6 Schrödinger operators in 1D

In this section we apply the theory developped in Section 5 to Schrödinger operators $-\frac{d^2}{dx^2} + V$ in $L^2(\mathbb{R})$.

We say that a function $f : \mathbb{R} \to \mathbb{C}$ is absolutely continuous, if $f|_{[a,b]}$ is absolutely continuous for all $[a,b] \subset \mathbb{R}$ (cf. Example 1.7) and set

$$\boxed{H^2(\mathbb{R}) := \{f \in L^2(\mathbb{R}) : f, f' \text{ are absolutely continuous}, f'' \in L^2(\mathbb{R})\}.}$$

The space $H^2(\mathbb{R})$ is called *Sobolev space of second order*. This space can also be defined via weak derivatives.

Recall: each absolutely continuous function $f : [a,b] \to \mathbb{R}$ is differentiable almost everywhere and the main theorem of calculus holds true. Moreover, for any interval $(\alpha,\beta) \subset [a,b]$ integration by parts in the form

$$\boxed{\int_\alpha^\beta g(x) f'(x)dx = g(\beta)f(\beta) - g(\alpha)f(\alpha) - \int_\alpha^\beta g'(x)f(x)dx}$$

holds. Eventually, if f is absolutely continuous and f' is continuous, then f is continuously differentiable. Hence, $\boxed{H^2(\mathbb{R}) \subset C^1(\mathbb{R})}$.

Lemma 6.1. For any $\varepsilon > 0$ there exists $C_\varepsilon > 0$ such that

$$\boxed{\int_{\mathbb{R}} |f'(t)|^2 dt \le \varepsilon \int_{\mathbb{R}} |f''(t)|^2 dt + C_\varepsilon \int_{\mathbb{R}} |f(t)|^2 dt}$$

holds for all $f \in H^2(\mathbb{R})$. In particular, one has $f' \in L^2(\mathbb{R})$ for all $f \in H^2(\mathbb{R})$.

Proof:
Fix $\varepsilon > 0$, define $L = L(\varepsilon) := \sqrt{\frac{\varepsilon}{2}} > 0$. Let (α,β) be an interval of length L and write $(\alpha,\beta) = J_1 \cup J_2 \cup J_3$ with $J_1 := (\alpha, \alpha + \frac{L}{3})$, $J_2 := [\alpha + \frac{L}{3}, \beta - \frac{L}{3}]$, $J_3 := (\beta - \frac{L}{3}, \beta)$.
Let $f \in H^2(\mathbb{R})$. Since $H^2(\mathbb{R}) \subset C^1(\mathbb{R})$, there exists for all $s \in J_1$ and all $t \in J_3$ a number $x_0 = x_0(s,t)$ such that

$$\boxed{f'(x_0) = \frac{f(t) - f(s)}{t - s}}$$

(mean value theorem of differential calculus) (*)

Since $t - s \ge \frac{L}{3}$: $\quad |f'(x_0)| \le \frac{|f(t)| + |f(s)|}{|t-s|} \le \frac{3}{L}\left(|f(t)| + |f(s)|\right).$

Now we have for arbitrary $x \in (\alpha,\beta)$ and all $s \in J_1, t \in J_3$

$$\underline{|f'(x)|} \overset{f'\,AC}{\underset{(*)}{=}} \left| f'(x_0(s,t)) + \int_{x_0}^{x} f''(y)\,dy \right|$$

$$\leq \underline{\frac{3}{L}\left(|f(s)| + |f(t)|\right) + \int_\alpha^\beta |f''(y)|\,dy}$$

Integration w.r.t. s over J_1 and w.r.t. t over J_3:

$$\int_{J_1}\int_{J_3} |f'(x)|\,dt\,ds = \left(\frac{L}{3}\right)^2 |f'(x)|$$

$$\leq \int_{J_1}\int_{J_3} \left[\frac{3}{L}\left(|f(s)| + |f(t)|\right) + \int_\alpha^\beta |f''(y)|\,dy\right) dt\,ds$$

$$= \underbrace{\int_{J_1} |f(s)|\,ds + \int_{J_3} |f(t)|\,dt}_{\leq \int_\alpha^\beta |f(s)|\,ds} + \left(\frac{L}{3}\right)^2 \int_\alpha^\beta |f''(y)|\,dy$$

$$\Rightarrow |f'(x)| \leq \frac{9}{L^2}\int_\alpha^\beta |f(s)|\,ds + \int_\alpha^\beta |f''(y)|\,dy$$

$$\Rightarrow \underline{|f'(x)|^2} \leq \left(\frac{9}{L^2}\int_\alpha^\beta |f(s)|\,ds + \int_\alpha^\beta |f''(y)|\,dy\right)^2$$

$(a+b)^2 \leq 2a^2 + 2b^2$

CS

$$\leq \underline{2\left(\frac{9}{L^2}\right)^2 \cdot L \int_\alpha^\beta |f(s)|^2\,ds + 2L \cdot \int_\alpha^\beta |f''(y)|^2\,dy}$$

$$\Rightarrow \underline{\int_\alpha^\beta |f'(x)|^2\,dx} \leq \int_\alpha^\beta \left[\frac{162}{L^3}\int_\alpha^\beta |f(s)|^2\,ds + 2L\int_\alpha^\beta |f''(y)|^2\,dy\right] dx$$

