

# 1 Theoretical Basics

We start with the set of test functions

$$\mathcal{D} = C_0^\infty(\mathbb{R}) = \{f \in C^\infty : \text{supp}(f) \text{ is compact in } \mathbb{R}\}$$

and endow it with the topology: a sequence  $(\varphi_j)_{j \in \mathbb{N}}$  with  $\varphi_j \in \mathcal{D}$  converges against  $\varphi$ , if there is a compact set  $K \subset \mathbb{R}$  with  $\text{supp}(\varphi_j) \subset K$  for all  $j$  and

$$\lim_{j \rightarrow \infty} \sup_{x \in K} \left| \frac{\partial^\alpha}{\partial x^\alpha} (\varphi_j(x) - \varphi(x)) \right| = 0$$

for all multi-indizes  $\alpha \in \mathbb{N}^n$ . The set  $\mathcal{D}$  is – endowed with this convergence concept – a complete locally convex topological vector space satisfying the Heine–Borel property (Rudin 1991, §6.4–5).

The set of linear functionals from  $\mathcal{D}$  to  $\mathbb{R}$  we call the set of distributions

$$\mathcal{D}' = \{f : \mathcal{D} \rightarrow \mathbb{R} : f \text{ is linear} \}$$

That is, a distribution  $T$  assigns to each test function  $\varphi$  a real (or complex) scalar  $T(\varphi)$  such that

$$T(c_1\varphi_1 + c_2\varphi_2) = c_1T(\varphi_1) + c_2T(\varphi_2)$$

for all test functions  $\varphi_1, \varphi_2$  and scalars  $c_1, c_2$ . Moreover,  $T$  is continuous if and only if

$$\lim_{k \rightarrow \infty} T(\varphi_k) = T\left(\lim_{k \rightarrow \infty} \varphi_k\right)$$

for every convergent sequence  $\varphi_k \in \mathcal{D}$ . (Even though the topology of  $\mathcal{D}$  is not metrizable, a linear functional on  $\mathcal{D}$  is continuous if and only if it is sequentially continuous.) Equivalently,  $T$  is continuous if and only if for every compact subset  $K$  of  $\mathbb{R}$  there exists a positive constant  $C_K$  and a non-negative integer  $N_K$  such that

$$|T(\varphi)| \leq C_K \sup_K |\partial^\alpha \varphi|$$

for all test functions  $\varphi$  with support contained in  $K$  and all multi-indices  $\alpha$  with  $|\alpha| \leq N_K$  (Grubb 2009, p. 14).

The duality pairing between a distribution  $T \in \mathcal{D}'$  and a test function  $\varphi \in \mathcal{D}$  is denoted using angle brackets by

$$\begin{cases} \mathcal{D}' \times \mathcal{D} \rightarrow \mathbb{R} \\ (T, \varphi) \mapsto \langle T, \varphi \rangle \end{cases}$$

so that  $\langle T, \varphi \rangle = T(\varphi)$ . One interprets this notation as the distribution  $T$  acting on the test function  $\varphi$  to give a scalar, or symmetrically as the test function  $\varphi$  acting on the distribution  $T$ .

Now taking at distributions a closer look, we distinguish between two kinds: we call a distribution

- **regular** if there is locally integrable function

$$f \in L^1_{loc}(\mathbb{R}) = \{f: \Omega \rightarrow \mathbb{C} \text{ measurable} : f|_K \in L_1(K) \ \forall K \subset \mathbb{R}, \ K \text{ compact}\}$$

such that the distribution  $T$  can be written as

$$\langle T_f, \varphi \rangle = \int_{\mathbb{R}} f(t) \varphi(t) dt \quad \forall \varphi \in D$$

Sometimes, one abuses notation by identifying  $T_f$  with  $f$ , provided no confusion can arise, and thus the pairing between  $T_f$  and  $\varphi$  is often written

$$\langle f, \varphi \rangle = \langle T_f, \varphi \rangle = \int_{\mathbb{R}} f(t) \varphi(t) dt \quad \forall \varphi \in D$$

- **singular** if the distribution is not regular, e.g. if there is no integral representation with a locally integrable function.

