Karlsruher Institut für Technologie

Bachelorthesis

On the spectra of Schrödinger operator with periodic delta potential

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Chapter 1

Introduction

In 1962 Erwin Schrödinger published his theory based on de Broglie's idea of understanding systems with discrete energies as standing waves. A wave function in classical mechanics and electrodynamics is a periodic function with the property that

$$\psi(x,t) = A \cdot \sin(\omega t - kx) \tag{1.1}$$

where x denotes the space, t the time, ω the circular frequency, k the wave number and A the amplitude. Differentiating the equation (1.1) twice with respect to x we get

$$\frac{\partial^2}{\partial x^2}\psi(x,t) = -k^2 A \sin(\omega t - kx) = -k^2 \psi(x,t)$$

and differentiating twice with respect to t yields

$$\frac{\partial^2}{\partial t^2}\psi(x,t) = -\omega^2 A \sin(\omega t - kx) = -\omega^2 \psi(x,t).$$

Therefore ψ satisfies the following differential equations

$$\frac{\partial^2}{\partial x^2}\psi(x,t) = \frac{k^2}{\omega^2}\frac{\partial^2}{\delta t^2}\psi(x,t) \tag{1.2}$$

Now, we are looking for a wave function for mass tainted particles, like electrons. For that use the de-Broglie relation $\lambda = \frac{h}{p}$ in the quotient of (1.2):

$$\frac{k^2}{\omega^2} = \frac{p^2}{\nu^2 h^2}. \tag{1.3}$$

The kinetic energy of such a particle is his total energy E without the potential energy V:

$$E_{kin} = \frac{p^2}{2m} = E - V$$

Solving this equation to the impulse squared p^2 yields:

$$p^2 = 2m \cdot (E - V),$$

and using this expression in (1.3) we conclude with the new differential equation:

$$\frac{\partial^2}{\partial x^2}\psi(x,t) = \frac{2m(E-V)}{h^2\nu^2}\frac{\partial^2}{\partial t^2}\psi(x,t). \tag{1.4}$$

For simplicity, let us consinder only time-independent solutions of the differential eqation (1.4) and focus on systems for which the total energy stays constant. Because of $E = h\nu$, the frequency will stay constant too; hence the quotient $\frac{2m/(E-V)}{h^2v^2}$ on the right-hand side of (1.4) is a constant as well. Solutions for such a differential equation can be split into one only space-dependent and one only time-dependent component:

$$\psi(x,t) = f(t) \cdot \psi(x).$$

Using the approach $f(t) = \sin(\omega t)$ with $\frac{\partial^2}{\partial x^2}\psi(x,t) = f(t)\psi''(x)$ and $\frac{\partial^2}{\partial t^2}\psi(x,t) = \psi(x)f''(t)$ shows that (1.4) is equivalent to

$$\begin{aligned} f(t)\psi''(x) &= \frac{2m(E-V)}{h^2\nu^2}\psi(x)f''(t) \\ \iff \; -\psi''(x) + \frac{2m\omega^2}{h^2\nu^2}V\psi(x) &= \frac{2m\omega^2 E}{h^2\nu^2}\psi(x) \end{aligned}$$

Based on this, we are interested in the one-dimensional Schrödinger operator with describes the simplified movement of a non-relativistic movement of a quantum particle in a potential, especially in the spectral problem of such an operator; meanwhile the potential in this thesis given by a delta-distribution, thereby this operator is formally defined through the operation

$$-\frac{d^2}{dx^2} + \rho\sum_{i\in\mathbb{Z}}\delta_{x_i} \tag{1.5}$$

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 $i \in \mathbb{Z}$.

In general, one cannot expect that (1.5) has a classical solution. For the existence of a classical solution, all parameters have to be in a sense sufficiently smooth, which, for our distributional potential, is never the case. Nevertheless a solution of the so called weak formulation which requires less regularity can still exist, consider for this for $\mu \in \mathbb{R}$ the problem

$$\int u'\overline{v'} + \rho \sum_{i \in \mathbb{Z}} u(x_i)\overline{v(x_i)} - \mu \int u\overline{v} = \int f\overline{v} \quad \forall v \in H^1(\mathbb{R}), \tag{1.6}$$

where $u \in H^1(\mathbb{R})$ and $f \in L^2(\mathbb{R})$. This is obtained by multiplying

$$Au + \mu u = f$$

with some $v \in C_c^\infty(\mathbb{R})$, partial integration and using the fact that $C_c^\infty(\mathbb{R})$ is dense in $H^1(\mathbb{R})$.

