Chapter 2

Unbounded operators

In this chapter we define the notions of unbounded operators, their adjoint, their resolvent and their spectrum. Perturbation theory will also be considered. As in the previous chapter, $\mathcal{H}$ denotes an arbitrary Hilbert space.

2.1 Unbounded, closed, and self-adjoint operators

In this section, we define an extension of the notion of bounded linear operators. Obviously, the following definitions and results are also valid for bounded linear operators.

Definition 2.1.1. *A* linear operator on $\mathcal{H}$ *is a pair* $\big(A, \mathsf{D}(A)\big)$*, where* $\mathsf{D}(A)$ *is a linear manifold of* $\mathcal{H}$ *and* A *is a linear map from* $\mathsf{D}(A)$ *to* $\mathcal{H}$*.* $\mathsf{D}(A)$ *is called* the domain of A*. One says that the operator* $\big(A, \mathsf{D}(A)\big)$ *is* densely defined *if* $\mathsf{D}(A)$ *is dense in* $\mathcal{H}$*.*

Note that one often just says *the linear operator* A, but that its domain $\mathsf{D}(A)$ is implicitly taken into account. For such an operator, its range $\mathsf{Ran}(A)$ is defined by

$$\mathsf{Ran}(A) := A\,\mathsf{D}(A) = \{f \in \mathcal{H} \mid f = Ag \text{ for some } g \in \mathsf{D}(A)\}.$$

In addition, one defines the kernel $\mathsf{Ker}(A)$ of A by

$$\mathsf{Ker}(A) := \{f \in \mathsf{D}(A) \mid Af = 0\}.$$

Let us also stress that the sum $A + B$ for two linear operators is *a priori* only defined on the subspace $\mathsf{D}(A) \cap \mathsf{D}(B)$, and that the product AB is *a priori* defined only on the subspace $\{f \in \mathsf{D}(B) \mid Bf \in \mathsf{D}(A)\}$. These two sets can be very small.

Example 2.1.2. *Let* $\mathcal{H} := L^2(\mathbb{R})$ *and consider the operator* X *defined by* $[Xf](x) = xf(x)$ *for any* $x \in \mathbb{R}$*. Clearly,* $\mathsf{D}(X) = \{f \in \mathcal{H} \mid \int_{\mathbb{R}} |xf(x)|^2\,\mathrm{d}x < \infty\} \subsetneq \mathcal{H}$*. In addition, by considering the family of functions* $\{f_y\}_{y\in\mathbb{R}} \subset \mathsf{D}(X)$ *with* $f_y(x) := 1$ *in* $x \in [y, y+1]$ *and* $f_y(x) = 0$ *if* $x \notin [y, y+1]$*, one easily observes that* $\|f_y\| = 1$ *but* $\sup_{y\in\mathbb{R}} \|Xf_y\| = \infty$*, which can be compared with* (1.8)*.*

Clearly, a linear operator A can be defined on several domains. For example the operator X of the previous example is well-defined on the Schwartz space $\mathcal{S}(\mathbb{R})$, or on the set $C_c(\mathbb{R})$ of continuous functions on $\mathbb{R}$ with compact support, or on the space $\mathsf{D}(X)$ mentioned in the previous example. More generally, one has:

Definition 2.1.3. *For any pair of linear operators $\big(A,\mathsf{D}(A)\big)$ and $\big(B,\mathsf{D}(B)\big)$ satisfying $\mathsf{D}(A)\subset\mathsf{D}(B)$ and $Af=Bf$ for all $f\in\mathsf{D}(A)$, one says that $\big(B,\mathsf{D}(B)\big)$ is* an extension *of $\big(A,\mathsf{D}(A)\big)$ to $\mathsf{D}(B)$, or that $\big(A,\mathsf{D}(A)\big)$ is the restriction of $\big(B,\mathsf{D}(B)\big)$ to $\mathsf{D}(A)$.*

Let us now note that if $\big(A,\mathsf{D}(A)\big)$ is densely defined and if there exists $c\in\mathbb{R}$ such that $\|Af\|\leq c\|f\|$ for all $f\in\mathsf{D}(A)$, then there exists a natural continuous extension $\overline{A}$ of A with $\mathsf{D}(\overline{A})=\mathcal{H}$. This extension satisfies $\overline{A}\in\mathscr{B}(\mathcal{H})$ with $\|\overline{A}\|\leq c$, and is called *the closure of the operator A*.