## 1.1 The dirac delta distribution

$$f = \delta_{x_0}, \quad \langle \delta_{x_0}, \varphi \rangle = \varphi(x_0)$$

It is easy to see that  $f^\epsilon(x) \rightarrow 0$  almost everywhere and

$$\int f(y) dy = \alpha \neq 0$$

but

$$\int f^\epsilon dx = \frac{1}{\epsilon} \int f\left(\underbrace{\frac{x}{\epsilon}}_{=:y}\right) dx = \int f(y) dy$$

### Definition 1.1

For  $f \in \mathcal{D}'$  we say  $f^\epsilon \rightharpoonup f \in \mathcal{D}'$  if

$$\langle f^\epsilon, \varphi \rangle \rightarrow \langle f, \varphi \rangle \quad \forall \varphi \in \mathcal{D}$$

### Example 1.2

Let  $f^\epsilon(x) = \frac{1}{\epsilon} f\left(\frac{x-x_0}{\epsilon}\right)$ ,  $f \in C_c^\infty(\mathbb{R})$  with

$$\int_{\mathbb{R}} f(y) dy = \alpha < \infty$$

$$f^\epsilon \rightharpoonup \alpha \delta_{x_0}$$

## 1.2 The Schrödinger Operator

An Operator  $A$  is defined by three properties:

- space, i.e. a Hilbertspace  $H$
- domain,  $dom A \subset H$
- operation,  $Au$  with  $u \in dom A$

The Schrödinger Operator is defined on the space  $H = L^2(\mathbb{R})$  by

$$Au = -u'' + Vu$$

Now the question what is the domain of  $A$  arises.

### Example 1.3

$$i \cdot \frac{\partial \psi}{\partial t} A\psi$$

For  $\Omega \subset \mathbb{R}$  the probability of an particle being with  $\Omega$  in  $t$  can be described as

$$\int_{\Omega} |\psi(x, t)|^2$$

One now often is interested in quantum states of such particle and we therefore formulate the spectral problem

$$Au = \lambda u$$

Now assume  $V$  is rather good, e.g.  $V \in L^\infty(\mathbb{R})$  and  $dom A = H^2(\mathbb{R})$ .

### Definition 1.4

We call an operator  $A$  symmetric if

$$(Au, v)_H = (u, Av) \quad \forall u, v \in dom H$$

### Example 1.5

Let  $A = -\frac{d^2}{dx^2} + V$  for  $V: \mathbb{R} \rightarrow \mathbb{R}$

$$\begin{aligned} (Au, v) &= \int -u'' \bar{v} dx + \int V u \bar{v} dx \\ &= \int u' \bar{v}' dx + \int V u \bar{v} dx \end{aligned}$$

$$\begin{aligned} (u, Av) &= \int -u \overline{v''} dx + \int u \overline{V v} dx \\ &= \int u' \bar{v}' dx + \int V u \bar{v} dx \end{aligned}$$

And therefore  $A$  is symmetric.

**Definition 1.6**

For an operator  $A$  the adjoint  $A^*$  is the unique operator such that  $\forall v, v^* \in H$  where

$$(Au, v)_H = (u, v^*) \quad \forall u \in \text{dom} A$$

Then define  $\text{dom} A^* = \{v \in H\}$  and  $A^*v = v^*$ .

**Definition 1.7**

An operator  $A$  is self-adjoint if  $A = A^*$ .

If  $A$  is a self-adjoint operator then  $A$  is already symmetric but not the other way round. But as soon as  $A$  is bounded and symmetric then the operator is self-adjoint.

**Example 1.8**

Let  $H = L^2(0, 1)$  and define  $A = -\frac{d^2}{dx^2}$  on  $\text{dom} A = C_0^\infty(0, 1)$ . As  $A$  is symmetric  $A^*$  is an extension of  $A$ , e.g.  $A^* \supset A$ .

Now for  $v, v^* \in L^2$

$$\int -u'' \bar{v} dx = \int u \overline{v^*} \forall u \in C_0^\infty(0, 1)$$

Let  $v \in C^\infty(0, 1)$ :  $v^* := -v''$

$$\int -u'' \bar{v} dx = - \int u' \bar{v}' dx = - \int u \overline{v''} dx = \int u \overline{v^*} dx$$

$\Rightarrow H^2(0, 1) \cap H_0^1(0, 1) \Rightarrow A$  is self-adjoint.