One should note that left-hand side of problem (1.6) is actually convergent, as for arbitrary $\tilde{x}_i \in \Omega_i$

$$\begin{aligned}
\sum_{i \in \mathbb{Z}} |u(x_i)|^2 &\leq \sum_{i \in \mathbb{Z}} \left(\left| u(\tilde{x}_i) + \int_{\tilde{x}_i}^{x_i} u'(\tau) d\tau \right| \right)^2 \\
&\leq 2 \sum_{i \in \mathbb{Z}} \left(\int_{\Omega_i} |u(x)|^2 dx + \int_{\Omega_i} \left| u'(\tau) \right|^2 d\tau \right) \\
&\leq 2 \cdot \|u\|_{H^1(\mathbb{R})}^2. \qquad (1.7)
\end{aligned}$$

Chapter 2

The Schrödinger operator A

In this chapter we will examine the Schrödinger operator in more detail, show that it is self-adjoint and describe it's domain for later purpose. Given the $f \in L^2(\mathbb{R})$ from the requirements in (1.6), we define a functional $l\colon H^1 \to \mathbb{R}$ through Riesz' Representation Theorem with

$$l(v) := \int_{\mathbb{R}} fv$$

and the bilinear form $B_\mu\colon H^1(\mathbb{R}) \times H^1(\mathbb{R}) \to \mathbb{R}$ for $\mu \in \mathbb{R}$ through

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

Such that (1.6) is equivalent to finding $u \in H^1(\mathbb{R})$ such that

$$B_\mu[u,v] = l(v) \quad \forall v \in H^1(\mathbb{R}). \tag{2.1}$$

The existence of an unique element $u \in H^1(\mathbb{R})$ satisfying (2.1) is asserted by Lax Milgram's Theorem asserts if the bilinear form B is bounded and coercive.

Theorem 2.1. *The bilinear form $B_\mu[u,v]$ as left-hand of* (1.6) *has for all $u, v \in H^1(\mathbb{R})$ the properties*

i) $B_\mu[u,v]$ is bounded, i.e. there exists a constant $\alpha > 0$ such that

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

ii) $B_\mu[u,u]$ is coercive, i.e. there exists a constant $\beta > 0$ such that

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

Proof:

i) The boundedness follows from

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

ii) For the coercivity assume first $\rho \geq 0$, in order that for $\mu < -1$:

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

Same for $\rho < 0$, where $\mu < 2\rho$:

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

□

Thus, there is a function $u \in H^1(\mathbb{R})$ as the unique solution to the problem (2.1) and the operator $R_\mu\colon L^2(\mathbb{R}) \to H^1(\mathbb{R})$, $f \mapsto u$ is for $\mu \in \mathbb{R}$ small enough well-defined; obviously the mapping is one-to-one since for $u_1 = u_2$

$$0 = B_\mu[u_1, v] - B_\mu[u_2, v] = \int (f_1 - f_2)\overline{v} \quad \forall v \in H^1(\mathbb{R}). \tag{2.2}$$

As $H^1(\mathbb{R})$ is dense in $L^2(\mathbb{R})$ this yields that the equation (2.2) holds also for all $v \in L^2(\mathbb{R})$ and therefore $f_1 = f_2$ almost everywhere. Accordingly R_μ is bijective and we can define the Schrödinger operator as follows

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

from which follows that R_μ is the resolvent of A.

2.1 The Domain of A

Even though Lax Milgram's Theorem guarantees a solution $u \in H^1(\mathbb{R})$ the operator A yields additional properties for the solution, i.e. the domain of A.