Exercise 2.1.4. *Work on the details of this extension.*

Let us now consider a similar construction but in the absence of a constant $c\in\mathbb{R}$ such that $\|Af\|\leq c\|f\|$ for all $f\in\mathsf{D}(A)$. More precisely, consider an arbitrary densely defined operator $\big(A,\mathsf{D}(A)\big)$. Then for any $f\in\mathcal{H}$ there exists a sequence $\{f_n\}_{n\in\mathbb{N}}\subset\mathsf{D}(A)$ strongly converging to f. Note that the sequence $\{Af_n\}_{n\in\mathbb{N}}$ will not be Cauchy in general. However, let us assume that this sequence is strongly Cauchy, *i.e.* for any $\varepsilon>0$ there exists $N\in\mathbb{N}$ such that $\|Af_n-Af_m\|<\varepsilon$ for any $n,m\geq N$. Since $\mathcal{H}$ is complete, this Cauchy sequence has a limit, which we denote by h, and it would then be natural to set $\overline{A}f=h$. In short, one would have $\overline{A}f:=\text{s-}\lim_{n\to\infty}Af_n$. It is easily observed that this definition is meaningful if and only if by choosing a different sequence $\{f_n'\}_{n\in\mathbb{N}}\subset\mathsf{D}(A)$ strongly convergent to f and also defining a Cauchy sequence $\{Af_n'\}_{n\in\mathbb{N}}$ then $\text{s-}\lim_{n\to\infty}Af_n'=\text{s-}\lim_{n\to\infty}Af_n$. If this condition holds, then $\overline{A}f$ is well-defined. Observe in addition that the previous equality can by rewritten as $\text{s-}\lim_{n\to\infty}A(f_n-f_n')=0$, which leads naturally to the following definition.

Definition 2.1.5. *A linear operator $\big(A,\mathsf{D}(A)\big)$ is* closable *if for any sequence $\{f_n\}_{n\in\mathbb{N}}\subset\mathsf{D}(A)$ satisfying $\text{s-}\lim_{n\to\infty}f_n=0$ and such that $\{Af_n\}_{n\in\mathbb{N}}$ is strongly Cauchy, then $\text{s-}\lim_{n\to\infty}Af_n=0$.*

As shown before this definition, in such a case one can define an extension $\overline{A}$ of A with $\mathsf{D}(\overline{A})$ given by the sets of $f\in\mathcal{H}$ such that there exists $\{f_n\}_{n\in\mathbb{N}}\subset\mathsf{D}(A)$ with $\text{s-}\lim_{n\to\infty}f_n=f$ and such that $\{Af_n\}_{n\in\mathbb{N}}$ is strongly Cauchy. For such an element f one sets $\overline{A}f=\text{s-}\lim_{n\to\infty}Af_n$, and the extension $\big(\overline{A},\mathsf{D}(\overline{A})\big)$ is called the closure of A.

In relation with the previous construction the following definition is now natural:

Definition 2.1.6. *An linear operator $\big(A,\mathsf{D}(A)\big)$ is* closed *if for any sequence $\{f_n\}_{n\in\mathbb{N}}\subset\mathsf{D}(A)$ with $\text{s-}\lim_{n\to\infty}f_n=f\in\mathcal{H}$ and such that $\{Af_n\}_{n\in\mathbb{N}}$ is strongly Cauchy, then one has $f\in\mathsf{D}(A)$ and $\text{s-}\lim_{n\to\infty}Af_n=Af$.*

Exercise 2.1.7. *Prove the following assertions:*

(i) A bounded linear operator is always closed,

(ii) *If* $\big(A, \mathsf{D}(A)\big)$ *is closable and* $B \in \mathscr{B}(\mathcal{H})$*, then* $\big(A+B, \mathsf{D}(A)\big)$ *is closable,*

(iii) *f* $\big(A, \mathsf{D}(A)\big)$ *is closed and* $B \in \mathscr{B}(\mathcal{H})$*, then* $\big(A+B, \mathsf{D}(A)\big)$ *is closed,*

(iv) *If* $\big(A, \mathsf{D}(A)\big)$ *admits a closed extension* $\big(B, \mathsf{D}(B)\big)$*, then* $\big(A, \mathsf{D}(A)\big)$ *is closable and its closure satisfies* $\big(\overline{A}, \mathsf{D}(\overline{A})\big) \subset \big(B, \mathsf{D}(B)\big)$.

Let us still introduce the notion of the graph of an operator: For any linear operator $\big(A, \mathsf{D}(A)\big)$ one sets

$$\Gamma(A) := \{(f, Af) \mid f \in \mathsf{D}(A)\} \subset \mathcal{H} \oplus \mathcal{H} \tag{2.1}$$

and call it *the graph of* A. Note that the norm of an element (A, Af) in $\mathcal{H} \oplus \mathcal{H}$ is given by $(\|f\|^2 + \|Af\|^2)^{1/2}$. It is also clear that $\Gamma(A)$ is a linear manifold in $\mathcal{H} \oplus \mathcal{H}$, and one observes that $\big(A, \mathsf{D}(A)\big)$ is closed if and only if the graph $\Gamma(A)$ is closed in $\mathcal{H} \oplus \mathcal{H}$. On the other hand, $\big(A, \mathsf{D}(A)\big)$ is closable if and only if the closure of its graph does not contain any element of the form $(0, h)$ with $h \neq 0$. Let us finally observe that if one sets for any $f, g \in \mathsf{D}(A)$

$$\langle f, g\rangle_A := \langle f, g\rangle + \langle Af, Ag\rangle, \tag{2.2}$$

and if $\big(A, \mathsf{D}(A)\big)$ is a closed operator, then the linear manifold $\mathsf{D}(A)$ equipped with the scalar product (2.2) is a Hilbert space, with the natural norm deduced from this scalar product.

