Let us put the space H^2 in a more general context:

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 $|k|^m \hat{f} \in L^2(\mathbb{R}^d)$. ($1 + |k|^m \leq (1+k^2)^{\frac{m}{2}}$ and $(1+k^2)^{\frac{m}{2}} \leq 2^{\frac{m}{2}} (1+|k|^m)$)
- 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 of norm/scalar product are possible.)
- $$H^m(\mathbb{R}^d) := \Big\{ f \in L^2(\mathbb{R}^d) : \underbrace{\partial_x^\alpha f \in L^2(\mathbb{R}^d)}_{\partial_x^\alpha f \text{ is the distributional derivative}} \ \forall \overbrace{\alpha \in \mathbb{N}_0^d}^{\text{multi-index}}, |\alpha| \leq m \Big\}.$$
- Similarly to above, we could define for any $m \in \mathbb{R}$:

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

These spaces are sometimes called Bessel potential spaces.

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

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

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:

$\boxed{\begin{array}{l}\underline{\text{Lemma 3.37 (Sobolev Lemma):}} \text{ Let } \ell \in \mathbb{N}_0 \text{ and } f \in H^m(\mathbb{R}^d) \text{ with } m > \ell + \frac{d}{2}. \\ \text{Then } f \in C^\ell(\mathbb{R}^d) \text{ and } \partial^\alpha f \in C_\infty(\mathbb{R}^d)\ \forall\, |\alpha| \le \ell.\end{array}}$

Proof: HW7, 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 $m \le \ell + \frac{d}{2}$.

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.

3.2 Unitary Groups and their Generators

Let us now summarize the important properties of the free propagator $P_f(t)$. These will provide a good framework to define propagators also for the interacting Schrödinger equation:

a) $P_f(t)$ is unitary $\forall t \in \mathbb{R}$.

b) P_f is strongly continuous.

c) P_f is a group homomorphism:

$$P_f(t)P_f(s) = \mathcal{F}^{-1}e^{-i\frac{k^2}{2}t}\mathcal{F}\,\mathcal{F}^{-1}e^{-i\frac{k^2}{2}s}\mathcal{F} = \mathcal{F}^{-1}e^{-i\frac{k^2}{2}(t+s)}\mathcal{F} = P_f(t+s) \quad \forall s,t\in\mathbb{R}.$$

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

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.

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) and e), let us make the connection to the Schrödinger equation $i\frac{d}{dt}\psi(t)=H\psi(t)$.

For the free SE, $-\frac{\Delta}{2}\psi$ is only defined for $\psi\in H^2$, i.e., $\overbrace{-\frac{\Delta}{2}}^{\text{this operator is unbounded}}: H^2\to L^2$. More generally, let us consider bounded or unbounded operators $H: D(H)\to\mathcal{H}$, where $D(H)\subset\mathcal{H}$ is the domain of H.

We will require $D(H)$ to be dense (note: H^2 is dense in L^2).

Definition 3.31: A densly defined linear operator H with domain $\mathcal{D}(H) \subset \mathcal{H}$ is called generator of a strongly continuous unitary group $U(t)$ if

i) $\mathcal{D}(H) = \{ \psi \in \mathcal{H} : t \mapsto U(t)\psi \text{ is differentiable} \}$ → SE holds as equality of vectors in $\mathcal{H}$ for $\psi_0 \in \mathcal{D}(H)$

ii) For $\psi \in \mathcal{D}(H)$, we have $i \frac{d}{dt} U(t)\psi = \underbrace{U(t) H \psi}$

we show below that this $= H\, U(t)\psi$ (but a-priori we only know how to apply H to ψ)

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

Let us collect some important properties of generators:

Proposition 3.33: Let H be generator of $U(t)$. Then

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

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

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

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

Proof: HW 8

Example: Translation operator on $L^2(\mathbb{R})$

Let us consider $T(t): L^2(\mathbb{R}) \to L^2(\mathbb{R})$, where $(T(t)\psi)(x) := \psi(x-t)$.

We already introduced this operator on $\mathcal{S}$ as the pseudodifferential operator $e^{-it(-i\frac{d}{dx})}$. So we would guess that $D_0 = -i\frac{d}{dx}$ with domain $\mathcal{D}(D_0) = H^1(\mathbb{R})$ is the generator of the strongly continuous unitary one-parameter group $T(t)$. This is indeed so; proof in HW 8.