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

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

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

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]

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

This linear transform maps the Schwartz space $\mathcal{S}(\mathbb{R}^d)$ onto itself, and its inverse is provided by the formula $[\mathcal{F}^{-1}f](x) \equiv \check{f}(x) := \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{i\xi\cdot x} f(\xi)\,\mathrm{d}\xi$. 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 $d \leq 3$ 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*

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

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 $d \leq 3$. 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

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

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

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

□

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 $f \in D(-\Delta)$ 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 $X_1, \dots, X_d, D_1, \dots, D_d$ 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

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

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

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

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 $\hat{\mathbb{R}}^d \ni \xi \mapsto V_\xi := e^{-iX\cdot\xi} \in \mathscr{U}(\mathcal{H})$, acting on $\mathcal{H}$ as

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

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

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

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

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

which satisfies the relation $W(\mathsf{x})W(\mathsf{y}) = e^{\frac{i}{2}\sigma(\mathsf{x},\mathsf{y})}\, W(\mathsf{x}+\mathsf{y})$ 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

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

Now, recall that for a family of m commuting self-adjoint operators $S_1, \dots, S_m$ one usually defines a functional calculus by the formula $f(S) := \frac{1}{(2\pi)^{m/2}} \int_{\mathbb{R}^m} \check{f}(t) e^{-it\cdot S} \mathrm{d}t$, where $t \cdot S = t_1 S_1 + \ldots + t_m S_m$ 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

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

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 $x \to 0$:

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

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 $H_{m,\kappa}$:

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

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

$$\mathsf{D}(H_0^\nu) = \big\{f \in \mathsf{D}(L_0^{\max}) \mid \text{ for some } c \in \mathbb{C}, \tag{3.9}$$
$$f(x) - c\big(x^{1/2}\ln(x) + \nu x^{1/2}\big) \in \mathsf{D}(L_0^{\min}) \text{ around } 0\big\}, \qquad \nu \neq \infty;$$
$$\mathsf{D}(H_0^\infty) = \big\{f \in \mathsf{D}(L_0^{\max}) \mid \text{ for some } c \in \mathbb{C}, \tag{3.10}$$
$$f(x) - cx^{1/2} \in \mathsf{D}(L_0^{\min}) \text{ around } 0\big\}.$$

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 $m \in]-1,1[\setminus\{0\}$, 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

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

(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].