Let us now come back to the notion of the adjoint of an operator. This concept is slightly more subtle for unbounded operators than in the bounded case.

Definition 2.1.8. *Let* $\big(A, \mathsf{D}(A)\big)$ *be a densely defined linear operator on* $\mathcal{H}$. The adjoint A^* of A *is the operator defined by*

$$\mathsf{D}(A^*) := \big\{f \in \mathcal{H} \mid \exists f^* \in \mathcal{H} \text{ with } \langle f^*, g\rangle = \langle f, Ag\rangle \text{ for all } g \in \mathsf{D}(A)\big\}$$

and $A^* f := f^*$ *for all* $f \in \mathsf{D}(A^*)$.

Let us note that the density of $\mathsf{D}(A)$ is necessary to ensure that A^* is well defined. Indeed, if f_1^*, f_2^* satisfy for all $g \in \mathsf{D}(A)$

$$\langle f_1^*, g\rangle = \langle f, Ag\rangle = \langle f_2^*, g\rangle,$$

then $\langle f_1^* - f_2^*, g\rangle = 0$ for all $g \in \mathsf{D}(A)$, and this equality implies $f_1^* = f_2^*$ only if $\mathsf{D}(A)$ is dense in $\mathcal{H}$. Note also that once $\big(A^*, \mathsf{D}(A^*)\big)$ is defined, one has

$$\langle A^* f, g\rangle = \langle f, Ag\rangle \qquad \forall f \in \mathsf{D}(A^*) \text{ and } \forall g \in \mathsf{D}(A).$$

Exercise 2.1.9. *Show that if* $\big(A, \mathsf{D}(A)\big)$ *is closable, then* $\mathsf{D}(A^*)$ *is dense in* $\mathcal{H}$.

Some relations between A and its adjoint A^* are gathered in the following lemma.

Lemma 2.1.10. *Let* $\big(A, \mathsf{D}(A)\big)$ *be a densely defined linear operator on* $\mathcal{H}$*. Then* *(i)* $\big(A^*, \mathsf{D}(A^*)\big)$ *is closed,*

(ii) *One has* $\mathsf{Ker}(A^*) = \mathsf{Ran}(A)^\perp$,

(iii) *If* $\big(B, \mathsf{D}(B)\big)$ *is an extension of* $\big(A, \mathsf{D}(A)\big)$, *then* $\big(A^*, \mathsf{D}(A^*)\big)$ *is an extension of* $\big(B^*, \mathsf{D}(B^*)\big)$.

Proof. a) Consider $\{f_n\}_{n\in\mathbb{N}} \subset \mathsf{D}(A^*)$ such that $\text{s}-\lim_{n\to\infty} f_n = f \in \mathcal{H}$ and $\text{s}-\lim_{n\to\infty} A^* f_n = h \in \mathcal{H}$. Then for each $g \in \mathsf{D}(A)$ one has

$$\langle f, Ag\rangle = \lim_{n\to\infty} \langle f_n, Ag\rangle = \lim_{n\to\infty} \langle A^* f_n, g\rangle = \langle h, g\rangle.$$

Hence $f \in \mathsf{D}(A^*)$ and $A^* f = h$, which proves that A^* is closed.

b) Let $f \in \mathsf{Ker}(A^*)$, *i.e.* $f \in \mathsf{D}(A^*)$ and $A^* f = 0$. Then, for all $g \in \mathsf{D}(A)$, one has

$$0 = \langle A^* f, g\rangle = \langle f, Ag\rangle$$

meaning that $f \in \mathsf{Ran}(A)^\perp$. Conversely, if $f \in \mathsf{Ran}(A)^\perp$, then for all $g \in \mathsf{D}(A)$ one has

$$\langle f, Ag\rangle = 0 = \langle 0, g\rangle$$

meaning that $f \in \mathsf{D}(A^*)$ and $A^* f = 0$, by the definition of the adjoint of A.

