Hilbert space methods for quantum mechanics

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Spring Semester 2016

Contents

Chapter 1

Hilbert space and bounded linear operators

This chapter is mainly based on the first two chapters of the book [Amr]. Its content is quite standard and this theory can be seen as a special instance of bounded linear operators on more general Banach spaces.

1.1 Hilbert space

Definition 1.1.1. A (complex) Hilbert space $\mathcal{H}$ *is a vector space on* $\mathbb{C}$ *with a strictly positive scalar product (or inner product) which is complete for the associated norm*[1] *and which admits a countable orthonormal basis. The scalar product is denoted by* $\langle \cdot, \cdot \rangle$ *and the corresponding norm by* $\| \cdot \|$.

In particular, note that for any $f, g, h \in \mathcal{H}$ and $\alpha \in \mathbb{C}$ the following properties hold:

(i) $\langle f, g \rangle = \overline{\langle g, f \rangle}$,

(ii) $\langle f, g + \alpha h \rangle = \langle f, g \rangle + \alpha \langle f, h \rangle$,

(iii) $\|f\|^2 = \langle f, f \rangle \geq 0$, and $\|f\| = 0$ if and only if $f = 0$.

Note that $\overline{\langle g, f \rangle}$ means the complex conjugate of $\langle g, f \rangle$. Note also that the linearity in the second argument in (ii) is a matter of convention, many authors define the linearity in the first argument. In (iii) the norm of f is defined in terms of the scalar product $\langle f, f \rangle$. We emphasize that the scalar product can also be defined in terms of the norm of $\mathcal{H}$, this is the content of the *polarisation identity*:

$$4\langle f, g \rangle = \|f + g\|^2 - \|f - g\|^2 - i\|f + ig\|^2 + i\|f - ig\|^2. \tag{1.1}$$

[1] Recall that $\mathcal{H}$ is said to be complete if any Cauchy sequence in $\mathcal{H}$ has a limit in $\mathcal{H}$. More precisely, $\{f_n\}_{n \in \mathbb{N}} \subset \mathcal{H}$ is a Cauchy sequence if for any $\varepsilon > 0$ there exists $N \in \mathbb{N}$ such that $\|f_n - f_m\| < \varepsilon$ for any $n, m \geq N$. Then $\mathcal{H}$ is complete if for any such sequence there exists $f_\infty \in \mathcal{H}$ such that $\lim_{n \to \infty} \|f_n - f_\infty\| = 0$.

From now on, the symbol $\mathcal{H}$ will always denote a Hilbert space.

Examples 1.1.2. *(i)* $\mathcal{H} = \mathbb{C}^d$ *with* $\langle \alpha, \beta\rangle = \sum_{j=1}^d \overline{\alpha_j}\beta_j$ *for any* $\alpha, \beta \in \mathbb{C}^d$*,*

(ii) $\mathcal{H} = l^2(\mathbb{Z})$ *with* $\langle a, b\rangle = \sum_{j\in\mathbb{Z}} \overline{a_j} b_j$ *for any* $a, b \in l^2(\mathbb{Z})$*,*

(iii) $\mathcal{H} = L^2(\mathbb{R}^d)$ *with* $\langle f, g\rangle = \int_{\mathbb{R}^d} \overline{f(x)}\, g(x)\,\mathrm{d}x$ *for any* $f, g \in L^2(\mathbb{R}^d)$*.*

Let us recall some useful inequalities: For any $f, g \in \mathcal{H}$ one has

$$|\langle f, g\rangle| \leq \|f\|\,\|g\| \qquad \text{Schwarz inequality,} \tag{1.2}$$
$$\|f + g\| \leq \|f\| + \|g\| \qquad \text{triangle inequality,} \tag{1.3}$$
$$\|f + g\|^2 \leq 2\|f\|^2 + 2\|g\|^2, \tag{1.4}$$
$$\big|\|f\| - \|g\|\big| \leq \|f - g\|. \tag{1.5}$$

The proof of these inequalities is standard and is left as a free exercise, see also [Amr, p. 3-4]. Let us also recall that $f, g \in \mathcal{H}$ are said to be *orthogonal* if $\langle f, g\rangle = 0$.

Definition 1.1.3. *A sequence* $\{f_n\}_{n\in\mathbb{N}} \subset \mathcal{H}$ *is* strongly convergent *to* $f_\infty \in \mathcal{H}$ *if* $\lim_{n\to\infty} \|f_n - f_\infty\| = 0$*, or is* weakly convergent *to* $f_\infty \in \mathcal{H}$ *if for any* $g \in \mathcal{H}$ *one has* $\lim_{n\to\infty}\langle g, f_n - f_\infty\rangle = 0$*. One writes* $\mathrm{s-}\lim_{n\to\infty} f_n = f_\infty$ *if the sequence is strongly convergent, and* $\mathrm{w-}\lim_{n\to\infty} f_n = f_\infty$ *if the sequence is weakly convergent.*

Clearly, a strongly convergent sequence is also weakly convergent. The converse is not true.

Exercise 1.1.4. *In the Hilbert space* $L^2(\mathbb{R})$*, exhibit a sequence which is weakly convergent but not strongly convergent.*

Lemma 1.1.5. *Consider a sequence* $\{f_n\}_{n\in\mathbb{N}} \subset \mathcal{H}$*. One has*

$$\mathrm{s-}\lim_{n\to\infty} f_n = f_\infty \quad\Longleftrightarrow\quad \mathrm{w-}\lim_{n\to\infty} f_n = f_\infty \ \ \textit{and}\ \ \lim_{n\to\infty}\|f_n\| = \|f_\infty\|.$$

Proof. Assume first that $\mathrm{s-}\lim_{n\to\infty} f_n = f_\infty$. By the Schwarz inequality one infers that for any $g \in \mathcal{H}$:

$$|\langle g, f_n - f_\infty\rangle| \leq \|f_n - f_\infty\|\,\|g\| \to 0 \qquad \text{as } n\to\infty,$$

which means that $\mathrm{w-}\lim_{n\to\infty} f_n = f_\infty$. In addition, by (1.5) one also gets

$$\big|\|f_n\| - \|f_\infty\|\big| \leq \|f_n - f_\infty\| \to 0 \quad \text{as} \quad n\to\infty,$$

and thus $\lim_{n\to\infty}\|f_n\| = \|f_\infty\|$.

For the reverse implication, observe first that

$$\|f_n - f_\infty\|^2 = \|f_n\|^2 + \|f_\infty\|^2 - \langle f_n, f_\infty\rangle - \langle f_\infty, f_n\rangle. \tag{1.6}$$

If $\mathrm{w-}\lim_{n\to\infty} f_n = f_\infty$ and $\lim_{n\to\infty}\|f_n\| = \|f_\infty\|$, then the right-hand side of (1.6) converges to $\|f_\infty\|^2 + \|f_\infty\|^2 - \|f_\infty\|^2 - \|f_\infty\|^2 = 0$, so that $\mathrm{s-}\lim_{n\to\infty} f_n = f_\infty$. □

Let us also note that if $\text{s}-\lim_{n\to\infty} f_n = f_\infty$ and $\text{s}-\lim_{n\to\infty} g_n = g_\infty$ then one has

$$\lim_{n\to\infty} \langle f_n, g_n\rangle = \langle f_\infty, g_\infty\rangle$$

by a simple application of the Schwarz inequality.

Exercise 1.1.6. *Let $\{e_n\}_{n\in\mathbb{N}}$ be an orthonormal basis of an infinite dimensional Hilbert space. Show that $\text{w}-\lim_{n\to\infty} e_n = 0$, but that $\text{s}-\lim_{n\to\infty} e_n$ does not exist.*

Exercise 1.1.7. *Show that the limit of a strong or a weak Cauchy sequence is unique. Show also that such a sequence is bounded,* i.e. *if $\{f_n\}_{n\in\mathbb{N}}$ denotes this Cauchy sequence, then $\sup_{n\in\mathbb{N}} \|f_n\| < \infty$.*

For the weak Cauchy sequence, the boundedness can be obtained from the following quite general result which will be useful later on. Its proof can be found in [Kat, Thm. III.1.29]. In the statement, Λ is simply a set.

Theorem 1.1.8 (Uniform boundedness principle)**.** *Let $\{\varphi_\lambda\}_{\lambda\in\Lambda}$ be a family of continuous maps*[2] *$\varphi_\lambda : \mathcal{H} \to [0,\infty)$ satisfying*

$$\varphi_\lambda(f+g) \le \varphi_\lambda(f) + \varphi_\lambda(g) \qquad \forall f, g \in \mathcal{H}.$$

If the set $\{\varphi_\lambda(f)\}_{\lambda\in\Lambda} \subset [0,\infty)$ is bounded for any fixed $f \in \mathcal{H}$, then the family $\{\varphi_\lambda\}_{\lambda\in\Lambda}$ is uniformly bounded, i.e. *there exists $c > 0$ such that $\sup_\lambda \varphi_\lambda(f) \le c$ for any $f \in \mathcal{H}$ with $\|f\| = 1$.*

In the next definition, we introduce the notion of a linear manifold and of a subspace of a Hilbert space.

Definition 1.1.9. A linear manifold *$\mathcal{M}$ of a Hilbert space $\mathcal{H}$ is a linear subset of $\mathcal{H}$, or more precisely $\forall f, g \in \mathcal{M}$ and $\alpha \in \mathbb{C}$ one has $f + \alpha g \in \mathcal{M}$. If $\mathcal{M}$ is closed ($\Leftrightarrow$ any Cauchy sequence in $\mathcal{M}$ converges strongly in $\mathcal{M}$), then $\mathcal{M}$ is called a* subspace *of $\mathcal{H}$.*

Note that if $\mathcal{M}$ is closed, then $\mathcal{M}$ is a Hilbert space in itself, with the scalar product and norm inherited from $\mathcal{H}$. Be aware that some authors call *subspace* what we have defined as a linear manifold, and call *closed subspace* what we simply call a subspace.

Examples 1.1.10. *(i) If $f_1, \dots, f_n \in \mathcal{H}$, then $\mathsf{Vect}(f_1, \dots, f_n)$ is the closed vector space generated by the linear combinations of $f_1, \dots f_n$. $\mathsf{Vect}(f_1, \dots, f_n)$ is a subspace.*

(ii) If $\mathcal{M}$ is a subset of $\mathcal{H}$, then

$$\mathcal{M}^\perp := \{f \in \mathcal{H} \mid \langle f, g\rangle = 0, \forall g \in \mathcal{M}\} \tag{1.7}$$

is a subspace of $\mathcal{H}$.

[2] φ_λ is continuous if $\varphi_\lambda(f_n) \to \varphi_\lambda(f_\infty)$ whenever $\text{s}-\lim_{n\to\infty} f_n = f_\infty$.

Exercise 1.1.11. *Check that in the above example the set $\mathcal{M}^\perp$ is a subspace of $\mathcal{H}$.*

Exercise 1.1.12. *Check that a linear manifold $\mathcal{M} \subset \mathcal{H}$ is dense in $\mathcal{H}$ if and only if $\mathcal{M}^\perp = \{0\}$.*

If $\mathcal{M}$ is a subset of $\mathcal{H}$ the subspace $\mathcal{M}^\perp$ is called *the orthocomplement of $\mathcal{M}$ in $\mathcal{H}$*. The following result is important in the setting of Hilbert spaces. Its proof is not complicated but a little bit lengthy, we thus refer to [Amr, Prop. 1.7].

Proposition 1.1.13 (Projection Theorem)**.** *Let $\mathcal{M}$ be a subspace of a Hilbert space $\mathcal{H}$. Then, for any $f \in \mathcal{H}$ there exist a unique $f_1 \in \mathcal{M}$ and a unique $f_2 \in \mathcal{M}^\perp$ such that $f = f_1 + f_2$.*

Let us close this section with the so-called Riesz Lemma. For that purpose, recall first that the dual $\mathcal{H}^*$ of the Hilbert space $\mathcal{H}$ consists in the set of all bounded linear functionals on $\mathcal{H}$, *i.e.* $\mathcal{H}^*$ consists in all mappings $\varphi : \mathcal{H} \to \mathbb{C}$ satisfying for any $f, g \in \mathcal{H}$ and $\alpha \in \mathbb{C}$

(i) $\varphi(f + \alpha g) = \varphi(f) + \alpha\varphi(g)$, (linearity)

(ii) $|\varphi(f)| \leq c\|f\|$, (boundedness)

where c is a constant independent of f. One then sets

$$\|\varphi\|_{\mathcal{H}^*} := \sup_{0 \neq f \in \mathcal{H}} \frac{|\varphi(f)|}{\|f\|}.$$

Clearly, if $g \in \mathcal{H}$, then g defines an element φ_g of $\mathcal{H}^*$ by setting $\varphi_g(f) := \langle g, f\rangle$. Indeed φ_g is linear and one has

$$\|\varphi_g\|_{\mathcal{H}^*} := \sup_{0 \neq f \in \mathcal{H}} \frac{1}{\|f\|}|\langle g, f\rangle| \leq \sup_{0 \neq f \in \mathcal{H}} \frac{1}{\|f\|}\|g\|\,\|f\| = \|g\|.$$

In fact, note that $\|\varphi_g\|_{\mathcal{H}^*} = \|g\|$ since $\frac{1}{\|g\|}\varphi_g(g) = \frac{1}{\|g\|}\|g\|^2 = \|g\|$.

The following statement shows that any element $\varphi \in \mathcal{H}^*$ can be obtained from an element $g \in \mathcal{H}$. It corresponds thus to a converse of the previous construction.

Lemma 1.1.14 (Riesz Lemma)**.** *For any $\varphi \in \mathcal{H}^*$, there exists a unique $g \in \mathcal{H}$ such that for any $f \in \mathcal{H}$*

$$\varphi(f) = \langle g, f\rangle.$$

In addition, g satisfies $\|\varphi\|_{\mathcal{H}^*} = \|g\|$.

Since the proof is quite standard, we only sketch it and leave the details to the reader, see also [Amr, Prop. 1.8].

Sketch of the proof. If $\varphi \equiv 0$, then one can set $g := 0$ and observe trivially that $\varphi = \varphi_g$.

If $\varphi \neq 0$, let us first define $\mathcal{M} := \{f \in \mathcal{H} \mid \varphi(f) = 0\}$ and observe that $\mathcal{M}$ is a subspace of $\mathcal{H}$. One also observes that $\mathcal{M} \neq \mathcal{H}$ since otherwise $\varphi \equiv 0$. Thus, let $h \in \mathcal{H}$ such that $\varphi(h) \neq 0$ and decompose $h = h_1 + h_2$ with $h_1 \in \mathcal{M}$ and $h_2 \in \mathcal{M}^\perp$ by Proposition 1.1.13. One infers then that $\varphi(h_2) = \varphi(h) \neq 0$.

For arbitrary $f \in \mathcal{H}$ one can consider the element $f - \frac{\varphi(f)}{\varphi(h_2)} h_2 \in \mathcal{H}$ and observe that $\varphi\big(f - \frac{\varphi(f)}{\varphi(h_2)} h_2\big) = 0$. One deduces that $f - \frac{\varphi(f)}{\varphi(h_2)} h_2$ belongs to $\mathcal{M}$, and since $h_2 \in \mathcal{M}^\perp$ one infers that

$$\varphi(f) = \frac{\varphi(h_2)}{\|h_2\|^2} \langle h_2, f \rangle.$$

One can thus set $g := \overline{\frac{\varphi(h_2)}{\|h_2\|^2}} h_2 \in \mathcal{H}$ and easily obtain the remaining parts of the statement. □

As a consequence of the previous statement, one often identifies $\mathcal{H}^*$ with $\mathcal{H}$ itself.

Exercise 1.1.15. *Check that this identification is not linear but* anti-linear.

1.2 Vector-valued functions

Let $\mathcal{H}$ be a Hilbert space and let Λ be a set. A *vector-valued function* if a map $f : \Lambda \to \mathcal{H}$, *i.e.* for any $\lambda \in \Lambda$ one has $f(\lambda) \in \mathcal{H}$. In application, we shall mostly consider the special case $\Lambda = \mathbb{R}$ or $\Lambda = [a, b]$ with $a, b \in \mathbb{R}$ and $a < b$.

The following definitions are mimicked from the special case $\mathcal{H} = \mathbb{C}$, but different topologies on $\mathcal{H}$ can be considered:

Definition 1.2.1. *Let $J := (a, b)$ with $a < b$ and consider a vector-valued function $f : J \to \mathcal{H}$.*

(i) f is strongly continuous *on J if for any $t \in J$ one has $\lim_{\varepsilon \to 0} \|f(t+\varepsilon) - f(t)\| = 0$,*

(ii) f is weakly continuous *on J if for any $t \in J$ and any $g \in \mathcal{H}$ one has*

$$\lim_{\varepsilon \to 0} \big\langle g, f(t+\varepsilon) - f(t) \big\rangle = 0,$$

(iii) f is strongly differentiable *on J if there exists another vector-valued function $f' : J \to \mathcal{H}$ such that for any $t \in J$ one has*

$$\lim_{\varepsilon \to 0} \big\| \tfrac{1}{\varepsilon}\big(f(t+\varepsilon) - f(t)\big) - f'(t) \big\| = 0,$$

(iii) f is weakly differentiable *on J if there exists another vector-valued function $f' : J \to \mathcal{H}$ such that for any $t \in J$ and $g \in \mathcal{H}$ one has*

$$\lim_{\varepsilon \to 0} \big\langle g, \tfrac{1}{\varepsilon}\big(f(t+\varepsilon) - f(t)\big) - f'(t) \big\rangle = 0,$$

The map f' is called the strong derivative*, respectively the* weak derivative*, of f.*

Integrals of vector-valued functions can be defined in several senses, but we shall restrict ourselves to Riemann-type integrals. The construction is then similar to real or complex-valued functions, by considering finer and finer partitions of a bounded interval J. Improper Riemann integrals can also be defined in analogy with the scalar case by a limiting process. Note that these integrals can exist either in the strong sense (strong topology on $\mathcal{H}$) or in the weak sense (weak topology on $\mathcal{H}$). In the sequel, we consider only the existence of such integrals in the strong sense.

Let us thus consider $J := (a, b]$ with $a < b$ and let us set $\Pi = \{s_0, \dots, s_n; u_1, \dots u_n\}$ with $a = s_0 < u_1 \leq s_1 < u_2 \leq s_2 < \cdots < u_n \leq s_n = b$ for a partition of J. One also sets $|\Pi| := \max_{k\in\{1,\dots,n\}} |s_k - s_{k-1}|$ and the Riemann sum

$$\Sigma(\Pi, f) := \sum_{k=1}^{n} (s_k - s_{k-1}) f(u_k).$$

If one considers then a sequence $\{\Pi_i\}_{i\in\mathbb{N}}$ of partitions of J with $|\Pi_i| \to 0$ as $i \to \infty$ one writes

$$\int_J f(t)\mathrm{d}t \equiv \int_a^b f(t)\mathrm{d}t = \text{s}-\lim_{i\to\infty} \Sigma(\Pi_i, f)$$

if this limit exists and is independent of the sequence of partitions. In this case, one says that f is *strongly integrable* on $(a, b]$. Clearly, similar definitions hold for $J = (a, b)$ or $J = [a, b]$. Infinite intervals can be considered by a limiting process as long as the corresponding limits exist.

The following statements can then be proved in a way similar to the scalar case.

Proposition 1.2.2. *Let $(a, b]$ and $(b, c]$ be finite or infinite intervals and suppose that all the subsequent integrals exist. Then one has*

(i) $\int_a^b f(t)\mathrm{d}t + \int_b^c f(t)\mathrm{d}t = \int_a^c f(t)\mathrm{d}t$,

(ii) $\int_a^b \big(\alpha f_1(t) + f_2(t)\big)\mathrm{d}t = \alpha \int_a^b f_1(t)\mathrm{d}t + \int_a^b f_2(t)\mathrm{d}t$,

(iii) $\Big\| \int_a^b f(t)\mathrm{d}t\Big\| \leq \int_a^b \|f(t)\|\mathrm{d}t$.

For the existence of these integrals one has:

Proposition 1.2.3. *(i) If $[a, b]$ is a finite closed interval and $f : [a, b] \to \mathcal{H}$ is strongly continuous, then $\int_a^b f(t)\mathrm{d}t$ exists,*

(ii) If $a < b$ are arbitrary and $\int_a^b \|f(t)\|\mathrm{d}t < \infty$, then $\int_a^b f(t)\mathrm{d}t$ exists,

(iii) If f is strongly differentiable on (a, b) and its derivative f' is strongly continuous and integrable on $[a, b]$ then

$$\int_a^b f'(t)\mathrm{d}t = f(b) - f(a).$$

1.3 Bounded linear operators

First of all, let us recall that a linear map B between two complex vector spaces $\mathcal{M}$ and $\mathcal{N}$ satisfies $B(f + \alpha g) = Bf + \alpha Bg$ for all $f, g \in \mathcal{M}$ and $\alpha \in \mathbb{C}$.

Definition 1.3.1. *A map $B : \mathcal{H} \to \mathcal{H}$ is* a bounded linear operator *if $B : \mathcal{H} \to \mathcal{H}$ is a linear map, and if there exists $c > 0$ such that $\|Bf\| \leq c\|f\|$ for all $f \in \mathcal{H}$. The set of* all bounded linear operators on $\mathcal{H}$ *is denoted by $\mathscr{B}(\mathcal{H})$.*

For any $B \in \mathscr{B}(\mathcal{H})$, one sets

$$\begin{aligned} \|B\| &:= \inf\{c > 0 \mid \|Bf\| \leq c\|f\| \ \forall f \in \mathcal{H}\} \\ &= \sup_{0 \neq f \in \mathcal{H}} \frac{\|Bf\|}{\|f\|}. \end{aligned} \tag{1.8}$$

and call it *the norm of B*. Note that the same notation is used for the norm of an element of $\mathcal{H}$ and for the norm of an element of $\mathscr{B}(\mathcal{H})$, but this does not lead to any confusion. Let us also introduce the *range* of an operator $B \in \mathscr{B}(\mathcal{H})$, namely

$$\mathsf{Ran}(B) := B\mathcal{H} = \{f \in \mathcal{H} \mid f = Bg \text{ for some } g \in \mathcal{H}\}. \tag{1.9}$$

This notion will be important when the inverse of an operator will be discussed.

Exercise 1.3.2. *Let $\mathcal{M}_1, \mathcal{M}_2$ be two dense linear manifolds of $\mathcal{H}$, and let $B \in \mathscr{B}(\mathcal{H})$. Show that*

$$\|B\| = \sup_{f \in \mathcal{M}_1, g \in \mathcal{M}_2 \text{ with } \|f\| = \|g\| = 1} |\langle f, Bg\rangle|. \tag{1.10}$$

Exercise 1.3.3. *Show that $\mathscr{B}(\mathcal{H})$ is a complete normed algebra and that the inequality*

$$\|AB\| \leq \|A\| \, \|B\| \tag{1.11}$$

holds for any $A, B \in \mathscr{B}(\mathcal{H})$.

An additional structure can be added to $\mathscr{B}(\mathcal{H})$: an involution. More precisely, for any $B \in \mathscr{B}(\mathcal{H})$ and any $f, g \in \mathcal{H}$ one sets

$$\langle B^* f, g\rangle := \langle f, Bg\rangle. \tag{1.12}$$

Exercise 1.3.4. *For any $B \in \mathscr{B}(\mathcal{H})$ show that*

(i) *B^* is uniquely defined by* (1.12) *and satisfies $B^* \in \mathscr{B}(\mathcal{H})$ with $\|B^*\| = \|B\|$,*

(ii) $(B^*)^* = B$,

(iii) $\|B^*B\| = \|B\|^2$,

(iv) *If $A \in \mathscr{B}(\mathcal{H})$, then $(AB)^* = B^*A^*$.*

The operator B^* is called *the adjoint of* B, and the proof the unicity in (i) involves the Riesz Lemma. A complete normed algebra endowed with an involution for which the property (iii) holds is called a C^*-algebra. In particular $\mathscr{B}(\mathcal{H})$ is a C^*-algebra. Such algebras have a well-developed and deep theory, see for example [Mur]. However, we shall not go further in this direction in this course.

We have already considered two distinct topologies on $\mathcal{H}$, namely the strong and the weak topology. On $\mathscr{B}(\mathcal{H})$ there exist several topologies, but we shall consider only three of them.

Definition 1.3.5. *A sequence $\{B_n\}_{n\in\mathbb{N}} \subset \mathscr{B}(\mathcal{H})$ is* uniformly convergent *to $B_\infty \in \mathscr{B}(\mathcal{H})$ if $\lim_{n\to\infty} \|B_n - B_\infty\| = 0$, is* strongly convergent *to $B_\infty \in \mathscr{B}(\mathcal{H})$ if for any $f \in \mathcal{H}$ one has $\lim_{n\to\infty} \|B_n f - B_\infty f\| = 0$, or is* weakly convergent *to $B_\infty \in \mathscr{B}(\mathcal{H})$ if for any $f, g \in \mathcal{H}$ one has $\lim_{n\to\infty}\langle f, B_n g - B_\infty g\rangle = 0$. In these cases, one writes respectively $u - \lim_{n\to\infty} B_n = B_\infty$, $s - \lim_{n\to\infty} B_n = B_\infty$ and $w - \lim_{n\to\infty} B_n = B_\infty$.*

Clearly, uniform convergence implies strong convergence, and strong convergence implies weak convergence. The reverse statements are not true. Note that if $\{B_n\}_{n\in\mathbb{N}} \subset \mathscr{B}(\mathcal{H})$ is weakly convergent, then the sequence $\{B_n^*\}_{n\in\mathbb{N}}$ of its adjoint operators is also weakly convergent. However, the same statement does not hold for a strongly convergent sequence. Finally, we shall not prove but often use that $\mathscr{B}(\mathcal{H})$ is also weakly and strongly closed. In other words, any weakly (or strongly) Cauchy sequence in $\mathscr{B}(\mathcal{H})$ converges in $\mathscr{B}(\mathcal{H})$.

Exercise 1.3.6. *Let $\{A_n\}_{n\in\mathbb{N}} \subset \mathscr{B}(\mathcal{H})$ and $\{B_n\}_{n\in\mathbb{N}} \subset \mathscr{B}(\mathcal{H})$ be two strongly convergent sequence in $\mathscr{B}(\mathcal{H})$, with limits A_∞ and B_∞ respectively. Show that the sequence $\{A_n B_n\}_{n\in\mathbb{N}}$ is strongly convergent to the element $A_\infty B_\infty$.*

Let us close this section with some information about the inverse of a bounded operator. Additional information on the inverse in relation with unbounded operators will be provided in the sequel.

Definition 1.3.7. *An operator $B \in \mathscr{B}(\mathcal{H})$ is* invertible *if the equation $Bf = 0$ only admits the solution $f = 0$. In such a case, there exists a linear map $B^{-1} : \mathsf{Ran}(B) \to \mathcal{H}$ which satisfies $B^{-1}Bf = f$ for any $f \in \mathcal{H}$, and $BB^{-1}g = g$ for any $g \in \mathsf{Ran}(B)$. If B is invertible and $\mathsf{Ran}(B) = \mathcal{H}$, then $B^{-1} \in \mathscr{B}(\mathcal{H})$ and B is said to be* invertible in $\mathscr{B}(\mathcal{H})$ *(or* boundedly invertible*).*

Note that the two conditions B invertible and $\mathsf{Ran}(B) = \mathcal{H}$ imply $B^{-1} \in \mathscr{B}(\mathcal{H})$ is a consequence of the Closed graph Theorem. In the sequel, we shall use the notation $\mathbf{1} \in \mathscr{B}(\mathcal{H})$ for the operator defined on any $f \in \mathcal{H}$ by $\mathbf{1}f = f$, and $\mathbf{0} \in \mathscr{B}(\mathcal{H})$ for the operator defined by $\mathbf{0}f = 0$.

The next statement is very useful in applications, and holds in a much more general context. Its proof is classical and can be found in every textbook.

Lemma 1.3.8 (Neumann series)**.** *If $B \in \mathscr{B}(\mathcal{H})$ and $\|B\| < 1$, then the operator $(\mathbf{1}-B)$ is invertible in $\mathscr{B}(\mathcal{H})$, with*

$$(\mathbf{1} - B)^{-1} = \sum_{n=0}^{\infty} B^n,$$

and with $\|(\mathbf{1} - B)^{-1}\| \leq (1 - \|B\|)^{-1}$. The series converges in the uniform norm of $\mathscr{B}(\mathcal{H})$.

Note that we have used the identity $B^0 = \mathbf{1}$.

1.4 Special classes of bounded linear operators

In this section we provide some information on some subsets of $\mathscr{B}(\mathcal{H})$. We start with some operators which will play an important role in the sequel.

Definition 1.4.1. *An operator $B \in \mathscr{B}(\mathcal{H})$ is called* self-adjoint *if $B^* = B$, or equivalently if for any $f, g \in \mathcal{H}$ one has*

$$\langle f, Bg\rangle = \langle Bf, g\rangle. \tag{1.13}$$

For these operators the computation of their norm can be simplified (see also Exercise 1.3.2) :

Exercise 1.4.2. *If $B \in \mathscr{B}(\mathcal{H})$ is self-adjoint and if $\mathcal{M}$ is a dense linear manifold in $\mathcal{H}$, show that*

$$\|B\| = \sup_{f\in\mathcal{M},\ \|f\|=1} |\langle f, Bf\rangle|. \tag{1.14}$$

A special set of self-adjoint operators is provided by the set of orthogonal projections:

Definition 1.4.3. *An element $P \in \mathscr{B}(\mathcal{H})$ is* an orthogonal projection *if $P = P^2 = P^*$.*

It not difficult to check that there is a one-to-one correspondence between the set of subspaces of $\mathcal{H}$ and the set of orthogonal projections in $\mathscr{B}(\mathcal{H})$. Indeed, any orthogonal projection P defines a subspace $\mathcal{M} := P\mathcal{H}$. Conversely by taking the projection Theorem (Proposition 1.1.13) into account one infers that for any subspace $\mathcal{M}$ one can define an orthogonal projection P with $P\mathcal{H} = \mathcal{M}$.

In the sequel, we might simply say projection instead of orthogonal projection. However, let us stress that in other contexts a projection is often an operator P satisfying only the relation $P^2 = P$.

We gather in the next exercise some easy relations between orthogonal projections and the underlying subspaces. For that purpose we use the notation $P_\mathcal{M}, P_\mathcal{N}$ for the orthogonal projections on the subspaces $\mathcal{M}$ and $\mathcal{N}$ of $\mathcal{H}$.

Exercise 1.4.4. *Show the following relations:*

(i) If $P_{\mathcal{M}}P_{\mathcal{N}} = P_{\mathcal{N}}P_{\mathcal{M}}$*, then* $P_{\mathcal{M}}P_{\mathcal{N}}$ *is a projection and the associated subspace is* $\mathcal{M} \cap \mathcal{N}$*,*

(ii) If $\mathcal{M} \subset \mathcal{N}$*, then* $P_{\mathcal{M}}P_{\mathcal{N}} = P_{\mathcal{N}}P_{\mathcal{M}} = P_{\mathcal{M}}$*,*

(iii) If $\mathcal{M} \perp \mathcal{N}$*, then* $P_{\mathcal{M}}P_{\mathcal{N}} = P_{\mathcal{N}}P_{\mathcal{M}} = \mathbf{0}$*, and* $P_{\mathcal{M}\oplus\mathcal{N}} = P_{\mathcal{M}} + P_{\mathcal{N}}$*,*

(iv) If $P_{\mathcal{M}}P_{\mathcal{N}} = \mathbf{0}$*, then* $\mathcal{M} \perp \mathcal{N}$*.*

Let us now consider unitary operators, and then more general isometries and partial isometries. For that purpose, we recall that $\mathbf{1}$ denotes the identify operator in $\mathscr{B}(\mathcal{H})$.

Definition 1.4.5. *An element* $U \in \mathscr{B}(\mathcal{H})$ *is* a unitary operator *if* $UU^* = \mathbf{1}$ *and if* $U^*U = \mathbf{1}$*.*

Note that if U is unitary, then U is invertible in $\mathscr{B}(\mathcal{H})$ with $U^{-1} = U^*$. Indeed, observe first that $Uf = 0$ implies $f = U^*(Uf) = U^*0 = 0$. Secondly, for any $g \in \mathcal{H}$, one has $g = U(U^*g)$, and thus $\mathsf{Ran}(U) = \mathcal{H}$. Finally, the equality $U^{-1} = U^*$ follows from the unicity of the inverse.

More generally, an element $V \in \mathscr{B}(\mathcal{H})$ is called *an isometry* if the equality

$$V^*V = \mathbf{1} \tag{1.15}$$

holds. Clearly, a unitary operator is an instance of an isometry. For isometries the following properties can easily be obtained.

Proposition 1.4.6. *a) Let* $V \in \mathscr{B}(\mathcal{H})$ *be an isometry. Then*

(i) V *preserves the scalar product, namely* $\langle Vf, Vg\rangle = \langle f, g\rangle$ *for any* $f, g \in \mathcal{H}$*,*

(ii) V *preserves the norm, namely* $\|Vf\| = \|f\|$ *for any* $f \in \mathcal{H}$*,*

(iii) If $\mathcal{H} \neq \{0\}$ *then* $\|V\| = 1$*,*

(iv) VV^* *is the projection on* $\mathsf{Ran}(V)$*,*

(v) V *is invertible (in the sense of Definition 1.3.7),*

(vi) The adjoint V^* *satisfies* $V^*f = V^{-1}f$ *if* $f \in \mathsf{Ran}(V)$*, and* $V^*g = 0$ *if* $g \perp \mathsf{Ran}(V)$*.*

b) An element $W \in \mathscr{B}(\mathcal{H})$ *is an isometry if and only if* $\|Wf\| = \|f\|$ *for all* $f \in \mathcal{H}$*.*

Exercise 1.4.7. *Provide a proof for the previous proposition (as well as the proof of the next proposition).*

More generally one defines *a partial isometry* as an element $W \in \mathscr{B}(\mathcal{H})$ such that

$$W^*W = P \tag{1.16}$$

with P an orthogonal projection. Again, unitary operators or isometries are special examples of partial isometries.

As before the following properties of partial isometries can be easily proved.

Proposition 1.4.8. *Let $W \in \mathscr{B}(\mathcal{H})$ be a partial isometry as defined in* (1.16)*. Then*

(i) one has $WP = W$ and $\langle Wf, Wg\rangle = \langle Pf, Pg\rangle$ for any $f, g \in \mathcal{H}$,

(ii) If $P \neq \mathbf{0}$ then $\|W\| = 1$,

(iii) WW^* is the projection on $\mathsf{Ran}(W)$.

For a partial isometry W one usually calls *initial set projection* the projection defined by W^*W and by *final set projection* the projection defined by WW^*.

Let us now introduce a last subset of bounded operators, namely the ideal of *compact operators*. For that purpose, consider first any family $\{g_j, h_j\}_{j=1}^N \subset \mathcal{H}$ and for any $f \in \mathcal{H}$ one sets

$$Af := \sum_{j=1}^{N} \langle g_j, f\rangle\, h_j. \tag{1.17}$$

Then $A \in \mathscr{B}(\mathcal{H})$, and $\mathsf{Ran}(A) \subset \mathsf{Vect}(h_1, \dots, h_N)$. Such an operator A is called *a finite rank operator*. In fact, any operator $B \in \mathscr{B}(\mathcal{H})$ with $\dim\big(\mathsf{Ran}(B)\big) < \infty$ is a finite rank operator.