$(**)$

$$= \underbrace{\frac{162}{L^2}}_{\frac{324}{\varepsilon}} \underline{\int_\alpha^\beta |f(s)|^2\,ds + \underbrace{2L^2}_{\varepsilon}\int_\alpha^\beta |f''(y)|^2\,dy}$$

Now decompose $\mathbb{R}$ as infinite union of intervals of length L, $\mathbb{R} = \bigcup_{k=1}^{\infty} (\alpha_k, \beta_k)$ with $\beta_k - \alpha_k = L$,

and apply $(**)$ for each interval (α_k, β_k):

$$\int_{\mathbb{R}} |f'(x)|^2 dx = \sum_{k=1}^{\infty} \int_{\alpha_k}^{\beta_k} |f'(x)|^2 dx$$

$$\overset{(**)}{\leq} \sum_{k=1}^{\infty} \left[\frac{324}{\varepsilon} \int_{\alpha_k}^{\beta_k} |f(s)|^2 ds + \varepsilon \int_{\alpha_k}^{\beta_k} |f''(y)|^2 dy \right]$$

$$= \frac{324}{\varepsilon} \int_{\mathbb{R}} |f(x)|^2 dx + \varepsilon \int_{\mathbb{R}} |f''(x)|^2 dx \qquad \square$$

Lemma 6.2. For each $f \in H^2(\mathbb{R})$ one has

$$\lim_{x\to-\infty} f(x) = 0 = \lim_{x\to\infty} f(x) \quad \text{and} \quad \lim_{x\to-\infty} f'(x) = 0 = \lim_{x\to\infty} f'(x).$$

Proof:

Let $c \in \mathbb{R}$. Then we have for all $x < c$

$$\int_x^c f(s) \cdot f'(s)\, ds \overset{\text{int. by parts}}{=} \left(f(c)^2 - f(x)^2 \right) - \int_x^c f'(s) f(s) ds$$

$$\rightsquigarrow \int_x^c f(s) f'(s) ds = \frac{1}{2} \left(f(c)^2 - f(x)^2 \right)$$

Since $f' \in L^2(\mathbb{R})$ for $f \in H^2(\mathbb{R})$, the integral on the left hand side converges for $x \to -\infty$ and hence also $f(x)$ has to converge for $x \to -\infty$.

$$\Rightarrow \int_{-\infty}^c f(s) f'(s) ds = \frac{1}{2} \left(f(c)^2 - \lim_{x\to-\infty} f(x)^2 \right)$$

Since $f \in L^2(\mathbb{R})$, it must hold $\lim_{x\to-\infty} f(x) = 0$, as otherwise $\int_{-\infty}^c |f(x)|^2 dx = \infty$.

The other claims can be shown with the same arguments $\square$

In the following we consider $-\frac{d^2}{dx^2}$ as differential operator in $L^2(\mathbb{R})$.

i.e. $\exists k_f > 0 : f(x) = 0 \ \forall |x| \geq k_f$

Definition 6.3. The operator $T_0 : L^2(\mathbb{R}) \supset \operatorname{dom} T_0 \to L^2(\mathbb{R})$ defined by

$$T_0 f = -f'', \quad \boxed{\operatorname{dom} T_0 = C_0^\infty(\mathbb{R})} = \{f \in C^\infty(\mathbb{R}) : \operatorname{supp} f \text{ is compact}\}$$

is called *minimal operator* associated to $-\frac{d^2}{dx^2}$. Moreover, the operator $T : L^2(\mathbb{R}) \supset \operatorname{dom} T \to L^2(\mathbb{R})$ defined by

$$Tf = -f'', \quad \boxed{\operatorname{dom} T = H^2(\mathbb{R}),}$$

is called *maximal operator* associated to $-\frac{d^2}{dx^2}$.

First goal: show that T_0 is essentially self adjoint and that $\overline{T_0} = T$ is self adjoint.

Proposition 6.4. The operator T_0 is symmetric and

$$\boxed{\operatorname{ran} T_0 = \left\{ g \in C_0^\infty(\mathbb{R}) : \int_{\mathbb{R}} g(x)dx = \int_{\mathbb{R}} xg(x)dx = 0 \right\}}$$

Proof:

T_0 is symmetric, since for all $f \in \operatorname{dom} T_0 = C_0^\infty(\mathbb{R})$ one has

$$(T_0 f, f) = \int_{\cancel{-\infty}\ -k_f}^{\cancel{\infty}\ k_f} (-f''(x)) \cdot \overline{f(x)}\, dx = \int_{-k_f}^{k_f} \underbrace{|f'(x)|^2}_{\in \mathbb{R}} dx \in \mathbb{R}$$

"$\subset$" Let $g \in \operatorname{ran} T_0$. Then $\exists f \in C_0^\infty(\mathbb{R})$ s.t. $g = T_0 f = -f''$.

