

Recall: For $\psi_0 \in H^2$, $\psi(t)$ solves the free Schrödinger equation $\forall t$ in the L^2 sense.

If $L^2 \ni \psi_0 \notin H^2$, then $\psi(t)$ solves the free Schrödinger equation in the sense of distributions only (as noted before).

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 $|k|^m \hat{f} \in L^2(\mathbb{R}^d)$.
 $\left(\begin{array}{l} 1+|k|^m \leq (1+k^2)^{\frac{m}{2}} \\ \text{and } (1+k^2)^{\frac{m}{2}} \leq 2^{\frac{m}{2}}(1+|k|^m) \end{array} \right)$

• 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.)

• $H^m(\mathbb{R}^d) = \left\{ f \in L^2(\mathbb{R}^d) : \underbrace{\partial_x^\alpha f}_{\substack{\text{multi-index} \\ \partial_x^\alpha f \text{ is the distributional derivative}}} \in L^2(\mathbb{R}^d) \quad \forall \alpha \in \mathbb{N}_0^d, |\alpha| \leq m \right\}$.
 $= \left\{ T_f \in S'(\mathbb{R}^d) : \hat{f} \text{ measurable, } (1+k^2)^{\frac{m}{2}} \hat{f} \in L^2(\mathbb{R}^d) \right\}$.

• H^m for $m \in \mathbb{R}$ are sometimes called Bessel potential spaces.

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

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

So $W^{k,2} = H^k$. 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 $\partial^\alpha f \in C_0(\mathbb{R}^d) \forall |\alpha| \leq \ell$.

Proof: HW8, 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.

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 $U(t) \in \mathcal{L}(\mathcal{H})$ is called strongly continuous unitary one-parameter group if some Hilbert space

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

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

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., $-\frac{\Delta}{2}: H^2 \rightarrow L^2$. this operator is unbounded More generally, let us consider bounded or unbounded operators $H: \mathcal{D}(H) \rightarrow \mathcal{H}$, where $\mathcal{D}(H) \subset \mathcal{H}$ is the domain of H .

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

Definition 3.31: A densely 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) $\mathcal{D}(H) = \{ \psi \in \mathcal{H} : t \mapsto U(t)\psi \text{ is differentiable} \}$ \rightarrow 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 $i \frac{d}{dt} U(t)\psi = U(t)H\psi$

$\underbrace{U(t)H\psi}_{\text{we show below that this} = H U(t)\psi}$ (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 $P_f(t)$.