Exercise 1.4.9. *For the operator A defined in* (1.17)*, give an upper estimate for $\|A\|$ and compute A^*.*

Definition 1.4.10. *An element $B \in \mathscr{B}(\mathcal{H})$ is* a compact operator *if there exists a family $\{A_n\}_{n\in\mathbb{N}}$ of finite rank operators such that $\lim_{n\to\infty}\|B - A_n\| = 0$. The set of all compact operators is denoted by $\mathscr{K}(\mathcal{H})$.*

The following proposition contains sone basic properties of $\mathscr{K}(\mathcal{H})$. Its proof can be obtained by playing with families of finite rank operators.

Proposition 1.4.11. *The following properties hold:*

(i) $B \in \mathscr{K}(\mathcal{H}) \Longleftrightarrow B^* \in \mathscr{K}(\mathcal{H})$,

(ii) $\mathscr{K}(\mathcal{H})$ is a $*$-algebra, complete for the norm $\|\cdot\|$,

(iii) If $B \in \mathscr{K}(\mathcal{H})$ and $A \in \mathscr{B}(\mathcal{H})$, then AB and BA belong to $\mathscr{K}(\mathcal{H})$.

As a consequence, $\mathscr{K}(\mathcal{H})$ is a C^*-algebra and an ideal of $\mathscr{B}(\mathcal{H})$. In fact, compact operators have the nice property of improving some convergences, as shown in the next statement.

Proposition 1.4.12. *Let $K \in \mathscr{K}(\mathcal{H}))$.*

(i) If $\{f_n\}_{n\in\mathbb{N}} \subset \mathcal{H}$ is a weakly convergent sequence with limit $f_\infty \in \mathcal{H}$, then the sequence $\{Kf_n\}_{n\in\mathbb{N}}$ strongly converges to Kf_∞,

(ii) If the sequence $\{B_n\}_{n\in\mathbb{N}} \subset \mathscr{B}(\mathcal{H})$ strongly converges to $B_\infty \in \mathscr{B}(\mathcal{H})$, then the sequences $\{B_n K\}_{n\in\mathbb{N}}$ and $\{KB_n^*\}_{n\in\mathbb{N}}$ converge in norm to $B_\infty K$ and KB_∞^*, respectively.

Proof. a) Let us first set $\varphi_n := f_n - f_\infty$ and observe that $\mathrm{w-}\lim_{n\to\infty}\varphi_n = 0$. By an application of the uniform boundedness principle, see Theorem 1.1.8, it follows that $\{\|\varphi_n\|\}_{n\in\mathbb{N}}$ is bounded, *i.e.* there exists $M > 0$ such that $\|\varphi_n\| \leq M$ for any $n \in \mathbb{N}$. Since K is compact, for any $\varepsilon > 0$ there exists a finite rank operator A of the form given in (1.17) such that $\|K - A\| \leq \frac{\varepsilon}{2M}$. Then one has

$$\|K\varphi_n\| \leq \|(K-A)\varphi_n\| + \|A\varphi_n\| \leq \frac{\varepsilon}{2} + \sum_{j=1}^N |\langle g_j, \varphi_n\rangle| \, \|h_j\|.$$

Since $\mathrm{w-}\lim_{n\to\infty}\varphi_n = 0$ there exists $n_0 \in \mathbb{N}$ such that $\langle g_j, \varphi_n\rangle| \, \|h_j\| \leq \frac{\varepsilon}{2N}$ for any $j \in \{1,\dots,N\}$ and all $n \geq n_0$. As a consequence, one infers that $\|K\varphi_n\| \leq \varepsilon$ for all $n \geq n_0$, or in other words $\mathrm{s-}\lim_{n\to\infty} K\varphi_n = 0$.

b) Let us set $C_n := B_n - B_\infty$ such that $\mathrm{s-}\lim_{n\to\infty} C_n = \mathbf{0}$. As before, there exists $M > 0$ such that $\|C_n\| \leq M$ for any $n \in \mathbb{N}$. For any $\varepsilon > 0$ consider a finite rank operator A of the form (1.17) such that $\|K - A\| \leq \frac{\varepsilon}{2M}$. Then observe that for any $f \in \mathcal{H}$

$$\begin{aligned}
\|C_n K f\| &\leq M\|(K-A)f\| + \|C_n A f\| \\
&\leq M\|K-A\| \, \|f\| + \sum_{j=1}^N |\langle g_j, f\rangle| \, \|C_n h_j\| \\
&\leq \Big\{ M\|K-A\| \; + \sum_{j=1}^N \|g_j\| \, \|C_n h_j\| \Big\} \|f\|.
\end{aligned}$$

Since C_n strongly converges to $\mathbf{0}$ one can then choose $n_0 \in \mathbb{N}$ such that $\|g_j\| \, \|C_n h_j\| \leq \frac{\varepsilon}{2N}$ for any $j \in \{1,\dots N\}$ and all $n \geq n_0$. One then infers that $\|C_n K\| \leq \varepsilon$ for any $n \geq n_0$, which means that the sequence $\{C_n K\}_{n\in\mathbb{N}}$ uniformly converges to $\mathbf{0}$. The statement about $\{KB_n^*\}_{n\in\mathbb{N}}$ can be proved analogously by taking the equality $\|KB_n^* - KB_\infty^*\| = \|B_n K^* - B_\infty K^*\|$ into account and by remembering that K^* is compact as well. □

Exercise 1.4.13. *Check that a projection P is a compact operator if and only if $P\mathcal{H}$ is of finite dimension.*

Extension 1.4.14. *There are various subalgebras of $\mathscr{K}(\mathcal{H})$, for example the algebra of Hilbert-Schmidt operators, the algebra of trace class operators, and more generally the Schatten classes. Note that these algebras are not closed with respect to the norm $\|\cdot\|$ but with respect to some stronger norms $|||\cdot|||$. These algebras are ideals in $\mathscr{B}(\mathcal{H})$.*

1.5 Operator-valued maps

In analogy with Section 1.2 it is natural to consider function with values in $\mathscr{B}(\mathcal{H})$. More precisely, let J be an open interval on $\mathbb{R}$, and let us consider a map $F : J \to \mathscr{B}(\mathcal{H})$. The notion of continuity can be considered with several topologies on $\mathscr{B}(\mathcal{H})$, but as in Definition 1.3.5 we shall consider only three of them.

Definition 1.5.1. *The map F is* continuous in norm *on J if for all $t \in J$*

$$\lim_{\varepsilon\to 0} \big\|F(t+\varepsilon) - F(t)\big\| = 0.$$

The map F is strongly continuous *on J if for any $f \in \mathcal{H}$ and all $t \in J$*

$$\lim_{\varepsilon\to 0} \big\|F(t+\varepsilon)f - F(t)f\big\| = 0.$$

The map F is weakly continuous *on J if for any $f, g \in \mathcal{H}$ and all $t \in J$*

$$\lim_{\varepsilon\to 0} \big\langle g, \big(F(t+\varepsilon) - F(t)\big)f\big\rangle = 0.$$

One writes respectively $u - \lim_{\varepsilon\to 0} F(t+\varepsilon) = F(t)$, $s - \lim_{\varepsilon\to 0} F(t+\varepsilon) = F(t)$ and $w - \lim_{\varepsilon\to 0} F(t+\varepsilon) = F(t)$.

The same type of definition holds for the differentiability:

Definition 1.5.2. *The map F is* differentiable in norm *on J if there exists a map $F' : J \to \mathscr{B}(\mathcal{H})$ such that*

$$\lim_{\varepsilon\to 0} \Big\|\frac{1}{\varepsilon}\big(F(t+\varepsilon) - F(t)\big) - F'(t)\Big\| = 0.$$

The definitions for strongly differentiable *and* weakly differentiable *are similar.*

If J is an open interval of $\mathbb{R}$ and if $F : J \to \mathscr{B}(\mathcal{H})$, one defines $\int_J F(t)\,\mathrm{d}t$ as a Riemann integral (limit of finite sums over a partition of J) if this limiting procedure exists and is independent of the partitions of J. Note that these integrals can be defined in the weak topology, in the strong topology or in the norm topology (and in other topologies). For example, if $F : J \to \mathscr{B}(\mathcal{H})$ is strongly continuous and if $\int_J \|F(t)\|\mathrm{d}t < \infty$, then the integral $\int_J F(t)\,\mathrm{d}t$ exists in the strong topology.

Proposition 1.5.3. *Let J be an open interval of $\mathbb{R}$ and $F : J \to \mathscr{B}(\mathcal{H})$ such that $\int_J F(t)\,\mathrm{d}t$ exists (in an appropriate topology). Then,*

(i) For any $B \in \mathscr{B}(\mathcal{H})$ one has

$$B\int_J F(t)\,\mathrm{d}t = \int_J BF(t)\,\mathrm{d}t \quad \textit{and} \quad \Big(\int_J F(t)\,\mathrm{d}t\Big)B = \int_J F(t)B\,\mathrm{d}t,$$

(ii) *One has* $\left\| \int_J F(t)\,\mathrm{d}t \right\| \leq \int_J \|F(t)\|\,\mathrm{d}t$,

(iii) *If* $\mathscr{C} \subset \mathscr{B}(\mathcal{H})$ *is a subalgebra of* $\mathscr{B}(\mathcal{H})$, *closed with respect to a norm* $|||\cdot|||$, *and if the map* $F : J \to \mathscr{C}$ *is continuous with respect to this norm and satisfies* $\int_J |||F(t)|||\,\mathrm{d}t < \infty$, *then* $\int_J F(t)\,\mathrm{d}t$ *exists, belongs to* $\mathscr{C}$ *and satisfies*

$$\left|\left|\left| \int_J F(t)\,\mathrm{d}t \right|\right|\right| \leq \int_J |||F(t)|||\,\mathrm{d}t.$$

Note that the last statement is very useful, for example when $\mathscr{C} = \mathscr{K}(\mathcal{H})$ or for any Schatten class.

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 $\big(B^*, \mathsf{D}(B^*)\big)$. □

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. □

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 $z \in \rho(A) \cap \rho(A + B)$:*

$$(A-z)^{-1} - (A+B-z)^{-1} = (A-z)^{-1}B(A+B-z)^{-1} \tag{2.9}$$
$$= (A+B-z)^{-1}B(A-z)^{-1}. \tag{2.10}$$

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. □

Chapter 3

Examples

In this chapter we present some examples of operators which often appear in the literature. Most of them are self-adjoint and were first introduced in relation with quantum mechanics. Indeed, any physical system is described with such an operator. Self-adjoint operators are the natural generalization of Hermitian matrices. Obviously, the following list of examples is only very partial, and many other operators should be considered as well.

3.1 Multiplication and convolution operators

In this section, we introduce two natural classes of operators on $\mathbb{R}^d$. This material is standard and can be found for example in the books [Amr] and [Tes]. We start by considering multiplication operators on the Hilbert space $L^2(\mathbb{R}^d)$.

For any measurable complex function φ on $\mathbb{R}^d$ let us define the *multiplication operator* $\varphi(X)$ on $\mathcal{H}(\mathbb{R}^d) := L^2(\mathbb{R}^d)$ by

$$[\varphi(X)f](x) = \varphi(x)f(x) \qquad \forall x \in \mathbb{R}^d$$

for any

$$f \in \mathsf{D}\big(\varphi(X)\big) := \big\{g \in \mathcal{H}(\mathbb{R}^d) \mid \int_{\mathbb{R}^d} |\varphi(x)|^2|g(x)|^2\mathrm{d}x < \infty\big\}.$$

Clearly, the properties of this operator depend on the function φ. More precisely:

Lemma 3.1.1. *Let $\varphi(X)$ be the multiplication operator on $\mathcal{H}(\mathbb{R}^d)$. Then $\varphi(X)$ belongs to $\mathscr{B}\big(\mathcal{H}(\mathbb{R}^d)\big)$ if and only if $\varphi \in L^\infty(\mathbb{R}^d)$, and in this case $\|\varphi(X)\| = \|\varphi\|_\infty$.*

Proof. One has

$$\|\varphi(X)f\|^2 = \int_{\mathbb{R}^d} |\varphi(x)|^2|f(x)|^2\mathrm{d}x \le \|\varphi\|_\infty^2 \int_{\mathbb{R}^d} |f(x)|^2\mathrm{d}x = \|\varphi\|_\infty^2\|f\|^2.$$

Thus, if $\varphi \in L^\infty(\mathbb{R}^d)$, then $\mathsf{D}\big(\varphi(X)\big) = \mathcal{H}(\mathbb{R}^d)$ and $\|\varphi(X)\| \le \|\varphi\|_\infty$.

Now, assume that $\varphi \notin L^\infty(\mathbb{R}^d)$. It means that for any $n \in \mathbb{N}$ there exists a measurable set $W_n \subset \mathbb{R}^d$ with $0 < |W_n| < \infty$ such that $|\varphi(x)| > n$ for any $x \in W_n$. We then set $f_n = \chi_{W_n}$ and observe that $f_n \in \mathcal{H}(\mathbb{R}^d)$ with $\|f_n\|^2 = |W_n|$ and that

$$\|\varphi(X)f_n\|^2 = \int_{\mathbb{R}^d} |\varphi(x)|^2 |f_n(x)|^2 \mathrm{d}x = \int_{W_n} |\varphi(x)|^2 dx > n^2 \|f_n\|^2,$$

from which one infers that $\|\varphi(X)f_n\|/\|f_n\| > n$. Since n is arbitrary, the operator $\varphi(X)$ can not be bounded.

Let us finally show that if $\varphi \in L^\infty(\mathbb{R}^d)$, then $\|\varphi(X)\| \geq \|\varphi\|_\infty$. Indeed, for any $\varepsilon > 0$, there exists a measurable set $W_\varepsilon \subset \mathbb{R}^d$ with $0 < |W_\varepsilon| < \infty$ such that $|\varphi(x)| > \|\varphi\|_\infty - \varepsilon$ for any $x \in W_\varepsilon$. Again by setting $f_\varepsilon = \chi_{W_\varepsilon}$ one gets that $\|\varphi(X)f_\varepsilon\|/\|f_\varepsilon\| > \|\varphi\|_\infty - \varepsilon$, from which one deduces the required inequality. □

If $\varphi \in L^\infty(\mathbb{R}^d)$, one easily observes that $\varphi(X)^* = \overline{\varphi}(X)$, and thus $\varphi(X)$ is self-adjoint if and only if φ is a real function. The operator $\varphi(X)$ is a projection if and only if $\varphi(x) \in \{0,1\}$ for almost every $x \in \mathbb{R}^d$. Similarly, the operator $\varphi(X)$ is unitary if and only if $|\varphi(x)| = 1$ for almost every $x \in \mathbb{R}^d$. Observe also that $\varphi(X)$ is a partial isometry if and only if $|\varphi(x)| \in \{0,1\}$ for almost every $x \in \mathbb{R}^d$. However, since $\varphi(X)$ and $\overline{\varphi}(X)$ commute, it is impossible to obtain $\varphi(X)^*\varphi(X) = \mathbf{1}$ without getting automatically that $\varphi(X)$ is a unitary operator. In other words, there does not exist any isometry $\varphi(X)$ which is not unitary.

If φ is real but does not belong to $L^\infty(\mathbb{R}^d)$, one can show that $\big(\varphi(X), \mathsf{D}\big(\varphi(X)\big)\big)$ defines a self-adjoint operator in $\mathcal{H}(\mathbb{R}^d)$, see also [Ped, Example 5.1.15]. In particular, if $\varphi \in C(\mathbb{R}^d)$ or if $|\varphi|$ is polynomially bounded, then the mentioned operator is self-adjoint, see [Amr, Prop. 2.29]. For example, for any $j \in \{1, \dots, d\}$ the operator X_j defined by $[X_j f](x) = x_j f(x)$ is a self-adjoint operator with domain $\mathsf{D}(X_j)$. Note that the d-tuple $(X_1, \dots, X_d)$ is often referred to as the *position operator* in $\mathcal{H}(\mathbb{R}^d)$. More generally, for any $\alpha \in \mathbb{N}^d$ one also sets

$$X^\alpha = X_1^{\alpha_1} \dots X_d^{\alpha_d}$$

and this expression defines a self-adjoint operator on its natural domain. Other useful multiplication operators are defined for any $s > 0$ by the functions

$$\mathbb{R}^d \ni x \mapsto \langle x \rangle^s := \Big(1 + \sum_{j=1}^d x_j^2\Big)^{s/2} \in \mathbb{R}.$$

The corresponding operators $\big(\langle X \rangle^s, \mathcal{H}_s(\mathbb{R}^d)\big)$, with

$$\mathcal{H}_s(\mathbb{R}^d) := \Big\{ f \in \mathcal{H}(\mathbb{R}^d) \mid \langle X \rangle^s f \in \mathcal{H}(\mathbb{R}^d) \Big\} = \Big\{ f \in \mathcal{H}(\mathbb{R}^d) \mid \int_{\mathbb{R}^d} \langle x \rangle^{2s} |f(x)|^2 \mathrm{d}x < \infty \Big\},$$

are again self-adjoint operators on $\mathcal{H}(\mathbb{R}^d)$. Note that one usually calls $\mathcal{H}_s(\mathbb{R}^d)$ *the weighted Hilbert space with weight s* since it is naturally a Hilbert space with the scalar product $\langle f, g \rangle_s := \int_{\mathbb{R}^d} \overline{f(x)} g(x) \langle x \rangle^{2s} \mathrm{d}x$.

Exercise 3.1.2. *For any real $\varphi \in C(\mathbb{R}^d)$ or $\varphi \in L^\infty(\mathbb{R}^d)$, show that the spectrum of the self-adjoint multiplication operator $\varphi(X)$ coincides with the closure of $\varphi(\mathbb{R}^d)$ in $\mathbb{R}$.*

We shall now introduce a new type of operators on $\mathcal{H}(\mathbb{R}^d)$, but for that purpose we need to recall a few results about the usual Fourier transform on $\mathbb{R}^d$. The Fourier transform $\mathcal{F}$ is defined on any $f \in C_c(\mathbb{R}^d)$ by the formula[1]

$$[\mathcal{F}f](\xi) \equiv \hat{f}(\xi) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{e}^{-i\xi\cdot x} f(x)\,\mathrm{d}x. \tag{3.1}$$

This linear transform maps the Schwartz space $\mathcal{S}(\mathbb{R}^d)$ onto itself, and its inverse is provided by the formula $[\mathcal{F}^{-1}f](x) \equiv \check{f}(x) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{e}^{i\xi\cdot x} f(\xi)\,\mathrm{d}\xi$. In addition, by taking Parseval's identity $\int_{\mathbb{R}^d} |f(x)|^2 \mathrm{d}x = \int_{\mathbb{R}^d} |\hat{f}(\xi)|^2 \mathrm{d}\xi$ into account, one obtains that the Fourier transform extends continuously to a unitary map on $\mathcal{H}(\mathbb{R}^d)$. We shall keep the same notation $\mathcal{F}$ for this continuous extension, but one must be aware that (3.1) is valid only on a restricted set of functions.

Let us use again the multi-index notation and set for any $\alpha \in \mathbb{N}^d$

$$(-i\partial)^\alpha = (-i\partial_1)^{\alpha_1} \dots (-i\partial_d)^{\alpha_d} = (-i)^{|\alpha|} \partial_1^{\alpha_1} \dots \partial_d^{\alpha_d}$$

with $|\alpha| = \alpha_1 + \dots + \alpha_d$. With this notation at hand, the following relations hold for any $f \in \mathcal{S}(\mathbb{R}^d)$ and any $\alpha \in \mathbb{N}^d$:

$$\mathcal{F}(-i\partial)^\alpha f = X^\alpha \mathcal{F} f,$$

or equivalently $(-i\partial)^\alpha f = \mathcal{F}^* X^\alpha \mathcal{F} f$. Keeping these relations in mind, one defines for any $j \in \{1, \dots, d\}$ the self-adjoint operator $D_j := \mathcal{F}^* X_j \mathcal{F}$ with domain $\mathcal{F}^* \mathsf{D}(X_j)$. Similarly, for any $s > 0$, one also defines the operator $\langle D \rangle^s := \mathcal{F}^* \langle X \rangle^s \mathcal{F}$ with domain

$$\mathcal{H}^s(\mathbb{R}^d) := \big\{ f \in \mathcal{H}(\mathbb{R}^d) \mid \langle X \rangle^s \mathcal{F} f \in \mathcal{H}(\mathbb{R}^d) \big\} \equiv \big\{ f \in \mathcal{H}(\mathbb{R}^d) \mid \langle X \rangle^s \hat{f} \in \mathcal{H}(\mathbb{R}^d) \big\}. \tag{3.2}$$

Note that the space $\mathcal{H}^s(\mathbb{R}^d)$ is called *the Sobolev space of order* s, and $(D_1, \dots, D_d)$ is usually called *the momentum operator*[2].

We can now introduce the usual *Laplace operator* $-\Delta$ acting on any $f \in \mathcal{S}(\mathbb{R}^d)$ as

$$-\Delta f = -\sum_{j=1}^d \partial_j^2 f = \sum_{j=1}^d (-i\partial_j)^2 f = \sum_{j=1}^d D_j^2 f. \tag{3.3}$$

This operator admits a self-adjoint extension with domain $\mathcal{H}^2(\mathbb{R}^d)$, *i.e.* $\big(-\Delta, \mathcal{H}^2(\mathbb{R}^d)\big)$ is a self-adjoint operator in $\mathcal{H}(\mathbb{R}^d)$. However, let us stress that the expression (3.3) is not valid (pointwise) on all the elements of the domain $\mathcal{H}^2(\mathbb{R}^d)$. On the other hand, one has

[1] Even if the group $\mathbb{R}^d$ is identified with its dual group, we will keep the notation ξ for points of its dual group.

[2] In physics textbooks, the position operator is often denoted by $(Q_1, \dots, Q_d)$ while $(P_1, \dots, P_d)$ is used for the momentum operator.

$-\Delta = \mathcal{F}^* X^2 \mathcal{F}$, with $X^2 = \sum_{j=1}^d X_j^2$, from which one easily infers that $\sigma(-\Delta) = [0, \infty)$. Indeed, this follows from the content of Exercise 3.1.2 together with the invariance of the spectrum through the conjugation by a unitary operator.

Before going on with other operators of the form $\varphi(D)$, let us provide some additional information on the space $\mathcal{H}^2(\mathbb{R}^d)$ for $d \in \{1, 2, 3\}$.

Lemma 3.1.3. *Let $d \le 3$ and assume that $f \in \mathcal{H}^2(\mathbb{R}^d)$. Then $f \in C_0(\mathbb{R}^d)$, and for any $\alpha > 0$ there exists $\beta > 0$ such that*

$$\|f\|_\infty \le \alpha \|\Delta f\| + \beta \|f\|, \qquad f \in \mathcal{H}^2(\mathbb{R}^d).$$

In the following proof we shall denote by $\|g\|_1$ the L^1-norm of $g \in L^1(\mathbb{R}^d)$, *i.e.*

$$\|g\|_1 = \int_{\mathbb{R}^d} |g(x)| \mathrm{d}x. \tag{3.4}$$

Proof. For any $\gamma > 0$ let us set $g_\gamma : \mathbb{R}^3 \to \mathbb{R}$ defined by $g_\gamma(\xi) := (\xi^2 + \gamma^2)^{-1}$. The key observation is that g_γ belongs to $L^2(\mathbb{R}^d)$ if $d \le 3$. Then, for $f \in \mathcal{H}^2(\mathbb{R}^d)$ one has

$$(X^2 + \gamma^2)\hat{f} = \Big[(X^2 + \gamma^2)\langle X\rangle^{-2}\Big] \langle X\rangle^2 \hat{f} \in L^2(\mathbb{R}^d)$$

by (3.2), and one infers by the Cauchy-Schwarz inequality that

$$\|\hat{f}\|_1 = \int_{\mathbb{R}^d} \big|(\xi^2 + \gamma^2)^{-1}(\xi^2 + \gamma^2)\hat{f}(\xi)\big| \mathrm{d}\xi \;\le\; \|g_\gamma\| \, \|(X^2 + \gamma^2)\hat{f}\| < \infty$$

which implies that $\hat{f}$ belongs to $L^1(\mathbb{R}^d)$. By the Riemann-Lebesgue lemma (as presented for example in [Tes, Lem. 7.6]) one deduces that $f \in C_0(\mathbb{R}^d)$, and more precisely that

$$\begin{aligned}
\|f\|_\infty &\le (2\pi)^{-d/2} \|g_\gamma\| \, \|(X^2 + \gamma^2)\hat{f}\| \\
&\le (2\pi)^{-d/2} \gamma^{-2+d/2} \|g_1\| \left(\|\Delta f\| + \gamma^2 \|f\|\right) \\
&= (2\pi)^{-d/2} \|g_1\| \Big(\gamma^{-2+d/2} \|\Delta f\| + \gamma^{d/2} \|f\|\Big).
\end{aligned}$$

□

For any measurable function φ on $\mathbb{R}^d$ let us now set $\varphi(D) := \mathcal{F}^* \varphi(X) \mathcal{F}$, with domain $\mathsf{D}\big(\varphi(D)\big) = \big\{f \in \mathcal{H}(\mathbb{R}^d) \mid \hat{f} \in \mathsf{D}\big(\varphi(X)\big)\big\}$, and as before this operator is self-adjoint in $\mathcal{H}(\mathbb{R}^d)$, as for example for a continuous function φ or for a polynomially bounded function φ. Then, if one defines the convolution of two (suitable) functions on $\mathbb{R}^d$ by the formula

$$[k * f](x) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} k(y) f(x - y) \, \mathrm{d}y$$

and if one takes the equality $\check{g} * f = \mathcal{F}^*(g\hat{f})$ into account, one infers that the operator $\varphi(D)$ corresponds to *a convolution operator*, namely

$$\varphi(D) f = \check{\varphi} * f. \tag{3.5}$$

Obviously, the meaning of such an equality depends on the class of functions f and g considered.

Exercise 3.1.4. *Show that the following relations hold on the Schwartz space* $\mathcal{S}(\mathbb{R}^d)$*:* $[iX_j, X_k] = \mathbf{0} = [D_j, D_k]$ *for any* $j, k \in \{1, \dots, d\}$ *while* $[iD_j, X_k] = \mathbf{1}\delta_{jk}$.

3.1.1 The harmonic oscillator

An example of an operator which can be expressed easily in terms of the families of operators $\{X_j\}$ and $\{D_j\}$ is the harmonic oscillator, namely the operator

$$H = -\Delta + \omega^2 X^2 = \sum_{j=1}^{d} D_j^2 + \omega^2 \sum_{j=1}^{d} X_j^2 = \sum_{j=1}^{d} \big(D_j^2 + \omega^2 X_j^2\big),$$

where ω is a strictly positive constant. This operator can be defined on several domain, as for example on $C_c^\infty(\mathbb{R}^d)$ or on the Schwartz space $\mathcal{S}(\mathbb{R}^d)$. An other domain which is quite convenient is the following:

$$\mathsf{D}(H) := \mathsf{Vect}\big(\mathbb{R}^d \ni x \mapsto x^\alpha \,\mathrm{e}^{-x^2/2} \in \mathbb{R} \mid \alpha \in \mathbb{N}^d\big) \subset L^2(\mathbb{R}^d).$$

It is easily observed that the operator H is symmetric on $\mathsf{D}(H)$, and it can be shown that this operator is in fact essentially self-adjoint on the domain $\mathsf{D}(H)$, see Definition 2.1.14 for the notion of essential self-adjointness. In addition, H can be completely studied by some algebraic methods, by considering the so-called creation and annihilation operators. Let us simply mention that

$$\sigma(H) = \{(2n+d)\omega \mid n \in \mathbb{N}\}$$

and that the corresponding eigenfunctions can be expressed in terms of the Hermite polynomials.

Extension 3.1.5. *Work on the details of the algebraic methods for the harmonic oscillator. In particular, describe the eigenvalues, the corresponding eigenfunctions and determine the multiplicity of each eigenvalue.*

3.2 Schrödinger operators

In this section, we introduce some well-studied operators

First of all, let $h : \mathbb{R}^d \to \mathbb{R}$ be a continuous real function which diverges at infinity. Equivalently, we assume that h satisfies $(h - z)^{-1} \in C_0(\mathbb{R}^d)$ for some $z \in \mathbb{C} \setminus \mathbb{R}$. The corresponding convolution operator $h(D)$, defined by $\mathcal{F}^* h(X)\mathcal{F}$, is a self-adjoint operator with domain $\mathcal{F}^*\mathsf{D}\big(h(X)\big)$. Clearly, the spectrum of such an operator is equal to the closure of $h(\mathbb{R}^d)$ in $\mathbb{R}$.

Some examples of such a function h which are often considered in the literature are the functions defined by $h(\xi) = \xi^2$, $h(\xi) = |\xi|$ or $h(\xi) = \sqrt{1+\xi^2} - 1$. In these cases, the operator $h(D) = -\Delta$ corresponds to *the free Laplace operator*, the operator $h(D) = |D|$ is *the relativistic Schrödinger operator without mass*, while the operator

$h(D) = \sqrt{1-\Delta} - 1$ corresponds to *the relativistic Schrödinger operator with mass.* In these three cases, one has $\sigma\big(h(D)\big) = [0,\infty)$ while $\sigma_p\big(h(D)\big) = \emptyset$.

Let us now perturb this operator $h(D)$ with a multiplication operator $V(X)$. If the measurable function $V : \mathbb{R}^d \to \mathbb{R}$ is not essentially bounded, then the operator $h(D)+V(X)$ can only be defined on the intersection of the two domains, and checking that there exists a self-adjoint extension of this operator is not always an easy task. On the other hand, if one assumes that $V \in L^\infty(\mathbb{R}^d)$, then we can define the operator

$$H := h(D) + V(X) \qquad \text{with} \qquad \mathsf{D}(H) = \mathsf{D}\big(h(D)\big) \tag{3.1}$$

and this operator is self-adjoint. A lot of investigations have been performed on such an operator H when V vanishes at infinity, in a suitable sense. On the other hand, much less is known on this operator when the multiplication operator $V(X)$, also called *the potential*, has an anisotropic behavior. Let us just mention that a C^*-algebraic framework has been developed for dealing with this anisotropic behavior and that it involves crossed product C^*-algebras.

3.2.1 The hydrogen atom

Let us briefly introduce the operator used for describing a simple model of an atom with a single electron in $\mathbb{R}^3$. It is assumed that the nucleus of the atom is fixed at the origin, and the electron moves in the external potential generated by the nucleus. If the electrostatic force is taken into account, the resulting operator has the form

$$H = -\Delta - \frac{\gamma}{|X|} \tag{3.2}$$

where $-\Delta$ is the Laplace operator introduced in (3.3), $\gamma > 0$ is called the coupling constant, and $\frac{1}{|X|}$ is the operator of multiplication by the function $\mathbb{R}^3 \ni x \mapsto \frac{1}{|x|} \in \mathbb{R}$. *A priori*, the operator exhibited in (3.2) is well-defined only on $\mathsf{D}(-\Delta) \cap \mathsf{D}(|X|^{-1})$. However, it follows from Lemma 3.1.3 that $\mathsf{D}(-\Delta) \subset \mathsf{D}(|X|^{-1})$. Indeed, since any $f \in \mathsf{D}(-\Delta)$ also belongs to $C_0(\mathbb{R}^3)$ one has ($B_1(0)$ denotes the open ball centered at 0 and of radius 1)

$$\begin{aligned}
\int_{\mathbb{R}^3} \Big|\frac{1}{|x|}f(x)\Big|^2 \mathrm{d}x &= \int_{B_1(0)} \Big|\frac{1}{|x|}f(x)\Big|^2 \mathrm{d}x + \int_{\mathbb{R}^3\setminus B_1(0)} \Big|\frac{1}{|x|}f(x)\Big|^2 \mathrm{d}x \\
&\leq \|f\|_\infty^2 \int_{B_1(0)} \frac{1}{|x|^2}\mathrm{d}x + \int_{\mathbb{R}^3\setminus B_1(0)} |f(x)|^2 \mathrm{d}x \\
&< \infty.
\end{aligned}$$

As a consequence, $\mathsf{D}(-\Delta) \cap \mathsf{D}(|X|^{-1}) = \mathsf{D}(-\Delta)$.

In order to check that the operator H is self-adjoint on $\mathsf{D}(-\Delta) = \mathcal{H}^2(\mathbb{R}^3)$, let us decompose the function $x \mapsto -\gamma\frac{1}{|x|}$ into $V_1 + V_2$ with $V_1(x) = -\gamma\frac{1}{|x|}$ if $|x| < 1$ and 0 otherwise, and $V_2(x) = -\gamma\frac{1}{|x|}$ if $|x| \geq 1$ and 0 otherwise. Clearly, V_2 defines a bounded self-adjoint operator, and adding it to $-\Delta$ will not cause any problem. For V_1, one can observe that for any $c > 0$ the function

$$\mathbb{R}^3 \times \mathbb{R}^3 \ni (x, \xi) \mapsto V_1(x)(\xi^2 + c)^{-1} \in \mathbb{R}$$

belongs to $L^2(\mathbb{R}^3 \times \mathbb{R}^3)$. Since an operator with L^2-kernel corresponds to a Hilbert-Schmidt operator, the operator $V_1(X)(-\Delta + c)^{-1}$ is Hilbert-Schmidt (see Extension 1.4.14) and thus is compact. As a consequence of Proposition 2.3.5 one deduces that $V_1(X)$ is a multiplication operator which is $-\Delta$-bounded with relative bound equal to 0. By the Rellich-Kato theorem (see Theorem 2.3.3) one infers that $-\Delta + V_1(X)$ is self-adjoint on $\mathcal{H}^2(\mathbb{R}^3)$, and then that $-\Delta + V_1(X) + V_2(X) = -\Delta - \gamma\frac{1}{|X|}$ is self-adjoint on $\mathcal{H}^2(\mathbb{R}^3)$.

Let us add a few information about the operator (3.2) and refer to [Tes, Chap. 10] for more information. One has $[0, \infty) \subset \sigma(H)$. In fact, $[0, \infty)$ corresponds to the essential spectrum of H, as defined in the next chapter. In addition, the operator H possesses an infinite number of eigenvalues, which can be computed explicitly. More precisely, by a decomposition of this operator into the spherical harmonics $\{Y_l^m\}$ where $l \in \mathbb{N}$, $m \in \mathbb{Z}$ with $|m| \leq l$, and by studying the resulting operator for each index l one can get that

$$\sigma_p(H) = \Big\{ -\big(\tfrac{\gamma}{2(n+1)}\big)^2 \mid n \in \mathbb{N}\Big\}.$$

Each eigenvalue has a multiplicity $(n+1)^2$, which means that there are $(n+1)^2$ linearly independent functions in $\mathcal{H}^2(\mathbb{R}^3)$ satisfying $Hf = -\big(\frac{\gamma}{2(n+1)}\big)^2 f$. These functions can be expressed in terms of the Laguerre polynomials.

Extension 3.2.1. *Work on the details of the Hydrogen atom, and in particular study its eigenvalues and the corresponding eigenfunctions.*

3.3 The Weyl calculus

In section 3.1 we have seen how to define multiplication operators $\varphi(X)$ and convolution operators $\varphi(D)$ on the Hilbert space $\mathcal{H} := L^2(\mathbb{R}^d)$. A natural question is how to define a more general operator $f(X, D)$ on $L^2(\mathbb{R}^d)$ for a function $f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{C}$.