For every fixed $k \in \mathbb{Z}$ consider in (1.6) a test function $v \in C^\infty(\mathbb{R})$ such that $\operatorname{supp} v = \Omega_k$, then

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

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

Next, again in (1.6) for an arbitrary $k \in \mathbb{Z}$ a test function $v \in C^\infty(\mathbb{R})$ with $\operatorname{supp} v = \Omega_k$ yields through integration by parts on both sides of x_k

$$-\left(\int_{x_k-1/2}^{x_k} + \int_{x_k}^{x_k+1/2}\right) u'' \cdot \overline{v} + \left(u'(x_k - 0)\overline{v(x_k)} - u'(x_k + 0)\overline{v(x_k)}\right)$$

$$+\rho u(x_k)\overline{v(x_k)} = -\int_{x_k-1/2}^{x_k} u''\overline{v} - \int_{x_k}^{x_k+1/2} u''\overline{v}.$$

But as $v \in C^\infty(\mathbb{R})$, this is equivalent to

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

such that

$$\mathcal{D}(A) \subset \Big\{ u \in \bigcap_{i\in\mathbb{Z}} H^2(x_i, x_{i+1}), u'(x_i - 0) - u'(x_i + 0) + \rho u(x_i) = 0,\ \forall i \in \mathbb{Z} \Big\} =: B. \quad (2.3)$$

The action of the operator is defined by

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

We can even the opposite inclusion in (2.3), as $\mathcal{R}(R_\mu) = \mathcal{D}(A)$, by proving for $u \in B$ that is also in the range of R_μ. More specifically, as $\mathcal{D}(R_\mu) = L^2(\mathbb{R})$ define $f := Au$. To show $u = R_\mu(f - \mu u)$ consider

$$\int_{\mathbb{R}} u'\overline{v'} + \rho \sum_{i\in\mathbb{Z}} u(x_i)\overline{v(x_i)} - \mu \int_{\mathbb{R}} u\overline{v} = \int_{\mathbb{R}} (f - \mu u)\overline{v}$$

$$\iff \sum_{i\in\mathbb{Z}} \int_{\Omega_i} u'\overline{v'} + \rho u(x_i)\overline{v(x_i)} = -\sum_{i\in\mathbb{Z}} \int_{x_i - 1/2}^{x_i} u''\overline{v} + \int_{x_i}^{x_i+1/2} u''\overline{v}.$$

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

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

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

such that we conclude

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

Theorem 2.2. *R_μ is a symmetric operator.*

Proof: First, focus on $R_\mu^{-1} = (A - \mu I)$. As for all $v \in D(A)$:

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

R_μ^{-1} is symmetric. Now, as $\mathcal{D}(R_\mu) = L^2(\mathbb{R})$ and $\mathcal{R}(R_\mu) = \mathcal{D}(R_\mu^{-1})$ for each $f, g \in L^2(\mathbb{R})$ it follows

$$\langle R_\mu f, g\rangle = \langle R_\mu f, R_\mu^{-1} R_\mu g\rangle = \langle f, R_\mu g\rangle$$

such that R_μ is also symmetric. □

The last property of A we will need later is its self-adjointness. This reveals that A is also a symmetric and closed operator and that its eigenvalues are entirely real.

Theorem 2.3. *A is a self-adjoint operator.*

Proof: As we already know that R_μ and R_μ^{-1} are symmetric, showing that R_μ^{-1} is self-adjoint is equivalent to show that if $v \in \mathcal{D}(R_\mu^{-1*})$ and $v^* \in L^2(\mathbb{R})$ are such that

$$\langle R_\mu^{-1} u, v\rangle = \langle u, v^*\rangle, \quad \forall u \in \mathcal{D}(R_\mu^{-1}) \tag{*}$$

then $v \in \mathcal{D}(R_\mu^{-1})$ and $R_\mu^{-1} v = v^*$. In $(*)$ we define $u := R_\mu f$ for $f \in L^2$ and use that R_μ is symmetric and defined on the whole of $L^2(\mathbb{R})$:

$$\langle f, v\rangle = \langle R_\mu f, v^*\rangle = \langle f, R_\mu v^*\rangle, \quad \forall u \in \mathcal{D}(R_\mu^{-1})$$

Which means that $v \in \mathcal{R}(R_\mu) = \mathcal{D}(R_\mu^{-1})$ and $R_\mu^{-1} v = v^*$, i.e. R_μ^{-1} is self-adjoint. As the operator A is simply R_μ^{-1} shifted by $\mu \in \mathbb{R}$, A is self-adjoint as well. □

