Mathematical Quantum Theory

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Abstract

These are the lecture notes for the courses *Mathematical Quantum Theory* and *Advanced Topics in Quantum Mechanics*, both given at the University of Tübingen in the academic year 2018/2019.

Contents

1 Introduction

1.1 The Schrödinger equation

Let us consider the evolution of one particle in $\mathbb{R}^d$, with $d = 1, 2, 3$ the physically relevant choices of the dimension d. We will assume the particle to be pointlike. We suppose that the particle is exposed to the action of an external potential $V : \mathbb{R}^d \to \mathbb{R}$.

In quantum mechanics, the state of the system is described by the wave function $\psi(t, x)$, $\psi : \mathbb{R} \times \mathbb{R}^d \mapsto \mathbb{C}$, square integrable:

$$\|\psi(t,\cdot)\|_2^2 := \int_{\mathbb{R}^d} |\psi(t,x)|^2 dx = 1 . \tag{1.1}$$

The physical interpretation of $|\psi(t,x)|^2$ is that of probability distribution for finding the particle at (x,t). That is, the probability for finding the particle at the time t in the region $A \subset \mathbb{R}^d$ is:

$$\mathbb{P}^{\psi_t}(A) = \int_A |\psi(t,x)|^2 dx . \tag{1.2}$$

The evolution of the particle is defined by the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t}\psi(t,x) = -\frac{\hbar^2}{2m}\Delta_x \psi(t,x) + V(x)\psi(t,x) =: H\psi(t,x) , \tag{1.3}$$

where $\hbar$ is called the (reduced) Planck constant, and it has the dimensions of an action, $[\hbar] = [\text{energy}] \times [\text{time}]$. The Laplace operator is defined as:

$$\Delta_x = \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2} . \tag{1.4}$$

The differential operator H is called the Hamiltonian of the system. The Schrödinger equation is an example of partial differential equation, and the discussion of existence and uniqueness of solutions will be part of the present course.

Given a Hamiltonian H, the corresponding time-independent Schrödinger equation is:

$$H\psi = E\psi , \tag{1.5}$$

where the (real) number E has the interpretation of energy of the system. A square integrable solution of the time-independent Schrödinger equation is called an eigenstate of the Hamiltonian H. Notice that if ψ is an eigenstate of H, then $\psi(t) = e^{-iEt/\hbar}\psi$ is a solution of the time-dependent Schrödinger equation.

Comparison with classical mechanics. Recall the motion of particle in classical mechanics. The trajectory $q(t) \in \mathbb{R}^d$ of a classical particle is determined by Newton's equation:

$$m\ddot{q}(t) = F(q(t)) = -\nabla V(q(t)) , \qquad (q(0), \dot{q}(0)) = (q_0, \dot{q}_0) . \tag{1.6}$$

This second order ordinary differential equation can be rewritten as a first order differential equation for the pair $(p(t), q(t))$, with $p(t) = m\dot{q}(t)$ the momentum of the particle. The Hamilton's equation of motion for the particle is:

$$\frac{d}{dt}\begin{pmatrix} p(t) \\ q(t) \end{pmatrix} = \begin{pmatrix} -\nabla V(q(t)) \\ \frac{1}{m}p(t) \end{pmatrix} \equiv \begin{pmatrix} -\nabla_q H(q,p) \\ \nabla_p H(p,q) \end{pmatrix} , \tag{1.7}$$

with $H(p,q) = \frac{|p|^2}{m} + V(q)$ the Hamiltonian of the particle. The Hamiltonian appearing in the Schrödinger equation is called the canonical quantization of the classical Hamiltonian, obtained by replacing the position variable q by a multiplication operator x, and the momentum variable p by the differential operator $-i\hbar\nabla_x$.

Quantum mechanics is a more fundamental theory of nature than classical mechanics. A natural question is to understand how classical mechanics emerges from quantum mechanics. This question will be discussed later in the course, while introducing semiclassical analysis.

The main goal of this course is to develop the mathematical theory of the Schrödinger equation, for one particle and for many particle systems. Notice that the Schrödinger equation is a linear evolution equation, in contrast to Hamilton's equation of motion; this seems to suggest that its mathematical study should be "easy". This is not true, due to the fact that the solution of the equation lives in an infinite dimensional space, and that the operator H is unbounded.

2 Function spaces

In this section we shall introduce function spaces that will play an important role in the mathematical formulation of quantum mechanics. We shall only review some basic results, and we will refer the reader to [3, 5] for more details.

2.1 C^k spaces

Definition 2.1. *A multiindex $\alpha \in \mathbb{N}_0^d$ is a d-tuple $\alpha = (\alpha_1, \ldots, \alpha_d)$, with $\alpha_j \in \mathbb{N}_0$, and $|\alpha| = \sum_{j=1}^d \alpha_j$. For $x \in \mathbb{R}^d$ we define:*

$$x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_d^{\alpha_d} \qquad \textit{and} \qquad \partial_x^\alpha := \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}} \,. \tag{2.1}$$

Definition 2.2. *Let $A \subseteq \mathbb{R}^d$, $k \in \mathbb{N}_0$. We define:*

$$C^k(A) = \Big\{ f \mid f : A \to \mathbb{C},\ \partial_x^\alpha f \textit{ is continuous for all } \alpha \textit{ such that } |\alpha| \leqslant k \Big\} \,. \tag{2.2}$$

Also, we denote by $C_b^k(A)$ the restriction of $C^k(A)$ to functions with bounded derivatives:

$$C_b^k(A) = \Big\{ f \mid f \in C^k(A) \textit{ and there exists } c_\alpha > 0 \textit{ such that } \forall |\alpha| \leqslant k \ \sup_{x \in A} |\partial_x^\alpha f(x)| \leqslant c_\alpha \Big\} \,. \tag{2.3}$$

Remark 2.3. *It turns out that the space $C_b^k(A)$ is a Banach space, if endowed with the following norm:*

$$\|f\|_{C_b^k(A)} = \sum_{n=0}^k \sum_{\alpha : |\alpha| = n} \sup_{x \in A} |\partial_x^\alpha f(x)| \,. \tag{2.4}$$

We also define the space of C^k functions with compact support.

Definition 2.4. *Let:*

$$\textit{supp}(f) = \overline{\{x \in \textit{Dom}(f) \mid f(x) \neq 0\}} \tag{2.5}$$

be the support of the function f. Let $A \subseteq \mathbb{R}^d$, $k \in \mathbb{N}_0$. We define:

$$C_c^k(A) = \Big\{ f \mid f \in C^k(A) \textit{ s.t. } \textit{supp}(f) \cap A \textit{ is compact.} \Big\} \tag{2.6}$$

Remark 2.5. $C_c^k(A) \subseteq C_b^k(A) \subseteq C^k(A)$.

Example 2.6. *(i) Let $A = \mathbb{R}$, and $f(x) = x$. We have $f \in C^\infty(\mathbb{R})$. However, $f \notin C_b^\infty(\mathbb{R})$, since f is unbounded. Also, $f \notin C_c^\infty(\mathbb{R})$, since supp$(f) = \mathbb{R}$.*

(ii) Consider the "bump function":

$$f(x) = \begin{cases} \exp\big(-1/(1 - x^2)\big) & x \in (-1, 1) \\ 0 & \textit{otherwise.} \end{cases} \tag{2.7}$$

It is easy to see that all derivatives of f are continuous in $x \in \mathbb{R}$, and are compactly supported in $(-1, 1)$. Thus, $f \in C_c^\infty(\mathbb{R})$.

2.2 L^p spaces

Definition 2.7. *Let $A \subseteq \mathbb{R}^d$, measurable. Let $p \in \mathbb{R}$, $1 \leqslant p < \infty$. We define:*

$$L^p(A) := \left\{ f \mid f : A \to \mathbb{C},\ f \text{ measurable},\ \int_A dx\, |f(x)|^p < \infty \right\} . \tag{2.8}$$

Remark 2.8. *The integral $\int_A dx \cdots$ has to be understood as a Lebesgue integral. If the function f is Riemann integrable, then it coincides with the standard Riemann integral. More generally, one could replace dx by a Lebesgue measure $\mu(dx)$. In that case, we shall denote the corresponding L^p space by $L^p(A, d\mu)$. One can check that L^p is a vector space.*

Besides being vector spaces, L^p spaces are also Banach spaces, if endowed with the following norm.

Definition 2.9. *Let $f \in L^p(A)$, $1 \leqslant p < \infty$. We define:*

$$\|f\|_{L^p(A)} := \left(\int_A dx\, |f(x)|^p \right)^{1/p} . \tag{2.9}$$

One can check that the map $\| \cdot \|_{L^p(A)}$ has the following properties.

(i) $\|\lambda f\|_{L^p(A)} = |\lambda| \|f\|_{L^p(A)}$, $\lambda \in \mathbb{C}$.

(ii) $\|f\|_{L^p(A)} = 0 \Leftrightarrow f(x) = 0$ a.e.

(iii) $\|f + g\|_{L^p(A)} \leqslant \|f\|_{L^p(A)} + \|g\|_{L^p(A)}$ (Minkowki inequality).

These properties imply that $\| \cdot \|_{L^p(A)}$ is a semi-norm. The reason why it is not a norm is that it is easy to imagine functions such that $\|f\|_{L^p(A)} = 0$ and $f(x) \neq 0$ (take f to be zero everywhere except at a point). To ensure that $\| \cdot \|_{L^p(A)}$ defines a norm, one has to redefine L^p by identifying functions that differ on a zero measure set (e.g., on a countable set of points). Given $f \in L^p$, we define an equivalent class of functions as

$$\tilde{f} = \left\{ f' \in L^p \mid f - f' = 0 \text{ a.e.} \right\} \tag{2.10}$$

We redefine L^p as the set of the equivalence classes of functions $\tilde{f}$.

The L^∞ space is defined as follows.

Definition 2.10.

$$L^\infty(A) := \{ f \mid f : A \to \mathbb{C}\, , f \text{ measurable}\, , \exists K > 0 \text{ s.t. } |f(x)| \leqslant K \text{ a.e. } \} . \tag{2.11}$$

A norm on L^∞ is defined by taking the essential supremum of f:

$$\|f\|_{L^\infty(A)} := \inf \{ K \mid |f(x)| \leqslant K \text{ a.e. in } A \} . \tag{2.12}$$

Here we shall list some important facts about L^p spaces, without proof. We refer the reader to [3] for details. Whenever it does not generate ambiguity, we might replace $\| \cdot \|_{L^p(A)}$ by $\| \cdot \|_p$.

Theorem 2.11 (Completeness)**.** *Let $1 \leqslant p \leqslant \infty$, and let f^i, $i = 1, 2, 3, \cdots$ be a Cauchy sequence in $L^p(A)$:*

$$\lim_{i,j \to \infty} \|f^i - f^j\|_p = 0. \tag{2.13}$$

Then, there exists $f_* \in L^p(A)$ such that

$$\lim_{i \to \infty} \|f_i - f_*\|_p = 0 . \tag{2.14}$$

Remark 2.12. *We use the notation $f_i \to f_*$ and we say that f^i converges strongly to f_* in L^p.*

Another important property of L^p spaces, for $p < \infty$, is that their elements can be approximated arbitrarily well by smooth, compactly supported functions. In other words, $C^\infty_{\mathrm{c}}(A)$ is dense in $L^p(A)$.

Theorem 2.13 (Approximation by C^∞_{c} functions.)**.** *Let $f \in L^p(\mathbb{R}^d)$, $1 \leqslant p < \infty$. Then, there exists a sequence of functions $\{f^i\}_{i \in \mathbb{N}}$, $f^i \in C^\infty_{\mathrm{c}}(\mathbb{R}^d)$ such that $f^i \to f$ in L^p.*

2.3 Hilbert spaces

Let $\mathcal{H}$ be a vector space over $\mathbb{C}$. A map $\langle\cdot,\cdot\rangle : \mathcal{H}\times\mathcal{H}\to\mathbb{C}$ is called a scalar product (or a inner product) over $\mathcal{H}$ if:

(i) it is linear in its second variable, that is:

$$\langle\psi, \alpha\varphi_1 + \beta\varphi_2\rangle = \alpha\langle\psi,\varphi_1\rangle + \beta\langle\psi,\varphi_2\rangle \tag{2.15}$$

(ii) it is antisymmetric, that is:

$$\langle\psi,\varphi\rangle = \overline{\langle\varphi,\psi\rangle} \tag{2.16}$$

(iii) it is positive definite, that is:

$$\langle\psi,\psi\rangle \geqslant 0 \tag{2.17}$$

for all $\psi\in\mathcal{H}$, with $\langle\psi,\psi\rangle = 0$ if and only if $\psi = 0$.

Every scalar product induces a norm on $\mathcal{H}$, defined through:

$$\|\psi\| = \sqrt{\langle\psi,\psi\rangle}\,. \tag{2.18}$$

The triangle inequality for $\|\cdot\|$ follows from the Cauchy-Schwartz inequality

$$|\langle\psi,\varphi\rangle| \leqslant \|\psi\|\|\varphi\|\,. \tag{2.19}$$

In fact:

$$\begin{aligned}\|\psi+\varphi\| &= \sqrt{\langle\psi+\varphi,\psi+\varphi\rangle}\\ &= \sqrt{\|\psi\|^2+\|\varphi\|^2+2\mathrm{Re}\langle\psi,\varphi\rangle}\\ &\leqslant \sqrt{\|\psi\|^2+\|\varphi\|^2+2\|\psi\|\|\varphi\|}\\ &= \|\psi\|+\|\varphi\|\,.\end{aligned} \tag{2.20}$$

If the vector space $\mathcal{H}$ equipped with the scalar product $\langle\cdot,\cdot\rangle$ is complete, the pair $(\mathcal{H},\langle\cdot,\cdot\rangle)$ is called a Hilbert space.

Example 2.14. *(a) The space $\mathbb{C}^n$ equipped with the scalar product:*

$$\langle x,y\rangle_{\mathbb{C}^n} = \sum_{j=1}^{n}\bar{x}_j y_j \tag{2.21}$$

is a Hilbert space.

(b) The space ℓ^2 of the square summable sequences $(x_j)_{j\in\mathbb{N}}$, equipped with the scalar product:

$$\langle x,y\rangle_{\ell^2} = \sum_{j=1}^{\infty}\bar{x}_j y_j \tag{2.22}$$

is a Hilbert space.

Example 2.15 (L^2 space.)**.** *In quantum mechanics, a special role is played by the space of square integrable functions, $L^2(A)$. This space turns out to be a Hilbert space, if equipped with the following scalar product:*

$$\langle f,g\rangle = \int dx\,\overline{f(x)}g(x)\,. \tag{2.23}$$

It is easy to see that the scalar product $\langle f,g\rangle$ is well defined, for all $f,g\in L^2(A)$:

$$\begin{aligned}|\langle f,g\rangle| &\leqslant \int dx\,|f(x)||g(x)|\\ &\leqslant \frac{1}{2}\int dx\,|f(x)|^2 + \frac{1}{2}\int dx\,|g(x)|^2\\ &\equiv \frac{1}{2}\|f\|_{L^2(A)} + \frac{1}{2}\|g\|_{L^2(A)} < \infty\,.\end{aligned} \tag{2.24}$$

Also, it is easy to see that Eq. (2.23) fulfills the properties (i)–(iii) spelled above.

3 The free Schödinger equation

To start our mathematical study of the Schrödinger equation we shall consider the simplest possible situation, corresponding to a free particle in $\mathbb{R}^d$. We look for a solution $\psi : \mathbb{R} \times \mathbb{R}^d \to \mathbb{C}$ of the equation:

$$i\partial_t \psi(t,x) = -\frac{1}{2}\Delta_x \psi(t,x) \ , \tag{3.1}$$

where we set $\hbar = 1$ and $m = 1$. A special solution can be found by separation of variables. Consider first the time-independent Schrödinger equation:

$$-\frac{1}{2}\Delta_x \phi(x) = \lambda \phi(x) \ . \tag{3.2}$$

Then, a solution of Eq. (3.1) is obtained by setting $\psi(t,x) = e^{-i\lambda t}\phi(x)$. We are left with finding a solution of the time-independent equation (3.2). A family of solutions for such equation is given by the plane waves on $\mathbb{R}^d$:

$$\phi_k(x) = e^{ik\cdot x} = e^{i(k_1 x_1 + \ldots + k_d x_d)} \qquad \text{for } k \in \mathbb{R}^d \ . \tag{3.3}$$

In fact:

$$-\Delta_x \phi_k(x) = \frac{1}{2}(k_1^2 + \ldots + k_d^2)e^{ik\cdot x} \equiv \frac{|k|^2}{2}\phi_k(x) \ . \tag{3.4}$$

Thus, we found a first solution of the free Schrödinger equation, Eq. (3.1):

$$\psi_k(x,t) = e^{-i\frac{k^2}{2}t}e^{ik\cdot x} \ . \tag{3.5}$$

However, the above solution does not make sense in quantum mechanics, since $\psi(t,\cdot) \notin L^2(\mathbb{R}^d)$ for all t:

$$\int dx\, |\psi_k(t,x)|^2 = +\infty \ . \tag{3.6}$$

Nevertheless, we can use the above unphysical solutions to construct physical solutions of the Schrödinger equation, by using the fact that the Schrödinger equation is a linear equation: a linear combination of solutions of Eq. (3.1) is a solution of Eq. (3.1). More precisely, we shall consider solutions of the form:

$$\psi(x,t) = \int_{\mathbb{R}^d} \rho(k)\psi_k(x,t)dk \equiv \int_{\mathbb{R}^d} \rho(k) e^{-i(\frac{k^2}{2}t - k\cdot x)}dk \ . \tag{3.7}$$

Formally, $\psi(x,t)$ is a solution of Eq. (3.1), with initial datum at $t = 0$:

$$\psi(x,0) \equiv \psi_0(x) = \int_{\mathbb{R}^d} \rho(k)e^{ik\cdot x}dk \ . \tag{3.8}$$

The questions we will address here are: for which class of $\rho(k)$ does the function $\psi(t,x)$ makes sense from a quantum mechanical viewpoint, namely $\psi(t,\cdot) \in L^2(\mathbb{R}^d)$?

3.1 The Fourier transform on L^1

We are now ready to introduce the Fourier transform for L^1 functions.

Definition 3.1. *Let $f \in L^1(\mathbb{R}^d)$. We define the Fourier transform $\hat{f} \equiv \mathcal{F}f$ as*

$$(\mathcal{F}f)(k) \equiv \hat{f}(k) = \frac{1}{(2\pi)^{\frac{d}{2}}}\int dx\, e^{-ik\cdot x}f(x), \qquad k \in \mathbb{R}^d. \tag{3.9}$$

We define the inverse Fourier transform $\check{f} \equiv \mathcal{F}^{-1}f$ as:

$$(\mathcal{F}^{-1}f)(k) \equiv \check{f}(k) = \frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d} dx\, e^{ik\cdot x}f(x) \ . \tag{3.10}$$

Remark 3.2. *Since* $|e^{-ik\cdot x}| = 1$ *and* $f \in L^1(\mathbb{R}^d)$, $\hat{f}$ *and* $\check{f}$ *are well defined:*

$$|\hat{f}(k)| \leqslant \frac{1}{(2\pi)^{\frac{d}{2}}} \int dx\, |f(x)| = \frac{1}{(2\pi)^{\frac{d}{2}}} \|f\|_1 \ . \tag{3.11}$$

The next lemma will be useful to study the regularity properties of the Fourier transform.

Lemma 3.3. *Let* $\Gamma \subset \mathbb{R}$ *be an open interval, and* $f : \mathbb{R}^d \times \Gamma \to \mathbb{C}$ *such that* $f(x,\gamma) \in L^1(\mathbb{R}^d_x)$ *for all* $\gamma \in \Gamma$. *Let* $I(\gamma) = \int_{\mathbb{R}^d} f(x,\gamma)dx$. *Then, the following is true.*

(a) If the map $\gamma \mapsto f(x,\gamma)$ *is continuous for almost all* $x \in \mathbb{R}^d$, *and if there exists a function* $g \in L^1(\mathbb{R}^d)$ *such that* $\sup_{\gamma\in\Gamma} |f(x,\gamma)| \leqslant g(x)$ *for almost all* $x \in \mathbb{R}^d$, *then* $I(\gamma)$ *is also continuous.*

(b) If the map $\gamma \mapsto f(x,\gamma)$ *is continuously differentiable for almost all* $x \in \mathbb{R}^d$, *and if there exists a function* $g \in L^1(\mathbb{R}^d)$ *such that* $\sup_{\gamma\in\Gamma} |\partial_\gamma f(x,\gamma)| \leqslant g(x)$ *for almost all* $x \in \mathbb{R}^d$, *then* $I(\gamma)$ *is also continuously differentiable. Moreover:*

$$\frac{dI}{d\gamma}(\gamma) = \frac{d}{d\gamma} \int_{\mathbb{R}^d} f(x,\gamma)dx = \int_{\mathbb{R}^d} \frac{\partial}{\partial\gamma} f(x,\gamma)dx \ . \tag{3.12}$$

Proof. The proof immediately follows from the dominated convergence theorem, see [3]. ∎

Lemma 3.3 has important consequences on the behavior of the Fourier transform.

Theorem 3.4 (Riemann-Lebesgue.)**.** *Let* $f \in L^1(\mathbb{R}^d)$. *Then:*

$$\hat{f} \in C_\infty(\mathbb{R}^d) := \Big\{ f \in C(\mathbb{R}^d) \mid \lim_{R\to\infty} \sup_{|x|>R} |f(x)| = 0 \Big\} \ . \tag{3.13}$$

Proof. The continuity immediately follows from Lemma 3.3. The falloff at infinity will follow from a result we will discuss later on. ∎

Next, we will focus on the properties of the "nicest possible" functions, namely the Schwartz functions. Later, we will come back on a more general class of functions, by using approximation arguments.

Definition 3.5 (Schwartz functions.)**.** *The Schwartz space* $\mathcal{S}(\mathbb{R}^d)$ *is the set of functions* $f \in C^\infty(\mathbb{R}^d)$ *such that:*

$$\|f\|_{\alpha,\beta} := \|x^\alpha \partial_x^\beta f\|_\infty < \infty \ , \tag{3.14}$$

for all multiindices α, β.

That is, the functions in $\mathcal{S}(\mathbb{R}^d)$ decay faster than any inverse polynomial in x, and the same is true for all their partial derivatives. Obviously, if $f \in \mathcal{S}$ then $x^\alpha \partial_\beta f \in \mathcal{S}$ for all multiindices α and β. Also, $\mathcal{S}(\mathbb{R}^d) \subset L^p(\mathbb{R}^d)$. Finally, the maps $\|\cdot\|_{\alpha,\beta} : \mathcal{S} \to [0,\infty)$ are norms.

Remark 3.6. *Notice that* $C_c^\infty(\mathbb{R}^d) \subset \mathcal{S}(\mathbb{R}^d)$, *which means that* $\mathcal{S}(\mathbb{R}^d)$ *is dense in* $L^p(\mathbb{R}^d)$, $1 \leqslant p < \infty$.

Definition 3.7. *We say that* $f_n \to f$ *in* $\mathcal{S}$ *if* $\lim_{n\to\infty} \|f - f_n\|_{\alpha,\beta} \to 0$ *for all* $\alpha, \beta \in \mathbb{N}_0^d$.

Proposition 3.8 ($\mathcal{S}$ is a metric space.)**.** *Convergence in* $\mathcal{S}$ *is equivalent to convergence with respect to the metric:*

$$d_{\mathcal{S}}(f,g) = \sum_{n=0}^\infty 2^{-n} \sup_{|\alpha|+|\beta|=n} \frac{\|f-g\|_{\alpha,\beta}}{1+\|f-g\|_{\alpha,\beta}} \ . \tag{3.15}$$

Remark 3.9. *Notice that* $d_{\mathcal{S}}(f,g) \leqslant 2$.

Proof. Let us first check that $d_{\mathcal{S}}(f,g)$ is a metric. Positivity is trivial, and also symmetry: $d_{\mathcal{S}}(f,g) = d_{\mathcal{S}}(g,f)$. From the definition, we see that $d_{\mathcal{S}}(f,g) = 0$ implies $\|f-g\|_{0,0} = \|f-g\|_{\infty} = 0$, that is $f = g$. Also, the triangle inequality holds true: $d_{\mathcal{S}}(f,g) \leqslant d_{\mathcal{S}}(f,h)+d_{\mathcal{S}}(h,g)$, since $\|\cdot\|_{\alpha,\beta}$ satisfies the triangle inequality and the function $h(x) = x/(1+x)$ is monotone increasing and satisfies $h(x+y) \leqslant h(x)+h(y)$. This shows that d_{S} is a metric. Convergence in $\mathcal{S}$ immediately implies convergence with respect to $d_{\mathcal{S}}(f,g)$. On the other hand, suppose that $d_{\mathcal{S}}(f_n,f) \to 0$. To prove convergence in $\mathcal{S}$ we use that, for all α,β there exists a constant $C_{\alpha,\beta} > 0$ such that:

$$\|f_n - f\|_{\alpha,\beta} \leqslant C_{\alpha,\beta} d_{\mathcal{S}}(f_n,f)\ . \tag{3.16}$$

Therefore, convergence with respect to $d_{\mathcal{S}}$ implies convergence in $\mathcal{S}$. ∎

Theorem 3.10. *The Schwartz space is complete.*

Proof. Let (f_m) be a Cauchy sequence in $\mathcal{S}$. Then, (f_m) is a Cauchy sequence with respect to the (semi-)norms $\|\cdot\|_{\alpha,\beta}$. Also, convergence in $\mathcal{S}$ implies that $x^{\alpha}\partial_x^{\beta} f_m \to g_{\alpha,\beta}(x)$ in L^{∞} norm, with $g_{\alpha,\beta} \in C_{\mathrm{b}}(\mathbb{R}^d)$, the space of continuous, bounded functions. This last fact is implied by the completeness of $C_{\mathrm{b}}(\mathbb{R}^d)$ with respect to the $\|\cdot\|_{\infty}$ norm, recall Remark 2.3.

We are left with showing that $g := g_{0,0} \in C^{\infty}(\mathbb{R}^d)$, and that $x^{\alpha}\partial_x^{\beta} g = g_{\alpha,\beta}$. If so, $g \in \mathcal{S}$ and $d_{\mathcal{S}}(f_m,g) \to 0$. For simplicity, let us consider the case $d = 1$. We would like to show that $g \in C^1(\mathbb{R})$ and that $\partial_x g = g_{0,1}$. Higher derivatives and higher dimensions can be studied in the same way. For $f_m \in \mathcal{S}$, we write:

$$f_m(x) = f_m(0) + \int_0^x f_m'(y)\, dy\ . \tag{3.17}$$

We know that $f_m \to g$ and $f_m' \to g_{0,1}$ uniformly. Therefore, the $m \to \infty$ limit of Eq. (3.17) is:

$$g(x) = g(0) + \int_0^x g_{0,1}(y)\, dy\ . \tag{3.18}$$

This proves that $g \in C^1(\mathbb{R})$ with $g' = g_{0,1}$. ∎

Lemma 3.11 (Properties of $\mathcal{F}$ on $\mathcal{S}$.)**.** *The maps $\mathcal{F}$ and $\mathcal{F}^{-1}$ are continuous, linear maps from $\mathcal{S}$ into itself. Moreover, for all α,β it holds:*

$$\Big((ik)^{\alpha}\partial_k^{\beta}\mathcal{F}f\Big)(k) = \Big(\mathcal{F}\partial_x^{\alpha}(-ix)^{\beta} f\Big)(k)\ . \tag{3.19}$$

Remark 3.12. *In particular,*

$$\widehat{(xf)}(k) = i(\nabla_k \hat{f})(k) \qquad \textit{and} \qquad \widehat{(\nabla_x f)}(k) = ik\hat{f}(k)\ . \tag{3.20}$$

Proof. Let $f \in \mathcal{S}$. Recall:

$$\hat{f}(k) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} f(x) e^{-ik\cdot x} dx\ . \tag{3.21}$$

Then:

$$\begin{aligned}
(2\pi)^{d/2}\Big((ik)^{\alpha}\partial_k^{\beta}\mathcal{F}f\Big)(k) &= \int_{\mathbb{R}^d} (ik)^{\alpha}\partial_k^{\beta} e^{-ik\cdot x} f(x)\, dx \\
&= \int_{\mathbb{R}^d} (ik)^{\alpha}(-ix)^{\beta} e^{-ik\cdot x} f(x)\, dx \\
&= \int_{\mathbb{R}^d} (-1)^{|\alpha|}(\partial_x^{\alpha} e^{-ik\cdot x})(-ix)^{\beta} f(x)\ .
\end{aligned} \tag{3.22}$$

Integrating by parts:

$$\begin{aligned}
(2\pi)^{d/2}\Big((ik)^{\alpha}\partial_k^{\beta}\mathcal{F}\Big)(k) &= \int_{\mathbb{R}^d} e^{-ik\cdot x}\big(\partial_x^{\alpha}(-ix)^{\beta} f(x)\big)\, dx \\
&\equiv (2\pi)^{d/2}\Big(\mathcal{F}\partial_x^{\alpha}(-ix)^{\beta} f\Big)(k)\ .
\end{aligned} \tag{3.23}$$

This shows that, in particular, $\mathcal{F}f \in C^\infty$. Moreover:

$$\begin{aligned}
\|\hat{f}\|_{\alpha,\beta} &= \left\|k^\alpha \partial_k^\beta \hat{f}\right\|_\infty \leqslant \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} |\partial_x^\alpha x^\beta f(x)| \frac{(1+|x|^2)^d}{(1+|x|^2)^d}\, dx \\
&\leqslant \frac{1}{(2\pi)^{d/2}} \sup_{x\in\mathbb{R}^d} \left|(1+|x|^2)^d \partial_x^\alpha x^\beta f(x)\right| \int_{\mathbb{R}^d} \frac{1}{(1+|x|^2)^d}\, dx \\
&\leqslant C \sum_{j=0}^{m} \sup_{|\tilde{\alpha}|+|\tilde{\beta}|=j} \|f\|_{\tilde{\alpha},\tilde{\beta}} , \qquad (3.24)
\end{aligned}$$

with $m = \max\{|\alpha|, |\beta|\} + 2d$, and for $C > 0$ independent of f. Therefore, $\mathcal{F}f \in \mathcal{S}$. Eq. (3.24) also shows that $f_n \to f$ in $\mathcal{S}$ implies $\hat{f}_n \to \hat{f}$ in $\mathcal{S}$. In particular, Eq. (3.24) can be used to show that $\mathcal{F} : \mathcal{S} \to \mathcal{S}$ is continuous, with respect to the topology induced by $d_{\mathcal{S}}(\cdot,\cdot)$. In fact, suppose that $f_n \to f$ with respect to $d_{\mathcal{S}}$. Then, by Eq. (3.24), there exists $C_{\alpha.\beta} > 0$ such that:

$$\|\hat{f}_n - \hat{f}\|_{\alpha,\beta} \leqslant C_{\alpha,\beta} d_{\mathcal{S}}(f_n, f) . \qquad (3.25)$$

∎

Theorem 3.13. *The map $\mathcal{F} : \mathcal{S} \to \mathcal{S}$ is a continuous bijection, with inverse $\mathcal{F}^{-1}$.*

Proof. We will show that $\mathcal{F}^{-1} \circ \mathcal{F} = \mathbb{1}_{\mathcal{S}}$ (the same proof gives $\mathcal{F} \circ \mathcal{F}^{-1} = \mathbb{1}_{\mathcal{S}}$). Since $\mathcal{F}^{-1} \circ \mathcal{F}$ and $\mathbb{1}_{\mathcal{S}}$ are both continuous in $\mathcal{S}$, it is sufficient to prove their equality on a dense subset of $\mathcal{S}$.

Lemma 3.14. *$C_c^\infty(\mathbb{R}^d)$ is dense in $\mathcal{S}(\mathbb{R}^d)$.*

Proof. (of Lemma 3.14.) Let:

$$G(x) = \begin{cases} \exp\big(-1/(1-|x|^2)+1\big) & \text{for } |x| < 1 \\ 0 & \text{otherwise.} \end{cases} \qquad (3.26)$$

Let $f \in \mathcal{S}(\mathbb{R}^d)$, and let $f_n(x) = f(x)G(x/n)$. Clearly, $f_n \in C_c^\infty(\mathbb{R}^d)$. Moreover, $\lim_{n\to\infty} \|f_n - f\|_{\alpha,\beta} = 0$ for all α, β. ∎

Let us now come back to the proof of Theorem 3.13. By Lemma 3.14, it is sufficient to prove the claim of Theorem 3.13 on $C_c^\infty(\mathbb{R}^d)$. Let $f \in C_c^\infty(\mathbb{R}^d)$. Let us denote by $W_m \subset \mathbb{R}^d$ a cube in $\mathbb{R}^d$, centered in the origin, with side $2m$. Let us choose m large enough so that $\mathrm{supp}(f) \subset W_m$. Let $K_m = \pi/m\mathbb{Z}^d$. We can express the function f on W_m as the uniformly convergent Fourier series:

$$f(x) = \sum_{k\in K_m} f_k e^{ik\cdot x} , \qquad (3.27)$$

with Fourier coefficients:

$$f_k = \frac{1}{\mathrm{Vol}(W_m)} \int_{W_m} f(x) e^{-ik\cdot x} dx = \frac{1}{\mathrm{Vol}(W_m)} \int_{\mathbb{R}^d} f(x) e^{-ik\cdot x} dx = \frac{(2\pi)^{d/2}}{(2m)^d} (\mathcal{F}f)(k) . \qquad (3.28)$$

Therefore we have:

$$f(x) = \sum_{k\in K_m} \frac{(\mathcal{F}f)(k) e^{ik\cdot x}}{(2\pi)^{d/2}} \Big(\frac{\pi}{m}\Big)^d . \qquad (3.29)$$

The observation is that the right-hand side of Eq. (3.29) is a Riemann sum, over cubes of volume $(\pi/m)^d$ and with k the center of the cube. Therefore, we have:

$$f(x) = \lim_{m\to\infty} \sum_{k\in K_m} \frac{(\mathcal{F}f)(k) e^{ik\cdot x}}{(2\pi)^{d/2}} \Big(\frac{\pi}{m}\Big)^d = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} (\mathcal{F}f)(k) e^{ik\cdot x} dk = (\mathcal{F}^{-1} \circ \mathcal{F}f)(x) . \qquad (3.30)$$

This proves that $\mathcal{F}^{-1} \circ \mathcal{F} = \mathbb{1}_{C_c^\infty(\mathbb{R}^d)}$. ∎

Proposition 3.15. *Let $f, g \in \mathcal{S}(\mathbb{R}^d)$. Then:*

$$\int_{\mathbb{R}^d} \hat{f}(x)g(x)dx = \int_{\mathbb{R}^d} f(x)\hat{g}(x)dx \; . \tag{3.31}$$

Moreover,

$$\|f\|_2 = \|\hat{f}\|_2 \; . \tag{3.32}$$

Proof. By Fubini's theorem,

$$\int_{\mathbb{R}^d} \Big(\int_{\mathbb{R}^d} e^{-ik\cdot x} f(k)dk \Big) g(x)dx = \int_{\mathbb{R}^d} \Big(\int_{\mathbb{R}^d} e^{-ik\cdot x} g(x)dx \Big) f(k)dk \; . \tag{3.33}$$

Therefore, $(2\pi)^{d/2} \int dx\, \hat{f}(x)g(x) = (2\pi)^{d/2} \int dk\, \hat{g}(k)f(k)$. This proves Eq. (3.33). To prove Eq. (3.32), we use that $\overline{\mathcal{F}f(x)} = \mathcal{F}^{-1}\overline{f(x)}$, which can be easily checked. Thus, Eq. (3.32) follows as a special case of Eq. (3.33), choosing $g(x) = \overline{\mathcal{F}f(x)}$.

∎

Example 3.16 (The Fourier transform of a Gaussian.). *Let $\lambda > 0$, and let $g_\lambda(x) = \exp\big(-\lambda\frac{|x|^2}{2}\big)$ be the Gaussian function. Then, we claim that:*

$$\hat{g}_\lambda(k) = \lambda^{-\frac{d}{2}} \exp\left(-\frac{|k|^2}{2\lambda} \right) \; . \tag{3.34}$$

To prove Eq. (3.34), we proceed as follows. By scaling, it is enough to consider the case $\lambda = 1$. Also, since $g_1(x) = \prod_{i=1}^d \exp\left(-\frac{x_i^2}{2}\right)$, it is enough to consider the case $n = 1$. We have:

$$\hat{g}_1(k) = \frac{1}{(2\pi)^{\frac{1}{2}}} \int dx e^{-ik\cdot x} e^{-\frac{x^2}{2}} = \frac{1}{(2\pi)^{\frac{1}{2}}} \int dx e^{-\frac{(x+ik)^2}{2} - \frac{k^2}{2}} \equiv g_1(k)f(k), \tag{3.35}$$

where we defined $f(k) = \frac{1}{(2\pi)^{\frac{1}{2}}} \int dx e^{-\frac{(x+ik)^2}{2}}$. By dominated convergence, we can differentiate under the integral sign:

$$\frac{d}{dk} f(k) = \int_{\mathbb{R}} \frac{dx}{(2\pi)^{\frac{1}{2}}} (-(x+ik))ie^{-\frac{(x+ik)^2}{2}} = \int_{\mathbb{R}} \frac{dx}{(2\pi)^{\frac{1}{2}}} i\frac{d}{dx} e^{-\frac{(x+ik)^2}{2}} = 0. \tag{3.36}$$

This means that $f(k)$ is a constant and, in particular, $f(k) = f(0) = 1$. This proves Eq. (3.34).

3.2 Solution of the free Schrödinger equation

Let us now come back to the Schrödinger equation for one free particle in $\mathbb{R}^d$:

$$i\partial_t \psi(t,x) = -\frac{1}{2}\Delta_x \psi(t,x) \; . \tag{3.37}$$

Let us take the Fourier transform in both sides. Proceeding formally, we get:

$$i\partial_t \hat{\psi}(t,k) = \frac{1}{2}|k|^2 \hat{\psi}(t,k) \; . \tag{3.38}$$

The advantage of taking the Fourier transform is that now we are left with an ordinary differential equation of the first order. The solution is:

$$\hat{\psi}(t,k) = e^{-i\frac{|k|^2}{2}t} \hat{\psi}(0,k) \; . \tag{3.39}$$

To get a solution of the original equation (3.37), we have to take the inverse Fourier transform. We get:

$$\psi(t,x) = (\mathcal{F}^{-1} e^{-i\frac{|k|^2}{2}t} \mathcal{F}\psi_0)(x) \; , \tag{3.40}$$

with initial datum $\psi(0,x) = \psi_0(x)$. The next theorem shows that the above formal manipulation can be made rigorous for a suitable class of regular initial data.

Theorem 3.17 (Existence of a unique global solution for the free Schrödinger equation.)**.** *Let $\psi_0 \in \mathcal{S}(\mathbb{R}^d)$. Then, there exists a global solution $\psi \in C^\infty(\mathbb{R}_t, \mathcal{S}(\mathbb{R}^d))$ of the free Schrödinger equation with $\psi(0,x) = \psi_0(x)$ for $t \neq 0$, given by the expression:*

$$\psi(t,x) = \frac{1}{(2\pi i t)^{d/2}} \int_{\mathbb{R}^d} e^{i\frac{|x-y|^2}{2t}} \psi_0(y) dy \; . \tag{3.41}$$

Moreover, $\|\psi(t,\cdot)\|_{L^2(\mathbb{R}^d)} = \|\psi_0\|_{L^2(\mathbb{R}^d)}$.

Proof. To begin, notice first that, for $\psi_0 \in \mathcal{S}$, the expression (3.40) is well defined. Hence, Eq. (3.40) is a solution of the free Schrödinger equation (3.37). Next, we shall show that $\psi \in C^\infty(\mathbb{R}_t, \mathcal{S}(\mathbb{R}^d))$. Let us start by showing that $t \mapsto \psi(t)$ is differentiable. Let: $\dot{\psi}(t,x) := -i(\mathcal{F}^{-1}\frac{|k|^2}{2}e^{-i\frac{|k|^2}{2}t}\mathcal{F}\psi_0)(x)$. Then, $\dot{\psi}(t,\cdot) \in \mathcal{S}(\mathbb{R}^d)$. Furthermore, we claim that:

$$\lim_{h\to 0} \Big\| \frac{\psi(t+h) - \psi(t)}{h} - \dot{\psi}(t) \Big\|_{\alpha,\beta} = 0 \tag{3.42}$$

with respect to any $\|\cdot\|_{\alpha,\beta}$. By continuity of $\mathcal{F}$ and of $\mathcal{F}^{-1}$, this is equivalent to:

$$\lim_{h\to 0} \Big\| \frac{\hat{\psi}(t+h) - \hat{\psi}(t)}{h} - \hat{\dot{\psi}}(t) \Big\|_{\alpha,\beta} = 0 \; , \tag{3.43}$$

for all α, β. This follows from the smoothness of $e^{-i\frac{|k|^2}{2}t}$ and from the decay of $\hat{\psi}_0(k)$:

$$\begin{aligned}\Big\| \frac{\hat{\psi}(t+h) - \hat{\psi}(t)}{h} - \hat{\dot{\psi}}(t) \Big\|_{\alpha,\beta} &= \sup_{k\in\mathbb{R}^d} \Big| k^\alpha \partial_k^\beta \Big(\frac{e^{-i\frac{|k|^2}{2}(t+h)} - e^{-i\frac{|k|^2}{2}t}}{h} + i\frac{|k|^2}{2} e^{-i\frac{|k|^2}{2}t} \Big) (\mathcal{F}\psi_0)(k) \Big| \\ &\to 0 \qquad \text{as } h \to 0.\end{aligned} \tag{3.44}$$

In the same way, one can prove that $\psi(t,x) \in C^k(\mathbb{R}_t, \mathcal{S}(\mathbb{R}^d))$ for any $k \geqslant 1$, and hence that $\psi(t,x) \in C^\infty(\mathbb{R}_t, \mathcal{S}(\mathbb{R}^d))$. The uniqueness of the solution for $\psi_0 \in \mathcal{S}$ follows from the uniqueness of the solution of (3.38). The formula (3.41) follows from an explicit computation, using that:

$$\lim_{R\to\infty} \int_{-R}^{R} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}} \; , \tag{3.45}$$

for all $\alpha \in \mathbb{C}$ such that $\mathrm{Re}\,\alpha = 0$. Finally, the isometry in L^2 follows from the isometry property of the maps $\mathcal{F}$ and $\mathcal{F}^{-1}$, proven in Eq. (3.32), and from the fact that $|e^{-i|k|^2t/2}| = 1$. ∎

Remark 3.18 (Decay of the solutions of the Schrödinger equation.)**.** *The formula (3.41) immediately implies that:*

$$\sup_{x\in\mathbb{R}^d} |\psi(t,x)| \leqslant \frac{\|\psi_0\|_{L^1}}{(2\pi t)^{d/2}} \to 0 \qquad \text{as } t \to \infty. \tag{3.46}$$

However, as we just proved, the L^2 norm stays constant. This means that the solution of the Schrödinger equation spreads in space. One speaks about the "spreading of the wave packet".

Definition 3.19 (Polynomially bounded functions.)**.** *Let $C^\infty_{pol}(\mathbb{R}^d)$ be the space of the polynomially bounded smooth functions: $g \in C^\infty_{pol}(\mathbb{R}^d)$ if $g \in C^\infty(\mathbb{R}^d)$ and if:*

$$|\partial^\alpha g(x)| \leqslant C_\alpha \langle x \rangle^{n(\alpha)} := C_\alpha (1 + |x|^2)^{\frac{n(\alpha)}{2}} \; , \tag{3.47}$$

for all α.

Motivated by Lemma 3.11, we introduce the notion of pseudodifferential operator.

Definition 3.20 (Pseudodifferential operator.)**.** *Let $f \in C^\infty_{pol}(\mathbb{R}^d)$. Let $M_f : \mathcal{S} \to \mathcal{S}$ be the multiplication operator $\psi(x) \to f(x)\psi(x)$. We define the pseudodifferential operator $f(-i\nabla_x) : \mathcal{S} \to \mathcal{S}$ as:*

$$(f(-i\nabla_x)\psi)(x) := (\mathcal{F}^{-1} M_f \mathcal{F}\psi)(x) = (\mathcal{F}^{-1} f(k) \mathcal{F}\psi)(x) \; . \tag{3.48}$$

Remark 3.21. *Notice that the mapping $M_f : \mathcal{S} \to \mathcal{S}$ is continuous. The continuity of M_f and of $\mathcal{F}$ implies the continuity of $f(-i\nabla_x)$. For $f(k) = k^\alpha$, one naturally has $f(-i\nabla) = (-i)^{|\alpha|}\partial_x^\alpha$. For polynomial functions f, the corresponding pseudodifferential operators are differential operators.*

Example 3.22 (Translations and the free propagator.)**.** *Let $a \in \mathbb{R}^d$ and $T_a = e^{-ia\cdot k}$. One has $T_a \in C^\infty_{pol}$ and for $\psi \in \mathcal{S}(\mathbb{R}^d)$ one has:*

$$(T_a(-i\nabla)\psi)(x) = \frac{1}{(2\pi)^{d/2}}\int dk\, e^{-ik\cdot a}e^{ik\cdot x}\hat{\psi}(k)dk = \frac{1}{(2\pi)^{d/2}}\int e^{ik\cdot(x-a)}\hat{\psi}(k)dk = \psi(x-a)\ . \tag{3.49}$$

The operator $T_a(-i\nabla)$ is called the translation operator. Another example is $P_f(t,k) = e^{-i\frac{|k|^2}{2}t}$. One has $P_f(t,\cdot) \in C^\infty_{\text{pol}}(\mathbb{R}^d)$ and hence:

$$\psi(t,x) = (P_f(t,-i\nabla_x)\psi_0)(x)\ . \tag{3.50}$$

This operator is also called the free propagator, and one also writes:

$$\psi(t) = e^{\frac{i}{2}\Delta_x t}\psi_0\ . \tag{3.51}$$

Example 3.23 (The heat equation and diffusion.)**.** *We can apply the previous theory to solve the heat equation:*

$$\partial_t f(t,x) = \frac{1}{2}\Delta_x f(t,x)\ , \tag{3.52}$$

for $f(0,\cdot) = f_0 \in \mathcal{S}(\mathbb{R}^d)$. Let $t > 0$. The solution of Eq. (A.38) reads:

$$f(t) = e^{\frac{1}{2}\Delta_x t}f(0) = W(t,-i\nabla_x)f_0\ , \tag{3.53}$$

with $W(t,k) = e^{-\frac{k^2}{2}t}$. Notice that $W(t) \in C^\infty_{pol}$ only for $t \geqslant 0$. In general, one cannot establish existence of solutions of the heat equation for $t < 0$. However, if $\hat{f}_0$ has compact support, the corresponding solution of the heat equation exists for all times.

Definition 3.24 (Convolutions.)**.** *Let $f, g \in \mathcal{S}$. We define the convolution $f * g$ as:*

$$(f*g)(x) := \int_{\mathbb{R}^d} f(x-y)g(y)dy\ . \tag{3.54}$$

Here we list some properties of the convolution operation.

Theorem 3.25. *Let $f, g, h \in \mathcal{S}$. The following is true.*

(i) $(f*g)*h = f*(g*h)$ *and* $f*g = g*f$.

(ii) The map $g \mapsto f*g$ from $\mathcal{S}$ to $\mathcal{S}$ is continuous.

(iii) It follows that:

$$\widehat{f*g} = (2\pi)^{d/2}\hat{f}\cdot\hat{g}\ , \tag{3.55}$$

and also $\widehat{fg} = (2\pi)^{-d/2}\hat{f}*\hat{g}$. Moreover, one has:

$$g(-i\nabla)f = \mathcal{F}^{-1}(g\hat{f}) = (2\pi)^{-d/2}\check{g}*f\ . \tag{3.56}$$

Proof. The properties (i) and (iii) easily follows from the definition. Concerning (ii), continuity follows from:

$$f*g = (2\pi)^{d/2}\mathcal{F}^{-1}\hat{f}\mathcal{F}g\ ; \tag{3.57}$$

that is, the convolution with f corresponds to the combination of Fourier transform, multiplication by f, and inverse Fourier transform. All these maps are continuous, and their composition preserves continuity. Thus (ii) holds true. ■

Example 3.26 (The heat equation.)**.** *Consider:*

$$G(t,x) := (2\pi)^{-d/2}(\mathcal{F}^{-1}W)(t,x) = \frac{1}{(2\pi t)^{d/2}}e^{-\frac{|x|^2}{2t}}\ . \tag{3.58}$$

The function $G(t,x)$ is called the fundamental solution of the heat equation, and can be used to construct more general solutions. In fact:

$$f(t,x) = (W(t,-i\nabla_x)f_0)(x) = (G(t)*f_0)(x) = \frac{1}{(2\pi t)^{d/2}}\int_{\mathbb{R}^d} e^{-\frac{|x-y|^2}{2t}}f_0(y)dy\ . \tag{3.59}$$

3.2.1 Comparison between Schrödinger, heat and wave equations

To conclude this section, let us compare the free Schrödinger equation to the heat equation and the wave equation. For simplicity, we shall consider the case $d = 1$.

The wave equation. The wave equation can be used to describe the motion of an oscillating string of length L. Let $f(x,t)$ be the wave deflection. The equation reads:

$$\frac{\partial^2}{\partial t^2} f(t,x) = \frac{\partial^2}{\partial x^2} f(t,x) \; , \tag{3.60}$$

with boundary conditions:

$$f(t,0) = f(t,L) = 0 \; . \tag{3.61}$$

The acceleration of the string at the point is x is proportional to the curvature at the same point, and this explains why the string oscillates.

The heat equation. The temperature profile for the temperature $f(x,t)$ in a rod of length L, which temperature is kept to zero at both ends, satisfies the heat equation:

$$\frac{\partial}{\partial t} f(t,x) = \frac{\partial^2}{\partial x^2} f(t,x) \; , \tag{3.62}$$

with boundary condition:

$$f(t,0) = f(t,L) = 0 \; . \tag{3.63}$$

The rate at which the temperature changes at the position x is proportional to the curvature at that point. Therefore, the temperature converges to the constant value $f(x) = 0$.

The Schrödinger equation. The motion of one free quantum particle in one dimension is described by the Schrödinger equation:

$$\frac{\partial}{\partial t} \psi(t,x) = i \frac{\partial^2}{\partial x^2} \psi(t,x) \; , \tag{3.64}$$

with boundary condition:

$$\psi(t,0) = \psi(t,L) = 0 \; . \tag{3.65}$$

As for the heat equation, it depends on the first time derivative. However, due to the presence of the factor i, it gives rise to an oscillatory behavior of the solution. In fact, the function $\psi(t,x)$ is now complex values, which we can picture as a time-dependent vector field in $\mathbb{R}^2$. Even though the rate of change of the wave function is proportional to the curvature at the point x, because of the i factor it is described by an orthogonal vector to $\psi(x)$. Therefore, in general both the argument and the modulus of $\psi(t,x)$ change in time.

3.3 Tempered distribution

The goal of this section is to extend the notion of partial differential equation to functions that are not smooth, in fact not even differentiable in the standard sense. In particular, we shall be interested in formulating the Schrödinger equation for initial data which are only in $L^2(\mathbb{R}^d)$.

Definition 3.27. *The elements of the dual space $\mathcal{S}'(\mathbb{R}^d)$ of $\mathcal{S}(\mathbb{R}^d)$ are called tempered distribution.*

Remark 3.28. *The dual space V' of a topological vector space V is the space of continuous linear maps from V to $\mathbb{C}$. For $f \in V$ and $T \in V'$, one defines the pairing of f and T as:*

$$(f,T)_{V,V'} := T(f) \; . \tag{3.66}$$

Example 3.29. *Let us discuss some examples of tempered distributions.*

(a) *Let $g : \mathbb{R}^d \mapsto \mathbb{C}$ such that $(1 + |x|^2)^{-m} g(x) \in L^1(\mathbb{R}^d)$ for $m \in \mathbb{N}$. Then, the mapping*

$$T_g : \mathcal{S} \mapsto \mathbb{C} , \qquad f \mapsto \int_{\mathbb{R}^d} g(x) f(x)\, dx \tag{3.67}$$

is linear and continuous, hence $T_g \in \mathcal{S}'$.

Proof. Let $f_n \to f$ in $\mathcal{S}$. Then,

$$\begin{aligned} \lim_{n\to\infty} |T_g(f_n - f)| &\leqslant \lim_{n\to\infty} \int_{\mathbb{R}^d} |g(x)||f_n(x) - f(x)|\, dx \\ &\leqslant \|(1 + |x|^2)^{-m} g\|_1 \lim_{n\to\infty} \|(1 + |x|^2)^m |f_n - f|\|_\infty = 0 \, . \end{aligned} \tag{3.68}$$

■

(b) *The delta-distribution is defined as:*

$$\delta : \mathcal{S} \to \mathbb{C} , \qquad f \mapsto \delta(f) := f(0) \, . \tag{3.69}$$

Therefore, $\delta \in \mathcal{S}'$. One also writes:

$$\delta(f) = \int_{\mathbb{R}^d} \delta(x) f(x)\, dx \tag{3.70}$$

and:

$$\int_{\mathbb{R}^d} \delta(x - a) f(x)\, dx = f(a) \, . \tag{3.71}$$

The expression Eq. (A.37) is formal: there exists no function $\delta : \mathbb{R}^d \mapsto \mathbb{C}$ that gives (A.37). Nevertheless, one can approximate $\delta \in \mathcal{S}'$ by functions, more and more "peaked" at a, such that in the limit Eq. (A.37) holds true. For example, let $g \in L^1(\mathbb{R})$ with $\int dx\, g(x) = 1$. Let:

$$g_n(x) := n^d g(nx) \, . \tag{3.72}$$

Then, by dominated convergence, for any continuous bounded function f, and in particular for all $f \in \mathcal{S}$, one has:

$$\begin{aligned} \lim_{n\to\infty} T_{g_n}(f) &= \lim_{n\to\infty} \int_{\mathbb{R}} g_n(x) f(x)\, dx = \lim_{n\to\infty} \Big(\int_{\mathbb{R}} g_n(x) f(0)\, dx + \int_{\mathbb{R}} g_n(x)(f(x) - f(0))\, dx \Big) \\ &= f(0) + \lim_{n\to\infty} \int_{\mathbb{R}} g(y)(f(y/n) - f(0))\, dy = f(0) \equiv \delta(f) \, . \end{aligned} \tag{3.73}$$

In the last step we used that the argument of the integral converges to zero pointwise in x, as $n \to \infty$, and dominated convergence theorem to bring the limit inside the integral.