This can be seen as the problem of constructing a functional calculus $f \mapsto f(X, D)$ for the family $X_1, \ldots, X_d, D_1, \ldots, D_d$ of $2d$ self-adjoint, non-commuting operators. One also would like to define a multiplication $(f, g) \mapsto f \circ g$ satisfying $(f \circ g)(X, D) = f(X, D)g(X, D)$ as well as an involution $f \to f^\circ$ leading to $f^\circ(X, D) = f(X, D)^*$. The deviation of $\circ$ from pointwise multiplication is imputable to the fact that X and D do not commute.

The solution of these problems is called *the Weyl calculus*, or simply *the pseudodifferential calculus*. In order to define it, let us set $\Xi := \mathbb{R}^d \times \hat{\mathbb{R}}^d \cong \mathbb{R}^d \times \mathbb{R}^d$, which corresponds to the direct product of a locally compact Abelian group G and of its dual group $\hat{G}$. Elements of Ξ will be denoted by $\mathsf{x} = (x, \xi)$, $\mathsf{y} = (y, \eta)$ and $\mathsf{z} = (z, \zeta)$. We also set

$$\sigma(\mathsf{x}, \mathsf{y}) := \sigma\big((x, \xi), (y, \eta)\big) = y \cdot \xi - x \cdot \eta$$

for the standard *symplectic form* on Ξ. The prescription for $f(X, D) \equiv \mathfrak{Op}(f)$ with $f : \Xi \to \mathbb{C}$ is then defined for $u \in \mathcal{H}$ and $x \in \mathbb{R}^d$ by

$$[\mathfrak{Op}(f)u](x) := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \int_{\hat{\mathbb{R}}^d} \mathrm{e}^{i(x-y)\cdot\eta} f\left(\frac{x+y}{2}, \eta\right) u(y)\, \mathrm{d}y\, \mathrm{d}\eta, \tag{3.1}$$

the involution is $f^\circ(\mathsf{x}) := \overline{f(\mathsf{x})}$ and the multiplication (called *the Moyal product*) is

$$(f \circ g)(\mathsf{x}) := \frac{4^d}{(2\pi)^{2d}} \int_\Xi \int_\Xi \mathrm{e}^{-2i\sigma(\mathsf{x}-\mathsf{y}, \mathsf{x}-\mathsf{z})} f(\mathsf{y})\, g(\mathsf{z})\, \mathrm{d}\mathsf{y}\, \mathrm{d}\mathsf{z}. \tag{3.2}$$

Obviously, these formulas must be taken with some care: for many symbols f and g they need a suitable reinterpretation. Also, the normalization factors should always be checked once again, since they mainly depend on the conventions of each author.

Exercise 3.3.1. *Check that if $f(x, \xi) = f(\xi)$ (f is independent of x), then $\mathfrak{Op}(f) = f(D)$, while if $f(x, \xi) = f(x)$ (f is independent of ξ), then $\mathfrak{Op}(f) = f(X)$.*

Beside the encouraging results contained in the previous exercise, let us try to show where all the above formulas come from. We consider the strongly continuous unitary maps $\mathbb{R}^d \ni x \mapsto U_x \in \mathscr{U}(\mathcal{H})$ and $\hat{\mathbb{R}}^d \ni \xi \mapsto V_\xi := \mathrm{e}^{-iX\cdot\xi} \in \mathscr{U}(\mathcal{H})$, acting on $\mathcal{H}$ as

$$[U_x u](y) = u(y + x) \quad \text{and} \quad [V_\xi u](y) = \mathrm{e}^{-iy\cdot\xi}\, u(y), \qquad u \in \mathcal{H},\ y \in \mathbb{R}^d.$$

These operators satisfy the *Weyl form of the canonical commutation relations*

$$U_x V_\xi = \mathrm{e}^{-ix\cdot\xi}\, V_\xi U_x, \qquad x \in \mathbb{R}^d,\ \xi \in \hat{\mathbb{R}}^d, \tag{3.3}$$

as well as the identities $U_x U_{x'} = U_{x'} U_x$ and $V_\xi V_{\xi'} = V_{\xi'} V_\xi$ for $x, x' \in \mathbb{R}^d$ and $\xi, \xi' \in \hat{\mathbb{R}}^d$. These can be considered as a reformulation of the content of Exercise 3.1.4 in terms of bounded operators.

A convenient way to condense the maps U and V in a single one is to define *the Schrödinger Weyl system* $\{W(x, \xi) \mid x \in \mathbb{R}^d,\ \xi \in \hat{\mathbb{R}}^d\}$ by

$$W(\mathsf{x}) \equiv W(x, \xi) := \mathrm{e}^{\frac{i}{2}x\cdot\xi}\, U_x V_\xi = \mathrm{e}^{-\frac{i}{2}x\cdot\xi}\, V_\xi U_x, \tag{3.4}$$

which satisfies the relation $W(\mathsf{x})W(\mathsf{y}) = \mathrm{e}^{\frac{i}{2}\sigma(\mathsf{x},\mathsf{y})}\, W(\mathsf{x}+\mathsf{y})$ for any $\mathsf{x}, \mathsf{y} \in \Xi$. This equality encodes all the commutation relations between the basic operators X and D. Explicitly, the action of W on $u \in \mathcal{H}$ is given by

$$[W(x, \xi)u](y) = \mathrm{e}^{-i\left(\frac{1}{2}x + y\right)\cdot\xi}\, u(y + x), \qquad x, y \in \mathbb{R}^d,\ \xi \in \hat{\mathbb{R}}^d. \tag{3.5}$$

Now, recall that for a family of m commuting self-adjoint operators $S_1, \ldots, S_m$ one usually defines a functional calculus by the formula $f(S) := \frac{1}{(2\pi)^{m/2}} \int_{\mathbb{R}^m} \check{f}(t)\, \mathrm{e}^{-it\cdot S}\, \mathrm{d}t$, where $t \cdot S = t_1S_1 + \ldots + t_mS_m$ and $\check{f}$ is the inverse Fourier transform of f, see the next chapter for a simplified version of this formula. The prescription (3.1) can be obtained by a similar computation. For that purpose, let us define the *symplectic Fourier transformation* $\mathcal{F}_\Xi : \mathcal{S}'(\Xi) \to \mathcal{S}'(\Xi)$ by

$$(\mathcal{F}_\Xi f)(\mathsf{x}) := \frac{1}{(2\pi)^d} \int_\Xi \mathrm{e}^{i\sigma(\mathsf{x},\mathsf{y})} f(\mathsf{y})\, \mathrm{d}\mathsf{y}.$$

Now, for any function $f : \Xi \to \mathbb{C}$ belonging to the Schwartz space $\mathcal{S}(\Xi)$, we set

$$\mathfrak{Op}(f) := \frac{1}{(2\pi)^d} \int_\Xi (\mathcal{F}_\Xi^{-1} f)(\mathsf{x})\, W(\mathsf{x})\, \mathrm{d}\mathsf{x}. \tag{3.6}$$

By using (3.5), one gets formula (3.1). Then it is easy to verify that the relation $\mathfrak{Op}(f)\mathfrak{Op}(g) = \mathfrak{Op}(f \circ g)$ holds for $f, g \in \mathcal{S}(\Xi)$ if one uses the Moyal product introduced in (3.2).

Exercise 3.3.2. *Check that the above statements are correct, and in particular that the normalization factors are suitably chosen.*

3.4 Schrödinger operators with $\frac{1}{x^2}$-potential

In this section we consider various realizations of an operator on $\mathcal{H} := L^2(\mathbb{R}_+)$, and study some properties of the resulting operators. Our aim is to emphasize the role played by the realization, or in other words by the choice of the domain for this operator. As mentioned at the end of the section, depending on the realization, this operator can have zero eigenvalue, a finite number of eigenvalues, or even an infinite number of eigenvalues. On the other hand, the rest of the spectrum is stable and corresponds to the half-line $[0, \infty)$.

For any $\alpha \in \mathbb{C}$ we consider the differential expression

$$L_\alpha := -\partial_x^2 + \big(\alpha - \frac{1}{4}\big)x^{-2}$$

acting on distributions on $\mathbb{R}_+$, and denote by $L_\alpha^{\min}$ and $L_\alpha^{\max}$ the corresponding minimal and maximal operators associated with it in $\mathcal{H}$, see [BDG, Sec. 4 & App. A] for details. We simply recall from this reference that

$$\mathsf{D}(L_\alpha^{\max}) = \{f \in \mathcal{H} \mid L_\alpha f \in \mathcal{H}\}$$

and that $\mathsf{D}(L_\alpha^{\min})$ is the closure of the restriction of L_α to $C_c^\infty(\mathbb{R}_+)$. In fact, it can be shown that the following relation holds:

$$\big(L_\alpha^{\min}\big)^* = L_{\bar{\alpha}}^{\max}.$$

Let us recall some additional results which have been obtained in [BDG, Sec. 4]. For that purpose, we say that $f \in \mathsf{D}(L_\alpha^{\min})$ around 0, (or, by an abuse of notation,

$f(x) \in \mathsf{D}(L_\alpha^{\min})$ around 0) if there exists $\zeta \in C_c^\infty\big([0,\infty[\big)$ with $\zeta = 1$ around 0 such that $f\zeta \in \mathsf{D}(L_\alpha^{\min})$. In addition, it turns out that it is useful to introduce a parameter $m \in \mathbb{C}$ such that $\alpha = m^2$, even though there are two m corresponding to a single $\alpha \neq 0$. In other words, we shall consider from now on the operator

$$L_{m^2} := -\partial_x^2 + \big(m^2 - \frac{1}{4}\big)x^{-2}.$$

With this notation, if $\Re(m) \geq 1$ (we use the notation $\Re(m)$ for the real part of the complex number m) then $L_{m^2}^{\min} = L_{m^2}^{\max}$, while if $|\Re(m)| < 1$ then $L_{m^2}^{\min} \subsetneq L_{m^2}^{\max}$ and $\mathsf{D}(L_{m^2}^{\min})$ is a closed subspace of codimension 2 of $\mathsf{D}(L_{m^2}^{\max})$. More precisely, if $|\Re(m)| < 1$ and if $f \in \mathsf{D}(L_{m^2}^{\max})$ then there exist $a, b \in \mathbb{C}$ such that:

$$\begin{aligned} &f(x) - ax^{1/2-m} - bx^{1/2+m} \in \mathsf{D}(L_{m^2}^{\min}) \text{ around } 0 \qquad \text{if } m \neq 0,\\ &f(x) - ax^{1/2}\ln(x) - bx^{1/2} \in \mathsf{D}(L_0^{\min}) \text{ around } 0. \end{aligned}$$

In addition, the behavior of any function $g \in \mathsf{D}(L_{m^2}^{\min})$ is known, namely $g \in \mathcal{H}_0^1(\mathbb{R}_+)$ (the completion of $C_c^1(\mathbb{R}_+)$ with the $\mathcal{H}^1$-norm) and as $x \to 0$:

$$\begin{aligned} &g(x) = o\big(x^{3/2}\big) \text{ and } g'(x) = o\big(x^{1/2}\big) \qquad \text{if } m \neq 0,\\ &g(x) = o\big(x^{3/2}\ln(x)\big) \text{ and } g'(x) = o\big(x^{1/2}\ln(x)\big) \qquad \text{if } m = 0. \end{aligned}$$

3.4.1 Two families of Schrödinger operators

Let us first recall from [BDG, Def. 4.1] that for any $m \in \mathbb{C}$ with $\Re(m) > -1$ the operator H_m has been defined as the restriction of $L_{m^2}^{\max}$ to the domain

$$\begin{aligned} \mathsf{D}(H_m) = \big\{f \in \mathsf{D}(L_{m^2}^{\max}) \mid &\text{ for some } c \in \mathbb{C},\\ &f(x) - cx^{1/2+m} \in \mathsf{D}(L_{m^2}^{\min}) \text{ around } 0\big\}. \end{aligned}$$

It is then proved in this reference that $\{H_m\}_{\Re(m)>-1}$ is a holomorphic family of closed operators in $\mathcal{H}$. In addition, if $\Re(m) \geq 1$, then

$$H_m = L_{m^2}^{\min} = L_{m^2}^{\max}.$$

For this reason, we shall concentrate on the case $-1 < \Re(m) < 1$, considering a larger family of operators.

For $|\Re(m)| < 1$ and for any $\kappa \in \mathbb{C} \cup \{\infty\}$ we define a family of operators $H_{m,\kappa}$:

$$\begin{aligned} \mathsf{D}(H_{m,\kappa}) = \big\{f \in \mathsf{D}(L_{m^2}^{\max}) \mid &\text{ for some } c \in \mathbb{C}, \qquad (3.7)\\ &f(x) - c\big(\kappa x^{1/2-m} + x^{1/2+m}\big) \in \mathsf{D}(L_{m^2}^{\min}) \text{ around } 0\big\}, \qquad \kappa \neq \infty;\\ \mathsf{D}(H_{m,\infty}) = \big\{f \in \mathsf{D}(L_{m^2}^{\max}) \mid &\text{ for some } c \in \mathbb{C}, \qquad (3.8)\\ &f(x) - cx^{1/2-m} \in \mathsf{D}(L_{m^2}^{\min}) \text{ around } 0\big\}. \end{aligned}$$

For $m = 0$, we introduce an additional family of operators H_0^ν with $\nu \in \mathbb{C} \cup \{\infty\}$:

$$\begin{aligned}\mathsf{D}(H_0^\nu) = \big\{ f \in \mathsf{D}(L_0^{\max}) \mid \ &\text{for some } c \in \mathbb{C}, \\ &f(x) - c\big(x^{1/2}\ln(x) + \nu x^{1/2}\big) \in \mathsf{D}(L_0^{\min}) \text{ around } 0\big\}, \qquad \nu \neq \infty; \end{aligned} \tag{3.9}$$

$$\begin{aligned}\mathsf{D}(H_0^\infty) = \big\{ f \in \mathsf{D}(L_0^{\max}) \mid \ &\text{for some } c \in \mathbb{C}, \\ &f(x) - cx^{1/2} \in \mathsf{D}(L_0^{\min}) \text{ around } 0\big\}.\end{aligned} \tag{3.10}$$

The following properties of these families of operators are immediate:

Lemma 3.4.1. *(i) For any $|\Re(m)| < 1$ and any $\kappa \in \mathbb{C} \cup \{\infty\}$,*

$$H_{m,\kappa} = H_{-m,\kappa^{-1}}. \tag{3.11}$$

(ii) The operator $H_{0,\kappa}$ does not depend on κ, and all these operators coincide with H_0^∞.

As a consequence of (ii), all the results about the case $m = 0$ will be formulated in terms of the family H_0^ν.

Let us now derive an additional result for this family of operators. For its proof, we recall that the Wronskian $W(f, g)$ of two continuously differentiable functions f, g on $\mathbb{R}_+$ is given by the expression

$$W_x(f, g) \equiv W(f, g)(x) := f(x)g'(x) - f'(x)g(x). \tag{3.12}$$

Proposition 3.4.2. *For any $m \in \mathbb{C}$ with $|\Re(m)| < 1$ and for any $\kappa, \nu \in \mathbb{C} \cup \{\infty\}$, one has*

$$(H_{m,\kappa})^* = H_{\bar{m},\bar{\kappa}} \qquad \text{and} \qquad (H_0^\nu)^* = H_0^{\bar{\nu}} \tag{3.13}$$

with the convention that $\bar{\infty} = \infty$.

Proof. Recall from [BDG, App. A] that for any $f \in \mathsf{D}(L_{m^2}^{\max})$ and $g \in \mathsf{D}(L_{\bar{m}^2}^{\max})$, the functions f, f', g, g' are continuous on $\mathbb{R}_+$, and that the equality

$$\langle L_{m^2}^{\max} f, g\rangle - \langle f, L_{\bar{m}^2}^{\max} g\rangle = -W_0(\bar{f}, g)$$

holds with $W_0(\bar{f}, g) = \lim_{x\to 0} W_x(\bar{f}, g)$ and W_x defined in (3.12). In particular, if $f \in \mathsf{D}(H_{m,\kappa})$ one infers that

$$\langle H_{m,\kappa} f, g\rangle = \langle f, L_{\bar{m}^2}^{\max} g\rangle - W_0(\bar{f}, g).$$

Thus, $g \in \mathsf{D}\big((H_{m,\kappa})^*\big)$ if and only if $W_0(\bar{f}, g) = 0$, and then $(H_{m,\kappa})^* g = L_{\bar{m}^2}^{\max} g$. Then, by taking into account the explicit description of $\mathsf{D}(H_{m,\kappa})$, straightforward computations show that $W_0(\bar{f}, g) = 0$ if and only if $g \in \mathsf{D}(H_{\bar{m},\bar{\kappa}})$. One then deduces that $(H_{m,\kappa})^* = H_{\bar{m},\bar{\kappa}}$.

A similar computation leads to the equality $(H_0^\nu)^* = H_0^{\bar{\nu}}$. □

Corollary 3.4.3. *(i) The operator $H_{m,\kappa}$ is self-adjoint for $m \in]-1,1[$ and $\kappa \in \mathbb{R} \cup \{\infty\}$, and for $m \in i\mathbb{R}$ and $|\kappa| = 1$.*

(ii) The operator H_0^ν is self-adjoint for $\nu \in \mathbb{R} \cup \{\infty\}$.

Proof. For the operators $H_{m,\kappa}$ one simply has to take formula (3.13) into account for the first case, and the same formula together with (3.11) in the second case. Finally for the operators H_0^ν, taking formula (3.13) into account leads directly to the result. □

Let us finally state the a result about the point spectrum for the self-adjoint operators. In this statement, Γ denotes the Γ-function.

Theorem 3.4.4. *(i) If $m \in]-1,1[\backslash\{0\}$, then $H_{m,\kappa}$ is self-adjoint if and only if $\kappa \in \mathbb{R} \cup \{\infty\}$, and then*

$$\sigma_p(H_{m,\kappa}) = \Big\{ -4\Big(\kappa\frac{\Gamma(-m)}{\Gamma(m)}\Big)^{-1/m}\Big\} \quad \text{for } \kappa \in]-\infty, 0[,$$
$$\sigma_p(H_{m,\kappa}) = \emptyset \quad \text{for } \kappa \in [0,\infty],$$

(ii) If $m = im_i \in i\mathbb{R} \setminus \{0\}$, then $H_{im_i,\kappa}$ is self-adjoint if and only if $|\kappa| = 1$, and then

$$\sigma_p(H_{im_i,\kappa}) = \Bigg\{ -4\exp\Bigg(-\frac{\arg\big(\kappa\frac{\Gamma(-im_i)}{\Gamma(im_i)}\big) + 2\pi j}{m_i}\Bigg) \mid j \in \mathbb{Z}\Bigg\}$$

(iii) H_0^ν is self-adjoint if and only if $\nu \in \mathbb{R} \cup \{\infty\}$, and then

$$\sigma_p(H_0^\nu) = \big\{ -4\,\mathrm{e}^{2(\nu-\gamma)}\big\} \quad \text{for } \nu \in \mathbb{R},$$
$$\sigma_p(H_0^\infty) = \emptyset.$$

The proof of this theorem, as well as much more information about these families of operators, can be found in the preprint [DR].

Chapter 4

Spectral theory for self-adjoint operators

In this chapter we develop the spectral theory for self-adjoint operators. As already seen in Lemma 2.2.6, these operators have real spectrum, however much more can be said about them, and in particular the spectrum can be divided into several parts having distinct properties. Note that this chapter is mainly inspired from Chapter 4 of [Amr] to which we refer for additional information.

4.1 Stieltjes measures

We start by introducing Stieltjes measures, since they will be the key ingredient for the spectral theorem. For that purpose, let us consider a function $F : \mathbb{R} \to \mathbb{R}$ satisfying the following properties:

(i) F is monotone non-decreasing, *i.e.* $\lambda \geq \mu \Longrightarrow F(\lambda) \geq F(\mu)$,

(ii) F is right continuous, *i.e.* $F(\lambda) = F(\lambda + 0) := \lim_{\varepsilon \searrow 0} F(\lambda + \varepsilon)$ for all $\lambda \in \mathbb{R}$,

(iii) $F(-\infty) := \lim_{\lambda \to -\infty} F(\lambda) = 0$ and $F(+\infty) := \lim_{\lambda \to +\infty} F(\lambda) < \infty$.

Note that $F(\lambda + 0) := \lim_{\varepsilon \searrow 0} F(\lambda + \varepsilon)$ and $F(\lambda - 0) := \lim_{\varepsilon \searrow 0} F(\lambda - \varepsilon)$ exist since F is a monotone and bounded function.

Exercise 4.1.1. *Show that such a function has at most a countable set of points of discontinuity. For that purpose you can consider for fixed $n \in \mathbb{N}$ the set of points $\lambda \in \mathbb{R}$ for which $F(\lambda) - F(\lambda - 0) > 1/n$.*

With a function F having these properties, one can associate a bounded Borel measure m_F on $\mathbb{R}$, called *Stieltjes measure*, starting with

$$m_F\big((a, b]\big) := F(b) - F(a), \qquad a, b \in \mathbb{R} \tag{4.1}$$

and extending then this definition to all Borel sets of $\mathbb{R}$ (we denote by $\mathcal{A}_B$ the set of all Borel sets on $\mathbb{R}$). More precisely, for any set $V \in \mathcal{A}_B$ one sets

$$m_F(V) = \inf \sum_k m_F(J_k)$$

with $\{J_k\}$ any sequence of half-open intervals covering the set V, and the infimum is taken over all such covering of V. With this definition, note that $m_F(\mathbb{R}) = F(+\infty)$ and that

$$m_F\big((a,b)\big) = F(b-0) - F(a), \qquad m_F\big([a,b]\big) = F(b) - F(a-0)$$

and therefore $m_F\big(\{a\}\big) = F(a) - F(a-0)$ is different from 0 if F is not continuous at the point a.

Note that starting with a bounded Borel measure m on $\mathbb{R}$ and setting $F(\lambda) := m\big((-\infty,\lambda]\big)$, then F satisfies the conditions (i)-(iii) and the associated Stieltjes measure m_F verifies $m_F = m$. Observe also that if the measure is not bounded one can not have $F(+\infty) < \infty$. Less restrictively, if the measure is not bounded on any bounded Borel set, then the function F can not even be defined.

Exercise 4.1.2. *Work on the examples of functions F introduced in Examples 4.1 to 4.5 of [Amr], and describe the corresponding Stieltjes measures.*

Let us now recall the three types of measures on $\mathbb{R}$that are going to play an important role in the decomposition of any self-adjoint operator. First of all, a Borel measure is called *pure point* or *atomic* if the measure is supported by points only. More precisely, a Borel measure m is of this type if for any Borel set V there exists a collection of points $\{x_j\} \subset V$ such that

$$m(V) = \sum_j m(\{x_j\}).$$

Note that for Stieltjes measure, this set of points is at most countable. Secondly, a Borel measure m is absolutely continuous with respect to the Lebesgue measure if there exists a non-negative measurable function f such that for any Borel set V one has

$$m(V) = \int_V f(x)\mathrm{d}x$$

where $\mathrm{d}x$ denotes the Lebesgue measure on $\mathbb{R}$. Thirdly, a Borel measure m is singular continuous with respect to the Lebesgue measure if $m(\{x\}) = 0$ for any $x \in \mathbb{R}$ and if there exists a Borel set V of Lebesgue measure 0 such that the support of m is concentrated on V. Note that examples of such singular continuous measure can be constructed with Cantor functions, see for example [Amr, Ex. 4.5].

The following theorem is based on the Lebesgue decomposition theorem for measures.

Theorem 4.1.3. *Any Stieltjes measure m admits a unique decomposition*

$$m = m_p + m_{ac} + m_{sc}$$

where m_p *is* a pure point measure *(with at most a countable support),* m_{ac} *is* an absolutely continuous measure *with respect to the Lebesgue measure on* $\mathbb{R}$*, and* m_{sc} *is* a singular continuous measure *with respect to the Lebesgue measure* $\mathbb{R}$*.*

4.2 Spectral measures

We shall now define a spectral measure, by analogy with the Stieltjes measure introduced in the previous section. Indeed, instead of considering non-decreasing functions F defined on $\mathbb{R}$ and taking values in $\mathbb{R}$, we shall consider non-decreasing functions defined on $\mathbb{R}$ but taking values in the set $\mathcal{P}(\mathcal{H})$ of orthogonal projections on a Hilbert space $\mathcal{H}$.

Definition 4.2.1. A spectral family*, or* a resolution of the identity*, is a family* $\{E_\lambda\}_{\lambda\in\mathbb{R}}$ *of orthogonal projections in* $\mathcal{H}$ *satisfying:*

(i) The family is non-decreasing, i.e. $E_\lambda E_\mu = E_{\min\{\lambda,\mu\}}$*,*

(ii) The family is strongly right continuous, i.e. $E_\lambda = E_{\lambda+0} = s-\lim_{\varepsilon\searrow 0} E_{\lambda+\varepsilon}$*,*

(iii) $s-\lim_{\lambda\to-\infty} E_\lambda = \mathbf{0}$ *and* $s-\lim_{\lambda\to\infty} E_\lambda = \mathbf{1}$*,*

It is important to observe that the condition (i) implies that the elements of the families are *commuting, i.e.* $E_\lambda E_\mu = E_\mu E_\lambda$. We also define *the support of the spectral family* as the following subset of $\mathbb{R}$:

$$\operatorname{supp}\{E_\lambda\} = \big\{\mu\in\mathbb{R} \mid E_{\mu+\varepsilon} - E_{\mu-\varepsilon} \neq \mathbf{0},\ \forall\varepsilon>0\big\}.$$

Given such a family and in analogy with (4.1), one first defines

$$E\big((a,b]\big) := E_b - E_a, \qquad a,b\in\mathbb{R}, \tag{4.2}$$

and extends this definition to all sets $V\in\mathcal{A}_B$. As a consequence of the construction, note that

$$E\Big(\bigcup_k V_k\Big) = \sum_k E(V_k) \tag{4.3}$$

whenever $\{V_k\}$ is a countable family of disjoint elements of $\mathcal{A}_B$. Thus, one ends up with a projection-valued map $E:\mathcal{A}_B\to\mathcal{P}(\mathcal{H})$ which satisfies $E(\emptyset)=\mathbf{0}$, $E(\mathbb{R})=\mathbf{1}$, $E(V_1)E(V_2)=E(V_1\cap V_2)$ for any Borel sets V_1,V_2. In addition,

$$E\big((a,b)\big) = E_{b-0} - E_a, \qquad E\big([a,b]\big) = E_b - E_{a-0}$$

and therefore $E\big(\{a\}\big) = E_a - E_{a-0}$.

Definition 4.2.2. *The map* $E:\mathcal{A}_B\to\mathcal{P}(\mathcal{H})$ *defined by* (4.2) *is called* the spectral measure *associated with the family* $\{E_\lambda\}_{\lambda\in\mathbb{R}}$*. This spectral measure is* bounded from below *if there exists* $\lambda_-\in\mathbb{R}$ *such that* $E_\lambda=\mathbf{0}$ *for all* $\lambda<\lambda_-$*. Similarly, this spectral measure is* bounded from above *if there exists* $\lambda_+\in\mathbb{R}$ *such that* $E_\lambda=\mathbf{1}$ *for all* $\lambda>\lambda_+$*.*

Let us note that for any spectral family $\{E_\lambda\}_{\lambda\in\mathbb{R}}$ and any $f \in \mathcal{H}$ one can set

$$F_f(\lambda) := \|E_\lambda f\|^2 = \langle E_\lambda f, f\rangle.$$

Then, one easily checks that the function F_f satisfies the conditions (i)-(iii) of the beginning of Section 4.1. Thus, one can associate with each element $f \in \mathcal{H}$ a Stieltjes measure m_f on $\mathbb{R}$ which satisfies

$$m_f(V) = \|E(V)f\|^2 = \langle E(V)f, f\rangle \tag{4.4}$$

for any $V \in \mathcal{A}_B$. Note in particular that $m_f(\mathbb{R}) = \|f\|^2$. Later on, this Stieltjes measure will be decomposed according the content of Theorem 4.1.3.

Our next aim is to define integrals of the form

$$\int_a^b \varphi(\lambda)\, E(\mathrm{d}\lambda) \tag{4.5}$$

for a continuous function $\varphi : [a, b] \to \mathbb{C}$ and for any spectral family $\{E_\lambda\}_{\lambda\in\mathbb{R}}$. Such integrals can be defined in the sense of Riemann-Stieltjes by first considering a partition $a = x_0 < x_1 < ... < x_n = b$ of $[a, b]$ and a collection $\{y_j\}$ with $y_j \in (x_{j-1}, x_j)$ and by defining the operator

$$\sum_{j=1}^n \varphi(y_j)E\big((x_{j-1}, x_j]\big). \tag{4.6}$$

It turns out that by considering finer and finer partitions of $[a, b]$, the corresponding expression (4.6) strongly converges to an element of $\mathscr{B}(\mathcal{H})$ which is independent of the successive choice of partitions. The resulting operator is denoted by (4.5).

The following statement contains usual results which can be obtained in this context. The proof is not difficult, but one has to deal with several partitions of intervals. We refer to [Amr, Prop. 4.10] for a detailed proof.

Proposition 4.2.3 (Spectral integrals)**.** *Let $\{E_\lambda\}_{\lambda\in\mathbb{R}}$ be a spectral family, let $-\infty < a < b < \infty$ and let $\varphi : [a, b] \to \mathbb{C}$ be continuous. Then one has*

(i) $\Big\|\int_a^b \varphi(\lambda)\, E(\mathrm{d}\lambda)\Big\| = \sup_{\mu\in[a,b]\cap \mathrm{supp}\{E_\lambda\}} |\varphi(\mu)|$,

(ii) $\Big(\int_a^b \varphi(\lambda)\, E(\mathrm{d}\lambda)\Big)^* = \int_a^b \overline{\varphi}(\lambda)\, E(\mathrm{d}\lambda)$,

(iii) For any $f \in \mathcal{H}$, $\Big\|\int_a^b \varphi(\lambda)\, E(\mathrm{d}\lambda)f\Big\|^2 = \int_a^b |\varphi(\lambda)|^2\, m_f(\mathrm{d}\lambda)$,

(iv) If $\psi : [a, b] \to \mathbb{C}$ is continuous, then

$$\int_a^b \varphi(\lambda)\, E(\mathrm{d}\lambda) \cdot \int_a^b \psi(\lambda)\, E(\mathrm{d}\lambda) = \int_a^b \varphi(\lambda)\, \psi(\lambda)\, E(\mathrm{d}\lambda).$$

Let us now observe that if the support $\mathrm{supp}\{E_\lambda\}$ is bounded, then one can consider

$$\int_{-\infty}^{\infty} \varphi(\lambda)\, E(\mathrm{d}\lambda) = s - \lim_{M\to\infty} \int_{-M}^{M} \varphi(\lambda)\, E(\mathrm{d}\lambda). \tag{4.7}$$

Similarly, by taking property (iii) of the previous proposition into account, one observes that this limit can also be taken if $\varphi \in C_b(\mathbb{R})$. On the other hand, if φ is not bounded on $\mathbb{R}$, the r.h.s. of (4.7) is not necessarily well defined. In fact, if φ is not bounded on $\mathbb{R}$ and if $\mathrm{supp}\{E_\lambda\}$ is not bounded either, then the r.h.s. of (4.7) is an unbounded operator and can only be defined on a dense domain of $\mathcal{H}$.

Lemma 4.2.4. *Let $\varphi : \mathbb{R} \to \mathbb{C}$ be continuous, and let us set*

$$\mathsf{D}_\varphi := \Big\{f \in \mathcal{H} \mid \int_{-\infty}^{\infty} |\varphi(\lambda)|^2\, m_f(\mathrm{d}\lambda) < \infty\Big\}.$$

Then the pair $\Big(\int_{-\infty}^{\infty} \varphi(\lambda)\, E(\mathrm{d}\lambda), \mathsf{D}_\varphi\Big)$ defines a closed linear operator on $\mathcal{H}$. This operator is self-adjoint if and only if φ is a real function.

Proof. Observe first that $\mathsf{D}_\varphi = \mathsf{D}_{\overline{\varphi}}$, and set $A := \int_{-\infty}^{\infty} \varphi(\lambda)\, E(\mathrm{d}\lambda)$. A is densely defined because its domain contains all elements with compact support with respect to $\{E_\lambda\}$, *i.e.* it contains all $g \in \mathcal{H}$ satisfying $g = E\big((-N,N]\big)g$ for some $N < \infty$. Thus, for $f, g \in \mathsf{D}_\varphi$ one has by the point (ii) of Proposition 4.2.3

$$\begin{aligned}\langle f, Ag\rangle &= \lim_{M\to\infty} \Big\langle f, \int_{-M}^{M} \varphi(\lambda)\, E(\mathrm{d}\lambda) g\Big\rangle \\ &= \lim_{M\to\infty} \Big\langle \int_{-M}^{M} \overline{\varphi}(\lambda)\, E(\mathrm{d}\lambda) f, g\Big\rangle = \Big\langle \int_{-\infty}^{\infty} \overline{\varphi}(\lambda)\, E(\mathrm{d}\lambda) f, g\Big\rangle.\end{aligned}$$

It thus follows that $\mathsf{D}_{\overline{\varphi}} \subset \mathsf{D}(A^*)$, and that $A^* f = \int_{-\infty}^{\infty} \overline{\varphi}(\lambda)\, E(\mathrm{d}\lambda) f$ for any $f \in \mathsf{D}_{\overline{\varphi}}$. As a consequence A^* is an extension of $\int_{-\infty}^{\infty} \overline{\varphi}(\lambda)\, E(\mathrm{d}\lambda)$, and in order to show that these two operators are equal it is sufficient to show that $\mathsf{D}(A^*) \subset \mathsf{D}_{\overline{\varphi}}$.

For that purpose, recall that if $f \in \mathsf{D}(A^*)$ there exists $f^* \in \mathcal{H}$ such that for any $g \in \mathsf{D}_\varphi$

$$\langle f, Ag\rangle = \langle f^*, g\rangle.$$

In particular this equality holds if g has compact support with respect to $\{E_\lambda\}$. One then gets for any $M \in (0,\infty)$

$$\begin{aligned}
\big\|E\big((-M,M]\big)f^*\big\| &= \sup_{g\in\mathcal{H},\|g\|=1} \big|\big\langle E\big((-M,M]\big)f^*, g\big\rangle\big| \\
&= \sup_{g\in\mathcal{H},\|g\|=1} \big|\big\langle f^*, E\big((-M,M]\big)g\big\rangle\big| \\
&= \sup_{g\in\mathcal{H},\|g\|=1} \Big|\Big\langle f, \int_{-M}^{M} \varphi(\lambda)\, E(\mathrm{d}\lambda)g\Big\rangle\Big| \\
&= \sup_{g\in\mathcal{H},\|g\|=1} \Big|\Big\langle \int_{-M}^{M} \overline{\varphi}(\lambda)\, E(\mathrm{d}\lambda)f, g\Big\rangle\Big| \\
&= \Big\|\int_{-M}^{M} \overline{\varphi}(\lambda)\, E(\mathrm{d}\lambda)f\Big\| = \Big(\int_{-M}^{M} |\varphi(\lambda)|^2 m_f(\mathrm{d}\lambda)\Big)^{1/2}.
\end{aligned}$$

As a consequence, one has

$$\sup_{M>0} \int_{-M}^{M} |\varphi(\lambda)|^2 m_f(\mathrm{d}\lambda) \leq \|f^*\|^2 < \infty$$

from which one infers that $\int_{-\infty}^{\infty} |\varphi(\lambda)|^2 m_f(\mathrm{d}\lambda) < \infty$. This shows that if $f \in \mathsf{D}(A^*)$ then $f \in \mathsf{D}_{\overline{\varphi}}$.

