... Thus there is a sequence $R_n \to \infty$ such that for a.e. $k \in \mathbb{R}^d$

$$(\mathcal{F}\psi)(k) = \lim_{n\to\infty} \int_{|x|\le R_n} dx\, e^{-i2\pi x\cdot k}\psi(x).$$

## 6.6. Differential operators on $L^2(\mathbb{R}^d)$

**1. Lemma** Suppose $A$ is a closed, densely defined operator, and $U$ is a unitary operator. Then $AU$ and $UA$ are closed and densely defined. In addition,

$$(AU)^* = U^*A^*, \quad (UA)^* = A^*U^*.$$

**Proof.** The products are defined with their natural domains:

$$D(AU) = \{\psi \in \mathcal{H} \mid U\psi \in D(A)\} = U^*D(A)$$

$$D(UA) = D(A).$$

For any unitary map $\mathcal{U} : \tilde{\mathcal{H}} \to \tilde{\mathcal{H}}$ and subset $S \subset \tilde{\mathcal{H}}$ we have $\overline{\mathcal{U}S} = \mathcal{U}\overline{S}$. Thus both $D(A)$ and $U^*D(A)$ are dense. Now

$$\mathcal{G}(AU) = \{((\psi, AU\psi)) \mid U\psi \in D(A)\} = \{((U^*\phi, A\phi)) \mid \phi \in D(A)\} = \mathcal{U}_1\mathcal{G}(A) \text{ with}$$

$$\mathcal{U}_1((\psi,\phi)) := ((U^*\psi, \phi)).$$

Clearly, $\mathcal{U}_1 : \mathcal{H}\oplus\mathcal{H} \circlearrowleft$ is unitary, and thus $\overline{\mathcal{G}(AU)} = \mathcal{U}_1\overline{\mathcal{G}(A)} = \mathcal{U}_1\mathcal{G}(A) = \mathcal{G}(AU)$ and $AU$ is closed and densely def.

Similarly, $\mathcal{G}(UA) = \mathcal{U}_2\mathcal{G}(A)$, with $\mathcal{U}_2((\psi,\phi)) := ((\psi, U\phi))$ which is unitary. Thus also $UA$ is closed and densely def.

Suppose $\tilde{\phi}, \phi \in \mathcal{H}$. Then $\phi \in D((AU)^*)$, $\tilde{\phi} = (AU)^*\phi$

$\Leftrightarrow \forall \psi \in D(AU) : \ (\phi, AU\psi) = (\tilde{\phi}, \psi) = (U\tilde{\phi}, U\psi)$

$\Leftrightarrow \forall \varphi \in D(A) : \ (\phi, A\varphi) = (U\tilde{\phi}, \varphi)$

$\Leftrightarrow \ \phi \in D(A^*)$ and $U\tilde{\phi} = A^*\phi$

$\Leftrightarrow \quad \phi \in D(A^*) = D(U^*A^*)$ and $\tilde{\phi} = U^*A^*\phi$.

This proves that $(AU)^* = U^*A^*$.

Similarly, $\phi \in D((UA)^*)$, $\tilde{\phi} = (UA)^*\phi$

$\Leftrightarrow \forall \psi \in D(UA) : (\tilde{\phi}, \psi) = (\phi, UA\psi) = (U^*\phi, A\psi)$

$\Leftrightarrow \forall \psi \in D(A) : (\tilde{\phi}, \psi) = (U^*\phi, A\psi)$

$\Leftrightarrow U^*\phi \in D(A^*)$ and $\tilde{\phi} = A^*(U^*\phi)$

$\Leftrightarrow \phi \in U\,D(A^*) = (U^*)^* D(A^*) = D(A^*U^*)$

and $\tilde{\phi} = A^*U^*\phi$

and thus $(UA)^* = A^*U^*$ $\Box$

2. Corollary If $A$ is self-adjoint, and $U$ is unitary, then $U^*AU$ and $UAU^*$ are self-adjoint.

3. Definition: Let $\alpha$ be a multi-index. Then $V_\alpha(k) = (i2\pi k)^\alpha$ defines a closed multiplication operator $M_{V_\alpha}$ on $L^2(\mathbb{R}^d)$.

We define the operator $\partial^\alpha$ on $L^2(\mathbb{R}^d)$ by the formula $\partial^\alpha := \mathcal{F}_{L^2}^{-1} M_{V_\alpha} \mathcal{F}_{L^2}$.

