


1 On the spectra of Schrödinger operator with periodic delta potential

1.1 Periodic differential operator

Let A be the one-dimensional Schrödinger operator with a periodic delta potential, i.e. $\exists (x_k)_{k \in \mathbb{Z}}$ periodically distributed such that 

$$A = -\Delta + \rho \cdot \sum_{i \in \mathbb{Z}} \delta_{x_i} \quad (1.1)$$

Moreover, identify with Ω_k the periodicity cell containing delta point x_k and let w.o.l.g. $x_0 = 0$ and $|\Omega_i| = 1 \ \forall i \in \mathbb{Z}$. For this topic, one is interested in the weak formulation of the corresponding differential equation, i.e. for $\mu \in \mathbb{R}$ small enough and for a $f \in L^2(\mathbb{R})$ consider the equation

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

First, one has to notice that this formulation is well defined as for arbitrary $\tilde{x}_i \in \Omega_i$

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

Next, to show that for all $f \in L^2(\mathbb{R})$ there exists a unique $u \in H^1(\mathbb{R})$ such that (1.2) holds we want to use Lax-Milgram's theorem¹. It would guarantee the existence and uniqueness of a solution as $H^1(\mathbb{R})$ is a

¹formulation and prove in appendix A

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Hilbert space if the left-hand side of (1.2) as bilinear form

$$B[u, v] := \langle u', v' \rangle + \rho \sum_{i \in \mathbb{Z}} u(x_i) \overline{v(x_i)} - \mu \langle u, v \rangle$$

is bounded and $B[u, u]$ is coercive.

Theorem 1.1. *The bilinear form $B[u, v]$ is bounded.*

Proof. Using ((1.3)) we can estimate the norm of $B[u, v]$ by

$$\begin{aligned} |B(u, \varphi)|^2 &\leq \|u'\| \cdot \|v'\| + 2\rho \sum_{i \in \mathbb{Z}} |u(x_i)|^2 |v(x_i)|^2 - \mu \|u\| \cdot \|v\| \\ &\stackrel{(1.3)}{\leq} \|u'\| \cdot \|v'\| + 8\rho \cdot \|u\|_{H^1(\mathbb{R})}^2 \|v\|_{H^1(\mathbb{R})}^2 - \mu \|u\| \cdot \|v\| \\ &= (8\rho - \mu) \|u\| \cdot \|v\| + 8\rho (\|u\| \cdot \|v'\| + \|u'\| \cdot \|v\|) + (8\rho + 1) \|u'\| \cdot \|v'\| \\ &\leq \alpha \cdot \|u\|_{H^1} \cdot \|\varphi\|_{H^1} \end{aligned}$$

□

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 $\rho < 0$:

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

□

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All in all, Lax-Milgram's theorem now guarantees a unique element $u \in H$ such that

$$B[u, v] = \langle f, v \rangle$$

for all $v \in H^1(\mathbb{R})$.

As we now have a map $R_\mu f \mapsto u$, $R_\mu: L^2(\mathbb{R}) \rightarrow \mathcal{R}(R_\mu) \subset H^1(\mathbb{R})$ one can show that the inverse is well defined as R_μ is one-to-one since for $u_1 = u_2$

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

As H^1 is dense in L^2 this means that this equation holds also for all $v \in L^2(\mathbb{R})$ and therefore $f_1 = f_2$ almost everywhere. Accordingly R_μ is bijective and in turn

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

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

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

Such that $u'' = -Au \in L^2$ on $(x_k-1/2, x_k)$ and analogously on $(x_k, x_k+1/2)$. As $k \in \mathbb{Z}$ was arbitrary one can therefore fix