Further, we are going to examine small or even singular particles more closely. The potential  $V$  is a vector such that  $\text{grad} V = F$  whereas  $F$  denotes the force acting upon a particle.

As in this case  $V$  has only a small support one could approximate  $V$  with a single-point potential.

But the operator itself is harder to understand

$$Au = -u'' + \delta_{x_0} u$$

For  $f, g$ :

$$\int (f \cdot g) \varphi dx = \int f (g \cdot \varphi) dx$$

Now suppose  $f \in \mathcal{D}$ ,  $g \in C^\infty(\mathbb{R})$ :

$$\langle g \cdot f, \varphi \rangle \stackrel{\text{def}}{=} \langle f, \underbrace{g \cdot \varphi}_{\in \mathcal{D}} \rangle$$

### 1.3 Main Problem

For a differential equation we distinguish between three different solution concepts

- classical  $u \in C^2$
- strong  $u \in H^2$
- weak  $u \in H^1$

With some conditions to the potential those terms can be equivalent.

### 1.3.1 I:

Define  $A^\epsilon$  on  $\text{dom} A^\epsilon = H^2(\mathbb{R})$  with

$$A^\epsilon u = -u'' + \frac{1}{\epsilon} f\left(\frac{x}{\epsilon}\right)u, \quad f \in C_c^\infty(\mathbb{R})$$

while  $\int_{\mathbb{R}} f(x)dx = \alpha \neq 0$ . Now the question arises:  $A^\epsilon \xrightarrow{\epsilon \rightarrow 0} ?$

### 1.3.2 II:

$Au - \mu u = f \in L^2, u \in \mathbb{C} \setminus \mathbb{R}$  with  $A = -u'' + V$  the resolvent.

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

*todo check* if  $A$  is self-adjoint  $\Rightarrow$  has solution for  $\mathbb{C} \setminus \mathbb{R}$  defined and bounded arbitrary  $f$   
Partial integration yields

$$\int u' \bar{v}' dx + \int V u \bar{v} dx + \mu \int u \bar{v} dx = \int f \bar{v} dx \quad (*)$$

which holds for an arbitrary  $v \in C_0^\infty(\mathbb{R})$

We say,  $u$  is a weak solution if  $u \in H^1(\mathbb{R})$  and  $(*)$  holds. If the potential is even in  $L^\infty$  then the solution is also a strong solution (i.e.  $u \in H^2$ ) *todo proof*

For  $f \in L^2(\mathbb{R})$ ,  $Au - \mu u = f$  If we take a potential  $V$ , then  $\int V u \bar{v} dx$  could be also written as  $V(u\bar{v})$ .

Now suppose  $H = L^2(\mathbb{R})$ ,  $A = -\frac{d^2}{dx^2} + \alpha \delta_{x_0}$

$$\int u' \bar{v}' dx + \alpha u(x_0) \bar{v}(x_0) + \mu \int u \bar{v} dx = \int f \bar{v} dx \quad \forall v \in C_0^\infty(\mathbb{R}) \quad (1)$$

Since this formula only evaluations  $v$  and  $u$  in  $x_0 \Rightarrow \forall v \in H^1(\mathbb{R}), u \in H^1(\mathbb{R})$  is enough.

For  $d = 1$ :  $H^1(\mathbb{R}) \subset C(\mathbb{R})$  *todo proof*

## 2 The definition of our operator

### 2.0.1 I:

Now, we want to show that (1) has a unique solution using the Lax-Milgram theorem:

Let  $\mathcal{H} = H^1(\mathbb{R})$  and define  $a[u, v]$  as LHS and  $\langle f, v \rangle$  as RHS of (1):

$$\begin{aligned} a[u, v] &:= \int u' \bar{v}' dx + \alpha u(x_0) \bar{v}(x_0) + \mu \int u \bar{v} dx \\ \langle f, v \rangle &:= \int f \bar{v} dx \end{aligned}$$