Chapter 3

Fundamental domain of periodicity and the Brillouin zone

Let Ω be the fundamental domain of periodicity associated with (1.5), 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 denoted by the operation

$$-\frac{d^2}{dx^2} + \rho\delta_{x_0}.$$

Again, define A_k by considering the weak formulation to this problem, i.e. for $f \in L^2(\Omega)$ find a function $u \in H_k^1$ such that the equation

$$\int_\Omega u'\overline{v'} + \rho u(x_0)\overline{v(x_0)} - \mu \int_\Omega u\overline{v} = \int_\Omega f\overline{v}$$

holds for all $v \in H_k^1$ where

$$H_k^1 \;\; \coloneqq \;\; \Big\{\psi \in H^1(\Omega) : \; \psi(\frac{1}{2}) = e^{ik}\psi(-\frac{1}{2})\Big\}. \tag{3.1}$$

Due to the fact that convergence in H_k^1 implies the convergence on the trace of Ω, H_k^1 is a closed subspace of $H^1(\mathbb{R})$, and one can therefore apply the same arguments as above to show that $R_{\mu,k} \colon L^2(\Omega) \to H_k^1, f \mapsto u$ is well-defined and define in return

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

such that $R_{\mu,k}$ is the resolvent of A_k.

In this chapter we are going to analyse the operator $R_{\mu,k}$ in more detail, see that its eigenfunctions form form a complete and orthonormal system in H_k^1 and use this fact to deduce properties about the spectrum of A_k and also A in chapter 4.

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

Proof: For each bounded sequence $(f_j)_{j\geq 1} \in L^2(\Omega)$ there exist $(u_j)_{j\geq 1} \in H_k^1$ by

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

Each such u_j has to satisfy

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

Now, choosing in (3.2) $v = u_j$ yields with (1.7) 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 means that $(u_j)_{j\geq 1}$ is bounded in $H^1(\Omega)$. As $H^1(\Omega) \subset C(\Omega)$ we can further estimate

$$|f(x) - f(y)| \leq c|x-y|^{1/2} \text{ for some } c > 0, \tag{3.3}$$

from which for $f \in B_{H^1} \coloneqq \{f \in H_k^1(\Omega) : \|f\| \leq 1\}$ follows that

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

For an arbitrary $\epsilon > 0$ we now partition Ω into n_ϵ equidistant, disjoint intervals I_k, i.e. $\Omega = \bigcup_{j=1}^{n_\epsilon} I_j$. As all $f \in B_{H_k^1}$ are by (1.7) uniformly bounded on Ω, there exist for each subinterval I_k a finite number of constants $c_{1,k}, \ldots, c_{\nu_\epsilon,k}$ such that

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

Hence, there are finitly many simple functions such that for all $f \in L^2(\Omega)$ one of those simple functions, let's call it $g \in L^2(\Omega)$, with function value c_k on interval I_k for all $k \in \{1, \ldots, n_\epsilon\}$

sucht that

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

In conclusion this means that $B_{H_k^1}$ is totally bounded in $L^2(\Omega)$ and with the closure of H_k^1 this yields the compact embedding of H_k^1 in $L^2(\Omega)$. Thus, $R_{\mu,k}$ is compact. □

3.1 The Spectrum of A_k

As from now, consider the eigenvalue problem

$$A_k\psi = \lambda\psi \text{ on } \Omega \text{ for } \psi \in H_k^1. \tag{3.4}$$

In writing the boundary condition in (3.1), we understand ψ extended to the whole of $\mathbb{R}$. In fact, (3.1) forms boundary conditions on $\partial\Omega$, so-called semi-periodic boundary conditions.

Obviously, A_k has the same sequence of eigenfunctions as $R_{\mu,k}$, and if $\tilde{\lambda}$ is an eigenvalue for the eigenfunction ψ of $R_{\mu,k}$ then so is

$$\lambda = \frac{1}{\tilde{\lambda}} - \mu$$

for the operator A. Since Ω is bounded, and $R_{\mu,k}$ is a compact and symmetric operator, A_k has also a purely discrete spectrum satisfying

$$\lambda_1(k) \leq \lambda_2(k) \leq \ldots \leq \lambda_s(k) \to \infty \text{ as } s \to \infty.$$

and the corresponding eigenfunction can be chosen such that they depend on k in a measurable way[1] and that they form a $\langle\cdot,\cdot\rangle$-orthonormal and complete system $(\psi_s(\cdot,k))_{s\in\mathbb{N}}$ of eigenfunctions for (3.1). Therefore, we transform the eigenvalue problem (3.4) such that the