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

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

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

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But this is equivalent to


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

Such that

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

and the action of the operator is defined by

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

which also means that the definition of A is independent of μ .  The opposite inclusion one shows, as $\mathcal{R}(R_\mu) = \mathcal{D}(A)$, by proving that such a u is in the range of R_μ . More specifically, as $\mathcal{D}(R_\mu) = L^2(\mathbb{R})$ a particular choice of such an element in $\mathcal{D}(\mathbb{R}_\mu)$ would be

$$f := Au \in L^2$$

and left to show that $u = R_\mu(f - \mu u)$:

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

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

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

such that

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

Theorem 1.3. *A is a self-adjoint operator*

Proof. Last but not least, to show that A is self-adjoint, we focus first on R_μ^{-1} which is given by

$$R_\mu(A)^{-1} = (A - \mu I)$$

First one has to notice that R_μ^{-1} is symmetric, as $\forall v \in H^1$:

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


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 $f, g \in L^2(\mathbb{R})$ and for

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

it must hold that $\gamma = 0$. 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_μ is therefore symmetric.

All in all we can use this to show that R_μ is self-adjoint, as we get for an arbitrary $v^* \in \mathcal{D}(R_\mu^{-1})$ there exists a $v \in \mathcal{R}(R_\mu^{-1}) = \mathcal{D}(R_\mu)$: 

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

So $v^* \in \mathcal{R}(R_\mu)$ which means that R_μ^{-1} is self-adjoint. As A is simply R_μ^{-1} shifted by the real constant μ , A is self-adjoint as well. \square

1.2 Fundamental domain of periodicity and the Brillouin zone

Let Ω be the fundamental domain of periodicity associated with (1.1), e.g. $\Omega = \Omega_0$. As commonly used by literature the reciprocal lattice for Ω is equal to $[-2\pi, 2\pi]$, this set is the so called one-dimensional Brillouin zone B . For fixed $k \in \overline{B}$, we now consider the operator 

$$A_k: H_k^1 \rightarrow L^2(\mathbb{R}), \quad \psi \mapsto -\Delta\psi + \rho \cdot \delta_{x_0}\psi \quad (1.4)$$

where

$$H_k^1 := \left\{ H^1(\mathbb{R}) : \psi\left(-\frac{1}{2}\right) = e^{ik}\psi\left(\frac{1}{2}\right) \right\} \quad (1.5)$$

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


$$A_k\psi = \lambda\psi \text{ on } \Omega, \quad (1.6)$$

In writing the boundary condition in the form, we understand ψ extended to the whole of \mathbb{R} . In fact, (1.5) forms boundary conditions on $\partial\Omega$, so-called semi-periodic boundary conditions. Furthermore we know that (1.6), (1.5) is a symmetric eigenvalue problem in $L^2(\Omega)$ and ψ from 1.6 extended to the whole of \mathbb{R} by (1.5) solves also the eigenvalue problem of A with the same eigenvalue.

Since Ω is bounded, the subsequently shown compactness can be used to prove that (1.6), (1.5) 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]. 

Theorem 1.4. *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

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

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

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

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 $\forall \epsilon > 0 \ \exists g_1, \dots, g_{n_\epsilon}$:

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

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

$$|f(x) - f(y)| \leq c|x - y|^{1/2} \text{ for some } c > 0 \quad (1.7)$$

Now, for a $f \in B_{H^1}$ follows from (1.7) 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 Ω into n_ϵ equidistant intervals. As our simple function is constant on each subinterval, we chose this constant c_k such that

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

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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 (1.6) and (1.5),

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

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

$$\tilde{A}_k \varphi = \lambda \varphi \text{ on } \Omega, \tag{1.8}$$

$$\varphi(x - \frac{1}{2}) = \varphi(x + \frac{1}{2}) \tag{1.9}$$

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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

$$(Uf)(x, k) := \frac{1}{\sqrt{|B|}} \sum_{n \in \mathbb{Z}} f(x - n) e^{ikn} \quad (x \in \Omega, k \in B) \quad (1.10)$$

