5. Unbounded operators

(See also Hall, chapter 9)

Defn 5.1. Graph of an operator.

The graph of any function $f: X \to Y$ is the subset $\{(x, f(x))\} \subset X \times Y$.
The graph of an operator $A: D \to \mathcal{H}$ is thus

$$\{((\psi, A\psi))\} \subset D \times \mathcal{H} \subset \mathcal{H} \times \mathcal{H}.$$

Note the unfortunate need for new notation; otherwise indistinguishable from a scalar product. A better choice, used sometimes in math. phys., is to use "$\langle \cdot, \cdot \rangle$" for scalar product.

Reminder: (2.13) * $\mathcal{H}_1 \times \mathcal{H}_2$ can be made into a Hilbert space by endowing it with a scalar product:

$$\left(((\psi_1, \psi_2)), ((\phi_1, \phi_2)) \right) := (\psi_1, \phi_1) + (\psi_2, \phi_2)$$

Proof: easy computation, since

$$\|((\psi_1, \psi_2))\|^2 = \|\psi_1\|^2 + \|\psi_2\|^2 \quad \square$$

The resulting Hilbert space is denoted by $\mathcal{H}_1 \oplus \mathcal{H}_2$ (= external direct sum) which is true also in the previous sense of $\oplus$ (= internal direct sum, defn. 2.8.) after we identify

$$\mathcal{H}_1 \cong \{((\psi, 0)) \mid \psi \in \mathcal{H}_1\}$$
$$\mathcal{H}_2 \cong \{((0, \psi)) \mid \psi \in \mathcal{H}_2\}.$$

* For an operator A, its graph is def. as

$$\mathcal{G}(A) := \{((\psi, A\psi)) \mid \psi \in D(A)\} \subset \mathcal{H} \oplus \mathcal{H}.$$

Defn. 5.2. An operator A on $\mathcal{H}$ is closed, if its graph is closed, i.e.,

$$\mathcal{G}(A) = \overline{\mathcal{G}(A)}.$$

topology of $\mathcal{H} \oplus \mathcal{H}$

Observation 5.3. An operator A is closed if and only if (cc) holds:

(cc) For any sequence $\psi_n \in D(A)$, for which there are $\psi, \phi \in \mathcal{H}$ s.t. $\psi_n \to \psi$, and $A\psi_n \to \phi$ in norm, we have $\underbrace{}_{\psi \in D(A) \text{ and}}$ $\phi = A\psi$.

Proof. Assume A closed. Let (ψ_n) be a sequence as in (cc). Then

$$\|((\psi, \phi)) - ((\psi_n, A\psi_n))\|^2 = \|\psi - \psi_n\|^2 + \|\phi - A\psi_n\|^2 \xrightarrow{n\to\infty} 0,$$

and thus $((\psi, \phi)) \in \overline{G(A)} = G(A) \Rightarrow \phi = A\psi., \psi \in D(A)$.
Therefore, (cc) holds.

For the converse, assume (cc) holds.
Let $((\psi, \phi)) \in \overline{G(A)} \Rightarrow \exists$ seq. $((\psi_n, \phi_n)) \in G(A)$ s.t. $\|((\psi, \phi)) - ((\psi_n, \phi_n))\| \to 0$.
But since then $\phi_n = A\psi_n$ and $\|\psi - \psi_n\| \to 0$, $\|\phi - \phi_n\| \to 0$, (cc) implies that $\phi = A\psi.$, $\psi \in D(A)$.
$\Rightarrow ((\psi, \phi)) = ((\psi, A\psi)) \in G(A)$. Thus $G(A) = \overline{G(A)}$ and A is closed. $\square$

* Clearly, $A \subset B \Leftrightarrow G(A) \subset G(B)$, and $A = B \Leftrightarrow G(A) = G(B)$.
* Every $T \in \mathcal{B}(\mathcal{H})$ satisfies (cc), and is thus closed.

Defn. 5.4. An operator A is closable if it has a closed extension.

Thm. 5.5. If A is closable, then it has a unique smallest closed extension $\overline{A}$. In addition, $G(\overline{A}) = \overline{G(A)}$.