Since A^* is always closed by (i) of Lemma 2.1.10, one infers that $\int_{-\infty}^{\infty} \overline{\varphi}(\lambda)\, E(\mathrm{d}\lambda)$ on $\mathsf{D}_{\overline{\varphi}}$ is a closed operator. So the same holds for A on D_φ. Finally, since $\mathsf{D}_\varphi = \mathsf{D}_{\overline{\varphi}}$, the second statement is a direct consequence of the first one. □

A function φ of special interest is the function defined by the identity function id, namely $\mathrm{id}(\lambda) = \lambda$.

Definition 4.2.5. *For any spectral family $\{E_\lambda\}_{\lambda\in\mathbb{R}}$, the operator $\Big(\int_{-\infty}^{\infty} \lambda\, E(\mathrm{d}\lambda), \mathsf{D}_{\mathrm{id}}\Big)$ with*

$$\mathsf{D}_{\mathrm{id}} := \Big\{f \in \mathcal{H} \mid \int_{-\infty}^{\infty} \lambda^2\, m_f(\mathrm{d}\lambda) < \infty\Big\}$$

is called the self-adjoint operator associated with $\{E_\lambda\}$.

By this procedure, any spectral family defines a self-adjoint operator on $\mathcal{H}$. *The spectral Theorem* corresponds to the converse statement:

Theorem 4.2.6 (Spectral Theorem)**.** *With any self-adjoint operator $(A, \mathsf{D}(A))$ on a Hilbert space $\mathcal{H}$ one can associate a unique spectral family $\{E_\lambda\}$, called* the spectral family of A, *such that $\mathsf{D}(A) = \mathsf{D}_{\mathrm{id}}$ and $A = \int_{-\infty}^{\infty} \lambda\, E(\mathrm{d}\lambda)$.*

In summary, there is a bijective correspondence between self-adjoint operators and spectral families. This theorem extends the fact that any $n \times n$ hermitian matrix is diagonalizable. The proof of this theorem is not trivial and is rather lengthy. In the sequel, we shall assume it, and state various consequences of this theorem.

Extension 4.2.7. *Study the proof the Spectral Theorem, starting with the version for bounded self-adjoint operators.*

Based on this one-to-one correspondence it is now natural to set the following definition:

Definition 4.2.8. *Let A be a self-adjoint operator in $\mathcal{H}$ and $\{E_\lambda\}$ be the corresponding spectral family. For any bounded and continuous function $\varphi : \mathbb{R} \to \mathbb{C}$ one sets $\varphi(A) \in \mathscr{B}(\mathcal{H})$ for the operator defined by*

$$\varphi(A) := \int_{-\infty}^{\infty} \varphi(\lambda)\, E(\mathrm{d}\lambda). \tag{4.8}$$

Exercise 4.2.9. *For any self-adjoint operator A, prove the following equality:*

$$\operatorname{supp}\{E_\lambda\} = \sigma(A). \tag{4.9}$$

Note that part of the proof consists in showing that if $\varphi_z(\lambda) = (\lambda - z)^{-1}$ for some $z \in \rho(A)$, then $\varphi_z(A) = (A - z)^{-1}$, where the r.h.s. has been defined in Section 2.2. Let us also mention a useful equality which can be proved in this exercise: for any $z \in \rho(A)$ one has

$$\big\|(A - z)^{-1}\big\| = \big[\operatorname{dist}\big(z, \sigma(A)\big)\big]^{-1}. \tag{4.10}$$

For the next statement, we set $C_b(\mathbb{R})$ for the set of all continuous and bounded complex functions on $\mathbb{R}$.

Proposition 4.2.10. *a) For any $\varphi \in C_b(\mathbb{R})$ one has*

(i) $\varphi(A) \in \mathscr{B}(\mathcal{H})$ and $\|\varphi(A)\| = \sup_{\lambda \in \sigma(A)} |\varphi(\lambda)|$,

(ii) $\varphi(A)^* = \overline{\varphi}(A)$, and $\varphi(A)$ is self-adjoint if and only if φ is real,

(iii) $\varphi(A)$ is unitary if and only if $|\varphi(\lambda)| = 1$.

b) The map $C_b(\mathbb{R}) \ni \varphi \mapsto \varphi(A) \in \mathscr{B}(\mathcal{H})$ is a $*$-homomorphism.

c) If $\varphi \in C(\mathbb{R})$, then (4.8) defines a closed operator $\varphi(A)$ with domain

$$\mathsf{D}\big(\varphi(A)\big) = \Big\{ f \in \mathcal{H} \mid \int_{-\infty}^{\infty} |\varphi(\lambda)|^2\, m_f(\mathrm{d}\lambda) < \infty \Big\}. \tag{4.11}$$

In the point (iii) above, one can consider the function $\varphi_t \in C_b(\mathbb{R})$ defined by $\varphi_t(\lambda) := \mathrm{e}^{-i\lambda t}$ for any fixed $t \in \mathbb{R}$. Then, if one sets $U_t := \varphi_t(A)$ one first observes that $U_t U_s = U_{t+s}$. Indeed, one has

$$\begin{aligned} U_t U_s &= \int_{-\infty}^{\infty} \mathrm{e}^{i\lambda t}\, E(\mathrm{d}\lambda) \int_{-\infty}^{\infty} \mathrm{e}^{-i\lambda s}\, E(\mathrm{d}\lambda) = \int_{-\infty}^{\infty} \mathrm{e}^{-i\lambda t}\, \mathrm{e}^{-i\lambda s}\, E(\mathrm{d}\lambda) \\ &= \int_{-\infty}^{\infty} \mathrm{e}^{-i\lambda(t+s)}\, E(\mathrm{d}\lambda) = U_{t+s}. \end{aligned}$$

In addition, by an application of the dominated convergence theorem of Lebesgue, one infers that the map $\mathbb{R} \ni t \mapsto U_t \in \mathscr{B}(\mathcal{H})$ is strongly continuous. Indeed, since $\big| \mathrm{e}^{-i\lambda(t+\varepsilon)} - \mathrm{e}^{-i\lambda t} \big|^2 \leq 4$ one has

$$\|U_{t+\varepsilon}f - U_t f\|^2 = \int_{-\infty}^{\infty} \big| \mathrm{e}^{-i\lambda(t+\varepsilon)} - \mathrm{e}^{-i\lambda t} \big|^2 m_f(\mathrm{d}\lambda) \ \to\ 0 \quad \text{as} \quad \varepsilon \to 0.$$

As a consequence, such a family $\{U_t\}_{t\in\mathbb{R}}$ is called *a strongly continuous unitary group.* Note that since $\mathrm{e}^{-i\lambda t} = \sum_{k=0}^{\infty} \frac{(-i\lambda t)^k}{k!}$ one also infers that whenever A is a bounded operator

$$U_t = \sum_{k=0}^{\infty} \frac{(-itA)^k}{k!} \tag{4.12}$$

with a norm converging series. On the other hand, if A is not bounded, then this series converges on elements $f \in \cap_{k=0}^{\infty} \mathsf{D}(A^k)$. In particular, it converges strongly on elements of $\mathcal{H}$ which have compact support with respect to the corresponding spectral measure.

Let us now mention that the above construction is only one part of a one-to-one relation between strongly continuous unitary groups and self-adjoint operators. The proof of the following statement can be found for example in [Amr, Prop. 5.1].

Theorem 4.2.11 (Stone's Theorem)**.** *There exists a bijective correspondence between self-adjoint operators on $\mathcal{H}$ and strongly continuous unitary groups on $\mathcal{H}$. More precisely, if A is a self-adjoint operator on $\mathcal{H}$, then $\{\mathrm{e}^{-itA}\}_{t\in\mathbb{R}}$ is a strongly continuous unitary group, while if $\{U_t\}_{t\in\mathbb{R}}$ is a strongly continuous unitary group, one sets*

$$\mathsf{D}(A) := \Big\{ f \in \mathcal{H} \mid \exists\ s - \lim_{t\to 0} \frac{1}{t}[U_t - 1]f \Big\}$$

and for $f \in \mathsf{D}(A)$ one sets $Af = s - \lim_{t\to 0} \frac{i}{t}[U_t - 1]f$, and then $\big(A, \mathsf{D}(A)\big)$ is a self-adjoint operator.

Exercise 4.2.12. *Provide a precise proof of Stone's theorem.*

Let us close with section with two important observations. First of all, the map $\varphi \mapsto \varphi(A)$ can be extended from continuous and bounded φ to bounded and measurable functions φ. This extension can be realized by considering the Lebesgue-Stieltjes integrals in the weak form. In particular, this extension is necessary for defining $\varphi(A)$ whenever φ is the characteristic function on some Borel set V.

The second observation is going to provide an alternative formula for $\varphi(A)$ in terms of the unitary group $\{\mathrm{e}^{-itA}\}_{t\in\mathbb{R}}$. Indeed, assume that the inverse Fourier transform $\check{\varphi}$ of φ belongs to $L^1(\mathbb{R})$, then the following equality holds

$$\varphi(A) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \check{\varphi}(t)\ \mathrm{e}^{-itA}\ \mathrm{d}t. \tag{4.13}$$

Indeed, observe that

$$\langle f, \varphi(A) f\rangle = \int_{\mathbb{R}} \varphi(\lambda) m_f(\mathrm{d}\lambda) = \int_{\mathbb{R}} m_f(\mathrm{d}\lambda) \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{e}^{-i\lambda t}\ \check{\varphi}(t)\mathrm{d}t.$$

By application of Fubini's theorem one can interchange the order of integrations and obtain

$$\begin{aligned}\langle f, \varphi(A)f\rangle =& \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \mathrm{d}t\check{\varphi}(t)\int_{\mathbb{R}} \mathrm{e}^{-i\lambda t}\, m_f(\mathrm{d}\lambda)\\ =& \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \mathrm{d}t\,\check{\varphi}(t)\langle f, \mathrm{e}^{-itA} f\rangle = \Big\langle f, \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \mathrm{d}t\,\check{\varphi}(t)\,\mathrm{e}^{-itA} f\Big\rangle,\end{aligned}$$

and one gets (4.13) by applying the polarisation identity (1.1).

4.3 Spectral parts of a self-adjoint operator

In this section, we consider a fixed self-adjoint operator A (and its associated spectral family $\{E_\lambda\}$), and show that there exists a natural decomposition of the Hilbert space $\mathcal{H}$ with respect to this operator. First of all, recall from Lemma 2.2.6 that the spectrum of any self-adjoint operator is real. In addition, let us recall that for any $\mu \in \mathbb{R}$, one has

$$\mathsf{Ran}\,\big(E(\{\mu\})\big) = \{f \in \mathcal{H} \mid E(\{\mu\})f = f\}.$$

Then, one observes that the following equivalence holds:

$$f \in \mathsf{Ran}\,\big(E(\{\mu\})\big) \Longleftrightarrow f \in \mathsf{D}(A) \ \text{ with } Af = \mu f.$$

Indeed, this can be inferred from the equality

$$\|Af - \mu f\|^2 = \int_{-\infty}^{\infty} |\lambda - \mu|^2\, m_f(\mathrm{d}\lambda)$$

which itself can be deduced from the point (iii) of Proposition 4.2.3. In fact, since the integrand is strictly positive for each $\lambda \neq \mu$, one has $\|Af - \mu f\| = 0$ if and only if $m_f(V) = 0$ for any Borel set V on $\mathbb{R}$ with $\mu \notin V$. In other words, the measure m_f is supported only on $\{\mu\}$.

Definition 4.3.1. *The set of all $\mu \in \mathbb{R}$ such that* $\mathsf{Ran}\,\big(E(\{\mu\})\big) \neq 0$ *is called* the point spectrum of A *or* the set of eigenvalues of A. *One then sets*

$$\mathcal{H}_p(A) := \bigoplus \mathsf{Ran}\,\big(E(\{\mu\})\big)$$

where the sum extends over all eigenvalues of A.

In accordance with what has been presented in Theorem 4.1.3, we define two additional subspaces of $\mathcal{H}$.

Definition 4.3.2.

$$\begin{aligned}\mathcal{H}_{ac}(A) \;&:=\; \big\{f \in \mathcal{H} \mid m_f \textit{ is an absolutely continuous measure}\big\}\\ &=\; \big\{f \in \mathcal{H} \mid \textit{ the function } \lambda \mapsto \|E_\lambda f\|^2 \textit{ is absolutely continuous}\big\},\end{aligned}$$

$$\begin{aligned}\mathcal{H}_{sc}(A) &:= \big\{f \in \mathcal{H} \mid m_f \textit{ is a singular continuous measure}\big\}\\ &= \big\{f \in \mathcal{H} \mid \textit{ the function } \lambda \mapsto \|E_\lambda f\|^2 \textit{ is singular continuous}\big\},\end{aligned}$$

for which the comparison measure is always the Lebesgue measure on $\mathbb{R}$.

Note that one also uses the notation $\mathcal{H}_c(A)$ for the set of $f \in \mathcal{H}$ such that m_f is continuous, *i.e.* $m_f(\{x\}) = 0$ for any $x \in \mathbb{R}$. One also speaks then about the continuous subspace of $\mathcal{H}$ with respect to A.

The following statement provides the decomposition of any self-adjoint operator into three distinct parts. Note that depending on the operators, some parts of the following decomposition can be trivial. The proof of the statement is not difficult and consists in some routine computations.

Theorem 4.3.3. *Let A be a self-adjoint operator in a Hilbert space $\mathcal{H}$.*
a) This Hilbert space can be decomposed as follows

$$\mathcal{H} = \mathcal{H}_p(A) \oplus \mathcal{H}_{ac}(A) \oplus \mathcal{H}_{sc}(A),$$

and the restriction of the operator A to each of these subspaces defines a self-adjoint operator denoted respectively by A_p, A_{ac} and A_{sc}.
b) For any $\varphi \in C_b(\mathbb{R})$, one has the decomposition

$$\varphi(A) = \varphi(A_p) \oplus \varphi(A_{ac}) \oplus \varphi(A_{sc}).$$

Moreover, the following equality holds

$$\sigma(A) = \sigma(A_p) \cup \sigma(A_{ac}) \cup \sigma(A_{sc}).$$

Exercise 4.3.4. *Provide a full proof of the above statement.*

Note that one often writes $E_p(A)$, $E_{ac}(A)$ and $E_{sc}(A)$ for the orthogonal projection on $\mathcal{H}_p(A)$, $\mathcal{H}_{ac}(A)$ and $\mathcal{H}_{sc}(A)$, respectively, and with these notations one has $A_p = AE_p(A)$, $A_{ac} = AE_{ac}(A)$ and $A_{sc} = AE_{sc}(A)$. In addition, note that the relation between the set of eigenvalues $\sigma_p(A)$ introduced in Definition 2.2.4 and the set $\sigma(A_p)$ is

$$\sigma(A_p) = \overline{\sigma_p(A)}.$$

Two additional sets are often introduced in relation with the spectrum of A, namely $\sigma_d(A)$ and $\sigma_{ess}(A)$.

Definition 4.3.5. *An eigenvalue λ belongs to* the discrete spectrum $\sigma_d(A)$ of A *if and only if* $\mathsf{Ran}\big(E(\{\lambda\})\big)$ *is of finite dimension, and λ is isolated from the rest of the spectrum of A.* The essential spectrum $\sigma_{ess}(A)$ of A *is the complementary set of $\sigma_d(A)$ in $\sigma(A)$, or more precisely*

$$\sigma_{ess}(A) = \sigma(A) \setminus \sigma_d(A).$$

Since we have now all type of spectra at our disposal, let us come back to the examples of Chapter 3. As already mentioned in Exercise 3.1.2 the spectrum of any self-adjoint multiplication operator $\varphi(X)$ in $L^2(\mathbb{R}^d)$ is given by the closure of $\varphi(\mathbb{R}^d)$. Now, it is easily observed that $\lambda \in \sigma_p\big(\varphi(X)\big)$ if and only if there exists a Borel set V with strictly positive Lebesgue measure such that $\varphi(x) = \lambda$ for any $x \in V$. In this case, the multiplicity of the eigenvalue is infinite, since an infinite family of orthogonal eigenfunctions corresponding to the eigenvalue λ can easily be constructed. Obviously, the previous requirement is not necessary for $\lambda \in \sigma_{ess}\big(\varphi(X)\big)$. Let us also mention that if the function φ is continuously differentiable and if $\nabla\varphi(x) \neq 0$ for any $x \in \mathbb{R}^d$, then the operator $\varphi(X)$ has only absolutely continuous spectrum. Such a statement will be a consequence of the conjugate operator method introduced in subsequent chapters. Note also that for a convolution operator $\varphi(D)$ the situation is rather similar, and this can be deduced easily from Remark 4.3.6.

For the harmonic oscillator of Section 3.1.1, the corresponding operator has only discrete eigenvalues and no continuous spectrum, *i.e.* $\mathcal{H}_c(A) = \{0\}$. For Schrödinger operators, one has typically a mixture of continuous spectrum and of point spectrum. Note that the eigenvalues can be embedded in the continuous spectrum, but that the situation of eigenvalues below the continuous spectrum often appears for such operators. For the hydrogen atom of Section 3.2.1 this situation takes place, since the continuous spectrum corresponds to $[0, \infty)$ while the point spectrum consists in the eigenvalues which are all located below 0 and are converging to 0. For more general Schrödinger operators, it is also often expected that $\mathcal{H}_{sc}(A) = \{0\}$, but proving such a statement can be a difficult task. We shall come back to this question in the following chapters.

Let us still consider any compact self-adjoint operator A in a Hilbert space $\mathcal{H}$. It is easily observed that for any $\varepsilon > 0$ the subspace $E\big((-\infty, -\varepsilon]\big)\mathcal{H} \cup E\big([\varepsilon, \infty)\big)\mathcal{H}$ is of finite dimension, where $E(\cdot)$ corresponds to the spectral measure associated with A. In other words, away from 0 the spectrum of A consists of eigenvalues of finite multiplicity, and these eigenvalues can only converge to 0. On the other hand, 0 can be either an eigenvalue with finite or infinite multiplicity, or a point of accumulation of the spectrum without being itself a eigenvalue.

Remark 4.3.6. *If A is a self-adjoint operator in a Hilbert space $\mathcal{H}$ and if U is a unitary operator in $\mathcal{H}$, conjugating A by U does not change its spectral properties. More precisely, in one considers $A_U := UAU^*$ with domain $\mathsf{D}(A_U) = U\mathsf{D}(A)$, then this operator is self-adjoint and the following equalities hold: $\sigma(A_U) = \sigma(A)$, $\sigma_p(A_U) = \sigma_p(A)$, ... These facts are a consequence of the following observations: $\{UE_\lambda U^*\}$ corresponds to the spectral family for the operator A_U, and then for any Borel set V*

$$m_{Uf}(V) = \big\langle\big(UE(V)U^*\big)Uf, Uf\big\rangle = \langle E(V)f, f\rangle = m_f(V).$$

We end this section with a few results which are related to the essential spectrum of a self-adjoint operator. The first one provides another characterization of the spectrum or of the essential spectrum of a self-adjoint operator A.

Proposition 4.3.7 (Weyl's criterion). *Let A be a self-adjoint operator in a Hilbert space $\mathcal{H}$.*

a) A real number λ belongs to $\sigma(A)$ if and only if there exists a sequence $\{f_n\}_{n\in\mathbb{N}} \subset \mathsf{D}(A)$ such that $\|f_n\| = 1$ and $s - \lim_{n\to\infty}(A-\lambda)f_n = 0$.

b) A real number λ belongs to $\sigma_{ess}(A)$ if and only if there exists a sequence $\{f_n\}_{n\in\mathbb{N}} \subset \mathsf{D}(A)$ such that $\|f_n\| = 1$, $w - \lim_{n\to\infty} f_n = 0$ and $s - \lim_{n\to\infty}(A-\lambda)f_n = 0$.

Exercise 4.3.8. *Provide a proof of the above statement. For convenience, you can first provide such a proof in the special case of a multiplication operator in the Hilbert space $L^2(\mathbb{R})$.*

The second result deals with the conservation of the essential spectrum under a relatively compact perturbation. Before its statement, recall that the addition of a relatively compact perturbation does not change the self-adjointness property, see Proposition 2.3.5 in conjunction with Rellich-Kato theorem.

Proposition 4.3.9. *Let A be a self-adjoint operator in a Hilbert space $\mathcal{H}$, and let B be a symmetric operator in $\mathcal{H}$ which is A-compact. Then the following equality holds:*

$$\sigma_{ess}(A+B) = \sigma_{ess}(A). \tag{4.14}$$

Proof. Let us consider $\lambda \in \sigma_{ess}(A)$, and choose a sequence $\{f_n\}_{n\in\mathbb{N}} \subset \mathsf{D}(A)$ such that $\|f_n\| = 1$, $w - \lim_{n\to\infty} f_n = 0$ and $s - \lim_{n\to\infty}(A-\lambda)f_n = 0$. Note that the existence of such a sequence is provided by Proposition 4.3.7. By the same proposition, one would get $\lambda \in \sigma_{ess}(A+B)$ if one shows that $s - \lim_{n\to\infty}(A+B-\lambda)f_n = 0$, which is itself implied by $s - \lim_{n\to\infty} Bf_n = 0$.

For that purpose, let us fix $z \in \rho(A)$ such that $B(A-z)^{-1} \in \mathscr{K}(\mathcal{H})$ and write

$$\begin{aligned} Bf_n &= [B(A-z)^{-1}](A-z)f_n \\ &= [B(A-z)^{-1}](A-\lambda)f_n + (\lambda - z)[B(A-z)^{-1}]f_n. \end{aligned}$$

Observe now that both terms converge to 0 as $n \to \infty$. For the first term, this follows directly from the assumptions. For the second one, recall that $w - \lim_{n\to\infty} f_n = 0$ and that a compact operator transform a weak convergence into a strong convergence, see Proposition 1.4.12, which means that $s - \lim_{n\to\infty}[B(A-z)^{-1}]f_n = 0$. As a consequence one infers that $\sigma_{ess}(A) \subset \sigma_{ess}(A+B)$.

The converse statement $\sigma_{ess}(A+B) \subset \sigma_{ess}(A)$ can be obtained similarly by considering first $A+B$ and by perturbing this operator with the relatively compact operator $-B$. Note that the relative compactness of $-B$ with respect to $A+B$ is a direct consequence of the point (iii) of Proposition 2.3.5. □

In the previous statement we have obtained the stability of the essential spectrum under relatively compact perturbation. However, this stability does not imply anything about the conservation of the nature of the spectrum. In that respect the following statement shows that the nature of the spectrum can drastically change even under a small perturbation.

Proposition 4.3.10 (Weyl-von Neumann). *Let A be an arbitrary self-adjoint operator in a Hilbert space. Then, for any $\varepsilon > 0$ there exists a self-adjoint Hilbert-Schmidt operator B with its Hilbert-Schmidt norm $\|B\|_{HS}$ satisfying $\|B\|_{HS} < \varepsilon$ such that $A+B$ has only pure point spectrum.*

Exercise 4.3.11. *Study the proof of this proposition, as presented for example in [Kat, Sec. X.2].*

4.4 The resolvent near the spectrum

In this section we study the resolvent $(A-z)^{-1}$ of any self-adjoint operator A when z approaches a value in $\sigma(A)$. Such investigations lead quite naturally to the spectral theorem, but also allow us to deduce useful information on the spectrum of the operator A. The spectral family $\{E_\lambda\}$ associated with the operator A can also be deduced from such investigations.

As a motivation, consider the following function defined for any $\lambda \in \mathbb{R}$ and any $\varepsilon > 0$:

$$\mathbb{R} \ni \ x \mapsto \frac{1}{x-\lambda-i\varepsilon} - \frac{1}{x-\lambda+i\varepsilon} = \frac{2i\varepsilon}{(x-\lambda)^2+\varepsilon^2} \ \in \mathbb{C}.$$

It is known that this function converges as $\varepsilon \to 0$ and in the sense of distributions to $2\pi i\delta_0(x-\lambda)$. Thus, if we replace x by the self-adjoint operator A one formally infers that

$$\begin{aligned}\frac{1}{2\pi i}\int_a^b \big[(A-\lambda-i\varepsilon)^{-1} - (A-\lambda+i\varepsilon)^{-1}\big]\mathrm{d}\lambda \to \int_a^b \delta_0(A-\lambda)\mathrm{d}\lambda &= \chi_{(a,b)}(A)\\ &= E\big((a,b)\big).\end{aligned}$$

The next statement shows that this argument is almost correct, once the behavior of the operator A at the endpoints a and b is taken into account.

Proposition 4.4.1 (Stone's formula). *Let A be a self-adjoint operator with associated spectral family $\{E_\lambda\}$. Then for any $-\infty < a < b < \infty$ the following formulas hold:*

$$\begin{aligned}\frac{1}{2\pi i} s-\lim_{\varepsilon\searrow 0}\int_a^b \big[(A-\lambda-i\varepsilon)^{-1} - (A-\lambda+i\varepsilon)^{-1}\big]\mathrm{d}\lambda&\\ = E\big((a,b)\big) + \frac{1}{2}E(\{a\}) + \frac{1}{2}E(\{b\})& \qquad (4.15)\end{aligned}$$

and

$$E\big((a,b]\big) = \frac{1}{2\pi i}\ s-\lim_{\delta\searrow 0}\ s-\lim_{\varepsilon\searrow 0}\int_{a+\delta}^{b+\delta} \big[(A-\lambda-i\varepsilon)^{-1} - (A-\lambda+i\varepsilon)^{-1}\big]\mathrm{d}\lambda\ . \qquad (4.16)$$

Note that in the last formula the order of the two limits is important.

Proof. i) For any $\varepsilon > 0$ and $\lambda \in \mathbb{R}$ let us set

$$\begin{aligned}\Psi_\varepsilon(\lambda) =& \frac{1}{2\pi i}\int_a^b \Big(\frac{1}{x-\lambda-i\varepsilon} - \frac{1}{x-\lambda+i\varepsilon}\Big)\mathrm{d}x \\ =& \frac{1}{2\pi i}\int_a^b \frac{2i\varepsilon}{(x-\lambda)^2+\varepsilon^2}\mathrm{d}x \\ =& \frac{1}{\pi}\Big[\arctan\Big(\frac{b-\lambda}{\varepsilon}\Big) - \arctan\Big(\frac{a-\lambda}{\varepsilon}\Big)\Big].\end{aligned}$$

Clearly, Ψ_ε is continuous in λ and satisfies $|\Psi_\varepsilon(\lambda)| \leq 1$ for any $\lambda \in \mathbb{R}$. In addition, since $\lim_{\varepsilon\searrow 0}\arctan\big(\frac{x-\lambda}{\varepsilon}\big) = \frac{\pi}{2}$ if $\lambda < x$ and $\lim_{\varepsilon\searrow 0}\arctan\big(\frac{x-\lambda}{\varepsilon}\big) = -\frac{\pi}{2}$ if $\lambda > x$ one infers that

$$\Psi_0(\lambda) := \lim_{\varepsilon\searrow 0}\Psi_\varepsilon(\lambda) = \frac{1}{2}\Big(\chi_{(a,b)}(\lambda) + \chi_{[a,b]}(\lambda)\Big). \tag{4.17}$$

ii) For any $\varepsilon > 0$ the operator $\Psi_\varepsilon(A) := \int_{\mathbb{R}}\Psi_\varepsilon(\lambda)E(\mathrm{d}\lambda)$ is well-defined and belongs to $\mathscr{B}(\mathcal{H})$. Our aim is to show that this operator is strongly continuous in ε and strongly convergent for $\varepsilon \searrow 0$ to a limit corresponding to what is suggested by (4.17). For any $f \in \mathcal{H}$ one can write $f = E(\{a\})f + E(\{b\})f + f_0$ with $f_0 \in \big(E(\{a\})\mathcal{H} + E(\{b\})\mathcal{H}\big)^\perp$. One then has

$$\Psi_\varepsilon(A)E(\{a\})f = \Psi_\varepsilon(a)E(\{a\})f = \frac{1}{\pi}\arctan\Big(\frac{b-a}{\varepsilon}\Big)E(\{a\})f,$$

which converges strongly to $\frac{1}{2}E(\{a\})f$ as $\varepsilon \searrow 0$. Similarly,

$$s-\lim_{\varepsilon\searrow 0}\Psi_\varepsilon(A)E(\{b\})f = \frac{1}{2}E(\{b\})f.$$

On the other hand, since $E\big((a,b)\big)f_0 = E\big([a,b]\big)f_0 = \int_a^b E(\mathrm{d}\lambda)f_0$ one has

$$\begin{aligned}&E\big((a,b)\big)f_0 - \Psi_\varepsilon(A)f_0 \\ &= \int_a^b \big(1-\Psi_\varepsilon(\lambda)\big)E(\mathrm{d}\lambda)f_0 - \int_{-\infty}^a \Psi_\varepsilon(\lambda)E(\mathrm{d}\lambda)f_0 - \int_b^\infty \Psi_\varepsilon(\lambda)E(\mathrm{d}\lambda)f_0.\end{aligned}$$

By the dominated convergence theorem, one finds that each term on the right-hand side converges strongly to zero. Thus we have obtained that

$$\Psi_0(A) := s-\lim_{\varepsilon\searrow 0}\Psi_\varepsilon(A) = E\big((a,b)\big) + \frac{1}{2}E(\{a\}) + \frac{1}{2}E(\{b\}).$$

iii) To obtain the validity of (4.15) it is now sufficient to verify that for $\varepsilon > 0$ one has

$$\Psi_\varepsilon(A) = \frac{1}{2\pi i}\int_a^b \big[(A-\lambda-i\varepsilon)^{-1} - (A-\lambda+i\varepsilon)^{-1}\big]\mathrm{d}\lambda.$$

By the polarization identity, such an equality holds if one knows that for any $f \in \mathcal{H}$

$$\langle f, \Psi_\varepsilon(A) f\rangle = \frac{1}{2\pi i}\int_a^b \langle f, \big[(A-\lambda-i\varepsilon)^{-1} - (A-\lambda+i\varepsilon)^{-1}\big] f\rangle \mathrm{d}\lambda.$$

To prove this equality, one uses the first resolvent equation for the equality

$$\begin{aligned}(A-\lambda-i\varepsilon)^{-1} - (A-\lambda+i\varepsilon)^{-1} &= 2i\varepsilon(A-\lambda-i\varepsilon)^{-1}(A-\lambda+i\varepsilon)^{-1} \\ &= 2i\varepsilon\int_{\mathbb{R}} \frac{1}{(\mu-\lambda)^2+\varepsilon^2} E(\mathrm{d}\mu).\end{aligned}$$

It then follows that

$$\frac{1}{2\pi i}\int_a^b \big[(A-\lambda-i\varepsilon)^{-1} - (A-\lambda+i\varepsilon)^{-1}\big]\mathrm{d}\lambda = \frac{\varepsilon}{\pi}\int_a^b \mathrm{d}\lambda \int_{\mathbb{R}} \frac{1}{(\mu-\lambda)^2+\varepsilon^2} E(\mathrm{d}\mu)$$

and as a consequence

$$\frac{1}{2\pi i}\int_a^b \langle f, \big[(A-\lambda-i\varepsilon)^{-1} - (A-\lambda+i\varepsilon)^{-1}\big] f\rangle \mathrm{d}\lambda = \frac{\varepsilon}{\pi}\int_a^b \mathrm{d}\lambda \int_{\mathbb{R}} \frac{m_f(\mathrm{d}\mu)}{(\mu-\lambda)^2+\varepsilon^2}.$$

By an application of Fubini's theorem one deduces that

$$\begin{aligned}&\frac{1}{2\pi i}\int_a^b \langle f, \big[(A-\lambda-i\varepsilon)^{-1} - (A-\lambda+i\varepsilon)^{-1}\big] f\rangle \mathrm{d}\lambda \\ &= \int_{\mathbb{R}} m_f(\mathrm{d}\mu)\frac{\varepsilon}{\pi}\int_a^b \mathrm{d}\lambda \frac{1}{(\mu-\lambda)^2+\varepsilon^2} \\ &= \langle f, \Psi_\varepsilon(A) f\rangle,\end{aligned}$$

as expected.

iv) Let us finally deduce (4.16) from (4.15). As a consequence of the latter formula one has

$$\begin{aligned}&\frac{1}{2\pi i} s-\lim_{\delta\searrow 0}\int_{a+\delta}^{b+\delta} \big[(A-\lambda-i\varepsilon)^{-1} - (A-\lambda+i\varepsilon)^{-1}\big]\mathrm{d}\lambda \\ &= E\big((a+\delta,b+\delta)\big) + \frac{1}{2}E(\{a+\delta\}) + \frac{1}{2}E(\{b+\delta\}) \\ &= E_{b+\delta} - E_{a+\delta} + \frac{1}{2}E(\{a+\delta\}) - \frac{1}{2}E(\{b+\delta\}). \qquad (4.18)\end{aligned}$$

Observe also that if $\mu \in \mathbb{R}$ and $\delta > 0$, then by the right continuity of the spectral family one has

$$\|E(\{\mu+\delta\})f\|^2 \leq \big\|E\big((\mu,\mu+\delta]\big)f\big\|^2 = \|(E_{\mu+\delta}-E_\mu)f\|^2 \ \to\ 0 \ \text{ as } \ \delta\to 0,$$

or in other words $s-\lim_{\delta\searrow 0} E(\{\mu+\delta\}) = \mathbf{0}$. Thus, by taking the right continuity of $\{E_\lambda\}$ again into account, one infers that the strong limit as $\delta \searrow 0$ of (4.18) is $E_b - E_a \equiv E\big((a,b]\big)$, which proves (4.16). □

Let us now comment on the relation between the previous proposition and the proof of the spectral theorem, as stated in Theorem 4.2.6. First of all, observe that the uniqueness of the spectral family $\{E_\lambda\}$ is a consequence of Stone's formula. Indeed, if $\{E_\lambda\}$ and $\{E'_\lambda\}$ are two spectral families satisfying $A = \int_{\mathbb{R}} \lambda E(\mathrm{d}\lambda) = \int_{\mathbb{R}} \lambda E'(\mathrm{d}\lambda)$, then it would follow from the equality (4.16) that $E\big((a,b]\big) = E'\big((a,b]\big)$ (the l.h.s. of (4.16) depends only A). Hence,

$$E_\lambda = s - \lim_{a\to-\infty} E\big((a,\lambda]\big) = s - \lim_{a\to-\infty} E'\big((a,\lambda]\big) = E'_\lambda.$$

For the existence of the spectral family, the proof is much longer, and can be found in several textbooks. However, let us just sketch it. The starting point for such a proof is (almost) always the r.h.s. of (4.16), and one has to prove the existence of its r.h.s. at least in the weak sense, and to show that the corresponding operators have the properties of a spectral measure. For the existence of the limit, one has to consider

$$\begin{aligned}
&\frac{1}{2\pi i} \lim_{\delta\searrow 0} \lim_{\varepsilon\searrow 0} \Big(\int_{a+\delta}^{b+\delta} \langle f, (A-\lambda-i\varepsilon)^{-1} f\rangle \mathrm{d}\lambda - \int_{a+\delta}^{b+\delta} \langle f, (A-\lambda+i\varepsilon)^{-1} f\rangle \mathrm{d}\lambda \Big) \\
&= \lim_{\delta\searrow 0} \lim_{\varepsilon\searrow 0} \frac{1}{\pi} \int_{a+\delta}^{b+\delta} \Im \langle f, (A-\lambda-i\varepsilon)^{-1} f\rangle \mathrm{d}\lambda.
\end{aligned}$$

Thus, let us set $\Phi(z) := \langle f, (A-z)^{-1} f\rangle$ and observe that this $\mathbb{C}$-valued function is holomorphic in the upper half complex plane. Observe also that this function has a non-negative imaginary part and satisfies the estimate $|\Phi(z)| \leq c/\Im(z)$ for some finite constant c (which means that $\Phi(z)$ is a Nevanlinna function). Then one can use a theorem on analytic functions saying that in such a case there exists a finite Stieltjes measure m on $\mathbb{R}$ satisfying $\Phi(z) = \int_{\mathbb{R}} (\lambda - z)^{-1} m(\mathrm{d}\lambda)$. In addition, this measure satisfies

$$m\big((a,b]\big) = \lim_{\delta\searrow 0} \lim_{\varepsilon\searrow 0} \frac{1}{\pi} \int_{a+\delta}^{b+\delta} \Im \Phi(\lambda + i\varepsilon) \mathrm{d}\lambda.$$

As a consequence, the application of this theorem provides us for any $f \in \mathcal{H}$ the measure $m \equiv m_f$. The rest of the proof consists in routine computations.