Next, we shall introduce the notions of weak and weak* convergence.

Definition 3.30. *Let V be a topological vector space and V' its dual.*

(i) *A sequence (m_n) in V converges weakly to $m \in V$ if:*

$$\lim_{n\to\infty} T(m_n) = T(m) , \qquad \text{for all } T \in V' . \tag{3.74}$$

One also writes $w - lim_{n\to\infty} m_n = m$ or $m_n \rightharpoonup m$.

(ii) *A sequence (T_n) in V' converges in the weak* topology to $T \in V'$ if:*

$$\lim_{n\to\infty} T_n(m) = T(m) , \qquad \text{for all } m \in V . \tag{3.75}$$

One also writes $w^* - \lim_{n\to\infty} T_n = T$ or $T_n \overset{*}{\rightharpoonup} T$.

Theorem 3.31 (The adjoint map.)**.** *Let $A : \mathcal{S} \to \mathcal{S}$ be a linear and continuous map. Then, the map*

$$A' : \mathcal{S}' \to \mathcal{S}' , \qquad (A'T)(f) := T(Af) \qquad \text{for all } f \in \mathcal{S} \tag{3.76}$$

is weak continuous. The map A' is called the adjoint of A.*

Proof. One has $A'T \in \mathcal{S}'$, where $A'T \equiv T \circ A$ is a continuous map on $\mathcal{S}$. To prove the weak* continuity of $A' : \mathcal{S}' \to \mathcal{S}'$, we proceed as follows. Let $T_n \xrightarrow{*} T$. Then, for each $f \in \mathcal{S}$:

$$\lim_{n\to\infty}(A'T_n)(f) = \lim_{n\to\infty} T_n(Af) = T(Af) = (A'T)(f) , \tag{3.77}$$

that is $A'T_n \xrightarrow{*} A'T$. ■

Remark 3.32. *Strictly speaking, the above proof only shows sequential continuity in $\mathcal{S}'$. This does not immediately imply continuity in $\mathcal{S}'$, since the topology of $\mathcal{S}'$ is not defined through a metric. Nevertheless, the above argument can be repeated for a net on $\mathcal{S}'$, and net continuity would imply continuity.*

Next, we define the Fourier transform on $\mathcal{S}'$

Definition 3.33. *For $T \in \mathcal{S}'$, the Fourier transform $\widehat{T} \in \mathcal{S}'$ is defined as:*

$$\widehat{T}(f) := T(\hat{f}) \qquad \textit{for all } f \in \mathcal{S}. \tag{3.78}$$

Remark 3.34. *In other words, $\mathcal{F}_{\mathcal{S}'} := \mathcal{F}'_{\mathcal{S}}$. That is, the Fourier transform on $\mathcal{S}'$ is defined as the adjoint of the Fourier transform on $\mathcal{S}$.*

Lemma 3.35. *The Fourier transform $\mathcal{F} : \mathcal{S}' \to \mathcal{S}'$ is a weak* continuous bijection. Moreover, for $f \in \mathcal{S}$, $\widehat{T}_f = T_{\hat{f}}$.*

Proof. Since $\mathcal{F} : \mathcal{S} \to \mathcal{S}$ is continuous, it follows from Theorem 3.31 that $\mathcal{F} : \mathcal{S}' \to \mathcal{S}'$ is weak* continuous. Also, since $(\mathcal{F}^{-1}\mathcal{F}T)(f) = T(\mathcal{F}\mathcal{F}^{-1}f) = T(f)$, the Fourier transform on $\mathcal{S}'$ is also bijective, with inverse $\mathcal{F}^{-1}$. Finally, let $f \in L^1$. Then:

$$\widehat{T}_f(g) \equiv T_f(\hat{g}) = \int f(x)\hat{g}(x)\,dx = \int \hat{f}(x)g(x)\,dx = T_{\hat{f}}(g) , \tag{3.79}$$

where the second equality follows from Proposition 3.15. ■

Example 3.36 (The Fourier transform of the δ-distribution.)**.** *Let $\delta(f)$ be the delta distribution, $\delta(f) = f(0)$. Then:*

$$\hat{\delta}(f) = \delta(\hat{f}) = \hat{f}(0) = \frac{1}{(2\pi)^{d/2}}\int f(x)\,dx \equiv \int \frac{1}{(2\pi)^{d/2}} f(x)\,dx = T_g(f) , \tag{3.80}$$

with $g = (2\pi)^{-d/2}$ the constant function. That is, the Fourier transform of the delta distribution is the constant function g.

Let us now introduce the notion of derivative on the space of distributions $\mathcal{S}'$.

Definition 3.37 (The distributional derivative.)**.** *For $T \in \mathcal{S}'$, we define its distributional derivative $\partial_x^\alpha T \in \mathcal{S}'$ as:*

$$(\partial_x^\alpha T)(f) := T((-1)^{|\alpha|}\partial_x^\alpha f) . \tag{3.81}$$

Lemma 3.38. *The distributional derivative $\partial_x^\alpha : \mathcal{S}' \to \mathcal{S}'$ is weak* continuous and extends the notion of derivative on $\mathcal{S}$; that is, for $g \in \mathcal{S}$ we have:*

$$\partial_x^\alpha T_g = T_{\partial_x^\alpha g} . \tag{3.82}$$

Proof. As an adjoint map, the derivative ∂_x^α is continuous thanks to Theorem 3.31. The property Eq. (3.82) follows from the integration by parts formula:

$$(\partial_x^\alpha T_g)(f) = T_g((-1)^{|\alpha|}\partial_x^\alpha f) = \int g(x)(-1)^{|\alpha|}\partial_x^\alpha f(x)\,dx = \int f(x)\partial_x^\alpha g(x)\,dx = T_{\partial_x^\alpha g}(f) . \tag{3.83}$$

■

Example 3.39 (The derivative of the delta distribution.)**.** *It follows that:*

$$(\partial_x^\alpha \delta)(f) = \delta((-1)^{|\alpha|}\partial_x^\alpha f) = (-1)^{|\alpha|}\partial_x^\alpha f(0) . \tag{3.84}$$

For the Heaviside function $\theta(x) = \mathbf{1}_{[0,\infty)}(x)$ on $\mathbb{R}$ one has: $\frac{d}{dx}\theta = \delta$.

Lemma 3.40. *Let $g \in C^\infty_{pol}$. Then, $(gT)(f) = T(gf)$ defines a weak* continuous map from $\mathcal{S}'$ to $\mathcal{S}'$. In general, one cannot define the product of two distributions, but one can define the product of a distribution and of a function in C^∞_{pol}.*

Proof. Exercise. ■

Lemma 3.41. *Let $g \in \mathcal{S}$ and $\tilde{g}(x) = g(-x)$. Then $(g * T)(f) := T(\tilde{g} * f)$ defines a weak* continuous map from $\mathcal{S}'$ to $\mathcal{S}'$, which extends the convolution on $\mathcal{S}$: $g * T_h = T_{g*h}$ for $h \in \mathcal{S}$.*

Proof. Exercise. ■

This result allows to prove the following theorem.

Theorem 3.42. *$\mathcal{S}$ is dense in $\mathcal{S}'$ in the weak* topology.*

Proof. Let us give a sketch of the proof. We want to show that for all $T \in \mathcal{S}'$ there exists $(\varphi_n) \subset \mathcal{S}$ such that:

$$T_{\varphi_n} \xrightharpoonup{*} T \; . \tag{3.85}$$

We proceed as follows. Let $(g_n) \subset \mathcal{S}$ such that $(g_n * f) \to f$ in $\mathcal{S}$ (e.g., $g_n(x) = n^d g(nx)$, with $g \in \mathcal{S}$ and $\int g = 1$.) Then, we write:

$$\begin{aligned}
(g_n * T)(f) &= T(\tilde{g}_n * f) \\
&= T\Big(\int dy\, \tilde{g}_n(\cdot - y) f(y)\Big) \\
&= \int dy\, T(\tilde{g}_{n,y}) f(y) \; ,
\end{aligned} \tag{3.86}$$

with $\tilde{g}_{n,y}(\cdot) = \tilde{g}_n(\cdot - y)$. Thus, we would be tempted to say that $(g_n * T) = T_{\xi_n}$, with $\xi_n(y) = T(\tilde{g}_{n,y})$. To prove this, we simply notice that $\xi_n \in C^\infty_{\mathrm{pol}}(\mathbb{R}^d)$ (*exercise*), which implies that $\xi_n f \in \mathcal{S}$, and hence that it is an integrable function. Thus, by the weak* continuity of the convolution, Lemma 3.41, we just proved that for each $T \in \mathcal{S}'$ there exists $\xi_n \in C^\infty_{\mathrm{pol}}$ such that:

$$T_{\xi_n} \xrightharpoonup{*} T \; . \tag{3.87}$$

To conclude, we would like to show that the sequence (ξ_n) can be replaced by a sequence (φ_n) in $\mathcal{S}$. We proceed as follows. Let $G(x)$ as in Eq. (3.26). Let: $\varphi_n(x) = \xi_n(x) G(x/n)$. Then, being $G(x/n)$ compactly supported, $\varphi_n \in \mathcal{S}$. Notice that $T_{\varphi_n}(f) = T_{\xi_n}(G(\cdot/n) f)$. Fix $\varepsilon > 0$. By what we just proved, for n large enough:

$$\Big| T_{\xi_n}(G(\cdot/n) f) - T(G(\cdot/n) f) \Big| \leqslant \varepsilon/3 \; . \tag{3.88}$$

(Notice that the argument of the distributions is n-dependent. Nevertheless, this is not a problem, since the $\| \cdot \|_{\alpha,\beta}$ norms of $G(\cdot/n) f$ are all bounded uniformly in n.) Also, by the continuity of T:

$$\Big| T(G(\cdot/n) f) - T(f) \Big| \leqslant \varepsilon/3 \; , \tag{3.89}$$

where we used that $G(\cdot/n) f - f \to 0$ in $\mathcal{S}$, as $n \to \infty$. Finally, again by Eq. (3.87):

$$\Big| T(f) - T_{\xi_n}(f) \Big| \leqslant \varepsilon/3 \; . \tag{3.90}$$

All together, for any $f \in \mathcal{S}$ and for any $\varepsilon > 0$ there exists $n_0 \in \mathbb{N}$ such that for $n \geqslant n_0$:

$$\Big| T_{\xi_n}(f) - T_{\varphi_n}(f) \Big| \leqslant \varepsilon \; . \tag{3.91}$$

This, together with Eq. (3.87), implies that:

$$T_{\varphi_n} \xrightharpoonup{*} T \; . \tag{3.92}$$

■

Next, we discuss the solution of the free Schrödinger equation in the sense of distributions. We say that $\psi(t) \in C^\infty(\mathbb{R}_t, \mathcal{S}'(\mathbb{R}^d))$ is a distributional solution of the Schrödinger equation if:

$$i\frac{d}{dt}(f,\psi(t))_{\mathcal{S},\mathcal{S}'} = (f, -\frac{1}{2}\Delta\psi(t))_{\mathcal{S},\mathcal{S}'} \;, \tag{3.93}$$

for all functions $f \in \mathcal{S}(\mathbb{R}^d)$.

Proposition 3.43. *Let $\psi_0 \in \mathcal{S}'$. Then, there exists a unique, global solution $\psi(t) \in C^\infty(\mathbb{R}_t, \mathcal{S}'(\mathbb{R}^d))$ of the Schrödinger equation, given by*

$$\psi(t) = \mathcal{F}^{-1}e^{-i\frac{|k|^2}{2}t}\mathcal{F}\psi_0 \;. \tag{3.94}$$

Proof. By Lemma 3.35 and by the fact that $\mathcal{F}$ and $\mathcal{F}^{-1}$ are maps from $\mathcal{S}'$ to $\mathcal{S}'$, we know that $\psi(t) \in \mathcal{S}'(\mathbb{R}^d)$. To conclude, we show that $\psi(t)$ is a solution of the Schrödinger equation in the sense of distributions. Let $f \in \mathcal{S}$ be a test function. Then:

$$\begin{aligned}
i\frac{d}{dt}(f,\psi(t))_{\mathcal{S},\mathcal{S}'} &= i\frac{d}{dt}(\mathcal{F}e^{-i\frac{|k|^2}{2}t}\mathcal{F}^{-1}f,\psi_0)_{\mathcal{S},\mathcal{S}'} \\
&= (\mathcal{F}e^{-i\frac{|k|^2}{2}t}\frac{|k|^2}{2}\mathcal{F}^{-1}f,\psi_0)_{\mathcal{S},\mathcal{S}'} \\
&= (-\mathcal{F}e^{-i\frac{|k|^2}{2}t}\mathcal{F}^{-1}\frac{1}{2}\Delta f,\psi_0)_{\mathcal{S},\mathcal{S}'} \\
&= (-\frac{1}{2}\Delta f, \mathcal{F}^{-1}e^{-i\frac{|k|^2}{2}t}\mathcal{F}\psi_0)_{\mathcal{S},\mathcal{S}'} \\
&= (f, -\frac{1}{2}\Delta\psi(t))_{\mathcal{S},\mathcal{S}'} \;.
\end{aligned} \tag{3.95}$$

The regularity in time of the mapping $\psi(t) : \mathcal{S} \to \mathbb{C}$ can be easily checked. ∎

3.4 Long time asymptotics of the momentum operator

We have proven that, for $\psi_0 \in \mathcal{S}$, the solution of the free Schrödinger equation is given by:

$$\psi(t,x) = \frac{1}{(2\pi i t)^{d/2}}\int dy\, e^{i\frac{|x-y|^2}{2t}}\psi_0(y) \;. \tag{3.96}$$

The probability for finding the quantum particle in the region $A \subset \mathbb{R}^d$ is given by:

$$P(X(t) \in A) = \int_A |\psi(t,x)|^2\, dx \;. \tag{3.97}$$

Next, we want to determine the "velocity distribution" of the quantum particle. Since the velocity at a fixed time is not defined in standard quantum mechanics, we shall consider the asymptotic speed for large times, which we define as:

$$\lim_{t\to\infty} P\Big(\frac{X(t)}{t} \in A\Big) := \lim_{t\to\infty} P(X(t) \in tA) = \lim_{t\to\infty}\int_{tA} |\psi(t,x)|^2\, dx \;. \tag{3.98}$$

Notice that choice of the origin of the reference frame does not play any role. To get an expression for the above limit, we shall use the next lemma.

Lemma 3.44. *Let $\psi(t)$ be the solution of the free Schrödinger equation, with $\psi(0) = \psi_0 \in \mathcal{S}$. Then:*

$$\psi(t,x) = \frac{e^{i\frac{x^2}{2t}}}{(it)^{d/2}}\hat{\psi}_0(x/t) + r(t,x) \;, \tag{3.99}$$

with $\lim_{t\to\infty}\|r(t)\|_{L^2} = 0$.

Proof. We have, by Eq. (3.96):

$$\begin{aligned}\psi(t,x) &= \frac{e^{i\frac{x^2}{2t}}}{(it)^{d/2}}\frac{1}{(2\pi)^{d/2}}\int e^{-i\frac{x}{t}y}\Big(e^{i\frac{y^2}{2t}}+1-1\Big)\psi_0(y)\,dy \\ &= \frac{e^{i\frac{x^2}{2t}}}{(it)^{d/2}}\Big(\hat\psi_0(x/t)+\frac{1}{(2\pi)^{d/2}}\int e^{-i\frac{x}{t}y}\Big(e^{i\frac{y^2}{2t}}-1\Big)\psi_0(y)\,dy\Big) \\ &= \frac{e^{i\frac{x^2}{2t}}}{(it)^{d/2}}\Big(\hat\psi_0(x/t)+\hat h(t,x/t)\Big)\;, \qquad (3.100)\end{aligned}$$

and hence:

$$r(t,x)=\frac{e^{i\frac{x^2}{2t}}}{(it)^{d/2}}\hat h(t,x/t)\;. \qquad (3.101)$$

To prove the claim on the L^2 norm, we proceed as follows:

$$\|r(t,\cdot)\|^2_{L^2}=\int|r(t,x)|^2\,dx=\frac{1}{t^d}\int|\hat h(t,x/t)|^2\,dx=\int|\hat h(t,y)|^2dy=\int|h(t,y)|^2dy\;. \qquad (3.102)$$

Now, notice that $h(t,x)\to 0$ pointwise as $t\to\infty$. Also, $|h(t,x)|^2\leqslant 4|\psi_0(x)|^2$. Therefore, by dominated convergence theorem:

$$\lim_{t\to\infty}\int|h(t,x)|^2dx=0\;. \qquad (3.103)$$

This concludes the proof. ∎

Theorem 3.45. *Let $\psi(t,x)$ be a solution of the free Schrödinger equation and let $A\subset\mathbb{R}^d$ measurable. Then:*

$$\lim_{t\to\infty}P\Big(\frac{X(t)}{t}\in A\Big)=:\lim_{t\to\infty}\mathbb{P}^{\psi_t}(t\Lambda)=\int_A|\hat\psi_0(p)|^2dp\;. \qquad (3.104)$$

Proof. By Lemma 3.44, we have:

$$\int_{tA}|\psi(t,x)|^2dx=\frac{1}{t^d}\int_{tA}|\hat\psi_0(x/t)|^2dx+R(t)=\int_A|\hat\psi_0(p)|^2dp+R(t)\;, \qquad (3.105)$$

where, following the proof of the Lemma:

$$\begin{aligned}\lim_{t\to\infty}R(t) &= \lim_{t\to\infty}\int_{tA}|r(t,x)|^2\,dx+\lim_{t\to\infty}2\mathrm{Re}\Big(\frac{1}{t^d}\int_{tA}\overline{\hat\psi_0(x/t)}\hat h(t,x/t)dx\Big) \\ &= \lim_{t\to\infty}2\mathrm{Re}\Big(\int_A\overline{\hat\psi_0(p)}\hat h(t,p)\Big)\;. \qquad (3.106)\end{aligned}$$

By the Cauchy-Schwarz inequality we have:

$$\lim_{t\to\infty}\Big|\int_{tA}\overline{\hat\psi_0(p)}\hat h(t,p)dp\Big|\leqslant\lim_{t\to\infty}\|\hat\psi_0\|_{L^2}\|\hat h(t)\|_{L^2}=0\;. \qquad (3.107)$$

∎

Remark 3.46.
- *If we would not have set the mass m to 1, the probability in the left-hand side of Eq. (3.104) should have been replaced by $P(mX(t)/t\in\Lambda)$. Therefore, the above result allows to control the asymptotic distribution of the momentum of the quantum particle.*
- *The operator $P:=-i\nabla_x$ is called the momentum operator. The expectation value of the momentum operator is given by:*

$$\mathbb{E}^{\psi_t}(P):=\langle\psi_t,P\psi_t\rangle:=\int_{\mathbb{R}^d}\overline{\psi(t,x)}(P\psi)(t,x)dx=\int_{\mathbb{R}^d}\overline{\hat\psi(t,p)}p\hat\psi(t,p)dp=\int_{\mathbb{R}^d}p|\hat\psi(0,p)|^2dp\;, \qquad (3.108)$$

where we used that $|\hat\psi(t,p)|=|\hat\psi(0,p)|$. Thus, the quantum mechanical expectation value of the momentum operator is equal to its expectation value with respect to the asymptotic momentum distribution.

3.5 Properties of Hilbert spaces

Recall the definition of Hilbert space, given in Section 2.3. In this section we shall spell out some important properties of Hilbert spaces, that will play a role in the following discussion.

Definition 3.47. *Let $\mathcal{H}$ be a Hilbert space. A sequence (φ_n) in $\mathcal{H}$ is called an orthonormal sequence if $\langle \varphi_n, \varphi_m \rangle = \delta_{n,m}$.*

The next proposition is an immediate consequence of notion of orthogonality.

Proposition 3.48. *Let $(\varphi_j)_{j\in\mathbb{N}}$ be a orthonormal sequences in $\mathcal{H}$. For any $\psi \in \mathcal{H}$, let us rewrite:*

$$\begin{aligned} \psi &= \sum_{j=1}^{n} \langle \varphi_j, \psi \rangle \varphi_j + \Big(\psi - \sum_{j=1}^{n} \langle \varphi_j, \psi \rangle \varphi_j \Big) \\ &=: \psi_n + \psi_n^{\perp} \ . \end{aligned} \tag{3.109}$$

Then, $\langle \psi_n, \psi^{\perp} \rangle = 0$ and:

$$\langle \psi, \psi \rangle = \langle \psi_n, \psi_n \rangle + \langle \psi_n^{\perp}, \psi_n^{\perp} \rangle \ . \tag{3.110}$$

Proof. Exercise. ∎

Proposition 3.48 implies the validity of two important inequalities, the Cauchy-Schwarz inequality and the Bessel inequality.

Corollary 3.49. *(a) Let $(\varphi_j)_{j\in\mathbb{N}}$ be an orthonormal sequences in $\mathcal{H}$. Let $\psi \in \mathcal{H}$ and $n \in \mathbb{N}$. Then:*

$$\|\psi\|^2 \geqslant \sum_{j=1}^{n} |\langle \varphi_j, \psi \rangle|^2 \qquad \textit{(Bessel inequality)}. \tag{3.111}$$

(b) Let $\varphi, \psi \in \mathcal{H}$. Then:

$$|\langle \varphi, \psi \rangle| \leqslant \|\varphi\| \|\psi\| \ , \qquad \textit{(Cauchy-Schwarz inequality)}. \tag{3.112}$$

Proof. Eq. (3.111) immediately follows from Proposition 3.48. Eq. (3.112) follows from Eq. (3.111), after choosing $\varphi_1 = \varphi/\|\varphi\|$ and $n = 1$. ∎

Proposition 3.50 (Polarization identity.)**.** *Let $\mathcal{H}$ be a Hilbert space. Let $\psi, \varphi \in \mathcal{H}$. Then:*

$$\langle \varphi, \psi \rangle = \frac{1}{4} (\|\varphi + \psi\|^2 - \|\varphi - \psi\|^2 - i\|\varphi + i\psi\|^2 + i\|\varphi - i\psi\|^2) \ . \tag{3.113}$$

Proof. Eq. (3.113) follows from the following identity, valid for any sesquilinear form[1] $B : X \times X \to \mathbb{C}$, with X a complex vector space:

$$B(x, y) = \frac{1}{4} (B(x+y, x+y) - B(x-y, x-y) - iB(x+iy, x+iy) + iB(x-iy, x-iy)) \ . \tag{3.114}$$

∎

Definition 3.51. *An orthonormal sequence $(\varphi_j)_{j\in\mathbb{N}}$ in $\mathcal{H}$ is called an orthonormal basis if for all $\psi \in \mathcal{H}$:*

$$\psi = \sum_{j=1}^{\infty} \langle \varphi_j, \psi \rangle \varphi_j \ . \tag{3.115}$$

Remark 3.52. *Notice that the series converges in $\mathcal{H}$. In fact, by Bessel's inequality,*

$$\sum_{j=1}^{n} |\langle \varphi_j, \psi \rangle|^2 \leqslant \|\psi\|^2 \ .$$

[1] A map $B : X \times X \to \mathbb{C}$ is called a sesquilinear form if it is linear in the second variable and antilinear in the first variable.

Thus, $\lim_{n\to\infty}\sum_{j=1}^{n}|\langle\varphi_j,\psi\rangle|^2$ *exists. Consider the sequence of partial sums* $\Big(\sum_{j=1}^{n}\langle\varphi_j,\psi\rangle\varphi_j\Big)$. *Let* $n'>n$. *We have:*

$$\Big\|\sum_{j=1}^{n}\langle\varphi_j,\psi\rangle\varphi_j-\sum_{j=1}^{n'}\langle\varphi_j,\psi\rangle\varphi_j\Big\|^2=\sum_{j=n}^{n'}|\langle\varphi_j,\psi\rangle|^2\ , \tag{3.116}$$

which vanishes as $n\to\infty$. *Hence,* $\Big(\sum_{j=1}^{n}\langle\varphi_j,\psi\rangle\varphi_j\Big)$ *is a Cauchy sequence in* $\mathcal{H}$. *Being* $\mathcal{H}$ *complete,* $\sum_{j=1}^{\infty}\langle\varphi_j,\psi\rangle\varphi_j\in\mathcal{H}$.

Definition 3.53. *A topological vector space is called separable if it contains a countable, dense subset.*

Proposition 3.54. *A Hilbert space is separable if and only if it contains an orthonormal basis.*

Proof. Let (φ_j) be a ONB. Then, the following set is a dense and countable subset of $\mathcal{H}$:

$$\mathrm{span}_{\mathbb{Q}+i\mathbb{Q}}\{\varphi_j\mid j\in\mathbb{N}\}:=\Big\{\sum_{j=1}^{N}(a_j+ib_j)\varphi_j\mid N\in\mathbb{N}\ ,\quad a_j,b_j\in\mathbb{Q}\Big\}\ . \tag{3.117}$$

Let us now prove the converse statement. Suppose that $(\varphi_j)_{j\in\mathbb{N}}$ is a dense and countable subset of $\mathcal{H}$. Let $(\varphi_j)_{j\in J}\subseteq(\varphi_j)_{j\in\mathbb{N}}$ be a subset of linearly independent vectors in $(\varphi_j)_{j\in\mathbb{N}}$, dense in $\mathcal{H}$. This subset can be used to define a ONB, via the Gram-Schmidt method. ∎

Proposition 3.55. *Let* (φ_j) *be an orthonormal basis for* $\mathcal{H}$. *Then, the following inequality holds true:*

$$\|\psi\|^2=\sum_{j=1}^{\infty}|\langle\varphi_j,\psi\rangle|^2\qquad\textit{(Parseval equality.)} \tag{3.118}$$

Proof. Eq. (3.118) immediately follows from the definition and the continuity of the scalar product:

$$\begin{aligned}\|\psi\|^2&=\Big\langle\lim_{N\to\infty}\sum_{j=1}^{N}\langle\varphi_j,\psi\rangle\varphi_j,\lim_{M\to\infty}\sum_{i=1}^{M}\langle\varphi_i,\psi\rangle\varphi_i\Big\rangle\\&=\lim_{N\to\infty}\lim_{M\to\infty}\Big\langle\sum_{j=1}^{N}\langle\varphi_j,\psi\rangle\varphi_j,\sum_{i=1}^{M}\langle\varphi_i,\psi\rangle\varphi_i\Big\rangle=\lim_{N\to\infty}\sum_{j=1}^{N}|\langle\varphi_j,\psi\rangle|^2\ .\end{aligned} \tag{3.119}$$

∎

Remark 3.56 (ℓ^2 as a coordinate space for a separable Hilbert space.)**.** *Let* $(\varphi_j)\subset\mathcal{H}$ *be a ONB. Then, the Parseval equality implies that the following mapping is an isometry:*

$$U:\mathcal{H}\to\ell^2\ ,\qquad\varphi\mapsto(\langle\varphi_j,\psi\rangle)_{j\in\mathbb{N}}\ . \tag{3.120}$$

In particular, for each sequence $c\in\ell^2$ *we can associate a series* $\sum_{j=1}^{\infty}c_j\varphi_j$, *which converges in norm:*

$$\Big\|\sum_{j=N}^{\infty}c_j\varphi_j\Big\|^2=\sum_{j=N}^{\infty}|c_j|^2\to0\qquad\textit{as } N\to\infty; \tag{3.121}$$

this means that U *is also surjective, i.e. it is an isometric isomorphism. Therefore, each separable Hilbert space is isometrically isomorphic to* ℓ^2 *and each ONB generates an isometric isomorphism. Thus, we can identify* ℓ^2 *as the coordinate space for separable Hilbert spaces of infinite dimension.*

Example 3.57. *Consider* $L^2([0,2\pi])$. *It is a separable Hilbert space, and a ONB is provided by* $\varphi_k(x)=\frac{1}{\sqrt{2\pi}}e^{ikx}$, $k\in\mathbb{N}$. *Let* $\psi\in L^2([0,2\pi])$, *and consider its Fourier series:*

$$\psi=\sum_{k=-\infty}^{\infty}\langle\varphi_k,\psi\rangle\varphi_k\ . \tag{3.122}$$

The Fourier series provides an isometric isomorphism between ℓ^2 *and* L^2.

Proposition 3.58 (Characterization of an orthonormal basis.). *An orthonormal sequence $(\varphi_j)_{j\in I}$ in $\mathcal{H}$ is an orthonormal basis of $\mathcal{H}$ if and only if:*

$$\langle \varphi_j, \psi\rangle = 0 \quad \text{for all } j \in I \quad \Rightarrow \psi = 0\ . \tag{3.123}$$

Proof. Let $(\varphi_j)_{j\in I}$ be a ONB of $\mathcal{H}$. Suppose that $\langle \varphi_j, \psi\rangle = 0$ for all $j \in I$. Then, by definition of ONB, Eq. (3.115), $\psi = 0$. Let us now prove the converse implication. Let (φ_j) be an orthonormal sequence in $\mathcal{H}$, and let $\phi \in \mathcal{H}$. By Bessel's inequality, we have, for all $n \in \mathbb{N}$:

$$\sum_{j=1}^{n} |\langle \varphi_j, \phi\rangle|^2 \leqslant \|\phi\|^2\ . \tag{3.124}$$

Being the sequence $n \mapsto \sum_{j=1}^{n} |\langle \varphi_j, \phi\rangle|^2$ nondecreasing and bounded, the $n \to \infty$ limit exists: $\lim_{n\to\infty} \sum_{j=1}^{n} |\langle \varphi_j, \phi\rangle|^2 = \sum_{j\in I} |\langle \varphi_j, \phi\rangle|^2$. In particular, this implies that the series $\sum_{j\in I}\langle \varphi_j, \phi\rangle\varphi_j$ is convergent in $\mathcal{H}$. Consider the vector:

$$\psi = \phi - \sum_{j\in I}\langle \phi, \varphi_j\rangle\varphi_j\ . \tag{3.125}$$

By construction, $\langle \psi, \varphi_j\rangle = 0$ for all $j \in I$. By assumption, this implies that $\psi = 0$, hence:

$$\phi = \sum_{j\in I}\langle \phi, \varphi_j\rangle\varphi_j\ , \qquad \text{for all } \phi \in \mathcal{H}. \tag{3.126}$$

Therefore, $\{\varphi_j\}_{j\in I}$ is an ONB of $\mathcal{H}$. This concludes the proof. ∎

Definition 3.59. *Let $M \subset \mathcal{H}$. We define its orthogonal complement as:*

$$M^{\perp} := \Big\{\psi \in \mathcal{H} \mid \langle \varphi, \psi\rangle = 0 \quad \text{for all } \varphi \in M\Big\}\ . \tag{3.127}$$

Remark 3.60. *It follows that $M \cap M^{\perp} = \{0\}$. Also, being $\langle \varphi, \cdot\rangle$ linear and continuous, $M^{\perp}$ is a closed subspace of M.*

Theorem 3.61. *Let $M \subset \mathcal{H}$ be a closed subspace of $\mathcal{H}$. Then:*

$$\mathcal{H} = M \oplus M^{\perp}\ . \tag{3.128}$$

That is, every element $\psi \in \mathcal{H}$ can be rewritten in a unique way as $\psi = \varphi + \varphi^{\perp}$ with $\varphi \in M$ and $\varphi^{\perp} \in M^{\perp}$.

Proof. Let $\psi \in \mathcal{H}$. If $\psi \in M$, or $\psi \in M^{\perp}$, there is nothing to prove. Suppose that $\psi \notin M$, $\psi \notin M^{\perp}$. Let (v_k) be a minimizing sequence:

$$\lim_{k\to\infty} \|\psi - v_k\|^2 = \inf_{v\in M} \|\psi - v\|^2\ . \tag{3.129}$$

By using that $\|\cdot\|^2 = \langle \cdot, \cdot\rangle$, we have:

$$\|\psi - v\|^2 = F(v) + \|\psi\|^2\ , \quad F(v) := \|v\|^2 - 2\mathrm{Re}\,\langle \psi, v\rangle\ . \tag{3.130}$$

Therefore, $\lim_{k\to\infty} F(v_k) = \inf_{v\in M} F(v) =: \alpha$. Our preliminary goal is to show that $v_k \to v$ in M. To prove this, we write:

$$\begin{aligned} F(v_k) + F(v_l) &= \|v_k\|^2 - 2\mathrm{Re}\,\langle \psi, v_k\rangle + \|v_l\|^2 - 2\mathrm{Re}\,\langle \psi, v_l\rangle \\ &= \frac{1}{2}\Big(\|v_k + v_l\|^2 + \|v_k - v_l\|^2\Big) - 2\mathrm{Re}\,\langle \psi, v_k + v_l\rangle \\ &= 2\Big\|\frac{v_k + v_l}{2}\Big\|^2 - 4\mathrm{Re}\,\Big\langle \psi, \frac{v_k + v_l}{2}\Big\rangle + \frac{1}{2}\|v_k - v_l\|^2 \\ &= 2F\Big(\frac{v_k + v_l}{2}\Big) + \frac{1}{2}\|v_k - v_l\|^2 \geqslant 2\alpha + \frac{1}{2}\|v_k - v_l\|^2\ . \end{aligned} \tag{3.131}$$

Since $F(v_k), F(v_l) \to \alpha$ as $k, l \to \infty$, we get that $\|v_k - v_l\| \to 0$. Being (v_k) a Cauchy sequence, and since $\mathcal{H}$ is complete, $v_k \to v$ in $\mathcal{H}$. Also, since M is closed, $v \in M$. By continuity of the scalar product, $\alpha = F(v)$. Our next goal is to show that $\psi - v \in M^{\perp}$. If so, this provides one decomposition $\psi = v + v^{\perp}$, with $v \in M$ and $v^{\perp} \in M^{\perp}$.

Let $\tilde{v} \in M$ and let $f(t) := F(v + t\tilde{v})$. Then, by definition of v:

$$f(t) \geqslant F(v) \equiv f(0) , \qquad \text{for all } t \in \mathbb{R}. \tag{3.132}$$

Thus, $t = 0$ is a minimum of $f(t)$. In particular, $f'(0) = 0$. Let us compute the derivative. A simple computation shows that:

$$0 = f'(0) = 2\mathrm{Re}\langle \psi - v, \tilde{v} \rangle . \tag{3.133}$$

Replacing $\tilde{v}$ with $i\tilde{v}$, we get the same identity but with Re replaced by Ran. Hence:

$$0 = \langle \psi - v, \tilde{v} \rangle = 0 , \qquad \text{for all } \tilde{v} \in M. \tag{3.134}$$

In conclusion, $\psi - v \in M^{\perp}$, as claimed; thus, $\psi = v + \perp v$. Let us now prove uniqueness of the splitting. Suppose there exists $v_1, v_2 \in M$ and $v_1^{\perp}$, $v_2^{\perp}$ such that:

$$\psi = v_1 + v_1^{\perp} = v_2 + v_2^{\perp} . \tag{3.135}$$

Then, $v_1 - v_2 = v_2^{\perp} - v_1^{\perp}$, which means that $v_1 - v_2 = 0$ and $v_1^{\perp} - v_2^{\perp} = 0$, since $M \cap M^{\perp} = \{0\}$. ∎

3.6 The Fourier transform in L^2

Definition 3.62. *Let X and Y be two normed spaces. An operator $L : X \to Y$ between X and Y is called bounded if there exists $C < \infty$ such that:*

$$\|Lx\|_Y \leqslant C\|x\|_X , \qquad \textit{for all } x \in X. \tag{3.136}$$

Proposition 3.63. *Let X and Y be two normed spaces. Let $\mathcal{L}(X,Y)$ be the set of the bounded linear operators from X to Y. Let:*

$$\|L\|_{\mathcal{L}(X,Y)} := sup_{\|x\|_X = 1} \|Lx\|_Y . \tag{3.137}$$

Then, $\|\cdot\|_{\mathcal{L}(X,Y)}$ defines a norm on $\mathcal{L}(X,Y)$. Moreover, if Y is complete then $\mathcal{L}(X,Y)$ is complete as well, that is it is a Banach space.

Proof. It is easy to check that $\|\cdot\|_{\mathcal{L}(X,Y)}$ defines a norm on $\mathcal{L}(X,Y)$. Let now prove that if Y is complete then $\mathcal{L}(X,Y)$ is complete as well. Let (L_n) be a Cauchy sequence in $\mathcal{L}(X,Y)$:

$$\|L_n - L_m\|_{\mathcal{L}(X,Y)} \to 0 \qquad \text{as } n, m \to \infty. \tag{3.138}$$

Then, $(L_n x)$ is Cauchy sequence in Y, since

$$\|L_n x - L_m x\|_Y \leqslant \|L_n - L_m\|_{\mathcal{L}(X,Y)} \|x\|_Y . \tag{3.139}$$

Being Y complete, $L_n x \to y \in Y$, as $n \to \infty$. We define $Lx := y$. It is easy to show that L is a linear operator. Let us prove that L is a bounded operator. By the Cauchy property, we have, for all $\varepsilon > 0$, for n, m large enough:

$$\sup_{\|x\|_X = 1} \|L_n x - L_m x\|_Y \leqslant \varepsilon . \tag{3.140}$$

Therefore, dropping the sup and taking the $m \to \infty$ limit:

$$\|L_n x - Lx\|_Y \leqslant \varepsilon \Rightarrow \|Lx\|_Y \leqslant C , \tag{3.141}$$

uniformly in x, for all x such that $\|x\|_X = 1$. This proves that $L \in \mathcal{L}(X,Y)$. Due to the arbitrariness of ε, Eq. (3.141) also proves that $L_n \to L$ in $\mathcal{L}(X,Y)$. This concludes the proof. ∎

Theorem 3.64. *Let X and Y be two normed spaces. Let $L : X \to Y$ be a linear operator. Them, the following statements are equivalent:*

(i) L is continuous at 0.

(ii) L is continuous.

(iii) L is bounded.

Proof. $(iii) \Rightarrow (i)$. In fact, let $\|x_n\| \to 0$. Then, $\|Lx_n\| \leqslant \|L\|\|x_n\| \to 0$.

Let us now show that $(i) \Rightarrow (ii)$. Let $\|x_n - x\| \to 0$ and let L be continuous at 0. Then, $\|Lx_n - Lx\| = \|L(x_n - x)\| \to 0$.

Finally, let us prove that $(ii) \Rightarrow (iii)$. Suppose that L is continuous but not bounded: that is, there exists a sequence (x_n) with $\|x_n\| = 1$ such that $\|Lx_n\| \geqslant n$. Then, let $z_n := \frac{x_n}{\|Lx_n\|}$. It follows that $\|z_n\| \leqslant \frac{1}{n}$, but $\|Lz_n\| = 1$, which contradicts continuity. ■

Example 3.65 (Unbounded linear operators.)**.** *Let $\ell_0 = \{(x_n) \in \ell^1 \mid \exists N \in \mathbb{N} : x_n = 0\ \forall n \geqslant N\}$ be the space of finite sequences, equipped with the norm $\|x\|_{\ell^1} := \sum_{n=1}^{\infty} |x_n|$. Then, the operator $T : \ell_0 \to \ell_0$ such that $x \mapsto Tx = (x_1, 2x_2, 3x_3, \ldots)$ is unbounded, since $\|Te_n\| = n$ but $\|e_n\| = 1$.*

Theorem 3.66 (Extension of densely defined linear bounded operators.)**.** *Let $Z \subset X$ be a dense subspace of a normed space X and let Y be a Banach space. Let $L : Z \to Y$ be linear and bounded. Then, L admits a unique linear and bounded extension $\tilde{L} \in \mathcal{L}(X, Y)$ with $\tilde{L} \restriction_Z = L$ and*

$$\|\tilde{L}\|_{\mathcal{L}(X,Y)} = \|L\|_{\mathcal{L}(Z,Y)} \,. \tag{3.142}$$

Proof. Let $x \in X$. Then, there exists a sequence $(z_n) \subset Z$ such that $\|z_n - x\|_X \to 0$. Being (z_n) convergent, the sequence (z_n) is also a Cauchy sequence. Thus, $\|Lz_n - Lz_m\|_Y = \|L(z_n - z_m)\|_Y \leqslant \|L\|\|z_n - z_m\|_X$, which means that (Lz_n) is also a Cauchy sequence in Y. Since Y is complete, $Lz_n \to y \in Y$. Let us now prove that the limit y does not depend on the choice of the sequence (z_n) (provided it converges to x). Let (z'_n) be another sequence in Z, such that $\|z'_n - x\|_X \to 0$. Consider the new sequence $z_1, z'_1, z_2, z'_2, \ldots$. By assumption, also this new sequence converges to x, and by following the previous argument, $Lz_1, Lz'_1, Lz_2, Lz'_2 \ldots$ converges to $\tilde{y} \in Y$. But since every subsequence of a convergent sequence converges to the same limit, we have $y = \lim Lz_n = \lim Lz'_n = \tilde{y}$. Therefore, we can define $\tilde{L}x := y$. The linearity of L follows immediately from the previous construction. The boundedness follows from:

$$\|\tilde{L}x\|_Y = \lim_{n\to\infty} \|Lz_n\|_Y \leqslant \lim_{n\to\infty} \|L\|\|z_n\|_X = \|L\|\|x\|_X \,. \tag{3.143}$$

Therefore, $\tilde{L}$ is bounded, and also continuous, by Theorem 3.64. Finally, the extension $\tilde{L}$ of L is unique: this follows from the fact that two continuous maps which coincide on a dense subset are equal. ■

Next, we shall extend the Fourier transform on L^2.

Theorem 3.67 (The Fourier transform on L^2.)**.** *The Fourier transform $\mathcal{F} : (\mathcal{S}(\mathbb{R}^d), \|\cdot\|_{L^2}) \to L^2(\mathbb{R}^d)$ can be uniquely extended to a bounded linear operator on $L^2(\mathbb{R}^d)$. Moreover, for all $f \in L^2$:*

$$\|\mathcal{F}f\|_{L^2} = \|f\|_{L^2} \tag{3.144}$$

and $\mathcal{F}\mathcal{F}^{-1} = \mathcal{F}^{-1}\mathcal{F} = \mathbb{1}_{L^2}$.

Remark 3.68. *Eq. (3.144) takes the name of Plancherel's theorem.*

Proof. By Theorem 2.13, the space $\mathcal{S}$ is dense in L^2. The extension of $\mathcal{F}$ to a bounded linear operator on L^2 follows from Theorem 3.66. Moreover, as proven in Theorem 3.13,

$$\mathcal{F}^{-1}\mathcal{F} \restriction_{\mathcal{S}} = \mathcal{F}\mathcal{F}^{-1} \restriction_{\mathcal{S}} = \mathbb{1}_{\mathcal{S}} \,. \tag{3.145}$$

Being $\mathcal{F}, \mathcal{F}^{-1}, \mathbb{1}$ continuous, and being $\mathcal{S}$ dense in L^2, Eq. (3.145) holds as an identity on L^2. ■

Definition 3.69 (Unitary operator.). *A bounded linear operator $U \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$ is called unitary if it is surjective and isometric, that is $\|U\psi\|_{\mathcal{H}_2} = \|\psi\|_{\mathcal{H}_1}$ for all $\psi \in \mathcal{H}_1$.*

Remark 3.70. *By the polarisation identity, it immediately follows that U "preserves angles", that is:*

$$\langle U\psi, U\varphi\rangle_{\mathcal{H}_2} = \langle \psi, \varphi\rangle_{\mathcal{H}_1} \qquad \text{for all } \varphi, \psi \in \mathcal{H}_1. \tag{3.146}$$

Remark 3.71. *The Fourier transform $\mathcal{F} : L^2 \to L^2$ is unitary.*

As an application of the Fourier transform in L^2, consider the propagator of the free Schrödinger equation, defined in Eq. (3.50). By extending the Fourier transform to L^2, the free propagator can also be extended to an operator on L^2:

$$P_{\mathrm{f}}(t) : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d) , \quad P_{\mathrm{f}}(t) = \mathcal{F}^{-1} e^{-i\frac{k^2}{2}t} \mathcal{F} . \tag{3.147}$$

It follows that $P_{\mathrm{f}}(t)$ is a unitary operator, for all $t \in \mathbb{R}$. Moreover, it satisfies the following composition property:

$$P_{\mathrm{f}}(s)P_{\mathrm{f}}(t) = \mathcal{F}^{-1} e^{-i\frac{k^2}{2}s} \mathcal{F}\mathcal{F}^{-1} e^{-i\frac{k^2}{2}t} \mathcal{F} = \mathcal{F}^{-1} e^{-i\frac{k^2}{2}(s+t)} \mathcal{F} = P_{\mathrm{f}}(s+t) . \tag{3.148}$$

Therefore, one says that $P_{\mathrm{f}} : \mathbb{R} \to \mathcal{L}(L^2)$ is a unitary group. In the next section we will show that the function:

$$\psi(t) := P_{\mathrm{f}}(t)\psi_0 , \qquad \psi_0 \in L^2(\mathbb{R}^d) \tag{3.149}$$

solves the Schrödinger equation in the L^2 sense. Before doing that, let us first check that

$$\psi : \mathbb{R} \to L^2(\mathbb{R}^d) , \qquad \psi_0 \mapsto \psi(t) = P_{\mathrm{f}}(t)\psi_0 \tag{3.150}$$

is continuous. By dominated convergence:

$$\|\psi(t) - \psi(t_0)\|_{L^2}^2 = \|(P_{\mathrm{f}}(t) - P_{\mathrm{f}}(t_0))\psi_0\|_{L^2}^2 = \int_{\mathbb{R}^d} \left| e^{-i\frac{k^2}{2}t} - e^{-i\frac{k^2}{2}t_0} \right|^2 |\hat{\psi}_0(k)|^2 \, dk \to 0 \tag{3.151}$$

as $t \to t_0$. This proves the continuity of $\psi(t)$. Let us now check differentiability. Again by dominated convergence, we see that $\psi : \mathbb{R} \to L^2(\mathbb{R}^d)$ is differentiable if and only if:

$$|k|^4 |\hat{\psi}_0(k)|^2 \tag{3.152}$$

is integrable, that is when $|k|^2\hat{\psi}_0(k) \in L^2(\mathbb{R}^d)$. To conclude, let us discuss the continuity properties of the unitary group P_{f}. In particular, let us consider $\|P_{\mathrm{f}}(t) - P_{\mathrm{f}}(t_0)\|_{\mathcal{L}(L^2)}$, with $\|\cdot\|_{\mathcal{L}(L^2)}$ defined in Proposition 3.63. We have:

$$\|P_{\mathrm{f}}(t) - P_{\mathrm{f}}(t_0)\|_{\mathcal{L}(L^2)} = \left\| e^{-i\frac{k^2}{2}t} - e^{-i\frac{k^2}{2}t_0} \right\|_{\mathcal{L}(L^2)} = \sup_{k \in \mathbb{R}^d} \left| e^{-i\frac{k^2}{2}t} - e^{-i\frac{k^2}{2}t_0} \right| = 2 , \tag{3.153}$$

where we used that $\mathcal{F}$ is unitary, and that it leaves L^2 invariant. Therefore, the unitary group P_{f} is not continuous with respect to the topology of the bounded operators. However, one might have continuity with respect to different topologies.

Definition 3.72. *Let (A_n) be a sequences in $\mathcal{L}(\mathcal{H})$ and $A \in \mathcal{L}(\mathcal{H})$.*

(a) We say that A_n converges to A in norm if:

$$\lim_{n\to\infty} \|A_n - A\|_{\mathcal{L}(\mathcal{H})} = 0 . \tag{3.154}$$

One writes also $\lim_{n\to\infty} A_n = A$ or $A_n \to A$.

(b) We say that A_n converges strongly (or pointwise) to A if:

$$\lim_{n\to\infty} \|A_n\psi - A\psi\|_{\mathcal{H}} = 0 \qquad \text{for all } \psi \in \mathcal{H}. \tag{3.155}$$

One writes also $s - \lim_{n\to\infty} A_n = A$ or $A_n \xrightarrow{s} A$.

(c) *We say that A_n converges weakly to A if:*

$$\lim_{n\to\infty} |\langle\varphi, (A_n - A)\psi\rangle| = 0 \qquad \text{for all } \varphi, \psi \in \mathcal{H}. \tag{3.156}$$

One writes also $w - \lim_{n\to\infty} A_n = A$ or $A_n \xrightarrow{w} A$.

Remark 3.73. *These notions of convergence verify the following chain of implications:*

$$\text{norm convergence} \Rightarrow \text{strong convergence} \Rightarrow \text{weak convergence}. \tag{3.157}$$

The reverse implications are in general not correct.

3.7 Unitary groups and their generators

In this section we shall discuss in which sense $\psi(t) = P_{\mathrm{f}}(t)\psi_0$ with $\psi_0 \in L^2$ solves the free Schrödinger equation:

$$i\frac{d}{dt}\psi(t) = -\frac{1}{2}\Delta\psi(t)\ . \tag{3.158}$$

As we have seen in the previous section, $\psi(t)$ is differentiable in the strong sense if $|k|^2\hat{\psi}(t) \in L^2$. Moreover, the distributional derivative:

$$-\frac{1}{2}\Delta\psi(t) = \mathcal{F}^{-1}\frac{|k|^2}{2}\hat{\psi}(t) \tag{3.159}$$

is in L^2 if and only if $|k|^2\hat{\psi}(t) \in L^2$. Also,

$$|k|^2\hat{\psi}(t) = |k|^2 e^{-i\frac{k^2}{2}t}\hat{\psi}_0 \in L^2 \tag{3.160}$$

if and only if $|k|^2\hat{\psi}_0 \in L^2$. Therefore, if the initial datum satisfies $|k|^2\hat{\psi}_0 \in L^2$, then $|k|^2\hat{\psi}(t) \in L^2$ for all times, and $\psi(t)$ solves the Schrödinger equation in the L^2 sense: Eq. (3.158) holds as an identity between L^2 functions.

Definition 3.74 (Sobolev spaces.). *Let $m \in \mathbb{Z}$. The m-th Sobolev space $H^m(\mathbb{R}^d) \subset \mathcal{S}'(\mathbb{R}^d)$ is the set of distributions $f \in \mathcal{S}'(\mathbb{R}^d)$ such that $\hat{f}$ is a measurable function and:*

$$(1 + |k|^2)^{\frac{m}{2}}\hat{f} \in L^2(\mathbb{R}^d)\ . \tag{3.161}$$

For $m \geqslant 0$, it follows that $H^m \subset L^2$.

Remark 3.75. *Let us consider again the propagator of the free Schrödinger equation:*

$$P_f : \mathbb{R} \to \mathcal{L}(L^2)\ , \qquad t \mapsto P_f(t) = \mathcal{F}^{-1}e^{-i\frac{k^2}{2}t}\mathcal{F}\ . \tag{3.162}$$

It satisfies the following properties:

(a) *$P_f(t)$ is unitary for all $t \in \mathbb{R}$.*
(b) *P_f is strongly continuous: $t \mapsto P_f(t)\psi$ is continuous for all $\psi \in L^2$.*
(c) *P_f has the group property: $P_f(s)P_f(t) = P_f(t + s)$ for all $s, t \in \mathbb{R}$.*

Moreover,

(d) *For all $\psi_0 \in L^2$, $\psi(t) = P_f\psi_0$ is a solution in the sense of distributions.*
(e) *For all $\psi_0 \in H^2 \subset L^2$, $\psi(t) = P_f(t)\psi_0$ is a solution in the L^2 sense: the map $\mathbb{R} \ni t \mapsto \psi(t) \in L^2$ is differentiable and the derivative satisfies:*

$$i\frac{d}{dt}\psi(t) = -\frac{1}{2}\Delta\psi(t) \tag{3.163}$$

where $-\frac{1}{2}\Delta\psi(t) \in L^2$.

The items $(a) - (c)$ motivate the following definition.

Definition 3.76 (Strongly continuous one-parameter group.)**.** *A family $U(t)$, $t \in \mathbb{R}$, of unitary operators $U(t) \in \mathcal{L}(\mathcal{H})$ is called a strongly continuous one-parameter group if:*

(i) $U : \mathbb{R} \to \mathcal{L}(\mathcal{H})$, $t \mapsto U(t)$ *is strongly continuous.*

(ii) $U(t+s) = U(t)U(s)$ *for all* t, s *and moreover* $U(0) = \mathbb{1}_{\mathcal{H}}$.

The items $(d) - (e)$ motivate the following definition.

Definition 3.77 (Generator of a unitary group.)**.** *A densely defined linear operator H with domain $D(H) \subseteq \mathcal{H}$ is called a generator of a strongly continuous unitary group if:*

(i) $D(H) = \{\psi \in \mathcal{H} \mid t \mapsto U(t)\psi$ *is differentiable*$\}$.

(ii) For all $\psi \in D(H)$ *it follows that* $i\frac{d}{dt}U(t)\psi = U(t)H\psi$.

Example 3.78 (The free Hamilton operator.)**.** *Consider the free Hamilton operator:*

$$H_0 = -\frac{1}{2}\Delta \quad \textit{with} \quad D(H_0) = H^2(\mathbb{R}^d) \tag{3.164}$$

is the generator of the unitary group $P_f(t)$. This can easily be checked from the definition (3.162), and from the fact that $\mathcal{F}\mathcal{F}^{-1} = \mathcal{F}^{-1}\mathcal{F} = \mathbb{1}$.

Proposition 3.79 (Properties of the generators.)**.** *Let H be a generator for $U(t)$. Then:*

(i) $D(H)$ *is invariant under* $U(t)$, *that is* $U(t)D(H) = D(H)$ *for all* $t \in \mathbb{R}$.