$$\Rightarrow \int_{-\infty}^{\infty} x^j g(x)\, dx = \int_{-\infty}^{\infty} x^j (-f''(x))\, dx = -\int_{-\infty}^{\infty} \underbrace{(x^j)''}_{=0} f(x)\, dx = 0, \ j = 0, 1$$

"$\supset$" Let $g \in C_0^\infty(\mathbb{R})$ s.t. $\int_{-\infty}^{\infty} x^j g(x)\, dx = 0$, $j = 0, 1$. ($\square$)

Since $g \in C_0^\infty(\mathbb{R})$ there exist $\alpha < \beta$ s.t. $g(x) = 0$ $\forall x \in \mathbb{R} \setminus [\alpha, \beta]$

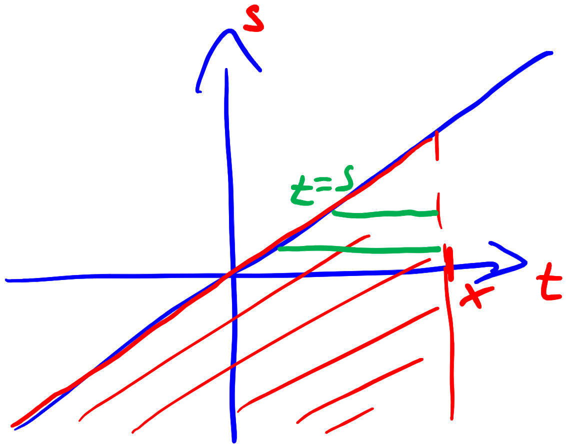
Define $\quad f(x) := -\int_{-\infty}^{x}\int_{-\infty}^{t} g(s)\,ds\,dt$

Then $f \in C^\infty(\mathbb{R})$ and $-f'' = g$.

For $x \le \alpha$ we have $g(s) = 0$ for all $s \le t \le x \le \alpha$

$$\Rightarrow f(x) = -\int_{-\infty}^{x}\int_{-\infty}^{t} \underbrace{g(s)}_{=0}\,ds\,dt = 0$$

Moreover, for $x \ge \beta$ we have



$$f(x) = -\int_{-\infty}^{x}\int_{-\infty}^{t} g(s)\,ds\,dt$$

Fubini

$$= -\int_{-\infty}^{x}\int_{s}^{x} \underline{g(s)}\,dt\,ds$$

$$= \int_{-\infty}^{x} g(s) \int_{s}^{x} dt\,ds = \int_{-\infty}^{x} g(s)(x-s)\,ds$$

$$= x\int_{-\infty}^{x} g(s)\,ds - \int_{-\infty}^{x} s\,g(s)\,ds$$

$$\overset{x \ge \beta}{=} x \underbrace{\int_{-\infty}^{\infty} g(s)\,ds}_{=0} - \underbrace{\int_{-\infty}^{\infty} s\,g(s)\,ds}_{=0} = 0 \quad \text{due to } (\square)$$

$\Rightarrow$ support of $f \subset [\alpha, \beta]$, i.e. $f \in C_0^\infty(\mathbb{R}) = \mathrm{dom}\, T_0$

and $T_0 f = -f'' = g \Rightarrow g \in \mathrm{ran}\, T_0$

$\square$

Lemma 6.5. Let X be a complex vector space and let $F, F_0, F_1 : X \to \mathbb{C}$ be linear (or anti-linear) functionals such that $\boxed{\ker F_0 \cap \ker F_1 \subset \ker F}$. Then there exist $c_0, c_1 \in \mathbb{C}$ such that

$$\boxed{Fx = c_0 F_0 x + c_1 F_1 x}$$

holds for all $x \in X$.

Proof:

Define $\tilde{F} : X \to \mathbb{C}^2$, $\tilde{F}x = \begin{pmatrix} F_0 x \\ F_1 x \end{pmatrix}$

Define on $\operatorname{ran} \tilde{F} \subset \mathbb{C}^2$ the map g_0 by

$$g_0(\tilde{F}x) := Fx$$

g_0 is well defined, as for $\begin{pmatrix} F_0 x \\ F_1 x \end{pmatrix} = \begin{pmatrix} F_0 y \\ F_1 y \end{pmatrix}$

$\Longleftrightarrow \begin{pmatrix} F_0 x - F_0 y \\ F_1 x - F_1 y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ i.e. $x - y \in \ker F_0 \cap \ker F_1 \subset \ker F$

$\Rightarrow F(x-y) = 0$, i.e. $Fx = Fy$.

g_0 is also linear. Hence, by the Hahn-Banach theorem the map g_0, which is defined on $\operatorname{ran} \tilde{F} \subset \mathbb{C}^2$, has continuation onto $\mathbb{C}^2$.

$\rightarrow g_0 \begin{pmatrix} y_0 \\ y_1 \end{pmatrix} = c_0 y_0 + c_1 y_1 \quad \forall (y_0, y_1) \in \mathbb{C}^2$

$$\Rightarrow \underset{\underset{Fx}{\shortparallel}}{g_0(\tilde{F}x)} = g_0 \begin{pmatrix} F_0 x \\ F_1 x \end{pmatrix} = c_0 F_0 x + c_1 F_1 x$$