Let us add another comment in relation with the previous proposition. As already mentioned in Exercise 4.2.9, and more precisely in (4.10), for any $\lambda \in \sigma(A)$ one has

$$\|(A - \lambda \mp i\varepsilon)^{-1}\| = \frac{1}{|\varepsilon|}.$$

However, for some particular $f \in \mathcal{H}$ the expressions $(A-\lambda\mp i\varepsilon)^{-1} f$ could be convergent as $\varepsilon \searrow 0$. In particular, this is the case if the associated measure m_f is supported away from the value λ, or equivalently if there exists $\kappa > 0$ such that $E([\lambda-\kappa, \lambda+\kappa])f = 0$. Indeed, in this situation one has

$$\begin{aligned}
\|(A - \lambda \mp i\varepsilon)^{-1} f\|^2 &= \int_{-\infty}^{\lambda-\kappa} |\mu - \lambda \mp i\varepsilon|^{-2} m_f(\mathrm{d}\mu) + \int_{\lambda+\kappa}^{\infty} |\mu - \lambda \mp i\varepsilon|^{-2} m_f(\mathrm{d}\mu) \\
&\leq \frac{1}{\kappa^2} \int_{\mathbb{R}} m_f(\mathrm{d}\mu) = \frac{1}{\kappa^2} \|f\|^2.
\end{aligned}$$

Since this estimate holds for any $\varepsilon > 0$, and even for $\varepsilon = 0$, one easily obtains from the dominated convergence theorem that $\lim_{\varepsilon\searrow 0} \|(A-\lambda\mp i\varepsilon)^{-1}f - (A-\lambda)^{-1}f\| = 0$.

Let us also observe that if $\lambda \notin \sigma_p(A)$, then the previous argument holds for a dense set of elements of $\mathcal{H}$. Indeed, in such a case one has $s-\lim_{\kappa\searrow 0} E([\lambda-\kappa,\lambda+\kappa]) = \mathbf{0}$. However, if $E(\{\lambda\}) \neq \mathbf{0}$ then the above set of vectors can not be dense since it is orthogonal to $E(\{\lambda\})\mathcal{H}$.

Let us still assume that $\lambda \notin \sigma_p(A)$. In the previous paragraphs, it was shown that the set of vectors such that the limit $s-\lim_{\varepsilon\searrow 0}(A-\lambda\mp i\varepsilon)^{-1}f$ exists is dense in $\mathcal{H}$, but the choice of this dense set was depending on λ. A more interesting situation would be when this set can be chosen independently of λ, or at least for any λ in some interval (a,b). In the next statement, we show that if this situation takes place, then the spectrum of A in (a,b) is absolutely continuous. In order to get a better understanding of the subsequent result, let us recall that if $\phi:\mathbb{R}\to\mathbb{C}$ is a smooth function, then

$$\lim_{\varepsilon\searrow 0}\int_{\mathbb{R}}\frac{\phi(\mu)}{\mu-\lambda-i\varepsilon}\mathrm{d}\mu = i\pi\phi(\lambda) + \mathrm{Pv}\int_{\mathbb{R}}\frac{\phi(\mu)}{\mu-\lambda}\mathrm{d}\mu, \tag{4.19}$$

where Pv denotes the principal value integral. In particular, let us now choose $f\in\mathcal{H}_{ac}(A)$, which implies that there exists a non-negative measurable function $\theta_f:\mathbb{R}\to\mathbb{R}_+$ such that $m_f(V) = \int_V \theta_f(\mu)\mathrm{d}\mu$. If we assume in addition some regularity on θ_f, as for example $\theta_f\in C^1$, then one infers from (4.19) that

$$\langle f,(A-\lambda-i\varepsilon)^{-1}f\rangle = \int_{\mathbb{R}}\frac{\theta_f(\mu)}{\mu-\lambda-i\varepsilon}\mathrm{d}\mu \to i\pi\theta_f(\lambda) + \mathrm{Pv}\int_R\frac{\theta_f(\mu)}{\mu-\lambda}\mathrm{d}\mu \quad \text{as } \varepsilon\searrow 0.$$

The next statement clarifies the link between the existence of a limit for $(A-\lambda-i\varepsilon)^{-1}$ as $\varepsilon\searrow 0$ and the existence of absolutely continuous spectrum for A.

Proposition 4.4.2. *Let A be a self-adjoint operator and let $J := (\alpha,\beta)\subset\mathbb{R}$.*

(i) Let $f\in\mathcal{H}$ such that for each $\lambda\in J$ the expression $\Im\langle f,(A-\lambda-i\varepsilon)^{-1}f\rangle$ admits a limit as $\varepsilon\searrow 0$ and that this convergence holds uniformly in λ on any compact subset of J. Then $E(J)f\in\mathcal{H}_{ac}(A)$,

(ii) Assume that there exists a dense set $\mathcal{D}\subset\mathcal{H}$ such that the assumptions of (i) hold for any $f\in\mathcal{D}$, then $E(J)\mathcal{H}\subset\mathcal{H}_{ac}(A)$. In particular, it follows that

$$\sigma_p(A)\cap J = \emptyset = \sigma_{sc}(A)\cap J.$$

Proof. i) First of all, for z in the upper half complex plane let us set

$$\phi(z) := \Im\langle f,(A-z)^{-1}f\rangle.$$

By assumption $\phi(\lambda) := \lim_{\varepsilon\searrow 0}\phi(\lambda+i\varepsilon)$ exists for any $\lambda\in J$ and defines a bounded and uniformly continuous function on any compact subset of J.

Let us also consider $\lambda \in [a,b] \subset J$ and deduce from Stone's formula that

$$\big\langle f, E\big((a,\lambda]\big)f\big\rangle = \frac{1}{\pi}\lim_{\delta\searrow 0}\lim_{\varepsilon\searrow 0}\int_{a+\delta}^{\lambda+\delta}\Im\big\langle f,(A-\mu-i\varepsilon)^{-1}f\big\rangle \mathrm{d}\mu$$

where we can choose δ small enough such that $[a+\delta,\lambda+\delta]\subset J$. Then, by the observation made in the previous paragraph and by an application of the dominated convergence theorem one infers that

$$\big\langle f, E\big((a,\lambda]\big)f\big\rangle = \frac{1}{\pi}\lim_{\delta\searrow 0}\int_{a+\delta}^{\lambda+\delta}\phi(\mu)\mathrm{d}\mu = \frac{1}{\pi}\int_a^\lambda \phi(\mu)\mathrm{d}\mu.$$

Since ϕ is continuous on $[a,b]$ if follows that $\phi\in L^1([a,b])$. Finally, since $E\big((a,\lambda]\big)f = E\big((a,\lambda]\big)E(J)f$ one infers that the map $\lambda\mapsto \big\langle f, E\big((a,\lambda]\big)f\big\rangle$ defines an absolutely continuous measure on $(a,b]$.

ii) One has $E(J)f\in\mathcal{H}_{ac}(A)$ for each $f\in\mathcal{D}$. Since $\mathcal{D}$ is assumed to be dense in $\mathcal{H}$, it easily follows that $\{E(J)f \mid f\in\mathcal{D}\}$ is dense in $E(J)\mathcal{H}$, and hence $E(J)\mathcal{H}\subset\mathcal{H}_{ac}(A)$. □

The following result will be at the root of the commutator methods introduced later on.

Theorem 4.4.3 (Putnam's theorem)**.** *Let H and A be bounded self-adjoint operators satisfying $[iH,A]\geq CC^*$ for some $C\in\mathscr{B}(\mathcal{H})$. Then for all $\lambda\in\mathbb{R}$, any $\varepsilon>0$ and each $f\in\mathcal{H}$ one has*

$$\Im\langle Cf,(H-\lambda-i\varepsilon)^{-1}Cf\rangle \leq 4\|A\|\,\|f\|^2, \tag{4.20}$$

and $\mathsf{Ran}(C)\subset\mathcal{H}_{ac}(H)$. In particular, if $\mathsf{Ker}(C^*)=\{0\}$, then the spectrum of H is purely absolutely continuous.

Proof. In this proof, we use the notation $R(z)$ for $(H-z)^{-1}$ when $z\in\rho(H)$.

i) For any $f\in\mathcal{H}$ one has

$$\begin{aligned}\Im\langle Cf,R(\lambda+i\varepsilon)Cf\rangle &= \frac{1}{2i}\big\langle Cf,[R(\lambda+i\varepsilon)-R(\lambda-i\varepsilon)]Cf\big\rangle\\ &= \varepsilon\big\langle Cf,R(\lambda+i\varepsilon)R(\lambda-i\varepsilon)Cf\big\rangle\\ &= \varepsilon\|R(\lambda-i\varepsilon)Cf\|^2\\ &\leq \varepsilon\|R(\lambda-i\varepsilon)C\|\,\|f\|^2.\end{aligned} \tag{4.21}$$

Since for any bounded operator T one has $\|T\|^2=\|TT^*\|$ one infers that

$$\begin{aligned}\|R(\lambda-i\varepsilon)C\|^2 &= \|R(\lambda-i\varepsilon)CC^*R(\lambda+i\varepsilon)\|\\ &= \sup_{f\in\mathcal{H},\|f\|=1}\big\langle R(\lambda+i\varepsilon)f,CC^*R(\lambda+i\varepsilon)f\big\rangle\\ &\leq \sup_{f\in\mathcal{H},\|f\|=1}\big\langle R(\lambda+i\varepsilon)f,[iH,A]R(\lambda+i\varepsilon)f\big\rangle\\ &= \big\|R(\lambda-i\varepsilon)[iH,A]R(\lambda+i\varepsilon)\big\|\\ &= \big\|R(\lambda-i\varepsilon)[i(H-\lambda+i\varepsilon),A]R(\lambda+i\varepsilon)\big\|\\ &\leq \|AR(\lambda+i\varepsilon)\|+\|R(\lambda-i\varepsilon)A\|+\|2i\varepsilon R(\lambda-i\varepsilon)AR(\lambda+i\varepsilon)\|.\end{aligned}$$

Finally, since $\|R(\lambda \pm i\varepsilon)\| \leq \varepsilon^{-1}$ one gets $\|R(\lambda - i\varepsilon)C\|^2 \leq 4\varepsilon^{-1}\|A\|$. By inserting this estimate into (4.21) one directly deduces the inequality (4.20).

ii) Let $\{E_\lambda\}$ be the spectral family of H. For any $J = (a,b]$ one has by Stone's formula

$$\big\langle Cf, E\big((a,b]\big)Cf\big\rangle = \frac{1}{\pi} \lim_{\delta \searrow 0} \lim_{\varepsilon \searrow 0} \int_{a+\delta}^{b+\delta} \Im\big\langle Cf, (H - \lambda - i\varepsilon)^{-1}Cf\big\rangle \mathrm{d}\lambda.$$

Now since one has

$$\int_{a+\delta}^{b+\delta} \Im\big\langle Cf, (H - \lambda - i\varepsilon)^{-1}Cf\big\rangle \mathrm{d}\lambda \leq 4\|A\|\, \|f\|^2\, (b-a)$$

one infers that

$$\langle Cf, E(J)Cf\rangle \equiv m_{Cf}(J) \leq 4\|A\|\, \|f\|^2\, |J|,$$

where $|J|$ means the Lebesgue measure of J. Such an inequality implies that $m_{Cf}(V) \leq 4\|A\|\ \|f\|^2\ |V|$ for any Borel set V of $\mathbb{R}$, and consequently that the measure m_{Cf} is absolutely continuous with respect to the Lebesgue measure. It thus follows that $Cf \in \mathcal{H}_{ac}(H)$. Finally, if $\mathsf{Ker}(C^*) = \{0\}$, then $\mathsf{Ran}(C)$ is dense in $\mathcal{H}$, as proved in (ii) of Lemma 2.1.10. As a consequence, one obtains that $\mathcal{H}_{ac}(H) = \mathcal{H}$. □

Chapter 5

Scattering theory

In this chapter we introduce the basic tools of scattering theory. This theory deals with the unitary group generated by any self-adjoint operator and corresponds to a comparison theory. More precisely, if A and B are self-adjoint operators in a Hilbert space $\mathcal{H}$, and if the corresponding unitary groups are denoted by $\{U_t\}_{t\in\mathbb{R}}$ and $\{V_t\}_{t\in\mathbb{R}}$, then one typically considers the product operator $V_t^* U_t$ and study its behavior for large $|t|$. Understanding the limit $\lim_{t\to\pm\infty} V_t^* U_t$ in a suitable sense, provides many information on the relation between the operator A and B.

Scattering theory was first developed in close relation with physics. However, it is now a mathematical subject on its own, and new developments are currently taking place in a more interdisciplinary framework.

5.1 Evolution groups

Let A be a self-adjoint operator in a Hilbert space $\mathcal{H}$. The elements of the corresponding strongly continuous unitary group $\{U_t\}_{t\in\mathbb{R}}$ provided by Stone's theorem in Theorem 4.2.11 are often denoted by $U_t = \mathrm{e}^{-itA}$. This group is called *the evolution group* associated with A. Let us also recall that if $\{U_t\}_{t\in\mathbb{R}}$ is a strongly continuous unitary group, then its *generator* corresponds to the self-adjoint operator $\big(A, \mathsf{D}(A)\big)$ defined by

$$\mathsf{D}(A) := \Big\{ f \in \mathcal{H} \mid \exists\ s-\lim_{t\to 0} \frac{1}{t}[U_t - 1]f \Big\}$$

and for $f \in \mathsf{D}(A)$ by $Af = s - \lim_{t\to 0} \frac{i}{t}[U_t - 1]f$. Obviously, the relation $U_t = \mathrm{e}^{-itA}$ then holds, and the domain $\mathsf{D}(A)$ is left invariant by the action of U_t for any $t \in \mathbb{R}$.

Given a strongly continuous unitary group $\{U_t\}_{t\in\mathbb{R}}$ it is often not so simple to compute explicitly $\mathsf{D}(A)$. However, in applications one can often guess a smaller domain $\mathcal{D} \subset \mathcal{H}$ on which the computation of $s - \lim_{t\to 0} \frac{1}{t}[U_t - 1]f$ is well-defined. The following statement provides a criterion for checking if the domain $\mathcal{D}$ is large enough for defining entirely the operator A.

Proposition 5.1.1 (Nelson's criterion)**.** *Let $\{U_t\}_{t\in\mathbb{R}}$ be a strongly continuous unitary group, and let A denotes its self-adjoint generator. Let $\mathcal{D}$ be a dense linear submanifold of $\mathcal{H}$ such that $\mathcal{D}$ is invariant under the action of U_t for any $t \in \mathbb{R}$ and such that $s-\lim_{t\to 0}\frac{1}{t}[U_t - 1]f$ has a limit for any $f \in \mathcal{D}$. Then A is essentially self-adjoint on $\mathcal{D}$.*

Proof. Let us denote by A_0 the restriction of A to $\mathcal{D}$. Since A is self-adjoint, A_0 is clearly symmetric. In order to show that A_0 is essentially self-adjoint, we shall use the criterion (ii) of Proposition 2.1.15. More precisely, A_0 is essentially self-adjoint if $\mathsf{Ran}(A_0 \pm i)$ are dense in $\mathcal{H}$, or equivalently if $\mathsf{Ker}(A_0^* \mp i) = \{0\}$. Note that we have also used Lemma 2.1.10 for the previous equivalence.

Let us show that $\mathsf{Ker}(A_0^* - i) = \{0\}$. For that purpose, assume that $h \in \mathsf{Ker}(A_0^* - i)$, *i.e.* $h \in \mathsf{D}(A_0^*)$ and $A_0^* h = ih$. For any $f \in \mathcal{D}$ one has

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle U_t f, h\rangle &= \langle -iAU_t f, h\rangle = i\langle A_0 U_t f, h\rangle \\ &= i\langle U_t f, A_0^* h\rangle = i\langle U_t f, ih\rangle = -\langle U_t f, h\rangle\end{aligned}$$

where the invariance of $\mathcal{D}$ under U_t has been used for the second equality. Thus if one sets $\phi(t) := \langle U_t f, h\rangle$ one gets the differential equation $\phi'(t) = -\phi(t)$, whose solution is $\phi(t) = \phi(0)\,\mathrm{e}^{-t}$. If $\phi(0) \neq 0$ it follows that $|\phi(t)| \to \infty$ as $t \to -\infty$ which is impossible since $|\phi(t)| \leq \|f\|\,\|h\|$. One deduces that $\phi(0) = 0$ which means that $\langle f, h\rangle = 0$. It follows that h is perpendicular to $\mathcal{D}$, but by density of $\mathcal{D}$ in $\mathcal{H}$ one concludes that $h = 0$. ☐

Remark 5.1.2. *Dealing with the group $\{\mathrm{e}^{-itA}\}_{t\in\mathbb{R}}$ let us provide two formulas which could also have been introduced in the previous chapter, namely*

$$(A - z)^{-1} = i\int_0^\infty \mathrm{e}^{izt}\,\mathrm{e}^{-itA}\,\mathrm{d}t, \qquad \text{for } \Im(z) > 0\ , \tag{5.1}$$

$$(A - z)^{-1} = -i\int_{-\infty}^0 \mathrm{e}^{izt}\,\mathrm{e}^{-itA}\,\mathrm{d}t, \qquad \text{for } \Im(z) < 0\ . \tag{5.2}$$

Since the map $t \mapsto \mathrm{e}^{izt}\,\mathrm{e}^{-itA}$ is strongly continuous and integrable in norm, the above integrals exist in the strong sense by Proposition 1.5.3. Their equality with the resolvent of A at z can be checked directly, as shown for example in the proof of [Amr, Prop. 5.1].

Let us now present a few examples of evolution groups and their corresponding self-adjoint generators.

Example 5.1.3. *In the Hilbert space $\mathcal{H} := L^2(\mathbb{R})$ we consider the* translation group, *namely $[U_t f](x) := f(x - t)$ for any $f \in \mathcal{H}$ and $x \in \mathbb{R}$. It is easily checked that $\{U_t\}_{t\in\mathbb{R}}$ defines a strongly continuous unitary group in $\mathcal{H}$. In addition, its self-adjoint generator can by computed on $C_c^\infty(\mathbb{R})$, according to Proposition 5.1.1. One then finds that the generator is $-i\frac{\mathrm{d}}{\mathrm{d}x}$, or in other words the operator D already considered in Chapter 3. Note that the operator D is indeed essentially self-adjoint on $C_c^\infty(\mathbb{R})$.*

Example 5.1.4. *In $\mathcal{H} := L^2(\mathbb{R}^d)$ we consider the* dilation group *acting on any $f \in \mathcal{H}$ by $[U_t f](x) = \mathrm{e}^{dt/2} f(\mathrm{e}^t x)$ for any $x \in \mathbb{R}^d$. It is also easily checked that $\{U_t\}_{t\in\mathbb{R}}$ defines a strongly continuous unitary group in $\mathcal{H}$. The self-adjoint generator of this group can by computed on the Schwartz space $\mathcal{S}(\mathbb{R}^d)$, according to Proposition 5.1.1. A direct computations shows that this generator A is given on $\mathcal{S}(\mathbb{R}^d)$ by the expression*

$$A = -\frac{1}{2}\sum_{j=1}^{d}(X_j D_j + D_j X_j) \equiv -\frac{1}{2}(X\cdot D + D\cdot X).$$

Example 5.1.5. *Consider the Hilbert space $\mathcal{H} := L^2(\mathbb{R}^d)$ and the Laplace operator $-\Delta = D^2$, as already introduced in equation (3.3). The unitary group generated by this operator has obviously a very simple expression once a Fourier transformation is performed, or more precisely $\big[\mathcal{F}\,\mathrm{e}^{-itD^2} f\big](\xi) = \mathrm{e}^{-it\xi^2}[\mathcal{F}f](\xi)$ for any $f \in \mathcal{H}$ and $\xi \in \mathbb{R}^d$. Without this Fourier transformation, this operator corresponds to the following integral operator:*

$$\big[\,\mathrm{e}^{-itD^2} f\big](x) = \frac{1}{(4\pi i t)^{d/2}}\int_{\mathbb{R}^d} \mathrm{e}^{\frac{i|x-y|^2}{4t}}\, f(y)\mathrm{d}y$$

with the square root given by

$$\Big(\frac{4\pi i t}{|4\pi i t|}\Big)^{-n/2} = \begin{cases} \mathrm{e}^{-in\pi/4} & \text{if} \quad t>0,\\ \mathrm{e}^{+in\pi/4} & \text{if} \quad t<0.\end{cases}$$

Exercise 5.1.6. *Work on the details of the results presented in the previous three examples.*

Later on, we shall often have to compute the derivative with respect to t of the product of two unitary groups. Since the generators of these groups are often unbounded operators, some care is necessary. In the next Lemma, we provide some conditions in order to deal with the Leibnitz rule in this setting. The proof of this Lemma is provided for example in [Amr, Prop. 5.5]. Note that the first statement can even be used in the special case $B = \mathbf{1}$.

Lemma 5.1.7. *Let $\big(A, \mathsf{D}(A)\big)$ and $\big(B, \mathsf{D}(B)\big)$ be self-adjoint operators in a Hilbert space $\mathcal{H}$.*

(i) Let $C \in \mathscr{B}(\mathcal{H})$ be such that $C\mathsf{D}(B) \subset \mathsf{D}(A)$. Then for any $f \in \mathsf{D}(B)$ the map $t \mapsto \mathrm{e}^{itA}\, C\, \mathrm{e}^{-itB} f$ is strongly differentiable and

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{itA}\, C\, \mathrm{e}^{-itB} f = i\,\mathrm{e}^{itA}\big(AC - CB\big)\,\mathrm{e}^{-itB} f\ . \tag{5.3}$$

(ii) Let C be B-bounded and such that $C\mathsf{D}(B^2) \subset \mathsf{D}(A)$. Then for any $f \in \mathsf{D}(B^2)$ the map $t \mapsto \mathrm{e}^{itA}\, C\, \mathrm{e}^{-itB} f$ is strongly differentiable and its derivative is again given by (5.3).

In the next statements, we study the asymptotic behavior of different parts of the Hilbert space under the evolution group. First of all, we consider the absolutely continuous subspace.

Proposition 5.1.8. *Let A be a self-adjoint operator and let $\{U_t\}_{t\in\mathbb{R}}$ be the corresponding unitary group. Let also $f \in \mathcal{H}_{ac}(A)$. Then,*

(i) $U_t f$ converges weakly to 0 as $t \to \pm\infty$,

(ii) If $B \in \mathscr{B}(\mathcal{H})$ is A-compact, then $\|BU_t f\| \to 0$ as $t \to \pm\infty$.

Proof. i) For any $h \in \mathcal{H}_{ac}(A)$ and since $m_h(\mathbb{R}) = \int_{\mathbb{R}} m_h(\mathrm{d}\lambda) = \|h\|^2$, one infers that there exists a non-negative function $\theta \in L^1(\mathbb{R})$ such that $m_h(V) = \int_V \theta(\lambda)\mathrm{d}\lambda$ for any $V \in \mathcal{A}_B$. It thus follows that

$$\varphi(t) := \langle h, U_t h\rangle = \int_{\mathbb{R}} \mathrm{e}^{-it\lambda}\, m_h(\mathrm{d}\lambda) = \int_{\mathbb{R}} \mathrm{e}^{-it\lambda}\, \theta(\lambda)\mathrm{d}\lambda.$$

Thus, φ is the Fourier transform of the function $\theta \in L^1(\mathbb{R})$, and consequently belongs to $C_0(\mathbb{R})$ by the Riemann-Lebesgue lemma. It follows that $\lim_{t\to\pm\infty}\langle h, U_t h\rangle = 0$.

We now show that $\lim_{t\to\pm\infty}\langle g, U_t f\rangle = 0$ for any $g \in \mathcal{H}$ and $f \in \mathcal{H}_{ac}(A)$. Since $U_t f \in \mathcal{H}_{ac}(A)$ for any $t \in \mathbb{R}$ it follows that $\langle g, U_t f\rangle = 0$ if $g \in \mathcal{H}_s(A) := \mathcal{H}_{ac}(A)^\perp$. Thus, one can assume that $g \in \mathcal{H}_{ac}(A)$. By the polarization identity, one then obtains that $\langle g, U_t f\rangle$ is the sum of four terms of the form $\langle g + \alpha f, U_t(g + \alpha f)\rangle$ for some $\alpha \in \mathbb{C}$, and since $g + \alpha f$ belongs to $\mathcal{H}_{ac}(A)$ one infers from the previous paragraph that these four contributions converge to 0 as $t \to \pm\infty$, and this proves the statement (i).

ii) Observe first that it is sufficient to prove the statement (ii) for a dense set of elements of $\mathcal{H}_{ac}(A)$. Let us take for this dense set the linear manifold $\mathcal{H}_{ac}(A) \cap \mathsf{D}(A)$, and for any f in this set we define $g := (A + i)f$. Clearly $g \in \mathcal{H}_{ac}(A)$ and one has $f = (A + i)^{-1}g$. It follows that

$$BU_t f = BU_t(A + i)^{-1}g = B(A + i)^{-1}U_t g. \tag{5.4}$$

Since $U_t g$ converges weakly to 0 by the statement (i) and since $B(A + i)^{-1}$ belongs to $\mathscr{K}(\mathcal{H})$, one deduces from Proposition 1.4.12 that $B(A+i)^{-1}U_t g$ converges strongly to 0 as $t \to \pm\infty$. By (5.4), it means that $BU_t f$ converges strongly to 0, as stated in (ii). □

For $f \in \mathcal{H}_{sc}(A)$, the previous result does not hold in general. However, once a certain average is taken, similar results can be deduced. Since t is often interpreted as the time, one speaks about a temporal mean. We state the result for arbitrary $f \in \mathcal{H}_c(A)$, and refer to [Amr, Prop. 5.9] for its proof.

Proposition 5.1.9. *Let A be a self-adjoint operator and let $\{U_t\}_{t\in\mathbb{R}}$ be the corresponding unitary group. Let also $f \in \mathcal{H}_c(A)$. Then,*

(i) For any $h \in \mathcal{H}$ one has

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T |\langle h, U_t f\rangle|^2 \mathrm{d}t = 0 \quad \textit{and} \quad \lim_{T\to\infty} \frac{1}{T}\int_{-T}^0 |\langle h, U_t f\rangle|^2 \mathrm{d}t = 0.$$

(ii) If $B \in \mathscr{B}(\mathcal{H})$ is A-compact, then one has

$$\lim_{T\to\infty}\int_0^T \frac{1}{T}\|BU_tf\|^2\mathrm{d}t = 0 \quad \textit{and} \quad \lim_{T\to\infty}\frac{1}{T}\int_{-T}^0 \|BU_tf\|^2\mathrm{d}t = 0.$$

The first result can in fact be deduced from a stronger statement, usually called *RAGE theorem* in honor of its authors Ruelle, Amrein, Georgescu and Enss.

Theorem 5.1.10 (RAGE Theorem)**.** *Let A be a self-adjoint operator and let $\{U_t\}_{t\in\mathbb{R}}$ be the corresponding unitary group. Let also $E(\{0\})$ denote the spectral projection onto $\mathsf{Ker}(A)$. Then for any $f \in \mathcal{H}$ one has*

$$s-\lim_{T\to\pm\infty}\frac{1}{T}\int_0^T U_tf\,\mathrm{d}t = E(\{0\})f.$$

In particular, if $f \perp \mathsf{Ker}(A)$, then the previous limit is 0.

Exercise 5.1.11. *Provide a proof of RAGE theorem, see for Example [RS3, Thm XI.115].*

Let us close this section with one more result about U_tf for any $f \in \mathcal{H}_c(A)$. Its proof can be found in [RS3, Corol. p. 343]. We emphasize that in the statement, the family $\{t_k\}$ can be chosen independently of the element $f \in \mathcal{H}_c(A)$.

Corollary 5.1.12. *Let A be a self-adjoint operator and let $\{U_t\}_{t\in\mathbb{R}}$ be the corresponding unitary group. Then there exists a sequence $\{t_k\}_{k\in\mathbb{N}} \subset \mathbb{R}$ with $t_k \to \infty$ as $k \to \infty$ such that $w-\lim_{k\to\infty} U_{t_k}f = 0$ for any $f \in \mathcal{H}_c(A)$. In addition, if $B \in \mathscr{B}(\mathcal{H})$ is A-compact, then $\lim_{k\to\infty}\|BU_{t_k}f\| = 0$ for any $f \in \mathcal{H}_c(A)$.*

5.2 Wave operators

Scattering theory is mainly a comparison theory. Namely, given a self-adjoint operator H on a Hilbert space $\mathcal{H}$ one wonders if the evolution group $\{\mathrm{e}^{-itH}\}_{t\in\mathbb{R}}$ can be approximated by a simpler evolution group $\{\mathrm{e}^{-itH_0}\}_{t\in\mathbb{R}}$ as $t \to \pm\infty$. More precisely, let $f \in \mathcal{H}$ and consider the family of elements $\mathrm{e}^{-itH} f \in \mathcal{H}$. The previous question reduces to looking for a "simpler" operator H_0 and for two elements $f_\pm \in \mathcal{H}$ such that

$$\lim_{t\to\pm\infty}\big\|\,\mathrm{e}^{-itH} f - \mathrm{e}^{-itH_0} f_\pm\big\| = 0. \tag{5.5}$$

Obviously, one has to be more precise in what "simpler" means, and about the set of f which admit such an approximation.

Observe first that there is not a single procedure which leads to a natural candidate for H_0. Such a choice depends on the framework and on the problem. However, the initial question can be rephrased very precisely. By using the unitarity of e^{itH}, observe that (5.5) is equivalent to

$$\lim_{t\to\pm\infty} \left\| f - e^{itH} e^{-itH_0} f_\pm \right\| = 0. \tag{5.6}$$

For that reason, a natural object to consider is $s - \lim_{t\to\pm\infty} e^{itH} e^{-itH_0}$. However, this limit has a better chance to exist if considered only on a subspace of the Hilbert space. So let E be an orthogonal projection and assume that $E\, e^{-itH_0} = e^{-itH_0} E$ for any $t \in \mathbb{R}$. Equivalently, this means that the subspace $E\mathcal{H}$ is left invariant by the unitary group $\{e^{-itH_0}\}_{t\in\mathbb{R}}$. We say in that case that E commutes with the evolution group $\{e^{-itH_0}\}_{t\in\mathbb{R}}$. Note that we have chosen the notation E for this projection because in most of the applications E is related to the spectral family of H_0. However, other choices can also appear.

Definition 5.2.1. *Let H, H_0 be two self-adjoint operators in a Hilbert space $\mathcal{H}$, and let E be an orthogonal projection which commutes with $\{e^{-itH_0}\}_{t\in\mathbb{R}}$. The* wave operators *are defined by*

$$W_\pm(H, H_0, E) := s - \lim_{t\to\pm\infty} e^{itH} e^{-itH_0} E \tag{5.7}$$

whenever these limits exit. If $E = \mathbf{1}$ then these operators are denoted by $W_\pm(H, H_0)$.

Note that we could have chosen two different projections $E_\pm$ for $t \to \pm\infty$. Since the general theory is not more difficult in this case, we do not mention it in the sequel. However, in applications this slight extension is often useful. We now provide some information about these operators. Recall that some properties of isometries and partial isometries have be introduced in Propositions 1.4.6 and 1.4.8.

Proposition 5.2.2. *Let $W := W_\pm(H, H_0, E)$ be one of the wave operators. Then*

(i) W is a partial isometry, with initial set $E\mathcal{H}$. In particular, W is an isometry if $E = \mathbf{1}$,

(ii) W intertwines the two operators H_0 and H, or more precisely $e^{-itH} W = W e^{-itH_0}$ for any $t \in \mathbb{R}$. More generally, $E^H(V)W = WE^{H_0}(V)$ for any Borel set V, and $\varphi(H)W = W\varphi(H_0)$ for any $\varphi \in C_b(\mathbb{R})$. The following equality also holds:

$$HWf = WH_0 f \qquad \forall f \in \mathsf{D}(H_0). \tag{5.8}$$

Proof. In this proof we consider only $W := W_+(H, H_0, E)$, the case $W = W_-(H, H_0, E)$ being similar.

i) If $f \perp E\mathcal{H}$ then clearly $Wf = 0$. On the other hand, if $f \in E\mathcal{H}$ then $\|Wf\| = \lim_{t\to\infty} \| e^{itH} e^{-itH_0} f\| = \lim_{t\to\infty} \|f\| = \|f\|$, where Lemma 1.1.5 has been used for the first equality. It follows that W is a partial isometry, or an isometry if $E = \mathbf{1}$.

ii) Observe that

$$\begin{aligned}
\mathrm{e}^{-itH} W &= \mathrm{e}^{-itH}\, s-\lim_{s\to\infty} \mathrm{e}^{isH}\, \mathrm{e}^{-isH_0} E \\
&= s-\lim_{s\to\infty} \mathrm{e}^{i(s-t)H}\, \mathrm{e}^{-isH_0} E \\
&= s-\lim_{s'\to\infty} \mathrm{e}^{-is'H}\, \mathrm{e}^{-i(s'+t)H_0} E \\
&= W\, \mathrm{e}^{-itH_0}
\end{aligned}$$

where we have used that E and e^{-itH_0} commute. This proves the first part of the statement (ii). Then, by multiplying this equality with $\pm i\, \mathrm{e}^{izt}$ and by integrating with respect to t on $[0,\infty)$ for $\Im(z) > 0$ or on $(-\infty, 0]$ if $\Im(z) < 0$, one gets as in Remark 5.1.2 the equality

$$(H-z)^{-1}W = W(H_0-z)^{-1} \qquad \text{for any } z \in \mathbb{C}\setminus\mathbb{R}.$$

One then also deduces for any $\alpha, \beta \in \mathbb{R}$ that

$$\begin{aligned}
&\int_\alpha^\beta \big((H-\lambda-i\varepsilon)^{-1} - (H-\lambda+i\varepsilon)^{-1}\big) W \,\mathrm{d}\lambda \\
&= W \int_\alpha^\beta \big((H_0-\lambda-i\varepsilon)^{-1} - (H_0-\lambda+i\varepsilon)^{-1}\big) \,\mathrm{d}\lambda
\end{aligned}$$

Thus, by considering $\alpha = a+\delta$, $\beta = b+\delta$ and by taking consecutively the two limits $\lim_{\varepsilon\searrow 0}$ and then $\lim_{\delta\searrow 0}$ one infers that $E^H\big((a,b]\big)W = WE^{H_0}\big((a,b]\big)$ for any $a < b$. Considering the limit $a \to -\infty$ one finds $E^H_\lambda W = WE^{H_0}_\lambda$ for any $\lambda \in \mathbb{R}$. The equality mentioned in the statement for any Borel set follows then from the equality for any elements of the spectral family. The equality $\varphi(H)W = W\varphi(H_0)$ follows also from the previous equality and from the definition of the function of an operator.