If  $\mu \in \mathbb{R}$  *todo check if that is really necessary since Lax-Milgram needs it, (and usse trace? inequality)*

since  $|u(x_0)|^2 = |u(x) + \int_x^{x_0} u'(\tau) d\tau|^2$  we can write with labech formula *todo which formalar is this?*

$$\begin{aligned} a[u, v] &= \int |u'|^2 + \alpha |u(x_0)|^2 - \mu \int |u|^2 \\ &\leq 2|u(x)|^2 + 2 \left| \int_{x_0}^x u'(\tau) d\tau \right|^2 \\ &\leq 2|u(x)|^2 + 2 \int_{x_0}^x |u'(\tau)|^2 d\tau (x_1 - x_0)^2 \\ &\leq 2|u(x)|^2 + 2 \int_{x_0}^{x_1} |u'(\tau)|^2 d\tau (x_1 - x_0)^2 \end{aligned}$$

$$\xrightarrow{\text{Integr.}} (x_1 - x_0) |u(x_0)|^2 \leq 2 \int_{x_0}^{x_1} |u(x)|^2 dx + 2(x_1 - x_0)^2 \int_{x_0}^{x_1} |u'(\tau)|^2 d\tau$$

*todo is there something missing? can't read what I've written there*

$$\Rightarrow |u(x_0)|^2 \leq \underbrace{\frac{2}{x_1 - x_0}}_{=:a} \int_{\mathbb{R}} |u(x)|^2 dx + \underbrace{2(x_1 - x_0)}_{=:b} \int_{\mathbb{R}} |u'(\tau)|^2 d\tau$$

Now  $a$  is not independent from  $b$ , a small  $a$  results in a large  $b$  and vice versa.

For  $\alpha \geq 0$ :

$$\begin{aligned} a[u, u] &\stackrel{\text{per def}}{\geq} \int |u'|^2 - \mu |u|^2 \\ &\stackrel{\mu < -1}{\geq} \int |u'|^2 + \int |u|^2 \\ &= \|u\|_{\mathcal{H}}^2 \end{aligned}$$

For  $\alpha < 0$

$$\begin{aligned} a[u, u] &\geq \int |u'|^2 - \mu \int |u| + \alpha a \int |u(x)|^2 dx + \alpha b \int_{\mathbb{R}} |u'(\tau)| d\tau \\ &= (1 + \alpha b) \int |u'|^2 + (\alpha a - \mu) \int |u|^2 \\ &= c \|u\|_{\mathcal{H}}^2 \end{aligned}$$

As we want that both coefficients in front of the integrals to be positive  $\Rightarrow$  we chose  $x_n$  correspondent *is it really  $x_n$*  We therefore generally choose  $\mu$  'relatively' close to  $-\infty$ .

### 2.0.2 II:

Now, we have to proof:

$$\begin{aligned} |a[u, v]| &\stackrel{\text{Cauchy-Schwarz}}{\underset{\text{ford}=1}{\leq}} \|u'\|_{L^2} \|v'\|_{L^2} + |\alpha| (a \|u\|_{L^2}^2 + b \|u'\|_{L^2}^2)^{\frac{1}{2}} (\dots \text{same vor } v?)^{\frac{1}{2}} + |\mu| \|u\|_{L^2} \|v\|_{L^2} \\ &\leq C \|u\|_{\mathcal{H}} \|v\|_{\mathcal{H}} \end{aligned}$$

### 2.0.3 III:

$$|\langle f, v \rangle| \leq c \|v\|_{\mathcal{H}}$$

Which follows from (1) RHS, Hölder  $\Rightarrow L^2$  Norm of both  $\leq H^1$  Norm! *todo proof*

Lax-Milgram gives as now the unique solution for the given problem.

## 2.1 Now to my homework

For  $f \xrightarrow{R_\mu} u$  solution of (1) and since (1) is the weak formulation of

$$\underbrace{-u'' + \alpha \delta_{x_0} u}_{=: Au} - \mu u = f \quad (2)$$

the mapping  $f \mapsto u$  gives us also a weak solution of (2).

Now we focus on this equation:  $Au - \mu u = f$ :

### Definition 2.1

$$\text{dom} A = \text{range} R_\mu \subset H^1(\mathbb{R})$$

$$Au := \underbrace{f}_{\in L^2} + \mu \underbrace{u}_{\in H^1} \in L^2$$

## 2 The definition of our operator

So the next steps would be to

- describe domain of  $A$  explicitly
- show that  $A = A^*$

**Homework:** Let  $u \in \text{dom} A$  and  $u \in C^2(-\infty, x_0]$  and also  $u \in C^2[x_0, \infty)$

$\Rightarrow$  find conditions on  $u$  at  $x_0$  such that our assumption holds

by the way  $u \in H^1(\mathbb{R})$ .