c) Consider $f \in \mathsf{D}(B^*)$ and observe that $\langle B^* f, g\rangle = \langle f, Bg\rangle$ for any $g \in \mathsf{D}(B)$. Since $\big(B, \mathsf{D}(B)\big)$ is an extension of $\big(A, \mathsf{D}(A)\big)$, one infers that $\langle B^* f, g\rangle = \langle f, Ag\rangle$ for any $g \in \mathsf{D}(A)$. Now, this equality means that $f \in \mathsf{D}(A^*)$ and that $A^* f = B^* f$, or more explicitly that A^* is defined on the domain of B^* and coincide with this operator on this domain. This means precisely that $\big(A^*, \mathsf{D}(A^*)\big)$ is an extension of $\big(B^*, \mathsf{D}(B^*)\big)$. $\square$

Extension 2.1.11. *Work on the additional properties of the adjoint operators as presented in Propositions 2.20 to 2.22 of [Amr].*

Let us finally introduce the analogue of the bounded self-adjoint operators but in the unbounded setting. These operators play a key role in quantum mechanics and their study is very well developed.

Definition 2.1.12. *A densely defined linear operator* $\big(A, \mathsf{D}(A)\big)$ *is* self-adjoint *if* $\mathsf{D}(A^*) = \mathsf{D}(A)$ *and* $A^* f = Af$ *for all* $f \in \mathsf{D}(A)$.

Note that as a consequence of Lemma 2.1.10.(i) a self-adjoint operator is always closed. Recall also that in the bounded case, a self-adjoint operator was characterized by the equality

$$\langle Af, g\rangle = \langle f, Ag\rangle \tag{2.3}$$

for any $f, g \in \mathcal{H}$. In the unbounded case, such an equality still holds if $f, g \in \mathsf{D}(A)$. However, let us emphasize that (2.3) does not completely characterize a self-adjoint operator. In fact, a densely defined operator $\big(A, \mathsf{D}(A)\big)$ satisfying (2.3) is called *a symmetric operator*, and self-adjoint operators are special instances of symmetric operators (but not all symmetric operators are self-adjoint). In fact, for a symmetric operator the adjoint operator $\big(A^*, \mathsf{D}(A^*)\big)$ is an extension of $\big(A, \mathsf{D}(A)\big)$, but the equality of these two operators holds only if $\big(A, \mathsf{D}(A)\big)$ is self-adjoint. Note also that for any symmetric operator the scalar $\langle f, Af\rangle$ is real for any $f \in \mathsf{D}(A)$.

Exercise 2.1.13. *Show that a symmetric operator is always closable.*

Let us add one more definition related to self-adjoint operators.

Definition 2.1.14. *A symmetric operator* $\big(A, \mathsf{D}(A)\big)$ *is* essentially self-adjoint *if its closure* $\big(\overline{A}, \mathsf{D}(\overline{A})\big)$ *is self-adjoint. In this case* $\mathsf{D}(A)$ *is called* a core *for* $\overline{A}$.

A following *fundamental criterion for self-adjointness* is important in this context, and its proof can be found in [Amr, Prop. 3.3].

Proposition 2.1.15. *Let* $\big(A, \mathsf{D}(A)\big)$ *be a symmetric operator in a Hilbert space* $\mathcal{H}$. *Then*

(i) $\big(A, \mathsf{D}(A)\big)$ *is self-adjoint if and only if* $\mathsf{Ran}(A+i) = \mathcal{H}$ *and* $\mathsf{Ran}(A-i) = \mathcal{H}$,

(ii) $\big(A, \mathsf{D}(A)\big)$ *is essentially self-adjoint if and only if* $\mathsf{Ran}(A+i)$ *and* $\mathsf{Ran}(A-i)$ *are dense in* $\mathcal{H}$.

We still mention that the general theory of extensions of symmetric operators is rather rich and can be studied on its own.

Extension 2.1.16. *Study the theory of extensions of symmetric operators (there exist several approaches for this study).*

2.2 Resolvent and spectrum

We come now to the important notion of the spectrum of an operator. As already mentioned in the previous section we shall often speak about a linear operator A, its domain $\mathsf{D}(A)$ being implicitly taken into account. Recall also that the notion of a closed linear operator has been introduced in Definition 2.1.6.

The notion of the inverse of a bounded linear operator has already been introduced in Definition 1.3.7. By analogy we say that any linear operator A is *invertible* if $\mathsf{Ker}(A) = \{0\}$. In this case, the inverse A^{-1} gives a bijection from $\mathsf{Ran}(A)$ onto $\mathsf{D}(A)$. More precisely $\mathsf{D}(A^{-1}) = \mathsf{Ran}(A)$ and $\mathsf{Ran}(A^{-1}) = \mathsf{D}(A)$. It can then be checked that if A is closed and invertible, then A^{-1} is also closed. Note also if A is closed and if $\mathsf{Ran}(A) = \mathcal{H}$ then $A^{-1} \in \mathscr{B}(\mathcal{H})$. In fact, the boundedness of A^{-1} is a consequence of the closed graph theorem[1] and one says in this case that A is *boundedly invertible* or *invertible in* $\mathscr{B}(\mathcal{H})$.