For (5.8) observe that if $f \in \mathsf{D}(H_0)$, then $W\,\mathrm{e}^{-itH_0} f$ is strongly differentiable at $t = 0$, with derivative $-iWH_0 f$. However, since $W\,\mathrm{e}^{-itH_0} f = \mathrm{e}^{-itH}\, Wf$, this function is also strongly differentiable at $t = 0$. It then follows from Stone's theorem that $Wf \in \mathsf{D}(H)$ and that the derivative at $t = 0$ is given by $-iHWf$. The equality (5.8) follows then directly. □

Note that the properties mentioned in the point (ii) are usually referred to as the *intertwining properties* of the wave operators. Note also that the different steps presented in the proof, namely how to go from an intertwining relation for the unitary group to an intertwining relation for arbitrary continuous and bounded functions, is a quite common procedure. One can prove similarly that if $B \in \mathscr{B}(\mathcal{H})$ satisfies $CU_t = U_tC$ for an arbitrary unitary group, then $C\varphi(A) = \varphi(A)C$ for any bounded and continuous function of its generator A.

Let us now state some additional properties of the wave operators.

Proposition 5.2.3. *Let* $W_\pm := W_\pm(H, H_0, E)$ *be the wave operators for the pair* (H, H_0) *and the initial set projection* E. *Let* $F_\pm$ *be the final range projection,* i.e. *the orthogonal projection on* $\mathsf{Ran}(W_\pm)$ *which is given by* $F_\pm := W_\pm W_\pm^*$. *Then* $F_\pm$ *commute with the elements of the unitary group* $\{\mathrm{e}^{-itH}\}_{t\in\mathbb{R}}$ *and the limits*

$$W_\pm(H_0, H, F_\pm) := s - \lim_{t\to\pm\infty} \mathrm{e}^{itH_0}\,\mathrm{e}^{-itH}\,F_\pm$$

exist and satisfy $W_\pm(H_0, H, F_\pm) = W_\pm(H, H_0, E)^*$. *In addition, the following implications hold:*

$$E\mathcal{H} \subset \mathcal{H}_{ac}(H_0) \Longrightarrow F_\pm\mathcal{H} \subset \mathcal{H}_{ac}(H),$$
$$E\mathcal{H} \subset \mathcal{H}_{c}(H_0) \Longrightarrow F_\pm\mathcal{H} \subset \mathcal{H}_{c}(H).$$

Proof. In this proof we consider only $W := W_+(H, H_0, E)$, the case $W = W_-(H, H_0, E)$ being similar. Accordingly, we simply write F for F_+.

i) Recall first that $\mathrm{e}^{-itH}\,W = W\,\mathrm{e}^{-itH_0}$ for any $t \in \mathbb{R}$. By taking the adjoint on both sides, and by switching t to $-t$ one infers that $W^*\,\mathrm{e}^{-itH} = \mathrm{e}^{-itH_0}\,W^*$ for any $t \in \mathbb{R}$. It then follows that

$$\mathrm{e}^{-itH}\,F = \mathrm{e}^{-itH}\,WW^* = W\,\mathrm{e}^{-itH_0}\,W^* = WW^*\,\mathrm{e}^{-itH} = F\,\mathrm{e}^{-itH},$$

which corresponds to the expected commutation relation.

ii) Let us now consider $g \in \mathsf{Ran}(W)$. There exists thus $f \in E\mathcal{H}$ such that $g = Wf$. Then we have

$$\begin{aligned}\|\,\mathrm{e}^{itH_0}\,\mathrm{e}^{-itH}\,g - f\| &= \big\|\,\mathrm{e}^{itH}\,\mathrm{e}^{-itH_0}\big(\mathrm{e}^{itH_0}\,\mathrm{e}^{-itH}\,g - f\big)\big\| \\ &= \|g - \mathrm{e}^{itH}\,\mathrm{e}^{-itH_0}\,f\| = \|Wf - \mathrm{e}^{itH}\,\mathrm{e}^{-itH_0}\,f\|,\end{aligned}$$

which converges to 0 as $t \to +\infty$. It thus follows that the operator $W_+(H_0, H, F)$ exists. One also deduces from the previous equalities that $s - \lim_{t\to+\infty} \mathrm{e}^{itH_0}\,\mathrm{e}^{-itH}\,W = E$, and as a consequence

$$\begin{aligned}W_+(H_0, H, F) &= s - \lim_{t\to+\infty} \mathrm{e}^{itH_0}\,\mathrm{e}^{-itH}\,F \\ &= s - \lim_{t\to+\infty} \mathrm{e}^{itH_0}\,\mathrm{e}^{-itH}\,WW^* = EW^* = (WE)^* = W^*,\end{aligned}$$

as mentioned in the statement.

iii) Let again $g \in \mathsf{Ran}(W)$ and let $f \in E\mathcal{H}$ such that $Wf = g$. One then infers from Proposition 5.2.2 that for any $V \in \mathcal{A}_B$ one has

$$\langle g, E^H(V)g\rangle = \langle Wf, E^H(V)Wf\rangle = \langle W^*Wf, E^{H_0}(V)f\rangle = \langle f, E^{H_0}(V)f\rangle.$$

Thus, if the measure $m_f^{H_0}$ is absolutely continuous, then the same property holds for the measure m_g^H. Similarly, if f belongs to $\mathcal{H}_c(H_0)$, then $g = Wf$ belongs to $\mathcal{H}_c(H)$. □

Up to now, we have studied some properties of the wave operators by assuming their existence. In the next statement, we give a criterion which ensures their existence. Its use is often quite easy, especially if the evolution group generated by H_0 is simple enough.

Proposition 5.2.4 (Cook criterion). *Let H_0, H be two self-adjoint operators in a Hilbert space $\mathcal{H}$, let $\mathcal{M}$ be a subspace of $\mathcal{H}$ invariant under the group $\{e^{-itH_0}\}_{t\in\mathbb{R}}$, and let $\mathcal{D}$ be a linear subset of $\mathcal{M}$ satisfying*

(i) The linear combinations of elements of $\mathcal{D}$ span a dense set in $\mathcal{M}$,

(ii) $e^{-itH_0} f \in \mathsf{D}(H) \cap \mathsf{D}(H_0)$ for any $f \in \mathcal{D}$ and $t \in \mathbb{R}$,

(iii) $\int_{\pm 1}^{\pm\infty} \|(H-H_0)\, e^{-i\tau H_0} f\| d\tau < \infty$ for any $f \in \mathcal{D}$.

Then $W_\pm(H, H_0, E)$ exists, with E the orthogonal projection on $\mathcal{M}$.

Proof. As in the previous proofs, we consider only $W_+(H, H_0, E)$, the proof for the other wave operator being similar.

For any $f \in \mathcal{D}$ and by the assumption (ii) one infers that

$$\begin{aligned}\frac{d}{dt}\big(e^{itH}\, e^{-itH_0} f\big) &= \big(\frac{d}{dt} e^{itH}\big)\, e^{-itH_0} f + e^{itH}\,\big(\frac{d}{dt} e^{-itH_0} f\big)\\ &= i\, e^{itH}(H-H_0)\, e^{-itH_0} f.\end{aligned}$$

By the result of Proposition 1.2.3.(iii) and for any $t > s > 1$ one gets that

$$\begin{aligned}e^{itH}\, e^{-itH_0} f - e^{isH}\, e^{-isH_0} f &= \int_s^t \frac{d}{d\tau}\big(e^{i\tau H}\, e^{-i\tau H_0} f\big) d\tau\\ &= i \int_s^t e^{i\tau H}(H-H_0)\, e^{-i\tau H_0} f d\tau\end{aligned}$$

from which one infers that

$$\begin{aligned}\big\| e^{itH}\, e^{-itH_0} f - e^{isH}\, e^{-isH_0} f\big\| &= \Big\| \int_s^t \frac{d}{d\tau}\big(e^{i\tau H}\, e^{-i\tau H_0} f\big) d\tau\Big\|\\ &\leq \int_s^t \big\| e^{i\tau H}(H-H_0)\, e^{-i\tau H_0} f\big\| d\tau\\ &= \int_s^t \big\|(H-H_0)\, e^{-i\tau H_0} f\big\| d\tau\ .\end{aligned}$$

Since the latter expression is arbitrarily small for s and t large enough, one deduces that the map $t \mapsto e^{itH}\, e^{-itH_0} f$ is strongly Cauchy for any $f \in \mathcal{D}$, and thus strongly convergent for any $f \in \mathcal{D}$. The strong convergence on $\mathcal{M}$ directly follows by a simple density argument. □

Let us still mention a rather famous result about trace-class perturbations, see also Extension 1.4.14. For its proof we refer for example to [Kat, Thm. X.4.4].

Theorem 5.2.5 (Kato-Rosenblum theorem). *Let H and H_0 be two self-adjoint operators in a Hilbert space such that $H - H_0$ is a trace class operator (or in particular a finite rank operator). Then the wave operators $W_\pm\big(H, H_0, E_{ac}(H_0)\big)$ exist.*

Extension 5.2.6. *Work on this theorem and on its proof.*

Let us now provide a few examples for which the existence of the wave operators has been shown. Note that most the time, the existence is proved by using Proposition 5.2.4 or a slightly improved version of it. The first example corresponds to a Schrödigner operator with a short-range potential.

Example 5.2.7. *In the Hilbert space $\mathcal{H} := L^2(\mathbb{R}^d)$, let H_0 be the Laplace operator $-\Delta$ and let $H := H_0 + V(X)$ with $V(X)$ a multiplication operator by a real valued measurable function which satisfies*

$$|V(x)| \leq c \frac{1}{(1+|x|)^{1+\varepsilon}}$$

for some constant $c > 0$ and some $\varepsilon > 0$. Then the projection E can be chosen equal to $\mathbf{1}$ and the wave operators $W_\pm(H, H_0)$ exist. Note that such a result is part of the folklore of scattering theory for Schrödinger operators and that the proof of such a statement can be found in many textbooks.

The second example is a very simple system on which all the computations can be performed explicitly, see [Yaf, Sec. 2.4].

Example 5.2.8. *Let $\mathcal{H} := L^2(\mathbb{R})$ and consider the operator H_0 defined by the operator D. The corresponding unitary group acts as $[\mathrm{e}^{-itH_0} f](x) = f(x-t)$ as mentioned in Example 5.1.3. Let also $q : \mathbb{R} \to \mathbb{R}$ belong to $L^1(\mathbb{R})$ and consider the unitary operator V defined by $[Vf](x) = \mathrm{e}^{-i\int_0^x q(y)\mathrm{d}y} f(x)$ for any $f \in \mathcal{H}$ and $x \in \mathbb{R}$. By setting $H := VH_0V^*$ one checks that H is the operator defined on*

$$\mathsf{D}(H) := \big\{f \in \mathcal{H} \mid f \text{ is absolutely continuous and } -if' + qf \in L^2(\mathbb{R})\big\}$$

with $Hf = -if' + qf$ for any $f \in \mathsf{D}(H)$. The unitary group generated by H can then be computed explicitly and one gets

$$[\mathrm{e}^{itH}\,\mathrm{e}^{-itH_0} f](x) = [V\,\mathrm{e}^{itH_0}\,V^*\,\mathrm{e}^{-itH_0} f](x) = \mathrm{e}^{i\int_x^{x+t} q(y)\mathrm{d}y} f(x).$$

We can then conclude that the wave operators $W_\pm(H, H_0)$ exist and are given by

$$[W_\pm(H, H_0)f](x) = \mathrm{e}^{i\int_x^{\pm\infty} q(y)\mathrm{d}y} f(x).$$

We add one more example for which all computations can be done explicitly and refer to [Ric, Sec. 2] for the details.

Example 5.2.9. *Let $\mathcal{H} := L^2(\mathbb{R}_+)$ and consider the Dirichlet Laplacian H_D on $\mathbb{R}_+$. More precisely, we set $H_D = -\frac{d^2}{dx^2}$ with the domain $\mathsf{D}(H_D) = \{f \in \mathcal{H}^2(\mathbb{R}_+) \mid f(0) = 0\}$. Here $\mathcal{H}^2(\mathbb{R}_+)$ means the usual Sobolev space on $\mathbb{R}_+$ of order 2. For any $\alpha \in \mathbb{R}$, let us also consider the operator H^α defined by $H^\alpha = -\frac{d^2}{dx^2}$ with $\mathsf{D}(H^\alpha) = \{f \in \mathcal{H}^2(\mathbb{R}_+) \mid f'(0) = \alpha f(0)\}$. It can easily be checked that if $\alpha < 0$ the operator H^α possesses only one eigenvalue, namely $-\alpha^2$, and the corresponding eigenspace is generated by the function $x \mapsto e^{\alpha x}$. On the other hand, for $\alpha \geq 0$ the operators H^α have no eigenvalue, and so does H_D.*

Let us also recall the action of the dilation group in $\mathcal{H}$, as already introduced in Example 5.1.4. This unitary group $\{U_t\}_{t\in\mathbb{R}}$ acts on $f \in \mathcal{H}$ as

$$[U_t f](x) = e^{t/2} f\big(e^t x\big), \qquad \forall x \in \mathbb{R}_+.$$

Its self-adjoint generator is denoted by A. For this model, the following equality can be proved

$$W_-(H^\alpha, H_D) = 1 + \tfrac{1}{2}\big(1 + \tanh(\pi A) - i\cosh(\pi A)^{-1}\big)\Big[\frac{\alpha + i\sqrt{H_D}}{\alpha - i\sqrt{H_D}} - 1\Big]. \qquad (5.9)$$

and a similar formula holds for $W_+(H^\alpha, H_D)$. Let us still mention that the function of A in the above formula is linked to the Hilbert transform.

5.3 Scattering operator and completeness

In this section we consider again two self-adjoint operators H and H_0 in a Hilbert space $\mathcal{H}$, and assume that the wave operators $W_\pm(H, H_0)$ exist. Note that for simplicity we have set $E = \mathbf{1}$ but the general theory can be considered without much additional efforts.

Definition 5.3.1. *In the framework mentioned above, the operator*

$$S \equiv S(H, H_0) := \big(W_+(H, H_0)\big)^* W_-(H, H_0)$$

is called the scattering operator *for the pair (H, H_0).*

We immediately state and prove some properties of this operator. For simplicity, we shall simply write $W_\pm$ for $W_\pm(H, H_0)$.

Proposition 5.3.2. *(i) The scattering operator commutes with H_0, or more precisely*

$$[S, e^{-itH_0}] = 0 \qquad \forall t \in \mathbb{R}, \qquad (5.10)$$

and for any $f \in \mathsf{D}(H_0)$ one has $Sf \in \mathsf{D}(H_0)$ and $SH_0 f = H_0 S f$.

(ii) S is an isometric operator if and only if $\mathsf{Ran}(W_-) \subset \mathsf{Ran}(W_+)$,

(iii) S is a unitary operator if and only if $\mathsf{Ran}(W_-) = \mathsf{Ran}(W_+)$.

Proof. i) The first statement directly follows from the intertwining relations as presented in Proposition 5.2.2 and in its proof for the adjoint operators. Indeed one has

$$S\,\mathrm{e}^{-itH_0} = W_+^* W_-\,\mathrm{e}^{-itH_0} = W_+^*\,\mathrm{e}^{-itH}\,W_- = \mathrm{e}^{-itH_0}\,W_+^* W_- = \mathrm{e}^{-itH_0}\,S.$$

Then, for any $f \in \mathsf{D}(H_0)$ observe that $\frac{i}{t}S(\mathrm{e}^{-itH_0}-1)f = \frac{i}{t}(\mathrm{e}^{-itH_0}-1)Sf$, and since the l.h.s. converges to SH_0f, the r.h.s. must also converge and it converges then to H_0Sf, which proves the second part of the statement (i).

ii) Let us set $F_\pm$ for the final range projection, *i.e.* $F_\pm := W_\pm W_\pm^*$. The assumption $\mathsf{Ran}(W_-) \subset \mathsf{Ran}(W_+)$ means $F_+W_- = W_-$. Under this hypothesis one has

$$S^*S = W_-^* W_+ W_+^* W_- = W_-^* F_+ W_- = W_-^* W_- = \mathbf{1},$$

which means that S is isometric. On the other hand if $\mathsf{Ran}(W_-) \subset \mathsf{Ran}(W_+)$ is not satisfied, then there exists $g \in \mathsf{Ran}(W_-)$ with $g \notin \mathsf{Ran}(W_+) \equiv \mathsf{Ran}(F_+)$. By setting $f = W_-^* g$ (so that $g = W_-f$) one infers that $\|F_+g\| < \|g\| = \|W_-f\| = \|f\|$, since W_- is an isometry. It follows that

$$\|Sf\| = \|W_+^* W_- f\| = \|W_+^* g\| = \|W_+ W_+^* g\| = \|F_+ g\| < \|f\|,$$

which means that S can not be isometric.

iii) S is unitary if and only if S and S^* are isometric. By (ii) S is isometric if and only if $\mathsf{Ran}(W_-) \subset \mathsf{Ran}(W_+)$. Since $S^* = W_-^* W_+$ one infers by exchanging the role of the two operators that S^* is isometric if and only if $\mathsf{Ran}(W_+) \subset \mathsf{Ran}(W_-)$. This naturally leads to the statement (iii). □

In relation with the previous statement, let us assume that H_0 is purely absolutely continuous. In that case, one often says that the scattering system for the pair (H, H_0) is *complete*[1] if $\mathsf{Ran}(W_-) = \mathcal{H}_{ac}(H)$ or if $\mathsf{Ran}(W_+) = \mathcal{H}_{ac}(H)$. We also say that *the asymptotic completeness* holds if $\mathsf{Ran}(W_-) = \mathsf{Ran}(W_+) = \mathcal{H}_p(H)^\perp$. Note that this latter requirement is a very strong condition. In particular it implies that H has not singular continuous spectrum, and that for any $f \in \mathcal{H}_{ac}(H)$ there exists $f_\pm$ such that

$$\lim_{t\to\pm\infty} \big\|\,\mathrm{e}^{-itH} f - \mathrm{e}^{-itH_0} f_\pm\big\| = 0. \tag{5.11}$$

In other words, the evolution of any element of $\mathcal{H}_{ac}(H)$ can be described asymptotically by the simpler evolution e^{-itH_0} on a vector $f_\pm$.

In the Examples 5.2.7, 5.2.8 and 5.2.9, the corresponding scattering systems are asymptotically complete. Note also that the Kato-Rosenblum theorem leads to the existence and to the completeness of the wave operators. On the other hand, Cook criterion, as presented in Proposition 5.2.4, does not provide any information about the completeness or the asymptotic completeness of the wave operators.

[1] Be aware that this terminology is not completely fixed and can still depend on the authors.

Let us close this section with a variant of the spectral theorem. The following formulation is a little bit imprecise because a fully rigorous version needs some more information on the structure of direct integrals of Hilbert spaces and on the notion of the multiplicity theory. We refer to [BM, Chap. 2] for the notion of multiplicity, and to the same book but Chapter 4 and 5 for more information on direct integral of Hilbert spaces and of operators. We also refer to [Yaf, Sec. 1.5] for a very short presentation of the same material.

For a σ-finite measure m on $(\mathbb{R}, \mathcal{A}_B)$ we define

$$\mathscr{H} := \int_{\mathbb{R}}^{\oplus} \mathfrak{H}(\lambda)\, m(\mathrm{d}\lambda) \tag{5.12}$$

as the Hilbert space of equivalence class of vector-valued functions $\mathbb{R} \ni \lambda \mapsto \mathfrak{f}(\lambda) \in \mathfrak{H}(\lambda)$ taking values in the Hilbert space $\mathfrak{H}(\lambda)$ and which are measurable and square integrable with respect to the measure m. The scalar product in $\mathscr{H}$ is given by

$$\langle \mathfrak{f}, \mathfrak{g}\rangle_{\mathscr{H}} := \int_{\mathbb{R}} \langle \mathfrak{f}(\lambda), \mathfrak{g}(\lambda)\rangle_\lambda\, m(\mathrm{d}\lambda)$$

with $\langle\cdot,\cdot\rangle_\lambda$ the scalar product in $\mathfrak{H}(\lambda)$. If the fiber $\mathfrak{H}(\lambda)$ is a constant Hilbert space $\mathfrak{H}$ independent of λ, then the above construction corresponds to $L^2(\mathbb{R}, m; \mathfrak{H}) \cong L^2(\mathbb{R}, m) \otimes \mathfrak{H}$.

In this context, one of the formulation of the spectral theorem can be expressed as a decomposition of any self-adjoint operator into a direct integral of operator. More precisely, for any self-adjoint operator H in a Hilbert space $\mathcal{H}$ there exists a measure σ-finite measure m on $\mathbb{R}$ and a unitary transformation $\mathscr{F} : \mathcal{H} \to \mathscr{H}$ such that

$$\langle E(V)f, g\rangle_{\mathcal{H}} = \int_V \langle [\mathscr{F} f](\lambda), [\mathscr{F} g](\lambda)\rangle_\lambda\, m(\mathrm{d}\lambda),$$

where $E(\cdot)$ is the spectral measure associated with H and V is any Borel set on $\mathbb{R}$. A different way of writing the same information is by saying that H is a diagonal operator in the direct integral representation provided by $\mathscr{H}$. In other words, the following equality holds:

$$\mathscr{F} H \mathscr{F}^* = \int_{\mathbb{R}}^{\oplus} \lambda\, m(\mathrm{d}\lambda).$$

Note that such a decomposition is called *the direct integral representation of* H. This representation is often highly non-unique, but in applications some natural choices often appear. In addition, if H is purely absolutely continuous, then the measure m can be chosen as the Lebesgue measure, as mentioned in [BM, Sec. 5.2.4]. In any case, the support of the measure m coincides with the spectrum of H, and thus we can restrict the above construction to the spectrum $\sigma(H)$ of H.

Once the notion of a direct integral Hilbert space $\mathscr{H}$ is introduced, as in (5.12), direct integral operators operators acting on this Hilbert space can naturally be studied.

We refer again to [BM] for more information, or to [RS4, XIII.16] for a short introduction to this theory and a few important results. Our only aim in this direction is the statement of the following result. Note that its proof is based on the commutation relation provided in (5.10) and that such an argument is quite standard.

Proposition 5.3.3. *Let H_0 be an absolutely continuous self-adjoint operator in a Hilbert space $\mathcal{H}$ and let $\mathscr{F}_0$ and $\mathscr{H}_0$ be a direct integral representation of H_0,* i.e. *$\mathscr{H}_0$ is a direct integral Hilbert space as constructed in* (5.12) *with m the Lebesgue measure, and $\mathscr{F}_0 : \mathcal{H} \to \mathscr{H}_0$ is a unitary map satisfying $\mathscr{F}_0 H_0 \mathscr{F}_0^* = \int_{\sigma(H_0)}^{\oplus} \lambda \,\mathrm{d}\lambda$. Let H be another self-adjoint operator in $\mathcal{H}$ such that the wave operators $W_\pm(H, H_0)$ exist and are asymptotically complete. Then there exists a family $\{S(\lambda)\}_{\lambda\in\sigma(H_0)}$ of unitary operator in $\mathfrak{H}(\lambda)$ for almost every λ such that*

$$\mathscr{F} S \mathscr{F}^* = \int_{\sigma(H_0)}^{\oplus} S(\lambda)\,\mathrm{d}\lambda.$$

The operator $S(\lambda)$ is called the *scattering matrix at energy* λ even if $S(\lambda)$ is usually not a matrix but a unitary operator in $\mathfrak{H}(\lambda)$. Note that there also exist expressions for the operators S and the operator $S(\lambda)$ in terms of the difference of the resolvent of H and the resolvent of H_0 on the real axis. Such expressions are usually referred to as *the stationary approach of scattering theory*. This approach will not be developed here, but the reference [Yaf] is one of the classical book on the subject.

Extension 5.3.4. *Work on the notion of multiplicity and on the theory of direct integral of Hilbert spaces and direct integral of operators.*

Chapter 6

Commutator methods

Let us consider a self-adjoint operator H in a Hilbert space $\mathcal{H}$. As seen in Section 4.4 the resolvent $(H - \lambda \mp i\varepsilon)^{-1}$ does not possess a limit in $\mathscr{B}(\mathcal{H})$ as $\varepsilon \searrow 0$ if $\lambda \in \sigma(H)$. However, the expression $\langle f, (H - \lambda \mp i\varepsilon)^{-1} f\rangle$ may have a limit as $\varepsilon \searrow 0$ for suitable f. In addition, if this limit exists for sufficiently many f, then H is likely to have only absolutely continuous spectrum around λ, see Proposition 4.4.2 for a precise statement.

Our aim in this chapter is to present a method which allows us to determine if the spectrum of H is purely absolutely continuous in some intervals. This method is an extension of Theorem 4.4.3 of Putnam which is valid if both operators H and A are unbounded. Again, the method relies on the positivity of the commutator $[iH, A]$, once this operator is well-defined and localized in the spectrum of H. In fact, it was E. Mourre who understood how the method of Putnam can be sufficiently generalized.

Since the proof of the main result is rather long and technical, we shall first state the main result in a quite general setting. Then, the various tools necessary for understanding this result will be presented, as well as some of its corollaries. Only at the end of the chapter, a proof will be sketched, or presented in a restricted setting.

6.1 Main result

As mentioned above, we will state the main results of the chapter even if it is not fully understandable yet. Additional explanations will be provided in the subsequent sections. Let us however introduce very few information. A self-adjoint operator H in a Hilbert space $\mathcal{H}$ has *a gap* if $\sigma(H) \neq \mathbb{R}$. In the sequel, we shall give a meaning to the requirement "H is of class $C^1(A)$ or of class $C^{1,1}(A)$", but let us mention that the condition H being of class $C^1(A)$, and *a fortiori* of class $C^{1,1}(A)$, ensures that the commutator $[iH, A]$, between two unbounded self-adjoint operators, is well-defined in a sense explained later on.

The following statement corresponds to [ABG, Thm. 7.4.2].

Theorem 6.1.1. *Let H be a self-adjoint operator in $\mathcal{H}$, of class $C^{1,1}(A)$ and having a spectral gap. Let $J \subset \mathbb{R}$ be open and bounded and assume that there exist $a > 0$ and*

$K \in \mathscr{K}(\mathcal{H})$ such that

$$E^H(J)[iH,A]E^H(J) \geq aE^H(J) + K.$$

Then H has at most a finite number of eigenvalues in J, multiplicity counted, and has no singular continuous spectrum in J.

In fact, this statement is already a corollary of a more general result that we provide below. For its statement, let us still introduce some information. If A is a second self-adjoint operator in $\mathcal{H}$, with domain $\mathsf{D}(A)$, let us set $\mathcal{G} := \big(\mathsf{D}(A), \mathcal{H}\big)_{1/2,1}$ for the Banach space obtained by interpolation between $\mathsf{D}(A)$ and $\mathcal{H}$ (explained later on). Its dual space is denoted by $\mathcal{G}^*$ and one has $\mathcal{G} \subset \mathcal{H} \subset \mathcal{G}^*$ with dense and continuous embeddings, as well as $\mathscr{B}(\mathcal{H}) \subset \mathscr{B}(\mathcal{G},\mathcal{G}^*)$. If H is of class $C^1(A)$ we also define the subset $\mu^A(H)$ by

$$\mu^A(H) := \big\{\lambda \in \mathbb{R} \mid \exists \varepsilon > 0, a > 0 \text{ s.t. } E(\lambda;\varepsilon)[iH,A]E(\lambda;\varepsilon) \geq aE(\lambda;\varepsilon)\big\}, \tag{6.1}$$

where $E(\lambda;\varepsilon) := E^H\big((\lambda-\varepsilon,\lambda+\varepsilon)\big)$.

The following statement is a slight reformulation of [ABG, Thm 7.4.1].

Theorem 6.1.2. *Let H be a self-adjoint operator in $\mathcal{H}$ and assume that H has a gap and is of class $C^{1,1}(A)$. Then, for each $\lambda \in \mu^A(H)$ the limits $\lim_{\varepsilon\searrow 0}\langle f,(H-\lambda\mp i\varepsilon)^{-1}f\rangle$ exist for any $f \in \mathcal{G}$ and uniformly on each compact subset of $\mu^A(H)$. In particular, if T is a linear operator from $\mathcal{H}$ to an auxiliary Hilbert space, and if T is continuous when $\mathcal{H}$ is equipped with the topology induced by $\mathcal{G}^*$, then T is locally H-smooth on the open set $\mu^A(H)$.*

Note that the notion of H-smooth operator will be introduced later on, but that these operators play an important role for proving the existence and the completeness of some wave operators.

Remark 6.1.3. *In the above two statements, it is assumed that H has a spectral gap, which is a restricting assumption since there also exist operators H with $\sigma(H) = \mathbb{R}$. For example, the operator X of multiplication by the variable in $L^2(\mathbb{R})$ has spectrum equal to $\mathbb{R}$. However, there also exists a version of the Theorems 6.1.1 and 6.1.2 which do not require the existence of a gap. The main interest in the gap assumption is that there exists $\lambda_0 \in \mathbb{R}$ such that $(H-\lambda_0)^{-1}$ is bounded and self-adjoint. This operator can then be used in the proofs and this fact is quite convenient. If such a λ_0 does not exist proofs are a little bit more involved.*

Our main task now is to introduce all the notions such that the above statements become fully understandable.

6.2 Regularity classes

Most of the material presented in this section is borrowed from Chapter 5 of [ABG] to which we refer for more information and for a presentation in a more general setting.

Let us consider a self-adjoint operator A in $\mathcal{H}$ which generates the strongly continuous unitary group $\{e^{-itA}\}_{t\in\mathbb{R}}$. We also consider a bounded operator S in $\mathcal{H}$. In this setting, the map

$$\mathbb{R} \ni \; t \mapsto \mathscr{U}_t[S] \equiv S(t) := e^{itA}\, S\, e^{-itA} \; \in \mathscr{B}(\mathcal{H}) \tag{6.2}$$

is well-defined and its regularity can be studied. In fact, $\mathscr{U}_t : \mathscr{B}(\mathcal{H}) \to \mathscr{B}(\mathcal{H})$ defines a weakly continuous representation of $\mathbb{R}$ in $\mathscr{B}(\mathcal{H})$.

We start by some conditions of regularity indexed by a positive integer k.

Definition 6.2.1. *Let $k \in \mathbb{N}$.*

(i) $C^k(A)$ denotes the Banach space of all $S \in \mathscr{B}(\mathcal{H})$ such that the map (6.2) *is k-times strongly continuously differentiable, and endowed with the norm*

$$\|S\|_{C^k} := \Big(\sum_{j=0}^{k} \|S^{(j)}(0)\|^2\Big)^{1/2}, \tag{6.3}$$

where $S^{(j)}(0)$ denotes the j^{th} derivative of $S(t)$ evaluated at $t = 0$.

(ii) $C^k_u(A)$ denotes the Banach space of all $S \in \mathscr{B}(\mathcal{H})$ such that the map (6.2) *is k-times continuously differentiable in norm, and endowed with the norm defined by* (6.3).

It can be shown that these spaces are indeed complete and that $C^k_u(A) \subset C^k(A)$. An equivalent description of the elements of $C^k(A)$ or $C^k_u(A)$ is provided in the following statement, see [ABG, Thm. 5.1.3] for its proof.

Proposition 6.2.2. *Let $k \in \mathbb{N}^*$ and $S \in \mathscr{B}(\mathcal{H})$. Then S belongs to $C^k(A)$ or to $C^k_u(A)$ if and only if $\lim_{t\searrow 0} t^{-k}(\mathscr{U}_t - \mathbf{1})^k[S]$ exists in the strong or in the norm topology of $\mathscr{B}(\mathcal{H})$.*

Note now that a formal computation of $\frac{\mathrm{d}}{\mathrm{d}t}S(t)|_{t=0}$ gives $S'(0) = [iA, S]$. However, this formula has to be taken with some care since it involves the operator A which is often unbounded. In fact, a more precise and alternative description of the $C^1(A)$ condition is often very useful, see [ABG, Lem. 6.2.9] for its proof.

Lemma 6.2.3. *The bounded operator S belongs to $C^1(A)$ if and only if there exists a constant $c < \infty$ such that*

$$\big|\langle Af, iSf\rangle - \langle S^*f, iAf\rangle\big| \le c\|f\|^2, \qquad \forall f \in \mathsf{D}(A). \tag{6.4}$$

In fact, the expression $\langle Af, iSf\rangle - \langle iS^*f, Af\rangle$ defines a quadratic form with domain $\mathsf{D}(A)$, and the condition (6.4) means precisely that this form is bounded. Since $\mathsf{D}(A)$ is dense in $\mathcal{H}$, this form extends to a bounded form on $\mathcal{H}$, and there exists a unique operator in $\mathscr{B}(\mathcal{H})$ which corresponds to this form. For an obvious reason we denote this bounded operator by $[iA, S]$ and the following equality holds for any $f \in \mathsf{D}(A)$

$$\langle Af, iSf\rangle - \langle S^*f, iAf\rangle = \langle f, [iA, S]f\rangle.$$

However, let us stress that the bounded operator $[iA, S]$ has *a priori* no explicit expression on all $f \in \mathcal{H}$.

Let us add some rather simple properties of the class $C^k(A)$ and $C^k_u(A)$.

Proposition 6.2.4. *(i) If S belongs to $C^k(A)$ then $S \in C^{k-1}_u(A)$,*

(ii) If $S, T \in C^k(A)$ then $ST \in C^k(A)$, and if $S, T \in C^k_u(A)$ then $ST \in C^k_u(A)$,

(iii) If S is boundedly invertible, then $S \in C^k(A) \iff S^{-1} \in C^k(A)$, and $S \in C^k_u(A) \iff S^{-1} \in C^k_u(A)$,

(iv) $S \in C^k(A) \iff S^* \in C^k(A)$, and $S \in C^k_u(A) \iff S^* \in C^k_u(A)$.

Exercise 6.2.5. *Provide a proof of the above statements. Note that compared with the general theory presented in [ABG, Sec. 5.1] we are dealing only with a one-parameter unitary group, and only in the Hilbert space $\mathcal{H}$. Multiparameter C_0-group acting on arbitrary Banach spaces are avoided in these notes.*

Let us now present some regularity classes of fractional order. Consider $s \geq 0$, $p \in [0, \infty]$ and let $\ell \in \mathbb{N}$ with $\ell > s$. We can then define

$$\|S\|^{(\ell)}_{s,p} := \|S\| + \Big(\int_{|t|\leq 1} \big\||t|^{-s}(\mathscr{U}_t - \mathbf{1})^\ell[S]\big\|^p \frac{\mathrm{d}t}{|t|}\Big)^{1/p},$$

with the convention that the integral is replaced by a sup when $p = \infty$. It can then be shown that if $\|S\|^{(\ell)}_{s,p} < \infty$ then $\|S\|^{(\ell')}_{s,p} < \infty$ for any integer $\ell' > s$. For that reason, the following definition is meaningful:

Definition 6.2.6. *For any $s \geq 0$ and $p \in [0, \infty]$ we set $C^{s,p}(A)$ for the set of $S \in \mathscr{B}(\mathcal{H})$ such that $\|S\|^{(\ell)}_{s,p} < \infty$ for some (and them for all) $\ell \in \mathbb{N}$ with $\ell > s$. For two different integers $\ell, \ell' > s$, the maps $S \mapsto \|S\|^{(\ell)}_{s,p}$ and $S \mapsto \|S\|^{(\ell')}_{s,p}$ define equivalent norms on $C^{s,p}(A)$. Endowed with any of these norms, $C^{s,p}(A)$ is a Banach space.*

Let us state some relations between these spaces and the spaces $C^k(A)$ and $C^k_u(A)$ introduced above. All these relations are proved in a larger setting in [ABG, Sec. 5.2].

