6.7. Free Schrödinger evolution on $\mathbb{R}^d$

Consider the following operators on $L^2(\mathbb{R}^d)$

$$\hat{p}_j := -i\partial_j \quad , \quad j = 1, \dots, d$$

$$\widehat{p_j^2} := -\partial_j^2 \quad , \quad j = 1, \dots, d$$

$$H_0 := -\frac{1}{2}\Delta = \frac{1}{2}\sum_{j=1}^{d} (-i\partial_j)^2$$

By 6.6.4. and 6.6.6. all are densely defined and self-adjoint.

1. Definition For $t \in \mathbb{R}$, let $U_t = F_t(-i\partial)$ with $F_t(p) = e^{-it\frac{1}{2}p^2}$, defined as in 6.6.5. Then $\psi(t) := U_t \psi(0)$ defines the free Schrödinger evolution on $L^2(\mathbb{R}^d)$.

2. Properties: $*$ Now $U_t = \mathcal{F}^{-1} M_{u_t} \mathcal{F}$ with

$$u_t(k) = e^{-it\frac{1}{2}(2\pi k)^2} = e^{-it\frac{(2\pi)^2}{2}k^2}.$$

Exercise 5.5. $\Rightarrow$ $(M_{u_t})_t$ is a strongly continuous unitary group, with generator M_V,

$V(k) = \frac{1}{2}(2\pi)^2 k^2$: Exercise 7.1. $\Rightarrow$ U_t is also a strongly continuous unitary group, with generator $A = \mathcal{F}^{-1} M_V \mathcal{F}$. Since $V(k) = \frac{p^2}{2}\Big|_{p = 2\pi k}$

$$\Rightarrow A = \frac{1}{2}\sum_{j=1}^{d}(-i\partial_j)^2 = -\frac{1}{2}\Delta = H_0.$$

Thus $U_t = e^{-itH_0}$ with $H_0 = -\frac{1}{2}\Delta = -\frac{1}{2}\nabla^2$.

$*$ In general, the natural domains of combinations of unbounded operators are not very useful. Here, however, we do have

$$H_0 = \frac{1}{2}\sum_{j=1}^{d}\widehat{p_j^2} \quad \text{and} \quad \widehat{p_j^2} = \hat{p}_j\,\hat{p}_j.$$

3. Proposition: a) If $\psi(t_0) \in \mathcal{S}$ for some t_0, then $\psi(t) \in \mathcal{S}$ $\forall t$, and $\forall t \neq 0$

$$\psi(x,t) := \psi(t)(x) = \int_{\mathbb{R}^d} dy\, \mathcal{K}(x,y;t)\, \psi(y,0)$$

where $\mathcal{K}$ is called the free propagator

and is given by

$$\mathcal{K}(x,y;t) = \frac{1}{(-i 2\pi t)^{d/2}}\, e^{i \frac{1}{2t}(x-y)^2}$$

In addition, $\psi(x,t)$ solves the free Schrödinger differential equation:

$$i\, \partial_t \psi(x,t) = -\frac{1}{2} \Delta_x \psi(x,t) \quad \forall t \in \mathbb{R},\ x \in \mathbb{R}^d.$$

b) If $\psi(0) \in L^1 \cap L^2$; $t \neq 0$, then

$$\psi(x,t) = \int_{\mathbb{R}^d} dy\, \mathcal{K}(x,y;t)\, \psi(y,0) \quad \text{a.e. } x \in \mathbb{R}^d$$

c) In general, $\forall \psi \in L^2$, $t \neq 0$, $\exists R_n > 0$, $n \in \mathbb{N}$, s.t. $R_n \to \infty$ and for a.e. $x \in \mathbb{R}^d$

$$\psi(x,t) = \lim_{n \to \infty} \int_{|y| \leq R_n} dy\, \mathcal{K}(x,y;t)\, \psi(y,0).$$

Proof. a) Assume $\psi(t_0) \in \mathcal{S}$, $t_0 \in \mathbb{R}$. By the group property of U_t, then $\forall t$

$$\psi(t) = U_t \psi(0) = U_{t-t_0} U_{t_0} \psi(0) = U_{t-t_0} \psi(t_0).$$

$$= \mathcal{F}_{L^2}^{-1} M_{u_{t-t_0}} \mathcal{F}_{L^2} \psi(t_0) = \mathcal{F}_{\mathcal{S}}^{-1} M_{u_{t-t_0}} \mathcal{F}_{\mathcal{S}} \psi(t_0)$$

$= \tilde{U}_{t-t_0} \psi(t_0)$, where $\tilde{U}_t$ denotes

the map "U_t" defined in Ex. 7.5.
Since then $\tilde{U}_{t-t_0}\psi(t_0) \in S$, we find that $\psi(t) \in S$ $\forall t \in \mathbb{R}$. But then also $\psi(0) \in S$

$$\Rightarrow \psi(t) = U_t \psi(0) = \tilde{U}_t \psi(0). \text{ Thus } \forall t \neq 0,\ x \in \mathbb{R}^d,$$

$$\Rightarrow \psi(x,t) = \int_{\mathbb{R}^d} dy\, \underbrace{K(x-y,t)}_{= \mathcal{K}(x,y;t)} \psi(y,0).$$

This proves the first part of "a)".