Definition 2.2.1. *For a closed linear operator A its* resolvent set $\rho(A)$ *is defined by*

$$\begin{aligned}\rho(A) :=& \big\{z \in \mathbb{C} \mid (A-z) \text{ is invertible in } \mathscr{B}(\mathcal{H})\big\} \\ =& \big\{z \in \mathbb{C} \mid \mathsf{Ker}(A-z) = \{0\} \text{ and } \mathsf{Ran}(A-z) = \mathcal{H}\big\}.\end{aligned}$$

[1] Closed graph theorem: If $\big(B, \mathcal{H}\big)$ is a closed operator, then $B \in \mathscr{B}(\mathcal{H})$, see for example [Kat, Sec. III.5.4]. This can be studied as an Extension.

For $z \in \rho(A)$ the operator $(A-z)^{-1} \in \mathscr{B}(\mathcal{H})$ is called the resolvent of A at the point z. The spectrum $\sigma(A)$ of A *is defined as the complement of $\rho(A)$ in $\mathbb{C}$,* i.e.

$$\sigma(A) := \mathbb{C} \setminus \rho(A). \tag{2.4}$$

The following statement summarized several properties of the resolvent set and of the resolvent of a closed linear operator.

Proposition 2.2.2. *Let A be a closed linear operator on a Hilbert space $\mathcal{H}$. Then*

(i) The resolvent set $\rho(A)$ is an open subset of $\mathbb{C}$,

(ii) If $z_1, z_2 \in \rho(A)$ then the first resolvent equation *holds, namely*

$$(A - z_1)^{-1} - (A - z_2)^{-1} = (z_1 - z_2)(A - z_1)^{-1}(A - z_2)^{-1} \tag{2.5}$$

(iii) If $z_1, z_2 \in \rho(A)$ then the operators $(A - z_1)^{-1}$ and $(A - z_2)^{-1}$ commute,

(iv) In each connected component of $\rho(A)$ the map $z \mapsto (A - z)^{-1}$ is holomorphic.

Exercise 2.2.3. *Provide the proof of the previous proposition.*

As a consequence of the previous proposition, the spectrum of a closed linear operator is always closed. In particular, $z \in \sigma(A)$ if $A-z$ is not invertible or if $\mathsf{Ran}(A-z) \neq \mathcal{H}$. The first situation corresponds to the definition of an eigenvalue:

Definition 2.2.4. *For a closed linear operator A, a value $z \in \mathbb{C}$ is* an eigenvalue of A *if there exists $f \in \mathsf{D}(A)$, $f \neq 0$, such that $Af = zf$. In such a case, the element f is called* an eigenfunction of A associated with the eigenvalue z. *The dimension of the vector space generated by all eigenfunctions associated with an eigenvalue z is called* the multiplicity of z. *The set of all eigenvalues of A is denoted by $\sigma_p(A)$.*

Let us still provide two properties of the spectrum of an operator in the special cases of a bounded operator or of a self-adjoint operator.

Exercise 2.2.5. *By using the Neumann series, show that for any $B \in \mathscr{B}(\mathcal{H})$ its spectrum is contained in the ball in the complex plane of center 0 and of radius $\|B\|$.*

Lemma 2.2.6. *Let A be a self-adjoint operator in $\mathcal{H}$.*

(i) Any eigenvalue of A is real,

(ii) More generally, the spectrum of A is real, i.e. $\sigma(A) \subset \mathbb{R}$,

(iii) Eigenvectors associated with different eigenvalues are orthogonal to one another.

Proof. a) Assume that there exists $z \in \mathbb{C}$ and $f \in \mathsf{D}(A)$, $f \neq 0$ such that $Af = zf$. Then one has

$$z\|f\|^2 = \langle f, zf\rangle = \langle f, Af\rangle = \langle Af, f\rangle = \langle zf, f\rangle = \overline{z}\|f\|^2.$$

Since $\|f\| \neq 0$, one deduces that $z \in \mathbb{R}$.

b) Let us consider $z = \lambda + i\varepsilon$ with $\lambda, \varepsilon \in \mathbb{R}$ and $\varepsilon \neq 0$, and show that $z \in \rho(A)$. Indeed, for any $f \in \mathsf{D}(A)$ one has

$$\begin{aligned}\|(A-z)f\|^2 &= \|(A-\lambda)f - i\varepsilon f\|^2 \\ &= \big\langle (A-\lambda)f - i\varepsilon f, (A-\lambda)f - i\varepsilon f\big\rangle \\ &= \|(A-\lambda)f\|^2 + \varepsilon^2\|f\|^2.\end{aligned}$$

It follows that $\|(A-z)f\| \geq |\varepsilon|\|f\|$, and thus $A - z$ is invertible.