Proof. Let B be a closed extension of A.
$\Rightarrow D(A) \subset D(B)$ and $\forall \psi \in D(A): B\psi = A\psi$.
Thus $G(A) \subset G(B) \Rightarrow \overline{G(A)} \subset \overline{G(B)} = G(B)$
Let

$$D' := \{\psi \in \mathcal{H} \mid \exists \phi \in \mathcal{H} \text{ s.t. } ((\psi, \phi)) \in \overline{G(A)}\}$$
$$(= P_1 \overline{G(A)})$$

For any $\alpha_i \in \mathbb{C}$, $((\psi_i, \phi_i)) \in G(A)$, we have $\psi_i \in D(A)$ and $\phi_i = A\psi_i$

$\Rightarrow \alpha_1((\psi_1, \phi_1)) + \alpha_2((\psi_2, \phi_2))$

$= ((\alpha_1\psi_1 + \alpha_2\psi_2, \alpha_1\phi_1 + \alpha_2\phi_2))$

$= ((\underbrace{\alpha_1\psi_1 + \alpha_2\psi_2}_{\in D(A)}, A(\alpha_1\psi_1 + \alpha_2\psi_2))) \in \mathcal{G}(A)$.

Therefore, $\mathcal{G}(A)$ is a subspace $\Rightarrow \overline{\mathcal{G}(A)}$ is a subspace

$\Rightarrow D' = P_1\overline{\mathcal{G}(A)}$ is a subspace. (& independent of B)

In addition, if $((\psi, \phi)) \in \overline{\mathcal{G}(A)} (\subset \mathcal{G}(B))$ then $\psi \in D(B)$ and $\phi = B\psi$.
Thus $D' \subset D(B)$ and $\{((\psi, B\psi)) \mid \psi \in D'\} = \overline{\mathcal{G}(A)}$.

We define $A'_B = B|_{D'}$. By the above results, A'_B is an operator for which $\mathcal{G}(A'_B) = \overline{\mathcal{G}(A)}$.
In addition, $\psi \in D(A) \Rightarrow ((\psi, A\psi)) \in \mathcal{G}(A) \subset \overline{\mathcal{G}(A)}$
$\Rightarrow \psi \in D'$ and $A'_B\psi = B\psi = A\psi$. Thus A'_B is a closed extension of A, and $A \subset A'_B \subset B$.
Let B' be some other closed extension on A.
Then we can construct $A'_{B'}$ for which $\mathcal{G}(A'_{B'}) = \overline{\mathcal{G}(A)} = \mathcal{G}(A'_B)$.
Thus $A'_{B'} = A'_B$ and $A \subset A'_{B'} \subset B'$. Therefore, we can choose any B, and define $\bar{A} = A'_B$. Then for any $B' \supset A$, closed, we have $A \subset \bar{A} \subset B'$, and $\bar{A}$ is closed. Thus $\bar{A}$ is a mimimal closed extension of A, and it is obviously unique.
By construction, $\mathcal{G}(\bar{A}) = \overline{\mathcal{G}(A)}$. □

Remarks

* $\bar{A}$ is called the closure of A.

* Bounded operators are closable.

* However, there are unbounded operators, which are not closable; it can even happen that $\overline{\mathcal{G}(A)} = \mathcal{H} \oplus \mathcal{H}$.

* If A is a closed operator, a subspace $C \subset D(A)$ is called a core for A if the restriction R of A to C satisfies $\bar{R} = A$; in short, if $\overline{A|_C} = A$.

5.6. Defn. Let A be a densely defined operator. Define

$$D^* := \{ \phi \in \mathcal{H} \mid \psi \mapsto (\phi, A\psi) \text{ is continuous } D(A) \to \mathbb{C} \}$$
$$= \{ \phi \in \mathcal{H} \mid \sup_{\substack{\psi \in D(A);\\ \|\psi\| = 1}} |(\phi, A\psi)| < \infty \}$$