(ii) H *commutes with* $U(t)$, *that is:*

$$[H, U(t)]\psi := HU(t)\psi - U(t)H\psi = 0 \quad \textit{for all } \psi \in D(H). \tag{3.165}$$

(iii) H *is symmetric, that is:*

$$\langle H\psi, \varphi\rangle = \langle \psi, H\varphi\rangle \qquad \textit{for all } \varphi, \psi \in D(H). \tag{3.166}$$

(iv) U *is uniquely determined by* H.

(v) H *is uniquely determined by* U.

Proof. (i) We notice that the map $s \mapsto U(s)U(t)\psi = U(s+t)\psi$ is differentiable if and only if the map $s \mapsto U(s)\psi = U(-t)U(s+t)\psi$ is differentiable. The derivative of the first map at $s = 0$ is: $(-i)U(t)H\psi$. The derivative of the second map at $s = 0$ is: $(-i)U(-t)U(t)H\psi$. Thus, $\psi \in D(H)$ if and only if $\psi \in U(t)D(H)$.

(ii) Let $\psi \in D(H)$. Then:

$$U(t)H\psi = U(t)i\frac{d}{ds}U(s)\psi\,|_{s=0} = i\frac{d}{ds}U(t)U(s)\psi\,|_{s=0} = i\frac{d}{ds}U(s)U(t)\psi\,|_{s=0} = HU(t)\psi\;. \tag{3.167}$$

To get the third equality we used that $U(t)U(s) = U(t+s) = U(s)U(t)$, and that $U(t)\psi$ is in $D(H)$, by what we proved before.

(iii) By unitarity, $\langle\psi, \varphi\rangle = \langle U(t)\psi, U(t)\varphi\rangle$ for all $\psi, \varphi \in \mathcal{H}$. Therefore,

$$\begin{aligned} 0 &= \frac{d}{dt}\langle\psi,\varphi\rangle = \frac{d}{dt}\langle U(t)\psi, U(t)\varphi\rangle = \langle -iHU(t)\psi, U(t)\varphi\rangle + \langle U(t)\psi, -iHU(t)\varphi\rangle \\ &= i\langle U(t)H\psi, U(t)\varphi\rangle - i\langle U(t)\psi, U(t)H\varphi\rangle = i\langle H\psi,\varphi\rangle - i\langle\psi, H\varphi\rangle\;. \end{aligned} \tag{3.168}$$

(iv) Suppose that $\widetilde{U}(t)$ is generated by H. Then, by symmetry of H:

$$\begin{aligned} \frac{d}{dt}\big\|(U(t) - \widetilde{U}(t))\psi\big\|^2 &= 2\frac{d}{dt}\Big(\|\psi\|^2 - \mathrm{Re}\,\langle U(t)\psi, \widetilde{U}(t)\psi\rangle\Big) \\ &= -2\mathrm{Re}\,\Big(\langle -iHU(t)\psi, \widetilde{U}(t)\psi\rangle + \langle U(t)\psi, -iH\widetilde{U}(t)\psi\rangle\Big) \\ &= -2\mathrm{Re}\,\Big(i\langle HU(t)\psi, \widetilde{U}(t)\psi\rangle - i\langle U(t)\psi, H\widetilde{U}(t)\psi\rangle\Big) \\ &= 0\;, \end{aligned} \tag{3.169}$$

for all $\psi \in D(H)$ (for the second term, we actually use that $\widetilde{U}(t)D(H) = D(H)$). Eq. (3.169) together with $U(0) = \widetilde{U}(0) = \mathbb{1}$, implies that $U(t) \restriction_{D(H)} = \widetilde{U}(t) \restriction_{D(H)}$ for all $t \in \mathbb{R}$. Moreover, from $\overline{D(H)} = \mathcal{H}$ (recall that, by definition, the generator H is densely defined in $\mathcal{H}$), we conclude that $U = \widetilde{U}$ on $\mathcal{H}$.

(v) This is an immediate consequence of the definition of H.

∎

Example 3.80 (Translations as unitary groups on L^2). *(a) Let $T(t) : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ with $\psi \mapsto (T(t)\psi)(x) := \psi(x-t)$ be the group of translations. It follows that $T(t)$ is a strongly continuous unitary group, generated by $D_0 = -i\frac{d}{dx}$, with domain $D(D_0) = H^1(\mathbb{R})$.*

(b) The definition of the translations on $L^2([0,1])$ is a bit more delicate. Let $0 \leqslant t < 1$ and $\theta \in [0, 2\pi)$. We define:

$$(T_\theta(t)\psi)(x) := \begin{cases} \psi(x-t) & \text{if } x-t \in [0,1] \\ e^{i\theta}\psi(x-t+1) & \text{if } x-t < 0. \end{cases} \tag{3.170}$$

This definition allows to define the translation to the right for all $t \geqslant 0$. Intuitively, whatever "exits the interval $[0,1]$ from the right", "comes back from the left" with a phase factor $e^{i\theta}$. One can easily check that $T_\theta(t)$ is unitary, and that it satisfies the group composition property. However notice that for $\theta \neq \theta'$ one has $T_\theta(t) \neq T_{\theta'}(t)$ for $t \neq 0$: different phase factors produce different translation groups. Thus, according to Proposition 3.79, these groups must have different generators.

However, for t small enough the function $(T_\theta(t)\psi)(x)$ does not depend on θ: how can this be, if the generators of T_θ, $T_{\theta'}(t)$ differ for different θ, θ'? The difference lies in the domains of D_θ, which differ for different values of θ. One has $D_\theta = -i\frac{d}{dx}$, with domain:

$$D(D_\theta) = \{\psi \in H^1([0,1]) \mid e^{i\theta}\psi(1) = \psi(0)\}\,. \tag{3.171}$$

One can check that $D(D_\theta)$ is invariant under $T_\theta(t)$, and that D_θ is the generator of T_θ. Here, $H^1([0,1])$ is the local Sobolev space, defined as follows:

$$H^1([0,1]) := \{\psi \in L^2([0,1]) \mid \text{such that there exists } \varphi \in H^1(\mathbb{R}) \text{ with } \varphi\restriction_{[0,1]} = \psi\}\,. \tag{3.172}$$

As we will prove later $H^1(\mathbb{R}) \subset C(\mathbb{R})$, which means that the pointwise constraint in the definition of $D(D_\theta)$ makes sense.

Remark 3.81. *The operator $-i\frac{d}{dx}$ equipped with the maximal definition domain $D_{max} = H^1([0,1])$ does not generate any unitary group, since H^1 is not invariant under T_θ. The same is true if one chooses a too small domain, for instance $D_{min} = \{\psi \in H^1([0,1]) \mid \psi(0) = \psi(1) = 0\}$.*

Remark 3.82. *For $\psi, \varphi \in H^1([0,1])$ it follows that:*

$$\begin{aligned} \langle \psi, -i\frac{d}{dx}\varphi\rangle &= \int_0^1 dx\, \overline{\psi(x)}(-i\frac{d}{dx}\varphi(x)) = -i(\overline{\psi(1)}\varphi(1) - \overline{\psi(0)}\varphi(0)) + \int_0^1 dx\, \overline{(-i\frac{d}{dx}\psi(x))}\varphi(x) \\ &= -i(\overline{\psi(1)}\varphi(1) - \overline{\psi(0)}\varphi(0)) + \langle -i\frac{d}{dx}\psi, \varphi\rangle\,. \end{aligned} \tag{3.173}$$

That is, the operator $-i\frac{d}{dx}$ on $D_{\max}$ is not symmetric. As we shall see later, this implies that $-i\frac{d}{dx}$ is not a generator. Instead, $-i\frac{d}{dx}$ on D_θ and on $D_{\min}$ is a symmetric operator, since the boundary term in Eq. (3.173) vanishes. However, $-i\frac{d}{dx}$ is a generator only if defined on D_θ. The symmetry of the operator is a necessary but not sufficient condition to define the generator of a unitary group.

Before discussing further how to characterize the generator of a unitary group, we conclude this section by discussing a regularity result for functions in Sobolev spaces.

Lemma 3.83 (Sobolev.). *Let $\ell \in \mathbb{N}_0$ and $f \in H^m(\mathbb{R}^d)$ with $m > \ell + \frac{d}{2}$. Then, $f \in C^\ell(\mathbb{R}^d)$ and $\partial^\alpha f \in C_\infty(\mathbb{R}^d)$ for all $|\alpha| \leqslant \ell$.*

Proof. We will prove that $k^\alpha \hat{f}(k) \in L^1(\mathbb{R}^d)$ for all $\alpha \in \mathbb{N}_0^d$ with $|\alpha| \leqslant \ell$. Then, $\partial^\alpha f \in C_\infty(\mathbb{R}^d)$ follows thanks to the Riemann-Lebesgue lemma, Theorem 3.4.

From the definition of H^m one has $(1+|k|^2)^{m/2}\hat{f}(k) \in L^2(\mathbb{R}^d)$, and therefore for all $\alpha \in \mathbb{N}_0^d$ with $|\alpha| \leqslant \ell$:

$$\begin{aligned}\int_{\mathbb{R}^d} |k^\alpha \hat{f}(k)|\, dk &\leqslant \int_{\mathbb{R}^d} (1+|k|^2)^{\ell/2} |\hat{f}(k)|\, dk \\ &= \int_{\mathbb{R}^d} (1+|k|^2)^{m/2} |\hat{f}(k)| (1+|k|^2)^{\frac{\ell-m}{2}}\, dk \\ &\leqslant \|(1+|k|^2)^{m/2}\hat{f}(k)\|_{L^2(\mathbb{R}^d)} \Big(\int_{\mathbb{R}^d} \frac{1}{(1+|k|^2)^{m-\ell}} dk \Big)^{1/2} ,\end{aligned} \quad (3.174)$$

where in the last step we used the Cauchy-Schwarz inequality. The last integral is finite if and only if $2(m-\ell) > d$. ■

4 Selfadjoint operators

4.1 The Hilbert space adjoint

Let V and W be normed spaces and $A \in \mathcal{L}(V, W)$. Then, the dual spaces V' and W' are Banach spaces and one can define the adjoint operators $A' : W' \to V'$ for $w' \in W'$:

$$(A'w')(v) := w'(Av) \qquad \text{for all } v \in V. \quad (4.1)$$

Therefore, $A' \in \mathcal{L}(W', V')$ and from the Hahn-Banach theorem one also has $\|A'\| = \|A\|$. For Hilbert spaces, it follows that $\mathcal{H}' \cong \mathcal{H}$, which means that if $A \in \mathcal{L}(\mathcal{H})$ then $A' \in \mathcal{L}(\mathcal{H}')$ can also be seen as an operator in $\mathcal{L}(\mathcal{H})$. We shall clarify these points in the following.

Theorem 4.1 (Riesz)**.** *Let $\mathcal{H}$ be a Hilbert space and $T \in \mathcal{H}'$. Then, there exists a unique $\psi_T \in \mathcal{H}$ such that:*

$$T(\varphi) = \langle \psi_T, \varphi \rangle_{\mathcal{H}} , \qquad \textit{for all } \varphi \in \mathcal{H}. \quad (4.2)$$

Proof. Let $T \in \mathcal{H}'$. We would like to prove that T can be understood as a "projection" over a vector $\psi_T \in \mathcal{H}$. If so, we can think $M := \mathrm{Ker}(T)$ as being the orthogonal complement of ψ_T. Since T is continuous, M is closed. If $M = \mathcal{H}$ then $T = 0$ and $\psi_T = 0$ provides the required vector.

Suppose that $M \neq \mathcal{H}$. Then, we claim that $M^\perp$ is one dimensional. Let $\psi_0, \psi_1 \in M^\perp \backslash \{0\}$. Let $\alpha := \frac{T(\psi_0)}{T(\psi_1)}$. We have:

$$T(\psi_0 - \alpha\psi_1) = T(\psi_0) - \alpha T(\psi_1) = 0 . \quad (4.3)$$

That is, $\psi_0 - \alpha\psi_1 \in M \cap M^\perp = \{0\}$, which proves that $\psi_0 = \alpha\psi_1$, and hence that $M^\perp$ is one-dimensional. Now, by Theorem 3.61, for any $\varphi \in \mathcal{H}$ there is a unique splitting:

$$\varphi = \varphi_M + \varphi_{M^\perp} = \varphi_M + \frac{\langle \psi_0, \varphi \rangle}{\|\psi_0\|^2} \psi_0 , \quad (4.4)$$

where the last step follows from the fact that $\dim(M^\perp) = 1$. Now, let $\psi_T := \frac{\overline{T(\psi_0)}}{\|\psi_0\|^2}\psi_0$. We have:

$$T(\varphi) = T(\varphi_M + \frac{\langle \psi_0, \varphi \rangle}{\|\psi_0\|^2}\psi_0) = \langle \psi_0, \varphi \rangle \frac{T(\psi_0)}{\|\psi_0\|^2} \equiv \langle \psi_T, \varphi \rangle , \quad (4.5)$$

where the second equality follows from the linearity of T, and from the fact that $\varphi_M \in \mathrm{Ker}(T)$. This proves the claim (4.2). The uniqueness follows from the definition of scalar product. ■

Riesz Theorem, together with the next proposition, shows that $\mathcal{H}$ and $\mathcal{H}'$ are isometrically isomorphic. In other words, $\mathcal{H}$ is selfdual.

Proposition 4.2 (Selfduality of Hilbert spaces)**.** *Consider the map:*

$$J : \mathcal{H} \to \mathcal{H}' , \qquad \varphi \mapsto J\varphi := \langle \varphi, \cdot \rangle . \tag{4.6}$$

J is a linear map. Moreover, J is an isometry:

$$\|J\varphi\|_{\mathcal{H}'} = \|\varphi\|_{\mathcal{H}} . \tag{4.7}$$

Remark 4.3. *Theorem 4.1 proves that $\mathcal{H}$ and $\mathcal{H}'$ are isomorphic. Proposition 4.2 proves that the isomorphism that associates to an element of $\mathcal{H}$ an element of $\mathcal{H}'$ is an isometry.*

Proof. The linearity of J immediately follows from its definition. Let us now prove Eq. (4.7). We have:

$$\begin{aligned} \|J\varphi\|_{\mathcal{H}'} &= \sup_{\psi \in \mathcal{H}} \frac{|J\varphi(\psi)|}{\|\psi\|_{\mathcal{H}}} \\ &= \sup_{\psi \in \mathcal{H}} \frac{|\langle \varphi, \psi \rangle|}{\|\psi\|_{\mathcal{H}}} \\ &= \|\varphi\|_{\mathcal{H}} , \end{aligned} \tag{4.8}$$

since $|\langle \varphi, \psi \rangle| \leqslant \|\varphi\|\|\psi\|$ by Cauchy-Schwarz inequality and $\langle \varphi, \varphi \rangle = \|\varphi\|^2$. ∎

Definition 4.4 (Hilbert space adjoint)**.** *Let $A \in \mathcal{L}(\mathcal{H})$. The Hilbert space adjoint operator $A^* : \mathcal{H} \to \mathcal{H}$ is defined as:*

$$A^* = J^{-1} A' J . \tag{4.9}$$

Proposition 4.5. *For $A \in \mathcal{L}(\mathcal{H})$ it follows:*

$$\langle \psi, A\varphi \rangle = \langle A^*\psi, \varphi \rangle \qquad \textit{for all } \psi, \varphi \in \mathcal{H}. \tag{4.10}$$

This relation defines A^* uniquely.

Proof. By the definition of A^* it follows that:

$$\langle \psi, A\varphi \rangle = J\psi(A\varphi) = A'J\psi(\varphi) = JJ^{-1}A'J\psi(\varphi) = JA^*\psi(\varphi) = \langle A^*\psi, \varphi \rangle . \tag{4.11}$$

Also, the map $\varphi \mapsto \langle \psi, A\varphi \rangle$ is continuous and linear. Therefore, by Theorem 4.1 there exists a unique vector $\eta \in \mathcal{H}$ with $\langle \psi, A\varphi \rangle = \langle \eta, \varphi \rangle$ for all $\varphi \in \mathcal{H}$. This proves uniqueness of A^*. ∎

Theorem 4.6 (Properties of the Hilbert space adjoint)**.** *Let $A, B \in \mathcal{L}(\mathcal{H})$ and $\lambda \in \mathbb{C}$. Then:*

(i) $(A + B)^* = A^* + B^*$ *and* $(\lambda A)^* = \overline{\lambda} A^*$.

(ii) $(AB)^* = B^* A^*$.

(iii) $\|A^*\| = \|A\|$.

(iv) $A^{**} = A$.

(v) $\|AA^*\| = \|A^*A\| = \|A\|^2$.

(vi) $Ker\, A = (Ran\, A^*)^\perp$ *and* $Ker\, A^* = (Ran\, A)^\perp$.

Proof. $(i) - (iii)$ follows immediately from the definition of Hilbert space adjoint. The property (iv) follows from:

$$\langle \psi, A\varphi \rangle = \langle A^*\psi, \varphi \rangle = \overline{\langle \varphi, A^*\psi \rangle} = \overline{\langle A^{**}\varphi, \psi \rangle} = \langle \psi, A^{**}\varphi \rangle \qquad \text{for all } \psi, \varphi \in \mathcal{H}. \tag{4.12}$$

The property (v) follows from:

$$\|A\varphi\|^2 = \langle A\varphi, A\varphi \rangle = \langle \varphi, A^*A\varphi \rangle \leqslant \|\varphi\|^2 \|A^*A\| , \tag{4.13}$$

therefore:

$$\|A\|^2 = \sup_{\|\varphi\|=1} \|A\varphi\|^2 \leqslant \|A^*A\| \leqslant \|A^*\|\|A\| = \|A\|^2 . \tag{4.14}$$

To conclude, the property (vi) follows from:

$$\begin{aligned}
\varphi \in \operatorname{Ker} A \quad &\Longleftrightarrow \quad A\varphi = 0 \\
&\Longleftrightarrow \quad \langle \psi, A\varphi \rangle = 0 \quad \text{for all } \psi \in \mathcal{H} && (4.15) \\
&\Longleftrightarrow \quad \langle A^*\psi, \varphi \rangle = 0 \quad \text{for all } \psi \in \mathcal{H} && (4.16) \\
&\Longleftrightarrow \quad \varphi \in (\operatorname{Ran} A^*)^\perp \, . && (4.17)
\end{aligned}$$

■

Example 4.7. *Let $T : \ell^2 \to \ell^2$ be the right shift, $(x_1, x_2, \ldots) \mapsto (0, x_1, x_2, \ldots)$. We have:*

$$\langle x, Ty \rangle = \sum_{j=2}^{\infty} x_j y_{j-1} = \sum_{j=1}^{\infty} x_{j+1} y_j =: \langle T^* x, y \rangle \, , \tag{4.18}$$

with T^* the left shift operator, $(x_1, x_2, \ldots) \mapsto (x_2, x_3, \ldots)$. Notice that the rightshift is isometric, but not surjective and hence not unitary. It follows that $T^*T = \mathbb{1}$, but $TT^* \neq \mathbb{1}$.

Proposition 4.8. *$U \in \mathcal{L}(\mathcal{H})$ is unitary if and only if $U^* = U^{-1}$.*

Proof. Suppose that U is unitary. Then:

$$(U^*U\psi - \psi, \varphi) = (U\psi, U\varphi) - \langle \psi, \varphi \rangle = 0 \qquad \text{for all } \psi, \varphi \in \mathcal{H}. \tag{4.19}$$

Therefore, $U^*U = \mathbb{1}$. Since U is surjective, for any $\varphi \in \mathcal{H}$ there exists $\psi \in \mathcal{H}$ such that $U\psi = \varphi$. Also, $UU^*\varphi = UU^*U\psi = U\psi = \varphi$. This implies that $UU^* = \mathbb{1}$. That is, $U^* = U^{-1}$.

Suppose now that $U^* = U^{-1}$. Then, U is surjective, and moreover:

$$\langle U\varphi, U\psi \rangle = \langle U^*U\varphi, \psi \rangle = \langle U^{-1}U\varphi, \psi \rangle = \langle \varphi, \psi \rangle \, . \tag{4.20}$$

This proves that U is unitary. ■

Definition 4.9 (Bounded selfadjoint operator)**.** *$A \in \mathcal{L}(\mathcal{H})$ is called selfadjoint if $A = A^*$.*

Proposition 4.10. *Let $A \in \mathcal{L}(\mathcal{H})$. Then:*

$$A \text{ is selfadjoint} \iff A \text{ is symmetric.} \tag{4.21}$$

Proof. The proof immediately follows from Proposition 4.5. ■

Remark 4.11. *In general, for unbounded operators the implication $\Leftarrow$ does not hold true.*

Theorem 4.12 (Bounded generator.)**.** *Let $H \in \mathcal{L}(\mathcal{H})$ with $H^* = H$. Then, the operator*

$$e^{-iHt} = \sum_{n=0}^{\infty} \frac{(-iHt)^n}{n!} \tag{4.22}$$

defines a unitary group with generator H, with $D(H) = \mathcal{H}$. Moreover, the map $\mathbb{R} \to \mathcal{L}(\mathcal{H}) : t \mapsto e^{-iHt}$ is differentiable.

Proof. Exercise. ■

Definition 4.13 (Unbounded operators.)**.** *(a) An unbounded operator is a pair $(T, D(T))$ of a subspace $D(T) \subset \mathcal{H}$ together with a linear operator $T : D(T) \to \mathcal{H}$. If $\overline{D(T)} = \mathcal{H}$, we say that T is densely defined.*

(b) An operator $(S, D(S))$ is called an extension of $(T, D(T))$ if $D(S) \supset D(T)$ and $S \restriction_{D(T)} = T$. We say that $T \subset S$.

(c) An operator $(T, D(T))$ is called symmetric if for all $\varphi, \psi \in D(T)$ it follows that:

$$\langle \varphi, T\psi \rangle_{\mathcal{H}} = \langle T\varphi, \psi \rangle_{\mathcal{H}} \, . \tag{4.23}$$

Example 4.14. *The free Hamilton operator* $H_0 = -\frac{1}{2}\Delta$ *on* $D(H_0) = H^2(\mathbb{R}^d)$ *is a symmetric unbounded operator, densely defined.*

As we have seen in Example 3.80, the solution of the Schrödinger equation generated by a symmetric operator H might leave $D(H)$, if $D(H)$ is chosen too small. We would like to understand what is exactly missing to imply that a given symmetric operator is the generator of a unitary group. Let $(H_0, D(H_0))$ be a symmetric operator, and let $(H_1, D(H_1))$ be a symmetric extension. Suppose that the equation:

$$i\frac{d}{dt}\psi(t) = H_1\psi(t) \ , \tag{4.24}$$

with initial datum $\psi(0) \in D(H_0)$ has, at least for small times, a solution $\psi(t)$ that belongs at least to $D(H_1)$ but not to $D(H_0)$. The question we ask is where does $\psi(t)$ go after leaving $D(H_0)$. For $\varphi \in D(H_0) \subset D(H_1)$ it follows that:

$$\langle H_1\psi(t), \varphi\rangle = \langle \psi(t), H_1\varphi\rangle = \langle \psi(t), H_0\varphi\rangle \ . \tag{4.25}$$

Therefore, if $\psi(t)$ does not belong to $D(H_0)$, then it is at least in the domain of the adjoint operator H_0^*, defined as follows.

Definition 4.15 (The adjoint operator)**.** *Let* T *be a densely defined linear operator on a Hilbert space* $\mathcal{H}$*. Then, the domain* $D(T^*)$ *of the adjoint operator* T^* *is defined as:*

$$D(T^*) := \{\psi \in \mathcal{H} \mid \exists \eta \in \mathcal{H} \ s.t. \ \langle \psi, T\varphi\rangle = \langle \eta, \varphi\rangle \ \forall \varphi \in D(T)\} \ . \tag{4.26}$$

Since $D(T)$ *is densely defined,* η *is uniquely defined and we define, for all* $\psi \in D(T^*)$*:*

$$T^* : D(T^*) \to \mathcal{H} \ , \qquad \psi \mapsto T^*\psi := \eta \ . \tag{4.27}$$

Remark 4.16. *By Theorem 4.1, Definition 4.15 is equivalent to:*

$$D(T^*) := \{\psi \in \mathcal{H} \mid \varphi \mapsto \langle \psi, T\varphi\rangle \text{ is continuous on } D(T).\} \tag{4.28}$$

Proposition 4.17. $(T^*, D(T^*))$ *is a linear (not necessarily densely defined) operator and:*

$$\langle \psi, T\varphi\rangle = \langle T^*\psi, \varphi\rangle \qquad \text{for all } \psi \in D(T^*) \text{ and } \varphi \in D(T). \tag{4.29}$$

Proof. It immediately follows from Definition 4.15. ∎

Definition 4.18 (Self-adjoint operator)**.** *Let* $(T, D(T))$ *be a densely defined linear operator. If* $D(T^*) = D(T)$ *and* $T = T^*$ *holds true on* $D(T)$*, then we say that* $(T, D(T))$ *is a selfadjoint operator.*

Example 4.19. *In order to clarify the above definition, let us come back to Example 3.80.*

(a) Let us consider first $D_{min} = -i\frac{d}{dx}$ *with:*

$$D(D_{min}) = \{\varphi \in H^1([0,1]) \mid \varphi(0) = \varphi(1) = 0\} \ . \tag{4.30}$$

For $\varphi \in D(D_{min})$ *we have:*

$$\langle \psi, D_{min}\varphi\rangle = \int_0^1 dx\, \overline{\psi(x)}\Big(-i\frac{d}{dx}\varphi(x)\Big) = \int_0^1 dx\, \overline{\Big(-i\frac{d}{dx}\psi(x)\Big)}\varphi(x) \quad = \quad \langle -i\frac{d}{dx}\psi, \varphi\rangle \\ =: \quad \langle \eta, \varphi\rangle \tag{4.31}$$

provided $\frac{d}{dx}\psi \in L^2([0,1])$*, which is implied by* $\psi \in H^1([0,1])$*. Therefore, one has* $D(D^*_{min}) = H^1([0,1]) \supsetneq D(D_{min})$ *which implies that* D_{min} *is not selfadjoint.*

(b) Let $D_\theta = -i\frac{d}{dx}$ *with:*

$$D(D_\theta) = \{\varphi \in H^1([0,1]) \mid e^{i\theta}\varphi(1) = \varphi(0)\} \ . \tag{4.32}$$

One has, for $\varphi \in D(D_\theta)$:

$$\begin{aligned}
\langle \psi, D_\theta \varphi \rangle &= \int_0^1 dx\, \overline{\psi(x)} \Big(-i \frac{d}{dx} \varphi(x) \Big) \\
&= i(\overline{\psi(0)}\varphi(0) - \overline{\psi(1)}\varphi(1)) + \int_0^1 dx\, \overline{\Big(-i \frac{d}{dx} \psi(x) \Big)} \varphi(x) = \langle -i \frac{d}{dx} \psi, \varphi \rangle \\
&\equiv \langle \eta, \varphi \rangle \,, \qquad (4.33)
\end{aligned}$$

provided that $\psi \in H^1([0,1])$ and that:

$$\overline{\psi(0)}\varphi(0) - \overline{\psi(1)}\varphi(1) = 0 \qquad \Longleftrightarrow \qquad \frac{\overline{\psi(0)}}{\overline{\psi(1)}} = \frac{\varphi(1)}{\varphi(0)} = e^{-i\theta} \,. \qquad (4.34)$$

It follows than that $D(D^*_\theta) = D(D_\theta)$ and that $D^*_\theta = -i\frac{d}{dx} = D_\theta$. That is, D_θ is selfadjoint.

Theorem 4.20 (Generator of a unitary group)**.** *A densely defined operator $(H, D(H))$ is a generator of a unitary group $U(t) = e^{-iHt}$ if and only if H is selfadjoint.*

Remark 4.21. *The Spectral Theorem, to be stated later, will imply that every selfadjoint operator generates a unitary group. The converse implication, that is that every unitary group is generated by a selfadjoint operator, is called the Stone Theorem. Both will be proven later; Theorem 4.20 will then follow as an immediate corollary.*

Definition 4.22 (Direct sum of Hilbert spaces)**.** *Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Hilbert spaces. Then, their direct sum is defined as:*

$$\mathcal{H}_1 \oplus \mathcal{H}_2 := \mathcal{H}_1 \times \mathcal{H}_2 \,, \qquad (4.35)$$

equipped with the scalar product

$$\langle \varphi, \psi \rangle_{\mathcal{H}_1 \oplus \mathcal{H}_2} := \langle \varphi_1, \psi_1 \rangle_{\mathcal{H}_1} + \langle \varphi_2, \psi_2 \rangle_{\mathcal{H}_2} \,. \qquad (4.36)$$

Remark 4.23. *$(\mathcal{H}_1 \oplus \mathcal{H}_2, \langle \cdot, \cdot \rangle_{\mathcal{H}_1 \oplus \mathcal{H}_2})$ is a Hilbert space.*

Definition 4.24 (Graph of an operator, closed operator, closure)**.** *(a) The graph of a linear operator $T : D(T) \to \mathcal{H}$ is the space:*

$$\Gamma(T) = \{(\varphi, T\varphi) \in \mathcal{H} \oplus \mathcal{H} \mid \varphi \in D(T)\} \subset \mathcal{H} \oplus \mathcal{H} \,. \qquad (4.37)$$

(b) An operator T is called closed if $\Gamma(T)$ is a closed subspace of $\mathcal{H} \oplus \mathcal{H}$.

(c) An operator T is called closable if it admits a closed extension. In this case, the smallest closed extension $\overline{T}$ is called the closure of T.

Remark 4.25. *It is easy to see that:*

$$\Gamma(\overline{T}) = \overline{\Gamma(T)} \,. \qquad (4.38)$$

Remark 4.26. *Therefore, an operator T is closed if for every sequence $(\varphi_n) \subset D(T)$ such that $\varphi_n \to \varphi$ and $T\varphi_n \to \eta$ in $\mathcal{H}$, then $\varphi \in D(T)$ and $T\varphi = \eta$.*

Theorem 4.27 (The adjoint of an operator is always closed.)**.** *Let $(T, D(T))$ be densely defined. Then, T^* is closed.*

Proof. We shall show that $\Gamma(T^*)$ is a closed subspace of $\mathcal{H} \oplus \mathcal{H}$. To do this, let us first notice that:

$$\begin{aligned}
(\psi, \eta) \in \Gamma(T^*) &\iff \langle \psi, T\varphi \rangle = \langle \eta, \varphi \rangle \qquad \text{for all } \varphi \in D(T) \\
&\iff \langle \psi, T\varphi \rangle - \langle \eta, \varphi \rangle = 0 \qquad \text{for all } \varphi \in D(T) \qquad (4.39) \\
&\iff \langle (\psi, \eta), (-T\varphi, \varphi) \rangle_{\mathcal{H} \oplus \mathcal{H}} = 0 \qquad \text{for all } \varphi \in D(T). \qquad (4.40)
\end{aligned}$$

Let us introduce the unitary map:

$$W : \mathcal{H} \oplus \mathcal{H} \to \mathcal{H} \oplus \mathcal{H} : (\varphi_1, \varphi_2) \mapsto (-\varphi_2, \varphi_1) \,. \qquad (4.41)$$

Therefore, we rewrite Eq. (4.39) as:

$$(\psi, \eta) \in \Gamma(T^*) \iff \langle(\psi, \eta), \phi\rangle_{\mathcal{H}\oplus\mathcal{H}} = 0 \quad \text{for all } \phi \in W(\Gamma(T)). \tag{4.42}$$

That is, $\Gamma(T^*) = (W(\Gamma(T)))^{\perp}$. Being the orthogonal complement a closed set, it follows that $\Gamma(T^*)$ is closed and hence that T^* is a closed operator. ∎

Proposition 4.28 (Extension of symmetric operators via their adjoint)**.** *A densely defined operator T is symmetric if and only if $T \subset T^*$.*

Proof. If T is symmetric, it follows that $D(T) \subset D(T^*)$, because for every $\psi \in D(T)$ one can set $\eta = T\psi =: T^*\psi$. Conversely, if $T \subset T^*$, then for every $\psi \in D(T) \subset D(T^*)$ we have $\langle\psi, T\varphi\rangle = \langle T^*\psi, \varphi\rangle = \langle T\psi, \varphi\rangle$ for all $\varphi \in D(T)$. ∎

Remark 4.29 (Symmetric operators are closable)**.** *Since for symmetric operators one has $T \subset T^*$ and T^* is closed, then the symmetric operators are always closable.*

Remark 4.30. *For general symmetric operators T, the identity $\overline{T} = T^*$ does not have to be true. In fact, it is not difficult to see that $\overline{T}$ is symmetric, while T^* may not be.*

Proposition 4.31. *Let T be densely defined and $T \subset S$. Then, $S^* \subset T^*$.*

Proof. With the notation of the proof of Theorem 4.27, one has $\Gamma(S^*) = (W\Gamma(S))^{\perp}$. Since $T \subset S$, one has $\Gamma(T) \subset \Gamma(S)$, and also $W\Gamma(T) \subset W\Gamma(S)$. Hence:

$$\Gamma(S^*) = (W\Gamma(S))^{\perp} \subset (W\Gamma(T))^{\perp} = \Gamma(T^*) \, . \tag{4.43}$$

∎

Proposition 4.32. *Let T be densely defined and closable. Then, T^* is also densely defined.*

Proof. We shall prove that $D(T^*)$ is dense in $\mathcal{H}$ by showing that $D(T^*)^{\perp} = 0$. Let $\eta \in D(T^*)^{\perp}$. Then (recall that the orthogonal complement is a closed set):

$$(\eta, 0) \in \Gamma(T^*)^{\perp} = (W\Gamma(T))^{\perp\perp} = \overline{W\Gamma(T)} \, . \tag{4.44}$$

Since $W\Gamma(T) = \{(-T\varphi, \varphi) \mid \varphi \in D(T)\}$, there exists a sequence (φ_n) in $D(T)$ with $\varphi_n \to 0$, such that $-T\varphi_n \to \eta$. Being T closable, we have that $\overline{T}0 = \eta = 0$. ∎

Proposition 4.33. *Let T densely defined and closable. Then:*

(a) $T^{**} = \overline{T}$.

(b) $(\overline{T})^* = T^* = T^{***}$.

Proof. Being W unitary, it follows that for every subspace $M \subset \mathcal{H} \oplus \mathcal{H}$ then $W(M^{\perp}) = (W(M))^{\perp}$.

(a) We already know that $\Gamma(T^*) = (W\Gamma(T))^{\perp}$. Replacing T with T^* we have:

$$\Gamma(T^{**}) = (W\Gamma(T^*))^{\perp} = (W((W\Gamma(T))^{\perp}))^{\perp} = W\circ W(\Gamma(T)^{\perp\perp}) = -\overline{\Gamma(T)} = -\Gamma(\overline{T}) = \Gamma(\overline{T}) \, . \tag{4.45}$$

(b) Thanks to the previous equality it turns out that $\overline{T}^* = T^{***}$. Moreover,

$$\Gamma(\overline{T}^*) = (W\Gamma(\overline{T}))^{\perp} = \overline{W\Gamma(T)}^{\perp} = (W\Gamma(T))^{\perp} = \Gamma(T^*) \, . \tag{4.46}$$

∎

4.2 Criteria for symmetry, selfadjointness and essential selfadjointness

Selfadjoint operators play an important role in quantum mechanics, since they are the only operators that can generate time evolution. Nevertheless, we would like to have criteria that allows to check whether a given operator is selfadjoint. Before doing this, let us discuss a simple criterion to determine whether an operator is symmetric.

Lemma 4.34 (Criterium for symmetry)**.** *Let T be a linear operator on a complex Hilbert space $\mathcal{H}$. Then:*

$$\langle \varphi, T\varphi \rangle \in \mathbb{R} \quad \text{for all } \varphi \in D(T) \qquad \Longleftrightarrow \qquad T \text{ is symmetric.} \tag{4.47}$$

Proof. The fact that T is symmetric immediately implies that $\langle \varphi, T\varphi \rangle \in \mathbb{R}$, since $\overline{\langle \varphi, T\varphi \rangle} = \langle T\varphi, \varphi \rangle$. Let us now prove the converse implication. Suppose that $\langle \varphi, T\varphi \rangle \in \mathbb{R}$ for all $\varphi \in D(T)$. We would like to show that

$$\langle \varphi, T\psi \rangle = \langle T\varphi, \psi \rangle \qquad \text{for all } \psi, \varphi \in D(T). \tag{4.48}$$

Consider the identity:

$$\begin{aligned} &\langle \varphi, T\psi \rangle = \\ &\frac{1}{4}(\langle \varphi + \psi, T(\varphi + \psi) \rangle - \langle \varphi - \psi, T(\varphi - \psi) \rangle - i\langle \varphi + i\psi, T(\varphi + i\psi) \rangle + i\langle \varphi - i\psi, T(\varphi - i\psi) \rangle) \end{aligned} \tag{4.49}$$

Let us take the complex conjugate of both sides, recalling that, by assumption, $\langle \varphi, T\varphi \rangle \in \mathbb{R}$ for all $\varphi \in D(T)$. We have:

$$\begin{aligned} &\overline{\langle \varphi, T\psi \rangle} = \langle T\psi, \varphi \rangle = \\ &\frac{1}{4}(\langle \varphi + \psi, T(\varphi + \psi) \rangle - \langle \varphi - \psi, T(\varphi - \psi) \rangle + i\langle \varphi + i\psi, T(\varphi + i\psi) \rangle - i\langle \varphi - i\psi, T(\varphi - i\psi) \rangle) \,. \end{aligned} \tag{4.50}$$

Therefore, interchaging ψ with φ:

$$\begin{aligned} &\langle T\varphi, \psi \rangle = \\ &\frac{1}{4}(\langle \varphi + \psi, T(\varphi + \psi) \rangle - \langle \varphi - \psi, T(\varphi - \psi) \rangle + i\langle \psi + i\varphi, T(\psi + i\varphi) \rangle - i\langle \psi - i\varphi, T(\psi - i\varphi) \rangle) \\ &= \frac{1}{4}(\langle \varphi + \psi, T(\varphi + \psi) \rangle - \langle \varphi - \psi, T(\varphi - \psi) \rangle + i\langle i\psi - \varphi, T(i\psi - \varphi) \rangle - i\langle i\psi + \varphi, T(i\psi + \varphi) \rangle) \\ &\equiv \langle \varphi, T\psi \rangle \end{aligned} \tag{4.51}$$

where the last step follows by comparison with Eq. (4.49). ∎

Example 4.35. *(i) Let $f : \mathbb{R} \to \mathbb{C}$ measurable. Consider the multiplication operator $(A_f\psi)(x) = f(x)\psi(x)$, for all $\psi \in D(A_f) = \{\psi \in L^2(\mathbb{R}) \mid f\psi \in L^2(\mathbb{R})\}$. We then have that A_f is a symmetric operator if and only if $f(x)$ is real valued.*
Let us compute the adjoint of A_f^*. To begin, notice that $D(A_f)$ is dense in $L^2(\mathbb{R})$. This follows from $C_c^\infty(\mathbb{R}) \subset D(A_f) \subset L^2(\mathbb{R})$. The adjoint operator on $D(A_f)$ is given by:

$$(A_f^*\psi)(x) = \overline{f(x)}\psi(x) \,. \tag{4.52}$$

Thus, $A_f^* = A_f$ if and only if f is real valued.

(ii) Consider the distributional Laplacian $-\Delta$ on $H^2(\mathbb{R}^d)$. For all $\psi \in H^2(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$:

$$\langle \psi, -\Delta\psi \rangle = \langle \mathcal{F}\psi, \mathcal{F} - \Delta\mathcal{F}^{-1}\mathcal{F}\psi \rangle = \int dk\, |\hat{\psi}(k)|^2 k^2 \in \mathbb{R} \,. \tag{4.53}$$

Hence, $-\Delta$ is a symmetric operator.

Sometimes, one has to deal with non-closed symmetric operators. Of course, these operators cannot be self-adjoint (self-adjoint operators are always closed). The relevant question here is whether the closure of a symmetric operator is selfadjoint.

Definition 4.36 (Essentially selfadjoint operator)**.** *A symmetric, densely defined operator is called essentially selfadjoint if its closure is selfadjoint.*

Corollary 4.37. *A symmetric, densely defined operator T is essentially selfadjoint if and only if T^* is symmetric. In this case $\overline{T} = T^*$ and $\overline{T}$ is the unique selfadjoint extension of T.*

Proof. Suppose that T^* is symmetric. We would like to show that $(\overline{T})^* = \overline{T}$, that is T is essentially selfadjoint. By Proposition 4.33 (b), $(\overline{T})^* = T^*$, hence it is enough to check that $T^* = \overline{T}$. By Theorem 4.27, T^* is closed. Moreover, being T symmetric, by Proposition 4.28 $T \subset T^*$. Thus, $\overline{T} \subset T^*$. To conclude, we would like to show that $T^* \subset \overline{T}$. We claim that $T^{***} \subset T^{**}$. If so, by Proposition 4.33, we have: $T^* = T^{***} \subset T^{**} = \overline{T}$, which proves that $T^* \subset \overline{T}$ and hence that $T^* = \overline{T}$. The claim $T^{***} \subset T^{**}$ follows from the fact that, for T symmetric, $T^{**} \subset T^*$. In fact: by Proposition 4.33 (b), we have $T^* = (\overline{T})^*$; since $\overline{T}$ is symmetric and densely defined, $(\overline{T})^* \supset \overline{T}$, by Proposition 4.28; finally, Proposition 4.33 (a) implies that $\overline{T} = T^{**}$.

Now, suppose that T is essentially selfadjoint. Then, $\overline{T}$ is selfadjoint, and in particular symmetric. Moreover, T^* is symmetric as well, since, by Proposition 4.33, $T^* = (\overline{T})^* = \overline{T}$, where the last equality follows from the definition of essential selfadjointness.

To conclude, we have to show that $\overline{T}$ is the unique selfadjoint extension of T. Suppose that S is another selfadjoint extension of T. Then, $T \subset S$ implies that $\overline{T} \subset \overline{S} = S$ (since, by Theorem 4.27, selfadjoint operators are closed). The reverse implication follows from Proposition 4.31: $S = S^* \subset T^* = \overline{T}$, *i.e.* $S = \overline{T}$. ■

Definition 4.38. *Let $(T, D(T))$ be a selfadjoint operator. A subspace $D_0 \subset D(T)$, dense in $\mathcal{H}$, is called core of T if (T, D_0) is essentially selfadjoint, that is if:*

$$\overline{T \restriction_{D_0}} = T \; . \tag{4.54}$$

Remark 4.39. *Equivalently, D_0 is a core for $(T, D(T))$ if and only if D_0 is dense in $D(T)$ with respect to the graph norm:*

$$\|\varphi\|^2_{\Gamma(T)} := \|T\varphi\|^2_{\mathcal{H}} + \|\varphi\|^2_{\mathcal{H}} \; . \tag{4.55}$$

Example 4.40. *(a) As we have seen in Example 4.19, the operator $(-i\frac{d}{dx}, D_{min})$ is symmetric but not selfadjoint. Let us check whether it is essentially selfadjoint. To do so, let us compute the closure of the operator, and check whether the closure is selfadjoint. Being $T = -i\frac{d}{dx}$ symmetric on its domain, we know that $\overline{T} = T^{**} \subset T^*$. Therefore, for all $\psi \in D(T^*) = H^1([0,1])$ and all $\varphi \in D(\overline{T})$, recalling that $\overline{T} \subset T^* = -i\frac{d}{dx}$:*

$$\begin{aligned} 0 &= \langle \psi, \overline{T}\varphi\rangle - \langle T^*\psi, \varphi\rangle \\ &= \langle \psi, -i\frac{d}{dx}\rangle - \langle -i\frac{d}{dx}\psi, \varphi\rangle = i[\varphi(0)\overline{\psi(0)} - \varphi(1)\overline{\psi(1)}] \; , \end{aligned} \tag{4.56}$$

which implies that $\varphi(0) = \varphi(1) = 0$ (because $\psi \in D(T^*) = H^1([0,1])$ does not need to satisfy any boundary condition). We conclude that $D(\overline{T}) \subset \{\psi \in D(T^*) \mid \psi(0) = \psi(1) = 0\} \equiv D_{min}$. On the other hand, it is easy to check that every $\psi \in H^1([0,1])$ with $\psi(0) = \psi(1) = 0$ is also in $D(T^{**}) = D(\overline{T})$. In fact, for any $\psi \in D_{min}$ and any $\varphi \in D(T^*) = H^1([0,1])$, integrating by parts:

$$\langle \psi, T^*\varphi\rangle = \langle \psi, -i\frac{d}{dx}\varphi\rangle = \langle -i\frac{d}{dx}\psi, \varphi\rangle =: \langle \eta, \varphi\rangle \; , \tag{4.57}$$

with $\eta \in L^2(\mathbb{R})$ given by $-i\frac{d}{dx}\psi$. Therefore, $D(\overline{T}) = D_{min}$, and $\overline{T}\psi = -i\frac{d}{dx}\psi$ for all $\psi \in D(\overline{T})$. Hence, $\overline{T}$ is a symmetric operator on D_{min}, but not selfadjoint; that is (T, D_{min}) is not essentially selfadjoint.

(b) We already know that $(-i\frac{d}{dx}, D_\theta)$ is selfadjoint. Hence, it is in particular essentially selfadjoint.

The distinction between closed symmetric operators and self-adjoint operators may seem just a technicality, but it is actually very important. The spectral theorem, which plays a very important role in quantum mechanics, only holds for selfadjoint operators, not for general closed symmetric operators. Similarly, only selfadjoint operators, and not general closed symmetric operators, generate a unitary evolution. Unfortunately, while it is easy to check whether an operator is symmetric, it is much more difficult to decide whether it is selfadjoint; we need criteria to prove selfadjointness. The basic criterium is stated in the following theorem.

Theorem 4.41 (Criteria for seldadjointness)**.** *Let $(H, D(H))$ be densely defined and symmetric. Then, the following statements are equivalent:*

(i) H is selfadjoint.

(ii) H is closed and $Ker(H^* \pm i) = \{0\}$.

(iii) $Ran(H \pm i) = \mathcal{H}$.

Proof. $(i) \Rightarrow (ii)$. Let H be selfadjoint. Then, H is closed (since H^* is closed, Theorem 4.27). Let $\varphi_\pm \in \mathrm{Ker}(H^* \pm i)$. Then, $H\varphi_\pm = \mp i\varphi_\pm$. Since the eigenvalues of a symmetric operators are always real, it follows that $\varphi_\pm = 0$.

$(ii) \Rightarrow (iii)$. This implication will be postponed to the next lemma.

$(iii) \Rightarrow (i)$. Being H symmetric, it follows that $H \subset H^*$, by Proposition 4.28. We are left with showing that $H^* \subset H$. To this end, let $\psi \in D(H^*)$. Then, by the assumption $\mathrm{Ran}(H \pm i) = \mathcal{H}$, there exists $\varphi \in D(H)$ such that

$$(H^* - i)\psi = (H - i)\varphi \; . \tag{4.58}$$

By $H \subset H^*$, it also follows that:

$$(H^* - i)\psi = (H^* - i)\varphi \; , \tag{4.59}$$

that is $\varphi - \psi \in \mathrm{Ker}\,(H^* - i)$. As the next lemma will show, this implies that $\varphi - \psi = 0$, that is $\psi = \varphi \in D(H)$, which shows that $D(H^*) \subset D(H)$. Also, by Eq. (4.58), $H = H^*$ on $D(H)$, which concludes the proof. ∎

Lemma 4.42. *Let $(T, D(T))$ be densely defined. Then:*

(a) For all $z \in \mathbb{C}$ it follows that $Ker\,(T^* \pm z) = Ran\,(T \pm \overline{z})^\perp$. In particular:

$$Ker\,(T^* \pm z) = \{0\} \iff \overline{Ran\,(T \pm z)} = \mathcal{H} \; . \tag{4.60}$$

(b) If T is closed and symmetric, then the sets $Ran\,(T \pm i)$ are closed.

Remark 4.43. *Let us check how this lemma allows to conclude the proof of Theorem 4.41. Let us check that $(ii) \Rightarrow (iii)$. Eq. (4.60) implies that: $Ker\,(H^* \pm i) = \{0\} \Rightarrow \overline{Ran\,(H \pm i)} = \mathcal{H}$. Finally, being H closed and symmetric, item (b) above implies that $Ran\,H$ is closed. This proves the implication $(ii) \Rightarrow (iii)$.*

To conclude the proof of the implication $(iii) \Rightarrow (i)$ above, we have to show that (iii) implies that $Ker\,(H^* - i) = \{0\}$. Since $Ran\,(H \pm i) \subset \overline{Ran\,(H \pm i)}$, and $Ran\,(H \pm i) = \mathcal{H}$ by assumption, Eq. (4.60) implies that $Ker\,(H^* - i) = \{0\}$, which concludes the proof of Theorem 4.41.

Proof. (of Lemma 4.42.) To prove (a), notice first that $(T + z)^* = T^* + \overline{z}$. Then:

$$\begin{aligned} \psi \in \mathrm{Ran}\,(T \pm z)^\perp \quad &\iff \quad \langle \psi, (T \pm z)\varphi \rangle = 0 \quad \text{for all } \varphi \in D(T) \\ &\iff \quad \psi \in D(T^*) \quad \text{and} \quad (T^* \pm \overline{z})\psi = 0 \\ &\iff \quad \psi \in \mathrm{Ker}\,(T^* \pm \overline{z}) \; . \end{aligned} \tag{4.61}$$

This proves (a). Let us now prove (b); we start by choosing $+i$. The proof for $-i$ is exactly the same. For symmetric T, it follows that $\langle \psi, T\psi \rangle = \langle T\psi, \psi \rangle = \overline{\langle \psi, T\psi \rangle}$, that is $\langle \psi, T\psi \rangle \in \mathbb{R}$. Therefore, for any $\psi \in D(T)$:

$$\begin{aligned} \|(T + i)\psi\|^2 &= \langle (T + i)\psi, (T + i)\psi \rangle = \|T\psi\|^2 + \|\psi\|^2 - 2\mathrm{Re}\, i\langle \psi, T\psi \rangle \\ &= \|T\psi\|^2 + \|\psi\|^2 \geqslant \|\psi\|^2 \; . \end{aligned} \tag{4.62}$$

Therefore, $T + i$ is injective and $(T + i)^{-1} : \mathrm{Ran}(T + i) \to D(T)$ exists and it is bounded. Let (ψ_n) be a sequence in $\mathrm{Ran}\,(T + i)$ such that $\psi_n \to \psi$. Let $\varphi_n := (T + i)^{-1}\psi_n$. The boundedness of $(T + i)^{-1}$ implies that ψ_n is a Cauchy sequence, which therefore converges to $\varphi \in \mathcal{H}$. Being T closed, $\Gamma(T)$ is a closed set; therefore, the sequence $(\varphi_n, \psi_n) \in \Gamma(T + i)$ converges to $(\varphi, \psi) = (\varphi, (T + i)\varphi) \in \Gamma(T + i)$, which shows that $\psi \in \mathrm{Ran}\,(T + i)$. ∎

Remark 4.44. *Suppose that H is nonnegative, that is $\langle\psi, H\psi\rangle \geqslant 0$ for all $\psi \in D(H)$. Then, it is not difficult to see that the condition for selfadjointness Ran $(H \pm i) = \mathcal{H}$ in Theorem 4.41 can be replaced by Ran $(H + 1) = \mathcal{H}$.*

From Theorem 4.41, we also obtain criteria for essential selfadjointness.

Corollary 4.45 (Criteria for essential selfadjointness)**.** *Let H be densely defined and symmetric. Then, the following statements are equivalent:*

(i) *H is essentially selfadjoint.*

(ii) *Ker $(H^* \pm i) = \{0\}$.*

(iii) $\overline{\mathrm{Ran}\,(H \pm i)} = \mathcal{H}$.

Proof. Exercise. ∎

Example 4.46. *(a) Let us give a simple proof of the fact that the operator $H = -i\frac{d}{dx}$ on $D_{min} = \{\psi \in H^1([0,1]) \mid \psi(1) = \psi(0) = 0\}$ is not essentially selfadjoint, based on Corollary 4.45. The equation:*

$$H^*\varphi_\pm = -i\frac{d}{dx}\varphi_\pm = \mp i\varphi_\pm \tag{4.63}$$

is solved by $\varphi_\pm = e^{\pm x}$, which lies in $D(H^*) = H^1([0,1])$. Therefore, Ker$(H^* \pm i) \neq \{0\}$, which disproves essential selfadjointess.

(b) For $H_0 = -\Delta$ on $C_c^\infty(\mathbb{R}^d)$ it follows that $D(H_0^*) = H^2(\mathbb{R}^d)$ and the equation

$$H_0^*\varphi_\pm = -\Delta\varphi_\pm = \mp i\varphi_\pm \tag{4.64}$$

has no solution in H^2, since $-\Delta$ is a symmetric operator. Therefore, Ker $(H_0^* \pm i) = \{0\}$ and H_0 is essentially selfadjoint on $C_c^\infty(\mathbb{R}^d)$.

To conclude this section, let us prove that $(-\Delta, H^2(\mathbb{R}^d))$ is a selfadjoint operator. We could use Theorem 4.41, by checking that $\Gamma(-\Delta)$ is closed. An easier proof will be provided by the following lemma.

Lemma 4.47. *Let $U : \mathcal{H}_1 \to \mathcal{H}_2$ be a unitary operator, and $(H, D(H))$ be a selfadjoint operator on $\mathcal{H}_1$. Then, $(UHU^*, UD(H))$ is selfadjoint on $\mathcal{H}_2$.*

Proof. Exercise. ∎

Let $\mathcal{H}_1 = \mathcal{H}_2 = L^2(\mathbb{R}^d)$, $H = -\Delta$ and $D(-\Delta) = H^2(\mathbb{R}^d)$. Choose $U = \mathcal{F}$, the Fourier transform on $L^2(\mathbb{R}^d)$. Then, $UHU^* = \mathcal{F} - \Delta\mathcal{F}^{-1} \equiv A_f$ with $f = k^2$ (multiplication operator). Being f measurable and real valued, selfadjointness immediately follows from Example 4.35.

4.3 Selfadjoint extensions

If a symmetric operator is nonnegative, there is a simple way of constructing a selfadjoint extension via the Friedrichs extension.