[1] see [M. Reed and B. Simon. Methods of modern mathematical physics I–IV]

boundary condition is independent from k:

$$\varphi_s(x,k) \coloneqq e^{-ikx}\psi_s(x,k).$$

Then,

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

Defining the operator $\tilde{A}_k\colon D(A_k) \to L^2(\mathbb{R})$ through

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

and using (3.4) and (3.1), yields

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

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

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

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

with the same eigenvalue sequence $(\lambda_s(s))_{s\in\mathbb{N}}$ as in (3.4).

We shall see in the next chapter 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. For that we need two results involving the Floquet transformation, an operator mapping from $L^2(\mathbb{R})$ to $L^2(\Omega \times B)$ as $\Omega \times B$ is compact.

3.2 The Floquet transformation

Theorem 3.2. *The Floquet transformation* $U\colon L^2(\mathbb{R}) \to L^2(\Omega \times B)$

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

is an isometric isomorphism, with inverse

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

If $g(\cdot,k)$ *is extended to the whole of* $\mathbb{R}$ *by the semi-periodicity condition* (3.1)*, we have*

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

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

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

where we used Beppo Levi's Theorem to exchange summation and integration, that shows that

$$\sum_{n\in\mathbb{Z}} |f(x-n)|^2 < \infty \text{ for almost every } x \in \Omega.$$

Thus, $(Uf)(x,k)$ is well-defined by (3.7) (as a Fourier series with variable k) for almost every $x \in \Omega$, and Parseval's equality gives for these x

$$\int_B |(Uf)(x,k)|^2 dk = \sum_{n\in\mathbb{Z}} |f(x-n)|^2.$$

This expression is by (3.10) in $L^2(\Omega)$, and

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

We still haven't shown that U is onto, and that U^{-1} is given by (3.8) or (3.9). Let $g \in L^2(\Omega \times B)$, then define

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

Parseval's Theorem gives for fixed $x \in \Omega$ that $\sum_{n\in\mathbb{Z}} |f(x-n)|^2 = \int_B |g(x,k)|^2 dk$. Integrating over Ω yields then

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

i.e. $f \in L^2(\mathbb{R})$. Now (3.7) gives, for almost every $x \in \Omega$,

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

whence (3.11) implies $Uf = g$ and (3.8). Now (3.9) follows from (3.8) using $g(x+n,k) = e^{ikn} g(x,k)$. □

3.3 Completeness of the Bloch waves

Using the transformation U, we can now prove the property of completeness of the Bloch waves $\psi_s(\cdot,k)$ in $L^2(\Omega)$ when we vary k over the Brillouin zone B.

Theorem 3.3. *For each $f \in L^2(\mathbb{R})$ and $l \in \mathbb{N}$, define*

$$f_l(x) := \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \langle (Uf)(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)} \psi_s(x,K) dk \quad (x \in \mathbb{R}). \tag{3.12}$$

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

Proof: The last theorem tells us that $Uf \in L^2(\Omega\times B)$, which in return means that $(Uf)(\cdot,k) \in L^2(\Omega)$ for almost all $k \in B$ by Fubini's Theorem. As $(\psi_s(\cdot,k))_{s\in\mathbb{N}}$ is an orthonormal and complete system of eigenfunction in $L^2(\Omega)$ for each $k \in B$, we derive

$$\lim_{l\to\infty} \|(Uf)(\cdot,k) - g_l(\cdot,k)\|_{L^2(\Omega)} = 0 \text{ for almost every } k \in B$$

where

$$g_l(x,k) := \sum_{s=1}^{l} \langle (Uf)(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)} \psi_s(x,k). \tag{3.13}$$

By Bessel's inequality, we get moreover

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

for all $l \in \mathbb{N}$ and almost every $k \in B$. Moreover $\|(Uf)(\cdot,k)\|^2_{L^2(\Omega)} \in L^1(B)$ as a function of k by Theorem 3.2. Thus, by Lebesgue's Dominated Convergence theorem

$$\lim_{l\to\infty} \int_B \|(Uf)(\cdot,k) - g_l(\cdot,k)\|^2_{L^2(\Omega)} dk = \int_B \lim_{l\to\infty} \|(Uf)(\cdot,k) - g_l(\cdot,k)\|^2_{L^2(\Omega)} dk = 0.$$