Suppose $\phi \in D^*$. Since $D(A)$ is a subsp., the map $\psi \mapsto (\phi, A\psi)$ has a continuous (bounded) extension $\Lambda : \mathcal{H} \to \mathbb{C}$, and Λ is linear and bounded. (Hahn-Banach Thm. (Rudin, Funct. Anal., 3.6.) or as in Exercise 2.4.). Thus by 3.1.a)
$\exists! \psi_0 \in \mathcal{H}$ s.t. $\Lambda\psi = (\psi_0, \psi)$.
Thus ψ_0 is such that

$$(*) \qquad (\psi_0, \psi) = (\phi, A\psi) \quad \forall \psi \in D(A).$$

Since $D(A)$ is dense, ψ_0 is the only vector in $\mathcal{H}$ which satisfies $(*)$.
Therefore, we can define $A^* : D^* \to \mathcal{H}$ by $A^* : \phi \mapsto \psi_0$, s.t. ψ_0 solves $(*)$.

Proposition: A^* is an operator.

Proof. $\alpha_1, \alpha_2 \in \mathbb{C}$ and $\phi_1, \phi_2 \in D^* \Rightarrow$
if $\psi \in D(A)$, then $|(\alpha_1\phi_1 + \alpha_2\phi_2, A\psi)|$
$\leq |\alpha_1| |(\phi_1, A\psi)| + |\alpha_2| |(\phi_2, A\psi)|$
$\Rightarrow \alpha_1\phi_1 + \alpha_2\phi_2 \in D^*$. $\therefore$ D^* subspace.
Also $(\alpha_1 A^*\phi_1 + \alpha_2 A^*\phi_2, \psi)$
$= \alpha_1^* (A^*\phi_1, \psi) + \alpha_2^* (A^*\phi_2, \psi)$
$= \alpha_1^* (\phi_1, A\psi) + \alpha_2^* (\phi_2, A\psi)$
$= (\alpha_1\phi_1 + \alpha_2\phi_2, A\psi) \quad \forall \psi \in D(A).$
$\Rightarrow$ (by uniq. of ψ_0) $A^*(\alpha_1\phi_1 + \alpha_2\phi_2)$
$= \alpha_1 A^*\phi_1 + \alpha_2 A^*\phi_2$.
$\therefore$ A^* is linear. $\square$

<u>Summary</u>: The <u>adjoint</u> A^* of a <u>densely defined</u> operator A is defined by:

$$D(A^*) := \{ \phi \in \mathcal{H} \mid \sup_{\substack{\psi \in D(A), \\ \|\psi\| = 1}} |(\phi, A\psi)| < \infty \}$$

and for $\phi \in D(A^*)$, $A^*\phi$ is the unique solution to the equation

$$(A) \qquad (A^*\phi, \psi) = (\phi, A\psi) \quad \forall \psi \in D(A).$$

<u>Remarks</u>: * If A is not densely defined, the solution to (A) is not unique: one can always add any vector in $D(A)^\perp$ to $A^*\phi$.

* If $A \in \mathcal{B}(\mathcal{H})$, let A_1^* denote its adjoint as defined in 3.2 and A_2^* the adjoint as def. above. Since $|(\phi, A\psi)| \leq \|\phi\| \, \|A\|$ for $\|\psi\| = 1$ it follows that $D(A_2^*) = \mathcal{H} = D(A_1^*)$. Also, if $\psi, \phi \in \mathcal{H}$, then $\phi \in D(A_2^*)$, $\psi \in D(A)$ and thus by (A) and 3.2.
$$(A_2^*\phi, \psi) = (\phi, A\psi) = (A\psi, \phi)^* = (\psi, A_1^*\phi)^* = (A_1^*\phi, \psi) \quad \forall \phi, \psi \in \mathcal{H}.$$
$\Rightarrow A_1^*\phi = A_2^*\phi \;\; \forall \phi \;\; \Rightarrow A_1^* = A_2^*$.
That is, the definitions of adjoint agree for $A \in \mathcal{B}(\mathcal{H})$.

* We assumed $D(A)$ is dense to define A^*. However, $D(A^*)$ need <u>not</u> be dense. It can even happen that $D(A^*) = \{0\}$.

* If $D(A)$ and $D(A^*)$ are both dense, we denote $A^{**} = (A^*)^*$.