Now, for any for any $g \in \mathsf{Ran}(A-z)$ let us observe that

$$\|g\| = \big\|(A-z)(A-z)^{-1}g\big\| \geq |\varepsilon|\big\|(A-z)^{-1}g\big\|.$$

Equivalently, it means for all $g \in \mathsf{Ran}(A-z)$, one has

$$\big\|(A-z)^{-1}g\big\| \leq \frac{1}{|\varepsilon|}\|g\|. \tag{2.6}$$

Let us finally observe that $\mathsf{Ran}(A-z)$ is dense in $\mathcal{H}$. Indeed, by Lemma 2.1.10 one has

$$\mathsf{Ran}(A-z)^\perp = \mathsf{Ker}\big((A-z)^*\big) = \mathsf{Ker}(A^* - \overline{z}) = \mathsf{Ker}(A - \overline{z}) = \{0\}$$

since all eigenvalues of A are real. Thus, the operator $(A-z)^{-1}$ is defined on the dense domain $\mathsf{Ran}(A-z)$ and satisfies the estimate (2.6). As explained just before the Exercise 2.1.4, it means that $(A-z)^{-1}$ continuously extends to an element of $\mathscr{B}(\mathcal{H})$, and therefore $z \in \rho(A)$.

c) Assume that $Af = \lambda f$ and that $Ag = \mu g$ with $\lambda, \mu \in \mathbb{R}$ and $\lambda \neq \mu$, and $f, g \in \mathsf{D}(A)$, with $f \neq 0$ and $g \neq 0$. Then

$$\lambda\langle f, g\rangle = \langle Af, g\rangle = \langle f, Ag\rangle = \mu\langle f, g\rangle,$$

which implies that $\langle f, g\rangle = 0$, or in other words that f and g are orthogonal. $\square$

2.3 Perturbation theory for self-adjoint operators

Let $\big(A, \mathsf{D}(A)\big)$ be a self-adjoint operator in a Hilbert space $\mathcal{H}$. The invariance of the self-adjoint property under the addition of a linear operator B is an important issue, especially in relation with quantum mechanics.

First of all, observe that if $\big(A, \mathsf{D}(A)\big)$ and $\big(B, \mathsf{D}(B)\big)$ are symmetric operator in $\mathcal{H}$ and if $\mathsf{D}(A) \cap \mathsf{D}(B)$ is dense in $\mathcal{H}$, then $A + B$ defined on this intersection is still a symmetric operator. Indeed, one has for any $f, g \in \mathsf{D}(A) \cap \mathsf{D}(B)$

$$\langle (A + B)f, g\rangle = \langle Af, g\rangle + \langle Bf, g\rangle = \langle f, Ag\rangle + \langle f, Bg\rangle = \langle f, (A + B)g\rangle.$$

However, even if both operators are self-adjoint, their sum is not self-adjoint in general. In the sequel we present some situations where the self-adjointness property is preserved.

In the simplest case, if $B \in \mathscr{B}(\mathcal{H})$ and B is self-adjoint, and if $\big(A, \mathsf{D}(A)\big)$ is a self-adjoint operator one easily observes that $\big(A + B, \mathsf{D}(A)\big)$ is still a self-adjoint operator. Indeed, this will automatically follow if one shows that $\mathsf{D}\big((A+B)^*\big) \subset \mathsf{D}(A+B) = \mathsf{D}(A)$. For that purpose, let $f \in \mathsf{D}\big((A+B)^*\big)$ and let $f^* \in \mathcal{H}$ such that $\langle f, (A+B)g\rangle = \langle f^*, g\rangle$ for any $g \in \mathsf{D}(A)$. Then one has

$$\langle f^*, g\rangle = \langle f, (A + B)g\rangle = \langle f, Ag\rangle + \langle f, Bg\rangle = \langle f, Ag\rangle + \langle Bf, g\rangle.$$

One thus infers that $\langle f, Ag\rangle = \langle f^* - Bf, g\rangle$ for any $g \in \mathsf{D}(A)$. Since $f^* - Bf \in \mathcal{H}$ this means that $f \in \mathsf{D}(A^*) \equiv \mathsf{D}(A)$.

Now, if B is not bounded, the question is more subtle. First of all, a notion of smallness of B with respect to A has to be introduced.

Definition 2.3.1. *Let $\big(A, \mathsf{D}(A)\big)$ and $\big(B, \mathsf{D}(B)\big)$ be two linear operators in $\mathcal{H}$. The operator B is said to be* A-bounded *or* relatively bounded with respect to A *if $\mathsf{D}(A) \subset \mathsf{D}(B)$ and if there exists $\alpha, \beta \geq 0$ such that for any $f \in \mathsf{D}(A)$*

$$\|Bf\| \leq \alpha\|Af\| + \beta\|f\|. \tag{2.7}$$

The infimum of all α satisfying this inequality is called the A-bound of B with respect to A, *or* the relative bound of B with respect to A.