Theorem 1.5. $U: L^2(\mathbb{R}) \rightarrow L^2(\Omega \times B)$ is an isometric isomorphism, with inverse

$$(U^{-1}g)(x - n) = \frac{1}{\sqrt{|B|}} \int_B g(x, k) e^{-ikn} dk \quad (x \in \Omega, n \in \mathbb{Z}) \quad (1.11)$$

If $g(\cdot, k)$ is extended to the whole of \mathbb{R} by the semi-periodicity condition (1.5), we have

$$U^{-1}g = \frac{1}{\sqrt{|B|}} \int_B g(\cdot, k) dk. \quad (1.12)$$

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

$$\int_{\mathbb{R}} |f(x)|^2 dx = \sum_{n \in \mathbb{Z}} \int_{\Omega} |f(x - n)|^2 dx. \quad (1.13)$$

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 (1.10) (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 (1.13), this expression is in $L^2(\Omega)$, and

$$\|Uf\|_{L^2(\Omega \times B)} = \|f\|_{L^2(\mathbb{R})}.$$

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We are left to show that U is onto, and that U^{-1} is given by (1.11) or (1.12). Let $g \in L^2(\Omega \times B)$, and define

$$f(x - n) := \frac{1}{\sqrt{|B|}} \int_B g(x, k) e^{-ikn} dk \quad (x \in \Omega, n \in \mathbb{Z}). \quad (1.14)$$

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 ,

$$\int_{\Omega \times B} |g(x, k)|^2 dx dk = \int_{\Omega} \sum_{n \in \mathbb{Z}} |f(x - n)|^2 dx \quad (1.15)$$

$$= \sum_{n \in \mathbb{Z}} \int_{\Omega} |f(x - n)|^2 dx \quad (1.16)$$

$$= \int_{\mathbb{R}} |f(x)|^2 dx, \quad (1.17)$$

i.e. $f \in L^2(\mathbb{R})$. Now (1.10) 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 (1.14) implies $Uf = g$ and (1.11). Now (1.12) follows from (1.11) using $g(x + n, k) = e^{ikn} g(x, k)$. \square

1.3 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 1.6. *For each $f \in L^2(\mathbb{R})$ and $l \in \mathbb{N}$, define*

$$f_l(x) := \frac{1}{\sqrt{|B|}} \sum_{s=1}^l \int_B \langle (Uf)(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)} \psi_s(x, K) dk \quad (x \in \mathbb{R}). \quad (1.18)$$

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

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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

$$g_l(x, k) := \sum_{s=1}^l \langle (Uf)(\cdot, k), \psi_s(\cdot, k) \rangle_{L^2(\Omega)} \psi_s(x, k). \quad (1.19)$$

Thus, for $\chi_l(k) := \|(Uf)(\cdot, k) - g_l(\cdot, k)\|_{L^2(\Omega)}^2$, 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 1.5. Altogether, Lebesgue's Dominated Convergence theorem implies

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

i.e.,

$$\|Uf - g_l\|_{L^2(\Omega \times B)} \rightarrow 0 \text{ as } l \rightarrow \infty \quad (1.20)$$

Using (1.18), (1.19) and (1.12), we find that $f_l = U^{-1}g_l$, whence (1.20) 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 (1.5). \square

1.4 The spectrum of A

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

$$\sigma(A) = \bigcup_{s \in \mathbb{N}} I_s \quad (1.21)$$

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where

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

For each $s \in \mathbb{N}$, λ_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 (1.8), (1.9) depend continuously on k . Thus, since B is compact and connected,

$$I_s \text{ is a compact real interval, for each } s \in \mathbb{N}. \quad (1.22)$$

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 (1.6) 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 (1.22) implies that

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

The first part of the statement (1.21) is

Theorem 1.7. $\sigma(A) \supset \bigcup_{s \in \mathbb{N}} I_s$.