5.7. Relations between closure and adjoint

Theorem Let A be a densely defined operator. Then all of the following are true:

a) A^* is closed.
b) A is closable $\Leftrightarrow$ $D(A^*)$ is dense.
c) If A is closable, then $\bar{A} = A^{**}$ and $(\bar{A})^* = A^*$.

Proof. Consider the map $V: \mathcal{H} \oplus \mathcal{H} \to \mathcal{H} \oplus \mathcal{H}$ defined by $V((\psi, \phi)) := ((-\phi, \psi))$.
Obviously V is linear, and a bijection. Also $\| V((\psi, \phi)) \|^2 = \| -\phi \|^2 + \| \psi \|^2 = \| ((\psi, \phi)) \|^2$ and thus (Exercise 3.4) V is unitary. Since clearly $V^2 = -1$, we thus have $V^* = V^{-1} = -V$. Now, if $E \subset \mathcal{H} \oplus \mathcal{H}$ is a subset, also $V(E^\perp) = (V(E))^\perp$.

(Proof: V is unitary, thus $x \in V(E)^\perp$
$\Leftrightarrow \forall y \in V(E): (x, y) = 0$
$\Leftrightarrow \forall x' \in E: (x, Vx') = 0$
$\overset{V^* \text{unit.}}{\Leftrightarrow} \forall x' \in E: (\underbrace{V^* x}_{= V^{-1} x}, \underbrace{V^* V x'}_{= x'}) = 0 \Leftrightarrow V^{-1} x \in E^\perp$
$\Leftrightarrow x \in V(E^\perp)$ $\blacksquare$)

On the other hand, $((\psi, \phi)) \in V(\mathcal{G}(A))^\perp$
$\Leftrightarrow \forall ((\psi', \phi')) \in \mathcal{G}(A): (V((\psi', \phi')), ((\psi, \phi))) = 0$
$\Leftrightarrow \forall \psi' \in D(A): (((-A\psi', \psi')), ((\psi, \phi))) = 0$
$\Leftrightarrow \forall \psi' \in D(A): -(A\psi', \psi) + (\psi', \phi) = 0$
$\Leftrightarrow \forall \psi' \in D(A): (\phi, \psi') = (\psi, A\psi')$.
$\Leftrightarrow \psi \in D(A^*), \phi = A^* \psi \Leftrightarrow ((\psi, \phi)) \in \mathcal{G}(A^*)$

Therefore, $\mathcal{G}(A^*) = V(\mathcal{G}(A))^\perp$ = closed subset.
$\Rightarrow A^*$ is a closed operator. $\Rightarrow$ a).

To prove b), note that $\mathcal{G}(A)$ is a subspace of $\mathcal{H} \oplus \mathcal{H}$ (see p. 44), and thus (Exercise 3.2.)

$$\overline{\mathcal{G}(A)} = (\mathcal{G}(A)^\perp)^\perp = (V^*[V(\mathcal{G}(A)^\perp)])^\perp = (V^*[(V\mathcal{G}(A))^\perp])^\perp$$
$$= (V^*[\mathcal{G}(A^*)])^\perp = ((-V)[\mathcal{G}(A^*)])^\perp = (V\mathcal{G}(A^*))^\perp.$$

Thus if $D(A^*)$ is dense, we have $\mathcal{G}(A^{**}) = V(\mathcal{G}(A^*))^\perp = \overline{\mathcal{G}(A)}$ $\Rightarrow$ A^{**} is a closed

$\longrightarrow$

extension of A $\Rightarrow$ A is closable
and $\mathcal{G}(\bar{A}) = \overline{\mathcal{G}(A)} = \mathcal{G}(A^{**}) \Rightarrow \bar{A} = A^{**}$.

Conversely, if $D(A^*)$ is not dense $\Rightarrow \exists\, \psi_0 \in D(A^*)^\perp$ with $\psi_0 \neq 0$. $\Rightarrow$ for any $((\psi, \phi)) \in \mathcal{G}(A^*)$, we have

$$(((\psi,\phi)), ((\psi_0, 0))) = (\psi, \psi_0) = 0$$

$$\Rightarrow ((\psi_0, 0)) \in \mathcal{G}(A^*)^\perp$$

$$\Rightarrow ((0, \psi_0)) = V((\psi_0, 0)) \in V(\mathcal{G}(A^*)^\perp) = (V\mathcal{G}(A^*))^\perp = \overline{\mathcal{G}(A)}.$$

If A is closable, $\mathcal{G}(\bar{A}) = \overline{\mathcal{G}(A)}$ and $((0,\psi_0)) \in \mathcal{G}(\bar{A})$ implies $\psi_0 = \bar{A}(0) = 0$, which would be a contradiction.