Clearly, if $B \in \mathscr{B}(\mathcal{H})$, then B is A-bounded with relative bound 0. In fact, such a A-bound can be 0 even if B is not bounded. More precisely, the following situation can take place: For any $\varepsilon > 0$ there exists $\beta = \beta(\varepsilon)$ such that

$$\|Bf\| \leq \varepsilon\|Af\| + \beta\|f\|.$$

In such a case, the A-bound of B with respect to A is 0, but obviously one must have $\beta(\varepsilon) \to \infty$ as $\varepsilon \to 0$.

Exercise 2.3.2. *Consider two linear operators $\big(A, \mathsf{D}(A)\big)$ and $\big(B, \mathsf{D}(B)\big)$ with $\mathsf{D}(A) \subset \mathsf{D}(B)$, and assume that A is self-adjoint.*

(i) Let also $a, b \geq 0$. Show that

$$\|Bf\|^2 \leq a^2\|Af\|^2 + b^2\|f\|^2 \qquad \forall f \in \mathsf{D}(A)$$

is equivalent to

$$\big\|B\big(A \pm i\tfrac{b}{a}\big)^{-1}\big\| \leq a,$$

(ii) *Show that if $B(A-z)^{-1} \in \mathscr{B}(\mathcal{H})$ for some $z \in \rho(A)$, then B is A-bounded,*

(iii) *Show that if B is A-bounded, then $B(A-z)^{-1} \in \mathscr{B}(\mathcal{H})$ for any $z \in \rho(A)$. In addition, if α denotes the A-bound of B, then*

$$\alpha = \inf_{z\in\rho(A)} \|B(A-z)^{-1}\| = \inf_{\kappa>0} \|B(A-i\kappa)^{-1}\| = \inf_{\kappa>0} \|B(A+i\kappa)^{-1}\|. \tag{2.8}$$

Let us still mention that a self-adjoint operator A is said to be *lower semibounded* or *bounded from below* if there exists $\lambda \in \mathbb{R}$ such that $(-\infty, \lambda) \subset \rho(A)$, or in other words if A has no spectrum below the value λ. Similarly, A is upper semibounded if there exists $\lambda' \in \mathbb{R}$ such that A has no spectrum above λ'.

Theorem 2.3.3 (Rellich-Kato theorem)**.** *Let $\big(A, \mathsf{D}(A)\big)$ be a self-adjoint operator and let $\big(B, D(B)\big)$ be a A-bounded symmetric operator with A-bound $\alpha < 1$. Then*

(i) *The operator $A+B$ is self-adjoint on $\mathsf{D}(A)$,*

(ii) *B is also $(A+B)$-bounded,*

(iii) *If A is semibounded, then $A+B$ is also semibounded.*

The proof of this theorem is left as an exercise since some preliminary work is necessary, see [Amr, Prop. 2.44] for the proof. Also one notion from the functional calculus for self-adjoint operator is used in the proof, and this concept will only be studied later on.

The following statement is often called *the second resolvent equation.*

Proposition 2.3.4. *Let $\big(A, \mathsf{D}(A)\big)$ be a self-adjoint operator and let $\big(B, D(B)\big)$ be a symmetric operator which is A-bounded with A-bound $\alpha < 1$. Then the following equality holds for any $z \in \rho(A) \cap \rho(A+B)$:*

$$\begin{aligned} (A-z)^{-1} - (A+B-z)^{-1} &= (A-z)^{-1}B(A+B-z)^{-1} && (2.9)\\ &= (A+B-z)^{-1}B(A-z)^{-1}. && (2.10)\end{aligned}$$

Proof. By assumption, both operators $(A-z)^{-1}$ and $(A+B-z)^{-1}$ belong to $\mathscr{B}(\mathcal{H})$. In addition, $B(A+B-z)^{-1}$ and $B(A-z)^{-1}$ also belong to $\mathscr{B}(\mathcal{H})$, as a consequence of the previous theorem and of Exercise 2.3.2. Since $(A+B-z)^{-1}$ maps $\mathcal{H}$ onto $\mathsf{D}(A)$ one has

$$\begin{aligned} B(A+B-z)^{-1} &= (A+B-z)(A+B-z)^{-1} - (A-z)(A+B-z)^{-1}\\ &= \mathbf{1} - (A-z)(A+B-z)^{-1}. \end{aligned}$$

By multiplying this equality on the left by $(A-z)^{-1}$ one infers the first equality of the statement.