Definition 4.48. *A densely defined linear operator $(T, D(T))$ on a Hilbert space $\mathcal{H}$ is called nonnegative, $T \geqslant 0$, if:*

$$q_T(\psi) := \langle\psi, T\psi\rangle \geqslant 0 \qquad \textit{for all } \psi \in D(T). \tag{4.65}$$

It is called positive, $T > 0$, if $q_T(\psi) > 0$ for all $\psi \in D(T)$.

Remark 4.49. *The functional $q_T(\cdot)$ is called the quadratic form associated to T.*

Remark 4.50. *Lemma 4.34 implies that every nonnegative operator is symmetric.*

Proposition 4.51. *Let $(T, D(T))$ be a densely defined, linear, nonnegative operator. Given $\psi, \varphi \in D(T)$, let $\langle\varphi, \psi\rangle_T := \langle\varphi, T\psi\rangle + \langle\varphi, \psi\rangle$. Then, $\langle\cdot,\cdot\rangle_T$ defines a scalar product on $D(T)$.*

Proof. Exercise. ∎

Remark 4.52. *Therefore, $\|\cdot\|_T := \sqrt{\langle\cdot,\cdot\rangle_T}$ defines a norm on $D(T)$. Being T nonnegative, we have $\|\psi\|_T^2 = \langle\psi, T\psi\rangle \geqslant \langle\psi, \psi\rangle = \|\psi\|^2$.*

Definition 4.53. *The completion $\mathcal{H}_T$ of $D(T)$ is the set of equivalence classes of sequences in $D(T)$ which are Cauchy with respect to the $\|\cdot\|_T$ norm. Two sequences (ψ_n), (φ_n) belong to the same equivalence class in $\mathcal{H}_T$ if $\|\psi_n - \varphi_n\|_T \to 0$.*

Remark 4.54. *If a sequence is Cauchy with respect to the $\|\cdot\|_T$ norm, it is also Cauchy with respect to the $\|\cdot\|$ norm (recall Remark 4.52).*

Proposition 4.55. *Let $[(\varphi_n)_{n\in\mathbb{N}}] \in \mathcal{H}_T$, such that $\varphi_n \to \varphi \in \mathcal{H}$. The map $[(\varphi_n)_{n\in\mathbb{N}}] \mapsto \varphi$ is well defined and injective.*

Proof. Let us start by proving that the map is well defined. Let (φ_n), (ψ_n) be two sequences in $\mathcal{H}_T$, with $\|\varphi_n - \psi_n\|_T \to 0$. That is, the two sequences belong to the same equivalence class, and have the same limit φ in $\mathcal{H}$ since, by Remark 4.52, $\|\varphi_n - \psi_n\| \to 0$. Thus, the map $[(\varphi_n)_{n\in\mathbb{N}}] \mapsto \varphi$ is well defined.

Let us now prove that the map is injective. Suppose that (ψ_n), (φ_n) are two sequences in $\mathcal{H}_T$. Suppose that they converge to the same limit, $\|\varphi_n - \psi_n\| \to 0$. Then, we claim that $\|\varphi_n - \psi_n\|_T \to 0$, that is they belong to the same equivalence class. This follows from:

$$\begin{aligned}
\|\psi_n - \varphi_n\|_T^2 &= \langle\psi_n - \varphi_n, \psi_n - \varphi_n - (\psi_m - \varphi_m)\rangle_T + \langle\psi_n - \varphi_n, \psi_m - \varphi_m\rangle_T \\
&\leqslant \|\psi_n - \varphi_n\|_T \|\psi_n - \varphi_n - (\psi_m - \varphi_m)\|_T + \|(T+1)(\psi_n - \varphi_n)\|\|\psi_m - \varphi_m\| \\
&\leqslant C\|\psi_n - \varphi_n - (\psi_m - \varphi_m)\|_T + \|(T+1)(\psi_n - \varphi_n)\|\|\psi_m - \varphi_m\| \,,
\end{aligned} \tag{4.66}$$

where we used that every Cauchy sequence is bounded and that T is a symmetric operator. For any $\varepsilon > 0$, by choosing n, m large enough, $C\|\psi_n - \varphi_n - (\psi_m - \varphi_m)\|_T \leqslant \varepsilon/2$. Also, for any n we can choose m large enough so that $\|(T+1)(\psi_n - \varphi_n)\|\|\psi_m - \varphi_m\| \leqslant \varepsilon/2$. Therefore, $\|\psi_n - \varphi_n\|_T^2 \leqslant \varepsilon$, that is $\|\varphi_n - \psi_n\|_T \to 0$. ∎

Remark 4.56.
(i) This proposition is useful because it allows to identify $\mathcal{H}_T$ with a subspace $Q(T) \subset \mathcal{H}$, by associating to each equivalence class $[(\varphi_n)_n]$ its limit $\varphi \in \mathcal{H}$. Obviously, $D(T) \subset Q(T) \subset \mathcal{H}$ (every element of $D(T)$ is the limit of a sequence in $\mathcal{H}_T$: just take the constant sequence).

(ii) The scalar product $\langle\cdot,\cdot\rangle_T$, originally defined on $D(T)$, can be naturally extended to $Q(T)$. This is done by using the continuity of the scalar product on $\mathcal{H}$, and the fact that every element of $Q(T)$ is the limit of a sequence in $D(T)$. (Exercise).

Definition 4.57. *The subspace $Q(T)$ is called the form domain T. The extension of the quadratic form q_T to $Q(T)$ is defined as:*

$$q_T(\psi) := \langle\psi, \psi\rangle_T - \|\psi\|^2 \qquad \text{for all } \psi \in Q(T), \tag{4.67}$$

where $\langle\cdot,\cdot\rangle_T$ is the extension of the scalar product induced by T to $Q(T) \times Q(T)$.

Remark 4.58. *If $\psi \in D(T)$, then $q_T(\psi) = \langle\psi, T\psi\rangle$.*

Theorem 4.59 (Friedrichs extension)**.** *Let $(T, D(T))$ be a linear, symmetric, densely defined operator, bounded from below by γ: $\langle\psi, T\psi\rangle \geqslant \gamma$ for all $\psi \in D(T)$. Let:*

$$\begin{aligned}
D(\widetilde{T}) &:= D(T^*) \cap Q(T - \gamma) \\
\widetilde{T}\psi &:= T^*\psi \qquad \text{for all } \psi \in D(\widetilde{T}).
\end{aligned} \tag{4.68}$$

Then:

(i) $\widetilde{T}$ *is an extension of* T*, and* $\widetilde{T} \geqslant \gamma$*.*

(ii) $\widetilde{T}$ *is selfadjoint.*

(iii) $\widetilde{T}$ *is the only selfadjoint extension of* T *with* $D(\widetilde{T}) \subset Q(T-\gamma)$*.*

Proof. For simplicity, we shall set $\gamma = 0$. If not, replace T by $T-\gamma$ in what follows.

(i) We claim that $T \subset \widetilde{T}$. By Proposition 4.28, we have that $T \subset T^*$. Since $D(T^*) \supset D(T)$ and $Q(T) \supset D(T)$, then $D(T) \subset D(\widetilde{T})$. Moreover, $T = \widetilde{T}$ on $D(T)$, since $T = T^*$ on $D(T)$. This proves that $T \subset \widetilde{T}$. Let us now prove that $\widetilde{T} \geqslant 0$. Let $\psi \in D(\widetilde{T})$, and $(\psi_n) \subset D(T)$ such that $\psi_n \to \psi$ and (ψ_n) is Cauchy in $\|\cdot\|_T$. Then:

$$\langle \psi, \widetilde{T}\psi\rangle = \lim_{n\to\infty} \langle \psi_n, \widetilde{T}\psi\rangle \,. \tag{4.69}$$

We further write:

$$\begin{aligned} \langle \psi_n, \widetilde{T}\psi\rangle &= \langle \psi_n, T^*\psi\rangle \\ &= \langle T\psi_n, \psi\rangle \\ &= \langle T\psi_n, \psi_m\rangle + \langle T\psi_n, \psi - \psi_m\rangle \\ &= \langle T\psi_m, \psi_m\rangle + \langle T(\psi_n - \psi_m), \psi_m\rangle + \langle T\psi_n, \psi - \psi_m\rangle =: \mathrm{I} + \mathrm{II} + \mathrm{III}\,. \end{aligned} \tag{4.70}$$

Clearly, $\mathrm{I} \geqslant 0$. Pick $\varepsilon > 0$. Consider II. We have, for n, m large enough:

$$|\mathrm{II}| \leqslant \|\psi_n - \psi_m\|_T \|\psi_m\|_T \leqslant \frac{\varepsilon}{2}\,, \tag{4.71}$$

where we used that (ψ_n) is Cauchy in $\|\cdot\|_T$ and that every Cauchy sequence is bounded. Consider now III. We have, for m large enough:

$$|\mathrm{III}| \leqslant \|\psi_n - \psi_m\|_T \|\psi - \psi_m\| \leqslant \frac{\varepsilon}{2}\,. \tag{4.72}$$

Therefore, $\langle \psi, \widetilde{T}\psi\rangle \geqslant 0$.

(ii) Let us now show that $\widetilde{T}$ is selfadjoint. We shall use Theorem 4.41 (*ii*). Being $\widetilde{T} \geqslant 0$, $\widetilde{T}$ is symmetric. Our goal is to show that $\mathrm{Ran}\,(T+1) = \mathcal{H}$ (recall Remark 4.44). Recall:

$$D(\widetilde{T}) := \{\psi \in Q(T) \mid \exists \eta \in \mathcal{H} \quad \text{s.t.} \quad \langle \psi, T\varphi\rangle = \langle \eta, \varphi\rangle \quad \text{for all } \varphi \in D(T)\}\,, \tag{4.73}$$

where the vector η is unique (by density of $D(T)$ is $\mathcal{H}$). From the definition $\langle\cdot,\cdot\rangle_T$, this is equivalent to:

$$D(\widetilde{T}) = \{\psi \in Q(T) \mid \exists \eta \in \mathcal{H} \quad \text{s.t.} \quad \langle \psi, \varphi\rangle_T = \langle \eta, \varphi\rangle \quad \text{for all } \varphi \in D(T)\}\,. \tag{4.74}$$

Also, being $D(T)$ dense in $Q(T)$:

$$D(\widetilde{T}) = \{\psi \in Q(T) \mid \exists \eta \in \mathcal{H} \quad \text{s.t.} \quad \langle \psi, \varphi\rangle_T = \langle \eta, \varphi\rangle \quad \text{for all } \varphi \in Q(T)\}\,, \tag{4.75}$$

where now $\langle\cdot,\cdot\rangle$ is the extension of $\langle\cdot,\cdot\rangle_T$ to $Q(T)\times Q(T)$ (see Remark 4.56). By definition, $\widetilde{T}\psi = T^*\psi = \eta - \psi$ for all $\psi \in D(\widetilde{T})$, that is:

$$(\widetilde{T} + 1)\psi = \eta\,. \tag{4.76}$$

We will show that for every $\eta \in \mathcal{H}$ there exists ψ such that Eq. (4.76) holds true, *i.e.* that $\mathrm{Ran}\,(\widetilde{T}+1) = \mathcal{H}$, as claimed. For any $\eta \in \mathcal{H}$, the map $Q(T) \ni \varphi \mapsto \langle \eta, \varphi\rangle$ is a bounded linear functional on $Q(T)$, with respect to $\|\cdot\|$ and hence to $\|\cdot\|_T$. Thus, by Riesz theorem (Theorem 4.1), there exists $\xi \in Q(T)$ such that $\langle \eta, \varphi\rangle = \langle \xi, \varphi\rangle_T$ for all $\varphi \in Q(T)$. Comparing this equation with Eq. (4.75), we find that $\xi \in D(\widetilde{T})$. Also, by Eq. (4.76), we have $(\widetilde{T}+1)\xi = \eta$, which shows that $\mathrm{Ran}\,(\widetilde{T}+1) = \mathcal{H}$; therefore, Theorem 4.41 and Remark 4.44 imply that $\widetilde{T}$ is selfadjoint.

(iii) To conclude, let us prove uniqueness of the selfadjoint extension. Suppose that $\widehat{T}$ is another selfadjoint extension of T with $D(\widehat{T}) \subset Q(T)$. Let $\psi \in D(\widehat{T})$ and $\varphi \in D(T) \subset D(\widehat{T})$. Then:

$$\langle\varphi, (\widehat{T}+1)\psi\rangle = \langle(\widehat{T}+1)\varphi, \psi\rangle = \langle(T+1)\varphi, \psi\rangle = \overline{\langle\psi, (T+1)\varphi\rangle} = \overline{\langle\psi, \varphi\rangle_T} = \langle\varphi, \psi\rangle_T \,. \tag{4.77}$$

By density of $D(T)$ in $Q(T)$ and continuity of the scalar product, taking the complex conjugate:

$$\langle(\widehat{T}+1)\psi, \varphi\rangle = \langle\psi, \varphi\rangle_T \qquad \text{for all } \psi, \varphi \in D(\widehat{T}). \tag{4.78}$$

This implies that $\psi \in D(\widetilde{T})$, since $\psi \in Q(T)$ and $\langle\psi, \varphi\rangle_T = \langle\eta, \varphi\rangle$ holds for all $\varphi \in D(T) \subset D(\widehat{T})$, with $\eta = (\widehat{T}+1)\psi$. Thus, $D(\widehat{T}) \subset D(\widetilde{T})$. Moreover, by Eq. (4.76), $(\widetilde{T}+1)\psi = \eta$: therefore, $\widetilde{T}\psi = \widehat{T}\psi$ for all $\psi \in D(\widehat{T})$. In other words, $\widehat{T} \subset \widetilde{T}$. By taking the adjoint, and recalling Proposition 4.31, we also have $\widetilde{T}^* \subset \widehat{T}^*$, but then $\widetilde{T} = \widehat{T}$, since $\widetilde{T}^* = \widetilde{T}$ and $\widehat{T} = \widehat{T}^*$.

■

4.4 From quadratic forms to operators

Theorem 4.59 shows how to construct a selfadjoint extension of a nonnegative operator using the quadratic form associated with the operator. Later, we will be interested in defining a selfadjoint operator given a certain quadratic form.

Proposition 4.60. *Let $Q \subset \mathcal{H}$, let $s(\varphi, \psi)$ be a sesquilinear form on $Q \times Q$, with quadratic form $q(\psi) = s(\psi, \psi)$. Suppose that q is real valued and that q is semibounded: there exists $\gamma \in \mathbb{R}$ such that $q(\psi) \geqslant \gamma\|\psi\|^2$. Let:*

$$\langle\psi, \varphi\rangle_q := s(\psi, \varphi) + (1-\gamma)\langle\psi, \varphi\rangle \,. \tag{4.79}$$

Then, $\langle\cdot, \cdot\rangle_q$ is a scalar product on Q.

Proof. Exercise. ■

Remark 4.61. *Recall that a map $s(\cdot, \cdot) : Q \times Q \to \mathbb{C}$ is called a sesquilinear form if it is linear in the second variable and antilinear in the first variable.*

We would like to know whether $\langle\cdot, \cdot\rangle_q$ can be thought as the scalar product generated by an operator T with quadratic form $q_T = q$ and form domain $Q = Q(T)$. This is true, provided we make some assumptions on q.

Definition 4.62. *A real valued quadratic form q is called closable if for any sequence $(\psi_n) \subset Q$ such that $\|\psi_n\| \to 0$ and which is Cauchy with respect to $\|\cdot\|_q$ then $\|\psi_n\|_q \to 0$.*

Remark 4.63. *This is the analog of the property that allowed us to identify $\mathcal{H}_T$ with $Q(T) \subset \mathcal{H}$, recall Eq.(4.66).*

Let $\mathcal{H}_q$ be the completion of Q with respect to $\|\cdot\|_q$. For closable q, this space can be identified with a subspace of $\mathcal{H}$, that we shall denote by Q_q.

Definition 4.64. *The extension of q to Q_q is called the closure of q. The quadratic form is called closed if $Q_q = Q$.*

Theorem 4.65. *For every densely defined, closed, semibounded form $q : Q \to \mathbb{R}$ there is a unique selfadjoint operator T such that $Q = Q(T)$ and $q = q_T$. If s is the sesquilinear form associated with q, then:*

$$D(T) = \{\psi \in Q \mid \exists\eta \in \mathcal{H} \quad s.t. \quad s(\psi, \varphi) = \langle\eta, \varphi\rangle \quad \text{for all } \varphi \in Q\} \tag{4.80}$$

and $T\psi = \eta$.

Proof. For simplicity, we assume that $q \geqslant 0$ (that is, $\gamma = 0$). Since Q is dense, T is well defined (there cannot be two different η_1, η_2 with $s(\psi, \varphi) = \langle \eta_1, \varphi \rangle = \langle \eta_2, \varphi \rangle$ for all $\varphi \in Q$). By construction, we have $q_T(\psi) = q(\psi)$ for all $\psi \in D(T)$. It follows that T is symmetric and nonnegative. Proceeding as in the proof of Theorem 4.59, we find that $\mathrm{Ran}\,(T + 1) = \mathcal{H}$ and hence T is selfadjoint. Uniqueness is proven again as in the proof of Theorem 4.59. ∎

Definition 4.66. *A quadratic form is called bounded if $|q(\psi)| \leqslant C\|\psi\|^2$. The norm of q is given by:*

$$\|q\| = \sup_{\|\psi\|=1} |q(\psi)| \; . \tag{4.81}$$

Remark 4.67. *For bounded quadratic forms, the norm induced by $\langle \cdot, \cdot \rangle_q$ is equivalent to the standard norm. In this case, we obtain $\mathcal{H}_q = \mathcal{H}$ and the operator T associated with q is bounded, by the Hellinger-Toeplitz theorem (every symmetric operator defined on the full Hilbert space $\mathcal{H}$ is bounded). Together with the polarization identity, it is not difficult to check that a closed semibounded form q is bounded if and only if the corresponding selfadjoint operator T is bounded. In this case, $\|T\| = \|q\|$. In particular, it follows that:*

$$\|A\| = \sup_{\|\psi\|=1} |\langle \psi, A\psi \rangle| \tag{4.82}$$

for all symmetric operators.

5 The spectral theorem

5.1 The spectrum

Definition 5.1 (Resolvent, resolvent set and spectrum)**.** *Let $(T, D(T))$ be a linear operator on $\mathcal{H}$. We define the resolvent set of T as:*

$$\rho(T) := \{z \in \mathbb{C} \mid (T - z) : D(T) \to \mathcal{H} \quad \textit{is a bijection with continuous inverse.}\} \tag{5.1}$$

For $z \in \rho(T)$ we define the resolvent of T at z as:

$$R_z(T) := (T - z)^{-1} \in \mathcal{L}(\mathcal{H}) \; . \tag{5.2}$$

The spectrum of T is defined as the complement of the resolvent set:

$$\sigma(T) := \mathbb{C}\backslash\rho(T) \; . \tag{5.3}$$

Remark 5.2. *For closed operators, the continuity requirement in Eq. (5.1) can be dropped. This is a consequence of the closed graph theorem, stating that a linear map $T : X \to Y$ between two Banach spaces X, Y is continuous if and only if T is closed.*

Proposition 5.3. *If T is not closed, then $\rho(T) = \varnothing$.*

Proof. Suppose that $(T - z) : D(T) \to \mathcal{H}$ is a bijection. Then, $(T - z)$ is invertible, and it is not difficult to see that $\Gamma(T) = \Gamma(T - z) = \Gamma((T - z)^{-1})$ (modulo switching the order of the pairs in the definition of graph). Thus, if $\Gamma(T)$ is not closed, $\Gamma((T - z)^{-1})$ is not closed as well. This means that there exists $(\varphi_n) \subset \mathcal{H}$ such that $\varphi_n \to 0$ but $\lim_{n\to\infty}(T - z)^{-1}\varphi_n \neq 0$. Therefore, $(T - z)^{-1}$ is not continuous. Hence, $\rho(T) = \varnothing$. ∎

Definition 5.4. *Let $(T, D(T))$ be a closed, linear operator. Then, its spectrum $\sigma(T)$ is partitioned according to the following criteria:*

(a) $\sigma_p(T) := \{z \in \mathbb{C} \mid T - z \quad \textit{is not injective}\}$
is called the point spectrum, and it coincides with the set of eigenvalues of the operator.

(b) $\sigma_c(T) := \{z \in \mathbb{C} \mid T - z \quad \textit{is injective, not surjective, with dense range}\}$
is called the continuous spectrum.

(c) $\sigma_r(T) := \{z \in \mathbb{C} \mid T - z \quad \textit{is injective, not surjective, with no dense range}\}$
is called the residual spectrum.

Remark 5.5. *In conclusion, for closed operators:*

$$\sigma(T) = \sigma_p(T) \cup \sigma_c(T) \cup \sigma_r(T) \ , \tag{5.4}$$

and if $\dim \mathcal{H} < \infty$ *then* $\sigma(T) = \sigma_p(T)$ *is the set of eigenvalues.*

Example 5.6. *(i) Consider the position operator* $\hat{x}$*, with domain:*

$$\hat{D}(x) = \{\psi \in L^2(\mathbb{R}) \mid x\psi(x) \in L^2(\mathbb{R})\} \tag{5.5}$$

defined via $\hat{x} : \psi \mapsto x\psi$*. It follows that* $(\hat{x} - z)^{-1}$ *is the multiplication by the function* $(x-z)^{-1}$*, which is bounded for all* $z \in \mathbb{C}\backslash\mathbb{R}$*. Therefore,* $\sigma(\hat{x}) = \mathbb{R}$*.*
The map $(\hat{x} - \lambda)$ *has a dense range for all* $\lambda \in \mathbb{R}$*. To see this, for all* $\psi \in L^2$ *we define:*

$$\varphi_n := \chi_{\mathbb{R}\backslash[\lambda-\frac{1}{n},\lambda+\frac{1}{n}]}\frac{\psi}{x-\lambda} \ . \tag{5.6}$$

Then, $(x-\lambda)\varphi_n \to \psi$ *in* L^2*, and hence the range of* $x - \lambda$ *is dense. Therefore,* $\sigma(\hat{x}) = \sigma_c(\hat{x}) = \mathbb{R}$*.*

(ii) Let $U \in \mathcal{L}(\mathcal{H})$ *unitary. Then,* $\sigma(T) = \sigma(UTU^{-1})$*. This follows from the fact that* $T - z$ *is bijective if and only if* $U(T-z)U^{-1} = UTU^{-1} - z$ *is bijective.*
Therefore, the momentum operator $\hat{p} = -i\frac{d}{dx}$ *on* $L^2(\mathbb{R})$ *has real continuous spectrum,* $\sigma(\hat{p}) = \sigma_c(\hat{p}) = \mathbb{R}$*, since* $\hat{p} = \mathcal{F}\hat{x}\mathcal{F}^{-1}$ *and the Fourier transform is unitary.*

Theorem 5.7 (Properties of the resolvent and of the spectrum)**.** *Let* $(T, D(T))$ *be a densely defined operator on a Hilbert space* $\mathcal{H}$*. Then:*

(a) $\rho(T)$ *is open, that is the spectrum* $\sigma(T)$ *is closed.*

(b) The resolvent map:

$$\rho(T) \to \mathcal{L}(\mathcal{H}) \ , \qquad z \mapsto R_z(T) := (T-z)^{-1} \tag{5.7}$$

is analytic, that is $R_z(T)$ *can be written locally as a pointwise convergent series with coefficients in* $\mathcal{L}(\mathcal{H})$*.*

(c) If $T \in \mathcal{L}(\mathcal{H})$*, then* $|z| \leqslant \|T\|$ *for all* $z \in \sigma(T)$*. In particular, the spectrum is compact.*

(d) For $z, w \in \rho(T)$ *the first resolvent identity holds true:*

$$R_z(T) - R_w(T) = (z-w)R_w(T)R_z(T) \ . \tag{5.8}$$

In particular, the resolvents commute:

$$R_w(T)R_z(T) = R_z(T)R_w(T) \ . \tag{5.9}$$

The proof of this theorem is based on the following proposition.

Proposition 5.8 (Neumann series)**.** *Let* X *be a Banach space and* $T \in \mathcal{L}(X)$ *with* $\|T\| < 1$*. Then,* $1 - T$ *is continuously invertible and:*

$$(1-T)^{-1} = \sum_{n=0}^{\infty} T^n \ , \tag{5.10}$$

and:

$$\|(1-T)^{-1}\| \leqslant (1 - \|T\|)^{-1} \ . \tag{5.11}$$

Proof. Exercise. ■

Proof. (of Theorem 5.7.)

(a) Let $z_0 \in \rho(T)$ and $|z - z_0| < \|R_{z_0}\|^{-1}$. Then,

$$T - z = T - z_0 - (z - z_0) = (T - z_0)(1 - (z-z_0)R_{z_0}(T)) \ . \tag{5.12}$$

Then, the next proposition implies that $\|(z-z_0)R_{z_0}\| < 1$, which means that $1 - (z-z_0)R_{z_0}$ is continuously invertible, and hence $(T - z)$ is continuously invertible. Therefore, $z \in \rho(T)$.

(b) Thanks to the Neumann series :

$$R_z = (1 - (z - z_0)R_{z_0})^{-1} R_{z_0} = \sum_{n=0}^{\infty} (z - z_0)^n R_{z_0}^{n+1} , \tag{5.13}$$

where the coefficients $R_{z_0}^{n+1}$ belong to $\mathcal{L}(\mathcal{H})$.

(c) Let $|z| > \|T\|$. Then, $1 - \frac{T}{z}$ is invertible, and $T - z$ as well. Therefore, $z \in \rho(T)$.

(d) We have:

$$R_z(T) - R_w(T) = R_z(T)(T - w)R_w(T) - R_z(T)(T - z)R_w(T) = (z - w)R_z(T)R_w(T) . \tag{5.14}$$

■

Theorem 5.9 (Spectrum of a selfadjoint operator)**.** *Let $(H, D(H))$ be a selfadjoint operator. Then, $\sigma(H) \subset \mathbb{R}$ and for all $z \in \mathbb{C}\backslash\mathbb{R}$:*

$$\|(H - z)^{-1}\| \leqslant \frac{1}{|Im(z)|} . \tag{5.15}$$

Proof. Let $z = \lambda + i\mu$, with $\lambda, \mu \in \mathbb{R}$ and $\mu \neq 0$. Then, $(H - \lambda)/\mu$ is selfadjoint on $D(H)$ and, by Theorem 4.41:

$$\mathrm{Ker}\left(\frac{H - \lambda}{\mu} - i\right) = \mathrm{Ker}\,(H - \lambda - i\mu) = \{0\} \tag{5.16}$$

and:

$$\mathrm{Ran}\left(\frac{H - \lambda}{\mu} - i\right) = \mathrm{Ran}\,(H - \lambda - i\mu) = \mathcal{H} . \tag{5.17}$$

Eq. (5.16) implies that $H - z : D(H) \to \mathcal{H}$ is injective, while Eq. (5.17) implies that it is surjective, Therefore, $H - z : D(H) \to \mathcal{H}$ is a bijection. Moreover, the inverse is bounded, since:

$$\|(H - \lambda - i\mu)\psi\|^2 = \|(H - \lambda)\psi\|^2 + \|\mu\psi\|^2 \geqslant \mu^2\|\psi\|^2 , \tag{5.18}$$

which implies that $\|(H - z)^{-1}\| \leqslant 1/|\mu|$. Therefore, $z \in \rho(H)$. ■

Lemma 5.10. *Let $T : D(T) \to \mathcal{H}$ be a symmetric operator, and suppose that $\sigma(T) \subset \mathbb{R}$. Then, T is selfadjoint.*

Proof. If $\sigma(T) \subset \mathbb{R}$, then $T - z : D(T) \to \mathcal{H}$ is a bijection for all $z \in \mathbb{C}\backslash\mathbb{R}$. In particular, $\mathrm{Ran}(T - z) = \mathcal{H}$; being T symmetric, Theorem 4.41 implies that it is selfadjoint. ■

Remark 5.11. *Therefore, Theorem 5.9 and Lemma 5.10 imply that a symmetric operator T is selfadjoint if and only if $\sigma(T) \subset \mathbb{R}$.*

Lemma 5.12. *Let $T : D(T) \to \mathcal{H}$ be a closed, densely defined operator. Then,*

$$\|R_{z_0}(T)\| \geqslant dist(z_0, \sigma(T))^{-1} \tag{5.19}$$

for all $z_0 \in \mathbb{C}$.

Remark 5.13. *If T is bounded, we have $\{z \in \mathbb{C} \mid |z| > \|T\|\} \subset \rho(T)$.*

Proof. The radius of convergence of the Neumann series (5.13) is $\|R_{z_0}(T)\|^{-1}$. Also, the series cannot converge if $z \in \sigma(T)$; therefore, $\|R_{z_0}(T)\|^{-1} \leqslant \mathrm{dist}(z_0, \sigma(T))$. ■

Remark 5.14. *For selfadjoint operator, one actually has:*

$$\|(H - z)^{-1}\| = \frac{1}{dist(z, \sigma(H))} . \tag{5.20}$$

The next theorem provides a useful criterion to decide whether $z \in \sigma(A)$.

Theorem 5.15 (Weyl criterion.). *Let $T : D(T) \to \mathcal{H}$ be a closed densely defined operator. Suppose that there exists a sequence $\psi_n \in D(T)$ with $\|\psi_n\| = 1$ for all $n \in \mathbb{N}$ and such that $\|(T-z)\psi_n\| \to 0$ (such a sequence is known as a Weyl sequence at z). Then, $z \in \sigma(T)$. Conversely, if $z \in \partial\rho(T) \subset \sigma(T)$ (recall that $\sigma(T)$ is closed), then there exists a Weyl sequence at z.*

Proof. Let ψ_n be a Weyl sequence at z. If $z \in \rho(T)$, we would have

$$\|\psi_n\| = \|R_z(T)(T-z)\psi_n\| \leqslant \|R_z(T)\|\|(T-z)\psi_n\| \leqslant C\|(T-z)\psi_n\| \to 0 \; , \tag{5.21}$$

thus giving a contradiction. Hence, $z \in \sigma(T)$. On the other hand, suppose that $z \in \partial\sigma(T)$. Then, there exists a sequence $z_n \in \rho(T)$ with $z_n \to z$. From Theorem 5.12, we have $\|R_{z_n}(T)\| \to \infty$. Hence, there exists $(\varphi_n) \subset \mathcal{H}$ such that $\|R_{z_n}(T)\varphi_n\|/\|\varphi_n\| \to \infty$. Let $\psi_n = R_{z_n}(T)\varphi_n/\|R_{z_n}(T)\varphi_n\|$. Then, $\|\psi_n\| = 1$ for all n and:

$$\|(T-z)\psi_n\| \leqslant \|(T-z_n)\psi_n\| + |z-z_n|\|\psi_n\| = \frac{\|\varphi_n\|}{\|R_{z_n}(T)\varphi_n\|} + |z-z_n| \to 0 \; . \tag{5.22}$$

Hence ψ_n is a Weyl sequence. ∎

Another useful result is the following lemma, that establishes a relation between the spectrum of T and the one of its inverse T^{-1} (which is a densely defined operator on $\mathcal{H}$, if T is injective and Ran$T$ is dense).

Lemma 5.16. *Let T be injective and RanT be dense. Then, T^{-1} : RanT $\to \mathcal{H}$ is such that:*

$$\sigma(T^{-1})\backslash\{0\} = (\sigma(T)\backslash\{0\})^{-1} \; . \tag{5.23}$$

Furthermore, $T\psi = \lambda\psi$ if and only if $T^{-1}\psi = \lambda^{-1}\psi$.

Proof. Let $z \in \rho(T)\backslash\{0\}$. Since, for every $\varphi \in \mathcal{H}$:

$$(T^{-1} - z^{-1})(-z)TR_z(T)\varphi = (T-z)R_z(T)\varphi = \varphi \tag{5.24}$$

and for all $\psi \in D(T^{-1}) = \mathrm{Ran}\,(T)$ we can write $\psi = T\varphi$, we have:

$$\begin{aligned} (-z)TR_z(T)(T^{-1} - z^{-1})\psi &= (-z)TR_z(T)(T^{-1} - z^{-1})T\varphi \\ &= TR_z(T)(T-z)\varphi = T\varphi = \psi \; . \end{aligned} \tag{5.25}$$

This shows that $T^{-1} - z^{-1} : D(T^{-1}) \to \mathcal{H}$ is a bijection, with inverse given by $(-z)TR_z(T)$. Therefore, $z^{-1} \in \rho(T^{-1})$ and:

$$R_{z^{-1}}(T^{-1}) = -zTR_z(T) = -z - z^2R_z(T) \; . \tag{5.26}$$

Inverting the roles of T and T^{-1} we have that $z^{-1} \in \rho(T^{-1})\backslash\{0\}$ implies $z \in \rho(T)$. Thus, recalling that $\sigma(T) = \mathbb{C}\backslash\rho(T)$, we have that $z \in \sigma(T)\backslash\{0\}$ if and only if $z^{-1} \in \sigma(T^{-1})\backslash\{0\}$.

To prove the relation between point spectra, notice that if $T\psi = \lambda\psi$ holds, then $\lambda\psi$ is in the range of T, and hence ψ is in the range of T. Therefore, we can apply T^{-1} to both sides of the equation and obtain $\psi = \lambda A^{-1}\psi$, that is $\lambda^{-1}\psi = A^{-1}\psi$. ∎

5.2 Postulates of quantum mechanics

5.2.1 Observables

As discussed already in Section 1, quantum mechanical systems are described by vector in Hilbert spaces. Physically measurable quantities, called observables, correspond to self-adjoint operators on $\mathcal{H}$. The expected value associated with the self-adjoint operator T in the state ψ is given by $\langle\psi, T\psi\rangle$.

The vector ψ does not only determine the expectation of T, but also the distribution of its possible values. Let us consider the simple case in which A has the decomposition:

$$T = \sum_j \lambda_j P_{\varphi_j} \; , \tag{5.27}$$

with $\lambda_j \in \mathbb{R}$ the eigenvalues of T, and P_{φ_j} the orthogonal projection onto the normalized eigenvector φ_j. That is:

$$P_\varphi \psi = \langle \varphi, \psi \rangle \varphi \ . \tag{5.28}$$

One also uses the notation $P_\varphi = |\varphi\rangle\langle\varphi|$. Then, we have:

$$\langle \psi, T\psi \rangle = \sum_j \lambda_j |\langle \psi, \varphi_j \rangle|^2 \ . \tag{5.29}$$

Eq. (5.27) is called the spectral representation of the operator T. The spectral theorem for unbounded operators, that will be discussed later on, implies that the vectors φ_j form an ONB for $\mathcal{H}$ (this is clear if $\dim \mathcal{H} < \infty$, from the spectral theorem for matrices). In particular, $\sum_j |\langle \psi, \varphi_j \rangle|^2 = 1$. So far, we are assuming that the spectrum of the observable T coincides with its point spectrum. As we shall see, the spectral theorem will allow to generalize the expression (5.27) to cases in which $\sigma_{\mathrm{p}}(T) \neq \sigma(T)$, introducing the concept of projection-valued measure.

The interpretation of the identity (5.29) is the following: the eigenvalues λ_j are the possible values of the observable T and $|\langle \psi, \varphi_j \rangle|^2$ is the probability that, if the system is in the state ψ, a measurement of T gives the value λ_j. If for example $\psi = \varphi_j$, then a measurement of T will produce the value λ_j with probability 1. In general, however, ψ will be a linear combination of different φ_j's. Hence, a measurement of T will give different values with different probabilities. It makes sense, therefore, to define the variance of T in the state ψ by setting:

$$\Delta T_\psi = \langle \psi, (T - \langle \psi, T\psi \rangle)^2 \psi \rangle = \langle \psi, T^2 \psi \rangle - \langle \psi, T\psi \rangle^2 \ . \tag{5.30}$$

If, as before, $T = \sum_j \lambda_j P_{\varphi_j}$, a simple computation shows that:

$$\Delta T_\psi = \sum_j (\lambda_j - \langle \psi, T\psi \rangle)^2 |\langle \psi, \varphi_j \rangle|^2 \ . \tag{5.31}$$

An important property of quantum systems is that noncommuting observables cannot be measured simultaneously with arbitrary precision.

Theorem 5.17 (Heisenberg's uncertainty principle.)**.** *Let A, B be two self-adjoint operators acting on $\mathcal{H}$. Then, we have:*

$$\Delta A_\psi \Delta B_\psi \geqslant \frac{1}{4} |\langle \psi, [A, B]\psi \rangle|^2 \ . \tag{5.32}$$

Proof. For simplicitly, suppose that $\langle \psi, A\psi \rangle = \langle \psi, B\psi \rangle = 0$ (if not, redefine A, B by subtracting their average values on ψ). Then,

$$\langle \psi, [A, B]\psi \rangle = \langle \psi, AB\psi \rangle - \langle \psi, BA\psi \rangle = 2i \mathrm{Im} \langle \psi, AB\psi \rangle \ . \tag{5.33}$$

Therefore,

$$|\langle \psi, [A, B]\psi \rangle| \leqslant 2|\langle \psi, AB\psi \rangle| \leqslant 2|\langle A\psi, B\psi \rangle| \leqslant 2\|A\psi\|\|B\psi\| = 2(\Delta A_\psi)^{\frac{1}{2}} (\Delta B_\psi)^{\frac{1}{2}} \ . \tag{5.34}$$

That is:

$$\Delta A_\psi \Delta B_\psi \geqslant \frac{1}{4} |\langle \psi, [A, B]\psi \rangle|^2 \ . \tag{5.35}$$

∎

In particular, choosing $A = \hat{x}_i$ (position operator) and $B = \hat{p}_j \equiv -i\nabla_j$ (momentum operator), assuming that $\|\psi\|_2 = 1$, we obtain the relation:

$$\Delta x_{i,\psi} \Delta p_{j,\psi} \geqslant \frac{\delta_{ij}}{4} \ . \tag{5.36}$$

5.2.2 Time evolution

In every quantum system there is an observable that plays a particularly important role, the Hamiltonian. It generates time evolution via the Schrödinger equation:

$$i\partial_t \psi(t) = H\psi(t) \ . \tag{5.37}$$

If H is a bounded operator, the unique solution of the Schrödinger equation can be written as

$$\psi(t) = e^{-iHt}\psi(0) \ , \tag{5.38}$$

where the exponential of H is defined via its Taylor expansion, which converges for all times for bounded operators. More generally, if H has the spectral decomposition $H = \sum_j \lambda_j P_{\varphi_j}$, the exponential map is defined as:

$$e^{-iHt} = \sum_j e^{-i\lambda_j t} P_{\varphi_j} \ . \tag{5.39}$$

In particular, the solution of the Schrödinger equation associated to the initial datum $\psi(0) = \varphi_j$ is simply given by:

$$\psi(t) = e^{-i\lambda_i t}\varphi_i \ . \tag{5.40}$$

In this case, the expectation of an arbitrary self-adjoint operator T is given by:

$$\langle \psi(t), T\psi(t)\rangle = \langle \varphi_i, T\varphi_i\rangle \ , \tag{5.41}$$

and does not depend on t. Physically, the vectors $\psi(t) = e^{-i\lambda_j t}\varphi_j$ describe the same state for all times.

The spectral theorem will allow to introduce a spectral decomposition for any self-adjoint operators, even unbounded ones, and will allow to make sense of the exponential of the Hamilton operator. This in particular proves existence and uniqueness of the solution of the Schrödinger equation for general Hamiltonians.

5.3 Projection valued measures

As explained in Section 5.2.1, the spectral representation of a self-adjoint operator T is often useful in quantum mechanics. It tells us what are the possible outcomes of a measurement of the observable associated to T, and the probability with which possible values are assumed. Moreover, as we shall see later, it allows to define a functional calculus, that is to make sense of functions of operators. An important example is the unitary evolution e^{-iHT} associated to the Hamiltonian H.

In this section we will discuss how to define functions of self-adjoint operators, satisfying the properties:

$$(f+g)(T) = f(T) + g(T) \ , \qquad (fg)(T) = f(T)g(T) \ , \qquad \overline{f}(T) = f(T)^* \ . \tag{5.42}$$

The question is, for which class of functions f do we want to define $f(T)$. As long as f is a polynomial, we can define $f(T)$ by simply takinng powers of T. However, for several purposes, including solving the Schrödinger equation, taking powers of T is not enough. The next guess would be to consider functions that can be approximated by polynomials, like analytic functions. This works for bounded operators, but does not work well for unbounded operators: taking high powers of an unbounded operator typically makes the domain smaller and smaller.

A better approach consists in defining $\chi_\Omega(T)$ for all characteristic functions of Borel sets $\Omega \subset \mathbb{R}$, and then in using the bounded operators $\chi_\Omega(T)$ to construct measurable functions of A. The main advantage of this approach is that, since $\chi_\Omega^2 = \chi_\Omega = \overline{\chi}_\Omega$, the operator $\chi_\Omega(T)$ is an orthogonal projection, for all Borel sets $\Omega \subset \mathbb{R}$. On the other hand, we have to show how to use the orthogonal projections $\chi_\Omega(T)$ to define $f(T)$ for a general measurable function f, We start by discussing the second step, and we postpone the first.

Definition 5.18 (Projection-valued measure)**.** *Let $\mathcal{H}$ be a Hilbert space. Let $\mathcal{B}(\mathbb{R})$ be the Borel σ-algebra over $\mathbb{R}$. We say that a map $P : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ is a projection valued measure if:*

(i) $P(\Omega)^2 = P(\Omega) = P(\Omega)^*$, *for all* $\Omega \in \mathcal{B}(\mathbb{R})$.

(ii) $P(\mathbb{R}) = \mathbb{1}_{\mathcal{H}}$.

(iii) (Strong σ-additivity) If $\Omega = \bigcup_{n\in\mathbb{N}} \Omega_n$ *with* $\Omega_n \cap \Omega_m = \emptyset$ *for all* $n \neq m$*, then:*

$$\sum_{n\in\mathbb{N}} P(\Omega_n)\psi = \lim_{N\to\infty} \sum_{n=0}^{N} P(\Omega_n)\psi = P(\Omega)\psi \,, \tag{5.43}$$

for all $\psi \in \mathcal{H}$.

Example 5.19. *(a) Let $\mathcal{H} = \mathbb{C}^d$ and $T \in \mathcal{L}(\mathbb{C}^d)$ be a symmetric $d \times d$ matrix. Let $\lambda_1 < \lambda_2 < \ldots < \lambda_d$ be the eigenvalues of T, and $P_1, \ldots, P_d$ be the corresponding eigenprojectors (for simplicity, we assume the eigenvalues to be simple). Then, we can define:*

$$P(\Omega) = \sum_{j:\lambda_j\in\Omega} P_j \,. \tag{5.44}$$

It is easy to check that $P : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathbb{C}^d)$ is a projection-valued measure.

(b) Let $\mathcal{H} = L^2(\mathbb{R})$ and set $P(\Omega) = \chi_\Omega(x)$, with χ_Ω the characteristic function of the set Ω. Also in this case, P defines a projection valued measure on $\mathcal{H}$.

Remark 5.20. *In the definition of projection valued measure we request σ-additivity to hold in a strong sense (that is, after application to a fixed $\psi \in \mathcal{H}$), and not in norm (that is, taking the supremum over all ψ). This is an important point. Already in the simple example discussed above, where $P(\Omega) = \chi_\Omega(x)$ is a multiplication operator over $L^2(\mathbb{R})$, we do not have σ-additivity in norm, because the operator norm of multiplication operators is the L^∞ norm and thus:*

$$\|P(\Omega) - P(\Omega')\| = \|\chi_{\Omega\Delta\Omega'}\|_\infty = \begin{cases} 0 & \text{if } \mu(\Omega\Delta\Omega') = 0 \\ 1 & \text{if } \mu(\Omega\Delta\Omega') > 0 \end{cases} \tag{5.45}$$

where $\Omega\Delta\Omega' = (\Omega\backslash\Omega') \cup (\Omega'\backslash\Omega)$ is the symmetric difference of the two sets and $\mu(\cdot)$ denotes the Lebesgue measure on $\mathbb{R}$. Eq. (5.45) implies that σ-additivity does not hold in norm.

Remark 5.21. *In Definition 5.18, strong σ-additivity is actually equivalent to weak σ-additivity. In other words, Eq. (5.43) is equivalent to the condition:*

$$\sum_{n\in\mathbb{N}} \langle\psi, P(\Omega_n)\varphi\rangle = \langle\psi, P(\Omega)\varphi\rangle \,, \qquad \text{for all } \psi, \varphi \in \mathcal{H}. \tag{5.46}$$

This follows from the fact that, if P_n is a sequennce of orthogonal projections and P is an orthogonal projection with $w - \lim_{n\to\infty} P_n = P$ then, for any $\psi \in \mathcal{H}$:

$$\|P_n\psi\|^2 = \langle P_n\psi, P_n\psi\rangle = \langle\psi, P_n\psi\rangle \to \langle\psi, P\psi\rangle = \|P\psi\|^2 \,. \tag{5.47}$$

The weak convergence $P_n \to P$ together with $\|P_n\psi\| \to \|P\psi\|$ implies that $P_n\psi \to P\psi$. Hence, $P_n \to P$ strongly.

Next, we discuss some important properties of projection-valued measures.

Proposition 5.22. *The following properties are true.*

(i) $P(\emptyset) = 0$ *and* $P(\Omega^c) = 1 - P(\Omega)$

(ii) $P(\Omega_1 \cup \Omega_2) = P(\Omega_1) + P(\Omega_2) - P(\Omega_1 \cap \Omega_2)$.

(iii) $P(\Omega_1 \cap \Omega_2) = P(\Omega_1)P(\Omega_2)$

(iv) $P(\Omega_1) \leqslant P(\Omega_2)$ *if* $\Omega_1 \subset \Omega_2$.

Proof. Exercise. ∎

Definition 5.23 (Resolution of the identity). *For every projection-valued measure P we define the resolution of the identity $p : \mathbb{R} \to \mathcal{L}(\mathcal{H})$ via $p(\lambda) := P((-\infty; \lambda])$.*

Remark 5.24. *Then, $p(\lambda)$ is clearly an orthogonal projection for all $\lambda \in \mathbb{R}$. Monotonicity of P implies that $p(\lambda_1) \leqslant p(\lambda_2)$ if $\lambda_1 \leqslant \lambda_2$. Also, strong σ-additivity implies that for every $\psi \in \mathcal{H}$ and every sequence λ_n such that $\lambda_n \leqslant \lambda$ for all $n \in \mathbb{N}$ and such that $\lambda_n \to \lambda$ as $n \to \infty$,*

$$\lim_{n\to\infty} p(\lambda_n)\psi = p(\lambda)\psi \ . \tag{5.48}$$

That is, $s - \lim_{n\to-\infty} p(\lambda_n) = p(\lambda)$. Another consequence of strong σ-additivity is that:

$$s - \lim_{\lambda\to-\infty} p(\lambda) = 0 \ , \qquad s - \lim_{\lambda\to\infty} p(\lambda) = 1 \ . \tag{5.49}$$

As above, strong convergence of an orthogonal projection towards an orthogonal projection is equivalent to weak convergence.

Definition 5.25 (Measure and distribution associated to a projection-valued measure). *For any fixed $\psi \in \mathcal{H}$, we define the finite measure $\mu_\psi : \mathcal{B}(\mathbb{R}) \to [0; \infty)$ via $\mu_\psi(\Omega) = \langle \psi, P(\Omega)\psi \rangle$ for all $\Omega \in \mathcal{B}(\mathbb{R})$. The corresponding distribution function $d_\psi : \mathbb{R} \to [0; \infty)$ is given by $d_\psi(\lambda) = \mu_\psi((-\infty, \lambda])$.*

Remark 5.26. *Notice that $\mu_\psi(\Omega) \leqslant \|\psi\|^2$. Therefore, $d_\psi(\lambda) \leqslant \|\psi\|^2$. Also, $d_\psi(\lambda) = \|P((-\infty; \lambda])\psi\|^2 = \langle \psi, p(\lambda)\psi \rangle$.*

More generally, starting from the projection valued measure we can also introduce, for every $\psi, \varphi \in \mathcal{H}$, the complex measures $\mu_{\psi,\varphi}(\Omega) = \langle \psi, P(\Omega)\varphi \rangle$. They are related to the positive measures μ_ψ via the polarization identity:

$$\mu_{\psi,\varphi}(\Omega) = \frac{1}{4}[\mu_{\psi+\varphi}(\Omega) - \mu_{\psi-\varphi}(\Omega) + i\mu_{\psi-i\varphi}(\Omega) - i\mu_{\psi+i\varphi}(\Omega)] \ . \tag{5.50}$$

Also, they satisfy $|\mu_{\psi,\varphi}(\Omega)| \leqslant \|P(\Omega)\psi\|\|P(\Omega)\varphi\| \leqslant \|\psi\|\|\varphi\|$.

Remark 5.27. *Every distribution function is associated with a unique measure on the Borel σ-algebra $\mathcal{B}(\mathbb{R})$. One can also show that every resolution of the identity $p : \mathbb{R} \to \mathcal{L}(\mathcal{H})$ with the properties listed above is associated with a unique projection valued measure. This follows from the fact that the resolution of the identity allows us to define distribution functions d_ψ, which in turn can be used to reconstruct the measure μ_ψ. Then, it is easy to check that for all $\Omega \in \mathcal{B}(\mathbb{R})$ there is a unique orthogonal projection $P(\Omega)$ such that $\mu_\psi(\Omega) = \langle \psi, P(\Omega)\psi \rangle$. This follows from the fact that a linear operator can be reconstructed from the corresponding quadratic form, via the polarization identity.*

5.4 Functional calculus

We shall now use the projection valued measure $P : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ to define a functional calculus, that is a map from a class of functions to operators. We start with the set of measurable simple functions.

Definition 5.28 (Simple function.). *We say that the function f is a simple measurable function on $\mathbb{R}$ if*

$$f = \sum_{j=1}^{n} \alpha_j \chi_{\Omega_j} \ , \qquad n \in \mathbb{N} \ , \quad \alpha_j \in \mathbb{C} \ , \quad \Omega_j \in \mathcal{B}(\mathbb{R}) \ , \tag{5.51}$$

with $\Omega_j \cap \Omega_\ell = \varnothing$ for all $j \neq \ell$. We denote by $S(\mathbb{R})$ the space of simple measurable functions on $\mathbb{R}$ (or simple functions, for short).

Definition 5.29 (Functional calculus for simple functions.). *Let $f \in S$, $f = \sum_j \alpha_j \chi_{\Omega_j}$. Let $P : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ be a PVM. We define the functional calculus $\Phi : S \to \mathcal{L}(\mathcal{H})$ as:*

$$\Phi(f) := \sum_{j=1}^{n} \alpha_j P(\Omega_j) \ . \tag{5.52}$$

Remark 5.30. *We shall also define:*

$$\int f(\lambda)dp(\lambda) := \sum_{j=1}^{n} \alpha_j P(\Omega_j) \ . \tag{5.53}$$

Remark 5.31. *Notice that for arbitrary $\varphi, \psi \in \mathcal{H}$ we have:*

$$\langle \varphi, \Phi(f)\psi \rangle = \sum_{j=1}^{n} \alpha_j \langle \varphi, P(\Omega_j)\psi \rangle = \sum_{j=1}^{n} \alpha_j \mu_{\varphi,\psi}(\Omega_j) =: \int f(\lambda) d\mu_{\varphi,\psi}(\lambda) \ . \tag{5.54}$$

The right-hand side is the Lebesgue integral with respect to the complex measure $\mu_{\varphi,\psi}$ (which is just a linear combination of real measures, according to the polarization identity (5.50)).

Proposition 5.32. *The functional calculus $\Phi : (S, \|\cdot\|_\infty) \to \mathcal{L}(\mathcal{H})$ is a bounded linear map, with $\|\Phi\| \leqslant 1$.*

Proof. Linearity immediately follows from the definition. Let us prove boundedness. For $\psi \in \mathcal{H}$, we have:

$$\begin{aligned} \|\Phi(f)\psi\|^2 &= \Big\| \sum_{j=1}^{n} \alpha_j P(\Omega_j)\psi \Big\| \\ &= \sum_{j=1}^{n} |\alpha_j|^2 \|P(\Omega_j)\psi\|^2 \\ &= \sum_{j=1}^{n} |\alpha_j|^2 \mu_\psi(\Omega_j) \\ &= \int |f(\lambda)|^2 d\mu_\psi(\lambda) \ . \end{aligned} \tag{5.55}$$

In particular,

$$\|\Phi(f)\psi\| \leqslant \|f\|_\infty \|\psi\| \ , \tag{5.56}$$

where we used that $\mu_\psi(\Omega_j) \leqslant \|\psi\|^2$. Therefore:

$$\|\Phi\| := \frac{\|\Phi(f)\|}{\|f\|_\infty} \leqslant 1 \ . \tag{5.57}$$

■

Recall the notion of Borel measurable function on $\mathbb{R}$. We say that a function $f : \mathbb{R} \to \mathbb{C}$ is called Borel measurable if for any Borel set $\Omega \subset \mathcal{B}(\mathbb{C})$ one has $f^{-1}(\Omega) \subset \mathcal{B}(\mathbb{R})$. We denote by $\mathcal{M}_\mathrm{b}$ the space of bounded Borel functions.