All in all, this means

$$\|Uf - g_l\|_{L^2(\Omega\times B)} \to 0 \text{ as } l \to \infty \tag{3.14}$$

If $g(\cdot,k)$ is extended to the whole of $\mathbb{R}$ by the semi-periodicity condition (3.1), using (3.12), (3.13) and (3.9), we find that $f_l = U^{-1}g_l$, whence (3.14) gives

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

and the assertion follows since $U\colon L^2(\mathbb{R}) \to L^2(\Omega \times B)$ is isometric by Lemma 3.2. $\square$

Chapter 4

The spectrum of A

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

$$\sigma(A) = \bigcup_{s \in \mathbb{N}} I_s \tag{4.1}$$

where $I_s \coloneqq \{\lambda_s(k) : k \in \overline{B}\}$ $(s \in \mathbb{N})$. As B is compact and connected, for each of those sets I_s holds that

$$I_s \text{ is a compact real interval for each } s \in \mathbb{N}, \tag{4.2}$$

as λ_s is a continuous function of $k \in \overline{B}$ fo.r all $s \in \mathbb{N}$, which follows by standard arguments from the fact that the coefficients in the transformed eigenvalue problem (3.5), (3.6) depend continuously on k.

Moreover, Poincare's min-max principle for eigenvalues implies that $\mu_s \leq \lambda_s(k)$ for all $s \in \mathbb{N}, k \in \overline{B}$ with $(\mu_s)_{s \in \mathbb{N}}$ denoting the sequence of eigenvalues of problem (3.4) with Neumann ("free") boundary conditions. Since $\mu_s \to \infty$ as $s \to \infty$, we obtain

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

which together with (4.2) implies that

$$\bigcup_{s \in \mathbb{N}} I_s \text{ is close.} \tag{4.3}$$

The first part of the statement (4.1) is

Theorem 4.1. $\sigma(A) \supset \bigcup_{s\in\mathbb{N}} I_s$.

Proof: Let $\lambda \in \bigcup_{s\in\mathbb{N}} I_s$, i.e. $\lambda = \lambda_s(k)$ for some $s \in \mathbb{N}$ and some $k \in \overline{B}$, and

$$A_k \psi_s(\cdot, k) = \lambda \psi_s(\cdot, k) \tag{4.4}$$

We regard $\psi_s(\cdot, k)$ as extended to the whole of $\mathbb{R}$ by the boundary condition (3.1), whence, due to the periodicity of A, (4.4) holds for all $x \in \mathbb{R}$ and $\psi_s \in H^2_{loc}(\mathbb{R})$
We choose a function $\eta \in H^2(\mathbb{R})$ such that

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

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

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

Then,

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

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

$$\|R\| \leq \frac{c}{l}\|\psi_s(\cdot, k)\|_{H^1(K_l)} \leq c\frac{1}{\sqrt{l}}, \tag{4.6}$$

with K_l denoting the ball in $\mathbb{R}$ with radius l centered at x_0. Together with (4.4), (4.5) and (4.6), this gives

$$\|(A - \lambda I)u_l\| \leq \frac{c}{\sqrt{l}}$$

Again, by the semiperiodicity of $\psi_s(\cdot, k)$,

$$\|u_l\| \geq c\|\psi_s(\cdot, k)\| \geq c\sqrt{l}$$

with $c > 0$. We obtain therefore

$$\frac{1}{\|u_l\|}\|(A - \lambda I)u_l\| \leq \frac{c}{l}$$

Because moreover $u_l \in D(A)$, this results in

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

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

Theorem 4.2. $\sigma(A) \subset \bigcup_{s\in\mathbb{N}} I_s$.