Thus A is not closable. $\therefore$ b) holds.

For c), assume A is closable. We proved above that $\bar{A} = A^{**}$. Since A^* is closed,

also $A^* = \overline{A^*} = (A^*)^{**} = ((A^*)^*)^* = (A^{**})^* = \bar{A}^*$. $\square$

5.8. Definition: An operator A is <u>symmetric</u> if

$$(\phi, A\psi) = (A\phi, \psi) \quad \forall \phi, \psi \in D(A).$$

5.9. Definition: An operator A is <u>self-adjoint</u> if it is densely defined and $A^* = A$.

5.10. Thm: Let S, T be densely defined operators.
(Proof: Exercises 4.2. & 5.1.)
Then a) $S \subset T \Rightarrow T^* \subset S^*$
b) S symmetric $\Leftrightarrow S \subset S^*$
c) S symmetric $\Rightarrow$ S closable, and $\bar{S}$ symmetric.

5.11. Defn. A densely defined operator S is called <u>essentially self-adjoint</u>, if S is symmetric and $\bar{S}$ is self-adjoint.

5.12. Remark: 5.8. looks like the most natural generalization of the concept of self-adjointness from bounded operators to densely defined ones. In theorem 5.14. (Stone's theorem) we will find out why the definition in 5.6. is the one relevant to Q.M.

* Examples (some of the proofs later in exercises, see also Hall's book):

Consider $\mathcal{H} := L^2([0,1])$ and

$$D := \{\psi \in \mathcal{H} \mid \psi \text{ is differentiable at every point, and } \psi' : [0,1] \to \mathbb{C} \text{ is continuous}\}$$

If $\psi \in D$, obviously $\psi' \in \mathcal{H}$. Define operators A_0, A_1, A_2 by the formula

$$A_\ell \psi := -i\psi' \quad , \quad \ell = 0, 1, 2$$

using the following subsets of D as domains

$$D(A_0) := \{\psi \in D \mid \psi(0) = 0 = \psi(1)\}$$

$$D(A_1) := \{\psi \in D \mid \psi(0) = \psi(1)\}$$

$$D(A_2) := D.$$

Clearly, $A_0 \subset A_1 \subset A_2 \overset{5.10.}{\Rightarrow} A_2^* \subset A_1^* \subset A_0^*$, since each of the domains is dense in $\mathcal{H}$.
It turns out that

a) A_0 is symmetric but $\bar{\bar{A}}_0$ is not self-adjoint. (Hall, Proposition 9.27; see c) below)
b) A_1 is symmetric and $\bar{A}_1$ is self-adjoint (Hall, end of Section 9.6.)
c) $A_2 \subset A_0^*$ (Hall, Lemma 9.28)
$\overset{5.5.}{\Rightarrow} \bar{A}_0 \subset \bar{A}_2 \subset A_0^*$. Since $\bar{A}_0 \neq \bar{A}_2$ (Hall, p. 184), $\bar{A}_0 \neq A_0^*$.

* However, the operator A' analogous to A_0 on $L^2(\mathbb{R})$,

$$D(A') := C_c^\infty(\mathbb{R}) \quad \text{and} \quad A'\psi := -i\psi' \quad (\in C_c^\infty(\mathbb{R}) \subset L^2(\mathbb{R})),$$

is essentially self-adjoint on $L^2(\mathbb{R})$. (Hall, Prop. 9.29)

For theorem 9.6., we need the following Lemma:

9.8. Lemma Suppose T is a densely defined closed operator on $\mathcal{H}$.
Then for any $\phi, \phi' \in \mathcal{H}$ there are unique $\psi \in D(T)$, $\psi' \in D(T^*)$ s.t.

$$(*) \begin{cases} -T\psi + \psi' = \phi \\ \psi + T^*\psi' = \phi' \end{cases}$$