Proposition 5.33. *The functional calculus $\Phi : (S, \|\cdot\|_\infty) \to \mathcal{L}(\mathcal{H})$ extends uniquely to a bounded linear map $\Phi : (\mathcal{M}_b, \|\cdot\|_\infty) \to \mathcal{L}(\mathcal{H})$.*

Proof. The proof is an application of Theorem 3.66. To begin, recall that any bounded measurable function can be approximated in L^∞ norm by simple function. Therefore, $\mathcal{S}$ is dense is $\mathcal{M}_\mathrm{b}$ with respect to the $\|\cdot\|_\infty$ norm. By Theorem 3.66, there is a unique extension of Φ to a bounded linear map $\Phi : \mathcal{M}_\mathrm{b} \to \mathcal{L}(\mathcal{H})$, with norm $\|\Phi\| \leqslant 1$. This defines Φ for all $f \in \mathcal{M}_\mathrm{b}$. ■

The Lebesgue integral of functions in $\mathcal{M}_\mathrm{b}$ is defined as the limit of the Lebesgue integral of simple functions. We have, for any $f \in \mathcal{M}_\mathrm{b}$:

$$\langle \psi, \Phi(f)\varphi \rangle = \int f(\lambda) d\mu_{\varphi,\psi}(\lambda) \ . \tag{5.58}$$

We shall also generalize the definition (5.53) by setting:

$$\int f(\lambda)dp(\lambda) = \Phi(f) \ . \tag{5.59}$$

Theorem 5.34. *Let $P : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ be a projection-valued measure. Then, $\Phi : \mathcal{M}_b \to \mathcal{L}(\mathcal{H})$ is a C^*-algebra homomorphism with norm one. Moreover, for every sequence $f_n \in \mathcal{M}_b$ and $f \in \mathcal{M}_b$ such that $f_n \to f$ pointwise and with $\|f_n\|_\infty$ bounded, we have $\Phi(f_n) \to \Phi(f)$ strongly.*

Remark 5.35. *The fact that Φ is a C^*-algebra homomorphism means that Φ is linear, that $\Phi(1) = 1$, that $\Phi(fg) = \Phi(f)\Phi(g)$ for all $f, g \in \mathcal{M}_b$ and that $\Phi(\overline{f}) = \Phi(f)^*$.*

Proof. For simple measurable functions, It is easy to check that Φ is linear, that it satisfies $\Phi(fg) = \Phi(f)\Phi(g)$ and that $\Phi(\overline{f}) = \Phi(f)^*$. For general bounded measurable f, these properties follow by approximation.

If $f_n \to f$ pointwise and $\|f\|_\infty \leqslant K$, then, by dominated convergence theorem:

$$\langle \varphi, \Phi(f_n)\psi\rangle = \int f_n(\lambda) d\mu_{\varphi,\psi}(\lambda) \to \int f(\lambda) d\mu_{\varphi,\psi}(\lambda) = \langle \varphi, \Phi(f)\psi\rangle . \tag{5.60}$$

This shows that $\Phi(f_n)\psi \to \Phi(f)\psi$ weakly, as $n \to \infty$. Moreover, again by dominated convergence theorem:

$$\|\Phi(f_n)\psi\|^2 = \int |f_n(\lambda)|^2 d\mu_\psi(\lambda) \to \int |f(\lambda)|^2 d\mu_\psi(\lambda) = \|\Phi(f)\psi\|^2 . \tag{5.61}$$

This implies that $\Phi(f_n)\psi \to \Phi(f)\psi$, which means that $\Phi(f_n) \to \Phi(f)$ strongly. ∎

Remark 5.36. *Since $\Phi : \mathcal{M}_b \to \mathcal{L}(\mathcal{H})$ is a C^*-homomorphism, we find that:*

$$\begin{aligned} \langle \Phi(g)\varphi, \Phi(f)\psi\rangle &= \langle \varphi, \Phi(g)^*\Phi(f)\psi\rangle \\ &= \langle \varphi, \Phi(\overline{g}f)\psi\rangle = \int (\overline{g}f)(\lambda) d\mu_{\varphi,\psi}(\lambda) = \int \overline{g}(\lambda) f(\lambda) d\mu_{\varphi,\psi} , \end{aligned} \tag{5.62}$$

for all $f, g \in \mathcal{M}_b$ and for all $\varphi, \psi \in \mathcal{H}$. Hence, we have:

$$\mu_{\Phi(g)\varphi,\Phi(f)\psi}(\Omega) = \langle \Phi(g)\varphi, \Phi(\chi_\Omega)\Phi(f)\psi\rangle = \int \chi_\Omega(\lambda)\overline{g}(\lambda) f(\lambda) d\mu_{\varphi,\psi}(\lambda) , \tag{5.63}$$

which implies that

$$d\mu_{\Phi(g)\varphi,\Phi(f)\psi} = \overline{g} f d\mu_{\varphi,\psi} . \tag{5.64}$$

Example 5.37. *Let $\mathcal{H} = \mathbb{C}^d$. Let $T \in \mathbb{C}^{d\times d}$ matrix. Let $\lambda_1 < \lambda_2 \ldots < \lambda_d$ be the eigenvalues of T, that we assume to be disjoint. Let $P_1, \ldots, P_d$ be the corresponding (rank 1) eigenprojectors. We already defined the projection valued measure associated to T as:*

$$P_T(\Omega) = \sum_{j:\lambda_j\in\Omega} P_j . \tag{5.65}$$

Let $\mathcal{M}_b$ be the space of bounded measurable functions on $\sigma(T)$. The functional calculus associated to this space of functions is the map $\Phi_T : \mathcal{M}_b \to \mathcal{L}(\mathbb{C}^d)$:

$$\Phi_T(f) = \sum_{j=1}^{d} f(\lambda_j) P_j . \tag{5.66}$$

We have, for any $\psi \in \mathbb{C}^d$:

$$\mu_\psi((-\infty, \lambda]) = \sum_{j:\lambda_j\leqslant\lambda} \|P_j\psi\|^2 \tag{5.67}$$

or equivalently:

$$\langle \psi, \Phi_T(f)\psi\rangle = \int f(\lambda) d\mu_\psi(\lambda) = \sum_{j=1}^{d} f(\lambda_j)\|P_j\psi\|^2 . \tag{5.68}$$

The above discussion allows to define a functional calculus for bounded functions. Next, we shall introduce a functional calculus for unbounded functions; this is relevant for unbounded self-adjoint operators (like the Laplacian).

For f unbounded, we expect $\Phi(f)$ to be an unbounded operator. Hence, we first have to define its domain. Recall that. for every bounded measurable function f, we have:

$$\|\Phi(f)\psi\|^2 = \int |f(\lambda)|^2 d\mu_\psi(\lambda) \ . \tag{5.69}$$

Hence, we expect that even for unbounded f, the operator $\Phi(f)$ can be applied on it, if $f \in L^2(\mathbb{R}, d\mu_\psi)$.

Definition 5.38. *Given $f : \mathbb{R} \to \mathbb{C}$, we define the domain of the functional calculus associated to f as:*

$$\mathcal{D}_f := \{\psi \in \mathcal{H} \mid f \in L^2(\mathbb{R}, d\mu_\psi)\} \ . \tag{5.70}$$

Proposition 5.39. *$\mathcal{D}_f$ is a linear subspace, dense in $\mathcal{H}$.*

Proof. For every Borel set $\Omega \subset \mathbb{R}$, we have $\mu_{\alpha\psi}(\Omega) = |\alpha|^2 \mu_\psi(\Omega)$ and:

$$\mu_{\psi+\varphi}(\Omega) \leqslant 2\mu_\psi(\Omega) + 2\mu_\varphi(\Omega) \ . \tag{5.71}$$

This bound implies that $f \in L^2(\mathbb{R}, d\mu_{\alpha\psi+\varphi})$ if $f \in L^2(\mathbb{R}, d\mu_\psi) \cap L^2(\mathbb{R}, d\mu_\varphi)$ and $\alpha \in \mathbb{C}$. Hence $\alpha\psi + \varphi \in \mathcal{D}_f$ if $\psi, \varphi \in \mathcal{D}_f$ and $\alpha \in \mathbb{C}$.

To prove that $\mathcal{D}_f$ is dense in $\mathcal{H}$ we proceed as follows. Let $\Omega_n = \{\lambda \in \mathbb{R} \mid |f(\lambda)| \leqslant n\}$. Then, for any $\psi \in \mathcal{H}$, we define $\psi_n = P(\Omega_n)\psi$. Since $d\mu_{\psi_n} = \chi_{\Omega_n} d\mu_\psi$, we have $\psi_n \in \mathcal{D}_f$ for any n. Moreover, since $\chi_{\Omega_n} \to 1$ pointwise, it follows that $\psi_n \to \psi$ strongly. This proves that $\mathcal{D}_f$ is dense. ∎

Proposition 5.40. *Let f be a Borel measurable function on $\mathbb{R}$. Let $\psi \in \mathcal{D}_f$. Let $(f_n) \subset \mathcal{M}_b$, such that $f_n \to f$ pointwise and such that $\|f_n\|_{L^2(\mathbb{R}, d\mu_\psi)}$ is bounded uniformly in n. Then, the limit $\lim_{n\to\infty} \Phi(f_n)\psi =: \Phi(f)\psi$ exists in $\mathcal{H}$ and does not depend on the sequence (f_n). It defines a linear map $\Phi(f)$ on $\mathcal{D}_f$, such that for all $\psi, \varphi \in \mathcal{D}_f$:*

$$\|\Phi(f)\psi\|^2 = \int |f(\lambda)|^2 d\mu_\psi(\lambda) \ , \qquad \langle \psi, \Phi(f)\varphi \rangle = \int f(\lambda) d\mu_{\psi,\varphi}(\lambda) \ . \tag{5.72}$$

Remark 5.41. *The first integral makes sense by definition of $\mathcal{D}_f$. The second integral also makes sense, since by Cauchy-Schwarz $L^2(\mathbb{R}, d\mu_\psi) \subset L^1(\mathbb{R}, d\mu_\psi)$ (recall that $d\mu_\psi$ is a finite measure, that is it has finite mass).*

Proof. By dominated convergence, we have $f_n \to f$ in $L^2(\mathbb{R}, d\mu_\psi)$. Therefore,

$$\|\Phi(f_n)\psi - \Phi(f_m)\psi\| = \|\Phi(f_n - f_m)\psi\|^2 = \int |f_n(\lambda) - f_m(\lambda)|^2 d\mu_\psi(\lambda) \tag{5.73}$$

which implies that $\Phi(f_n)\psi$ is a Cauchy sequence in $\mathcal{H}$. Therefore, the limit exists and we set:

$$\Phi(f)\psi := \lim_{n\to\infty} \Phi(f_n)\psi \ . \tag{5.74}$$

It is easy to see that the limit does not depend on the sequence. Therefore, it defines a linear map $\Phi(f)$ on $\mathcal{D}_f$, and moreover:

$$\|\Phi(f)\psi\|^2 = \int |f(\lambda)|^2 d\mu_\psi(\lambda) \tag{5.75}$$

for all $\psi \in \mathcal{D}_f$. Since μ_ψ is a finite measure, we have that $L^2(\mathbb{R}, d\mu_\psi) \subset L^1(\mathbb{R}, d\mu_\psi)$ and therefore:

$$\langle \psi, \Phi(f)\psi \rangle = \int f(\lambda) d\mu_\psi(\lambda) \ , \tag{5.76}$$

or more generally:

$$\langle \psi, \Phi(f)\varphi \rangle = \int f(\lambda) d\mu_{\psi,\varphi}(\lambda) \ . \tag{5.77}$$

∎

Remark 5.42. *We shall set:*

$$\Phi(f) =: \int f(\lambda)dp(\lambda) \ . \tag{5.78}$$

Theorem 5.43. *For every Borel measurable function $f : \mathbb{R} \to \mathbb{C}$, the operator $\Phi(f) : D_f \to \mathcal{H}$ is a normal operator (meaning that $D(\Phi(f)) = D(\Phi(f)^*)$) and $\|\Phi(f)\psi\| = \|\Phi(f)^*\psi\|$ for all $\psi \in D_f$. Moreover, for f, g Borel measurable and $\alpha, \beta \in \mathbb{C}$, we have $\Phi(f)^* = \Phi(\overline{f})$,*

$$\alpha\Phi(f) + \beta\Phi(g) \subset \Phi(\alpha f + \beta g) \ , \tag{5.79}$$

with $D(\alpha\Phi(f) + \beta\Phi(g)) = \mathcal{D}_{|f|+|g|}$ and:

$$\Phi(f)\Phi(g) \subset \Phi(fg) \tag{5.80}$$

where $D(\Phi(f)\Phi(g)) = \mathcal{D}_g \cap \mathcal{D}_{fg}$.

Proof. Fix a Borel measurable function $f : \mathbb{R} \to \mathbb{C}$. For $n \in \mathbb{N}$, let $\Omega_n = \{\lambda \in \mathbb{R} \mid |f(\lambda)| < n\}$ and let $f_n = f\chi_{\Omega_n}$. Then, $f_n \in \mathcal{M}_\mathrm{b}$ and thus $\Phi(f_n)^* = \Phi(\overline{f_n})$ by Theorem 5.34. For any $\varphi, \psi \in \mathcal{D}_f = \mathcal{D}_{\overline{f}} = \mathcal{D}_{|f|}$, we have:

$$\langle \varphi, \Phi(f)\psi \rangle = \lim_{n\to\infty} \langle \varphi, \Phi(f_n)\psi \rangle = \lim_{n\to\infty} \langle \Phi(\overline{f_n})\varphi, \psi \rangle = \langle \Phi(\overline{f})\varphi, \psi \rangle \ . \tag{5.81}$$

This implies that $D(\Phi(f)^*) \supset D(\Phi(\overline{f})) = D(\Phi(f)) = \mathcal{D}_f$, and that, for all $\varphi \in \mathcal{D}_f$, one has $\Phi(f)^*\varphi = \Phi(\overline{f})\varphi$. To conclude that $\Phi(f)^* = \Phi(\overline{f})$ we still have to show that $D(\Phi(f)^*) \subset \mathcal{D}_f$. To this end, let us fix $\varphi \in D(\Phi(f)^*)$. Then, there exists $\widetilde{\varphi} \in \mathcal{H}$ such that $\langle \varphi, \Phi(f)\psi \rangle = \langle \widetilde{\varphi}, \psi \rangle$ for all $\psi \in D(\Phi(f))$. By definition of $\Phi(f)$ we find, for every $\xi \in \mathcal{H}$:

$$\Phi(f)\Phi(\chi_{\Omega_n})\xi = \lim_{m\to\infty} \Phi(f_m)\Phi(\chi_{\Omega_n})\xi = \lim_{m\to\infty} \Phi(f\chi_{\Omega_m}\chi_{\Omega_n})\xi = \Phi(f_n)\xi \ , \tag{5.82}$$

since $\chi_{\Omega_m}\chi_{\Omega_n} = \chi_{\Omega_n}$ for all $m \geqslant n$. Hence, we find:

$$\langle \Phi(\overline{f}_n)\varphi, \xi \rangle = \langle \varphi, \Phi(f_n)\xi \rangle = \langle \varphi, \Phi(f)\Phi(\chi_{\Omega_n})\xi \rangle = \langle \widetilde{\varphi}, \Phi(\chi_{\Omega_n})\xi \rangle = \langle \Phi(\chi_{\Omega_n})\widetilde{\varphi}, \xi \rangle \tag{5.83}$$

for all $\xi \in \mathcal{H}$. This implies that $\Phi(\overline{f_n})\varphi = \Phi(\chi_{\Omega_n})\widetilde{\varphi}$ and therefore that:

$$\int |f_n(\lambda)|^2 d\mu_\varphi(\lambda) = \|\Phi(\overline{f_n})\varphi\|^2 = \|\Phi(\chi_{\Omega_n})\widetilde{\varphi}\|^2 \to \|\widetilde{\varphi}\|^2 \ , \qquad \text{as } n \to \infty. \tag{5.84}$$

Since f is the pointwise limit of f_n, the monotone convergence theorem implies that $f \in L^2(\mathbb{R}, d\mu_\psi)$, with:

$$\int |f(\lambda)|^2 d\mu_\varphi(\lambda) = \|\widetilde{\varphi}\|^2 \ . \tag{5.85}$$

Hence $\varphi \in \mathcal{D}_f$. We obtain $\Phi(f)^* = \Phi(\overline{f})$, for all Borel measurable functions f over $\mathbb{R}$. This also implies that:

$$\|\Phi(f)\psi\|^2 = \int |f(\lambda)|^2 d\mu_\psi(\lambda) = \|\Phi(\overline{f})\psi\|^2 = \|\Phi(f)^*\psi\|^2 \tag{5.86}$$

for all $\psi \in \mathcal{D}_f = \mathcal{D}_{\overline{f}}$. Hence, $\Phi(f)$ is a normal operator.

Next, we observe that for two Borel measurable functions $f, g : \mathbb{R} \to \mathbb{C}$ and for $\alpha, \beta \in \mathbb{C}$, we have $D(\alpha\Phi(f) + \beta\Phi(g)) = D(\Phi(f)) \cap D(\Phi(g)) = \mathcal{D}_f \cap \mathcal{D}_g = \mathcal{D}_{|f|+|g|}$, because $|f| + |g| \in L^2(\mathbb{R}, d\mu_\psi)$ if and only if $f \in L^2(\mathbb{R}, d\mu_\psi)$ and $g \in L^2(\mathbb{R}, d\mu_\psi)$. Since $|\alpha f + \beta g| \leqslant C(|f| + |g|)$, it is easy to check that $\mathcal{D}_{|f|+|g|} \subset \mathcal{D}_{\alpha f+\beta g}$. It remains to show that $\alpha\Phi(f)\psi + \beta\Phi(g)\psi = \Phi(\alpha f + \beta g)\psi$ for all $\psi \in \mathcal{D}_{|f|+|g|}$. To this end, for $n \in \mathbb{N}$, set:

$$\Omega_n = \{\lambda \in \mathbb{R} \mid |f(\lambda)| + |g(\lambda)| \leqslant n\} \ , \qquad f_n = f\chi_{\Omega_n} \ , \qquad g_n = g\chi_{\Omega_n} \ . \tag{5.87}$$

For $\psi \in \mathcal{D}_{|f|+|g|}$, we have $\Phi(f_n)\psi \to \Phi(f)\psi$, $\Phi(g_n)\psi \to \Phi(g)\psi$, $\alpha\Phi(f_n)\psi + \beta\Phi(g_n)\psi = \Phi(\alpha f_n + \beta g_n)\psi = \Phi((\alpha f + \beta g)\chi_{\Omega_n})\psi \to \Phi(\alpha f + \beta g)\psi$.

Finally, we prove Eq. (5.80). To this end, assume first that g is bounded. Then:

$$\begin{aligned} D(\Phi(f)\Phi(g)) &= \{\psi \in \mathcal{H} \mid \Phi(g)\psi \in \mathcal{D}_f\} = \{\psi \in \mathcal{H} \mid f \in L^2(\mathbb{R}, d\mu_{\Phi(g)\psi})\} \\ &= \{\psi \in \mathcal{H} \mid f \in L^2(\mathbb{R}, |g|^2 d\mu_\psi)\} \\ &= \{\psi \in \mathcal{H} \mid fg \in L^2(\mathbb{R}, d\mu_\psi)\} = D(\Phi(fg)) \equiv \mathcal{D}_{fg} \ . \end{aligned} \tag{5.88}$$

Thus, for all $\psi \in D(\Phi(fg))$, we have $\Phi(g)\psi \in D(\Phi(f))$ and (recalling that $f_n = \chi_{\Omega_n} f$, with $\Omega_n = \{\lambda \in \mathbb{R} \mid |f(\lambda)| \leqslant n\}$):

$$\Phi(f)\Phi(g)\psi = \lim_{n\to\infty} \Phi(f_n)\Phi(g)\psi = \lim_{n\to\infty} \Phi(f_n g)\psi = \Phi(fg)\psi \ . \tag{5.89}$$

This shows that, if g is bounded, $\Phi(fg) = \Phi(f)\Phi(g)$. If now g is not necessarily bounded, we define $\Omega_n = \{\lambda \in \mathbb{R} \mid |g(\lambda)| \leqslant n\}$, $g_n = g\chi_{\Omega_n}$. Suppose that $\psi \in \mathcal{D}_g \cap \mathcal{D}_{fg}$. Then, we have $\Phi(g_n)\psi \to \Phi(g)\psi$. Moreover, $\psi \in \mathcal{D}_{fg_n} = D(\Phi(fg_n)) = D(\Phi(f)\Phi(g_n))$ implies (from the case considered above) that $\Phi(f)\Phi(g_n)\psi = \Phi(fg_n)\psi \to \Phi(fg)\psi$. Since $\Phi(f)$ is closed (which follows from $\overline{\Phi(f)} = \Phi(f)^{**} = \Phi(\bar{\bar{f}}) = \Phi(f)$), this shows that $\Phi(g)\psi \in \mathcal{D}_f$ and that $\Phi(f)\Phi(g)\psi = \Phi(fg)\psi$. ∎

5.5 Construction of projection valued measures

The discussion of the previous section allowed us to define the functional calculus, given a family of projection valued measures. In particular, given $P : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$, we can associate a self-adjoint operator $T = \int \lambda dp(\lambda)$ with domain:

$$D(T) = \{\psi \in \mathcal{H} \mid \int \lambda^2 d\mu_\psi(\lambda) < \infty\} \ . \tag{5.90}$$

The question we shall consider is this section is: given a self-adjoint operator T, is it possible to find a projection valued measure P such that T can be expressed as $T = \int \lambda dp(\lambda)$? If yes, this provides a spectral representation for the operator T. We shall first answer this question for the resolvent of T, $R_z(T)$, and later for T.

Definition 5.44. *Let $\mu(\cdot) : \mathcal{B}(\mathbb{R}) \to \mathbb{R}$ be a Borel measure. For all $z \in \mathbb{C}\backslash supp\mu$, we define the Borel transform F of μ as:*

$$F(z) = \int \frac{1}{\lambda - z} d\mu(\lambda) \ . \tag{5.91}$$

Remark 5.45. *The support of the measure is defined as:*

$$supp\mu = \{\lambda \in \mathbb{R} \mid \mu(O) > 0 \quad \textit{for all open neighbourhoods } O \textit{ of } \lambda\} \ . \tag{5.92}$$

Remark 5.46. *Since*

$$ImF(z) = Imz \int \frac{1}{|\lambda - z|^2} d\mu(\lambda) \ , \tag{5.93}$$

we conclude that $z \mapsto F(z)$ is a holomorphic function mapping the upper half complex plane $\{z \in \mathbb{C} \mid Imz > 0\}$ into itself. Such functions are called Herglotz or Nevanlinna functions.

Theorem 5.47. *Every Herglotz function F has the form:*

$$F(z) = bz + a + \int_{\mathbb{R}} \Big[\frac{1}{\lambda - z} - \frac{\lambda}{1 + \lambda^2}\Big] d\mu(\lambda) \ , \tag{5.94}$$

with $b \geqslant 0$, $a \in \mathbb{R}$ and μ a Borel measure on $\mathbb{R}$ with:

$$\int \frac{1}{1 + \lambda^2} d\mu(\lambda) < \infty \ . \tag{5.95}$$

Conversely, for every $b \geqslant 0$, $a \in \mathbb{R}$ and for every Borel measure μ satisfying Eq. (5.95), the function (5.94) is holomorphic on $\mathbb{C}\backslash supp\mu$. It is such that $F(\bar{z}) = \overline{F(z)}$ and:

$$ImF(z) = Imz \Big[b + \int \frac{1}{|\lambda - z|^2} d\mu(\lambda)\Big] \tag{5.96}$$

for all $z \in \mathbb{C}\backslash supp\mu$. Moreover, if F is a Herglotz function, the triple (a, b, μ) satisfying (5.94) is uniquely determined by

$$a = ReF(i)\ , \qquad b = ImF(i) - \int \frac{1}{\lambda^2+1} d\mu(\lambda) \tag{5.97}$$

and by the Stieltjes inversion formula:

$$\frac{1}{2}\big[\mu((\lambda_1,\lambda_2)) + \mu([\lambda_1,\lambda_2])\big] = \lim_{\varepsilon\to 0^+} \frac{1}{\pi}\int_{\lambda_1}^{\lambda_2} ImF(\lambda+i\varepsilon)d\lambda\ . \tag{5.98}$$

Remark 5.48. *That is, this theorem allows us to construct a measure starting from a Herglotz function. Later, we shall take as Herglotz function the quadratic form associated to $R_z(T)$, and use this theorem to construct the projection valued measure.*

Proof. Let $f(z) = i(i-z)/(i+z)$. It is easy to see that f is holomorphic in $\mathbb{D} = \{z \in \mathbb{C} \mid |z| < 1\}$ and that it takes values in $\mathbb{C}_+ = \{z \in \mathbb{C} \mid \text{Im}z > 0\}$. More precisely, f maps the lower disk $\mathbb{D}_- = \{z \in \mathbb{D} \mid \text{Im}z < 0\}$ into $\mathbb{C}_+\backslash\mathbb{D}$ and it maps the upper disk $\mathbb{D}_+ = \{z \in \mathbb{D} \mid \text{Im}z > 0\}$ into itself. Also, the map is invertible, and $f^{-1} : \mathbb{C}_+ \to \mathbb{D}$ is simply $f^{-1}(z) = f(z)$. Let:

$$C(z) := -iF(f(z)) \tag{5.99}$$

One easily sees that if the map F is Herglotz then C is a Caratheodory function, that is an holomorphic function on $\mathbb{D}$ with $\text{Re}\, C(z) \geqslant 0$ for all $z \in \mathbb{D}$. Also, we can invert Eq. (5.99) and obtain:

$$F(z) = iC(f(z))\ , \tag{5.100}$$

which shows that if C is a Caratheodory function then F is a Herglotz function. Thus, F is Herglotz if and only if C is Caratheodory.

We claim now that every Caratheodory function $C : \mathbb{D} \to \mathbb{C}$ has the form:

$$C(z) = ic + \int_{-\pi}^{\pi} \frac{e^{i\varphi}+z}{e^{i\varphi}-z} d\nu(\varphi) \tag{5.101}$$

for $c = \text{Im}\, C(0) \in \mathbb{R}$ and for a finite measure ν, with:

$$\int_{-\pi}^{\pi} d\nu(\varphi) = \text{Re}\, C(0)\ . \tag{5.102}$$

To prove this claim, let $C : \mathbb{D} \to \mathbb{C}$ be a Caratheodory function and fix $0 < r < 1$. Fix $z \in \mathbb{D}$ with $|z| < r$. By Cauchy theorem, we have the identity:

$$\begin{aligned} C(z) &= \frac{1}{4\pi i}\int_{|\xi|=r} \Big[\frac{\xi+z}{\xi-z} + \frac{r^2/\xi + z}{r^2/\xi - \overline{z}}\Big] C(\xi)\frac{d\xi}{\xi} \\ &= \frac{1}{2\pi i}\int_{|\xi|=r} \text{Re}\,\Big(\frac{\xi+z}{\xi-z}\Big) C(\xi)\frac{d\xi}{\xi} \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \text{Re}\Big(\frac{re^{i\varphi}+z}{re^{i\varphi}-z}\Big) C(re^{i\varphi})d\varphi\ . \end{aligned} \tag{5.103}$$

We take the real part:

$$\text{Re}\, C(z) = \int_{-\pi}^{\pi} P_{|z|/r}(\arg(z) - \varphi) d\nu_r(\varphi)\ , \tag{5.104}$$

where we set:

$$P_r(\varphi) = \text{Re}\,\frac{1+re^{i\varphi}}{1-re^{i\varphi}}\ , \qquad d\nu_r(\varphi) = \text{Re}\, C(re^{i\varphi})\frac{d\varphi}{2\pi}\ . \tag{5.105}$$

Notice that $d\nu_r$ is a Borel measure, thanks to $\text{Re}\, C \geqslant 0$. Setting $z = 0$, we obtain:

$$\int_{-\pi}^{\pi} d\nu_r(\varphi) = \text{Re}\, C(0) < \infty\ , \tag{5.106}$$

uniformly in $r < 1$. This implies that there exists a sequence $r_n \to 1$ and finite Borel measure ν on $[-\pi;\pi]$ such that, as $n \to \infty$:

$$\int_{[-\pi;\pi]} f(\varphi) d\nu_{r_n}(\varphi) \to \int_{[-\pi;\pi]} f(\varphi) d\nu(\varphi) \tag{5.107}$$

for all $f \in C([-\pi;\pi])$. In fact, uniform boundedness implies the existence of a subsequence of measures converging vaguely, that is after testing with compactly supported continuous functions; this can be proven approximating compactly supported continuous functions with simple functions, and from the convergence of $\nu_{r_n}([\lambda_1;\lambda_2])$ on subsequences, for any interval $[\lambda_1;\lambda_2]$.

For $|z| < 1$, we also have $P_{|z|/r}(\arg z - \varphi) \to P_{|z|}(\arg z - \varphi)$ as $r \to 1$, uniformly in φ. We conclude that:

$$\begin{aligned}
\operatorname{Re} C(z) &= \lim_{n\to\infty} \int_{-\pi}^{\pi} P_{|z|/r_n}(\arg(z) - \varphi) d\nu_{r_n}(\varphi) \\
&= \lim_{n\to\infty} \int_{-\pi}^{\pi} P_{|z|}(\arg(z) - \varphi) d\nu_{r_n}(\varphi) \\
&= \int_{-\pi}^{\pi} P_{|z|}(\arg(z) - \varphi) d\nu(\varphi) \\
&= \int_{-\pi}^{\pi} \operatorname{Re}\Big[\frac{e^{i\varphi} + z}{e^{i\varphi} - z}\Big] d\nu(\varphi) \ .
\end{aligned} \tag{5.108}$$

The claim (5.101) now follows because every holomorphic function is determined by its real part, up to an imaginary constant. In fact, let $f(z)$ be a holomorphic function, such that $\mathrm{Re} f = 0$. Then, the Cauchy-Riemann equation implies that $\mathrm{Im} f =$ constant. Therefore, $f(z) = ic$. This proves Eq. (5.101).

Let now F be an arbitrary Herglotz function and C the corresponding Caratheodory function, defined as in (5.99). Then we can write $F(z) = iC(i(i-z)/(i+z))$, or $F(z) = i\widetilde{C}((i-z)/(i+z))$ for the function $\widetilde{C}(z) = C(iz)$, which is also a Caratheodory function and therefore admits a representation as in (5.101). Hence:

$$\begin{aligned}
F(z) &= i\widetilde{C}((i-z)/(i+z)) \\
&= -c + i\int_{[-\pi;\pi]} \frac{e^{i\varphi} + \frac{i-z}{i+z}}{e^{i\varphi} - \frac{i-z}{i+z}} d\nu(\varphi) \\
&= -c + i\int_{[-\pi;\pi]} \frac{i(e^{i\varphi}+1) + z(e^{i\varphi}-1)}{i(e^{i\varphi}-1) + z(e^{i\varphi}+1)} d\nu(\varphi) \\
&= -c + i\int_{[-\pi;\pi]} \frac{i + z\frac{e^{i\varphi}-1}{e^{i\varphi}+1}}{i\frac{(e^{i\varphi}-1)}{e^{i\varphi}+1} + z} d\nu(\varphi) \\
&= -c + \nu(\{-\pi,\pi\})z + \int_{-\infty}^{\infty} \frac{1+\lambda z}{\lambda - z} d\widetilde{\mu}(\lambda) \ ,
\end{aligned} \tag{5.109}$$

where we changed variables, setting $\lambda = f(\varphi)$ with the function $f : (-\pi;\pi) \to \mathbb{R}$ defined through $f(\varphi) = i(1-e^{i\varphi})/(1+e^{i\varphi})$, we introduced the Borel measure $\widetilde{\mu}$ over $\mathbb{R}$ such that $\widetilde{\mu}(A) = \nu(f^{-1}(A))$, and we took into account the weight of ν at $\pm\pi$. Setting $a = -c$, $b = \nu(\{\pm\pi\})$ and $d\mu(\lambda) = (1+\lambda^2)d\widetilde{\mu}(\lambda)$, we obtain the desired representation of F.

Suppose now that a Herglotz function F has the form (5.94). Then, we find

$$\begin{aligned}
&\lim_{\varepsilon\to 0^+}\frac{1}{\pi}\int_{\lambda_1}^{\lambda_2}\operatorname{Im}F(\lambda+i\varepsilon)d\lambda \\
&\quad=\lim_{\varepsilon\to 0}\frac{1}{\pi}\int_{\lambda_1}^{\lambda_2}\int\frac{\varepsilon}{(x-\lambda)^2+\varepsilon^2}d\mu(x)d\lambda \qquad (5.110)\\
&\quad=\lim_{\varepsilon}\int\frac{1}{\pi}\int_{\lambda_1}^{\lambda_2}\frac{\varepsilon}{(x-\lambda)^2+\varepsilon^2}d\lambda d\mu(x)\\
&\quad=\lim_{\varepsilon\to 0}\int\frac{1}{\pi}[\operatorname{arctg}((\lambda_2-x)/\varepsilon)-\operatorname{arctg}((\lambda_1-x)/\varepsilon)]d\mu(x)\\
&\quad=\int\frac{1}{2}[\chi_{[\lambda_1,\lambda_2]}(x)+\chi_{(\lambda_1,\lambda_2)}(x)]d\mu(x)\\
&\quad=\frac{1}{2}(\mu([\lambda_1;\lambda_2])+\mu((\lambda_1;\lambda_2))) \qquad (5.111)
\end{aligned}$$

where we used the dominated convergence theorem to take the limit $\varepsilon\to 0$, since

$$\frac{1}{\pi}[\operatorname{arctg}((\lambda_2-x)/\varepsilon)-\operatorname{arctg}((\lambda_1-x)/\varepsilon)]\to\frac{1}{2}[\chi_{[\lambda_1,\lambda_2]}(x)+\chi_{(\lambda_1,\lambda_2)}(x)] \qquad (5.112)$$

pointwise, and

$$\frac{1}{\pi}[\operatorname{arctg}((\lambda_2-x)/\varepsilon)-\operatorname{arctg}((\lambda_1-x)/\varepsilon)]\leqslant\frac{C}{1+x^2} \qquad (5.113)$$

for an appropriate constant C depending on λ_1,λ_2. The formula for a,b follows evaluating (5.94) at $z=i$. ■

The next proposition allows to establish a link with the resolvent of selfadjoint operators.

Proposition 5.49. *Let $(T,D(T))$ be a selfadjoint operator. Let $F_\psi^T(z)$ be the quadratic form associated to $R_z(T)$:*

$$F_\psi^T(z)=\langle\psi,R_z(T)\psi\rangle\ . \qquad (5.114)$$

Then, $F_\psi^T(z)$ is a Herglotz function, and it can be written as:

$$F_\psi^T(z)=\int_{\mathbb{R}}\frac{1}{\lambda-z}d\mu(\lambda)\ , \qquad (5.115)$$

for a unique finite Borel measure μ.

Proof. By the analyticity of $z\mapsto R_z(T)$, recall Theorem 5.7, we see that $F_\psi^T(z)$ is analytic in $\rho(T)$, and in particular in $\mathbb{C}_+$. Also, $F_\psi^T(z)$ maps $\mathbb{C}_+$ into itself, since:

$$\begin{aligned}
\operatorname{Im}F_\psi^T(z) &= \frac{1}{2i}[\langle\psi,R_z(T)\psi\rangle-\overline{\langle\psi,R_z(T)\psi\rangle}]\\
&= \frac{1}{2i}\langle\psi,(R_z(T)-R_z(T)^*)\psi\rangle\\
&= \frac{1}{2i}\langle\psi,(R_z(T)-R_{\overline{z}}(T))\psi\rangle\\
&= \frac{z-\overline{z}}{2i}\langle\psi,R_{\overline{z}}(T)R_z(T)\psi\rangle \qquad (5.116)
\end{aligned}$$

where in the last step we used Eq. (5.8). Therefore, $\operatorname{Im}F_\psi^T(z)=\operatorname{Im}z\|R_z(T)\psi\|^2\geqslant 0$ for $z\in\mathbb{C}_+$. Hence, $F_\psi^T(z)$ is a Herglotz function, which means that it can be rewritten as in Eq. (5.94), for some (a,b,μ). We clam that $a=b=0$, and that μ is a finite Borel measure. In fact, by Eq. (5.15) one has $\|R_z(T)\|\leqslant 1/|\operatorname{Im}z|$, which implies that

$$|yF_\psi^T(iy)|\leqslant\|\psi\|^2\ ,\qquad\forall y\in\mathbb{R}\ . \qquad (5.117)$$

This implies that $F_\psi^T(z)$ has the form:

$$F_\psi^T(z) = \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu(\lambda) \ . \tag{5.118}$$

The fact that the measure is finite, $\mu(\mathbb{R}) < \infty$, follows from

$$y\mathrm{Im}F(iy) = \int \frac{y^2}{\lambda^2 + y^2} d\mu(\lambda) \leqslant \|\psi\|^2 \ , \tag{5.119}$$

and from dominated convergence. ■

Remark 5.50. *Moreover, theorem 5.47 tells us that we can reconstruct the Borel measure associated to F_ψ^T by the inverse Stieltjes transform. In particular, the distribution function $d_\psi^T(\lambda) = \mu((-\infty;\lambda])$ is:*

$$d_\psi^T(\lambda) = \lim_{\delta \to 0^+} \lim_{\varepsilon \to 0^+} \frac{1}{\pi} \int_{-\infty}^{\lambda+\delta} Im\, F_\psi^T(t + i\varepsilon) dt \ . \tag{5.120}$$

Since this is a distribution function, it can be used to reconstruct the corresponding Borel measure $\mu_\psi^T : \mathcal{B}(\mathbb{R}) \to [0;\infty)$ (write the measure of any Borel set via the complement, countable union or intersection of sets $(-\infty, \lambda]$, $\lambda \in \mathbb{R}$).

We are now left with constructing the projection valued measure. For every $\Omega \in \mathcal{B}(\mathbb{R})$, we define the quadratic form:

$$q_\Omega^T(\psi) = \mu_\psi^T(\Omega) = \int \chi_\Omega(\lambda) d\mu_\psi^T(\lambda) \ . \tag{5.121}$$

Through the polarization identity, we also find a sesquilinear form $s_\Omega^T(\varphi, \psi)$ such that $q_\Omega^T(\psi) = s_\Omega^T(\psi, \psi)$. Clearly,

$$s_\Omega^T(\psi, \varphi) = \mu_{\psi,\varphi}^T(\Omega) \ , \tag{5.122}$$

with $\mu_{\psi,\varphi}^T$ defined from μ_ψ^T via the polarization identity. Since $0 \leqslant q_T(\psi) \leqslant \|\psi\|^2$, we have, by the Cauchy-Schwarz inequality for sesquilinear forms:

$$|s_\Omega^T(\psi, \varphi)| \leqslant q_\Omega^T(\psi)^{\frac{1}{2}} q_\Omega^T(\varphi)^{\frac{1}{2}} \leqslant \|\psi\| \|\varphi\| \ . \tag{5.123}$$

By Riesz' representation theorem, we can write the map $\varphi \mapsto s_\Omega^T(\psi, \varphi)$ as $s_\Omega^T(\psi, \varphi) = \langle \eta, \varphi \rangle$, for a unique $\eta \in \mathcal{H}$. By the antilinearity of the sesquilinear form, it is not difficult to see that $\eta = Q^T(\Omega)^* \psi$, for a bounded linear operator $Q^T(\Omega)$ with $\|Q^T(\Omega)\| \leqslant 1$. We then have:

$$s_\Omega^T(\psi, \varphi) = \mu_{\psi,\varphi}^T(\Omega) = \langle \psi, Q^T(\Omega)\varphi \rangle \ , \qquad q_\Omega^T(\psi) = \mu_\psi^T(\Omega) = \langle \psi, Q^T(\Omega)\psi \rangle \ . \tag{5.124}$$

Lemma 5.51. *The map $Q^T : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ is a projection valued measure.*

Proof. That is, we have to prove that:

(i) $Q^T(\Omega)^2 = Q^T(\Omega) = Q^T(\Omega)^*$.

(i) $Q^T(\mathbb{R}) = \mathbb{1}_{\mathcal{H}}$.

(iii) Strong σ-additivity.

We prove first that $Q^T(\Omega_1)Q^T(\Omega_2) = Q^T(\Omega_1 \cap \Omega_2)$ for all $\Omega_1, \Omega_2 \in \mathcal{B}(\mathbb{R})$. This implies, in particular, that for $\Omega_1 = \Omega_2$:

$$Q^T(\Omega)^2 = Q^T(\Omega) \ . \tag{5.125}$$

To this end, we observe that, for all $z, \tilde{z} \in \mathbb{C} \backslash \mathbb{R}$, by definition of $d\mu_{R_{\tilde{z}}(T)\varphi,\psi}^T(\lambda)$:

$$\begin{aligned} \int \frac{1}{\lambda - \tilde{z}} d\mu_{R_{\bar{z}}(T)\varphi,\psi}^T(\lambda) &= \langle R_{\bar{z}}(T)\varphi, R_{\tilde{z}}(T)\psi \rangle = \langle \varphi, R_z(T) R_{\tilde{z}}(T)\psi \rangle \\ &= \frac{1}{z - \tilde{z}} [\langle \varphi, R_z(T)\psi \rangle - \langle \varphi, R_{\tilde{z}}(T)\psi \rangle] \ , \end{aligned} \tag{5.126}$$

where we used the resolvent identity:

$$R_z(T) - R_{\tilde{z}}(T) = (z - \tilde{z}) R_z(T) R_{\tilde{z}}(T) \; . \tag{5.127}$$

We conclude that:

$$\begin{aligned} \int \frac{1}{\lambda - \tilde{z}} d\mu^T_{R_{\bar{z}}(T)\varphi,\psi}(\lambda) &= \frac{1}{z - \tilde{z}} \int \Big[\frac{1}{\lambda - z} - \frac{1}{\lambda - \tilde{z}} \Big] d\mu^T_{\psi,\varphi}(\lambda) \\ &= \int \frac{1}{\lambda - \tilde{z}} \frac{1}{\lambda - z} d\mu^T_{\psi,\varphi}(\lambda) \; . \end{aligned} \tag{5.128}$$

Since this identity holds for all $\tilde{z} \in \mathbb{C} \backslash \mathbb{R}$, we must have:

$$d\mu^T_{R_{\bar{z}}(T)\varphi,\psi}(\lambda) = \frac{1}{\lambda - z} d\mu^T_{\psi,\varphi}(\lambda) \; . \tag{5.129}$$

Therefore,

$$\begin{aligned} \int \frac{1}{\lambda - z} d\mu^T_{\varphi, Q(\Omega)\psi} &= \int d\mu^T_{R_{\bar{z}}(T)\varphi, Q(\Omega)\psi}(\lambda) \\ &= \langle \varphi, R_z(T) Q^T(\Omega)\psi \rangle \\ &= \int \chi_\Omega(\lambda) d\mu_{R_{\bar{z}}(T)\varphi,\psi}(\lambda) \\ &= \int \frac{1}{\lambda - z} \chi_\Omega(\lambda) d\mu_{\varphi,\psi}(\lambda) \; , \end{aligned} \tag{5.130}$$

which means that:

$$d\mu_{\varphi, Q^T(\Omega)\psi}(\lambda) = \chi_\Omega(\lambda) d\mu_{\varphi,\psi} \; . \tag{5.131}$$

Hence:

$$\begin{aligned} \langle \psi, Q^T(\Omega_1) Q^T(\Omega_2)\varphi \rangle &= \int d\mu_{\varphi,\psi}(\lambda) \chi_{\Omega_1}(\lambda) \chi_{\Omega_2}(\lambda) \\ &= \int \chi_{\Omega_1 \cap \Omega_2}(\lambda) d\mu_{\varphi,\psi}(\lambda) \\ &= \langle \varphi, Q^T(\Omega_1 \cap \Omega_2)\psi \rangle \; , \end{aligned} \tag{5.132}$$

which means that $Q^T(\Omega_1 \cap \Omega_2) = Q^T(\Omega_1) Q^T(\Omega_2)$. Also, we claim that $Q^T(\Omega)^* = Q^T(\Omega)$. This easily follows from $Q^T(\Omega) \geqslant 0$. Therefore, Q^T is an orthogonal projection.

Let us now prove that $Q^T(\mathbb{R}) = \mathbb{1}_{\mathcal{H}}$. Suppose it is false, $Q^T(\mathbb{R})\psi \neq \psi$. Then, we write:

$$\psi = Q^T(\mathbb{R})\psi + \varphi \tag{5.133}$$

with $\varphi \in \operatorname{Ker} Q^T(\mathbb{R})$. Then we have, for any $\xi \in \mathcal{H}$:

$$0 = d\mu_{\xi, Q^T(\mathbb{R})\varphi} = \chi_{\mathbb{R}}(\lambda) d\mu_{\xi,\varphi}(\lambda) \tag{5.134}$$

which implies $\langle \xi, R_z(T)\varphi \rangle = 0$ for all $\xi \in \mathcal{H}$ and for all $z \in \mathbb{C} \backslash \mathbb{R}$. Since $\mathbb{C} \backslash \mathbb{R} \subset \rho(T)$, $R_z(T)$ is invertible: for any $\eta \in \mathcal{H}$ there exists ξ such that $R_{\bar{z}}(T)\xi = \eta$. Therefore, $\varphi = 0$, thus implying a contradiction: $Q^T(\mathbb{R})\psi = \psi$.

Finally, we have to prove the strong σ-additivity. For orthogonal projection, the strong σ-additivity is equivalent to the weak σ-additivity, since $\|Q\psi\| = \langle \psi, Q\psi \rangle$ (hence $\|Q_n\psi\| \to \|Q\psi\|$ is implied by weak convergence). Let $(\Omega_n) \subset \mathcal{B}(\mathbb{R})$, such that $\Omega_n \cap \Omega_m = \varnothing$ for $n \neq m$. Let $\Omega = \cup_n \Omega_n$. Therefore, for all $\psi \in \mathcal{H}$, for $N \to \infty$:

$$\sum_{n=1}^N \langle \psi, Q^T(\Omega_n)\psi \rangle = \sum_{n=1}^N \mu_\psi(\Omega_n) \to \mu_\psi(\Omega) = \langle \psi, Q^T(\Omega)\psi \rangle \; , \tag{5.135}$$

where the convergence follows from the strong σ-additivity of the measure μ_ψ. By polarization,

$$\sum_{n=1}^N \langle \psi, Q^T(\Omega_n)\varphi \rangle \to \langle \psi, Q^T(\Omega)\varphi \rangle \tag{5.136}$$

for all ψ, φ, which implies strong σ-additivity. ∎

In conclusion, starting from a self-adjoint operator $T(,D(T))$ we constructed a PVM $P : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ such that, for all $z \in \mathbb{C}\backslash\mathbb{R}$:

$$R_z(T) = \int dp(\lambda)\frac{1}{\lambda - z} \ . \tag{5.137}$$

This easily implies the spectral theorem for unbounded self-adjoint operators.

Theorem 5.52. *For any self-adjoint operator $(T, D(T))$ there exists a unique PVM P^T such that:*

$$D(T) = \{\psi \in \mathcal{H} \mid \int \lambda^2 d\mu_\psi(\lambda) < \infty\} \ , \tag{5.138}$$

and:

$$T = \int \lambda dp(\lambda) \ . \tag{5.139}$$

Proof. Given the PVM constructed before, we know that $A = \int \lambda dp(\lambda)$ defines an unbounded self-adjoint operator, with domain $D(A) = \mathcal{D}_\lambda$. We claim that $A = T$. By construction:

$$R_z(T) = (T - z)^{-1} = \int dp(\lambda)\frac{1}{\lambda - z} \ , \qquad \text{for } z \in \mathbb{C}\backslash\mathbb{R}, \tag{5.140}$$

with $R_z(T) : \mathcal{H} \to D(T)$. We claim that $D(T) \subset \mathcal{D}_\lambda$. This follows from the fact that for any $\varphi \in D(T)$ there exists $\psi \in \mathcal{H}$ such that: $\Phi(\lambda - z)\varphi = \Phi(\lambda - z)\Phi(1/(\lambda - z))\psi = \psi$. Also, $\Phi(\lambda - z) \supset T - z$, since, for any $\psi \in \mathcal{D}_\lambda$,

$$\Phi(\lambda - z)\Phi(1/(\lambda - z))\psi = \Phi(1/(\lambda - z))\Phi(\lambda - z)\psi = \psi \ . \tag{5.141}$$

This shows that $\Phi(\lambda - z) = T - z$ on $D(T)$, hence $\Phi(\lambda) \supset T$. Using that both operators are self-adjoint, we get $\Phi(\lambda) = T$. To prove uniqueness, notice that the measure μ_ψ is uniquely determined by $R_z(T)$ via the Stieltjes inversion formula. Uniqueness of P^T follows from the fact that it is uniquely determined by μ_ψ. ∎

Finally, as one could expect, the projection valued measure associated with T is supported on the spectrum of T.

Theorem 5.53. *Let $T : D(T) \to \mathcal{H}$ be a self-adjoint operator, with projection-valued measure $P^T : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$. Then:*

$$\sigma(T) = \{\lambda \in \mathbb{R} \mid P^T((\lambda - \varepsilon, \lambda + \varepsilon)) \neq 0 \ , \qquad \forall\varepsilon > 0\} \ . \tag{5.142}$$

Also,

$$P^T(\sigma(T)) = \mathbb{1}_\mathcal{H} \ , \qquad P^T(\mathbb{R}\backslash\sigma(T)) = P^T(\mathbb{R} \cap \rho(T)) = 0 \ . \tag{5.143}$$

Remark 5.54. *The condition $P^T(\Omega) \neq 0$ has to be understood as there exists $\psi \in \mathcal{H}$ such that $P^T(\Omega)\psi \neq 0$.*

Proof. Let $\lambda_0 \in \mathbb{R}$, $\Omega_n = \{\lambda_0 - 1/n, \lambda_0 + 1/n\}$. Suppose that $P^T(\Omega_n) \neq 0$ for all $n \in \mathbb{N}$. Then, for all $n \in \mathbb{N}$ we can find $\psi_n \in \mathrm{Ran}P^T(\Omega_n)$ with $\|\psi_n\| = 1$. We have:

$$\begin{aligned} \|(T - \lambda_0)\psi_n\|^2 &= \|(T - \lambda_0)P^T(\Omega_n)\psi_n\|^2 \\ &= \int |\lambda - \lambda_0|^2 \chi_{\Omega_n}(\lambda) d\mu_{\psi_n}(\lambda) \leqslant \frac{1}{n^2} \ . \end{aligned} \tag{5.144}$$

Therefore, from the Weyl criterium, $\lambda_0 \in \sigma(T)$. This proves that $\{\lambda \in \mathbb{R} \mid P^T((\lambda - \varepsilon, \lambda + \varepsilon)) \neq 0 \ , \ \ \forall\varepsilon > 0\} \subset \sigma(T)$. On the other hand, suppose that there exists $\varepsilon > 0$ such that $P^T((\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)) = 0$. Define:

$$f_\varepsilon(\lambda) = \frac{1}{\lambda - \lambda_0}\chi_{\mathbb{R}\backslash\{\lambda_0 - \varepsilon, \lambda_0 + \varepsilon\}}(\lambda) \ . \tag{5.145}$$

By the properties of the functional calculus,

$$\begin{aligned}
(T-\lambda_0)\Phi^T(f_\varepsilon) &= \Phi^T((\lambda-\lambda_0)f_\varepsilon) \\
&= P^T(\mathbb{R}\backslash(\lambda_0-\varepsilon,\lambda_0+\varepsilon)) \\
&= \mathbb{1}_{\mathcal{H}} - P^T((\lambda_0-\varepsilon,\lambda_0+\varepsilon)) \\
&= \mathbb{1}_{\mathcal{H}} \ . \qquad (5.146)
\end{aligned}$$

Analogously, $\Phi^T(f_\varepsilon)(T-\lambda_0)\psi = \psi$ for all $\psi \in D(T)$. Therefore $(T-\lambda_0)$ is invertible, and $\lambda_0 \in \rho(T)$. This proves Eq. (5.142).

Let us now prove that $P^T(\mathbb{R}\cap\rho(T)) = 0$. For all $\lambda \in \mathbb{R}\cap\rho(T)$, let $I_\lambda \ni \lambda$ be an open neighbourhood of λ and $P^T(I_\lambda) = 0$ (otherwise $\lambda \in \sigma(T)$, as we just proved). Let us cover $\mathbb{R}\cap\rho(T)$ with intervals I_λ, and let $\{J_n\}_{n\in\mathbb{N}}$ be a countable subcovering. Let $\Omega_n = J_n\backslash\cup_{i=1}^{n-1}J_i$. so that $\{\Omega_n\}$ is a disjoint covering. By σ-additivity of the projection valued measure,

$$P^T(\mathbb{R}\cap\rho(T)) = \lim_{N\to\infty}\sum_{n=0}^{N} P^T(\Omega_n) = 0 \ . \qquad (5.147)$$

■

Remark 5.55. *Therefore,* $\Phi^T(f) = P(\sigma(T))\Phi^T(f) = \Phi^T(\chi_{\sigma(T)}f)$. *That is, changing* f *on* $\mathbb{R}\backslash\sigma(T)$ *does not change* $\Phi^T(f)$.

5.6 Unitary equivalence of self-adjoint operators with multiplication operators

In this section we shall show that self-adjoint operators are unitarily equivalent to multiplication operators. We say that two operators T on $\mathcal{H}$ and $\widetilde{T}$ on $\widetilde{H}$ are unitarily equivalent if there exists a unitary operator $U : \mathcal{H} \to \widetilde{\mathcal{H}}$ such that $UT = \widetilde{T}U$, with $UD(T) = D(\widetilde{T})$.

Let $\psi \in \mathcal{H}$. Let P be a projection valued measure, generating a functional calculus Φ, and a Borel measure $\mu_\psi = \langle\psi, P(\Omega)\psi\rangle$. Let

$$\mathcal{H}_\psi = \{\Phi(g)\psi \mid g \in L^2(\mathbb{R}, d\mu_\psi)\} \subset \mathcal{H} \ . \qquad (5.148)$$

It is not difficult to see that $\mathcal{H}_\psi$ is closed. Therefore, by Theorem 3.61, we can split the original Hilbert space as $\mathcal{H} = \mathcal{H}_\psi \oplus \mathcal{H}_\psi^\perp$. In what follows, we shall denote by P_ψ the projection onto $\mathcal{H}_\psi$.