Proof: Let $\lambda \in \mathbb{R} \setminus \bigcup_{s\in\mathbb{N}} I_s$, we have to prove that $\lambda \in \rho(A)$, i.e. that for each $f \in L^2(\mathbb{R})$ some $u \in D(A)$ exists satisfying $(A - \lambda I)u = f$. For given $f \in L^2(\mathbb{R})$, we define, for $l \in \mathbb{N}$,

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

and

$$u_l := \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int_B \frac{1}{\lambda_s(k) - \lambda} \langle (Uf)(\cdot, k), \psi_s(\cdot, k)\rangle_{L^2(\Omega)} \psi_s(x, k) dk \tag{4.7}$$

Here, note that, due to (4.3) some $\delta > 0$ exists such that

$$|\lambda_s(k) - \lambda| \geq \delta \text{ for all } s \in \mathbb{N}, k \in B \tag{4.8}$$

In particular, consider for fixed $k \in B$ and $v \in \mathcal{D}(A_k)$:

$$(A_k - \lambda I)v(\cdot, k) = (Uf)(\cdot, k) \text{ on } \Omega, \tag{4.9}$$

which has a unique solution as $\lambda \in \mathbb{R} \setminus \bigcup_{s\in\mathbb{N}} I_s$. Parseval gives

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

Since both $v(\cdot,k)$ and $\psi_s(\cdot,k)$ satisfy semi-periodic boundary conditions, $A-\lambda I$ can be moved to $\psi_s(\cdot,k)$ in the inner product, and hence (3.4) and (4.8) give

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

By Theorem 3.2, this implies $v \in L^2(\Omega \times B)$, and we can define $u := U^{-1}v \in L^2(\mathbb{R})$. Thus, (4.9) gives

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

whence (4.7) implies

$$u_l(x) = \frac{1}{\sqrt{|B|}} \sum_{s=1}^{l} \int \langle (Uu)(\cdot,k), \psi_s(\cdot,k)\rangle_{L^2(\Omega)} \psi_s(x,k) dk,$$

and Theorem 3.3 gives

$$u_l \to u, \quad f_l \to f \quad \text{ in } L^2(\mathbb{R}). \tag{4.10}$$

We will now prove that in the distributional sense

$$(A-\lambda I)u_l = f_l \text{ for all } l \in \mathbb{N} \tag{4.11}$$

which implies that $\langle u_l, (A-\lambda I)v\rangle = \langle f_l, v\rangle$ for all $v \in D(A)$, whence Theorem 3.13 implies $u_l \in D(A)$, and

$$(A-\lambda I)u_l = f_l \quad \forall l \in \mathbb{N}$$

Since A is closed, (4.10) now implies

$$u \in D(A), \text{ and } (A - \lambda I)u = f$$

which is the desired result.

Left to prove is (4.11), i.e. that

$$\langle u_l, (A - \lambda I)\varphi \rangle_{L^2(\mathbb{R})} = \langle f_l, \varphi \rangle_{L^2(\mathbb{R})} \quad \forall \varphi \in C_0^\infty(\mathbb{R}). \tag{4.12}$$

Let $\varphi \in C_0^\infty(\mathbb{R})$ be fixed, and let $K \subseteq \mathbb{R}$ denote an open interval containing $\mathrm{supp}(\varphi)$ in its interior. Both the functions

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

are in $L^2(K \times B)$ by Fubini's THeorem, since (4.8) and the fact that $(A_k - \lambda I)\varphi \in L^\infty(K)$ and $\varphi \in L^\infty(K)$, imply both

$$\|r_s(x,k)\|_{L^2(K \times B)} \leq c \|(Uf)(\cdot,k)\|^2_{L^2(\Omega)} \|\psi_s(\cdot,k)\|^2_{L^2(K)}$$

and

$$\|t_s(x,k)\|_{L^2(K \times B)} \leq \tilde{c} \|(Uf)(\cdot,k)\|^2_{L^2(\Omega)} \|\psi_s(\cdot,k)\|^2_{L^2(K)},.$$

the latter factor is bounded as a function of k because K is covered by a finite number of copies of Ω, and the former is in $L^1(B)$ by Theorem 3.2.

Since $K \times B$ is bounded, r and t are also in $L^1(K \times B)$. Therefore, Fubini's Theorem implies that the order of integration with respect to x and l may be exchanged for r and t.

Thus, by (4.7),

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

Since φ has compact support in the interior of K, $(A-\lambda I)$ may be moved to $\psi_s(\cdot,k)$, and hence (3.4) gives

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

i.e. (4.12). □

Bibliography

[1] a

Erklärung

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

Ort, den Datum