

## The spectrum of A

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

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

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 (3.5), (3.6) depend continuously on  $k$ . Thus, since  $B$  is compact and connected,

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

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 (3.3) 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 (5.2) implies that

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

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

$$A\psi_s(\cdot, k) = \lambda\psi_s(\cdot, k) \tag{5.3}$$

We regard  $\psi_s(\cdot, k)$  as extended to the whole of  $\mathbb{R}$  by the boundary condition (3.2), whence, due to the periodicity of  $A$ , (5.3) 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,

$$\begin{aligned}
(A - \lambda I)u_l &= \sum_{j \in \mathbb{N}} \left[ \left( -\frac{d^2}{dx^2} - \lambda \right) u_l|_{(x_j, x_{j+1})} \cdot \mathbb{1}_{(x_j, x_{j+1})} \right] \\
&= \sum_{j \in \mathbb{N}} \left[ \left( -\frac{d^2}{dx^2} - \lambda \right) \left( \eta \left( \frac{|\cdot|}{l} \right) \psi_s(\cdot, k) \right) \Big|_{(x_j, x_{j+1})} \cdot \mathbb{1}_{(x_j, x_{j+1})} \right] \\
&= \sum_{j \in \mathbb{N}} \left[ \eta \left( \frac{|\cdot|}{l} \right) \left( -\frac{d^2}{dx^2} - \lambda \right) \psi_s(\cdot, k)|_{(x_j, x_{j+1})} \cdot \mathbb{1}_{(x_j, x_{j+1})} \right] \\
&\quad - \frac{2}{l} \sum_{j \in \mathbb{N}} \left[ \left( \eta' \left( \frac{|\cdot|}{l} \right) \psi'_s(\cdot, k) \right) \Big|_{(x_j, x_{j+1})} \cdot \mathbb{1}_{(x_j, x_{j+1})} \right] \\
&\quad - \frac{1}{l^2} \sum_{j \in \mathbb{N}} \left[ \left( \eta'' \left( \frac{|\cdot|}{l} \right) \psi_s(\cdot, k) \right) \Big|_{(x_j, x_{j+1})} \cdot \mathbb{1}_{(x_j, x_{j+1})} \right] \\
&= \sum_{j \in \mathbb{N}} \left[ \eta \left( \frac{|\cdot|}{l} \right) \left( -\frac{d^2}{dx^2} - \lambda \right) \psi_s(\cdot, k)|_{(x_j, x_{j+1})} \cdot \mathbb{1}_{(x_j, x_{j+1})} \right] + R
\end{aligned} \tag{5.4}$$

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

$$\|R\| \leq \frac{c}{l} \|\psi_s(\cdot, k)\|_{H^1(K_l)} \leq c \frac{1}{\sqrt{l}}, \tag{5.5}$$

with  $K_l$  denoting the ball in  $\mathbb{R}$  with radius  $l$ , centered at  $x_0$ . Together with (5.3), (5.4) and (5.5), 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,  $\lambda \in \sigma(A)$ . □

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

*Proof.* todo □

TODO Theorem 3.6.3.

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