Lemma 5.56. *The subspace* $\mathcal{H}_\psi$ *reduces* $\Phi(f)$*:*

$$P_\psi\Phi(f) \subset \Phi(f)P_\psi \ . \qquad (5.149)$$

Remark 5.57. *That is, if* $\varphi \in \mathcal{D}_f$ *then* $P_\psi\varphi \in \mathcal{D}_f$, *i.e.* $P_\psi\mathcal{D}_f \subset \mathcal{D}_f$. *Also, for all* $\varphi \in \mathcal{D}_f$, $P_\psi\Phi(f) = \Phi(f)P_\psi\varphi$. *We shall also say that* $\mathcal{H}_\psi$ *is invariant under* $\Phi(f)$.

Proof. (Sketch). Suppose f is bounded. Any $\varphi \in \mathcal{H}$ can be written as $\varphi = P_\psi\varphi + \varphi^\perp$, with $P_\psi\varphi = \Phi(g)\psi$ for some $g \in L^2(\mathbb{R}, d\mu_\psi)$. We claim that $\Phi(f)\varphi^\perp \in \mathcal{H}_\psi^\perp$. In fact:

$$\langle\Phi(f)\varphi^\perp, \Phi(h)\psi\rangle = \langle\varphi^\perp, \Phi(\bar{f}h)\psi\rangle = 0 \ , \qquad (5.150)$$

because $\bar{f}h \in L^2(\mathbb{R}, d\mu_\psi)$ since f is bounded. It follows that:

$$\begin{aligned}
P_\psi\Phi(f)\varphi &= P_\psi\Phi(f)\Phi(g)\psi = P_\psi\Phi(fg)\psi \\
&= \Phi(fg)\psi = \Phi(f)\Phi(g)\psi = \Phi(f)P_\psi\varphi \ . \qquad (5.151)
\end{aligned}$$

This proves the claim for bounded f. The case of unbounded f follows by an approximation argument, we omit the details. ■

Therefore, we can decompose $\Phi(f) = \Phi(f)|_{\mathcal{H}_\psi} \oplus \Phi(f)|_{\mathcal{H}_\psi^\perp}$; this means that if $\varphi = \varphi_1 + \varphi_2$ with $\varphi_1 \in \mathcal{H}_\psi$ and $\varphi_2 \in \mathcal{H}_\psi^\perp$, then $\Phi(f)\varphi = \Phi(f)\varphi_1 + \Phi(f)\varphi_2$ with $\Phi(f)\varphi_1 \in \mathcal{H}_\psi$ and $\Phi(f)\varphi_2 \in \mathcal{H}_\psi^\perp$.

The domain of $\Phi(f)|_{\mathcal{H}_\psi}$ is defined as:

$$P_\psi \mathcal{D}_f = \mathcal{D}_f \cap \mathcal{H}_\psi = \{\Phi(g)\psi \mid g, fg \in L^2(\mathbb{R}, d\mu_\psi)\} . \tag{5.152}$$

On $P_\psi \mathcal{D}_f$ the action of $\Phi(f)$ is then given by:

$$\Phi(f)\Phi(g)\psi = \Phi(fg)\psi \tag{5.153}$$

This implies that the operator $\Phi(f)$ can be interpreted, when considering its action of $\mathcal{H}_\psi$, as a multiplication operator by f. To be more precise, we can define the map:

$$U_\psi : \mathcal{H}_\psi \to L^2(\mathbb{R}, d\mu_\psi) , \tag{5.154}$$

by setting $U_\psi \Phi(f)\psi = f$. Since $\|\Phi(f)\psi\| = \|f\|_2$, the map U_ψ is unitary. Furthermore, it follows that:

$$U_\psi D(\Phi(f)|_{\mathcal{H}_\psi}) = U_\psi P_\psi \mathcal{D}_f = U_\psi(\mathcal{D}_f \cap \mathcal{H}_\psi) = \{g \in L^2(\mathbb{R}, d\mu_\psi) \mid fg \in L^2(\mathbb{R}, d\mu_\psi)\} \tag{5.155}$$

and:

$$U_\psi \Phi(f)|_{\mathcal{H}_\psi} = f U_\psi , \tag{5.156}$$

where f also denotes the multiplication operator, $(fg)(\lambda) = f(\lambda)g(\lambda)$, with domain $D(f) = U_\psi D(\Phi(f)|_{\mathcal{H}_\psi})$.

We say that the vector ψ is cyclic if $\mathcal{H}_\psi = \mathcal{H}$. In this case the picture is complete: the operator $\Phi(f)$ is unitarily equivalent to the multiplication operator f, acting on its domain $D(f) = U_\psi \mathcal{D}_f$. In general however $\mathcal{H}_\psi \neq \mathcal{H}$, and Eq. (5.156) only shows that the restriction of $\Phi(f)$ on the space $\mathcal{H}_\psi$ (more precisely, on the dense domain $\mathcal{H}_\psi \cap \mathcal{D}_f$) is unitarily equivalent to multiplication with f.

What can we say about the restriction of $\Phi(f)$ on the orthogonal complement $\mathcal{H}_\psi^\perp$? Also on $\mathcal{H}_\psi^\perp$ we can choose a vector ψ'; the corresponding space $\mathcal{H}_{\psi'}$ will again be invariant with respect to the action of $\Phi(f)$. We can iterate the procedure; $\{\psi_j\}_{j\in J}$ is called a family of spectral vectors, if $\mathcal{H}_{\psi_i} \perp \mathcal{H}_{\psi_j}$ for all $i \neq j$. We say that a family of spectral vectors if a spectral basis of $\mathcal{H}$ if $\mathcal{H} = \bigoplus_{j\in J} \mathcal{H}_{\psi_j}$. Such family always exists.

Lemma 5.58. *Let $\mathcal{H}$ be a separable Hilbert space, and P and projection valued measure. Then there exists a, at most countable, spectral basis $\{\psi_j\}_{j\in J}$ with $\mathcal{H} = \bigoplus_{j\in J} \mathcal{H}_{\psi_j}$. We can define a unitary map $U = \bigoplus_{j\in J} U_{\psi_j} : \mathcal{H} \to \bigoplus_{j\in J} L^2(\mathbb{R}, d\mu_{\psi_j})$, where U_{ψ_j} is defined as in Eq. (5.154), through the identity $U_{\psi_j}\Phi(f)\psi_j = f$. Then, for any Borel measurable $f : \mathbb{R} \to \mathbb{C}$:*

$$U\mathcal{D}_f = D(f) = \bigoplus_{j\in J} \{g \in L^2(\mathbb{R}, d\mu_{\psi_j}) \mid fg \in L^2(\mathbb{R}, d\mu_{\psi_j})\} , \tag{5.157}$$

and $U\Phi(f) = fU$, where f acts as a multiplication on each component of $\bigoplus_{j\in J} L^2(\mathbb{R}, d\mu_{\psi_j})$.

This last lemma shows, in particular, that any selfadjoint operator is unitarily equivalent to the multiplication operator $\hat{\lambda}$: $(\hat{\lambda}g)(\lambda) = \lambda g(\lambda)$.

Remark 5.59. *Notice that the spectral basis is not unique, and its cardinality is not well defined: there might exists different spectral bases with different cardinality. However, since we are only considering separable Hilbert spaces, the cardinality of every spectral basis is at most countable. The minimal cardinality of a spectral basis for a given self-adjoint operator T, or more generally for a given projection valued measure P, is called the spectral multiplicity of T (or of P). We shall say that the spectrum of T is simple if the spectral multiplicity of T is one (this means that there exists a cyclic vector).*

5.7 Decomposition of the spectrum

Let us start by reminding some well-known facts about Borel measures. For any Borel measure μ there exists a decomposition $\mu = \mu_{\rm ac} + \mu_{\rm s}$, where $\mu_{\rm ac}$ is absolutely continuous with respect to the Lebesgue measure (meaning that $\mu_{\rm ac}(\Omega) = 0$ for all $\Omega \in \mathcal{B}(\mathbb{R})$ with Lebesgue measure $|\Omega| = 0$) while $\mu_{\rm s}$ is singular with respect to the Lebesgue measure (meaning that there exists a set Ω with $|\Omega| = 0$ and $\mu_{\rm s}(\mathbb{R}\backslash\Omega) = 0$).

The singular measure $\mu_{\rm s}$ can be further decomposed as $\mu_{\rm s} = \mu_{\rm pp} + \mu_{\rm sc}$, where $\mu_{\rm pp}$ is pure point (meaning that the distribution function $d_{\rm pp}(\lambda)$ is a step function on $\mathbb{R}$) and $\mu_{\rm sc}$ is singular continuous (meaning that the distribution function is continuous on $\mathbb{R}$).

The measures $\mu_{\rm ac}, \mu_{\rm sc}, \mu_{\rm pp}$ are mutually singular: there exist disjoint sets $M_{\rm ac}, M_{\rm pp}, M_{\rm sc} \subset \mathbb{R}$ such that $\mu_{\rm ac}$ is supported on $M_{\rm ac}$, $\mu_{\rm pp}$ is supported on $M_{\rm pp}$ and $\mu_{\rm sc}$ is supported on $M_{\rm sc}$. Observe that the choice of the sets $M_{\rm ac}, M_{\rm sc}, M_{\rm pp}$ is not unique: one can always add sets with zero μ measure. We will choose $M_{\rm pp}$ as the set of all jump points of the distribution function $\mu(\lambda)$ and $M_{\rm sc}$ with Lebesgue measure equal to zero.

At first, suppose that the spectrum of T is simple, and that ψ is a cyclic vector. Let $P \equiv P^T$ be the projection-valued measure associated to T, and let $\mu \equiv \mu^T_\psi$ be the corresponding spectral measure. We then introduce the orthogonal projections:

$$P_{\rm ac} = \Phi(\chi_{M_{\rm ac}}) \ , \quad P_{\rm sc} = \Phi(\chi_{M_{\rm sc}}) \ , \quad P_{\rm pp} = \Phi(\chi_{M_{\rm pp}}) \ , \tag{5.158}$$

such that $P_{\rm ac} + P_{\rm sc} + P_{\rm pp} = \mathbb{1}_{\mathcal{H}}$. By the orthogonality of the projections, we write:

$$\mathcal{H} = \mathcal{H}_{\rm ac} \oplus \mathcal{H}_{\rm sc} \oplus \mathcal{H}_{\rm pp} \ , \tag{5.159}$$

with $\mathcal{H}_\sharp = P_\sharp \mathcal{H}$. Recall that the Hilbert space $\mathcal{H} \equiv \mathcal{H}_\psi$ is unitarily equivalent to $L^2(\mathbb{R}, d\mu)$, $U_\psi \mathcal{H}_\psi = L^2(\mathbb{R}, d\mu_\psi)$. Writing $U_\psi \mathcal{H}_\psi = U_\psi(P_{\rm ac} + P_{\rm sc} + P_{\rm pp})\mathcal{H}_\psi$ and using that $U_\psi P_\sharp U^*_\psi = \chi_{M_\sharp}$, we get the following orthogonal splitting:

$$L^2(\mathbb{R}, d\mu) = L^2(\mathbb{R}, d\mu_{\rm ac}) \oplus L^2(\mathbb{R}, d\mu_{\rm sc}) \oplus L^2(\mathbb{R}, d\mu_{\rm pp}) \ . \tag{5.160}$$

This means that every function $g \in L^2(\mathbb{R}, d\mu)$ can be written as $g = g_{\rm ac} + g_{\rm sc} + g_{\rm pp}$, with $g_\sharp = g|_{M_\sharp}$. Being the sets $M_\sharp$ disjoint, the functions appearing in the splitting are orthogonal. Notice that, by construction, if $\varphi \in M_\sharp$, then $\mu_\varphi \equiv \mu_{\varphi,\sharp}$, with $\sharp =$ ac, sc, pp. In fact, being ψ cyclic, $\varphi = \Phi(g_\sharp)\psi$ for some $g_\sharp \in L^2(\mathbb{R}, d\mu_\sharp)$, and $d\mu_\psi(\lambda) = |g_\sharp(\lambda)|^2 d\mu_\psi(\lambda)$, with $g_\sharp$ supported in $M_\sharp$.

Also,

$$T = (TP_{\rm ac}) \oplus (TP_{\rm sc}) \oplus (TP_{\rm pp}) \ . \tag{5.161}$$

We define the absolutely continuous, singular continuous and pure point spectrum of T as:

$$\sigma_{\rm ac}(T) := \sigma(TP_{\rm ac}) \ , \qquad \sigma_{\rm sc}(T) := \sigma(TP_{\rm sc}) \ , \qquad \sigma_{\rm pp}(T) := \sigma(TP_{\rm pp}) \ . \tag{5.162}$$

Being the subspaces $\mathcal{H}_\sharp$ invariant under T, we have $P_\sharp T P_\sharp = TP_\sharp$. Hence, $TP_\sharp$ are selfadjoint, and $\sigma_\sharp(T)$ are closed subsets of $\mathbb{R}$.

Remark 5.60. *One has $\sigma_p(T) \subset \sigma_{pp}(T)$, with $\sigma_p(T)$ the set of eigenvalues of T. This also implies $\overline{\sigma_p(T)} \subset \sigma_{pp}(T)$. It is possible to prove that $\sigma_{pp}(T) = \overline{\sigma_p(T)}$. See next example.*

Example 5.61. *Let $\mathcal{H} = \ell^2(\mathbb{N})$, let $T\delta_n = \frac{1}{n}\delta_n$ with δ_n the sequence equal to 1 at the n-th place and zero otherwise. That is T is a diagonal matrix with elements $1/n$. Then, $\sigma_p(T) = \{1/n \mid n \in \mathbb{N}\}$. We claim that*

$$\sigma(T) = \sigma_{pp}(T) = \sigma_p(T) \cup \{0\} = \overline{\sigma_p(T)} \ . \tag{5.163}$$

We claim that $\{0\}$ belongs to $\sigma(T)$. To see this, notice that T is injective, but not surjective: not every vector in $\ell^2(\mathbb{N})$ can be written as $T\varphi$ for some $\varphi \in \ell^2(\mathbb{N})$. Finally, notice that all points $z \in \mathbb{C}$ which are not in $\{\frac{1}{n} \mid n \in \mathbb{N}\} \cup \{0\}$ are in $\rho(T)$. This simply follows by computing the resolvent:

$$(T - z)^{-1}\delta_n = \frac{n}{1 - zn}\delta_n \ , \tag{5.164}$$

and observing that $(T - z)^{-1}$ is bounded for all $z \in \{\frac{1}{n} \mid n \in \mathbb{N}\} \cup \{0\}$. Therefore, $\sigma(T) = \sigma_p(T) \cup \{0\}$. At the same time, we know that $\sigma(T) = \sigma_{pp}(T) \cup \sigma_{ac}(T) \cup \sigma_{sc}(T)$. Being $\sigma_p(T) \subset \sigma_{pp}(T)$ with $\sigma_p(T)$ open and $\sigma_{pp}(T)$ closed, it follows that $\sigma_p(T) \cup \{0\} = \sigma_{pp}(T)$.

Example 5.62. *An example of purely absolutely continuous spectrum is obtained taking μ to be the Lebesgue measure. An example with purely singular continuous spectrum is given by taking μ to be the Cantor measure.*

To conclude, we are left with discussing the case in which the spectrum of T is not simple. In this case there is no cyclic vector, and we need to introduce a spectral basis. After introducing such basis, the operator T is unitarily equivalent to a multiplication operator, after conjugating with the unitary map: $U\mathcal{H} \to \oplus_j L^2(\mathbb{R}, d\mu_{\psi_j})$. In general, however, it is difficult to exclude that the splitting (5.159) depend on the choice of the spectral basis. For this reason, we introduce the following definition of spectral subspaces of $\mathcal{H}$:

$$\begin{aligned} \mathcal{H}_{\mathrm{ac}} &:= \{\psi \in \mathcal{H} \mid \mu_\psi \text{ is absolutely continuous}\} \\ \mathcal{H}_{\mathrm{sc}} &:= \{\psi \in \mathcal{H} \mid \mu_\psi \text{ is singular continuous}\} \\ \mathcal{H}_{\mathrm{pp}} &:= \{\psi \in \mathcal{H} \mid \mu_\psi \text{ is pure point}\} \;. \end{aligned} \tag{5.165}$$

Lemma 5.63. *We have:*

$$\mathcal{H} = \mathcal{H}_{ac} \oplus \mathcal{H}_{sc} \oplus \mathcal{H}_{pp} \;. \tag{5.166}$$

As for the simple case, the absolutely continuous, singular continuous and pure point spectrum are defined as:

$$\sigma_\sharp(T) = \sigma(T|_{\mathcal{H}_\sharp}) = \sigma(TP_\sharp) \;, \tag{5.167}$$

where $P_\sharp$ is the projector over $\mathcal{H}_\sharp$.

To conclude, we discuss a simple consequence of the fact that $\sigma_{\mathrm{pp}}(T) = \overline{\sigma_{\mathrm{p}}(T)}$.

Proposition 5.64. *Let $(T, D(T))$ be a selfadjoint operator. Suppose that $\psi \in \mathcal{H}_{pp}$. Let $(\varphi_j)_{j\in\mathbb{N}}$ be the eigenvectors of T, $T\varphi_j = \lambda_j \varphi_j$. Then, there exists $(\alpha_j) \subset \mathbb{C}$ such that*

$$\lim_{N\to\infty} \Big\| \psi - \sum_{j=1}^{N} \alpha_j \varphi_j \Big\| = 0 \;. \tag{5.168}$$

Proof. The proof immediately follows from the fact that $M_{\mathrm{pp}} = \overline{M_{\mathrm{p}}}$, with $M_{\mathrm{p}} = \{\lambda \in \mathbb{R} \mid \lambda \text{ is an eigenvalue of } T\}$. Therefore, $\mathcal{H}_{\mathrm{p}} = \phi(\chi_{M_{\mathrm{p}}})\mathcal{H} \equiv P_{\mathrm{p}}\mathcal{H}$ is dense in $\mathcal{H}_{\mathrm{pp}}$. ∎

Remark 5.65. *Recall that $\lambda_j \neq \lambda_k$ implies that $\langle \varphi_j, \varphi_k \rangle = 0$. This follows from, for $\varepsilon > 0$:*

$$\begin{aligned} \langle \varphi_j, \varphi_k \rangle &= \frac{1}{\lambda_k + i\varepsilon} \langle \varphi_j, (H + i\varepsilon \mathbb{1}_{\mathcal{H}})\varphi_k \rangle \\ &= \frac{1}{\lambda_k + i\varepsilon} \langle (H - i\varepsilon \mathbb{1}_{\mathcal{H}})\varphi_j, \varphi_k \rangle \\ &= \frac{\lambda_j - i\varepsilon}{\lambda_k + i\varepsilon} \langle \varphi_j, \varphi_k \rangle \end{aligned} \tag{5.169}$$

which implies that $\langle \varphi_j, \varphi_k \rangle = 0$ (since $\lambda_j, \lambda_k \in \mathbb{R}$, the ratio in the r.h.s. is $\neq 1$).

To conclude, let us discuss a simple example of self-adjoint operator with purely absolutely continuous spectrum.

Example 5.66. *The Laplacian $(-\Delta, H^2(\mathbb{R}^d))$ is a selfadjoint operator, with:*

$$\sigma(-\Delta) = \sigma_{ac}(-\Delta) = [0, \infty) \;. \tag{5.170}$$

The selfadjointness of the Laplacian has been proved in Section 4.2, using that it is unitarily equivalent to multiplication by $|k|^2$ (real-valued measurable function), recall Lemma 4.47. Also, $\sigma(-\Delta) = [0,\infty)$, since $\sigma(-\Delta) = \sigma(\mathcal{F}(-\Delta)\mathcal{F}^{-1}) = \sigma(A_{k^2})$, and $\sigma(A_{k^2}) = [0,\infty)$, since $k \mapsto (k^2 - z)^{-1}$ is a bounded function for all $z \notin \mathbb{R}\backslash[0,\infty)$.

Let us now prove that $\sigma(-\Delta) = \sigma_{ac}(-\Delta)$. To do this, it is enough to show that the spectral measure μ_ψ is absolutely continuous with respect to the Lebesgue measure, for all $\psi \in H^2(\mathbb{R}^d)$. Observe that, for all $\psi \in L^2(\mathbb{R}^d)$, $z \in \rho(-\Delta)$:

$$\langle \psi, R_z(-\Delta)\psi \rangle = \langle \hat{\psi}, R_z(A_{k^2})\hat{\psi} \rangle = \int_{\mathbb{R}^d} \frac{|\hat{\psi}(k)|^2}{k^2 - z} dk = \int_{\mathbb{R}} \frac{1}{r^2 - z} d\tilde{\mu}_\psi(r) \tag{5.171}$$

where

$$d\widetilde{\mu}_\psi(r) = \chi_{[0,\infty)}(r)r^{d-1}\Big(\int_{S^{d-1}} |\hat{\psi}(r\omega)|^2 d\omega\Big)dr \; . \tag{5.172}$$

After a simple change of variables, we have:

$$\langle \psi, R_z(-\Delta)\psi\rangle = \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu_\psi(\lambda) \; , \tag{5.173}$$

with $\mu_\psi(\lambda)$ given by:

$$d\mu_\psi(\lambda) = \frac{1}{2}\chi_{[0,\infty)}(\lambda)\lambda^{\frac{d}{2}-1}\Big(\int_{S^{d-1}} |\hat{\psi}(\sqrt{\lambda}\omega)|^2 d\omega\Big)d\lambda \; . \tag{5.174}$$

This measure is absolutely continuous, since it is of the form $d\mu_\psi(\lambda) = f(\lambda)d\lambda$, with $f \in L^1(\mathbb{R}^d, d\lambda)$ given by:

$$f_\psi(\lambda) = \frac{1}{2}\chi_{[0,\infty)}(\lambda)\lambda^{\frac{d}{2}-1}\Big(\int_{S^{d-1}} |\hat{\psi}(\sqrt{\lambda}\omega)|^2 d\omega^{n-1}\Big) \; . \tag{5.175}$$

Absolute continuity of the measure follows from the fact that the integral of an L^p function over a set with zero Lebesgue measure is zero.

6 Quantum dynamics

In this section we shall apply the spectral theorem to study solutions of the Schrödinger equation:

$$i\partial_t \psi(t) = H\psi(t) \; , \tag{6.1}$$

where H is a selfadjoint operator, the Hamiltonian, defined on a domain $D(H) \subset \mathcal{H}$.

6.1 Existence and uniqueness of the solution of the Schrödinger equation

In the next theorem we shall prove that the solution to this equation is given by $\psi(t) = U(t)\psi(0)$, with $U(t) = \exp(-iHt)$, define via functional calculus:

$$e^{-iHt} = \int e^{-i\lambda t} dp(\lambda) \; , \tag{6.2}$$

with P the projection-valued measure associated to $(H, D(H))$.

Theorem 6.1. *Let $(H, D(H))$ be a selfadjoint operator and let $U(t) = e^{-iHt}$. Then:*

(i) $U(t)$ is a strongly continuous one-parameter unitary group.

(ii) The limit:

$$\lim_{t\to 0} \frac{1}{t}[U(t) - \mathbb{1}]\psi \tag{6.3}$$

exists if and only if $\psi \in D(H)$. In this case:

$$\lim_{t\to 0} \frac{1}{t}[U(t) - \mathbb{1}]\psi = -iH\psi \; . \tag{6.4}$$

(iii) We have $U(t)D(H) = D(H)$ and, on $D(H)$, $[U(t), H] = 0$ for all $t \in \mathbb{R}$.

Remark 6.2. *That is, H is the generator of $U(t)$, recall Definition 3.77.*

Proof. Let us prove (i). The spectral representation of $U(t)$, Eq. (6.2), together with the rules of functional calculus, implies that $U(t)^{-1} = U(t)^*$, and that $U(t+s) = U(t)U(s)$ for all $t, s \in \mathbb{R}$. To prove that $U(t)$ is strongly continuous, fix $\psi \in \mathcal{H}$ and consider:

$$\lim_{t\to t_0} \|e^{-iHt}\psi - e^{-iHt_0}\psi\|^2 = \lim_{t\to t_0} \int |e^{-i\lambda t} - e^{-i\lambda_0 t}|^2 d\mu_\psi(\lambda) = 0 \tag{6.5}$$

by dominated convergence. This proves (i). Let us now consider (ii). Suppose that $\psi \in D(H)$. Then, we have:

$$\lim_{t\to 0}\left\|\frac{1}{t}(e^{-iHt}-1)\psi + iH\psi\right\|^2 = \lim_{t\to 0}\int\left|\frac{1}{t}(e^{-i\lambda t}-1)+i\lambda t\right|^2 d\mu_\psi(\lambda) = 0\ , \tag{6.6}$$

again by dominated convergence. Here we used the bound $|e^{-i\lambda t}-1| \leqslant |t\lambda|$ and the fact that, since $\psi \in D(H)$:

$$\int \lambda^2 d\mu_\psi(\lambda) < \infty\ . \tag{6.7}$$

One the other hand, define the operator $\widetilde{H} : D(\widetilde{H}) \to \mathcal{H}$ by:

$$D(\widetilde{H}) = \{\psi : \lim_{t\to 0}\frac{i}{t}[U(t)\psi - \psi] \quad \text{exists}\} \tag{6.8}$$

and by:

$$\widetilde{H}\psi = \lim_{t\to 0}\frac{i}{t}[U(t)\psi - \psi] \tag{6.9}$$

for all $\psi \in D(\widetilde{H})$. The operator $\widetilde{H}$ is the generator of the one-parameter group $U(t)$. It follows from Eq. (6.6) that $H \subset \widetilde{H}$. Moreover, for all $\varphi, \psi \in D(\widetilde{H})$ we have:

$$\langle\varphi, \widetilde{H}\psi\rangle = \lim_{t\to 0}\langle\varphi, \frac{i}{t}[U(t)\psi - \psi]\rangle = \lim_{t\to 0}\langle\frac{(-i)}{t}[U(-t)\varphi - \varphi], \psi\rangle = \langle\widetilde{H}\varphi, \psi\rangle\ . \tag{6.10}$$

We conclude that $\widetilde{H}$ is a symmetric extension of H. However, self-adjoint operators are maximal: they do not have symmetric extensions[2], which means that $\widetilde{H} = H$. This proves (ii). The proof of (iii) follows from Proposition 3.79 (ii). ∎

Therefore, it follows from Eq. (6.4) that, for $\psi_0 \in D(H)$, the vector $\psi(t) \in U(t)\psi_0$ with $U(t) = e^{-iHt}$ is a solution of the Schrödinger equation with initial datum $\psi(0) = \psi_0$. In fact:

$$i\partial_t U(t)\psi_0 = \lim_{h\to 0}\frac{i}{h}[U(t+h) - U(t)]\psi_0 = \lim_{h\to 0}\frac{i}{h}[U(h) - \mathbb{1}]U(t)\psi_0 = HU(t)\psi_0 \tag{6.11}$$

because $U(t)\psi_0 \in D(H)$ if $\psi_0 \in D(H)$. It turns out that $U(t)\psi_0$ is the unique solution of the Schrödinger equation.

Lemma 6.3. *Let $\psi_0 \in D(H)$ and let $\psi(t)$ be a solution of the Schrödinger equation with initial datum $\psi(0) = \psi_0$. Then $\psi(t) = U(t)\psi_0$.*

Proof. Let $\psi(t)$ be a solution of the Schrödinger equation. In particular, $\psi(t)$ is differentiable and $\psi(t) \in D(H)$ for all $t \in \mathbb{R}$ (or for all t in the time-interval on which $\psi(t)$ is a solution). Let $\varphi(t) = U(-t)\psi(t)$. Then:

$$\begin{aligned} i\partial_t\varphi(t) &= \lim_{\varepsilon\to 0}\frac{i}{\varepsilon}[U(-t-\varepsilon)\psi(t+\varepsilon) - U(-t)\psi(t)] \\ &= \lim_{\varepsilon\to 0}\Big[iU(-t-\varepsilon)\frac{\psi(t+\varepsilon)-\psi(t)}{\varepsilon} + i\frac{U(-\varepsilon)-\mathbb{1}}{\varepsilon}U(-t)\psi(t)\Big]\ . \end{aligned} \tag{6.12}$$

Since ψ is differentiable and U is strongly continuous, we have, as $\varepsilon \to 0$:

$$iU(-t-\varepsilon)\frac{\psi(t+\varepsilon)-\psi(t)}{\varepsilon} \to iU(-t)\psi'(t) = U(-t)H\psi(t) = HU(-t)\psi(t)\ . \tag{6.13}$$

On the other hand, $\psi(t) \in D(H)$ implies that $U(-t)\psi(t) \in D(H)$ and therefore that:

$$i\frac{U(-\varepsilon)-\mathbb{1}}{\varepsilon}U(-t)\psi(t) \to -HU(-t)\psi(t)\ . \tag{6.14}$$

We conclude that $\varphi'(t) = 0$ for all t and therefore that $\varphi(t) = \varphi(0) = \psi(0) = \psi_0$. Hence, $\psi(t) = U(t)\psi_0$. ∎

Remark 6.4. *Since $D(U(t)) = \mathcal{H}$, the dynamics can be extended to all initial data $\psi_0 \in \mathcal{H}$. However, notice that $U(t)\psi_0$ is a solution of the Schrödinger equation if and only if $\psi_0 \in D(H)$.*

[2] Suppose that $H \subset \widetilde{H}$. Then, by Proposition 4.31 $\widetilde{H}^* \subset H$. Also, being $\widetilde{H}$ symmetric, by Proposition 4.28 $\widetilde{H} \subset \widetilde{H}^*$. That is, $\widetilde{H} \subset H$, hence $\widetilde{H} = H$.

6.2 Stone's theorem

In the previous section we proved that any self-adjoint operator generates a unitary evolution. Conversely, Stone's theorem shows that any strongly continuous one-parameter unitary group $U(t)$ is generated by a selfadjoint operator such that $U(t) = e^{-iHt}$.

Theorem 6.5. *Let $U(t)$ be a weakly continuous one-parameter unitary group. Let $H : D(H) \to \mathcal{H}$ be the generator of $U(t)$, defined by:*

$$D(H) = \{\psi \in \mathcal{H} \mid \lim_{t\to 0} \frac{1}{t}[U(t)\psi - \psi] \quad exist\} \tag{6.15}$$

and by:

$$H\psi = \lim_{t\to 0} \frac{i}{t}[U(t)\psi - \psi] \qquad \text{for all } \psi \in D(H). \tag{6.16}$$

Then, H is selfadjoint and $U(t) = e^{-iHt}$.

Proof. First of all, we notice that the weak continuity of $U(t)$ also implies strong continuity, since, for any $\psi \in \mathcal{H}$ and for $t \to t_0$:

$$\|U(t)\psi - U(t_0)\psi\|^2 = 2\|\psi\|^2 - 2\mathrm{Re}\,\langle\psi, U(t_0 - t)\psi\rangle \to 0 \tag{6.17}$$

if $U(t_0 - t) \to 1$ weakly. Next, we claim that $D(H)$ is dense in $\mathcal{H}$. For any $\psi \in \mathcal{H}$ and $\tau > 0$, we set:

$$\psi_\tau := \int_0^\tau U(t)\psi dt\ . \tag{6.18}$$

This implies that $\tau^{-1}\psi_\tau \to \psi$ as $\tau \to 0$. In fact, given $\varepsilon > 0$, by the strong continuity of $U(t)$ we can find $t_0 > 0$ such that $\|U(t)\psi - \psi\| \leqslant \varepsilon$ for all $0 < t < t_0$. Then, for all $0 < \tau < t_0$ we have:

$$\|\tau^{-1}\psi_\tau - \psi\| \leqslant \frac{1}{\tau}\int_0^\tau \|U(t)\psi - \psi\|dt \leqslant \varepsilon\ . \tag{6.19}$$

Since $\varepsilon > 0$ is arbitrary, this shows that $\tau^{-1}\psi_\tau \to \psi$. Moreover, we claim that $\psi_\tau \in D(H)$. In fact, for any $\tau > 0$, we have:

$$\begin{aligned}
\frac{1}{t}(U(t)\psi_\tau - \psi_\tau) &= \frac{1}{t}\Big[\int_t^{t+\tau} U(s)\psi ds - \int_0^\tau U(s)\psi ds\Big] \\
&= \frac{1}{t}\Big[\int_\tau^{\tau+t} U(s)\psi ds - \int_0^t U(s)\psi ds\Big] \\
&= (U(\tau) - \mathbb{1})\frac{1}{t}\int_0^t U(s)\psi ds \to [U(\tau) - 1]\psi\ , \qquad \text{as } t \to 0.
\end{aligned} \tag{6.20}$$

This implies that $\psi_\tau \in D(H)$. Hence, for arbitrary $\psi \in \mathcal{H}$, we found a sequence $\tau^{-1}\psi_\tau \in D(H)$ with $\tau^{-1}\psi_\tau \to \psi$. This proves that $D(H)$ is dense. Next, we show that H is essentially self-adjoint. From Corollary 4.45, it is enough to check that $\mathrm{Ker}\,(H^* \pm i) = \{0\}$. To this end, suppose that $H^*\varphi = \mp i\varphi$. Then, proceeding as in the proof of Theorem 6.1 (*iii*), for any $\psi \in D(H)$, we have $U(t)\psi \in D(H)$ for all $t \in \mathbb{R}$ and therefore:

$$\frac{d}{dt}\langle\varphi, U(t)\psi\rangle = \langle\varphi, -iHU(t)\psi\rangle = -i\langle H^*\varphi, U(t)\psi\rangle = \pm\langle\varphi, U(t)\psi\rangle\ . \tag{6.21}$$

Hence,

$$\langle\varphi, U(t)\psi\rangle = e^{\pm t}\langle\varphi, \psi\rangle\ . \tag{6.22}$$

Since the left-hand side is bounded, uniformly in $t \in \mathbb{R}$, we must have $\langle\varphi, \psi\rangle = 0$. Since $\psi \in D(H)$ is arbitrary and $D(H)$ is dense, we conclude that $\varphi = 0$. Therefore, H is essentially selfadjoint, and its closure $\overline{H}$ is selfadjoint. We can therefore define the one-parameter group $V(t) = e^{-i\overline{H}t}$. We claim now that $V(t) = U(t)$. This would also imply, by Theorem 6.1, that $\overline{H} = H$ (because it would imply that $D(\overline{H}) = D(H)$) and therefore it would conclude the proof of the theorem.

To show that indeed $V(t) = U(t)$, we pick $\psi \in D(H)$ and we set $\psi(t) = U(t)\psi - V(t)\psi$. Then, we compute:

$$\begin{aligned}\lim_{s\to 0} \frac{\psi(t+s)-\psi(t)}{s} &= \lim_{s\to 0} \frac{(U(s)-\mathbb{1})}{s} U(t)\psi - \lim_{s\to 0} \frac{V(s)-\mathbb{1}}{s} V(t)\psi \\ &= iHU(t)\psi - i\overline{H}V(t)\psi = i\overline{H}\psi(t) \;, \end{aligned} \tag{6.23}$$

where we used that $U(t)\psi \in D(H)$ if $\psi \in D(H)$, $V(t)\psi \in D(\overline{H})$ if $\psi \in D(H) \subset D(\overline{H})$, and that $HU(t)\psi = \overline{H}U(t)\psi$ for $\psi \in D(H)$ (because $\overline{H}$ is an extension of H). We obtain:

$$\frac{d}{dt}\|\psi(t)\|^2 = \frac{d}{dt}\langle \psi(t), \psi(t)\rangle = 2\mathrm{Re}\,\langle \psi(t), i\overline{H}\psi(t)\rangle = 0 \tag{6.24}$$

since $\langle \psi(t), \overline{H}\psi(t)\rangle \in \mathbb{R}$ (which follows from the fact that $\overline{H}$ is selfadjoint). With $\psi(0) = 0$, it follows that $\psi(t) = 0$ for all t and therefore that $U(t)\psi = V(t)\psi$ for all $\psi \in D(H)$. Since $D(H)$ is dense in $\mathcal{H}$ and $U(t)$, $V(t)$ are unitary (in particular, bounded), this also implies that $U(t) = V(t)$ on $\mathcal{H}$. ■

6.3 The RAGE theorem

There is an interesting relation between the spectrum of a selfadjoint operator H and the properties of the quantum dynamics $U(t) = e^{-iHt}$. This relation is summarized in a theorem due to Ruelle-Amrein-Georgescu-Enss. The goal here is to understand, based on the spectral properties of H, whether a quantum system whose evolution is generated by H remains confined in a bounded region for all times or whether instead it moves to infinity as $t \to \infty$.

A first simple observation is as follows. Let H be a selfadjoint operator, and $\mathcal{H}_{\text{ac}}$, $\mathcal{H}_{\text{sc}}$, $\mathcal{H}_{\text{pp}}$ the corresponding spectral subspaces, so that $\mathcal{H} = \mathcal{H}_{\text{ac}} \oplus \mathcal{H}_{\text{sc}} \oplus \mathcal{H}_{\text{pp}}$.

If $\psi \in \mathcal{H}_{\text{ac}}$, then the spectral measure μ_ψ is absolutely continuous with respect to the Lebesgue measure. This also implies that $\mu_{\varphi,\psi}$ is absolutely continuous with respect to Lebesgue, for all $\varphi \in \mathcal{H}$, since

$$|\mu_{\varphi,\psi}(\Omega)| = |\langle \varphi, P(\Omega)\psi\rangle| \leqslant \|\langle \varphi, P(\Omega)\rangle\|^{1/2} |\langle \psi, P(\Omega)\psi\rangle|^{1/2} = \mu_\varphi(\Omega)^{1/2}\mu_\psi(\Omega)^{1/2} \;. \tag{6.25}$$

Therefore, setting $U(t) = e^{-iHt}$ we find:

$$\langle \varphi, U(t)\psi\rangle = \int e^{-i\lambda t} d\mu_{\varphi,\psi}(\lambda) \to 0 \qquad \text{as } t \to \infty, \tag{6.26}$$

by the Riemann-Lebesgue lemma. This is because any Borel measure μ which is absolutely continuous with respect to Lebesgue can be written as $d\mu(\lambda) = f(\lambda)d\lambda$, with $f \in L^1(\mathbb{R}, d\lambda)$ and $d\lambda$ the volume measure. In fact, by Theorem 3.4:

$$\langle \varphi, U(t)\psi\rangle = \int e^{-i\lambda t} f_{\varphi,\psi}(\lambda) d\lambda \equiv \hat{f}_{\varphi,\psi}(t) \to 0 \qquad \text{as } t \to \infty. \tag{6.27}$$

This means that, if $\psi \in \mathcal{H}_{\text{ac}}$, the time evolved state $U(t)\psi$ becomes orthogonal to any fixed $\varphi \in \mathcal{H}$, as $t \to \infty$. This of course cannot be true for all $\psi \in \mathcal{H}$. In particular, if ψ is an eigenvector of H, that is if $H\psi = E\psi$, one has:

$$|\langle \varphi, U(t)\psi\rangle| = |\langle \varphi, \psi\rangle| \;, \qquad \text{for all } t \in \mathbb{R}. \tag{6.28}$$

A more exhaustive understanding of the asymptotic behavior of $\langle \varphi, U(t)\psi\rangle$ in the limit of large t is provided by the following theorem.

Theorem 6.6. *[Wiener] Let μ a finite complex Borel measure on $\mathbb{R}$ and:*

$$\hat{\mu}(t) := \int_{\mathbb{R}} e^{-it\lambda} d\mu(\lambda) \;. \tag{6.29}$$

Then,

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T |\hat{\mu}(t)|^2 dt = \sum_{\lambda\in\mathbb{R}} |\mu(\{\lambda\})|^2 \;, \tag{6.30}$$

where the sum on the r.h.s. is finite (because μ is a finite measure).

Remark 6.7. *Recall that any Borel measure has can be written as* $\mu = \mu_{ac} + \mu_{sc} + \mu_{pp}$. *Also, since* μ_{ac}, μ_{sc} *have continuous distribution,* $\mu(\{\lambda\}) = \mu_{pp}(\{\lambda\})$. *Therefore,* $\sum_{\lambda\in\mathbb{R}} |\mu(\{\lambda\})|^2 = \sum_{\lambda\in\mathbb{R}} |\mu_{pp}(\{\lambda\})|^2$. *The sum is over the support of* M_{pp} *of the pure point measure* μ_{pp}, *which is a countable set. This follows from the fact that* $M_{pp} = \bigcup_{n\in\mathbb{N}} M_n$ *with* $M_n = \{\lambda \in \mathbb{R} \mid \mu(\{\lambda\}) > 1/n\} \equiv \{\lambda \in \mathbb{R} \mid \mu_{pp}(\{\lambda\}) > 1/n\}$. *Each set* M_n *is countable and finite: otherwise,* $\mu(M_n) = \infty$, *which is impossible since* μ *is finite. Therefore,* M_{pp} *is the countable union of finite sets, and hence it is countable.*

Proof. We apply Fubini's theorem to write:

$$\begin{aligned}\frac{1}{T}\int_0^T |\widehat{\mu}(t)|^2 dt &= \frac{1}{T}\int_0^T \int_{\mathbb{R}}\int_{\mathbb{R}} e^{-i(x-y)t} d\mu(x) d\overline{\mu(y)} dt \\ &= \int_{\mathbb{R}}\int_{\mathbb{R}} \Big[\frac{1}{T}\int_0^T e^{-i(x-y)t} dt\Big] d\mu(x) d\overline{\mu(y)} \, . \end{aligned} \tag{6.31}$$

Since

$$\Big|\frac{1}{T}\int_0^T e^{-i(x-y)} dt\Big| \leqslant 1 \tag{6.32}$$

and, as $T \to \infty$:

$$\frac{1}{T}\int_0^T e^{-i(x-y)t} dt \to \begin{cases} 0 & \text{if } x \neq y \\ 1 & \text{if } x = y. \end{cases} \tag{6.33}$$

Therefore, by dominated convergence:

$$\frac{1}{T}\int_0^T |\widehat{\mu}(t)|^2 dt \to \int_{\mathbb{R}}\int_{\mathbb{R}} \chi_{\{0\}}(x-y) d\mu(x) d\overline{\mu(y)} = \int_{\mathbb{R}} \mu(\{y\}) d\overline{\mu(y)} = \sum_{y\in\mathbb{R}} |\mu(\{y\})|^2 \, . \tag{6.34}$$

■

Let us now apply this theorem to study the quantity $|\langle\varphi, U(t)\psi\rangle|$, describing the probability of finding the evolved state in the state φ at time t. If $\psi \in \mathcal{H}_{\mathrm{ac}} \oplus \mathcal{H}_{\mathrm{sc}}$ and $\varphi \in \mathcal{H}$ is arbitrary, the measure $\mu_{\varphi,\psi}$ has not atoms, *i.e.* it is such that $\mu_{\varphi,\psi}(\{\lambda\}) = 0$, for all $\lambda \in \mathbb{R}$. Therefore, by Theorem 6.6:

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T |\langle\varphi, e^{-iHt}\psi\rangle|^2 dt = 0 \, . \tag{6.35}$$

Hence the probability of finding the evolved state in φ tends to zero, but only in an averaged sense.

Notice that $|\langle\varphi, U(t)\psi\rangle|^2 = \|P_\varphi U(t)\psi\|^2$, with P_φ the orthogonal projection onto φ. We can extend Eq. (6.35) to a more general class of operators, called compact operators. Compact operators are the natural generalization of finite-rank operators, that is operators that can be written as finite linear combination of orthogonal projectors. In the following, we shall denote by $B_1(0)$ the unit ball in $\mathcal{H}$, that is:

$$B_1(0) = \{\psi \in \mathcal{H} \mid \|\psi\| \leqslant 1\} \, . \tag{6.36}$$

Definition 6.8. *An operator* $K \in \mathcal{L}(\mathcal{H})$ *is called compact if* $KB_1(0) \subset \mathcal{H}$ *is pre-compact in* $\mathcal{H}$, *that is if* $\overline{KB_1(0)}$ *is compact.*

Remark 6.9. *(i) Equivalently, an operator* $K \in \mathcal{L}(\mathcal{H})$ *is compact if and only if for any bounded sequence* $\psi_n \in \mathcal{H}$, $K\psi_n$ *has a convergent subsequence.*

(ii) The space of all compact operator $\mathcal{K}(\mathcal{H})$ *is a closed linear subspace of* $\mathcal{L}(\mathcal{H})$. *Also,* K^* *is compact if* K *is compact, and* KA, AK *are compact if* $K \in \mathcal{K}(\mathcal{H})$ *and* $A \in \mathcal{L}(\mathcal{H})$. *Furthermore, compact operators can be approximated in norm by sequences of finite rank operators.*

Definition 6.10. *An operator* $K : D(K) \to \mathcal{H}$ *is called relatively compact with respect to the self-adjoint operator* H *if there exists* $z \in \rho(H)$ *such that* $KR_z(H) = K(z-H)^{-1}$ *is compact.*

Remark 6.11. *(i) Using the first resolvent identity, $R_z(H)-R_{z_0}(H) = (z-z_0)R_z(H)R_{z_0}(H)$, one can check that if $KR_z(H)$ is compact for one $z \in \rho(H)$, then it is compact for all $z \in \rho(H)$.*

(ii) If K is relatively compact with respect to H, then $D(H) \subset D(K)$, because every $\psi \in D(H)$ can be written as $\psi = R_A(z)\varphi$ for a $\varphi \in \mathcal{H}$.

The results (6.27), (6.35) can now be extended as follows.

Theorem 6.12. *Let H be a selfadjoint operator. Let K be relatively compact with respect to H. Then, for all $\psi \in D(H)$:*

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \|Ke^{-iHt}P_c(H)\psi\|^2 dt = 0 \ , \tag{6.37}$$

where $P_c(H) = P_{ac}(H) + P_{sc}(H)$ is the orthogonal projection onto $\mathcal{H}_{ac} \oplus \mathcal{H}_{sc}$. Also, for all $\psi \in D(H)$:

$$\lim_{t\to\infty} \|Ke^{-itH}P_{ac}(H)\psi\|^2 = 0 \ . \tag{6.38}$$

If we also assume that K is bounded, then Eqs. (6.37), (6.38) hold true for any $\psi \in \mathcal{H}$.

Proof. To prove Eqs. (6.37), (6.38), we can assume that $\psi \in \mathcal{H}_{\mathrm{c}}$ and, respectively, that $\psi \in \mathcal{H}_{\mathrm{ac}}$, and drop the orthogonal projections. If K is a rank-one projector, the claims follow from Eqs. (6.27), (6.35). If K is a finite-rank operator, $K\psi = \sum_{j=1}^n \alpha_j\langle\psi_j,\psi\rangle\varphi_j$ for two orthonormal families $\{\varphi_1,\ldots,\varphi_n\}$, $\{\psi_1,\ldots,\psi_n\}$ then:

$$\|Ke^{-iHt}\psi\|^2 = \sum_{j=1}^n |\langle\psi_j, e^{-iHt}\psi\rangle|^2 \ , \tag{6.39}$$

and the problem reduces to the rank-1 case. If K is compact, we can find a sequence of finite-rank operators K_n with $\|K - K_n\| \leqslant 1/n$. Then:

$$\|Ke^{-iHt}\psi\|^2 \leqslant 2\|K_n e^{-iHt}\psi\|^2 + 2n^{-2}\|\psi\|^2 \ , \tag{6.40}$$

and the problem reduces to the finite-rank case (by choosing first n large enough, and then T or t large enough). Finally, it K is relatively compact with respect to H and $\psi \in D(H)$, we write $\psi = (H-z)^{-1}\xi$ for a $\xi \in \mathcal{H}$ (notice that, if $\psi \in \mathcal{H}_{\mathrm{c}}$ or $\psi \in \mathcal{H}_{\mathrm{ac}}$, then also $\xi \in \mathcal{H}_{\mathrm{c}}$ or, respectively, $\xi \in \mathcal{H}_{\mathrm{ac}}$). Thus, it is enough to apply the result for compact operators to the operator $K(H-z)^{-1}$, because the operator $(H-z)^{-1}$ commutes with e^{-iHt}. ∎

Example 6.13. *A simple application of these results is obtained by taking $H = -\Delta$ and K the multiplication operator $\chi_{B_R(0)}(x)$. It turns out that the operator K is relatively compact with respect to H. More generally, one can prove that all operators of the form $f(i\nabla)g(\hat{x})$, or $g(\hat{x})f(-i\nabla)$, for $f, g \in C_\infty(\mathbb{R}^n)$ and $g(-i\nabla) = \mathcal{F}^{-1}g(k)\mathcal{F}$ are compact. In our case, $g(x) = \chi_{B_R(0)}(x)$ and $f(k) = (k^2+z)^{-1}$, with $z \in \mathbb{C}\backslash\mathbb{R}$.*

Since H has purely absolutely continuous spectrum, we conclude that:

$$\|\chi_{B_R(0)}e^{it\Delta}\psi\| \to 0 \qquad \text{as } t\to\infty, \tag{6.41}$$

for every $\psi \in \mathcal{H}$ and for every $R > 0$. In other words, if the evolution is generated by the Laplace operator, the probability that the system is found in a ball of radius R around the origin decays to zero as $t \to \infty$, for all $R > 0$ and for all initial data $\psi \in \mathcal{H}$: the system moves to infinity.

As we will see later, more realistic Hamilton operators have the form $H = -\Delta + V$, for a potential V. Depending on the form of V, the spectrum of H may contain absolutely continuous, singular continuous and pure point parts. Taking again $K = \chi_{B_R(0)}(x)$ (which is still relatively compact with respect to H, at least for reasonable choices of V), we conclude that

$$\|\chi_{B_R(0)}(x)e^{-iHt}\psi\| \to 0 \qquad \text{as } t\to\infty, \tag{6.42}$$

if $\psi \in \mathcal{H}_{ac}$, that:

$$\frac{1}{T}\int_0^T \|\chi_{B_R(0)}(x)e^{-iHt}\psi\|^2 dt \to 0 \qquad \text{as } t\to\infty, \tag{6.43}$$

if $\psi \in \mathcal{H}_{ac} \oplus \mathcal{H}_{sc}$, and that:

$$\|\chi_{B_R(0)}(x)e^{-iHt}\psi\| = \|\chi_{B_R(0)}\psi\| \to \|\psi\| \tag{6.44}$$

as $R \to \infty$, if ψ is an eigenvector of H. In other words, if the initial data ψ is an eigenvector (hence, it belongs to $\mathcal{H}_{pp}$), its evolution remains localized within a ball of radius R, if R is large enough.

If ψ is contained in the spectral subspace $\mathcal{H}_{as}$ of H, the its evolution moves to infinity, while if it is contained in the spectral subspace $\mathcal{H}_c$, with possibly a component in $\mathcal{H}_{sc}$, the probability for finding the state within a ball of radius R still goes to zero, but only in an average sense.

It turns out that the behavior of $\|Ke^{-iHt}\psi\|$ can be used to dynamically characterize the spectral subspaces $\mathcal{H}_\mathrm{c}$ and $\mathcal{H}_\mathrm{pp}$ associated with H.

