5. Unbounded operators

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

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

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.,

$$\mathcal{G}(A) = \overline{\mathcal{G}(A)} \quad \leftarrow \text{topology of } \mathcal{H} \oplus \mathcal{H}.$$

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 $\underbrace{\phi = A\psi}_{\psi \in D(A) \text{ and}}$.

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 $((\psi, \phi)) \in \overline{\mathcal{G}(A)} = \mathcal{G}(A) \Rightarrow \phi = A\psi., \psi \in D(A)$

Therefore, (cc) holds.

For the converse, assume (cc) holds.

Let $((\psi, \phi)) \in \overline{\mathcal{G}(A)} \Rightarrow \exists$ seq. $((\psi_n, \phi_n)) \in \mathcal{G}(A)$ 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 $\phi = A\psi., \psi \in D(A)$.

$\Rightarrow ((\psi, \phi)) = ((\psi, A\psi)) \in \mathcal{G}(A)$. Thus $\mathcal{G}(A) = \overline{\mathcal{G}(A)}$ and A is closed. $\square$

* Clearly, $A \subset B \Leftrightarrow \mathcal{G}(A) \subset \mathcal{G}(B)$, and $A = B \Leftrightarrow \mathcal{G}(A) = \mathcal{G}(B)$.
* 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 $\bar{A}$. In addition, $\mathcal{G}(\bar{A}) = \overline{\mathcal{G}(A)}$.

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 $\mathcal{G}(A) \subset \mathcal{G}(B) \Rightarrow \overline{\mathcal{G}(A)} \subset \overline{\mathcal{G}(B)} = \mathcal{G}(B)$

Let

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

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

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

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

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

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

$\Rightarrow \quad D' = P_1 \overline{\mathcal{G}(A)}$ 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 minimal closed extension of A, and it is obviously unique.
By construction, $\mathcal{G}(\bar{A}) = \overline{\mathcal{G}(A)}$. $\square$

<u>Remarks</u>

* $\bar{A}$ is called the <u>closure</u> 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 <u>subspace $C \subset D(A)$</u> is called <u>a core</u> 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 <u>equation</u>

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

<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.
$$(A_2^* \phi, \psi) = (\phi, A\psi) = (A\psi, \phi)^*$$
$$= (\psi, A_1^* \phi)^* = (A_1^* \phi, \psi) \quad \forall \phi, \psi \in \mathcal{H}.$$
$$\Rightarrow A_1^* \phi = A_2^* \phi \quad \forall \phi \quad \Rightarrow A_1^* = A_2^*.$$
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

<u>Theorem</u> 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 $(\bar{A})^* = A^*$.

<u>Proof.</u> 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 $x \in V(E)^\perp$

$\Leftrightarrow \forall y \in V(E): (x,y) = 0$

$\Leftrightarrow \forall x' \in E: (x, Vx') = 0$

$\underset{V^* \text{unit.}}{\Leftrightarrow} \forall x' \in E: (\underbrace{V^*x}_{=V^{-1}x}, \underbrace{V^*Vx'}_{=x'}) = 0 \Leftrightarrow V^{-1}x \in E^\perp$

$\Leftrightarrow x \in V(E^\perp)$ ☑)

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

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

5.10. Thm: Let S, T be densely defined operators. 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.

(Proof: Exercises 4.2. & 5.1.)

5.11. Defn. A densely defined operator S is called essentially self-adjoint, 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. The following theorem, however, shows that the one in 5.6. is more relevant: