3.2 Unitary Groups and their Generators

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Let us discuss the free propagator on L^2 again. In what sense does $\psi(t) = P_f(t)\psi_0$ solve the free Schrödinger equation?

Let us check differentiability in t: $$\left(\frac{\|\psi(t+h)-\psi(t)\|_{L^2}}{h}\right)^2 = \frac{1}{h^2}\|P_f(t+h)\psi_0 - P_f(t)\psi_0\|_{L^2}^2$$
$$= \int \underbrace{\left|\frac{e^{-i\frac{k^2}{2}h}-1}{h}\right|^2}_{\xrightarrow{h\to 0} \frac{k^4}{4}} |\hat{\psi}_0(k)|^2 \, dk$$

i.e., $\psi(t)$ is differentiable iff $|k|^4 |\hat{\psi}_0(k)|^2$ is integrable (dominated convergence), i.e., $k^2\hat{\psi}_0(k) \in L^2$.

What about existence of the distributional derivative $-\frac{1}{2}\Delta$?

$$\hookrightarrow -\frac{1}{2}\Delta\psi(t) = -\frac{1}{2}\Delta\mathcal{F}^{-1}\underbrace{e^{-i\frac{k^2}{2}t}\mathcal{F}\psi_0}_{\hat{\psi}(t)} = \mathcal{F}^{-1}\frac{k^2}{2}\underbrace{e^{-i\frac{k^2}{2}t}\hat{\psi}_0}_{\hat{\psi}(t)} \in L^2 \text{ iff } k^2\hat{\psi}_0(k) \in L^2$$

Conclusion: If $k^2\hat{\psi}_0(k) \in L^2$ (i.e., also $k^2\hat{\psi}(t) \in L^2 \ \forall t$), then $\psi(t)$ solves the free Schrödinger equation $\forall t$ in the L^2 sense.

Let us define the corresponding spaces:

Definition 3.28: Let $m \in \mathbb{N}$. The *m-th Sobolev space* is

$$H^m(\mathbb{R}^d) := \left\{ f \in L^2(\mathbb{R}^d) : (1+k^2)^{\frac{m}{2}}\hat{f} \in L^2(\mathbb{R}^d) \right\}.$$

Notes: • By Cauchy-Schwarz, the condition $(1+k^2)^{\frac{m}{2}}\hat{f} \in L^2(\mathbb{R}^d)$ is equivalent to $\hat{f} \in L^2(\mathbb{R}^d)$ and $|k|^m\hat{f} \in L^2(\mathbb{R}^d)$.

- One can show that $H^m(\mathbb{R}^d)$ with norm $\|f\|_{H^m(\mathbb{R}^d)} := \|(1+k^2)^{\frac{m}{2}} \mathcal{F} f\|_{L^2(\mathbb{R}^d)}$ is a Banach space, and with scalar product $\langle f, g \rangle_{H^m(\mathbb{R}^d)} := \int \overline{\hat{f}(k)} (1+k^2)^m \hat{g}(k) dk$ a Hilbert space. (Note: Other equivalent choices are possible.)

- We could equivalently define

$$H^m(\mathbb{R}^d) := \Big\{ f \in L^2(\mathbb{R}^d) : \partial_x^\alpha f \in L^2(\mathbb{R}^d) \ \forall \underbrace{\alpha \in \mathbb{N}_0^d}_{\text{multi-index}}, |\alpha| \leq m \Big\}.$$

Here, $\partial_x^\alpha f$ is the distributional (also called "weak") derivative. What does this mean?

First, recall that for $f \in L^2(\mathbb{R}^d)$, $T_f \in S'(\mathbb{R}^d)$. Also, for any $T \in S'(\mathbb{R}^d)$, $\partial_x^\alpha T$ is defined by $\partial_x^\alpha T(g) = T((-1)^{|\alpha|} \partial_x^\alpha g) \ \forall g \in S(\mathbb{R}^d)$. In particular, recall that $\partial_x^\alpha T_f = T_{\partial_x^\alpha f}$ for $f \in S(\mathbb{R}^d)$.

Now, for $f \in L^2(\mathbb{R}^d)$, we can define $T_f \in S'(\mathbb{R}^d)$ and $\partial_x^\alpha T_f \in S'(\mathbb{R}^d)$. If there is $g \in L^2(\mathbb{R}^d)$ such that $\partial_x^\alpha T_f = T_g$, we write $g = \partial_x^\alpha f \in L^2(\mathbb{R}^d)$ and call it weak/distributional partial derivative.

Note that with this definition it is natural to define the norm

$$\|f\|^2_{H^m(\mathbb{R}^d)} = \sum_{i=0}^m \|D^i f\|^2_{L^2(\mathbb{R}^d)}.$$

- Similarly to above, we could therefore even define for any $m \in \mathbb{R}$:

$$H^m(\mathbb{R}^d) := \Big\{ T_f \in S'(\mathbb{R}^d) : \hat{f} \text{ measurable}, (1+k^2)^{\frac{m}{2}} \hat{f} \in L^2(\mathbb{R}^d) \Big\}.$$

These spaces are sometimes called Bessel potential spaces.

- Another generalization is the $W^{k,p}(\mathbb{R}^d)$ Sobolev spaces, here for $k \in \mathbb{N}_0$, $1 \leq p \leq \infty$.

$$W^{k,p}(\mathbb{R}^d) := \Big\{ f \in L^p(\mathbb{R}^d) : \partial_x^\alpha f \in L^p(\mathbb{R}^d) \text{ for all } |\alpha| \leq k \Big\}.$$

So $W^{k,2} = H^2$. Similar to above, these can be turned into Banach spaces, but only for $p=2$ into Hilbert spaces.