Theorem 6.14 (RAGE theorem)**.** *Let H be a selfadjoint operator and suppose that K_n is a sequence of relatively compact operators with respect to H, converging strongly to the identity. Then:*

$$\begin{aligned} \mathcal{H}_c &= \left\{\psi \in \mathcal{H} \mid \lim_{n\to\infty}\lim_{T\to\infty}\frac{1}{T}\int_0^T \|K_n e^{-iHt}\psi\| = 0\right\} \\ \mathcal{H}_{pp} &= \left\{\psi \in \mathcal{H} \mid \lim_{n\to\infty}\sup_{t\geqslant 0}\|(1-K_n)e^{-iHt}\psi\| = 0\right\} . \end{aligned} \tag{6.45}$$

Proof. Pick first $\psi \in \mathcal{H}_c$. By Cauchy-Schwarz and by Theorem 6.12, we find:

$$\frac{1}{T}\int_0^T \|K_n e^{-iHt}\psi\| dt \leqslant \left[\frac{1}{T}\int_0^T \|K_n e^{-iHt}\psi\|^2 dt\right]^{1/2} \to 0 \tag{6.46}$$

as $T \to \infty$. Hence:

$$\mathcal{H}_\mathrm{c} \subset \left\{\psi \in \mathcal{H} \mid \left\{\psi \in \mathcal{H} \mid \lim_{n\to\infty}\lim_{T\to\infty}\frac{1}{T}\int_0^T \|K_n e^{-iHt}\psi\| = 0\right\} . \tag{6.47}$$

On the other hand, suppose that $\psi \notin \mathcal{H}_\mathrm{c}$. We want to show that:

$$\frac{1}{T}\int_0^T \|K_n e^{-iHt}\psi\|^2 dt \tag{6.48}$$

does not converge to zero, if we let first $T \to \infty$ and then $n \to \infty$. Since $\psi \notin \mathcal{H}_\mathrm{c}$, we have $\psi = \psi_\mathrm{c} + \psi_\mathrm{pp}$, for a $\psi_\mathrm{c} \in \mathcal{H}_\mathrm{c}$ and for $\psi_\mathrm{pp} \in \mathcal{H}_\mathrm{pp}$, with $\psi_\mathrm{pp} \neq 0$. Since $\|K_n e^{-iHt}\psi\| \geqslant \|K_n e^{-iHt}\psi_\mathrm{pp}\| - \|K_n e^{-iHt}\psi_\mathrm{c}\|$ and since we know that:

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T \|K_n e^{-iHt}\psi_\mathrm{c}\| dt = 0 , \tag{6.49}$$

it is enough to show that

$$\frac{1}{T}\int_0^T \|K_n e^{-iHt}\psi_\mathrm{pp}\| dt \tag{6.50}$$

does not converge to zero, it $T \to \infty$ and then $n \to \infty$. To prove this, we shall show that:

$$\sup_{t\geqslant 0}\|K_n e^{-iHt}\psi_\mathrm{pp} - e^{-iHt}\psi_\mathrm{pp}\| \to 0 \tag{6.51}$$

as $n \to \infty$. If this is true, we obtain that:

$$\frac{1}{T}\int_0^T \|K_n e^{-iHt}\psi_\mathrm{pp}\| dt \geqslant \|\psi_\mathrm{pp}\| - \sup_{t\geqslant 0}\|K_n e^{-iHt}\psi_\mathrm{pp} - e^{-iHt}\psi_\mathrm{pp}\| \to \|\psi_\mathrm{pp}\| > 0 \tag{6.52}$$

as $n \to \infty$, which implies the claim. To show (6.51), we use that ψ_pp can be approximated by a sequence ψ_N, having the form:

$$\psi_N = \sum_{j=1}^N \alpha_j \varphi_j \tag{6.53}$$

where $(\varphi_j)_{j\in\mathbb{N}}$ are orthonormal eigenfunctions of H, associated with eigenvalues λ_j, recall Proposition 5.64. This implies that:

$$e^{-iHt}\psi_N = \sum_{j=1}^{N} \alpha_j e^{-i\lambda_j t}\varphi_j \ . \tag{6.54}$$

Hence, for every fixed N, as $n \to \infty$:

$$\sup_{t\in\mathbb{R}} \|K_n e^{-iHt}\psi_N - e^{-iHt}\psi_N\| \leqslant \sum_{j=1}^{N} |\alpha_j| \|K_n\varphi_j - \varphi_j\| \to 0 \ , \tag{6.55}$$

because $K_n \to \mathbb{1}_{\mathcal{H}}$ strongly. Since, on the other hand, $\|e^{-iHt}\psi_{\mathrm{pp}} - e^{-iHt}\psi_N\| = \|\psi_{\mathrm{pp}} - \psi_N\| \to 0$ and also:

$$\|K_n e^{-iHt}\psi_{\mathrm{pp}} - K_n e^{-iHt}\psi_N\| \leqslant \|K_n\| \|\psi_{\mathrm{pp}} - \psi_N\| \leqslant C\|\psi_{\mathrm{pp}} - \psi_N\| \to 0 \tag{6.56}$$

as $N \to \infty$, uniformly in t and in n, we obtain Eq. (6.51). (We used that strong convergence of K_n to $\mathbb{1}_{\mathcal{H}}$ implies that (K_n) is a bounded sequence, whose proof is left as an exercise). This proves the first identity in Eq. (6.45). Let us now prove the second identity. The inclusion:

$$\mathcal{H}_{\mathrm{pp}} \subset \left\{ \psi \in \mathcal{H} \mid \lim_{n\to\infty} \sup_{t\geqslant 0} \|(\mathbb{1}_{\mathcal{H}} - K_n)e^{-iHt}\psi\| = 0 \right\} \tag{6.57}$$

follows from Eq. (6.51). Conversely, it $\psi \notin \mathcal{H}_{\mathrm{pp}}$, then $\psi = \psi_{\mathrm{c}} + \psi_{\mathrm{pp}}$ for $\psi_{\mathrm{c}} \in \mathcal{H}_{\mathrm{c}}$, with $\psi_{\mathrm{c}} \neq 0$. Applying again Eq. (6.51), it is enough to show that

$$\sup_{t\geqslant 0} \|(\mathbb{1}_{\mathcal{H}} - K_n)e^{-iHt}\psi_{\mathrm{c}}\| \quad \text{does not converge to zero as } n \to \infty. \tag{6.58}$$

To this end, let us proceed by contradiction and assume that $\sup_{t\geqslant 0} \|(\mathbb{1}_{\mathcal{H}} - K_n)e^{-iHt}\psi_{\mathrm{c}}\| \to 0$ as $n \to \infty$. Then, we would conclude:

$$\begin{aligned} 0 &= \lim_{n\to\infty} \lim_{T\to\infty} \frac{1}{T} \int_0^T \|(\mathbb{1}_{\mathcal{H}} - K_n)e^{-iHt}\psi_{\mathrm{c}}\| dt \\ &\geqslant \|\psi_{\mathrm{c}}\| - \lim_{n\to\infty} \lim_{T\to\infty} \frac{1}{T} \int_0^T \|K_n e^{-iHt}\psi_{\mathrm{c}}\| dt = \|\psi_{\mathrm{c}}\| > 0 \end{aligned} \tag{6.59}$$

which is a contradiction. ∎

7 General Schrödinger operators

7.1 Kato-Rellich theorem

Often in quantum mechanics one has to deal with perturbations H of simple reference operators H_0. As an example, one might consider Hamiltonians of the form $H = H_0 + V$, with $H_0 = -\Delta$ and $V \equiv V(\hat{x})$ a multiplication operator, describing an external potential.

Perturbation theory aims at establishing properties of H, starting from the properties of H_0, assumed to be well-known. Of course, to reach this goal, we will also need some information about $H - H_0$. For example, it is easy to check that if $H - H_0$ is bounded and seldadjoint, then H is again selfadjoint (provided H_0 is selfadjoint). More generally, in this section we will show that relatively bounded perturbations of self-adjoint operators remain self adjoint (if the relative bound is less than one).

Definition 7.1. *Let $A : D(A) \to \mathcal{H}$, $B : D(B) \to \mathcal{H}$ be two densely defined linear operators. We say that B is relatively bounded with respect to A (or A-bounded) if $D(A) \subset D(B)$ and if there are constants $a, b > 0$ such that:*

$$\|B\psi\| \leqslant a\|A\psi\| + b\|\psi\| \tag{7.1}$$

for all $\psi \in D(A)$. If B is relatively bounded with respect to A, then the infimum over all $a > 0$ such that Eq. (7.1) holds true is called the relative bound of B with respect to A (or the A-bound of B). If the A-bound of B is zero, then we say that B is infinitesimally A-bounded.

The next theorem is the main result of this section.

Theorem 7.2 (Kato-Rellich)**.** *Let A be self-adjoint and B a symmetric operator, bounded with respect to A and with A-bound less than one. Then, $A+B$ defined on $D(A+B) = D(A)$ is selfadjoint. The statement remains true if we replace everywhere selfadjoint with essentially selfadjoint. In this case, we have $D(\overline{A}) \subset D(\overline{B})$ and $\overline{A} + \overline{B} = \overline{A+B}$.*

Proof. We shall only consider the case in which A is selfadjoint. We shall prove that $\mathrm{Ran}\,(A+B \pm i\lambda_0) = \mathcal{H}$ for a suitable $\lambda_0 > 0$. This implies that $(A+B)/\lambda_0$ is selfadjoint, hence that $A+B$ is selfadjoint.

Let $\varphi \in D(A)$. We have, for every $\lambda > 0$:

$$\|(A+i\lambda)\varphi\|^2 = \|A\varphi\|^2 + \lambda^2\|\varphi\|^2 . \tag{7.2}$$

Being A selfadjoint, $(A \pm i\lambda)^{-1}$ is bounded. Setting $\varphi = (A+i\lambda)^{-1}\psi$, we have, for all $\psi \in \mathcal{H}$:

$$\|\psi\|^2 \geqslant \|A(A+i\lambda)^{-1}\psi\|^2 \qquad \text{and} \qquad \|\psi\|^2 \geqslant \lambda^2\|(A+i\lambda)^{-1}\psi\|^2 . \tag{7.3}$$

Therefore, $\|A(A+i\lambda)^{-1}\| \leqslant 1$ and $\|(A+i\lambda)^{-1}\| \leqslant \lambda^{-1}$. From the relative boundedness, it follows that, for $\varphi = (A+i\lambda)^{-1}\psi$:

$$\|B(A+i\lambda)^{-1}\psi\| \leqslant a\|A(A+i\lambda)^{-1}\psi\| + b\|(A+i\lambda)^{-1}\psi\| \leqslant \Big(a + \frac{b}{\lambda}\Big)\|\psi\| . \tag{7.4}$$

Choosing $\lambda_0 > b/(1-a) > 0$ (recall that $a < 1$ by assumption), it follows that $\|B(A+i\lambda)^{-1}\| < 1$. Therefore, by the Neumann series

$$\mathbb{1}_{\mathcal{H}} + B(A+i\lambda_0)^{-1} = \mathbb{1}_{\mathcal{H}} - (-B(A+i\lambda_0)^{-1}) \tag{7.5}$$

is continuously invertible, and hence $\mathrm{Ran}\,(\mathbb{1}_{\mathcal{H}} + B(A+i\lambda_0)^{-1}) = \mathcal{H}$. Using that, for all $\varphi \in D(A)$:

$$(\mathbb{1}_{\mathcal{H}} + B(A+i\lambda_0)^{-1})(A+i\lambda_0)\varphi = (A+B+i\lambda_0)\varphi \tag{7.6}$$

and that $\mathrm{Ran}\,(A+i\lambda_0) = \mathcal{H}$ (recall that A is selfadjoint), we find $\mathrm{Ran}\,(A+B+i\lambda_0) = \mathcal{H}$. The same argument applies for $-i\lambda_0$; this proves that $A+B$ is selfadjoint. ∎

Let us now discuss applications of the above theorem. We will be interested in operators of the form $H = -\Delta + V(\hat{x})$. We will use the Kato-Rellich theorem to establish under which conditions on V the operator H is self-adjoint.

Theorem 7.3. ($-\Delta$-bounded potentials on $\mathbb{R}^3$.) *Let $V : \mathbb{R}^3 \to \mathbb{R}$, with $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, that is one can write $V = V_1 + V_2$ with $V \in L^2$ and $V_2 \in L^\infty$. Then, V is infinitesimally H_0-bounded, with $H_0 = -\Delta$ on $D(H_0) = H^2(\mathbb{R}^3)$. In particular, the operator $H = H_0 + V$ is selfadjoint on $D(H_0)$.*

Proof. Let $D(V) = \{\psi \in L^2 \mid V\psi \in L^2\}$. $D(V)$ contains $C_c^\infty(\mathbb{R}^d)$, and it is therefore dense in L^2. Let $V = V_1 + V_2$ with $V_1 \in L^2$ and $V_2 \in L^\infty$. Then, by the Sobolev lemma 3.83, any function $\varphi \in H^2(\mathbb{R}^3)$ is continuous and bounded. Therefore:

$$\|V\varphi\|_{L^2(\mathbb{R}^3)} \leqslant \|\varphi\|_\infty \|V_1\|_{L^2(\mathbb{R}^3)} + \|V_2\|_{L^\infty(\mathbb{R}^3)}\|\varphi\|_{L^2(\mathbb{R}^3)} , \tag{7.7}$$

that is, $H^2(\mathbb{R}^3) \subset D(V)$. The next lemma will allow us to complete the proof of infinitesimal boundedness of V with respect to $-\Delta$. ∎

Lemma 7.4. *For every $a > 0$ there exists $b > 0$ such that for all $\varphi \in H^2(\mathbb{R}^3)$:*

$$\|\varphi\|_\infty \leqslant a\|\Delta\varphi\|_{L^2} + b\|\varphi\|_{L^2} . \tag{7.8}$$

Remark 7.5. *Eq. (7.8) together with Eq. (7.7) concludes the proof of infinitesimal boundedness of V with respect to $-\Delta$.*

Proof. By Cauchy-Schwarz inequality:

$$\begin{aligned}\|\varphi\|_\infty &\leqslant \|\widehat{\varphi}\|_{L^1} = \|(1+k^2)(1+k^2)^{-1}\widehat{\varphi}\|_{L^1} \\ &\leqslant \|(1+k^2)^{-1}\|_{L^2}\|(1+k^2)\widehat{\varphi}\|_{L^2} \\ &\leqslant C(\|k^2\widehat{\varphi}\|_{L^2} + \|\widehat{\varphi}\|_{L^2})\ . \end{aligned} \tag{7.9}$$

Setting $\widehat{\varphi}_r(k) = r^3\widehat{\varphi}(rk)$, one has:

$$\|\widehat{\varphi}_r\|_{L^1(\mathbb{R}^3)} = \|\widehat{\varphi}\|_{L^1(\mathbb{R}^3)} \qquad \text{for all } r \neq 0. \tag{7.10}$$

At the same time, we also have:

$$\|\widehat{\varphi}_r\|_{L^2(\mathbb{R}^3)} = r^{\frac{3}{2}}\|\widehat{\varphi}\|_{L^2(\mathbb{R}^3)} \tag{7.11}$$

and:

$$\|k^2\widehat{\varphi}_r\|_{L^2(\mathbb{R}^3)} = r^{-\frac{1}{2}}\|k^2\widehat{\varphi}\|_{L^2(\mathbb{R}^3)}\ . \tag{7.12}$$

All together, we have:

$$\begin{aligned}\|\varphi\|_\infty &\leqslant \|\widehat{\varphi}\|_{L^1} = \|\widehat{\varphi}_r\|_{L^1} \leqslant C(\|k^2\widehat{\varphi}_r\|_{L^2} + \|\widehat{\varphi}_r\|_{L^2}) \\ &= Cr^{-\frac{1}{2}}\|k^2\widehat{\varphi}\|_{L^2} + Cr^{\frac{3}{2}}\|\widehat{\varphi}\|_{L^2} \\ &= Cr^{-\frac{1}{2}}\|\Delta\varphi\|_{L^2} + Cr^{\frac{3}{2}}\|\varphi\|_{L^2}\ . \end{aligned} \tag{7.13}$$

Being r a free parameter, the claim follows. ■

Example 7.6 (The Coulomb potential)**.** *Let $V(x) = -\frac{e}{|x|}$ be the Coulomb potential (and $-e$ the electric charge). We write:*

$$\begin{aligned}V(x) = -\frac{e}{|x|} &= -\chi_{|x|\leqslant R}\frac{e}{|x|} - \chi_{|x|>R}\frac{e}{|x|} \\ &\equiv V_1 + V_2\ , \end{aligned} \tag{7.14}$$

where $V_1 \in L^2(\mathbb{R}^3)$ and $V_2 \in L^\infty$. Therefore, the previous results imply that $H = -\Delta - \frac{e}{|x|}$ is selfadjoint on $H^2(\mathbb{R})$. Analogously, it is possible to check that the N-body Hamiltonian:

$$H = \sum_{j=1}^{N} -\Delta_j - \sum_{j<k}\frac{e_{jk}}{|x_j - x_k|} \tag{7.15}$$

is a selfadjoint operator on $H^2(\mathbb{R}^{3N})$.

If the operator A is bounded below, under the same assumptions of Kato-Rellich theorem one can also prove that $A + B$ is bounded below. We will not discuss the proof of this fact. Instead, we shall focus on a special important case, the one of the hydrogenic atom:

$$H = -\Delta - \frac{Z}{|x|}\ , \tag{7.16}$$

on $D(H) = H^2(\mathbb{R}^d)$. As we proved above, this operator is selfadjoint on $H^2(\mathbb{R}^d)$. The parameter $Z > 0$ plays the role of nuclear charge (here we set $e = 1$). We will prove that this model is stable, in the sense that the Hamiltonian is bounded below by a constant. We shall prove an optimal lower bound which matches the ground state energy of the model,

$$E_{\mathrm{GS}} = \inf_{\psi\in H^2(\mathbb{R}^d)}\frac{\langle\psi, H\psi\rangle}{\langle\psi,\psi\rangle}\ . \tag{7.17}$$

Notice that this is very much in contrast with what happens in classical mechanics. Classically, the Hamiltonian $H(p,q) = p^2 - Z/|q|$ is *not* bounded from below: one can lower the energy by taking the electron closer and closer to the nucleus (that is, sending $|q|$ to zero, and choosing $p = 0$). In quantum mechanics, we know from the uncertainty principle, Eq. (5.36), that particles cannot be simultaneously localized *both* in space and in velocity: this ultimately means that a particle that is very close to the nucleus should have a large kinetic energy. The compensation between these two energies is ultimately responsible for the stability of the hydrogenic atom, and more generally for the stability of matter. This heuristic principle is captured by the following inequality.

Lemma 7.7 (Coulomb uncertainty principle.). *Let $H \in H^1(\mathbb{R}^3)$. Then:*

$$\int dx \, \frac{1}{|x|}|\psi(x)|^2 \leqslant \|\nabla\psi\|_{L^2(\mathbb{R}^3)}\|\psi\|_{L^2(\mathbb{R}^3)} \, . \tag{7.18}$$

Before discussing the proof, let us use this lemma to prove the stability of the hydrogenic atom.

Proposition 7.8. *Let $\psi \in H^1(\mathbb{R}^d)$, $E_\psi = \langle\psi, H\psi\rangle$. Then, the following inequality holds true:*

$$E_\psi \geqslant -\frac{Z^2}{4}\|\psi\|_2^2 \, . \tag{7.19}$$

Equality is reached for $\psi = Ke^{-(Z/4)|x|}$.

In particular, this proposition proves that $E_{\mathrm{GS}} = -\frac{Z^2}{4}$ (recall that $H^2(\mathbb{R}^d) \subset H^1(\mathbb{R}^d)$, which follows from the definition of Sobolev space, Definition 3.74, together with $|k| \leqslant (1/2)(1 + |k|^2)$). This inequality proves the stability of the hydrogenic atom.

Proof. (of Proposition 7.8.) Suppose that $\|\psi\|_2 = 1$. By Lemma 7.7, we have:

$$E_\psi \geqslant \|\nabla\psi\|_2^2 - Z\|\nabla\psi\|_2 \geqslant -\frac{Z^2}{4} \, , \tag{7.20}$$

as it follows from $x^2 - Zx = (x - Z/2)^2 - Z^2/4$. Equality for $\psi = Ke^{-(Z/4)|x|}$ is left as an exercise. ∎

To conclude, let us prove Lemma 7.7.

Proof. (of Lemma 7.7.) The starting point is the following identity:

$$2\langle\psi, \frac{1}{|x|}\psi\rangle = \sum_{j=1,2,3}\langle\psi, [\partial_{x_j}, \frac{x_j}{|x|}]\psi\rangle \, , \tag{7.21}$$

where we used that:

$$\Big[\partial_{x_j}, \frac{x_j}{|x|}\Big] = \frac{1}{|x|} - \frac{x_j^2}{|x|^3} \, . \tag{7.22}$$

Therefore, integrating by parts:

$$\begin{aligned}
2\langle\psi, \frac{1}{|x|}\psi\rangle &= -\sum_{j=1,2,3}\Big(\langle\partial_{x_j}\psi, \frac{x_j}{|x|}\psi\rangle + \langle\frac{x_j}{|x|}\psi, \partial_{x_j}\psi\rangle\Big) \\
&= -2\mathrm{Re}\sum_{j=1,2,3}\langle\partial_{x_j}\psi, \frac{x_j}{|x|}\psi\rangle \\
&\leqslant 2\sum_j|\langle\partial_{x_j}\psi, \frac{x_j}{|x|}\psi\rangle| \, .
\end{aligned}$$

By Cauchy-Schwarz inequality:

$$\begin{aligned}
2\langle\psi, \frac{1}{|x|}\psi\rangle &\leqslant 2\sum_j\|\partial_{x_j}\psi\|_{L^2}\Big\|\frac{x_j}{|x|}\psi\Big\|_{L^2} \\
&\leqslant 2\Big(\sum_j\|\partial_{x_j}\psi\|_{L^2}^2\Big)^{1/2}\Big(\sum_j\Big\|\frac{x_j}{|x|}\psi\Big\|_{L^2}^2\Big)^{1/2} \\
&\leqslant 2\|\nabla\psi\|_{L^2}\|\psi\|_{L^2} \, .
\end{aligned} \tag{7.23}$$

This concludes the proof. ∎

7.2 Relatively compact perturbations and Weyl's theorem

Kato-Rellich theorem allowed us to prove that selfadjointness survives perturbations, if they are small enough. It is also natural to ask whether perturbations preserve other properties of self-adjoint operators. For example, how does the spectrum of an operators looks like after perturbation?

Let T be a selfadjoint operator, and let λ be an eigenvalue of T. Let φ be the eigenvector of T with eigenvalue λ, and consider the perturbation $T + \varepsilon P_\varphi$, where P_φ is the projector onto φ. Then, φ is still an eigenvector of $T+\varepsilon P_\varphi$, with new eigenvalue $\lambda+\varepsilon$. This shows that the eigenvalues of a selfadjoint operator are, in general, not invariant under perturbations. The question we would like to address here is whether there exists subsets of the spectrum that are invariant under a class of perturbations.

Given a selfadjoint operator T with projection-valued measure P_T, let us define the discrete spectrum:

$$\sigma_{\mathrm{d}}(T) = \{\lambda \in \mathbb{R} \mid \operatorname{rank} P_T((\lambda - \varepsilon; \lambda + \varepsilon)) < \infty \qquad \text{for some } \varepsilon > 0\} \tag{7.24}$$

and the essential spectrum:

$$\sigma_{\mathrm{ess}}(T) = \{\lambda \in \mathbb{R} \mid \operatorname{rank} P_T((\lambda - \varepsilon; \lambda + \varepsilon)) = \infty \qquad \text{for all } \varepsilon > 0\}\ . \tag{7.25}$$

Obviously, $\sigma(T) = \sigma_{\mathrm{d}}(T) \cup \sigma_{\mathrm{ess}}(T)$, and $\sigma_{\mathrm{d}}(T) \cap \sigma_{\mathrm{ess}}(T) = \varnothing$. The essential spectrum contains the absolutely continuous spectrum, the singular continuous spectrum, accumulation points of eigenvalues and isolated eigenvalues of infinite multiplicity. Instead, the discrete spectrum $\sigma_{\mathrm{d}}(T)$ contains isolated eigenvalues of finite multiplicity. From what we discussed above, we know that the discrete spectrum is not invariant under finite rank perturbations. Instead, as we shall show, the essential spectrum is invariant under finite rank and, more generally, compact perturbations.

Lemma 7.9 (Weyl criterion for the essential spectrum)**.** *Let T be a self-adjoint operator. Then, $\lambda \in \sigma_{ess}(T)$ if and only if there exists a sequence $\psi_n \in D(T)$ such that $\|\psi_n\| = 1$ for all $n \in \mathbb{N}$, ψ_n converges weakly to 0 as $n \to \infty$, $\|(T-\lambda)\psi_n\| \to 0$. Moreover, if $\lambda \in \sigma_{ess}(T)$, the sequence ψ_n can be chosen to be orthonormal. Such a sequence is called a singular Weyl sequence at λ.*

Remark 7.10. *With respect to the Weyl criterion we discussed with Theorem 5.15, here $\psi_n \to 0$ weakly.*

Proof. Let ψ_n be a Weyl sequence at λ. Then, by Theorem 5.15, $\lambda \in \sigma(T)$. It is therefore enough to show that $\lambda \notin \sigma_{\mathrm{d}}(T)$. We proceed by contradiction. Suppose that $\lambda \in \sigma_{\mathrm{d}}(T)$. Then, there is $\varepsilon > 0$ such that the spectral projection $P_\varepsilon := P_T((\lambda-\varepsilon, \lambda+\varepsilon))$ is of finite rank. Let $\varphi_n := P_\varepsilon \psi_n$. Since, by assumption, $\psi_n \to 0$ weakly and P_ε is finite rank, we have $\varphi_n = P_\varepsilon \psi_n \to 0$ strongly.[3] On the other hand, by the spectral theorem:

$$\begin{aligned}
\|\psi_n - \varphi_n\|^2 &= \langle \psi_n, P_T((\lambda-\varepsilon;\lambda+\varepsilon)^c)\psi_n\rangle \\
&= \int \chi((\lambda-\varepsilon;\lambda+\varepsilon)^c)(x) d\mu_{\psi_n}(x) \\
&\leqslant \frac{1}{\varepsilon^2}\int (x-\lambda)^2 d\mu_{\psi_n}(x) = \frac{1}{\varepsilon^2}\|(T-\lambda)\psi_n\|^2 \to 0\ .
\end{aligned} \tag{7.28}$$

[3]Since P_ε is finite rank, it can be written as $P_\varepsilon = \sum_{\ell=1}^M \alpha_\ell P_{\phi_\ell}$, where $\{\phi_\ell\}$ is an orthonormal family, P_{ϕ_ℓ} is the projector over ϕ_ℓ and M = rank of P_ε. Therefore,

$$P_\varepsilon \psi_n = \sum_{\ell=1}^M \alpha_\ell \phi_\ell \langle \phi_\ell, \psi_n\rangle\ , \tag{7.26}$$

and the norm $\|P_\varepsilon \psi_n\|$ is:

$$\|P_\varepsilon \psi_n\|^2 = \sum_{\ell=1}^M |\alpha_\ell|^2 |\langle \phi_\ell, \psi_n\rangle|^2\ . \tag{7.27}$$

By weak convergence, $\langle \phi_\ell, \psi_n\rangle \to 0$. Hence, $\|P_\varepsilon \psi_n\| \to 0$.

Since $\|\psi_n\| = 1$ by assumption, and $\|\psi_n\| - \|\psi_n - \varphi_n\| \leqslant \|\varphi_n\| \leqslant \|\psi_n\| + \|\psi_n - \varphi_n\|$, we conclude that $\|\varphi_n\| \to 1$. This gives rise to a contradition: P_ε cannot be of finite rank, hence $\lambda \notin \sigma_{\mathrm{d}}(T)$.

Conversely, suppose that $\lambda \in \sigma_{\mathrm{ess}}(T)$. We claim that there exists a singular Weyl sequence at λ. There are two possibilities: either λ is isolated, or it is not. Suppose that λ is isolated. Then, λ has to be an eigenvalue of infinite multiplicity. We can choose an orthonormal sequence ψ_n in the eigenspace of T associated to λ. It is clear that $\psi_n \to 0$ weakly. Thus, $\{\psi_n\}$ is a singular Weyl sequence.

Suppose that λ is not isolated. In this case, consider the sequence of orthogonal projections:

$$P_n = P_T([\lambda - 1/n; \lambda - 1/(n+1)) \cup (\lambda + 1/(n+1); \lambda + 1/n]) . \tag{7.29}$$

Since λ is not isolated, there must be an infinite subsequence n_j, such that $\operatorname{rank} P_{n_j} > 0$ for all j. Hence, we construct a singular Weyl sequence by choosing a normalized $\psi_j \in \operatorname{ran} P_{n_j}$, for all $j \in \mathbb{N}$. ∎

We are now ready to prove stability of the essential spectrum with respect to compact perturbations.

Corollary 7.11. *Let T be a selfadjoint operator and K selfadjoint and compact. Then, $\sigma_{ess}(T + K) = \sigma_{ess}(T)$.*

Remark 7.12. *In particular, if T is a compact selfadjoint operator, this theorem recovers the well-known result $\sigma_{ess}(T) = \{0\}$.*

Proof. Let $\lambda \in \sigma_{\mathrm{ess}}(T)$ and let ψ_n be a singular Weyl sequence at λ. Then, we have:

$$\|(T + K - \lambda)\psi_n\| \leqslant \|(T - \lambda)\psi_n\| + \|K\psi_n\| \to 0 \tag{7.30}$$

because $\psi_n \to 0$ weakly, which implies that $K\psi_n \to 0$ strongly. Therefore, ψ_n is also a singular Weyl sequence at λ for the operator $T+K$, and therefore $\lambda \in \sigma_{\mathrm{ess}}(T+K)$. Reversing the roles of T and $T + K$, we can also show that $\lambda \in \sigma_{\mathrm{ess}}(T + K)$ implies $\lambda \in \sigma_{\mathrm{ess}}(T)$. ∎

Since, as observed at the beginning of the section, any point in the discrete spectrum can be moved away by a finite rank perturbation, we obtain the following characterization of the essential spectrum, whose proof will be omitted.

Theorem 7.13. *Let T be a selfadjoint operator. Then,*

$$\sigma_{ess}(T) = \bigcap_{\substack{K \text{ compact} \\ \text{self-adjoint}}} \sigma(T + K) . \tag{7.31}$$

Before discussing applications, let us mention that the essential spectrum is not only preserved by compact operators, but even by relatively compact operators. Recall that for a selfadjoint operator T, we say that K is relatively compact with respect to T if $KR_T(z)$ is compact for a $z \in \rho(T)$.

Theorem 7.14 (Weyl.)**.** *Let A, B be selfadjoint operators such that $R_A(z) - R_B(z)$ is compact, for a $z \in \rho(A) \cap \rho(B)$. Then, $\sigma_{ess}(A) = \sigma_{ess}(B)$.*

Proof. Fix $z \in \rho(A) \cap \rho(B)$. Let $\lambda \in \sigma_{\mathrm{ess}}(A)$ and ψ_n be a singular Weyl sequence for A at λ. Then:

$$\Big[R_A(z) - \frac{1}{\lambda - z}\Big]\psi_n = -\frac{R_A(z)}{\lambda - z}(A - \lambda)\psi_n . \tag{7.32}$$

Since $R_A(z)$ is bounded, we obtain that ψ_n is also a singular Weyl sequence for $R_A(z)$ at the point $(\lambda - z)^{-1}$. We claim that this proves that $(\lambda - z)^{-1} \in \sigma_{\mathrm{ess}}(R_A(z))$. Notice that this does not directly follow from Lemma 7.9, since the operator $R_A(z)$ is not selfadjoint. Nevertheless, the proof of Lemma 7.9 directly applies to this case as well, since the spectral projector of A is, by construction, equal to the spectral projection of $R_A(z)$. Also, the proof of Corollary 7.11, together with the assumption that $R_A(z) - R_B(z)$ is compact, implies that $(\lambda - z)^{-1} \in \sigma_{\mathrm{ess}}(R_B(z))$.

We are left with showing that $\lambda \in \sigma_{\text{ess}}(B)$. Setting $\varphi_n = R_B(z)\psi_n$, we find that:

$$\|(B-\lambda)\varphi_n\| = |z-\lambda|\Big\|\Big(R_B(z) - \frac{1}{\lambda - z}\Big)\psi_n\Big\| \to 0 \qquad \text{as } n \to \infty. \tag{7.33}$$

Moreover, since

$$\lim_{n\to\infty} \|\varphi_n\| = \lim_{n\to\infty} \|(\lambda - z)^{-1}\psi_n + (R_B(z) - (\lambda - z)^{-1})\psi_n\| = |\lambda - z|^{-1} \neq 0 \tag{7.34}$$

it follows that $\widetilde{\varphi}_n = \varphi_n/\|\varphi_n\|$ is a singular Weyl sequence for B at λ and that $\lambda \in \sigma_{\text{ess}}(B)$. Reverting the roles of A and B, we conclude that $\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(B)$. ■

The invariance of the essential spectrum with respect to relatively bounded perturbations is now a simple corollary of the last theorem.

Corollary 7.15. *Let T be a selfadjoint operator and let K be selfadjoint and relatively compact with respect to T. Then, $\sigma_{ess}(T) = \sigma_{ess}(T + K)$.*

Proof. To begin, notice that $T + K$ is a selfadjoint operator. In fact:

$$KR_T(i\lambda) = (KR_T(i))(T - i)R_T(i\lambda) \tag{7.35}$$

from which we get $\|KR_T(i\lambda)\| \to 0$ as $\lambda \to \infty$, since K is relatively compact with respect to T. This implies that K is relatively bounded with respect to T, with relative bound 0: hence, $T + K$ is selfadjoint, and $R_{T+K}(z)$ is bounded for all $z \in \mathbb{C}\backslash\mathbb{R}$.

To prove the corollary, it is enough to observe that

$$R_{T+K}(z) - R_T(z) = R_{T+K}(z)KR_T(z) \tag{7.36}$$

is the product of a bounded operator $R_{T+K}(z)$ and a compact operator $KR_T(z)$, and it is therefore compact. The claim then follows from Theorem 7.14. ■

7.3 Two examples of Schrödinger operators

In this section we shall discuss applications of Kato-Rellich and Weyl's theorems. We shall consider operators of the form $H = -\Delta + V(x)$, for suitable, explicit choices of the external potential $V(x)$. As we shall see, the spectrum of H will depend dramatically on the behavior of the function V.

Operators of this form are called Schrödinger operators. They play an important role in quantum mechanics. The nature of the spectrum of H will allow us to understand the dynamics generated by H, via the Schrödinger equation.

7.3.1 The harmonic oscillator

Consider the operator $H_{\text{harm}} = -\Delta + \omega^2 x^2$, depending on a fixed parameter $\omega \in \mathbb{R}$. For simplicity, suppose first that the system is one-dimensional: $x \in \mathbb{R}$ and $\Delta = d^2/dx^2$. Observe that the perturbation $V(x) = \omega^2 x^2$ is not relatively bounded with respect to $-\Delta$. Nevertheless, using the positivity of $V(x)$, we can construct a selfadjoint extension of H_{harm} by means of the Friedrichs extension.

The spectrum. Next, remark that $(H_{\text{harm}} + 1)^{-1}$ is compact. Therefore, the spectrum of $(H_{\text{harm}} + 1)^{-1}$ is discrete, and can only accumulate at zero (recall that the essential spectrum is given by $\{0\}$). This implies that the spectrum of H_{harm} consists of isolated eigenvalues, diverging at infinity.

To determine the eigenvalues of H_{harm}, we define the operators:

$$A_\pm = \frac{1}{\sqrt{2}}\Big[\sqrt{\omega}x \mp \frac{1}{\sqrt{\omega}}\frac{d}{dx}\Big]\,. \tag{7.37}$$

Note that $A_+ = A_-^*$. A simple computation shows that $[A_-, A_+] = 1$ and that $H = \omega(2\mathcal{N} + 1)$ where $\mathcal{N} = A_+A_-$. Next, we observe that:

$$[\mathcal{N}, A_\pm] = \pm A_\pm\,. \tag{7.38}$$

Hence, if $\mathcal{N}\psi = n\psi$ for $\psi \neq 0$, then $\mathcal{N}A_\pm\psi = (n \pm 1)A_\pm\psi$. Moreover, we have $\|A_+\psi\|^2 = \langle\psi, A_-A_+\psi\rangle = (n+1)\|\psi\|^2$ and $\|A_-\psi\|^2 = \langle\psi, A_+A_-\psi\rangle = n\|\psi\|^2$. This implies that $n \geqslant 0$, and therefore that $\sigma(\mathcal{N}) \subset \mathbb{N}$, because if $n \notin \mathbb{N}$ was an eigenvalue, then applying A_- sufficiently many times we would find a negative eigenvalue of $\mathcal{N}$.

if $\mathcal{N}\psi_0 = 0$, we must have $A_-\psi_0 = 0$: if $A_-\psi_0 \neq 0$, it would be an eigenvector of $\mathcal{N}$ with eigenvalue -1. The condition $A_-\psi_0 = 0$ implies that:

$$\sqrt{\omega}x\psi_0(x) = \frac{1}{\sqrt{\omega}}\psi_0'(x) \tag{7.39}$$

which has a unique normalized solution (up to an irrelevant phase):

$$\psi_0(x) = (\omega/\pi)^{1/4}e^{-\omega x^2/2} \ . \tag{7.40}$$

Starting from ψ_0, we can construct eigenvectors ψ_n associated with the eigenvalue $n \in \mathbb{N}$ of $\mathcal{N}$ for all $n \in \mathbb{N}$, setting:

$$\psi_n(x) = \frac{1}{\sqrt{n}}A_+^n\psi_0(x) \ . \tag{7.41}$$

We find that:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}(\omega/\pi)^{1/4}H_n(\sqrt{\omega}x)e^{-\omega x^2/2} \ , \tag{7.42}$$

where H_n is the Hermite polynomial of degree n, given by:

$$H_n(x) = e^{x^2/2}\Big[x - \frac{d}{dx}\Big]^n e^{-x^2/2} = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2} \ . \tag{7.43}$$

It turns out that the eigenvectors $\{\psi_n\}$ form a basis of the Hilbert space $L^2(\mathbb{R})$. This might be checked from the properties of the Hermite polynomials, or from the spectral theorem: since H_{harm} is selfadjoint and has discrete spectrum, the set of eigenvectors must form a complete basis of the Hilbert space. Summarizing, the Hamiltonian of the harmonic oscillator has the spectrum:

$$\sigma(H_{\text{harm}}) = \sigma_{\text{pp}}(H_{\text{harm}}) = \{\omega(2n+1) : n \in \mathbb{N}\} \ . \tag{7.44}$$

Each eigenvalue $\lambda_n = \omega(2n+1)$ is simple, and it is associated with the normalized eigenvector ψ_n. Notice that the difference $\lambda_{n+1} - \lambda_n$ is independent of n. In other words, the energy is quantized: each quantum carries the energy 2ω. Applying the operator A_+, we generate an additional energy quantum, applying the operator A_- we annihilate a quantum of energy. The operator A_+ is therefore called a creation operator, while A_- is called an annihilation operator.

Properties of eigenvectors. In terms of the creation operator A_+, the eigenvectors can be written as $\psi_n = (\sqrt{n!})^{-1}A_+^n\psi_0$. A simple computation shows that the expectation values of the position and of the momentum operator on the state ψ_n vanish. In fact:

$$\begin{aligned}
\langle\psi_n, \hat{x}\psi_n\rangle &= \frac{1}{\sqrt{2\omega}}\langle\psi_n, (A_+ + A_-)\psi_n\rangle \\
&= \frac{1}{n!\sqrt{2\omega}}\langle A_+^n\psi_0, (A_+ + A_-)A_+^n\psi_0\rangle \\
&= \frac{2}{n!\sqrt{2\omega}}\mathrm{Re}\,\langle A_+^n\psi_0, A_+^{n+1}\psi_0\rangle = 0
\end{aligned} \tag{7.45}$$

and similarly, with the momentum operator $\hat{p} = id/dx$:

$$\begin{aligned}
\langle\psi_n, \hat{p}\psi_n\rangle &= i\sqrt{\omega/2}\langle\psi_n, (A_- - A_+)\psi_n\rangle \\
&= i\frac{\sqrt{\omega}}{n!\sqrt{2}}\langle A_+^n\psi_0, (A_- - A_+)A_+^n\psi_0\rangle \qquad (7.46) \\
&= \frac{\sqrt{2\omega}}{n!}\mathrm{Im}\,\langle A_+^n\psi_0, A_+^{n+1}\psi_0\rangle = 0 \ . \qquad (7.47)
\end{aligned}$$

To have an idea of the distribution of position and momentum in the state ψ_n, we have to consider the variance of these quantities. We find:

$$\begin{aligned}
\Delta x_{\psi_n} &= \langle \psi_n, \hat{x}^2 \psi_n \rangle \\
&= \frac{1}{2\omega n!} \langle A_+^n \psi_0, (A_+ + A_-)^2 A_+^n \psi_0 \rangle \\
&= \frac{1}{2\omega n!} \langle A_+^n \psi_0, (A_+ A_- + A_- A_+) A_+^n \psi_0 \rangle \\
&= \frac{1}{2\omega n!} \langle A_+^n \psi_0, (2A_- A_+ - 1) A_+^n \psi_0 \rangle \\
&= \frac{1}{\omega n!} \| A_+^{n+1} \psi_0 \|^2 - \frac{1}{2\omega n!} \| A_+^n \psi_0 \|^2 = \frac{1}{\omega} (n + 1/2) \; . \qquad (7.48)
\end{aligned}$$

Similarly,

$$\begin{aligned}
\Delta p_{\psi_n} &= \langle \psi_n, \hat{p}^2 \psi_n \rangle \\
&= -\frac{\omega}{2n!} \langle A_+^n \psi_0, (A_- - A_+)^2 A_+^n \psi_0 \rangle \\
&= \frac{\omega}{2n!} \langle A_+^n \psi_0, (A_+ A_- + A_- A_+) A_+^n \psi_0 \rangle = \omega (n + 1/2) \; . \qquad (7.49)
\end{aligned}$$

We conclude that:

$$\Delta x_{\psi_n} \Delta p_{\psi_n} = (n + 1/2)^2 \; . \qquad (7.50)$$

Observe that for $n = 0$, corresponding to the state ψ_0 with smallest energy (the vacuum state, with no energy quanta), the product of the variance is minimal, according to Heisenberg uncertainty principle. For larger n, on the other hand, the uncertainty in the state ψ_n grows.

7.3.2 Finite well potential

The harmonic oscillator is a special example, is the sense that the Hamiltonian operator H has a purely discrete spectrum. Here we shall consider a simple one-dimensional system, where the spectrum of the Hamilton operator has a discrete and continuous component. We consider a Schrödinger operator $H = -\Delta + V$, with $V : \mathbb{R} \to \mathbb{R}$ by setting:

$$V(x) = \begin{cases} -b & \text{if } |x| < a \\ 0 & \text{if } |x| \geqslant a \end{cases} \qquad (7.51)$$

for some $a, b > 0$. It is easy to check that $V(x)$ is relatively compact with respect the Laplace operator $-\Delta = -d^2/dx^2$. Therefore, it follows from Weyl's theorem that the Hamilton operator H is such that:

$$\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(-\Delta) = [0; \infty) \; . \qquad (7.52)$$

We can ask whether H has additional eigenvalues. To answer this question, we shall solve the eigenvalue problem (also known as the time-independent Schrödinger equation) $H\psi = E\psi$, *i.e.*:

$$\Big[-\frac{d^2}{dx^2} + V(x) \Big] \psi(x) = E \psi(x) \; . \qquad (7.53)$$

We find:

$$-\psi''(x) = E\psi(x) \qquad (7.54)$$

for $|x| \geqslant a$ and:

$$-\psi''(x) = (E + b)\psi(x) \qquad (7.55)$$

for $|x| < a$. It follows that, if $E \geqslant 0$, $\psi(x) = Ae^{i\sqrt{E}x} + \widetilde{A}e^{-i\sqrt{E}x}$ if $x > a$ and, similarly, $\psi(x) = Be^{i\sqrt{E}x} + \widetilde{B}e^{-i\sqrt{E}x}$ if $x < -a$. But then, $\psi \notin L^2(\mathbb{R})$. Hence, H has no positive eigenvalues.

Negative eigenvalues. Let us assume now $E < 0$. In this case, explucing exponentially increasing solutions, we obtain that:

$$\psi(x) = \begin{cases} Ae^{-\sqrt{|E|}(x-a)} & \text{if } x \geqslant a \\ Be^{\sqrt{|E|}(x+a)} & \text{if } x \leqslant -a \end{cases} \qquad (7.56)$$

for some constants A, B. For $|x| < a$, on the other hand, we find:

$$\psi(x) = C\cos(\omega x) + \widetilde{C}\sin(\omega x) \tag{7.57}$$

where we set $\omega = \sqrt{b - |E|}$ (the case $E < -b$ can be easily excluded, since $H \geqslant -b$ cannot have eigenvalues below $-b$). Next, we have to make sure that ψ and ψ' are continuous at $x = \pm a$ (otherwise ψ is not a solution of $H\psi = E\psi$ on $\mathbb{R}$). We obtain the conditions:

$$\begin{aligned} B &= C\cos(\omega a) - \widetilde{C}\sin(\omega a) \\ \sqrt{|E|}B &= \omega C\sin(\omega a) + \omega C\cos(\omega a) \end{aligned} \tag{7.58}$$

at $x = -a$ and

$$\begin{aligned} A &= C\cos(\omega a) + \widetilde{C}\sin(\omega a) \\ -\sqrt{|E|}A &= -\omega C\sin(\omega a) + \omega\widetilde{C}\cos(\omega a) \end{aligned} \tag{7.59}$$

at $x = a$. Thus:

$$\begin{aligned} C\cos(\omega a) - \widetilde{C}\sin(\omega a) &= \frac{\omega}{\sqrt{|E|}}C\sin(\omega a) + \frac{\omega}{\sqrt{|E|}}\widetilde{C}\cos(\omega a) \\ C\cos(\omega a) + \widetilde{C}\sin(\omega a) &= \frac{\omega}{\sqrt{|E|}}C\sin(\omega a) - \frac{\omega}{\sqrt{|E|}}\widetilde{C}\cos(\omega a) \end{aligned} \tag{7.60}$$

or equivalently

$$\begin{aligned} C - \widetilde{C}\tan(\omega a) &= \frac{\omega}{\sqrt{|E|}}C\tan(\omega a) + \frac{\omega}{\sqrt{|E|}}\widetilde{C} \\ C + \widetilde{C}\tan(\omega a) &= \frac{\omega}{\sqrt{|E|}}C\tan(\omega a) - \frac{\omega}{\sqrt{|E|}}\widetilde{C} \end{aligned} \tag{7.61}$$

To solve these equations, we must either have $\widetilde{C} = 0$ and $\sqrt{|E|} = \omega\tan(\omega a)$ or $C = 0$ and $\sqrt{|E|}\tan(\omega a) = -\omega$. Noticing that $\sqrt{|E|} = \sqrt{b - \omega^2}$ we can find solutions $\omega \in [0; \sqrt{b})$ of the equation $\sqrt{|E|} = \omega\tan(\omega a)$ intersecting the graphs $\sqrt{b - \omega^2}$ and of $\omega\tan(\omega a)$. Depending on the value of b, we find finitely many solutions $\omega_1, \dots, \omega_n$. It is interesting to notice that, no matter how small $b > 0$ is, we can always find a solutions $\omega_1 > 0$. Similarly, we can find solutions of $\sqrt{|E|}\tan(\omega a) = -\omega$, by looking at the intersections of the graphs of $\tan(\omega a)$ and of $-\omega/\sqrt{b - \omega^2}$. Also in this case, depending on the value of b, we obtain finitely many solutions $\widetilde{\omega}_1, \dots, \widetilde{\omega}_{n_2}$ (in this case, for b small enough, there is no solutions). For each value of $\omega \in \{\omega_1, \dots, \omega_{n_1}, \widetilde{\omega}_1, \dots, \widetilde{\omega}_{n_2}\}$, we can find the corresponding eigenvalue $E_1, \dots, E_{n_1+n_2}$ and a corresponding eigenvector $\psi_1, \dots, \psi_{n_1+n_2}$. Let us stress, once again, that the number of eigenvalues depend on the parameter a, b and that, no matter how small $a, b > 0$ are, there is always at least one negative eigenvalue.

Generalized eigenvectors for positive energies. We can ask whether we can find solutions of the equation $H\psi = E\psi$ for $E > 0$, that are associated with the continuous spectrum of H. As noticed above, for $E > 0$, that are associated with the continuous spectrum of H. As noticed above, for $E > 0$ solutions of $H\psi = E\psi$ are not in $L^2(\mathbb{R})$, they cannot be normalized. Still, we can look for so-called generalized eigenfunctions, oscillating at infinity, playing the same role as plane waves e^{ikx} play for the Laplace operator (notice that $-d^2/dx^2 e^{ikx} = k^2 e^{ikx}$; hence e^{ikx} is a solution of the eigenvalue equation $-\Delta f = Ef$, with $E = k^2 \geqslant 0$).

For $E > 0$, we find that solutions of $H\psi = E\psi$ must have the form

$$\psi(x) = \begin{cases} e_1 e^{ikx} + a_1 e^{-ikx} & \text{for } x < -a \\ c_1 e^{i\omega x} + c_2 e^{-i\omega x} & \text{for } |x| \leqslant a \\ e_2 e^{-ikx} + a_2 e^{ikx} & \text{for } x > a \end{cases} \tag{7.62}$$

for appropriate coefficients $e_1, e_2, a_1, a_2, c_1, c_2$ and where $k = \sqrt{E}$ and $\omega = \sqrt{E + b}$. The coefficients e_1 and e_2 are known as the incoming coefficients since they are associated to waves e^{ikx} for $x < -a$ and e^{-ikx} for $x > a$ that are moving towards the obstacle (described by the potential). The coefficients a_1, a_2 are known as outgoing coefficients, since they are associated to waves moving away from the obstacles, towards infinity.

The continuity of ψ, ψ' at $x = \pm a$ gives four conditions relating the six coefficients $e_1, e_2, a_1, a_2, c_1, c_2$. It follows that, for every $E > 0$, we can find two linearly independent solutions of the equation $H\psi = E\psi$. We can, for example, use the continuity relations to express c_1, c_2, a_1, a_2 as linear combinations of e_1, e_2 (of course, the coefficients of these combinations will depend on E and on the parameters a, b in the Hamilton operator). The 2×2 matrix $S = S(E)$ giving the outgoing coefficients as a functions of the incoming coefficients, *i.e.* such that $(a_1, a_2) = S(e_1, e_2)$, is known as the scattering matrix of the system. It can be shown to be a unitary matrix, describing the scattering of waves at the obstacle.

We can build two linearly independent solutions by fixing once $e_1 = 1$ and $e_2 = 0$ (this solution describes a wave incoming from the left), and then $e_1 = 0$ and $e_2 = 1$ (describing a solution incoming from the right). Alternatively, we can classify solutions according to their parity. In other words, we can find a solutions $\psi_{E,+}$ taking $e_1 = e_2 = 1$ (this solutions has positive parity, *i.e.* $\psi_{E,+}(x) = \psi_{E,+}(-x)$) and another solution $\psi_{E,-}$ taking $e_1 = 1$ and $e_2 = -1$ (this solution has negative parity, $\psi_{E,-}(-x) = -\psi_{E,-}(x)$). Comparing with the case $H = -\Delta$, the solution of $H\psi = E\psi$ incoming from the left is just e^{ikx} while the solution incoming from the right is e^{-ikx}. The solution with positive parity is $\cos(kx)$ and the solution with negative parity is just $\sin(kx)$. For the Laplace operator, the scattering matrix is just $S = \mathbb{1}$.

Completeness relation. One can prove that the states $\psi_{E,\pm}$ (or also the two states with energy $E > 0$ associated with $e_1 = 1$, $e_2 = 0$ and with $e_1 = 0$, $e_2 = 1$) build, together with the finitely many-eigenfunctions of H associated with negative energies, a complete set of functions, meaning that

$$\sum_{j=1}^{n} |\psi_j\rangle\langle\psi_j| + \int_0^\infty dk \, [|\psi_{E(k),+}\rangle\langle\psi_{E(k),+}| + |\psi_{E(k),-}\rangle\langle\psi_{E(k),-}|] = \mathbb{1}_{L^2(\mathbb{R})} \tag{7.63}$$

with $E(k) = k^2$. Futhermore, they satisfy the orthogonality relations:

$$\int dx \, \overline{\psi_{E(k),\pm}}(x)\psi_{E(k'),\pm}(x) = \delta(k-k') \qquad \text{while} \qquad \int dx \, \overline{\psi}_{E(k),\pm}(x)\psi_{E(k'),\mp}(x) = 0 \tag{7.64}$$

(of course, also the eigenfunctions $\psi_1, \ldots, \psi_n$ are orthonormal). Although the generalized eigenfunctions $\psi_{E,\pm}$ (or also the two states with energy $E > 0$ associated with $e_1 = 0$, $e_2 = 0$ and with $e_1 = 0$, $e_2 = 1$) are not in $L^2(\mathbb{R})$, they can nevertheless be used to construct singular Weyl sequences for H at every energy $E_0 > 0$. To this end, it is enough to consider linear combinations of the form

$$\int_0^\infty dk \, \alpha(k)\psi_{E(k),\pm}(x) \tag{7.65}$$

for a sequence of $\alpha \in L^2(\mathbb{R})$ with $\|\alpha\| = 1$ and concentrating closer and closer to the fixed value $k_0 = \sqrt{E_0}$. Hence, the existence of generalized eigenfunctions for all $E > 0$ is related to the fact that $\sigma_{\text{ess}}(H) = [0; \infty)$ (and the fact that we can find two linearly independent solutions $\psi_{E,\pm}$, for all $E > 0$, is related with the multiplicity of the essential spectrum).

Time-evolution of arbitrary initial data. Because of the completeness and of the orthogonality relations, we can also use the true eigenfunctions and the generalized eigenfunctions $\psi_{E,\pm}$ to compute the time-evolution of arbitrary initial data (similarly as we used Fourier transform to describe the free evolution generated by the Laplace operator). A given $\psi \in L^2(\mathbb{R})$ can be written, according to Eq. (7.63), as

$$\psi(x) = \sum_{j=1}^{n} \langle\psi_j, \psi\rangle\psi_j(x) + \sum_{\alpha=\pm} \int_0^\infty dk \, \langle\psi_{E(k),\alpha}, \psi\rangle\psi_{E(k),\alpha}(x) \tag{7.66}$$

with

$$\langle\psi_{E(k),\alpha}, \psi\rangle = \int dx \, \overline{\psi_{E(k)}(x)}\psi(x) \; . \tag{7.67}$$

Hence,

$$e^{-iHt}\psi(x) = \sum_{j=1}^{n} e^{-iE_j t}\langle\psi_j,\psi\rangle\psi_j(x) + \sum_{\alpha=\pm}\int_0^\infty dk\, e^{ik^2 t}\langle\psi_{E(k),\alpha},\psi\rangle\psi_{E(k),\alpha}(x) \tag{7.68}$$

in close analogy with the evolution generated by the Laplace operator, computed by means of Fourier transform.

7.4 General Schrödinger operators: existence of stationary states

So far, we considered two simple examples of Hamilton operators, whose eigenvalues and eigenvectors (and generalized eigenvectors) could be computed explicitly. For a general choice of the potential $V(x)$, we know, if $V(x)$ is relatively compact with respect to $-\Delta$, that $\sigma_{\text{ess}}(H) = [0;\infty)$, but it is impossible to determine explicitly the eigenvalues of $H = -\Delta + V(x)$. Still, it is often possible to show the existence of negative eigenvalues through the method of calculus of variations. This is the goal of the present section.

7.4.1 Energy functional

We consider a quantum system in d dimensions, described on $L^2(\mathbb{R}^d)$ by the Hamilton operator $H = -\Delta + V(x)$, assuming for now only that $V \in L^s_{\text{loc}}(\mathbb{R}^d)$, for a $1 \leqslant s \leqslant \infty$ (stronger conditions will come later). We consider the quadratic form associated with H, defining the energy functional

$$\varepsilon(\psi) = \langle\psi, H\psi\rangle = \int dx\, |\nabla\psi(x)|^2 + \int dx\, V(x)|\psi(x)|^2 \,. \tag{7.69}$$

We are going to establish conditions that guarantee that the functional ε attains a minimum on the unit sphere $\{\psi \in L^2(\mathbb{R}^d) \mid \|\psi\|_2 = 1\}$. We will show then that the minimizer ψ_0 of ε on the unit sphere is an eigenvector of H with eigenvalue $E_0 = \varepsilon(\psi_0)$. E_0 is going to be the ground state of H, *i.e.* the smallest eigenvalue of H. Later, we will show how to construct excited eigenvalues (if they exists) by similar minimization problems.