4. Properties: a) $\partial^\alpha$ is a closed, densely defined operator.

b) $A := (-i\partial)^\alpha$ is self-adjoint. If $\alpha_i$ is even $\forall i$, then $A$ is also positive. ($\Leftrightarrow$ $A$ self-adj. and $\sigma(A) \subset [0, \infty)$)

c) $\forall f \in \mathcal{S}$ : $\partial^\alpha_{L^2} f = \partial^\alpha f$ and, moreover, $\partial^\alpha_{L^2} = \overline{\partial^\alpha_{\mathcal{S}}}$.

d) "Partial integration" is possible: $\forall \phi, \psi \in D(\partial^\alpha)$

$$(\phi, \partial^\alpha\psi) = ((-\partial)^\alpha\phi, \psi).$$

Proof: By Lemma 6.6.1. above, and unitarity of $\mathcal{F}_{L^2}$, "a)" follows since $M_{V_\alpha}$ is closed and densely defined (Exercise 5.1.) "b)" is a consequence of the corresponding properties of $M_{V_\alpha}$ and Lemma 6.6.7. on page 77b.

Now $(-i)^{|\alpha|} V_\alpha(k) = (2\pi k)^\alpha \in \mathbb{R} \quad \forall k \in \mathbb{R}^d \Rightarrow M_{(-i)^{|\alpha|}V_\alpha}$ self-adjoint

Corollary 6.6.2.

$\Rightarrow \quad A := \mathcal{F}^* M_{(-i)^{|\alpha|}V_\alpha} \mathcal{F} = (-i\partial)^\alpha$ is self-adjoint.

If also $\quad \alpha_i = 2n_i \quad \forall i, \quad n \in \mathbb{N}_0^d,$

then

$$(\psi, A\psi) = (\psi, (-i\partial)^\alpha \psi) = (\hat\psi, (-i)^{|\alpha|} M_{V_\alpha} \hat\psi)$$
$$= \int dk\, |\hat\psi(k)|^2 \, (2\pi)^{|\alpha|} \prod_{j=1}^d k_j^{2n_j} \geq 0 \quad \forall \psi \in D(A)$$

Lemma 6.6.7.

$\Rightarrow \quad \sigma(A) \subset [0, \infty).$

To prove "c)", assume $f \in \mathcal{S}$. Then

Exercise 7.4b)

$$(M_{V_\alpha} \mathcal{F}_{L^2} f)(k) = (i2\pi k)^\alpha \hat f(k) \stackrel{!}{=} \mathcal{F}_\mathcal{S}(\partial^\alpha f)(k) \in \mathcal{S}$$

$$\Rightarrow \partial^\alpha_{L^2} f = \mathcal{F}_{L^2}^{-1} M_{V_\alpha} \mathcal{F}_{L^2} f = \mathcal{F}_\mathcal{S}^{-1}(\mathcal{F}_\mathcal{S}(\partial^\alpha f)) = \partial^\alpha f.$$

Thus $\partial^\alpha_{L^2}$ is a closed extension of the densely defined operator $\partial^\alpha_\mathcal{S} : \mathcal{S} \to L^2$

$\Rightarrow \partial^\alpha_\mathcal{S}$ is closable, and $\overline{\partial^\alpha_\mathcal{S}} \subset \partial^\alpha_{L^2}$.

To show the converse, suppose $\psi \in D(\partial^\alpha_{L^2})$.
Then $\hat\psi \in D(M_{V_\alpha}) \Rightarrow V_\alpha \hat\psi \in L^2$.
Since also $\hat\psi \in L^2 \Rightarrow \exists g_n \in \mathcal{S}, n \in \mathbb{N}$, s.t.
$g_n \to \hat\psi$ in norm. Let us then define $f_n = G_n g_n$ where

$$G_n(k) := e^{-\frac{1}{2}\varepsilon_n^2 k^{2\alpha}}, \quad \varepsilon_n = \|\hat\psi - g_n\|^{1/2}.$$

Clearly, also $f_n \in \mathcal{S} \ \forall n$, and $\varepsilon_n \xrightarrow{n\to\infty} 0$.
In addition,

$$\|\hat\psi - f_n\| = \|(1-G_n)\hat\psi + G_n(\hat\psi - g_n)\|$$
$$\leq \|(1-G_n)\hat\psi\| + \|G_n(\hat\psi - g_n)\|$$
$$\to 0 \text{ by easy applications of DCT.}$$