Interesting facts:

If we take the closure of  $C_0^\infty(\mathbb{R})$  but the Closure in  $H^1!!!$  we get:

$$\overline{[t]C_0^\infty(\mathbb{R})} = H^1$$



## 2 The definition of our operator

We want to construct the operator  $A$  in a smart way with

$$A = -\frac{d^2}{dx^2} + \alpha d_{x_0}, \quad \mathcal{H} = L^2(\mathbb{R})$$

Then we introduced the variational problem

$$\forall v \in H^1(\mathbb{R}) : \quad \int \nabla u \overline{\nabla v} dx - \mu \int u \bar{v} dx + \alpha u(x_0)v(x_0) = \int f \bar{v} dx \quad (1)$$

$\exists_1 u \in H^1(\mathbb{R})$  satisfying (1)

$$L^2(\mathbb{R}) \ni f \mapsto u =: R_\mu f$$

For  $f_1 \neq f_2 \Rightarrow u_1 \neq u_2$ , since:

$$\text{Suppose } u_1 = u_2 \Rightarrow \int (f_1 - f_2) \bar{v} = 0 \quad \forall \underbrace{v \in H^1(\mathbb{R})}_{\substack{\text{and therefore} \\ \forall v \in L^2(\mathbb{R})}} \Rightarrow f_1 = f_2$$

Since  $H^1$  is dense in  $L^2 \Rightarrow f_1 = f_2$

$$\Rightarrow \left. \begin{array}{l} f = R_\mu^{-1} u \\ Au - \mu u \end{array} \right\} Au = R_\mu^{-1} u + \mu u$$

$$\Rightarrow \text{dom } A = \text{range } A \mathbb{R}_{mu} \\ R_\mu^{-1} u = Au - \mu u =: g \text{ or } u = R_\mu g$$

$$\int u' v' - \mu \int u \bar{v} + \alpha u(x_0)v(x_0) = \int (Au - \mu u) \bar{v} \quad (2)$$

Lets take  $v \in C_0^\infty(-\infty, x_0)$ :

$$\Leftrightarrow \int_{-\infty}^{x_0} u' v' dx = \int_{-\infty}^{x_0} Au \bar{v} \\ \Leftrightarrow - \int_{-\infty}^{x_0} u \bar{v}'' dx = \int_{-\infty}^{x_0} Au \bar{v} dx$$

for  $u \in D'$ :

$$\langle u^{(m)}, v \rangle = (-1)^m \langle u, v^{(m)} \rangle \quad v \in C^\infty$$

$$\Rightarrow \langle u^{(m)}, v \rangle = \langle u, v'' \rangle = \int_{-\infty}^{x_0} u \bar{v}'' = - \int_{-\infty}^{x_0} Au \bar{v}$$

$$\Rightarrow u'' = \underbrace{-Au}_{\in L^2} \text{ on } (-\infty, x_0) \text{ Analogous argument on } (x_0, \infty)$$

Therefore we can fix the statement:

$$\boxed{\text{dom } A \supset \{u \in H^1(\mathbb{R}), u \in H^2(-\infty, x_0), u \in H^2(x_0, \infty)\}}$$

## 2 The definition of our operator

for an arbitrary  $b \in C_0^\infty(\mathbb{R})$ , therefore with the help of (2) since  $u \in H^2$  only on these two subintervals we integrate twice by parts on both sides of  $x_0$

$$\begin{aligned} & - \left( \int_{-\infty}^{x_0} + \int_{x_0}^{\infty} \right) u'' \bar{v} + (u'(x_0 - 0)v(x_0 - 0) - u'(x_0 + 0)v(x_0 + 0)) + \alpha u(x_0)\bar{v}(x_0) \\ & = - \int_{-\infty}^{x_0} u'' v - \int_{x_0}^{\infty} s u'' v \end{aligned}$$

which we can rewrite with the fact that  $v$  is continuous and  $v(x_0 + 0) = v(x_0 - 0)$ , after all we know that  $v \in C_0^\infty$

$$\Leftrightarrow u'(x_0 - 0) - u'(x_0 + 0) + \alpha u(x_0) = 0$$

$\Rightarrow \text{dom} \subset \{u \in H^1(\mathbb{R}), u \in H^2(-\infty, x_0), u \in H^2(x_0, \infty), u'(x_0 - 0) - u'(x_0 + 0) + \alpha u(x_0) = 0\} =: B$  And the action of the operator is defined by

$$Au = \begin{cases} -u'', & (-\infty, x_0) \\ -u'', & (x_0, \infty) \end{cases}$$