Proposition 6.2.7. *Let $k \in \mathbb{N}$, $s, t \geq 0$ and $p, q \in [1, \infty]$.*

(i) $C^{s,p}(A) \subset C^{t,q}(A)$ if $s > t$ and for p, q arbitrary,

(ii) $C^{t,p}(A) \subset C^{t,q}(A)$ if $q > p$ and in particular for any $p \in (1, \infty)$

$$C^{s,1}(A) \subset C^{s,p}(A) \subset C^{s,\infty}(A), \tag{6.5}$$

(iii) If $s = k$ is an integer one has

$$C^{k,1}(A) \subset C_u^k(A) \subset C^k(A) \subset C^{k,\infty}(A).$$

Note that a very precise formulation of the differences between $C^{k,1}(A)$, $C_u^k(A)$, $C^k(A)$ and $C^{k,\infty}(A)$ is presented in [ABG, Thm. 5.2.6]. Another relation between some of these spaces is also quite convenient:

Proposition 6.2.8. *Let $s \in (0, \infty)$ and $p \in [1, \infty]$, and write $s = k + \sigma$ with $k \in \mathbb{N}$ and $0 < \sigma \le 1$.*

(i) If $S \in C^{s,p}(A)$ and $j \le k$, then $S^{(j)}(0) \in C^{s-j,p}(A)$,

(ii) If $\|\cdot\|_{C^{\sigma,p}}$ is one norm on $C^{\sigma,p}(A)$, then

$$\|S\|_{C^k} + \|S^{(k)}(0)\|_{C^{\sigma,p}}$$

defines a norm on $C^{s,p}(A)$. In particular $S \in C^{s,p}(A)$ if and only if $S \in C^k(A)$ and $S^{(k)}(0)$ belongs to $C^{\sigma,p}(A)$.

Relations similar to the one presented in Proposition 6.2.4 also hold in the present context:

Proposition 6.2.9. *(i) If $S, T \in C^{s,p}(A)$, then $ST \in C^{s,p}(A)$,*

(ii) If S is boundedly invertible, then $S \in C^{s,p}(A) \iff S^{-1} \in C^{s,p}(A)$,

(iii) $S \in C^{s,p}(A) \iff S^* \in C^{s,p}(A)$.

Let us still mention one more regularity class with respect to A which is quite convenient in applications. The additional continuity condition is related to Dini continuity in classical analysis. For any integer $k \ge 1$ we set $C^{k+0}(A)$ for the set of $S \in C^k(A)$ and such that $S^{(k)}(0)$ satisfies

$$\int_{|t|\le 1} \big\|(\mathscr{U}_t - \mathbf{1})[S^{(k)}(0)]\big\| \frac{\mathrm{d}t}{|t|} < \infty.$$

Once endowed with the norm

$$\|S\|_{C^{k+0}} := \|S\| + \int_{|t|\le 1} \big\|(\mathscr{U}_t - \mathbf{1})[S^{(k)}(0)]\big\| \frac{\mathrm{d}t}{|t|}$$

the set $C^{k+0}(A)$ becomes a Banach space and the following relations hold for any $k \in \mathbb{N}$

$$C^{k+0}(A) \subset C^{k,1}(A) \subset C_u^k(A) \subset C^k(A) \subset C^{k,\infty}(A) \tag{6.6}$$

with $C^{0+0}(A) := C^{0,1}(A)$.

Up to now, we have considered only bounded elements S. In the next section we show how these notions can be useful for unbounded operators as well.

6.3 Affiliation

In this section we consider two self-adjoint operators A and H in a Hilbert space $\mathcal{H}$. The various regularity classes introduced before are defined in term of the unitary group generated by A, and the next definition gives a meaning to the regularity of the operator H with respect to A, even if H is unbounded. Before this definition, let us state a simple lemma whose proof depends only on the first resolvent equation and on some analytic continuation argument, see [ABG, Lem. 6.2.1] for the details.

Lemma 6.3.1. *Let $k \in \mathbb{N}$, $s \geq 0$ and $p \in [0, \infty]$, and let H, A be self-adjoint operators in $\mathcal{H}$. Assume that there exists $z_0 \in \mathbb{C}$ such that $(H - z_0)^{-1}$ belongs to $C^k(A)$, $C^k_u(A)$, or to $C^{s,p}(A)$. Then $(H - z)^{-1}$ belongs to the same regularity class for any $z \in \rho(H)$. In addition, if H is bounded, then H itself belongs to the same regularity class.*

The following definition becomes then meaningful.

Definition 6.3.2. *Let $k \in \mathbb{N}$, $s \geq 0$ and $p \in [0, \infty]$, and let H, A be self-adjoint operators in $\mathcal{H}$. We say that H* is of class $C^k(A)$, $C^k_u(A)$, or $C^{s,p}(A)$ *if $(H - z)^{-1}$ belongs to such a regularity class for some $z \in \rho(H)$, and thus for all $z \in \rho(H)$.*

Clearly, if the resolvent of H belongs to one of these regularity classes, then the same holds for linear combinations of the resolvent for different values of $z \in \rho(H)$. In fact, by functional calculus one can show that $\eta(H)$ belongs to the same regularity class for suitable function $\eta : \mathbb{R} \to \mathbb{R}$. We state such a result for a rather restricted class of functions η and refer to Theorem 6.2.5 and Corollary 6.2.6 of [ABG] for a more general statement. Note that the proof is rather technical and depends on an explicit formula for the operator $\eta(H)$ in terms of the resolvent of H. For completeness we provide such a formula but omit all the details and the explanations. For suitable functions $\eta : \mathbb{R} \to \mathbb{R}$ the following formula holds:

$$\begin{aligned}\eta(H) = &\sum_{k=0}^{r-1} \frac{1}{\pi k!} \int_{\mathbb{R}} \eta^{(k)}(\lambda) \Im\big(i^k (H - \lambda - i)^{-1}\big) \mathrm{d}\lambda \\ &+ \frac{1}{\pi (r-1)!} \int_0^1 \mu^{r-1} \mathrm{d}\mu \int_{\mathbb{R}} \eta^{(r)}(\lambda) \Im\big(i^r (H - \lambda - i\mu)^{-1}\big) \mathrm{d}\lambda. \end{aligned} \tag{6.7}$$

Proposition 6.3.3. *Assume that H is of class $C^k(A)$, $C^k_u(A)$, or $C^{s,p}(A)$, and let η be a real function belonging to $C^\infty_c(\mathbb{R})$. Then $\eta(H)$ belongs to the same regularity class.*

Let us now mention how the condition *H is of class $C^1(A)$* can be checked. For a bounded operator H, this has already been mentioned in Lemma 6.2.3. For an unbounded operator H the question is more delicate. We state below a quite technical result. Note that the invariance of the domain of H with respect to the unitary group generated by A is often assumed, and this assumption simplifies quite a lot the argumentation. However, in the following statement such an assumption is not made.

Theorem 6.3.4 (Thm. 6.2.10 of [ABG]). *Let H and A be self-adjoint operators in a Hilbert space $\mathcal{H}$.*

a) The operator H is of class $C^1(A)$ if and only if the following two conditions hold:

(i) There exists $c < \infty$ such that for all $f \in \mathsf{D}(A) \cap \mathsf{D}(H)$

$$\big|\langle Af, Hf\rangle - \langle Hf, Af\rangle\big| \leq c\big(\|Hf\|^2 + \|f\|^2\big),$$

(ii) For some $z \in \mathbb{C} \setminus \sigma(H)$ the set

$$\big\{f \in \mathsf{D}(A) \mid (H-z)^{-1} f \in \mathsf{D}(A) \text{ and } (H-\bar{z})^{-1} f \in \mathsf{D}(A)\big\}$$

is a core for A.

b) If H is of class $C^1(A)$, then the $\mathsf{D}(A) \cap \mathsf{D}(H)$ is a core for H and the form $[A, H]$ has a unique extension to a continuous sesquilinear form on $\mathsf{D}(H)$ endowed with the graph topology[1]*. If this extension is still denoted by $[A, H]$, then the following identify holds on $\mathcal{H}$:*

$$[A, (H-z)^{-1}] = -(H-z)^{-1}[A, H](H-z)^{-1}. \tag{6.8}$$

Let us still mention how the equality (6.8) can be understood. If we equip $\mathsf{D}(H)$ with the graph topology (it is then a Banach space), and denote by $\mathsf{D}(H)^*$ its dual space, then one has the following dense inclusions $\mathsf{D}(H) \subset \mathcal{H} \subset \mathsf{D}(H)^*$, and the operator $R(z)$ is bounded from $\mathcal{H}$ to $\mathsf{D}(\mathcal{H})$ and extends to a bounded operator from $\mathsf{D}(H)^*$ to $\mathcal{H}$. Then, the fact that $[A, H]$ has a unique extension to a sesquilinear form on $\mathsf{D}(H)$ means that its continuous extension $[A, H]$ is a bounded operator from $\mathsf{D}(H)$ to $\mathsf{D}(H)^*$. Thus, the r.h.s. of (6.8) corresponds to the product of three bounded operators

$$[A, (H-z)^{-1}] = -\underbrace{(H-z)^{-1}}_{\mathsf{D}(H)^* \to \mathcal{H}} \underbrace{[A, H]}_{\mathsf{D}(H) \to \mathsf{D}(H)^*} \underbrace{(H-z)^{-1}}_{\mathcal{H} \to \mathsf{D}(H)} \tag{6.9}$$

which corresponds to a bounded operator in $\mathcal{H}$. By setting $R(z) := (H-z)^{-1}$, formula (6.9) can also re rewritten as

$$[H, A] = (H-z)[A, R(z)](H-z) \tag{6.10}$$

where the r.h.s. is the product of three bounded operators, namely $(H-z) : \mathsf{D}(H) \to \mathcal{H}$, $[A, R(z)] : \mathcal{H} \to \mathcal{H}$ and $(H-z) : \mathcal{H} \to \mathsf{D}(H)^*$.

Another formula will also be useful later on. For $\tau \neq 0$ let us set $A_\tau := \frac{1}{i\tau}(\mathrm{e}^{i\tau A} - \mathbf{1})$, and observe that if H is of class $C^1(A)$ one has for any $z \in \rho(H)$

$$\begin{aligned} [A, R(z)] &= s - \lim_{\tau \to 0} \frac{1}{i\tau}\big(\mathrm{e}^{i\tau A} R(z) \mathrm{e}^{-i\tau A} - R(z)\big) \\ &= s - \lim_{\tau \to 0} \frac{1}{i\tau}\big[\mathrm{e}^{i\tau A}, R(z)\big] \mathrm{e}^{-i\tau A} = s - \lim_{\tau \to 0}[A_\tau, R(z)] \;. \end{aligned} \tag{6.11}$$

[1]The graph topology on $\mathsf{D}(H)$ corresponds to the topology obtained by the norm $\|f\|_{\mathsf{D}(H)} = \big(\|f\|^2 + \|Hf\|^2\big)^{1/2}$ for any $f \in \mathsf{D}(H)$.

In relation with formula (6.9) let us observe that if $J \subset \mathbb{R}$ is a bounded Borel set, then $E^H(J)$ is obviously an element of $\mathscr{B}(\mathcal{H})$ but it also belongs to $\mathscr{B}\big(\mathcal{H}, \mathsf{D}(H)\big)$. Indeed, this fact follows from the boundedness of the operator $HE^H(J)$. By duality, it also follows that the operator $E^H(J)$ extends to a bounded operator from $\mathsf{D}(H)^*$ to $\mathcal{H}$, or in short $E^H(J) \in \mathscr{B}\big(\mathsf{D}(H)^*, \mathcal{H}\big)$. This fact is of crucial importance. Indeed, if H is of class $C^1(A)$, then as shown above the operator $[iH, A]$ belongs to $\mathscr{B}\big(\mathsf{D}(H), \mathsf{D}(H)^*\big)$ and therefore the product

$$E^H(J)[iH, A]E^H(J)$$

belongs to $\mathscr{B}(\mathcal{H})$. Such a product was already mentioned in Section 6.1 for the special choice $J = (\lambda - \varepsilon, \lambda + \varepsilon)$ for some fixed $\lambda \in \mathbb{R}$ and $\varepsilon > 0$.

We now introduce an easy result which is often called *the Virial theorem*. Note that this result is often stated without the appropriate assumption.

Proposition 6.3.5. *Let H and A be self-adjoint operator in $\mathcal{H}$ such that H is of class $C^1(A)$. Then $E^H(\{\lambda\})[A, H]E^H(\{\lambda\}) = 0$ for any $\lambda \in \mathbb{R}$. In particular, if f is an eigenvector of H then $\langle f, [A, H]f\rangle = 0$.*

Proof. We must show that if $\lambda \in \mathbb{R}$ and $f_1, f_2 \in \mathsf{D}(H)$ satisfy $Hf_k = \lambda f_k$ for $k = 1, 2$, then $\langle f_1, [A, H]f_2\rangle = 0$. Since $f_1 = (\lambda - i)(H - i)^{-1}f_1$ and $f_2 = (\lambda + i)(H + i)^{-1}f_2$ we get by (6.10) and (6.11) that

$$\begin{aligned}\langle f_1, [A, H]f_2\rangle &= -(\lambda + i)^2\langle f_1, [A, (H + i)^{-1}]f_2\rangle \\ &= -(\lambda + i)^2 \lim_{\tau\to 0}\Big\{\langle f_1, A_\tau(H + i)^{-1}f_2\rangle - \langle (H - i)^{-1}f_1, A_\tau f_2\rangle\Big\}.\end{aligned}$$

We finally observe that for $\tau \neq 0$, the term into curly brackets is always equal to 0. □

In relation with the definition of $\mu^A(H)$ mentioned in (6.1) let us still introduce two functions which play an important role in Mourre theory. These functions are well defined if the operator H is of class $C^1(A)$. They provide what is called *the best Mourre estimate*, and the first one is defined for any $\lambda \in \mathbb{R}$ by

$$\varrho^A_H(\lambda) := \sup\big\{a \in \mathbb{R} \mid \exists\varepsilon > 0 \text{ s.t. } E(\lambda; \varepsilon)[iH, A]E(\lambda; \varepsilon) \geq aE(\lambda; \varepsilon)\big\}.$$

The second function looks similar to the previous one, but the inequality holds modulo a compact operator, namely

$$\begin{aligned}&\tilde\varrho^A_H(\lambda) \\ &:= \sup\big\{a \in \mathbb{R} \mid \exists\varepsilon > 0 \text{ and } K \in \mathscr{K}(\mathcal{H}) \text{ s.t. } E(\lambda; \varepsilon)[iH, A]E(\lambda; \varepsilon) \geq aE(\lambda; \varepsilon) + K\big\}.\end{aligned}$$

The relation between ϱ^A_H and $\mu^A(H)$ is rather clear. By looking back to the definition of (6.1) one gets

$$\mu^A(H) = \{\lambda \in \mathbb{R} \mid \varrho^A_H(\lambda) > 0\}.$$

Many properties of these functions have been deduced in [ABG, Sec. 7.2].

Proposition 6.3.6. *(i) The function* $\varrho_H^A : \mathbb{R} \to (-\infty, \infty]$ *is lower semicontinuous and* $\varrho_H^A(\lambda) < \infty$ *if and only if* $\lambda \in \sigma(H)$,

(ii) The function $\tilde{\varrho}_H^A : \mathbb{R} \to (-\infty, \infty]$ *is lower semicontinuous and satisfies* $\tilde{\varrho}_H^A \geq \varrho_H^A$. *Furthermore* $\tilde{\varrho}_H^A(\lambda) < \infty$ *if and only if* $\lambda \in \sigma_{ess}(H)$.

Let us now state and prove a corollary of the Virial theorem showing that when $\tilde{\varrho}_H^A$ is strictly positive, then only a finite number of eigenvalues can appear.

Corollary 6.3.7. *Let* H *and* A *be self-adjoint operator in* $\mathcal{H}$ *such that* H *is of class* $C^1(A)$. *If* $\tilde{\varrho}_H^A(\lambda) > 0$ *for some* $\lambda \in \mathbb{R}$ *then* λ *has a neighbourhood in which there is at most a finite number of eigenvalues of* H, *each of finite multiplicity.*

Proof. Let $\varepsilon > 0$, $a > 0$ and $K \in \mathscr{K}(\mathcal{H})$ such that

$$E(\lambda; \varepsilon)[iH, A]E(\lambda; \varepsilon) \geq aE(\lambda; \varepsilon) + K. \tag{6.12}$$

If g is an eigenvector of H associated with an eigenvalue in $(\lambda - \varepsilon, \lambda + \varepsilon)$ and if $\|g\| = 1$, then (6.12) and the Virial theorem imply that $\langle g, Kg \rangle < -a$. By contraposition, assume that the statement of the lemma is false. Then there exists an infinite orthogonal sequence $\{g_j\}$ of eigenvectors of H in $E(\lambda; \varepsilon)\mathcal{H}$. In particular, $w - \lim_{j\to\infty} g_j = 0$, as a consequence of the orthogonality of the sequence. However, since K is compact, Kg_j goes strongly to 0 as $j \to \infty$, and then one has $\langle g_j, Kg_j \rangle \to 0$ as $j \to \infty$. This contradicts the inequality $\langle g_j, Kg_j \rangle \leq -a < 0$. □

The previous result can then be used for showing that the two functions ϱ_H^A and $\tilde{\varrho}_H^A$ are in fact very similar. The proof of the following statement can be found in [ABG, Thm. 7.2.13].

Theorem 6.3.8. *Let* H *and* A *be self-adjoint operator in* $\mathcal{H}$ *such that* H *is of class* $C^1(A)$, *and let* $\lambda \in \mathbb{R}$. *If* λ *is an eigenvalue of* H *and* $\tilde{\varrho}_H^A(\lambda) > 0$, *then* $\varrho_H^A(\lambda) = 0$. *Otherwise* $\varrho_H^A(\lambda) = \tilde{\varrho}_H^A(\lambda)$.

As a conclusion of this section let us mention a result about the stability of the function $\tilde{\varrho}$. Once this stability is proved, the applicability of the previous corollary is quite enlarged.

Theorem 6.3.9. *Let* H, H_0 *and* A *be self-adjoint operators in a Hilbert space* $\mathcal{H}$ *and such that* H_0 *and* H *are of class* $C_u^1(A)$. *If the difference* $(H + i)^{-1} - (H_0 + i)^{-1}$ *is compact, then* $\tilde{\varrho}_H^A(\lambda) = \tilde{\varrho}_{H_0}^A(\lambda)$.

Note that the content of Proposition 6.3.3 for $\eta(H)$ is necessary for the proof of this statement, and that the $C_u^1(A)$-condition can not be weakened. We refer to [ABG, Thm. 7.2.9] for the details.

6.4 Locally smooth operators

An important ingredient for showing the absence of singular continuous spectrum and for proving the existence and the completeness of some wave operators is the notion of *locally smooth operators*. Such operators were already mentioned in the statement of Theorem 6.1.2 and we shall now provide more information on them. Note that an operator T is always smooth *with respect to another operator*, it is thus a relative notion.

Definition 6.4.1. *Let $J \subset \mathbb{R}$ be an open set, and let $\big(H, \mathsf{D}(H)\big)$ be a self-adjoint operator in $\mathcal{H}$. A linear continuous operator $T : \mathsf{D}(H) \to \mathcal{H}$ is* locally H-smooth on J *if for each compact subset $K \subset J$ there exists a constant $C_K < \infty$ such that*

$$\int_{-\infty}^{\infty} \|T\,\mathrm{e}^{-itH} f\|^2 \mathrm{d}t \le C_K \|f\|^2, \qquad \forall f \in E^H(K)\mathcal{H}. \tag{6.13}$$

In the next statement, we shall show that this notion can be recast in a time-independent framework. However some preliminary observations are necessary. As already mentioned in the previous section, by endowing $\mathsf{D}(H)$ with its graph norm, one gets the continuous and dense embeddings

$$\mathsf{D}(H) \subset \mathcal{H} \subset \mathsf{D}(H)^*,$$

and a continuous extension of $R(z) \equiv (H - z)^{-1} \in \mathscr{B}\big(\mathcal{H}, \mathsf{D}(H)\big)$ to an element $R(z) \in \mathscr{B}\big(\mathsf{D}(H)^*, \mathcal{H}\big)$, for any $z \in \rho(H)$. By choosing $z = \lambda + i\mu$ with $\mu > 0$ one observes that

$$\begin{aligned}\delta_{(\mu)}(H-\lambda) &:= \frac{1}{\pi}\Im R(\lambda + i\mu) \\ &= \frac{1}{2\pi i}\big(R(\lambda+i\mu) - R(\lambda - i\mu)\big) = \frac{\mu}{\pi} R(\lambda \mp i\mu) R(\lambda \pm i\mu)\end{aligned}$$

and infers that $\delta_{(\mu)}(H-\lambda) \in \mathscr{B}\big(\mathsf{D}(H)^*, \mathsf{D}(H)\big)$. Therefore, if $T \in \mathscr{B}\big(\mathsf{D}(H), \mathcal{H}\big)$ then $TR(z) \in \mathscr{B}(\mathcal{H})$ and $R(z)T^* = \big(TR(\bar{z})\big)^* \in \mathscr{B}(\mathcal{H})$, and consequently $T\delta_{(\mu)}(H-\lambda)T^* \in \mathscr{B}(\mathcal{H})$. Finally, by the C^*-property $\|S^*S\| = \|S^*\|^2 = \|S\|^2$ one deduces that

$$\|T\delta_{(\mu)}(H-\lambda)T^*\| = \frac{\mu}{\pi}\|TR(\lambda \mp i\mu)\|^2 = \frac{\mu}{\pi}\|R(\lambda \pm i\mu)T^*\|^2.$$

We are now ready to state:

Proposition 6.4.2. *A linear continuous operator $T : \mathsf{D}(H) \to \mathcal{H}$ is locally H-smooth on an open set J if and only if for each compact subset $K \subset J$ there exists a constant $C_K < \infty$ such that*

$$\big\|T \Im R(z) T^*\big\| \le C_K \qquad \text{if } \Re(z) \in K \text{ and } 0 < \Im(z) < 1. \tag{6.14}$$

The proof of this statement is not difficult but a little bit too long. The main ingredients are the equalities

$$R(\lambda \pm i\mu) = i \int_0^{\pm\infty} \mathrm{e}^{it\lambda}\, \mathrm{e}^{-itH-\mu|t|}\, \mathrm{d}t$$

and

$$\delta_{(\mu)}(H-\lambda) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{it\lambda}\, \mathrm{e}^{-itH-\mu|t|}\, \mathrm{d}t$$

which were already mentioned in Remark 5.1.2.

Exercise 6.4.3. *Provide the proof of the above statement, which can be borrowed from [ABG, Prop. 7.1.1].*

We shall immediately provide a statement which shows the importance of this notion of local smoothness for the existence and the completeness of the wave operators.

Theorem 6.4.4. *Let H_1, H_2 be two self-adjoint operators in a Hilbert space $\mathcal{H}$, with spectral measure denoted respectively by E_1 and E_2. Assume that for $j \in \{1,2\}$ there exist $T_j \in \mathscr{B}\big(\mathsf{D}(H_j),\mathcal{H}\big)$ which satisfy*

$$\langle H_1 f_1, f_2\rangle - \langle f_1, H_2 f_2\rangle = \langle T_1 f_1, T_2 f_2\rangle \qquad \forall f_j \in \mathsf{D}(H_j).$$

If in addition there exists an open set $J \subset \mathbb{R}$ such that T_j are locally H_j-smooth on J, then

$$W_\pm\big(H_1, H_2, E_2(J)\big) := s-\lim_{t\to\pm\infty} \mathrm{e}^{itH_1}\, \mathrm{e}^{-itH_2}\, E_2(J) \tag{6.15}$$

exist and are bijective isometries of $E_2(J)\mathcal{H}$ onto $E_1(J)\mathcal{H}$.

Proof. The existence of the limits (6.15) is a simple consequence of the following assertion: for any $f_2 \in \mathcal{H}$ such that $E_2(K_2)f_2 = f_2$ for some compact set $K_2 \subset J$, and for any $\theta_1 \in C_c^\infty(J)$ with $\theta_1(x) = 1$ for any x in a neighbourhood of K_2 the limit

$$s-\lim_{t\to\pm\infty} \theta_1(H_1)\, \mathrm{e}^{itH_1}\, \mathrm{e}^{-itH_2}\, f_2 \tag{6.16}$$

exists, and

$$s-\lim_{t\to\pm\infty} \big[1-\theta_1(H_1)\big]\, \mathrm{e}^{itH_1}\, \mathrm{e}^{-itH_2}\, f_2 = 0. \tag{6.17}$$

Let us now prove (6.16). For that purpose we set $W(t) := \theta_1(H_1)\, \mathrm{e}^{itH_1}\, \mathrm{e}^{-itH_2}$ and observe that for any $f_1 \in \mathcal{H}$ and $s < t$:

$$\begin{aligned}
|\langle f_1, [W(t)-W(s)]f_2\rangle| &= \Big|\int_s^t \langle T_1\, \mathrm{e}^{-i\tau H_1}\, \theta_1(H_1) f_1, T_2\, \mathrm{e}^{-i\tau H_2}\, f_2\rangle \mathrm{d}\tau\Big| \\
&\leq \Big[\int_s^t \|T_1\, \mathrm{e}^{-i\tau H_1}\, \theta_1(H_1) f_1\|^2 \mathrm{d}\tau\Big]^{1/2} \Big[\int_s^t \|T_2\, \mathrm{e}^{-i\tau H_2}\, f_2\|^2 \mathrm{d}\tau\Big]^{1/2} \\
&\leq C_{K_1}\|f\| \Big[\int_s^t \|T_2\, \mathrm{e}^{-i\tau H_2}\, f_2\|^2 \mathrm{d}\tau\Big]^{1/2}
\end{aligned}$$

with $K_1 = \operatorname{supp}\theta_1$. We thus obtain that $\|[W(t)-W(s)]f_2\| \to 0$ as $s \to \infty$ or $t \to -\infty$, which proves (6.16).

For the proof of (6.17) let $\theta_2 \in C_c^\infty(J)$ with $\theta_2(x) = 1$ if $x \in K_2$ and such that $\theta_1\theta_2 = \theta_2$. Then $f_2 = \theta_2(H_2)f_2$ and $[1-\theta_1(H_1)]\theta_2(H_2) = [1-\theta_1(H_1)][\theta_2(H_2) - \theta_2(H_1)]$. Hence (6.17) follows from

$$s - \lim_{|t|\to\infty} \big\|[\theta_2(H_2) - \theta_2(H_1)]\,\mathrm{e}^{-itH_2} f_2\big\| = 0. \tag{6.18}$$

In fact, we shall prove this estimate for any $\theta_2 \in C_0(\mathbb{R})$. Let us set $r_z(x) := (x-z)^{-1}$ for any $x \in \mathbb{R}$ and $z \in \mathbb{C}\setminus\mathbb{R}$. Since the vector space generated by the family of functions $\{r_z\}_{z\in\mathbb{C}\setminus\mathbb{R}}$ is a dense subset of $C_0(\mathbb{R})$ it is enough to show (6.18) with θ_2 replaced by r_z for any $z \in \mathbb{C}\setminus\mathbb{R}$. Set $R_j = (H_j - z)^{-1}$ for some fixed $z \in \mathbb{C}\setminus\mathbb{R}$ and observe that for any $g_j \in \mathcal{H}$

$$\begin{aligned}
|\langle g_1, (R_1 - R_2)g_2\rangle| &= |\langle R_1^* g_1, H_2R_2g_2\rangle - \langle H_1R_1^*g_1, R_2g_2\rangle| \\
&= |\langle T_1R_1^*g_1, T_2R_2g_2\rangle| \\
&\le \|T_1R_1^*\|\,\|g_1\|\,\|T_2R_2g_2\|.
\end{aligned}$$

Taking $g_2 = \mathrm{e}^{-itH_2} f_2$ we see that it is enough to prove that $\|T_2R_2\,\mathrm{e}^{-itH_2} f_2\| \to 0$ as $|t| \to \infty$. But this is an easy consequence of the fact that both the function $F(t) := T_2R_2\,\mathrm{e}^{-itH_2} f_2$ and its derivative are square integrable on $\mathbb{R}$.

As a consequence of the previous arguments, we have thus obtained that (6.16) exists. Clearly the same arguments apply for the existence of $W_\pm\big(H_2, H_1, E_1(J)\big)$. It then follows that $W_\pm\big(H_2, H_1, E_1(J)\big) = W_\pm\big(H_1, H_2, E_2(J)\big)^*$ from which one deduces the final statement, see also Proposition 5.2.3. □

6.5 Limiting absorption principle

Since the utility of locally smooth operators has been illustrated in the previous theorem, it remains to show how such operators can be exhibited. In this section, we provide this kind of information, and start with the so-called *limiting absorption principle*.

By looking back to the equation (6.14) and by assuming that $T \in \mathscr{B}(\mathcal{H})$, one observes that the main point is to obtain an inequality of the form

$$\big|\big\langle f, \Im R(\lambda + i\mu)f\big\rangle\big| \le C_K\|f\|_{\mathcal{G}}^2 \tag{6.19}$$

for some compact set $K \subset \mathbb{R}$, all $\lambda \in K$ and $\mu > 0$. Note that we have used the notation $\mathcal{G} := T^*\mathcal{H}$ endowed with the norm $\|f\|_{\mathcal{G}} := \inf\{\|g\| \mid T^*g = f\}$ for any $f \in \mathcal{G}$.

Let us be a little bit more general. Consider any Banach space $\mathcal{G}$ such that $\mathcal{G} \subset \mathsf{D}(H)^*$ continuously and densely. By duality it implies the existence of a continuous embedding $\mathsf{D}(H) \subset \mathcal{G}^*$, but this embedding is not dense in general. The closure of $\mathsf{D}(H)$ inside $\mathcal{G}^*$ is thus denoted by $\mathcal{G}^{*\circ}$, and is equipped with the Banach space structure inherited from $\mathcal{G}^*$. It then follows that $\mathscr{B}\big(\mathsf{D}(H)^*, \mathsf{D}(H)\big) \subset \mathscr{B}(\mathcal{G}, \mathcal{G}^{*\circ}) \subset \mathscr{B}(\mathcal{G}, \mathcal{G}^*)$ and in particular

$$\Im R(z) \in \mathscr{B}\big(\mathsf{D}(H)^*, \mathsf{D}(H)\big) \subset \mathscr{B}(\mathcal{G}, \mathcal{G}^{*\circ}) \subset \mathscr{B}(\mathcal{G}, \mathcal{G}^*), \qquad \forall z \in \rho(H).$$

Definition 6.5.1. *Let J be an open set, H a self-adjoint operator and $\mathcal{G} \subset \mathsf{D}(H)^*$.*

i) The generalized limiting absorption holds for H in $\mathcal{G}$ and locally on J *if for each compact subset $K \subset J$ there exists $C_K < \infty$ such that* (6.19) *holds for all $f \in \mathcal{G}$, any $\lambda \in K$ and $\mu > 0$, or equivalently if*

$$\sup_{\lambda \in K, \mu > 0} \|\Im R(\lambda + i\mu)\|_{\mathscr{B}(\mathcal{G}, \mathcal{G}^*)} < \infty$$

for any compact subset $K \subset J$.

ii) The strong generalized limiting absorption holds for H in $\mathcal{G}$ and locally on J *if*

$$\lim_{\mu \searrow 0} \langle f, \Im R(\lambda + i\mu) f\rangle =: \langle f, \Im R(\lambda + i0) f\rangle$$

exists for any $\lambda \in J$ and $f \in \mathcal{G}$, uniformly in λ on any compact subset of J.

Note that by an application of the uniform boundedness principle the generalized limiting absorption (GLAP) holds if the strong GLAP is satisfied. In the next statement we shall make the link between GLAP and locally smooth operators. For that purpose, we first recall a consequence of Stone's formula, see Proposition 4.4.1:

$$E\big((a,b)\big) + \frac{1}{2}E(\{a\}) + \frac{1}{2}E(\{b\}) = w - \lim_{\mu \searrow 0} \int_a^b \delta_{(\mu)}(H - \lambda)\mathrm{d}\lambda. \tag{6.20}$$

Namely, for any $a < b$ and $f \in \mathcal{H}$ one has

$$\begin{aligned} \frac{1}{b-a} m_f\big((a,b)\big) &= \frac{1}{b-a}\big\|E\big((a,b)\big)f\big\|^2 \\ &\le \sup_{a<\lambda<b, \mu>0} \langle f, \delta_{(\mu)}(H-\lambda) f\rangle = \sup_{a<\lambda<b, \mu>0} \frac{1}{\pi}\langle f, \Im R(\lambda + i\mu) f\rangle. \end{aligned} \tag{6.21}$$

Thus, if $J \subset \mathbb{R}$ is open and $|\frac{1}{\pi}\langle f, \Im R(\lambda + i\mu) f\rangle| \le C(f) < \infty$ for all $\lambda \in J$ and $\mu > 0$, then m_f is absolutely continuous on J and $\frac{\mathrm{d}}{\mathrm{d}\lambda}\|E_\lambda f\|^2 \le C(f)$ on J (recall that $E_\lambda = E\big((-\infty, \lambda]\big)$) If this holds for each f in a dense subset of $\mathcal{H}$ then the spectrum of H in J is purely absolutely continuous.

Proposition 6.5.2. *Let $\mathcal{G}$ be a Banach space with $\mathcal{G} \subset \mathsf{D}(H^*)$ continuously and densely, and let $J \subset \mathbb{R}$ be open.*

i) If the GLAP holds for H locally on J, then H has purely absolutely continuous spectrum in J. If the strong GLAP holds for H in $\mathcal{G}$ and locally on J, then for each $\lambda_0 \in \mathbb{R}$ the function $\lambda \mapsto E_\lambda - E_{\lambda_0} \in \mathscr{B}(\mathcal{G}, \mathcal{G}^*)$ is weak-continuously differentiable on J, and its derivative is equal to*

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} E_\lambda = \frac{1}{\pi}\Im R(\lambda + i0). \tag{6.22}$$

ii) Assume that $(\mathcal{G}^{*\circ})^* = \mathcal{G}$ and that the GLAP holds in $\mathcal{G}$ locally on J. Let $T : \mathsf{D}(H) \to \mathcal{H}$ be a linear operator which is continuous when $\mathsf{D}(H)$ is equipped with the topology induced by $\mathcal{G}^*$, or in other terms let $T \in \mathscr{B}(\mathcal{G}^{*\circ}, \mathcal{H})$, then T is locally H-smooth on J.