Also $\|V^\alpha \hat\psi - V^\alpha f_n\| \leq \|(1-G_n) V^\alpha \hat\psi\|$
$+ \|G_n V^\alpha(\hat\psi - g_n)\| \to 0$

since

$$\|G_n V^\alpha(\hat\psi - g_n)\|^2 \leq \int dk\, e^{-\varepsilon_n^2 k^{2\alpha}} (2\pi)^{2|\alpha|} k^{2\alpha} \times |\hat\psi(k) - g_n(k)|^2$$

$$\leq (2\pi)^{2|\alpha|} \frac{1}{\varepsilon_n^2} \int dk\, |\hat\psi(k) - g_n(k)|^2 \leq (2\pi)^{2|\alpha|} \|\hat\psi - g_n\|$$

$\to 0.$

where we have applied the inequality
$xe^{-x} \le e^{-1} < 1 \;\; \forall x \ge 0$.

Thus $f_n \to \hat{\psi}$ and $V_\alpha f_n \to V_\alpha \hat{\psi}$ in norm, with $f_n \in S \;\; \forall n$. Let

$\varphi_n = \mathcal{F}_S^{-1} f_n \in S. \Rightarrow \varphi_n \to \psi$ in $L^2$ and

also $\partial^\alpha \varphi_n = \mathcal{F}_S^{-1}(V_\alpha f_n) \to \mathcal{F}_{L^2}^{-1}(M_{V_\alpha}\hat{\psi}) = \partial^\alpha \psi$.

$$\text{Thus } (\psi, \partial^\alpha \psi) \in \overline{G(\partial^\alpha|_S)} \overset{\text{Thrm 5.5.}}{=} G(\overline{\partial^\alpha|_S}) \quad \forall \psi \in D(\partial^\alpha)$$

Hence, $G(\partial^\alpha|_{L^2}) = G(\overline{\partial^\alpha|_S}) \Rightarrow \partial^\alpha|_{L^2} = \overline{\partial^\alpha|_S}$.

"d)" follows from

$$(\phi, \partial^\alpha \psi) = (\mathcal{F}\phi, \mathcal{F}\partial^\alpha \psi) = (\hat{\phi}, M_{V_\alpha}\hat{\psi})$$

$$= \int dk \; \hat{\phi}(k)^* (i2\pi k)^\alpha \hat{\psi}(k)$$
$$= (-1)^{|\alpha|} \int dk \; \left((i2\pi k)^\alpha \hat{\phi}(k)\right)^* \hat{\psi}(k)$$
$$= (-1)^{|\alpha|} (M_{V_\alpha}\hat{\phi}, \hat{\psi}) = (-1)^{|\alpha|}(\partial^\alpha \phi, \psi) \quad \square$$

5. Definition Let $F: \mathbb{R}^d \to \mathbb{C}$ be Lebesgue measurable. We define then

$$F(-i\partial) := \mathcal{F}_{L^2}^{-1} M_{V_F} \mathcal{F}_{L^2}$$

where $V_F(k) := F(2\pi k)$.

6. Properties
a) $F(-i\partial)$ is a closed, densely defined operator.
b) If $F$ is real, $F(-i\partial)$ is self-adjoint.
c) If $F$ is positive, $F(-i\partial)$ is positive.

Proof Exactly as in 4. above. $\square$

<u>Lemma:</u> Suppose $A$ is self-adjoint operator on $\mathcal{H}$. Then

$$\sigma(A) \subset [0,\infty) \iff (\psi, A\psi) \geq 0 \quad \forall \psi \in D(A).$$

<u>Proof:</u> "$\Rightarrow$" If $\sigma(A) \subset [0,\infty)$, by spectral decomposition of $A$,

$$(\psi, A\psi) = \int_{\sigma(A)} E_{\psi,\psi}(d\lambda)\, \lambda \geq 0$$

since $E_{\psi,\psi}$ is a positive measure and $\lambda \in \sigma(A) \Rightarrow \lambda \geq 0$.