For the second equality, one starts with the equality

$$\begin{aligned} B(A-z)^{-1} &= (A+B-z)(A-z)^{-1} - (A-z)(A-z)^{-1}\\ &= (A+B-z)(A-z)^{-1} - \mathbf{1} \end{aligned}$$

and multiply it on the left by $(A+B-z)^{-1}$. □

Let us close this section with the notion of A-compact operator. More precisely, let $\big(A, \mathsf{D}(A)\big)$ be a closed linear operator, and let $\big(B, \mathsf{D}(B)\big)$ be a second operator. Then B is A-compact if $\mathsf{D}(A) \subset \mathsf{D}(B)$ and if there exists $z \in \rho(A)$ such that $B(A-z)^{-1}$ belongs to $\mathscr{K}(\mathcal{H})$. In such a case, the operator B is A-bounded with A-bound equal to 0, as shown in the next statement.

Proposition 2.3.5. *Let $\big(A, \mathsf{D}(A)\big)$ be self-adjoint, and let B be a symmetric operator which is A-compact. Then*

(i) $B(A-z)^{-1} \in \mathscr{K}(\mathcal{H})$ for any $z \in \rho(A)$,

(ii) B is A-bounded with A-bound equal to 0,

(iii) if $\big(C, \mathsf{D}(C)\big)$ is symmetric and A-bounded with A-bound $\alpha < 1$, then B is also $(A+C)$-compact.

Proof. a) By assumption, there exists $z_0 \in \rho(A)$ with $B(A-z_0)^{-1} \in \mathscr{K}(\mathcal{H})$. By the first resolvent equation (2.5) one then infers that

$$B(A-z)^{-1} = B(A-z_0)^{-1}\big(\mathbf{1} + (z-z_0)(A-z)^{-1}\big).$$

Since $B(A-z_0)^{-1}$ is compact and $\big(\mathbf{1}+(z-z_0)(A-z)^{-1}\big)$ is bounded, one deduces from Proposition 1.4.11.(iii) that $B(A-z)^{-1}$ is compact as well.

b) By (2.8) it is sufficient to show that for any $\varepsilon > 0$ there exists $z \in \rho(A)$ such that $\|B(A-z)^{-1}\| \leq \varepsilon$. For that purpose, we shall consider $z = i\mu$ and show that $\|B(A-i\mu)^{-1}\| \to 0$ as $\mu \to \infty$. Indeed observe first that

$$\begin{aligned} B(A-i\mu)^{-1} &= B(A-i)^{-1}\big((A-i)(A-i\mu)^{-1}\big) \\ &= B(A-i)^{-1}\big(\mathbf{1} + i(\mu-1)(A-i\mu)^{-1}\big). \end{aligned}$$

As a consequence of (2.6) one then deduces that $(A-i)(A-i\mu)^{-1} \in \mathscr{B}(\mathcal{H})$ with

$$\|(A-i)(A-i\mu)^{-1}\| \leq 1 + \frac{\mu-1}{\mu} \leq 2 \qquad \text{for any } \mu \geq 1. \tag{2.11}$$

If one shows that $\big((A-i)(A-i\mu)^{-1}\big)^*$ converges strongly to 0 as $\mu \to \infty$ then one gets from Proposition 1.4.12.(ii) and from the compactness of $B(A-i)^{-1}$ (as a consequence of the point (i) of this statement) that $\lim_{\mu\to\infty}\|B(A-i\mu)^{-1}\| = 0$.

One easily observes that for any $f \in \mathsf{D}(A)$ one has

$$\big((A-i)(A-i\mu)^{-1}\big)^* f = (A+i\mu)^{-1}(A+i)f$$

and that

$$\|\big(A+i\mu)^{-1}(A+i)f\| \leq \|(A+i\mu)^{-1}\|\,\|(A+i)f\| \leq \frac{1}{\mu}\|(A+i)f\| \tag{2.12}$$

where (2.6) has been used once again. Clearly, the r.h.s. of (2.12) converges to 0 as $\mu \to \infty$, and by the upper bound obtained in (2.11) one deduces by density that

$$\text{s-}\lim_{\mu \to 0} \big((A-i)(A-i\mu)^{-1}\big)^* = \mathbf{0},$$

as expected.

c) By the second resolvent equation (2.9) one gets

$$\begin{aligned} B(A+C-i)^{-1} &= B(A-i)^{-1} - B(A-i)^{-1}C(A+C-i)^{-1} \\ &= B(A-i)^{-1}\big(\mathbf{1} - C(A+C-i)^{-1}\big). \end{aligned}$$

Then $B(A-i)^{-1}$ is compact, by the point (i), and $C(A+C-i)^{-1}$ is bounded by Theorem 2.3.3.(ii) and by Exercise (2.3.2).(iii). As in (a) one deduces that $B(A+C-i)^{-1}$ is a compact operator. □