The connection to continuity and differentiability is the following:

Lemma 3.37 (Sobolev lemma): Let $\ell \in \mathbb{N}_0$ and $f \in H^m(\mathbb{R}^d)$ with $m > \ell + \frac{d}{2}$.

Then $f \in C^\ell(\mathbb{R}^d)$ and $\partial^\alpha f \in C_\infty(\mathbb{R}^d)$ $\forall\, |\alpha| \leq \ell$.

Proof: HW 6, Problem 3.

Note: The condition $m > \ell + \frac{d}{2}$ is generally sharp, i.e., $\exists\, f \in H^m(\mathbb{R}^d)$ s.t. $f \notin C^\ell(\mathbb{R}^d)$ for $m \leq \ell + \frac{d}{2}$.

Example: For $f \in H^1(\mathbb{R})$ we find $1 > \ell + \frac{1}{2}$, i.e., $f \in C^0(\mathbb{R})$. So any $f \in H^1(\mathbb{R})$, which a-priori is only defined almost everywhere, is actually continuous, i.e., defined pointwise. In $\mathbb{R}^3$, we need at least $f \in H^2(\mathbb{R}^3)$ to conclude continuity.

Let us get back to the free propagator $P_f : \mathbb{R} \to \mathcal{B}(L^2)$, $t \mapsto P_f(t) = \mathcal{F}^{-1} e^{-i\frac{k^2}{2}t} \mathcal{F}$.
It has the following properties:

a) $P_f(t)$ is unitary $\forall t \in \mathbb{R}$ (as noted in last section)

b) P_f is strongly continuous (as noted in last section)

c) P_f is a group homomorphism: $P_f(t) P_f(s) = \mathcal{F}^{-1} e^{-i\frac{k^2}{2}t} \mathcal{F}\, \mathcal{F}^{-1} e^{-i\frac{k^2}{2}s} \mathcal{F} = \mathcal{F}^{-1} e^{-i\frac{k^2}{2}(t+s)} \mathcal{F} = P_f(t+s)$ $\forall s,t \in \mathbb{R}$

d) For $\psi_0 \in L^2$, $\psi(t) = P_f(t)\psi_0$ solves the free SE in the sense of distributions (as noted before)

e) For $\psi_0 \in H^2 \subset L^2$, $\psi(t) = P_f(t)\psi_0$ solves the free SE in the L^2 sense (as noted above)

Next, recall that we are interested in the interacting Schrödinger equation with Hamiltonians of the form $H = -\frac{\Delta}{2} + V$. Therefore, we put what we know about the free Schrödinger equation in a general context. We make the connection between general unbounded operators H and objects like the propagator ($\psi(t) = P(t)\psi_0$) with the following two definitions.

The properties a), b), c) are fundamental, i.e., also propagators of any interacting SE should have them. Thus, we define:

Definition 3.30: A family $U(t)$, $t \in \mathbb{R}$, of unitary operators $U(t) \in \mathcal{L}(\underbrace{\mathcal{H}}_{\text{some Hilbert space}})$ is called strongly continuous unitary one-parameter group if

i) $U: \mathbb{R} \to \mathcal{L}(\mathcal{H})$, $t \mapsto U(t)$ is strongly continuous

ii) $U(t+s) = U(t)U(s)$ $\forall t, s \in \mathbb{R}$ (in particular $U(0) = \mathrm{id}_{\mathcal{H}}$)

Motivated by properties d), e), we make the connection to the Schrödinger-type equation $i\frac{d}{dt}\psi(t) = H\psi(t)$. Generally, H is an unbounded operator with some domain $D(H)$. But it will be very useful – and indeed general enough – if $D(H)$ is dense in $\mathcal{H}$. (So $H: D(H) \to \mathcal{H}$, but $H\varphi$ generally not defined for $\varphi \notin D(H)$.)

Definition 3.31: A densly defined linear operator H $\overbrace{\text{with domain } D(H) \subset \mathcal{H}}^{\text{i.e., } H \text{ not necessarily bounded}}$ is called generator of a strongly continuous unitary group $U(t)$ if

i) $D(H) = \{\psi \in \mathcal{H} : t \mapsto U(t)\psi \text{ is differentiable}\}$

ii) For $\psi \in D(H)$, we have $i\frac{d}{dt}U(t)\psi = \underbrace{U(t)H\psi}_{\text{we show below that this } = HU(t)\psi}$

So $H_0 = -\frac{1}{2}\Delta$ with $D(H_0) = H^2(\mathbb{R}^d)$ is generator of the unitary group $P_f(t)$.

Let us collect some important properties of generators:

<u>Proposition 3.33:</u> Let H be generator of $U(t)$. Then

i) $U(t)D(H) = D(H)$ $\forall t$, i.e., $D(H)$ is invariant under $U(t)$,

ii) $[H, U(t)]\psi = 0$ $\forall \psi \in D(H)$ (where $[A,B] := AB - BA$ is the commutator),

iii) H is symmetric, i.e., $\langle H\psi, \varphi\rangle = \langle \psi, H\varphi\rangle$ $\forall$ $\varphi, \psi \in D(H)$,

iv) U is uniquely determined by H, and H is uniquely determined by U.

Proof: HW 7