Now lets show " $\supset$ ":

Let  $u \in B$ , and since for  $u \in B$  it holds  $u \in H^2$  for both sides  $f := \begin{cases} -u'', & (-\infty, x_0) \\ -u'', & (x_0, \infty) \end{cases}$

Now we have to show that  $u$  is in Range of  $R_\mu$ .

Idea:  $Au = R_\mu^{-1}u + \mu u$

$$\begin{aligned} \Rightarrow u &= R_\mu Au - \mu R_\mu u \\ &= R_\mu(\underbrace{Au}_f - \mu u) \end{aligned}$$

We have to show  $u \in \text{dom} A = \text{range} R_\mu$

guess take  $u \in B$  construct  $f = \begin{cases} -u'', & (-\infty, x_0) \\ -u'', & (x_0, \infty) \end{cases}$  and further to show::

So we have to show  $u = R_\mu(f - \mu u)$ :

$$\begin{aligned} & \int u'v' - \mu \int uv + \alpha u(x_0)v(x_0) = \int (f - \mu u)v \\ & \int u'v' + \alpha u(x_0)v(x_0) = - \int_{-\infty}^{x_0} u''v - \int_{x_0}^{\infty} u''v \\ \Rightarrow & \int u'v' + \alpha u(x_0)v(x_0) = \int_{-\infty}^{x_0} u'v' + \int_{x_0}^{\infty} u'v' - u'(x_0 - 0)v(x_0) + u'(x_0 + 0)v(x_0) \\ & \alpha u(x_0)v(x_0) = u(x_0 + 0)v(x_0) - u(x_0 - 0)v(x_0) \end{aligned}$$

## 2 The definition of our operator

$\Rightarrow$  holds for  $B \Rightarrow \text{dom} A = B$ .

Now we are going to show the self-adjointness:

We know that  $A = R_\mu^{-1}u + \mu u$ . We are going to show that  $R_\mu^{-1}$  is symmetric and then  $A$  is of course symmetric as it is simply its shift.

As  $\text{dom} R_\mu = L^2(\mathbb{R})$  and  $\text{range} R_\mu = \text{dom} R_\mu^{-1}$  we are first going to focus on  $R_\mu$ , and proof that this operator is symmetric:

$(\underbrace{R_\mu f}_{=:u}, g) - (f, \underbrace{R_\mu g}_{=:v}) = \gamma$  We want to show that  $\gamma = 0$ :

$$\begin{aligned} \int u' \phi' - \mu u \bar{\phi} + \alpha u(x_0) \overline{\phi(x_0)} &= \underbrace{\int f \bar{\phi}}_v \\ \int v' \psi - \mu \int v \bar{\psi} + \alpha u(x_0) \overline{\psi(x_0)} &= \underbrace{\int g \bar{\psi}}_u \end{aligned}$$

Summing over lines yields:  $0 - 0 + 0 = \gamma$ .

Now as we know that  $R_\mu$  is symmetric we show that  $R_\mu^{-1}$  is also symmetric:

$$(R_\mu^{-1}u, v) = (u, v^*) \quad u \in \text{dom} R_\mu^{-1}$$

$u = R_\mu f$  for some  $f$  since  $\text{dom} R_\mu^{-1} = \text{range} R_\mu$ . Now we have to show that  $v \in \text{dom} R_\mu^{-1}$  and since self-adjoint and operator is defined on whole space

$$(f, v) = (R_\mu f, v^*) = (f, R_\mu v^*) \quad \text{for arbitrary } f \in C^2$$

$$v = R_\mu v^* \Rightarrow v \in \text{range} R_\mu = \text{dom} R_\mu^{-1}???$$