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

$$A\psi_s(\cdot, k) = \lambda\psi_s(\cdot, k) \quad (1.23)$$

We regard $\psi_s(\cdot, k)$ as extended to the whole of \mathbb{R} by the boundary condition (1.5), whence, due to the periodicity of A , (1.23) 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 $l \in \mathbb{N}$,

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

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Then,

$$\begin{aligned}
(A - \lambda I)u_l &= \sum_{j \in \mathbb{N}} \left[\left(-\frac{d^2}{dx^2} - \lambda \right) u_l|_{(x_j, x_{j+1})} \cdot \mathbf{1}_{(x_j, x_{j+1})} \right] \\
&= \sum_{j \in \mathbb{N}} \left[\left(-\frac{d^2}{dx^2} - \lambda \right) \left(\eta \left(\frac{|\cdot|}{l} \right) \psi_s(\cdot, k) \right) \Big|_{(x_j, x_{j+1})} \cdot \mathbf{1}_{(x_j, x_{j+1})} \right] \\
&= \sum_{j \in \mathbb{N}} \left[\eta \left(\frac{|\cdot|}{l} \right) \left(-\frac{d^2}{dx^2} - \lambda \right) \psi_s(\cdot, k) \Big|_{(x_j, x_{j+1})} \cdot \mathbf{1}_{(x_j, x_{j+1})} \right] \\
&\quad - \frac{2}{l} \sum_{j \in \mathbb{N}} \left[\left(\eta' \left(\frac{|\cdot|}{l} \right) \psi'_s(\cdot, k) \right) \Big|_{(x_j, x_{j+1})} \cdot \mathbf{1}_{(x_j, x_{j+1})} \right] \\
&\quad - \frac{1}{l^2} \sum_{j \in \mathbb{N}} \left[\left(\eta'' \left(\frac{|\cdot|}{l} \right) \psi_s(\cdot, k) \right) \Big|_{(x_j, x_{j+1})} \cdot \mathbf{1}_{(x_j, x_{j+1})} \right] \\
&= \sum_{j \in \mathbb{N}} \left[\eta \left(\frac{|\cdot|}{l} \right) \left(-\frac{d^2}{dx^2} - \lambda \right) \psi_s(\cdot, k) \Big|_{(x_j, x_{j+1})} \cdot \mathbf{1}_{(x_j, x_{j+1})} \right] + R
\end{aligned} \tag{1.24}$$

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 $\psi_s(\cdot, k) \in H_{loc}^2(\mathbb{R})$), and the semi-periodic structure of $\psi_s(\cdot, k)$ implies

$$\|R\| \leq \frac{c}{l} \|\psi_s(\cdot, k)\|_{H^1(K_l)} \leq c \frac{1}{\sqrt{l}}, \tag{1.25}$$

with K_l denoting the ball in \mathbb{R} with radius l , centered at x_0 . Together with (1.23), (1.24) and (1.25), 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

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

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

Proof. todo \square

TODO Theorem 3.6.3.

2 Appendix

Theorem 2.1 (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

$$B[u, v] = \langle w, v \rangle \tag{2.1}$$

Let us write $Au = w$ whenever (2.1) 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

$$\begin{aligned} \langle A(\lambda_1 u_1 + \lambda_2 u_2), v \rangle &= B[\lambda_1 u_1 + \lambda_2 u_2, v], \text{ (by (2.1))} \\ &= \lambda_1 B[u_1, v] + \lambda_2 B[u_2, v] \\ &= \lambda_1 \langle Au_1, v \rangle + \lambda_2 \langle Au_2, v \rangle, \text{ (by (2.1) again)} \\ &= \langle \lambda_1 Au_1 + \lambda_2 Au_2, v \rangle. \end{aligned}$$

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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

$$\begin{cases} A \text{ is one-to-one, and} \\ R(A), \text{ the range of } A, \text{ is close in } H. \end{cases} \quad (2.2)$$

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 (2.2).

We demonstrate now

$$R(A) = H \quad (2.3)$$

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 (2.2) and (2.3) 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 2.2 (Sobolev Embedding).

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

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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