Proof: Consider the proof of Theorem 5.7. There we defined the map $V((\psi, \phi)) = ((-\phi, \psi))$, which was unitary on $\mathcal{H} \oplus \mathcal{H}$, and showed that $G(T^*) = V(G(T))^\perp$.
Also since now $G(T)$ is closed, also $V(G(T))$ is a closed subspace, and thus by Ex. 3.2. $\Rightarrow V(G(T)) = [V(G(T))^\perp]^\perp = G(T^*)^\perp$
Since $G(T^*)$ is also a closed subspace, this implies (Theorem 2.11.) that

$$\mathcal{H} \oplus \mathcal{H} = G(T^*) \oplus G(T^*)^\perp = G(T^*) \oplus V(G(T)).$$

Thus for any $((\phi, \phi')) \in \mathcal{H} \oplus \mathcal{H}$ there are unique $a \in G(T^*)$, $b \in V(G(T))$ s.t. $((\phi, \phi')) = a + b$.
$\Rightarrow \exists \psi \in D(T)$ and $\psi' \in D(T^*)$ s.t.
$a = ((\psi', T^*\psi'))$, $b = ((-T\psi, \psi))$.
$\Rightarrow (*)$ holds. To see uniqueness, assume also $\tilde\psi$, and $\tilde\psi'$ satisfy $(*)$, and def.
$\tilde a = ((\tilde\psi', T^*\tilde\psi'))$, $\tilde b = ((-T\tilde\psi, \tilde\psi)) = V((\tilde\psi, T\tilde\psi))$
Then $\tilde a \in G(T^*)$, $\tilde b \in V(G(T))$ and
$\tilde a + \tilde b = ((\phi, \phi'))$. $\Rightarrow \tilde a = a$, $\tilde b = b$ □

9.9. Corollary Suppose T is densely defined and closed operator. Then

$$R(1 + T^*T) = \mathcal{H}.$$

Proof: Suppose $\phi' \in \mathcal{H}$ is given, and apply the lemma with $\phi = 0$, $\Rightarrow \exists \psi \in D(T)$, $\psi' \in D(T^*)$ s.t. $\psi' = T\psi$ and
$\phi' = \psi + T^*\psi' = \psi + T^*T\psi$
$\Rightarrow \psi \in D(1 + T^*T)$ and $\phi' = (1 + T^*T)\psi$ □

The following result is also a corollary of the earlier result $\mathcal{G}(T^*) = [V\mathcal{G}(T)]^\perp$ proven in Thrm 5.7.

It has also an easy direct proof, see Proposition 9.12. in Hall's book. (Note: in Hall's book "unbounded operator" means a densely defined operator, cf. Def. 3.1. of the book.)

<u>Proposition</u>: If T is a <u>densely defined</u> operator, then

$$\mathrm{Ker}(T^*) = R(T)^\perp .$$

<u>Proof</u>. Since $\mathcal{G}(T^*) = [V\mathcal{G}(T)]^\perp$, this follows by checking that the following equalities hold:

$$\psi \in R(T)^\perp \overset{(*)}{\Leftrightarrow} (\psi, 0) \in [V\mathcal{G}(T)]^\perp = \mathcal{G}(T^*)$$
$$\Leftrightarrow \psi \in D(T^*) \text{ and } T^*\psi = 0 \Leftrightarrow \psi \in \mathrm{Ker}(T^*).$$

Of these, only the first one "(*)" does not follow immediately from the definitions.
To see (*), note that $(\phi_1, \phi_2) \in V\mathcal{G}(T)$
$\overset{V^{-1}=-V}{\Leftrightarrow} -V(\phi_1, \phi_2) = (\phi_2, -\phi_1) \in \mathcal{G}(T)$
$\Leftrightarrow \phi_2 \in D(T)$ and $-\phi_1 = T\phi_2$
$\Leftrightarrow \exists \phi \in D(T)$ s.t. $\phi_1 = T\phi$, $\phi_2 = -\phi \Rightarrow \phi_1 \in R(T)$.
Since always

$$\langle (\phi_1, \phi_2) \,|\, (\psi, 0) \rangle_{\mathcal{H}\oplus\mathcal{H}} = \langle \phi_1 | \psi \rangle_{\mathcal{H}},$$