"$\Leftarrow$" Assume $(\psi, A\psi) \geq 0$ $\forall \psi \in D(A)$, and consider some $\lambda_0 < 0$. Define $B := \mathcal{O}(f_{\lambda_0})$ where $f_{\lambda_0}(\lambda) := \lambda_0 - \lambda$ on $\sigma(A)$. $\overset{5.24.}{\Rightarrow}$ $B$ is self-adjoint, since $\sigma(A) \subset \mathbb{R}$, and $D(B) = D(A)$. If $\psi \in D(B)$, and $\phi \in \mathcal{H}$, we also have $(\phi, B\psi)$
$= \int_{\sigma(A)} E_{\phi,\psi}(d\lambda)\,(\lambda_0 - \lambda) = \lambda_0 (\phi, \psi) - (\phi, A\psi)$
$= (\phi, (\lambda_0 - A)\psi)$. Therefore, $B = \lambda_0 - A$.
It follows from the assumption that if $\psi \in D(A)$
$0 \leq (-\lambda_0)\|\psi\|^2 \leq -\lambda_0(\psi,\psi) + (\psi, A\psi)$
$= -(\psi, (\lambda_0 - A)\psi) = -(\psi, B\psi)$
$\Rightarrow |\lambda_0|\, \|\psi\|^2 \leq \|\psi\|\, \|B\psi\| \quad \forall \psi \in D(B)$
$\Rightarrow |\lambda_0|\, \|\psi\| \leq \|B\psi\| \quad \forall \psi \in D(B)$.
If $\psi \neq 0 \Rightarrow B\psi \neq 0$. Hence, $B$ is one-to-one.
$\Rightarrow \exists B^{-1} : R(B) \to D(B)$, and if $\phi \in R(B)$ then $B^{-1}\phi \in D(B)$ satisfies $\|B^{-1}\phi\| \leq \frac{1}{|\lambda_0|}\|\phi\|$.
$\Rightarrow B^{-1}$ bounded, and if we can show $R(B) = \mathcal{H}$, then $B^{-1} = (\lambda_0 - A)^{-1} \in \mathcal{B}(\mathcal{H}) \Rightarrow \lambda_0 \notin \sigma(A)$.
Assume first $\phi \perp R(B)$.
$\Rightarrow \forall \psi \in D(B) : (\phi, B\psi) = 0 = (0, \psi)$
$\Rightarrow \phi \in D(B^*)$ and $B^*\phi = 0$. As $B^* = B$,
$\Rightarrow \phi \in D(B)$ with $B\phi = 0 \Rightarrow \phi = 0$.
Therefore, $\overline{R(B)} \overset{Ex\,3.2}{=} (R(B)^\perp)^\perp = \{0\}^\perp = \mathcal{H}$.
Suppose then $\phi \in \overline{R(B)} \Rightarrow \exists \psi_n \in D(B)$ s.t. $\|\phi - B\psi_n\| \to 0$.
But then $\|\psi_n - \psi_m\| \leq \frac{1}{|\lambda_0|}\|B\psi_n - B\psi_m\| \xrightarrow{n,m\to\infty} 0 \Rightarrow (\psi_n)$ is Cauchy
$\Rightarrow \exists \psi := \lim_{n\to\infty} \psi_n \in \mathcal{H}$. But since $B$ is closed $\overset{5.3.}{\Rightarrow} \psi \in D(B)$, $B\psi = \phi$
$\Rightarrow \phi \in R(B)$. Therefore, $R(B) = \overline{R(B)} = \mathcal{H}$ and thus $\lambda_0 < 0 \Rightarrow \lambda_0 \notin \sigma(A) \subset \mathbb{R}$. $\square$

## 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 $U_t = \mathcal{F}^{-1} M_{V_{F_t}} \mathcal{F}$ with

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

Exercise 5.5. $\Rightarrow$ $(V_{F_t})$ is a strongly continuous unitary group, with generator $M_V$,
$V(k) = \frac{(2\pi k)^2}{2}$. 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. <u>Proposition</u> a) If $\psi(t_0) \in S$ for some $t_0$, then $\psi(t) \in S$ $\forall t$, and $\forall t \neq 0$

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

where $K$ is called <u>the free propagator</u>

and is given by

$$K(x,y;t) = \frac{1}{(i2\pi t)^{d/2}}\, e^{i\frac{1}{2t}(x-y)^2}$$

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

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

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. $x \in \mathbb{R}^d$

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

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

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

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

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