By the inversion formula, we have for all $t, \varepsilon \in \mathbb{R}$, $x \in \mathbb{R}^d$,

$$\psi(x,t+\varepsilon) - \psi(x,t) =$$

$$= \int_{\mathbb{R}^d} dk\, e^{i2\pi x\cdot k} \left[\hat{\psi}(k,t+\varepsilon) - \hat{\psi}(k,t) \right]$$

Since $\hat{\psi}(k,t) = e^{-it\frac{1}{2}(2\pi k)^2} \hat{\psi}(k,0)$

$$\Rightarrow \psi(x,t+\varepsilon) - \psi(x,t) = \int dk\, e^{i2\pi x\cdot k} \left[e^{-i\varepsilon\frac{1}{2}(2\pi k)^2} - 1 \right] \hat{\psi}(k,t)$$

Since $\left| e^{-i\varepsilon\frac{1}{2}(2\pi k)^2} - 1 \right| \leq |\varepsilon| \frac{1}{2} (2\pi)^2 k^2$

and $k^2 \hat{\psi}(k,t) \in L^1$, DCT

$$\Rightarrow \lim_{\varepsilon \to 0} \frac{\psi(x,t+\varepsilon) - \psi(x,t)}{\varepsilon} = \int dk\, e^{i2\pi x\cdot k} \hat{\psi}(k,t) \times \underbrace{\lim_{\varepsilon \to 0} \frac{1}{\varepsilon}\left[e^{-i\varepsilon\frac{1}{2}(2\pi k)^2} - 1 \right]}_{= -i\frac{1}{2}(2\pi k)^2 = -i\left[-\frac{1}{2}(i2\pi k)^2\right]}$$

$$\Rightarrow i\partial_t \psi(x,t) = -\frac{1}{2} \int dk\, e^{i2\pi x\cdot k} \sum_{j=1}^{d} (i2\pi k_j)^2 \hat{\psi}(k,t)$$

$$= -\frac{1}{2} \nabla_x^2 \psi(x,t) \quad \text{by Exercise 7.4b)}$$

This completes the proof of "a)".

For "b)", Let $\psi(0) \in L^1 \cap L^2$, $t \neq 0$.

Then $\forall f \in S$: $(f, \psi(t)) = (f, U_t \psi(0))$

$$= (U_t^* f, \psi(0)) = (U_{-t} f, \psi(0))$$

$$= \int dx\, \psi(x,0) \Big[\int dy\, K(x,y;-t)\, f(y) \Big]^*$$

$$\overset{\text{Fubini}}{=} \int dy\, f(y)^* \Big[\int dx\, K(x,y;-t)^* \psi(x,0) \Big]$$

Since $K(x,y;-t)^* = K(y,x;t)$, this implies "b)" holds.

For "c)", let $R > 0$, and define $\psi_R(x,0) = \mathbb{1}(|x| \leq R)\psi(x,0)$ and $\psi_R(t) := e^{-itH_0}\psi_R(0)$. As $\psi_R(x,0) \in L^1 \cap L^2$ and

$$\| \psi_R(t) - \psi(t) \| = \| e^{-itH_0} (\psi_R(0) - \psi(0)) \|$$
$$= \| \psi_R(0) - \psi(0) \| \to 0, \quad R \to \infty.$$

$\Rightarrow \exists$ sequence $R_n \to \infty$ s.t. for a.e. $x \in \mathbb{R}^d$

$$\psi(t,x) = \lim_{n\to\infty} \psi_{R_n}(t,x)$$
$$= \lim_{n\to\infty} \int dy\, K(x,y;t)\, \mathbb{1}(|y| \leq R_n)\, \psi(y,0).$$

Thus "c)" holds, as well. $\square$

8. "Quantum phase space": Wigner transform and Weyl quantization

8.1. Definition: For $\phi, \psi \in L^2(\mathbb{R}^d)$,

we define the corresponding Wigner-Function $W[\phi,\psi] : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$,

$$W[\phi,\psi](x,k) :=$$

$$\int_{\mathbb{R}^d} dy \, e^{-i2\pi k\cdot y} \phi(x - \tfrac{y}{2})^* \psi(x + \tfrac{y}{2}).$$

The Wigner function of $\psi \in L^2(\mathbb{R}^d)$ is $W[\psi] := W[\psi,\psi]$.

8.2. Proposition (Basic properties) $\forall \phi, \psi \in L^2$:

a) (symmetry) $W[\phi,\psi]^* = W[\psi,\phi]$
b) (reality) $W[\psi](x,k) \in \mathbb{R} \quad \forall x,k$
c) (boundedness) $|W[\phi,\psi](x,k)| \leq 2^d \|\phi\| \, \|\psi\| \; \forall x,k$
d) (Fourier representation) If $\hat{\psi} = \mathcal{F}\psi$ and $\hat{\phi} = \mathcal{F}\phi$, then a.e. $x,k \in \mathbb{R}^d$

$$W[\phi,\psi](x,k) = W[\hat{\phi},\hat{\psi}](k,-x)$$

$$= \int dq \, e^{+i2\pi q\cdot x} \hat{\phi}(k - \tfrac{q}{2})^* \hat{\psi}(k + \tfrac{q}{2})$$

e) (recovery of inner products)
If $\psi, \phi \in \mathcal{S}$, then $W[\phi,\psi] \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$ and

$$\int_{\mathbb{R}^d} dk \, W[\phi,\psi](x,k) = \phi(x)^* \psi(x) \quad \forall x \in \mathbb{R}^d$$

$$\int_{\mathbb{R}^d} dx \, W[\phi,\psi](x,k) = \hat{\phi}(k)^* \hat{\psi}(k) \quad \forall k \in \mathbb{R}^d$$

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} dx\, dk \, W[\phi,\psi](x,k) = (\phi,\psi)$$