Clearly $\psi \in R(T)^\perp \Rightarrow (\psi, 0) \in [V\mathcal{G}(T)]^\perp$.
Also, if $\phi_1 \in R(T) \Rightarrow \exists \phi \in D(T)$ s.t. $\phi_1 = T\phi$
$\Rightarrow (\phi_1, -\phi) \in V\mathcal{G}(T)$. Hence, $(\psi, 0) \in [V\mathcal{G}(T)]^\perp$
$\Rightarrow \langle \phi_1 | \psi \rangle = 0 \quad \forall \phi_1 \in R(T)$
$\Rightarrow \psi \in R(T)^\perp$. $\square$

5.13. Suppose the map $Q: I \to \mathcal{B}(\mathcal{H})$, $I \subset \mathbb{R}$ interval, is strongly continuous. $Q(t)$ is said to be strongly differentiable at t_0 for $\psi_0 \in \mathcal{H}$, if the following norm-lim. exists

$$\exists \lim_{\substack{t \to t_0 \\ t \in I}} \frac{1}{t-t_0}\left(Q(t)\psi_0 - Q(t_0)\psi_0\right) =: \frac{d}{dt} Q(t)\psi_0 \Big|_{t=t_0}$$

Defn. Suppose $(U(t))_{t \geq 0}$ is a strongly continuous unitary semi-group. Its infinitesimal generator is a map $A : D(A) \to \mathcal{H}$ defined using

$$D(A) := \{ \psi \in \mathcal{H} \mid U(t) \text{ is strongly differentiable at } t=0 \text{ for } \psi \}$$

and for any $\psi \in D(A)$

$$A\psi := \lim_{\varepsilon \to 0^+} \frac{i}{\varepsilon}\left(U(\varepsilon)\psi - \psi\right) = i \frac{d}{dt} U(t)\psi \Big|_{t=0}$$

5.14. Theorem (Stone)

Suppose $(U(t))_{t \geq 0}$ is a strongly continuous unitary semigroup, and let A denote its infinitesimal generator, defined as above. Then A is a densely defined self-adjoint operator on $\mathcal{H}$ and $\forall t \geq 0$:

(Exp) $\quad U(t) = e^{-itA}$ (defined via spectral decomposition of A)

Denote $\psi(t) := U(t)\psi$ for $\psi \in \mathcal{H}$, $t \geq 0$. Then
- a) $t \mapsto \psi(t)$ is norm-continuous.
- b) If $\psi(0) \in D(A)$, then $\psi(t) \in D(A)$ $\forall t \geq 0$ and

$$i \frac{d}{dt} \psi(t) = A\psi(t) = U(t) A\psi(0).$$

c) $\forall \psi(0) \in \mathcal{H}: \quad \psi(t) = \lim_{\varepsilon \to 0^+} \exp\left(-it \frac{i}{\varepsilon}(U(\varepsilon)-1)\right)\psi(0).$

Conversely, if A is self-adjoint, and $U(t) = e^{-itA}$, then $(U(t))_{t\geq 0}$ is a strongly continuous semigroup and A is its infinitesimal generator.

<u>Proof</u>: Functional calculus with spectral representations. (See the Appendix on page 55.) For complete proofs, see Rudin, Funct. Anal., Th. 13.35 and Th. 13.37 or Reed & Simon I, chapter VIII.4. or Teschl, chapter 3. or Hall, chapter 10. □

<u>Remarks</u>: * The spectrum of a self-adjoint operator A, is a set $\sigma(A) \subset \mathbb{R}$. The spectral representation assigns to every Borel subset $\omega \subset \sigma(A)$ an orthogonal projection P_ω. so that for any $\phi, \psi \in \mathcal{H}$ the map $\mu_{\phi,\psi}: \omega \mapsto (\phi, P_\omega \psi)$ is a Borel measure, and $\forall \phi \in \mathcal{H}$, $\psi \in D(A)$

$$(\phi, A\psi) = \int_{\sigma(A)} \lambda \, \mu_{\phi,\psi}(d\lambda)$$

$$=: \int_{\sigma(A)} \lambda \, d(\phi, P_\lambda \psi)$$

The definition in (Exp) means

$\forall t \in \mathbb{R}, \phi, \psi \in \mathcal{H}:$

$$(\phi, e^{-itA}\psi) := \int_{\sigma(A)} e^{-it\lambda} \, d(\phi, P_\lambda \psi)$$

and the basic results of functional calculus show that then $D(e^{-itA}) = \mathcal{H}$ and e^{-itA} is unitary operator.