Proof. i) Let us first note that for any $f \in \mathsf{D}(H)^*$, the expression $\|E(\cdot)f\|^2$ is a well-defined positive Radon measure on $\mathbb{R}$, since for any bounded $J \in \mathcal{A}_B$ one has $E(J) \in \mathscr{B}\big(\mathsf{D}(H)^*, \mathsf{D}(H)\big)$. Note that this measure is usually unbounded if $f \in \mathsf{D}(H)^* \setminus \mathcal{H}$. As a consequence, (6.20) will hold in $\mathsf{D}(H)^*$, and by assumption (6.21) will hold for any $f \in \mathcal{G}$. It thus follows that m_f is absolutely continuous on J for any $f \in \mathcal{G}$. If the strong GLAP holds, then (6.22) is a direct consequence of (6.20).

ii) By assumption one has $T^* \in \mathscr{B}(\mathcal{H}, \mathcal{G})$. Since $\Im R(z)$ maps $\mathcal{G}$ into $\mathsf{D}(H) \subset \mathcal{G}^{*\circ}$ we get

$$\|T\Im R(z)T^*\| \leq \|T\|_{\mathcal{G}^*\to\mathcal{H}} \|\Im R(z)\|_{\mathcal{G}\to\mathcal{G}^*} \|T^*\|_{\mathcal{H}\to\mathcal{G}}$$

which means that T is locally H-smooth on J, by Proposition 6.4.2. □

Let us still mention that quite often, the limiting absorption principle is formally obtained by replacing $\Im R(\lambda + i\mu)$ by $R(\lambda + i\mu)$. However, since $R(\lambda + i\mu)$ does not belong to $\mathscr{B}\big(D(H)^*, \mathsf{D}(H)\big)$, the expression $\langle f, R(z)f\rangle$ is not *a priori* well-defined for f in the space $\mathcal{G}$ used before. One natural way to overcome this difficulty is to consider the space $\mathsf{D}\big(|H|^{1/2}\big)$, which is called *the form domain of* H. Then the following embeddings are continuous and dense

$$\mathsf{D}(H) \subset \mathsf{D}\big(|H|^{1/2}\big) \subset \mathcal{H} \subset \mathsf{D}\big(|H|^{1/2}\big)^* \subset \mathsf{D}(H)^*.$$

The main point in this construction is that $R(z) \in \mathscr{B}\Big(\mathsf{D}\big(|H|^{1/2}\big)^*, \mathsf{D}\big(|H|^{1/2}\big)\Big)$ for any $z \in \rho(H)$. So we can mimic the previous construction and consider $\mathcal{G} \subset \mathsf{D}\big(|H|^{1/2}\big)^*$ continuously and densely. Note that in the applications one often considers $\mathcal{G} \subset \mathcal{H} \subset \mathsf{D}\big(|H|^{1/2}\big)^*$. Then, it follows that that $\mathsf{D}\big(|H|^{1/2}\big) \subset \mathcal{G}^*$ continuously, and consequently

$$\mathscr{B}\Big(\mathsf{D}\big(|H|^{1/2}\big)^*, \mathsf{D}\big(|H|^{1/2}\big)\Big) \subset \mathscr{B}(\mathcal{G}, \mathcal{G}^{*\circ}) \subset \mathscr{B}(\mathcal{G}, \mathcal{G}^*).$$

In this context, the *limiting absorption principle* (LAP) or the strong LAP corresponds to the content of (6.5.1) with $\Im R(\lambda + i\mu)$ replaced by $R(\lambda + i\mu)$. Note that the LAP is usually a much stronger requirement than the GLAP since the the real part of $R(\lambda+i\mu)$ is a much more singular object (in the limit $\mu \searrow 0$) than its imaginary part.

Let us still reformulate the strong limiting absorption principle in different terms: Consider $\mathbb{C}_\pm := \{z \in \mathbb{C} \mid \pm\Im(z) > 0\}$ and observe that $\mathbb{C}_\pm \ni z \mapsto R(z) \in \mathscr{B}(\mathcal{G}, \mathcal{G}^*)$ is a holomorphic function. The strong LAP is equivalent to the fact that this function has a weak*-continuous extension to the set $\mathbb{C}_\pm \cup J$. The boundary values $R(\lambda \pm i0)$ of the resolvent on the real axis allow us to expression the derivative of the spectral measure on J as

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} E_\lambda = \frac{1}{2\pi i}\big[R(\lambda + i0) - R(\lambda - i0)\big]. \tag{6.23}$$

6.6 The method of differential inequalities

In this section we provide the proofs of Theorems 6.1.1 and 6.1.2. In fact, we shall mainly deal with a bounded operator S and show at the end how an unbounded operator H *with a spectral gap* can be treated in this setting. For an unbounded operator H without a spectral gap, we refer to [ABG, Sec. 7.5].

Our framework is the following: Let A be a self-adjoint (usually unbounded) operator in a Hilbert space $\mathcal{H}$ and let S be a bounded and self-adjoint operator in $\mathcal{H}$. We assume that S belongs to $C^{1,1}(A)$, as introduced in Section 6.2. Observe that this regularity condition means

$$\begin{aligned}
&\int_{|t|\leq 1} \big\|(\mathscr{U}_t - \mathbf{1})^2[S]\big\|\frac{\mathrm{d}t}{t^2} < \infty\\
\Longleftrightarrow &\int_{|t|\leq 1} \big\|\,\mathrm{e}^{2itA} S\,\mathrm{e}^{-2itA} - 2\,\mathrm{e}^{itA} S\,\mathrm{e}^{-itA} + S\big\|\frac{\mathrm{d}t}{t^2} < \infty\\
\Longleftrightarrow &\int_{|t|\leq 1} \big\|\,\mathrm{e}^{itA} S\,\mathrm{e}^{-itA} + \mathrm{e}^{-itA} S\,\mathrm{e}^{itA} - 2S\big\|\frac{\mathrm{d}t}{t^2} < \infty\\
\Longleftrightarrow &\int_0^1 \big\|\,\mathrm{e}^{itA} S\,\mathrm{e}^{-itA} + \mathrm{e}^{-itA} S\,\mathrm{e}^{itA} - 2S\big\|\frac{\mathrm{d}t}{t^2} < \infty.
\end{aligned}$$

Our first aim is to provide the proof the following theorem. In its statement, the space $\mathcal{G} := \big(\mathsf{D}(A), \mathcal{H}\big)_{1/2,1}$ appears, and we will explain its definition when necessary. The important information is that $\mathcal{G} \subset \mathcal{H}$ continuously and densely. We also recall that $\mu^A(S) = \{\lambda \in \mathbb{R} \mid \varrho_S^A(\lambda) > 0\}$.

Theorem 6.6.1. *Let S be a bounded and self-adjoint operator which belongs to $C^{1,1}(A)$. Then the holomorphic function $\mathbb{C}_\pm \ni z \mapsto (S - z)^{-1} \in \mathscr{B}(\mathcal{G}, \mathcal{G}^*)$ extends to a weak*-continuous function on $\mathbb{C}_\pm \cup \mu^A(S)$.*

As explained in the previous sections, such a statement means that a strong limiting absorption principle holds for S in $\mathcal{G}$ and locally on $\mu^A(S)$. Some consequences of this statement is that S has purely absolutely continuous spectrum on $\mu^A(S)$, that the derivative of its spectral measure can be expressed by the imaginary part of its resolvent on the real axis, as mentioned in (6.23), and that some locally S-smooth operators on $\mu^A(S)$ are automatically available.

The proof of Theorem 6.6.1 is divided into several lemmas. Note that since $S \in C^{1,1}(A) \subset C^1(A)$, then the commutator $B := [iS, A]$ is well-defined and belongs to $\mathscr{B}(\mathcal{H})$. Before starting with these lemmas, let us provide a heuristic explanation about the approach. Since the aim is to consider $\langle f, (S - \lambda \mp i\mu)^{-1} f\rangle$ and its limits when $\mu \searrow 0$, we shall consider a regularized version of such an expression, with an additional parameter ε, namely

$$\big\langle f_\varepsilon, \big(S_\varepsilon - \lambda \mp i(\varepsilon B_\varepsilon + \mu)\big)^{-1} f_\varepsilon\big\rangle. \tag{6.24}$$

Then, it is mainly a matter of playing with the ε-dependence of all these terms...

The following lemma is really technical, but it is of crucial importance since it is there that the assumption $\varrho_S^A(\lambda_0) > 0$ will play an essential role. For completeness we provide its proof. Note that the reason for getting an estimate of the form (6.25) will become clear only in the subsequent lemma.

Lemma 6.6.2. *Let $\{S_\varepsilon\}_{0<\varepsilon<1}$ and $\{B_\varepsilon\}_{0<\varepsilon<1}$ be two families of bounded self-adjoint operators satisfying $\|S_\varepsilon - S\| + \varepsilon\|B_\varepsilon\| \leq c\varepsilon$ for some constant c as well as the condition $\lim_{\varepsilon\to 0}\|B_\varepsilon - B\| = 0$. Let $\lambda_0 \in \mathbb{R}$ and $a \in \mathbb{R}$ such that $\varrho_S^A(\lambda_0) > a > 0$. Then there exist some strictly positive numbers δ, ε_0 and b such that for $|\lambda - \lambda_0| \leq \delta$, for $0 < \varepsilon \leq \varepsilon_0$ and for any $\mu \geq 0$ the following estimate holds for all $g \in \mathcal{H}$:*

$$a\|g\|^2 \leq \langle g, B_\varepsilon g\rangle + \frac{b}{\mu^2+\delta^2}\big\|\big[S_\varepsilon - \lambda \mp i(\varepsilon B_\varepsilon + \mu)\big]g\big\|^2. \tag{6.25}$$

Proof. Let us choose numbers $a < a_0 < a_1 < \varrho_S^A(\lambda_0)$ and $\delta > 0$ such that $a_1 E \leq EBE$ for $E = E^S\big((\lambda_0 - 2\delta, \lambda_0 + 2\delta)\big)$. Let us also choose $\varepsilon_1 > 0$ such that $\|B_\varepsilon - B\| \leq a_1 - a_0$ for any $0 < \varepsilon \leq \varepsilon_1$. This implies that $EB_\varepsilon E \geq EBE - (a_1 - a_0)E \geq a_0 E$. Let us set $E^\perp = \mathbf{1} - E$ and consider from now on λ and μ real with $|\lambda - \lambda_0| \leq \delta$ and $\mu \geq 0$. Observe then that $\|(S - \lambda \mp i\mu)^{-1}E^\perp\| \leq (\mu^2+\delta^2)^{-1/2}$, and hence

$$\begin{aligned}
\|E^\perp g\|^2 &= \big\|(S-\lambda\mp i\mu)^{-1}E^\perp\big[S_\varepsilon - \lambda \mp i(\varepsilon B_\varepsilon + \mu) + S - S_\varepsilon \pm i\varepsilon B_\varepsilon\big]g\big\|^2 \\
&\leq \frac{2}{\mu^2+\delta^2}\big\|\big[S_\varepsilon - \lambda \mp i(\varepsilon B_\varepsilon+\mu)\big]g\big\|^2 + \frac{2c^2\varepsilon^2}{\mu^2+\delta^2}\|g\|^2.
\end{aligned}$$

We then get for $\varepsilon \leq \varepsilon_1$ and for any $\nu > 0$:

$$\begin{aligned}
a_0\|g\|^2 &= a_0\langle g, Eg\rangle + a_0\|E^\perp g\|^2 \\
&\leq \langle g, EB_\varepsilon Eg\rangle + a_0\|E^\perp g\|^2 \\
&= \langle g, B_\varepsilon g\rangle - 2\Re\langle Eg, B_\varepsilon E^\perp g\rangle - \langle E^\perp g, B_\varepsilon E^\perp g\rangle + a_0\|E^\perp g\|^2 \\
&\leq \langle g, B_\varepsilon g\rangle + \nu\|g\|^2 + \nu^{-1}\|B_\varepsilon\|^2\|E^\perp g\|^2 + \|B_\varepsilon\|\,\|E^\perp g\|^2 + a_0\|E^\perp g\|^2 \\
&\leq \langle g, B_\varepsilon g\rangle + \nu\|g\|^2 + \big[\nu^{-1}\|B_\varepsilon\|^2 + \|B_\varepsilon\| + a_0\big]\frac{2c^2\varepsilon^2}{\mu^2+\delta^2}\|g\|^2 \\
&\quad + \big[\nu^{-1}\|B_\varepsilon\|^2 + \|B_\varepsilon\| + a_0\big]\frac{2}{\mu^2+\delta^2}\big\|\big[S_\varepsilon - \lambda \mp i(\varepsilon B_\varepsilon + \mu)\big]g\big\|^2.
\end{aligned}$$

Since we have $\|B_\varepsilon\| \leq c$ and since we may assume $c \geq 1$ and $\nu \leq 1$, it follows that

$$\Big[a_0 - \nu - \frac{2c^2\varepsilon^2(a_0+2c^2)}{\nu\delta^2}\Big]\|g\|^2 \leq \langle g, B_\varepsilon g\rangle + \frac{2a_0+4c^2}{\nu(\mu^2+\delta^2)}\big\|\big[S_\varepsilon - \lambda \mp i(\varepsilon B_\varepsilon + \mu)\big]g\big\|^2.$$

We can finally chose $\nu > 0$ and $\varepsilon_0 \in (0, \varepsilon_1)$ such that the term in the square brackets in the l.h.s. is bigger of equal to a for any $0 < \varepsilon \leq \varepsilon_0$. We then get (6.25) with $b = \nu^{-1}(2a_0 + 4c^2)$. □

Lemma 6.6.3. *Under the same assumptions as in the previous lemma, the operators* $S_\varepsilon - \lambda \mp i(\varepsilon B_\varepsilon + \mu)$ *are invertible in* $\mathscr{B}(\mathcal{H})$ *whenever* $|\lambda - \lambda_0| \le \delta$, $0 < \varepsilon \le \varepsilon_0$ *and* $\mu \ge 0$. *For any fixed* λ *and* μ *satisfying these conditions we set*

$$G_\varepsilon^\pm := \big[S_\varepsilon - \lambda \mp i(\varepsilon B_\varepsilon + \mu)\big]^{-1}$$

Then one has $(G_\varepsilon^\pm)^* = G_\varepsilon^\mp$ *and*

$$\|G_\varepsilon^\pm\| \le \frac{1}{a\varepsilon + \mu}\Big[1 + b\varepsilon \frac{c\varepsilon + \|S\| + |\lambda + i\mu|}{\mu^2 + \delta^2}\Big]. \tag{6.26}$$

Moreover, for any $h \in \mathcal{H}$

$$\|G_\varepsilon^\pm h\| \le \frac{1}{\sqrt{a\varepsilon}} |\Im\langle h, G_\varepsilon^+ h\rangle|^{1/2} + \frac{1}{\delta}\Big(\frac{b}{a}\Big)^{1/2}\|h\|. \tag{6.27}$$

Proof. Let us set

$$T_\varepsilon^\pm := S_\varepsilon - \lambda \mp i(\varepsilon B_\varepsilon + \mu)$$

and deduce from (6.25)

$$\begin{aligned}
(a\varepsilon + \mu)\|g\|^2 &\le \langle g, (\varepsilon B_\varepsilon + \mu) g\rangle + \frac{b\varepsilon}{\mu^2 + \delta^2}\|T_\varepsilon^\pm g\|^2 \\
&= \mp \Im\langle g, T_\varepsilon^\pm g\rangle + \frac{b\varepsilon}{\mu^2 + \delta^2}\|T_\varepsilon^\pm g\|^2 \\
&\le \|g\|\,\|T_\varepsilon^\pm g\|\Big\{1 + \frac{b\varepsilon}{\mu^2 + \delta^2}\|T_\varepsilon^\pm\|\Big\} \\
&\le \|g\|\,\|T_\varepsilon^\pm g\|\Big\{1 + b\varepsilon \frac{\|S\| + c\varepsilon + |\lambda + i\mu|}{\mu^2 + \delta^2}\Big\}.
\end{aligned}$$

It follows from this equality and from the boundedness (and thus closeness) of $T_\varepsilon^\pm$ that these operators are injective and with closed range, see also [Amr, Lem. 3.1]. In addition, since $(T_\varepsilon^\pm)^* = T_\varepsilon^\mp$ and since $\mathsf{Ker}\big((T_\varepsilon^\pm)^*\big) = \mathsf{Ran}(T_\varepsilon^\pm)^\perp$, one infers that $\mathsf{Ran}(T_\varepsilon^\pm) = \mathcal{H}$. One then easily deduces all assertions of the lemma, except the estimate (6.27).

To prove (6.27), let us set $g = G_\varepsilon^\pm h$ in (6.25) and observe that

$$a\varepsilon\|G_\varepsilon^\pm h\|^2 \le \langle G_\varepsilon^\pm h, (\varepsilon B_\varepsilon + \mu) G_\varepsilon^\pm h\rangle + \frac{b\varepsilon}{\mu^2 + \delta^2}\|h\|^2. \tag{6.28}$$

By taking the following identities into account,

$$\begin{aligned}
\langle G_\varepsilon^\pm h, (\varepsilon B_\varepsilon + \mu) G_\varepsilon^\pm h\rangle &= \pm(2i)^{-1}\langle h, G_\varepsilon^\mp (T_\varepsilon^\mp - T_\varepsilon^\pm) G_\varepsilon^\pm h\rangle \\
&= \pm(2i)^{-1}\langle h, (G_\varepsilon^\pm - G_\varepsilon^\mp) h\rangle \\
&= \Im\langle h, G_\varepsilon^+ h\rangle,
\end{aligned}$$

one directly obtains (6.27) from (6.28). □

We keep the assumptions and the notations of the previous two lemmas, and set simply G_ε and T_ε for G_ε^+ and T_ε^+. The derivative with respect to the variable ε will be denoted by $'$, *i.e.* $G'_\varepsilon = \frac{\mathrm{d}}{\mathrm{d}\varepsilon} G_\varepsilon$.

Lemma 6.6.4. *Assume that the maps $\varepsilon \mapsto S_\varepsilon$ and $\varepsilon \mapsto B_\varepsilon$ are C^1 in norm, and that for any fixed ε the operators B_ε and S_ε belong to $C^1(A)$. Then the map $\varepsilon \mapsto G_\varepsilon$ is C^1 in norm, and also $G_\varepsilon \in C^1(A)$ for any fixed ε.*

Proof. The differentiability of G_ε with respect to ε follows easily from the equality

$$G_{\varepsilon'} - G_\varepsilon = G_{\varepsilon'}(T_\varepsilon - T_{\varepsilon'})G_\varepsilon = G_{\varepsilon'}\big(S_\varepsilon - S_{\varepsilon'} - i(\varepsilon B_\varepsilon - \varepsilon' B_{\varepsilon'})\big)G_\varepsilon.$$

We thus get that $G'_\varepsilon = -G_\varepsilon T'_\varepsilon G_\varepsilon$. For the regularity of G_ε with respect to A, this follows from the statement (iii) of Proposition 6.2.4. In addition, one can also infer that $[A, G_\varepsilon] = -G_\varepsilon[A, T_\varepsilon]G_\varepsilon$, see [ABG, Prop. 6.1.6] for the details. Note that this equality can also be obtained with the operator A_τ, as already used in (6.11). □

Note that from the previous statement and from its proof, one deduces the following equality

$$G'_\varepsilon + [A, G_\varepsilon] = iG_\varepsilon\big\{B_\varepsilon - [iS_\varepsilon, A] + \varepsilon\big(i\varepsilon^{-1}S'_\varepsilon + B'_\varepsilon + [A, B_\varepsilon]\big)\big\}G_\varepsilon. \tag{6.29}$$

In the next lemma we provide a precise formulation of what had been mentioned in (6.24).

Lemma 6.6.5. *Let us keep the assumptions of the previous three lemmas, and let $\{f_\varepsilon\}_{0<\varepsilon<1}$ be a bounded family of elements of $\mathcal{H}$ such that $\varepsilon \mapsto f_\varepsilon$ is strongly C^1 and such that $f_\varepsilon \in \mathsf{D}(A)$ for any fixed ε. Set*

$$F_\varepsilon := \langle f_\varepsilon, G_\varepsilon f_\varepsilon\rangle.$$

Then the map $\varepsilon \mapsto F_\varepsilon$ is of class C^1 and its derivatives satisfies

$$F'_\varepsilon = \langle f_\varepsilon, (G'_\varepsilon + [A, G_\varepsilon])f_\varepsilon\rangle + \langle G^*_\varepsilon f_\varepsilon, f'_\varepsilon + Af_\varepsilon\rangle + \langle f'_\varepsilon - Af_\varepsilon, G_\varepsilon f_\varepsilon\rangle. \tag{6.30}$$

In addition, if we set

$$\ell(\varepsilon) := \|f'_\varepsilon\| + \|Af_\varepsilon\|, \qquad q(\varepsilon) := \|\varepsilon^{-1}(B_\varepsilon - [iS_\varepsilon, A]) + i\varepsilon^{-1}S'_\varepsilon + B'_\varepsilon + [A, B_\varepsilon]\|, \tag{6.31}$$

then F_ε satisfies the differential inequality

$$\frac{1}{2}|F'_\varepsilon| \leq \omega\|f_\varepsilon\|\big[\ell(\varepsilon) + \omega\varepsilon q(\varepsilon)\|f_\varepsilon\|\big] + \frac{\ell(\varepsilon)}{\sqrt{a\varepsilon}}|F_\varepsilon|^{1/2} + \frac{q(\varepsilon)}{a}|F_\varepsilon|, \tag{6.32}$$

with $\omega = a^{-1/2}b^{1/2}\delta^{-1}$ and $0 < \varepsilon \leq \varepsilon_0$.

Proof. The equality (6.30) is obvious, since the commutator can be opened on $\mathsf{D}(A)$. By using (6.29) it can then be rewritten as

$$\begin{aligned} F_\varepsilon' =& i\big\langle G_\varepsilon^* f_\varepsilon, \big\{B_\varepsilon - [iS_\varepsilon, A] + \varepsilon(i\varepsilon^{-1}S_\varepsilon' + B_\varepsilon' + [A, B_\varepsilon])\big\}G_\varepsilon f_\varepsilon\big\rangle \\ &+ \langle G_\varepsilon^* f_\varepsilon, f_\varepsilon' + Af_\varepsilon\rangle + \langle f_\varepsilon' - Af_\varepsilon, G_\varepsilon f_\varepsilon\rangle. \end{aligned} \tag{6.33}$$

As a consequence one infers that

$$|F_\varepsilon'| \leq \varepsilon q(\varepsilon)\|G_\varepsilon f_\varepsilon\|\,\|G_\varepsilon^* f_\varepsilon\| + \ell(\varepsilon)\big(\|G_\varepsilon f_\varepsilon\| + \|G_\varepsilon^* f_\varepsilon\|\big). \tag{6.34}$$

In addition it follows from (6.27) that

$$\|G_\varepsilon^\pm f_\varepsilon\| \leq \frac{1}{\sqrt{a\varepsilon}}|F_\varepsilon|^{1/2} + \omega\|f_\varepsilon\|.$$

By inserting these inequalities in (6.34) and by using the inequality $(p+q)^2 \leq 2p^2 + 2q^2$ for any $p, q \geq 0$ one directly obtains (6.32). □

The differential inequality (6.32), from which the method takes its name, is quite remarkable in that the spectral variable $\lambda + i\mu$ does not appear explicitly in the coefficients. In fact, the only conditions on these parameters are $|\lambda - \lambda_0| \leq \delta$ and $\mu \geq 0$.

Let us still rewrite (6.32) in the simple form

$$|F_\varepsilon'| \leq \eta(\varepsilon) + \varphi(\varepsilon)|F_\varepsilon|^{1/2} + \psi(\varepsilon)|F_\varepsilon|.$$

By using the trivial inequality $|F_s| \leq |F_{\varepsilon_0}| + \int_s^{\varepsilon_0} |F_\tau'|\mathrm{d}\tau$, we then obtain for $0 < \varepsilon < s < \varepsilon_0$

$$|F_s| \leq |F_{\varepsilon_0}| + \int_s^{\varepsilon_0} \eta(\tau)\mathrm{d}\tau + \int_s^{\varepsilon_0} \big[\varphi(\tau)|F_\tau|^{1/2} + \psi(\tau)|F_\tau|\big]\mathrm{d}\tau. \tag{6.35}$$

We shall now apply an extended version of the Gronwall lemma to this differential inequality. More precisely, let us first state such a result, and refer to [ABG, Lem. 7.A.1] for its proof.

Lemma 6.6.6 (Gronwall lemma)**.** *Let $(a, b) \subset \mathbb{R}$ and let f, φ, ψ be non-negative real functions on (a, b) with f bounded, and $\varphi, \psi \in L^1\big((a, b)\big)$. Assume that, for some constants $\omega \geq 0$ and $\theta \in [0, 1)$ and for all $\lambda \in (a, b)$ one has*

$$f(\lambda) \leq \omega + \int_\lambda^b \big[\varphi(\tau)f(\tau)^\theta + \psi(\tau)f(\tau)\big]\mathrm{d}\tau.$$

Then one has for each $\lambda \in (a, b)$

$$f(\lambda) \leq \Big[\omega^{1-\theta} + (1-\theta)\int_\lambda^b \varphi(\tau)\,\mathrm{e}^{(\theta-1)\int_\tau^b \psi(s)\mathrm{d}s}\,\mathrm{d}\tau\Big]^{1/(1-\theta)}\,\mathrm{e}^{\int_\lambda^b \psi(\tau)\mathrm{d}\tau}.$$

Thus, by applying this result for $\theta = 1/2$ to (6.35) one gets that

$$|F_\varepsilon| \leq \Big[\Big(|F_{\varepsilon_0}| + \int_\varepsilon^{\varepsilon_0} \eta(\tau)\mathrm{d}\tau\Big)^{1/2} + \frac{1}{2}\int_\varepsilon^{\varepsilon_0} \varphi(\tau)\,\mathrm{e}^{-\frac{1}{2}\int_\tau^{\varepsilon_0}\psi(s)\mathrm{d}s}\,\mathrm{d}\tau\Big]^2\,\mathrm{e}^{\int_\varepsilon^{\varepsilon_0}\psi(\tau)\mathrm{d}\tau}$$

for all $0 < \varepsilon < \varepsilon_0$. We can then deduce the simpler inequality

$$|F_\varepsilon| \leq 2\Big[|F_{\varepsilon_0}| + \int_\varepsilon^{\varepsilon_0} \eta(\tau)\mathrm{d}\tau + \Big(\int_\varepsilon^{\varepsilon_0}\varphi(\tau)\mathrm{d}\tau\Big)^2\Big]\,\mathrm{e}^{\int_\varepsilon^{\varepsilon_0}\psi(\tau)\mathrm{d}\tau}.$$

Our final purpose is to get a bound on $|F_\varepsilon| < const. < \infty$ independent of $z = \lambda + i\mu$ as $\varepsilon \to 0$. From the above estimate we see that this is satisfied if

$$\int_0^{\varepsilon_0}[\eta(\tau) + \varphi(\tau) + \psi(\tau)]\mathrm{d}\tau < \infty.$$

By coming back to the explicit formula for these functions, it corresponds to the condition

$$\int_0^{\varepsilon_0}\Big[\ell(\varepsilon)\|f_\varepsilon\| + \varepsilon q(\varepsilon)\|f_\varepsilon\|^2 + \frac{\ell(\varepsilon)}{\sqrt{\varepsilon}} + q(\varepsilon)\Big]\mathrm{d}\varepsilon < \infty.$$

In fact, it is easily observed (see also page 304 of [ABG]) that this condition is satisfied if the following assumption holds:

$$\int_0^1[\varepsilon^{-1/2}\ell(\varepsilon) + q(\varepsilon)]\mathrm{d}\varepsilon < \infty.$$

By looking back at the definitions of ℓ and q in (6.31) we observe that the condition on ℓ corresponds to a condition on the family of elements $\{f_\varepsilon\}$ while the condition on q corresponds to conditions on the families $\{S_\varepsilon\}$ and $\{B_\varepsilon\}$. For the condition on q let us just mention that a suitable choice for S_ε is given by

$$S_\varepsilon := \int_{-\infty}^{\infty}\mathrm{e}^{-i\varepsilon\tau A}\,S\,\mathrm{e}^{i\varepsilon\tau A}\,\mathrm{e}^{-\tau^2/4}\,\frac{\mathrm{d}\tau}{(4\pi)^{1/2}}.$$

Then by setting $B_\varepsilon := [iS_\varepsilon, A]$ and by assuming that $S \in C^{1,1}(A)$ it is shown in [ABG, Lem. 7.3.6] that all assumptions on the families $\{S_\varepsilon\}$ and $\{B_\varepsilon\}$ are satisfied. Note that the proof of this statement is rather technical and that we shall not comment on it.

For the condition involving ℓ, let us consider $f \in \mathcal{H}$ and set for any $\varepsilon > 0$

$$f_\varepsilon := (\mathbf{1} + i\varepsilon A)^{-1}f.$$

Then one has $f_\varepsilon \in \mathsf{D}(A)$, $f'_\varepsilon = -i(\mathbf{1} + i\varepsilon A)^{-1}Af_\varepsilon$, $\|f_\varepsilon\| \leq \|f\|$, $\|f_\varepsilon - f\| \to 0$ as $\varepsilon \to 0$, and $\ell(\varepsilon) \leq 2\|Af_\varepsilon\|$. Then the condition $\int_0^1 \varepsilon^{-1/2}\ell(\varepsilon)\mathrm{d}\varepsilon < \infty$ holds if

$$\int_0^1 \varepsilon^{1/2}\big\|A(\mathbf{1} + i\varepsilon A)^{-1}f\big\|\frac{\mathrm{d}\varepsilon}{\varepsilon} < \infty. \tag{6.36}$$

Such a condition corresponds to a regularity condition of f with respect to A. In fact, many Banach spaces of elements of $\mathcal{H}$ having a certain regularity with respect A can be defined, and Chapter 2 of [ABG] is entirely devoted to that question. Here, the elements of $\mathcal{H}$ satisfying condition (6.36) are precisely those belonging to the space $\big(\mathsf{D}(A),\mathcal{H}\big)_{1/2,1}$, as shown in [ABG, Prop. 2.7.2]. Note that this space is an interpolation space between $\mathsf{D}(A)$ and $\mathcal{H}$ and contains the space $\mathsf{D}(\langle A\rangle^{1/2+\epsilon})$ for any $\epsilon>0$.

By summing up, for any $f\in\mathcal{G}:=\big(\mathsf{D}(A),\mathcal{H}\big)_{1/2,1}$ one has $\int_0^1\varepsilon^{-1/2}\ell(\varepsilon)\mathrm{d}\varepsilon\le c_1\|f\|_{\mathcal{G}}$ for some $c_1<\infty$ independent of $f\in\mathcal{G}$. By looking at the explicit form of the functions η and φ one also obtains that there exists $c_2<\infty$ such that $\int_0^1\eta(\tau)\mathrm{d}\tau\le c_2\|f\|^2_{\mathcal{G}}$ and $\int_0^1\varphi(\tau)\mathrm{d}\tau\le c_2\|f\|_{\mathcal{G}}$. One then infers that $|F_\varepsilon|\le c\|f\|^2_{\mathcal{G}}$ for any $0<\varepsilon\le\varepsilon_0$, $|\lambda-\lambda_0|\le\delta$ and $\mu\ge0$ with a constant c independent of $f\in\mathcal{G}$, ε, λ and μ. The proof of Theorem 6.6.1 can now be provided:

Proof of Theorem 6.6.1. By all the previous arguments, there exists an integrable function $\kappa:(0,\varepsilon_0)\to\mathbb{R}$ such that $|F'_\varepsilon|\le\kappa(\varepsilon)$ for all ε, λ, μ as above. Now, fix $\mu>0$. Since $S_\varepsilon-\lambda-i(\varepsilon B_\varepsilon+\mu)$ converges to $S-\lambda-i\mu\equiv S-z$ in norm as $\varepsilon\to0$ we shall have $G_\varepsilon\to(S-z)^{-1}$ in norm too, and

$$\langle f,(S-z)^{-1}f\rangle=\lim_{\varepsilon\to0}\langle f_\varepsilon,G_\varepsilon f_\varepsilon\rangle=\langle f_{\varepsilon_0},G_{\varepsilon_0}(z)f_{\varepsilon_0}\rangle-\int_0^{\varepsilon_0}F'_\varepsilon(z)\mathrm{d}\varepsilon. \tag{6.37}$$

Note that we have explicitly indicated the dependence on $z=\lambda+i\mu$ of G_{ε_0} and F'_ε. Let us set $\Omega:=\{\lambda+i\mu\mid|\lambda-\lambda_0|<\delta,\mu\ge0\}$. It follows from (6.26) that $\|G_{\varepsilon_0}(z)\|\le$ *const.* $<\infty$ independently of $z\in\Omega$. For each $\varepsilon>0$ the continuity of $z\in\Omega$ of $F'_\varepsilon(z)$ follows from (6.33). By the dominated convergence theorem, with the fact that $|F'_\varepsilon|\le\kappa(\varepsilon)$, the equation (6.37) gives the existence of a continuous extension of the function $\langle f,(S-z)^{-1}f\rangle$ from the domain $\{z\in\Omega\mid\Im(z)=\mu>0\}$ to all Ω. The polarization principle shows that this holds for $\langle f,(S-z)^{-1}g\rangle$ for any $f,g\in\mathcal{G}$. $\square$

Let us finally show how the two theorems stated at the beginning of the chapter follow from the various results obtained subsequently. First of all we provide a proof of Theorem 6.1.2.

Proof of Theorem 6.1.2. Let $\lambda_0\in\mathbb{R}\setminus\sigma(H)$ and set $S:=(H-\lambda_0)^{-1}$. Then S is a bounded self-adjoint operator, and the resolvents of S and H are related by the identity

$$(H-z)^{-1}=(\lambda_0-z)^{-1}[S-(\lambda_0-z)^{-1}]^{-1}S,\qquad\Im(z)\neq0. \tag{6.38}$$

Let $J\subset\mu^A(H)$ be a compact set with $\lambda_0\notin J$ and set $\tilde J:=\{(\lambda_0-\lambda)^{-1}\mid\lambda\in J\}$. Note that there is no restriction on the generality if we assume that λ does not belong to a neighbourhood of λ_0, since $(H-z)^{-1}$ is holomorphic in such a neighbourhood. Then $S\in C^{1,1}(A)$ and $\tilde J$ is a compact subset of $\mu^A(S)$, see Proposition 7.2.5 of [ABG]. In addition, Theorem 6.6.1 says that the map $\zeta\mapsto(S-\zeta)^{-1}\in\mathscr{B}(\mathcal{G},\mathcal{G}^*)$ extends to a weak*-continuous function on $\mathbb{C}_\pm\cup\tilde J$. Since $z\mapsto\zeta=(\lambda_0-z)^{-1}$ is a homeomorphism of $\mathbb{C}_\pm\cup J$ onto $\mathbb{C}_\pm\sup\tilde J$, we see that $z\mapsto[S-(\lambda_0-z)^{-1}]^{-1}\in\mathscr{B}(\mathcal{G},\mathcal{G}^*)$ extends to a weak*-continuous function on $\mathbb{C}_\pm \cup J$. The result of the theorem now follows from the identity (6.38) and the fact that $S\mathcal{G} \subset \mathcal{G}$, as a consequence of [ABG, Thm. 5.3.3].

The second part of the statement is a direct consequence of what has been presented in Section 6.4. Note in particular that in the Definition 6.4.1 of a locally H-smooth operator, one could have considered $T : \mathsf{D}(H) \to \mathcal{K}$ with $\mathcal{K}$ an arbitrary Hilbert space. It is in this generality that the statement of Theorem 6.1.2 is provided, and this slight extension can easily be taken into account. □

In the same vein one has:

Proof of Theorem 6.1.1. The first assertion about the finiteness of the set of eigenvalues is a direct consequence of Corollary 6.3.7. For the second statement, observe that Theorem 6.3.8 implies the inclusion $J \setminus \sigma_p(H) \subset \mu^A(H)$, and then use the consequences of the limiting absorption principle, as presented in Section 6.5. □

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