* If $\mathcal{H} = \mathbb{C}^N$, A is a self-adjoint matrix, with eigenvalues $\lambda_n \in \mathbb{R}$ and (orthonormal) collection of eigenvectors $e_n \in \mathbb{C}^N$ ...

$\longrightarrow$

... and the spectral definition means

$$(\phi, e^{-itA}\psi) := \sum_{n=1}^{N} e^{-it\lambda_n} (\phi, e_n)(e_n, \psi).$$

* If A is a bounded operator,

$$e^{-itA} = \sum_{n=0}^{\infty} \frac{1}{n!} (-itA)^n, \qquad (*)$$

but for unbounded operators, using the sum is usually not a good idea. For instance, if A is self-adj, usually $D(A^2) \subset D(A)$ is a <u>proper</u> subset, and the sum in $(*)$ makes sense only for so called <u>analytic vectors</u>; for ψ s.t.

$$\psi \in C^\infty(A) := \bigcap_{n=1}^{\infty} D(A^n) \quad \text{and}$$

$$\sum_{n=0}^{\infty} \frac{1}{n!} \|A^n \psi\| \, t^n < \infty \quad \text{for some } t > 0.$$

* It is possible, that S is essentially self-adjoint, i.e., S is symmetric and $\bar{S}$ is self-adjoint, but although $C^\infty(\bar{S})$ is dense, $C^\infty(S)$ is empty.

* However, by c), e^{-itA} is a strong limit of

$$\sum_{n=0}^{\infty} \frac{1}{n!} (-itA_\varepsilon)^n \qquad \text{where } A_\varepsilon = \frac{i}{\varepsilon}(U(\varepsilon) - I) \text{ is a bounded operator.}$$

<u>5.15 Remark</u>: Stone's theorem shows that the best we can do to understand the original Schrödinger equation $i\frac{d}{dt}\psi(t) = S\psi(t)$ on page 3 is to find a dense subspace of $\mathcal{H}$ for which the right hand side makes sense, and then look for self-adjoint extensions of S. As we will see later, even if S is symmetric, any of the following can happen:

1) $\bar{S}$ is the unique self-adjoint extension (S.A.E.)
2) There are (infinitely) many S.A.E.
3) There are no S.A.E.

* If 1) happens, we should just be happy.
* 2) means that we forgot to "put in all the physics" in the Schrödinger equation. Typical examples are boundary conditions.
* 3) means that the (physical) system is not closed, and we are either forced to "leak" or "inject probability". (roughly speaking)

5.16. Examples : Three standard ways of defining operators on $\mathcal{H} = L^2(\Omega)$ when $\Omega \subset \mathbb{R}^d$, open subset: multiplication, integral, and differential operators.

1) Multiplication operators (potentials)

Let $V: \Omega \to \mathbb{C}$ be Lebesgue measable. The corresponding multiplication operator M_V (also denoted $\hat{V}$ or simply V) is a mapping $D(M_V) \to \mathcal{H}$ defined by

$$(M_V \psi)(x) = V(x)\psi(x), \quad x \in \Omega$$

on

$$D(M_V) := \{\psi \in \mathcal{H} \mid V\psi \in L^2(\Omega)\}.$$

M_V has the following properties: (Ex. 5.2.)

a) M_V is a closed, densely defined operator.

b) $(M_V)^* = M_{V^*}$

c) M_V self-adjoint $\Leftrightarrow$ $V(x) \in \mathbb{R}$ a.e. $x \in \Omega$.

* Thus every $V: \Omega \to \mathbb{R}$, which is Lebesgue measurable, generates a strongly cont. USG. With $U_t = e^{-itM_V} = M_{(e^{-itV})}$.