Boundedness from below. The first question we have to consider, to show the existence of a minimizer for Eq. (7.69), is whether ε is bounded below. Consider, for example, for $d = 3$, the potential $V(x) = -|x|^{-5/2}$. Then, $V \in L^s_{\text{loc}}(\mathbb{R}^3)$, for all $s < 6/5$. For every $\psi \in C_0^\infty(\mathbb{R}^d)$ with $\|\psi\|_2 = 1$ and for $\lambda > 0$ we set:

$$\psi_\lambda(x) = \lambda^{-3/2}\psi(x/\lambda) \,. \tag{7.70}$$

Then, $\|\psi_\lambda\|_2 = 1$ for all $\lambda > 0$ and

$$\begin{aligned} \varepsilon(\psi_\lambda) &= \int |\nabla\psi_\lambda(x)|^2 dx - \int |x|^{-5/2}|\psi_\lambda(x)|^2 \\ &= \lambda^{-2}\int |\nabla\psi(x)|^2 dx - \lambda^{-5/2}\int dx\, |x|^{-5/2}|\psi(x)|^2 \,. \end{aligned} \tag{7.71}$$

For $\lambda \to 0$ we notice that the second term dominates and that the energy takes arbitrarily large negative values. In this case, $\varepsilon(\psi)$ is not bounded below and the minimum cannot be attained. The following theorem provides sufficient conditions to make sure that the energy is bounded below. We use the notation

$$T(\psi) = \int dx\, |\nabla\psi(x)|^2 \tag{7.72}$$

for the kinetic energy of the particle.

Theorem 7.16. *Assume that $V \in L^\infty(\mathbb{R}^d) + L^{d/2}(\mathbb{R}^d)$, if $d \geqslant 3$, that $V \in L^\infty(\mathbb{R}^d) + L^{1+\varepsilon}(\mathbb{R}^d)$, if $d = 2$, for an arbitrary $\varepsilon > 0$, and that $V \in L^\infty(\mathbb{R}^d) + L^1(\mathbb{R}^d)$, if $d = 1$. Then, there exists constants $C, D > 0$ with*

$$\varepsilon(\psi) \geqslant CT(\psi) - D\|\psi\|^2 \,. \tag{7.73}$$

In particular,

$$E_0 := \inf\{\varepsilon(\psi) \mid \|\psi\|_2 = 1\} > -\infty \,. \tag{7.74}$$

Remark 7.17. *Here $V \in L^{p_1} + L^{p_2}$ means that there are $V_1 \in L^{p_1}$ and $V_2 \in L^{p_2}$ such that $V = V_1 + V_2$.*

Proof. We consider only the case $d \geqslant 3$ (the other cases can be handled analogously). By assumption, we have $V_1 \in L^\infty$, $V_2 \in L^{d/2}$ with $V = V_1 + V_2$. We claim that, for arbitrary $\delta > 0$, there exists $W_1 \in L^\infty$, $W_2 \in L^{d/2}$ with $V = W_1 + W_2$ and $\|W_2\|_{d/2} \leqslant \delta$. In fact, since $|V_2(x)|^{d/2}\chi(|V_2(x)| \geqslant \mu) \leqslant |V_2(x)|^{d/2}$ for all $x \in \mathbb{R}^d$ and since $|V_2(x)|^{d/2}\chi(|V_2(x)| \geqslant \mu) \to 0$ for almost all $x \in \mathbb{R}^d$, as $\mu \to \infty$, it follows from dominated convergence that

$$\int |V_2(x)|^{d/2}\chi(|V_2(x)| \geqslant \mu) \to 0 \tag{7.75}$$

as $\mu \to \infty$. Hence, there exists $\mu_0 > 0$ large enough with

$$\int |V_2(x)|^{d/2}\chi(|V_2(x)| \geqslant \mu) \leqslant \delta^{d/2} \,. \tag{7.76}$$

Then, $W_2(x) = V_2(x)\chi(|V_2(x)| \geqslant \mu_0)$ and $W_1(x) = V_1(x) + V_2(x)\chi(|V_2(x)| \leqslant \mu_0)$ have the desired properties. Thus

$$\begin{aligned}
\varepsilon(\psi) &= \int |\nabla\psi|^2 dx + \int V|\psi|^2 \\
&= \|\nabla\psi\|_2^2 + \int W_1(x)|\psi(x)|^2 + \int W_2(x)|\psi(x)|^2 \\
&\geqslant \|\nabla\psi\|_2^2 - \|W_1\|_\infty\|\psi\|_2^2 - \|W_2\|_{d/2}\|\psi\|_{2d/(d-2)}^2 \\
&\geqslant (1 - C\delta)\|\nabla\psi\|_2^2 - \|W_1\|_\infty\|\psi\|_2^2
\end{aligned} \tag{7.77}$$

where in the last bound we used the Sobolev inequality. The theorem follows by choosing δ small enough. ∎

For example, for $d = 3$, the last theorem can be applied to the hydrogen atom, where $V(x) = -1/|x| = -\chi(|x| \leqslant 1)/|x| - \chi(|x| \geqslant 1)/|x| \in L^p(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, for all $p < 3$. Theorem 7.16 implies that the spectrum of the hydrogen atom is bounded below, something we already knew from Proposition 7.8. We stress again that the stability of the hydrogen atom and of other quantum systems with attractive potentials (that is, the fact that the spectrum is bounded below) was a crucial success of quantum mechanics. In the classical counterpart of such systems, the energy can take arbitrarily negative values. In quantum mechanics, stability follows thanks to the fact that the negative potential energy is compensated by the positive kinetic energy, so that the total energy is always bounded below. In order to localize the electron close to the singularity of the potential, we pay a price in terms of kinetic energy (this is a formulation of Heisenberg's uncertainty principle).

7.4.2 Weak continuity of the potential energy

Next, we look for conditions that guarantee the existence of a minimum of the energy (boundedness from below is a necessary but not sufficient condition). We will make use of the following result.

Theorem 7.18. *Let $V : \mathbb{R}^d \to \mathbb{R}$ with $V \in L^\infty(\mathbb{R}^d) + L^{d/2}(\mathbb{R}^d)$, if $d \geqslant 3$, $V \in L^\infty(\mathbb{R}^d) + L^{1+\varepsilon}(\mathbb{R}^d)$, if $d = 2$, and $V \in L^\infty(\mathbb{R}^d) + L^1(\mathbb{R}^d)$, if $d = 1$. We assume moreover that $V \in L^\infty(\mathbb{R}^d \backslash B_R(0))$ for sufficiently large $R > 0$, with $\|V\|_{L^\infty(\mathbb{R}^d\backslash B_R(0))} \to 0$ as $R \to \infty$. The potential energy*

$$P(\psi) = \int dx\, V(x)|\psi(x)|^2 \tag{7.78}$$

is then weakly continuous in $H^1(\mathbb{R}^d)$. In other words, if $\psi_j \to \psi$ weakly in $H^1(\mathbb{R}^d)$, then $P(\psi_j) \to P(\psi)$ as $j \to \infty$.

Proof. We consider the case $n \geqslant 3$, the other cases can be handled analogously. Let ψ_j be a sequence in $H^1(\mathbb{R}^d)$ with $\psi_j \to \psi$ weakly in $H^1(\mathbb{R}^d)$. Then, the sequence ψ_j is bounded in $H^1(\mathbb{R}^d)$, *i.e.* $\|\psi_j\|_{H^1} \leqslant C$ for all $j \in \mathbb{N}$. Since

$$\int_{|x|\geqslant R} V(x)|\psi_j(x)|^2 \leqslant \|V\|_{L^\infty(B_R^c(0))}\|\psi_j\|_2^2 \leqslant C\|V\|_{L^\infty(B_R^c(0))} \to 0 \tag{7.79}$$

uniformly in j, it is enough to show that:

$$\int \chi_{B_R(0)}(x)V(x)|\psi_j(x)|^2 \to \int \chi_{B_R(0)}(x)V(x)|\psi(x)|^2 \tag{7.80}$$

as $j \to \infty$, for an arbitrary, but fixed $R > 0$. We write now $V(x) = V_1(x) + V_2(x)$, with $V_1 \in L^{d/2}(\mathbb{R}^d)$ and $V_2 \in L^\infty(\mathbb{R}^d)$. For $\delta > 0$ we set

$$V_{1,\delta}(x) = \begin{cases} V_1(x) & \text{if } |V_1(x)| \leqslant 1/\delta \\ 0 & \text{otherwise} \end{cases} \tag{7.81}$$

and $V_\delta = V_{1,\delta} + V_2$. Then, $|V_{1,\delta}(x)| \leqslant |V_1(x)|$ for all $\delta > 0$, and $V_{1,\delta}(x) \to V_1(x)$ almost everywhere. Dominated convergence implies that:

$$\int dx\,|V(x) - V_\delta(x)|^{d/2} = \int |V_1(x) - V_{1,\delta}(x)|^{d/2}dx \to 0 \qquad \text{as } \delta \to 0. \tag{7.82}$$

Therefore,

$$\begin{aligned} \left|\int \chi_{B_R(0)}(x)(V_\delta(x) - V(x))|\psi_j(x)|^2\right| &\leqslant \int |V_\delta(x) - V(x)||\psi_j(x)|^2dx \\ &\leqslant \|\psi_j\|_{2d/(d-2)}^2 \int |V_\delta(x) - V(x)|^{d/2}dx \\ &\leqslant \|\psi_j\|_{H^1}^2 \int |V_\delta(x) - V(x)|^{d/2}dx \to 0 \end{aligned} \tag{7.83}$$

where in the last step we used Sobolev inequality. This means that it is enough to show that:

$$\int \chi_{B_R(0)}V_\delta|\psi_j|^2 \to \int \chi_{B_R}(0)V_\delta|\psi|^2 \tag{7.84}$$

as $j \to \infty$, for all fixed $\delta, R > 0$. To this end, notice $\psi_j \to \psi$ weakly in $H^1(\mathbb{R}^d)$ implies that $\psi_j \to \psi$ strongly in $L^q(B_R(0))$ for all $1 \leqslant q < 2n/(n-2)$; see Theorem A.5. In particular, $|\psi_j|^2 \to |\psi|^2$ strongly in $L^{q/2}(B_R(0))$. Hence,

$$\left|\int \chi_{B_R(0)}V_\delta(|\psi_j|^2 - |\psi|^2)\right| \leqslant \|V_\delta\|_\infty\||\psi_j|^2 - |\psi|^2\|_{L^1(B_R(0))} \to 0 \tag{7.85}$$

as $j \to \infty$. ∎

7.4.3 Existence of minimizers

We are now ready to show the existence of a minimum of the energy functional.

Theorem 7.19. *Let $V : \mathbb{R}^d \to \mathbb{R}$ with $V \in L^\infty(\mathbb{R}^d) + L^{d/2}(\mathbb{R}^d)$, if $d \geqslant 3$, $V \in L^\infty(\mathbb{R}^d) + L^{1+\varepsilon}(\mathbb{R}^d)$, if $d = 2$, and $V \in L^\infty(\mathbb{R}^d) + L^1(\mathbb{R}^d)$, if $d = 1$. Moreover, let $V \in L^\infty(\mathbb{R}^d \backslash B_R(0))$ for R large enough, with $\|V\|_{L^\infty(B_R^c(0))} \to 0$ as $R \to \infty$. We assume that:*

$$E_0 = \inf\{\varepsilon(\psi) \mid \psi \in H^1(\mathbb{R}^d), \|\psi\|_2 = 1\} < 0\,. \tag{7.86}$$

Then, there exists $\psi_0 \in H^1(\mathbb{R}^d)$, with $\|\psi_0\|_2 = 1$ and $\varepsilon(\psi_0) = E_0$. Moreover, the function ψ_0 satisfies the Schrödinger equation in the sense of distributions:

$$(-\Delta + V)\psi_0 = E_0\psi_0\,. \tag{7.87}$$

Proof. Let ψ_j a sequence in $H^1(\mathbb{R}^d)$ with $\|\psi_j\|_2 = 1$ and $\varepsilon(\psi_j) \to E_0$ as $j \to \infty$. Theorem 7.16 implies that

$$\varepsilon(\psi_j) \geqslant \frac{1}{2}\|\nabla\psi_j\|_2^2 - C\ , \tag{7.88}$$

which implies that $\|\nabla\psi_j\|$ is bounded. Hence, $\|\psi_j\|_{H^1} \leqslant C$ for all j. By the Banach-Alaoglu theorem, this implies that there exists a subsequence ψ_{n_j} and $\psi_0 \in H^1(\mathbb{R}^d)$ such that $\psi_{n_j} \to \psi_0$ weakly in $H^1(\mathbb{R}^d)$ (in other words, $\psi_{n_j} \to \psi_0$ weakly in $L^2(\mathbb{R}^n)$ and $\nabla\psi_{n_j} \to \nabla\psi_0$ weakly in $L^2(\mathbb{R}^d)$). Since in the weak limit the norm can only get smaller, we obtain:

$$\|\psi_0\|_2 \leqslant 1\ , \qquad \|\nabla\psi_0\|_2 \leqslant \liminf_{j\to\infty} \|\nabla\psi_{n_j}\|_2\ . \tag{7.89}$$

From Theorem 7.18 we have that $P(\psi_0) = \lim_{j\to\infty} P(\psi_{n_j})$. This implies that

$$E_0\|\psi_0\|_2^2 \leqslant \varepsilon(\psi_0) = \|\nabla\psi_0\|_2^2 + P(\psi_0) \leqslant \liminf_{j\to\infty}(\|\nabla\psi_{n_j}\|_2^2 + P(\psi_{n_j})) = \liminf_{j\to\infty} \varepsilon(\psi_{n_j}) = E_0\ . \tag{7.90}$$

Since $E_0 < 0$, we find $\|\psi_0\|_2 \geqslant 1$. This means that $\|\psi_0\|_2 = 1$ and $\varepsilon(\psi_0) = E_0$. To show that ψ_0 satisfies the Schrödinger equation, we consider the variation of ψ_0. For $\delta \in \mathbb{R}$ and $f \in C_0^\infty(\mathbb{R}^d)$, let $\psi_\delta = \psi_0 + \delta f$ and $R(\delta) = \varepsilon(\psi_\delta)/\|\psi_\delta\|_2^2$. Then $R(\delta)$ has a minimum in $\delta = 0$. Hence, since R is differentiable in $\delta = 0$,

$$0 = \frac{dR(\delta)}{d\delta}\ |_{\delta=0} = \frac{d\varepsilon(\psi_\delta)}{d\delta}\ |_{\delta=0} - E_0\frac{d\|\psi_\delta\|_2^2}{d\delta}\ |_{\delta=0}\ . \tag{7.91}$$

A simple computation shows that

$$\frac{d\varepsilon(\psi_\delta)}{d\delta}\ |_{\delta=0} = 2\mathrm{Re}\int dx\, (\nabla\overline{f}\cdot\nabla\psi_0 + V\overline{f}\psi_0) \tag{7.92}$$

and that

$$\frac{d\|\psi_\delta\|_2^2}{d\delta}\ |_{\delta=0} = 2\mathrm{Re}\int dx\, \overline{f}\psi_0\ . \tag{7.93}$$

Thus,

$$\mathrm{Re}\int [(-\Delta + V - E_0)\overline{f}]\psi_0 = 0 \tag{7.94}$$

for all $f \in C_0^\infty(\mathbb{R}^d)$. If we replace f by if we conclude that

$$\int [(-\Delta + V - E_0)\overline{f}]\psi_0 = 0\ , \tag{7.95}$$

for all $f \in C_0^\infty(\mathbb{R}^n)$. This shows that ψ_0 solves the Schrödinger equation in the sense of distributions. ∎

Remark 7.20. *Since* $\inf\sigma(H) = \inf_{\psi\in D(H),\|\psi\|_2=1}\varepsilon(\psi)$, *and since* $D(H)$ *is dense in* H^1 *(*$D(H)$ *is dense in* H^2*, the domain of the Laplacian, which is dense in* H^1*), we conclude that* $E_0 = \inf\sigma(H)$.

7.4.4 Excited states

Theorem 7.19 gives a variational characterization of the smallest eigenvalue of H. It is also possible to give a variational characterization of higher eigenvalues and eigenfunctions. Let us assume that

$$E_0 = \inf\{\varepsilon(\psi) \mid \psi \in H^1(\mathbb{R}^d),\ \|\psi\|_2 = 1\} < 0\ . \tag{7.96}$$

Then Theorem 7.19 implies that the energy functional $\varepsilon(\varphi)$ has a minimizer ψ_0 on the unit sphere of $L^2(\mathbb{R}^d)$ which is an eigenvector of H with eigenvalue E_0. We can then define:

$$E_1 = \inf\{\varepsilon(\psi) \mid \psi \in H^1(\mathbb{R}^d),\ \|\psi\|_2 = 1 \text{ and } \langle\psi,\psi_0\rangle = 0\} \tag{7.97}$$

that is we look for the infimum of the energy functional among all normalized vectors, orthogonal to the eigenvector ψ_0. If this minimum is attained, we denote the minimizing vector by ψ_1. We can proceed recursively. Given that we already constructed the normalized vectors $\psi_0, \psi_1, \ldots, \psi_{k-1}$, we define:

$$E_k = \inf\{\varepsilon(\psi) \mid \psi \in H^1(\mathbb{R}^d),\ \|\psi\|_2 = 1 \text{ and } \langle\psi, \psi_j\rangle = 0, \text{ for all } j = 0, 1, \ldots, k-1\}\ . \quad (7.98)$$

In the next theorem, we show that if $E_k < 0$ then E_k is an eigenvalue of H and the minimizer ψ_k is the corresponding eigenvector.

Theorem 7.21. *Let V be as in Theorem 7.19. Assume $E_k < 0$. Then, the infimum in Eq. (7.98) is attained and the minimizer ψ_k is such that $H\psi_k = E_k\psi_k$.*

Proof. The proof of the existence of a minimizer follows the same ideas as the proof of Theorem 7.19. From a minimizing sequence ψ_k^j, we extract a weak limit ψ_k. As in the proof of Theorem 7.19, one can show that $\varepsilon(\psi_k) = E_k$ and that $\|\psi_k\| = 1$. The only additional observation here is that $\langle\psi_k, \psi_\ell\rangle = 0$, for all $\ell = 0, 1, \ldots, k-1$. This follows from $\psi_k^j \to \psi_k$ weakly, since $\langle\psi_k^j, \psi_\ell\rangle = 0$ for all $\ell = 0, \ldots, k-1$ and for all j.

To show that ψ_k solves the eigenvalue equation $H\psi_k = E_k\psi_k$, we first show, proceeding as in the proof of Theorem 7.19, that $\langle f, (H - E_k)\psi_k\rangle = 0$ for all $f \in C_0^\infty(\mathbb{R}^d)$ with $\langle f, \psi_\ell\rangle = 0$ for all $\ell = 0, 1, \ldots, k-1$. This implies that:

$$(H - E_k)\psi_k = \sum_{\ell=1}^{k-1} \alpha_\ell \psi_\ell\ , \quad (7.99)$$

for appropriate coefficients $\alpha_\ell \in \mathbb{C}$. Multiplying the equation with ψ_i and using the orthogonality $\langle\psi_i, \psi_k\rangle = 0$ for $i = 0, \ldots, k-1$ we conclude that $\alpha_i = 0$ for all $i = 0, \ldots, k-1$ and therefore that

$$H\psi_k = E_k\psi_k\ . \quad (7.100)$$

■

It follows from the recursion sketched above to define $E_0, E_1, \ldots$ only stops when it reaches $E_m = 0$. Also, it is not difficult to see that the eigenvalues have finite multiplicity. Let us sketch the proof. Suppose that E_k has infinite multiplicity, and let $(\psi_{k,j})$ be a orthonormal basis for the spectral subspace of E_k. Then, being orthonormal, the sequence $\psi_{k,j}$ converges to zero weakly in L^2. Weak convergence to zero in H^1 can be proven via an approximation argument, using that every element in the dual of H^1 can be approximated with a Schwartz function, and that $\|\psi_{k,j}\|_2 = 1$. By the continuity of the potential energy, we then have:

$$P(\psi_{k,j}) \to 0 \qquad \text{as } j \to \infty, \quad (7.101)$$

which implies that $E_k = \lim_{j\to\infty} \varepsilon(\psi_{k,j}) = \lim_{j\to\infty} T(\psi_{k,j}) \geqslant 0$, which contradicts $E_k < 0$. Therefore, E_k is in the discrete spectrum of H. Furthermore, it is not difficult to check that there cannot be any additional eigenvalues in $(-\infty; 0)$. In fact, if $E < 0$ and if $\psi \in L^2(\mathbb{R}^d)$ are such that $H\psi = E\psi$ and $\|\psi\| = 1$, and if $j > 0$ is such that $E_0 \leqslant E_1 \leqslant \cdots \leqslant E_j < E < E_{j+1}$, then $\langle\psi, \psi_\ell\rangle = 0$ for all $\ell = 0, 1, \ldots, j$ and:

$$\langle\psi, H\psi\rangle = \varepsilon(\psi) = \min\{\varepsilon(\varphi) \mid \|\varphi\| = 1 \text{ and } \langle\varphi, \psi_\ell\rangle = 0 \text{ for all } \ell = 0, 1, \ldots, j\} \quad (7.102)$$

which by definitions implies that $E = E_{j+1}$

Let us now comment on the essential spectrum of H. If V is a relatively compact perturbation of the Laplacian, we know from Weyl's theorem that $\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(-\Delta) = [0; \infty)$. The next theorem gives more general conditions under which this is true, that allow in particular to include the Coulomb potential.

Theorem 7.22. *Suppose that V is a Kato class potential, that is V can be written as $V_1 + V_2$ with $V_1 \in L^\infty(\mathbb{R}^d)$ and $V_2 \in L^p(\mathbb{R}^d)$, with $\|V_1\|_\infty < \varepsilon$. Here, $p = 2$ for $d \leqslant 3$ and $p > d/2$ for $d \geqslant 4$. Then, V is relatively compact with respect to $-\Delta$.*

Thus, under the slightly more restrictive condition that the potential is Kato class, $\sigma_{\text{ess}}(H) = [0; \infty)$.

To conclude the section, let us state, without proof, some important properties of eigenvectors of Schrödinger operators, that hold true in great generality.

1) **Uniqueness of the ground state.** Under the same assumption of Theorem 7.19, the normalized minimizer ψ_0 of the energy functional ε. (which by Theorem 7.19 is an eigenvector of H with eigenvalues $E_0 = \min\{\varepsilon(\psi) \mid \|\psi\| = 1\}$) can be chosen (by appropriate choice of the overall phase) to be a strictly positive function. Moreover, up to a constant phase, ψ_0 is the unique normalized minimizer. This implies that the ground state energy E_0 of H, that is the smallest eigenvalue of H, is nondegenerate.
2) **Elliptic regularity.** Let $B_1 \subset \mathbb{R}^d$ be an open ball and let ψ and V be functions on B with $(-\Delta+V)\psi = 0$ in the sense of distributions. Then, for any ball $B \subset \mathbb{R}^d$ concentric with B_1 and with strictly smaller radius, we have:
   (i) If $d = 1$, ψ is continuously differentiable on B.
   (ii) If $d = 2$, $\psi \in L^q(B)$ for all $q < \infty$.
   (iii) If $d = 3$, $\psi \in L^q(B)$ for all $q < d/(d-2)$.
   (iv) If $d \geqslant 2$ and $V \in L^p(B_1)$ for a $d/2 < p \leqslant d$, then ψ is Hölder continuous with exponent α in B, for all $\alpha < 2 - d/p$.
   (v) If $d \geqslant 1$ and $V \in L^p(B_1)$ for a $p > d$, ψ is continuously differentiable and the derivative is Hölder continuous with exponent α in B, for all $\alpha < 1 - d/p$.
   (vi) If $d \geqslant 1$ and $V \in C^{k,\alpha}(B_1)$ (this is the subspace of $C^k(B_1)$ of functions whose k-th derivative is Hölder continuous with exponent α) for some $k \geqslant 0$ and $0 < \alpha < 1$, then $\psi \in C^{k+2,\alpha}(B)$.

In other words, there is a gain in regularity of two derivatives between the potential and eigenvectors of Schrödinger operators (which by definition are only in L^2). Note that this regularity results hold locally. For example, this result implies that the eigenvectors of the hydrogen atom, with $V(x) = -Z/|x|$, are C^∞ in any ball away from the original. In a ball containing the origin, on the other hand, $V \in L^p$ for all $p < 3$; hence, the result above implies that eigenvectors of the hydrogen atom are Hölder continuous with exponent α, for any $\alpha < 1$.

7.4.5 Min-max principles

Theorem 7.22 gives a variational characterization of all negative eigenvalues of H. However, it is usually difficult to use in practice, since it defines E_k by using all the eigenvectors ψ_j associated with the eigenvalues $E_j < E_k$. To compute the eigenvalues of H, the following *min-max principles* are much more practical.

We denote as above by $E_0 \leqslant E_1 \leqslant E_2 \leqslant \cdots \leqslant E_N \leqslant \cdots < 0$ the eigenvalues of the Schrödinger operator $H = -\Delta + V$. If H has a finite number J of eigenvalues, we set $E_N = 0$ for all $N \geqslant J$.

Theorem 7.23 (Min-max principles.)**.** *Let V as in Theorem 7.21.*

Version 1. *Choose $\phi_0, \ldots, \phi_N \in H^1(\mathbb{R}^d)$ such that $V|\phi_i|^2 \in L^1(\mathbb{R}^d)$ for all i and such that $\langle \phi_i, \phi_j \rangle = \delta_{ij}$. We define the $(N+1) \times (N+1)$ self-adjoint matrix $h = (h_{ij})_{0 \leqslant i,j \leqslant N}$ by setting $h_{ij} = \langle \phi_i, H\phi_j \rangle$. Then, the eigenvalue problem $hv = \lambda v$ has $(N+1)$ eigenvalues $\lambda_0 \leqslant \lambda_1 \leqslant \cdots \leqslant \lambda_N$ such that $\lambda_i \geqslant E_i$ for all $i = 0, 1, \ldots, N$.*

Version 2. *If $N < J$,*

$$E_N = \max_{\phi_0,\ldots,\phi_{N-1}} \min\{\varepsilon(\phi_N) \mid \|\phi_N\| = 1 \text{ and } \langle \phi_N, \phi_j \rangle = 0, \text{ for all } j = 0, \ldots, N-1\} \quad (7.103)$$

where the maximum is taken over all orthonormal families $\phi_0, \ldots, \phi_{N-1}$.

Version 3. *If $N < J$,*

$$E_N = \min_{\phi_0,\ldots,\phi_N} \max\{\varepsilon(\phi) \mid \|\phi\| = 1 \text{ and } \phi \in span(\phi_0, \ldots, \phi_N)\} \quad (7.104)$$

where the minimum is taken over all orthonormal families $\phi_0, \ldots, \phi_N$.

If $N \geqslant J$, Version 2 and Version 3 hold true with max-min and min-max replaced by max-inf and inf-max.

Remark 7.24. *As it will be clear from the proof, the max and the min in the above expressions are attained.*

Proof. Let us assume $N < J$, which is the most interesting case. We begin with Version 1. Let $v_0, \dots, v_N$ be the orthonormal eigenvectors of the matrix h. We use these eigenvectors to define functions $\xi_i(x) = \sum_{j=0}^N v_i(j)\phi_j(x)$ for $i = 0, 1, \dots, N$. These functions are orthonormal, since

$$\langle \xi_i, \xi_k \rangle = \sum_{j,\ell} \overline{v}_i(j) v_k(\ell) \langle \phi_j, \phi_\ell \rangle = \sum_j \overline{v}_i(j) v_k(j) = \delta_{ik} \tag{7.105}$$

and moreover

$$\langle \xi_i, H\xi_j \rangle = \sum_{\ell,m=0}^N \overline{v}_i(\ell) v_j(m) \langle \phi_\ell, H\phi_m \rangle = \langle v_i, h v_j \rangle = \delta_{ij}\lambda_i \ . \tag{7.106}$$

We clearly have:

$$E_0 \leqslant \varepsilon(\xi_0) = \langle \xi_0, H\xi_0 \rangle = \lambda_0 \ . \tag{7.107}$$

Let us now assume that $E_i \leqslant \lambda_i$ for all $i \leqslant k-1$. We prove that $E_k \leqslant \lambda_k$. To this end, we observe that dim span$(\xi_0, \dots, \xi_k) = k+1$ and therefore that it must contain a function $\xi = \sum_{j=0}^k c_j \xi_j$ with $\|\xi\| = 1$ and such that $\langle \xi, \psi_i \rangle = 0$ for all $i = 0, 1, \dots, k-1$. By Theorem 7.22, we find:

$$E_k \leqslant \varepsilon(\xi) = \sum_{i,j=1}^k \overline{c}_i c_j \langle \xi_i, H\xi_j \rangle = \sum_{j=0}^k |c_j|^2 \lambda_j \leqslant \lambda_k \ . \tag{7.108}$$

This completes the proof of Version 1. To show Version 2, we set:

$$\gamma_N = \max_{\phi_0,\dots,\phi_{N-1}} \min\{\varepsilon(\phi_N) \mid \langle \phi_N, \phi_j \rangle = 0, \text{ for all } j = 0, \dots, N-1\} \ . \tag{7.109}$$

Clearly, by Theorem 7.22, we have:

$$\gamma_N \geqslant \min\{\varepsilon(\phi_N) \mid \|\phi_N\| = 1 \text{ and } \langle \phi_N, \psi_j \rangle = 0, \text{ for } j = 0, 1, \dots, N-1\} = E_N \ . \tag{7.110}$$

On the other hand, for an arbitrary choice of orthonormal $\phi_0, \dots, \phi_{N-1}$ we can find a linear combination $f = \sum_{j=0}^N c_j \psi_j$ such that f is normalized and orthogonal to all ϕ_j (because dim span$(\psi_0, \dots, \psi_N) = N+1$). Then, we have:

$$\varepsilon(f) = \langle f, Hf \rangle = \sum_{j=0}^N |c_j|^2 E_j \leqslant E_N \ . \tag{7.111}$$

Hence, $\gamma_N \leqslant E_N$. To prove Version 3, we define:

$$\widetilde{\gamma}_N = \min_{\phi_0,\dots,\phi_N} \max\{\varepsilon(\phi) \mid \|\phi\| = 1 \text{ and } \phi \in \text{span}(\phi_0, \dots, \phi_N)\} \tag{7.112}$$

Choosing $\phi_0, \dots, \phi_N$ to be $\psi_0, \dots, \psi_N$ and noticing that for $\phi = \sum_{j=0}^N c_j \psi_j$ with $\sum_{j=0}^N |c_j|^2 = 1$ we have

$$\varepsilon(\phi) = \langle \phi, H\phi \rangle = \sum_{j=0}^N |c_j|^2 E_j \leqslant E_N \tag{7.113}$$

we conclude that:

$$\widetilde{\gamma}_N \leqslant \max\{\varepsilon(\phi) \mid \|\phi\| = 1 \text{ and } \phi \in \text{span}(\psi_0, \dots, \psi_N)\} = E_N \ . \tag{7.114}$$

On the other hand, for arbitrary $\phi_0, \dots, \phi_N$, we can find $f \in \text{span}(\phi_0, \dots, \phi_N)$ with $\|f\| = 1$ such that $\langle f, \psi_j \rangle = 0$ for all $j = 0, 1, \dots, N-1$. This implies, from Theorem 7.21, that:

$$E_N = \inf\{\varepsilon(\phi) \mid \|\phi\| = 1 \text{ and } \langle \phi, \psi_j \rangle = 0 \text{ for all } j = 0, 1, \dots, N-1\} \leqslant \varepsilon(f) \ . \tag{7.115}$$

Therefore, $\widetilde{\gamma}_N \geqslant E_N$. ∎

7.4.6 Generalized min-max principle

Let us mention a simple extension of the min-max principle, which is very useful to get bounds on sums of eigenvalues. From Version 1 of Theorem 7.23, we find in particular that:

$$\sum_{j=0}^{N} E_j \leqslant \sum_{j=0}^{N} \lambda_j = \operatorname{Tr} h = \sum_{j=0}^{N} h_{jj} = \sum_{j=0}^{N} \varepsilon(\phi_j) \,. \tag{7.116}$$

for any orthonormal family $\phi_0, \ldots, \phi_N$. We can generalize this statement to the case where the functions ϕ_j are not orthonormal. Let $\phi_0, \ldots, \phi_L$ be the $(L+1)$ functions in $H^1(\mathbb{R}^d)$ such that $\theta_{ij} = \langle \phi_i, \phi_j \rangle$ defines a $(L+1) \times (L+1)$ matrix θ with $0 \leqslant \theta \leqslant 1$. Suppose that $\operatorname{Tr} \theta = \sum_{j=0}^{L} \theta_{jj} = N + 1 + \delta$, for a $\delta \in (0;1)$. Then, we have:

$$\sum_{j=0}^{L} \varepsilon(\phi_j) \geqslant \sum_{j=0}^{N} E_j + \delta E_{N+1} \,. \tag{7.117}$$

To prove Eq. (7.117), consider first the case in which the functions are orthogonal (but not necessarily normalized). Then, $T_j = \theta_{jj} = \|\phi_j\|^2 \leqslant 1$ (from the assumption $\theta \leqslant 1$). Let us reorder the indices $0, \ldots, L$ such that

$$0 < T_L \leqslant T_{L-1} \leqslant \cdots \leqslant T_0 \leqslant 1 \,. \tag{7.118}$$

Let $\psi_j = \phi_j / \sqrt{T_j}$ (then ψ_j in an orthonormal family). Then, by a telescopic rearrangement of sums:

$$\begin{aligned}
\sum_{j=0}^{L} \varepsilon(\phi_j) &= \sum_{j=0}^{L} T_j \varepsilon(\psi_j) && (7.119)\\
&= T_L \sum_{j=0}^{L} \varepsilon(\psi_j) + (T_{L-1} - T_L) \sum_{j=0}^{L-1} \varepsilon(\psi_j) + \\
&\quad \cdots + (T_1 - T_2) \sum_{j=0}^{1} \varepsilon(\psi_j) + (T_0 - T_1) \varepsilon(\psi_0) \\
&\geqslant T_L \sum_{j=0}^{L} E_j + (T_{L-1} - T_L) \sum_{j=0}^{L-1} E_j + \ldots + (T_0 - T_1) E_0 \\
&= \sum_{j=0}^{L} T_j E_j \\
&\geqslant \min \left\{ \sum_{j=0}^{L} T_j E_j \mid 0 \leqslant T_j \leqslant 1 \,, \sum_{j=0}^{L} T_j = N + 1 + \delta \right\} = \sum_{j=0}^{N} E_j + \delta E_{N+1} \,.
\end{aligned}$$

Now, let us consider the general case. Define μ_α and g_α to be the eigenvalues and the corresponding eigenvectors of the matrix θ. We denote by G the $(L+1) \times (L+1)$ matrix with the eigenvectors g_α as columns. We set $\Phi_\alpha = \sum_{j=0}^{L} g_\alpha(j) \phi_j$. Then, we have:

$$\begin{aligned}
\langle \Phi_\alpha, \Phi_\beta \rangle &= \sum_{i,j} \overline{g}_\alpha(i) g_\beta(j) \langle \phi_i, \phi_j \rangle \\
&= \sum_{i,j} \overline{g}_\alpha(i) g_\beta(j) \theta_{ij} \\
&= (G^* \theta G)_{\alpha,\beta} = \delta_{\alpha,\beta} \mu_\alpha \,. && (7.120)
\end{aligned}$$

Since $\sum_{\alpha=0}^{L} \operatorname{Tr} \theta = N + 1 + \delta$, we apply the result for the case of orthogonal (but not normalized) functions established above. We find that:

$$\sum_{j=0}^{N} E_j + \delta E_{N+1} \leqslant \sum_{\alpha=0}^{L} \varepsilon(\Phi_\alpha) = \sum_{\alpha,i,j} \overline{g}_\alpha(i) g_\alpha(j) \langle \phi_i, h \phi_j \rangle = \sum_{j=0}^{L} h_{jj} = \sum_{j=0}^{L} \varepsilon(\phi_j) \,, \tag{7.121}$$

which proves Eq. (7.117).

8 Semiclassical approximations

8.1 Dirichlet Laplacian

In the last section we gave a variational characterization for the eigenvalues of Schrödinger operators of the form $H = -\Delta + V$. The question we want to address in this section is whether it is possible to obtain information on the eigenvalues E_j by looking at the corresponding *classical* system, at least in some particular regime. To simplify the analysis, we will focus here on a special class of potentials V, For an open bounded subset $\Omega \subset \mathbb{R}^d$, we will consider the potential:

$$V_\Omega(x) = \begin{cases} 0 & \text{if } x \in \Omega \\ +\infty & \text{if } x \notin \Omega \end{cases} \tag{8.1}$$

This (mathematically not very precise) choice means that we look at the Laplace operator on Ω, imposing Dirichlet boundary conditions at the boundary of Ω. In other words, for a bounded open subset $\Omega \subset \mathbb{R}^d$, we will consider the operator $H_\Omega = -\Delta$, defined on the Hilbert space $H_0^2(\Omega)$, the closure of $C_0^\infty(\Omega)$ with respect to the H^2-norm. The eigenvalues have a variational characterization, similarly as the Schrödinger operators discussed in the previous section. Defining:

$$E_0 = \inf \Big\{ \int_\Omega |\nabla\varphi(x)|^2 dx \mid \varphi \in H_0^2(\Omega),\ \|\varphi\|_2 = 1 \Big\} \tag{8.2}$$

we can show (as in the proof of Theorem 7.19, using also the fact that $\psi_j \to \psi$ weakly in $H^1(\Omega)$ for a bounded set Ω implies also that $\psi_j \to \psi$ strongly in $L^2(\Omega)$) that E_0 is attained by a minimizer ψ_0 with $\|\psi_0\| = 1$, which is then a solution of $H_\Omega\psi_0 = E_0\psi_0$. Recursively, after constructing the eigenvectors $\psi_0, \ldots, \psi_{k-1}$, we find that:

$$E_k = \inf \Big\{ \int_\Omega |\nabla\varphi(x)|^2 dx \mid \varphi \in H_0^2(\Omega),\ \|\varphi\|_2 = 1,\ \langle\varphi, \psi_\ell\rangle = 0,\ \ell = 0, 1, \ldots, k-1 \Big\} \tag{8.3}$$

is attained by a normalized minimizer ψ_k such that $H_\Omega\psi_k = E_k\psi_k$. In this case, the recursion never stops, H_Ω has infinitely many eigenvalues (tending to infinity) and eigenvectors. Similarly as discussed in the previous section, alls eigenvalues and eigenvectors of H_Ω are obtained by this recursion. Finally, it is not difficult to see that the spectrum of H_Ω is purely discrete: $\sigma_{\text{ess}}(H_\Omega) = \varnothing$. To prove this, recall Weyl's characterization of the essential spectrum, Lemma 7.9. A number $E \in \mathbb{R}$ belongs to the essential spectrum of H_Ω if and only if there exists a singular Weyl sequence (ψ_n) at E, that is a sequence such that $\psi_n \to 0$ weakly in L^2, $\|\psi_n\|_2 = 1$ and $\|(H - E)\psi_n\|_2 \to 0$. This last condition, together with $\|\psi_n\|_2 = 1$, implies that $\|\psi_n\|_{H^1} \leqslant C$ uniformly in n. Therefore, we can extract a weakly convergent subsequence in H^1, $\psi_{n_j} \to \psi$. Suppose that $\psi \neq 0$. Then, $\|\psi\|_2^2 = \lim_{j\to\infty}\langle\psi, \psi_{n_j}\rangle = \lim_{n\to\infty}\langle\psi, \psi_n\rangle = 0$, which gives a contradiction. Therefore, $\psi = 0$.

By Theorem A.5, weak convergence in H^1 implies strong convergence in L^2 on bounded sets. Therefore, $\|\psi_{n_j}\|_2 \to 0$ as $n \to \infty$, which contradicts $\|\psi_{n_j}\|_2 = 1$. Thus, (ψ_n) is not a singular Weyl sequence. This shows that the spectrum is purely discrete, *i.e.* it is given by eigenvalues of finite multiplicity.

8.2 Lower bound on the sum of Dirichlet eigenvalues

Our goal in this section is to extract information about the eigenvalues E_j. It turns out that it is quite difficult to approximate the single eigenvalues E_j. Instead, it is easier to obtain information about sums of eigenvalues. Besides the mathematical interest for the question of approximation sums of eigenvalues, this is also a relevant question in physics, since, as we shall see later, this allows to estimate the energy of a system of many non-interacting fermions. The first result we want to discuss is a lower bound for the sum of the first N eigenvalues of H_Ω, a result due to Li-Yau and Berezin.

Theorem 8.1. *Let $\Omega \subset \mathbb{R}^d$ be open and bounded, $\phi_0, \ldots, \phi_{N-1} \in H_0^1(\Omega)$ an orthonormal family in $L^2(\Omega)$. Then:*

$$\sum_{j=1}^{N-1} \|\nabla\phi_j\|_2^2 \geqslant (2\pi)^2 \frac{d}{d+2} \Big(\frac{d}{|S_{d-1}|}\Big)^{2/d} N^{1+2/d} |\Omega|^{-2/d}\ , \tag{8.4}$$

where $|S_{d-1}|$ is the area of the $(d-1)$-dimensional unit sphere. In particular:

$$\sum_{j=0}^{N-1} E_j \geqslant (2\pi)^2 \frac{d}{d+2}\Big(\frac{d}{|S_{n-1}|}\Big)^{2/d} N^{1+2/d}|\Omega|^{2/d} \,. \tag{8.5}$$

Proof. Since $H_0^1(\Omega)$ is the closure of $C_0^\infty(\Omega)$ with respect to the H^1 norm, it is enough to show the statement for orthonormal families $\phi_0, \ldots, \phi_{N-1} \in C_0^\infty(\Omega)$, compactly supported away form the boundary of Ω. We extend $\phi_0, \ldots, \phi_{N-1}$ to functions in $C_0^\infty(\mathbb{R}^d)$, by setting them equal to zero outside of their support. Now, we can express the H^1 norm of ϕ_j by means of its Fourier transform. We find:

$$\|\nabla\phi_j\|_2^2 = \int k^2 |\widehat{\phi}_j(k)|^2 dk \,. \tag{8.6}$$

Hence,

$$\sum_{j=0}^{N-1} \|\nabla\phi_j\|_2^2 = \int k^2 \rho(k) dk \,, \tag{8.7}$$

where we set

$$\rho(k) = \sum_{j=0}^{N-1} |\widehat{\phi}_j(k)|^2 \,. \tag{8.8}$$

Notice that:

$$\int \rho(k) dk = N \,. \tag{8.9}$$

Moreover, with the definition $e_k(x) = e^{-ikx}\chi_\Omega(x)/(2\pi)^{d/2}$, we find:

$$\widehat{\phi}_j(k) = \langle \phi_j, e_k \rangle \,. \tag{8.10}$$

Extending $\phi_0, \ldots, \phi_{N-1}$ to an orthonormal basis $\{\phi_j\}_{j=0}^\infty$ of $L^2(\mathbb{R}^d)$, we find:

$$\hat{\phi}_j(k) = \langle \phi_j, e_k \rangle \,. \tag{8.11}$$

We conclude that, by the bathtub principle, see Appendix B:

$$\begin{aligned} \sum_{j=0}^{N-1} \|\nabla\phi_j\|_2^2 &= \int k^2 \rho(k) dk \\ &\geqslant \inf\Big\{ \int k^2 \rho(k) \mid \rho \in L^1(\mathbb{R}^d),\ \int \rho(k) dk = N \text{ and } 0 \leqslant \rho(k) \leqslant |\Omega|/(2\pi)^d \Big\} \\ &= \frac{|\Omega|}{(2\pi)^d} \int k^2 \chi(|k| \leqslant M) dk \,, \end{aligned} \tag{8.12}$$

where $M > 0$ is chosen so that

$$\int \chi(|k| \leqslant M) \frac{|\Omega|}{(2\pi)^d} dk = N \tag{8.13}$$

which implies that

$$M = (2\pi)\Big(\frac{d}{|S_{d-1}|}\Big)^{1/d} N^{1/d} |\Omega|^{-1/d} \,. \tag{8.14}$$

Therefore, Eq. (8.12) yields:

$$\begin{aligned} \sum_{j=0}^{N-1} \|\nabla\phi_j\|_2^2 &\geqslant \frac{|\Omega|}{(2\pi)^d} \int k^2 \chi\Big(|k| \leqslant (2\pi)\Big(\frac{d}{|S_{d-1}|}\Big)^{1/d} N^{1/d}|\Omega|^{-1/d}\Big) \\ &= (2\pi)^2 \frac{d}{d+2}\Big(\frac{d}{|S_{d-1}|}\Big)^{2/d} N^{1+2/d} |\Omega|^{-2/d} \,. \end{aligned} \tag{8.15}$$

■

As an example, let us consider the sum $S(N) = \sum_{j=0}^{N-1} E_j$ of the eigenvalues of the operator H_Ω, for the simple case in which $\Omega = [0; L]^d$ of a cube with side length L. In this case, eigenvectors of H_Ω are products of eigenvectors of the one-dimensional Laplace operator on the interval $[0; L]$, with Dirichlet boundary conditions. Hence, we look for solutions of:

$$-\psi''(x) = E\psi(x) , \qquad \text{with } \psi(0) = \psi(L) = 0. \tag{8.16}$$

The condition $\psi(0) = 0$ implies that $\psi(x) = A\sin(kx)$ with $k = \sqrt{E}$. The condition $\psi(L) = 0$ implies that $k = m\pi/L$, for an $m \in \mathbb{N}$. This gives the eigenvalues

$$E_m = \frac{(m\pi)^2}{L^2} , \tag{8.17}$$

and the eigenvector $\psi_m(x) = A\sin(m\pi/L)$ (for an appropriate normalization constant A), for $m \in \mathbb{N}$. The energy of the product wave function $\psi_{(m_1,\ldots,m_d)}(x_1, \ldots, x_d) = \prod_{j=1}^{d} \psi_{m_j}(x_j)$ is then given by:

$$E(m) = \frac{\pi^2}{L^2} \sum_{j=1}^{d} m_j^2 , \tag{8.18}$$

for any $m = (m_1, \ldots, m_d) \in \mathbb{N}^d$. Let us now fix $\kappa > 0$ such that the set

$$K_\kappa = \{x = (x_1, \ldots, x_d) \in \mathbb{R}^d \mid \|x\| \leqslant \kappa \text{ and } x_j \geqslant 0 \text{ for all } j = 1, \ldots, d\} \tag{8.19}$$

has volume N. In other words, we require that:

$$\frac{1}{2^d} |S_{d-1}| \frac{\kappa^d}{d} = N , \tag{8.20}$$

or equivalently, we fix:

$$\kappa = 2N^{1/d} \Big(\frac{d}{|S_{d-1}|} \Big)^{1/d} . \tag{8.21}$$

Then, the set K_κ certainly contains less than N points $(m_1, \ldots, m_d) \in \mathbb{N}^d$, because every such point can be associated uniquely with a square with unit volume (the square $\{(x_1, \ldots, x_n) \mid m_j - 1 \leqslant x_j \leqslant m_j\}$) contained in K_κ (the case with exactly N points can be excluded because one cannot cover a ball with finitely many nonoverlapping unit cubes). Hence (remember that we use the notation E_{N-1} for the N-th eigenvalue of H_Ω)

$$E_{N-1} \geqslant \frac{\pi^2}{L^2} \kappa^2 = (2\pi)^2 \Big(\frac{d}{|S_{d-1}|} \Big)^{2/d} N^{2/d} |\Omega|^{-2/d} \tag{8.22}$$

and

$$\begin{aligned} S(N) &= \sum_{j=0}^{N-1} E_j \geqslant (2\pi)^2 \Big(\frac{d}{|S_{d-1}|} \Big)^{2/d} |\Omega|^{-2/d} \sum_{j=1}^{N} j^{2/d} \\ &\geqslant (2\pi)^2 \frac{d}{d+2} \Big(\frac{d}{|S_{d-1}|} \Big)^{2/d} |\Omega|^{-2/d} N^{1+2/d} , \end{aligned} \tag{8.23}$$

in agreement with the result of Theorem 8.1. A famous conjecture in mathematics, due to George Polya, states that the bound (8.22) for the N-th eigenvalue of H_Ω holds not only if Ω is a cube but for arbitrary open bounded $\Omega \subset \mathbb{R}^d$. From the lower bound in Theorem 8.1 we obtain the bound:

$$E_{N-1} \geqslant \frac{1}{N} \sum_{j=0}^{N-1} E_j \geqslant (2\pi)^2 \frac{d}{d+2} \Big(\frac{d}{|S_{d-1}|} \Big)^{2/d} |\Omega|^{-2/d} N^{2/d} , \tag{8.24}$$

which however misses Polya's conjecture because of the factor $d/(d+2) < 1$. Although Polya's conjecture is known to hold true for special classes of domains Ω, it remains open in its full generality.

8.3 Asymptotic behavior of eigenvalues

For the cube $\Omega = [0; L]^d$, the right hand side of Eq. (8.23) is not only a lower bound for the sum $S(N)$. Instead, it really capture the leading behavior of $S(N)$, in the limit of large N. With κ as defined in Eq. (8.21), we have:

$$S(N) \simeq \sum_{m \in \mathbb{N}^d : |m| \leqslant \kappa} \frac{\pi^2}{L^2} |m|^2 \tag{8.25}$$

where $|m|^2 = \sum_{j=1}^d m_j^2$, for $m \in \mathbb{N}^d$. Defining $k = m/N^{1/d}$ and $\lambda = \kappa/N^{1/d} = 2(d/|S_{d-1}|)^{1/d}$, we find

$$S(N) \simeq \frac{\pi^2}{L^2} N^{1+2/d} \sum_{k \in \mathbb{N}^d/N^{1/d} : |k| \leqslant \lambda} \frac{1}{N} k^2 \; . \tag{8.26}$$

The sum on the right-hand side is a Riemann sum; as $N \to \infty$, it approaches

$$S(N) \simeq \frac{\pi^2}{L^2} N^{1+2/d} \int_{|k| \leqslant \lambda} k^2 dk = (2\pi)^2 \frac{d}{d+2} \Big(\frac{d}{|S_{d-1}|} \Big)^{2/d} |\Omega|^{-2/d} N^{1+2/d} \tag{8.27}$$

up to errors of lower order in N. It turns out that the same asymptotics behavior of the sum $S(N)$ holds for a more general class of domains. This important result is known as Weyl's law. In order to state Weyl's law, we need to introduce first the notion of boundary area. Let $\Omega \subset \mathbb{R}^d$ be a bounded set, $\partial\Omega$ its boundary. We define the boundary area $\mathcal{A}(\Omega)$ of $\partial\Omega$ by

$$\mathcal{A}(\Omega) = \limsup_{r \to 0^+} \frac{1}{2r} \big[|\{x \in \Omega^c \mid \mathrm{dist}(x, \Omega) < r\}| + |\{x \in \Omega \mid \mathrm{dist}(x, \Omega^c) < r\}| \big] \; . \tag{8.28}$$

Theorem 8.2. *Let $\Omega \subset \mathbb{R}^d$ open, bounded and with finite boundary area $\mathcal{A}(\Omega)$. Then:*

$$S(N) = \sum_{j=0}^{N-1} E_j = (2\pi)^2 \frac{d}{d+2} \Big(\frac{d}{|S_{d-1}|} \Big)^{2/d} |\Omega|^{-2/d} N^{1+2/d} + o(N^{1+2/d}) \tag{8.29}$$

in the limit $N \to \infty$.

In fact, the error $o(N^{1+2/d})$ in Eq. (8.29) can be estimated more precisely by:

$$0 \leqslant o(N^{1+2/d}) \leqslant CN(\mathcal{A}(\Omega)/|\Omega|)^{2/3} (d/|S_{d-1}|)^{4/3d} (N/|\Omega|)^{4/3d} \tag{8.30}$$

for a universal constant $C > 0$.

The result can be interpreted as a semiclassical estimate. The postulate of semiclassical analysis is that every quantum state occupies $(2\pi)^d$ in the classical phase space. We are interested in the total energy of the N states with the smallest possible energies. The classical counterpart of the Laplace operator with Dirichlet boundary boundary conditions is the classical Hamiltonian $\mathcal{H}(p, x) = p^2 \chi(x \in \Omega)$. To minimize the total energy, we fill the phase space with $x \in \Omega$ and $|p| \leqslant \kappa$, where $\kappa > 0$ is chosen, so that

$$\frac{\kappa^d}{d} |S_{d-1}| |\Omega| = (2\pi)^d N \; , \tag{8.31}$$

i.e. so that there is enough space for N quantum states (according to the postulate that every quantum state occupy the volume $(2\pi)^d$ in phase space). We find

$$\kappa = (2\pi) \Big(\frac{d}{|S_{d-1}|} \Big)^{1/d} N^{1/d} |\Omega|^{1/d} \; . \tag{8.32}$$

Hence, semiclassical analysis suggests that the total energy of the N states with smallest energy is given by:

$$\frac{1}{(2\pi)^d} \int_{\Omega \times \{|p| \leqslant \kappa\}} p^2 dp dx = (2\pi)^2 \frac{d}{d+2} \Big(\frac{d}{|S_{d-1}|} \Big)^{2/d} \frac{N^{1+2/d}}{|\Omega|^{2/d}} \tag{8.33}$$

which is exactly the statement of Theorem 8.2.

The goal of the rest of this section consists in proving Theorem 8.2. Since a lower bound for $S(N)$ has already been established in Theorem 8.1 (in fact, the lower bound holds for all N, not only in the limit $N \to \infty$), we need only to prove an upper bound for $S(N)$, coinciding to leading order with the right-hand side of Eq. (8.29). To find such an upper bound, we will use coherent states; this is not surprising, since we pointed out above that Weyl's law is a semiclassical estimate, and coherent states are as close as possible to classical states.

8.4 Upper bound on the sum of Dirichlet eigenvalues

8.4.1 Coherent states

In the present setting, coherent states are wave functions of the form

$$F_{k,y}(x) = e^{ik\cdot x} G(x-y) , \tag{8.34}$$

where G is centered Gaussian function, $y, k \in \mathbb{R}^d$. Since $|F_{k,y}(x)| = G(x-y)$ and $|\widehat{F}_{k,y}(p)| = \widehat{G}(p-k)$, the coherent state $F_{k,y}$ is localized around y in position space and it is localized around k in momentum space. In the sequel, we will not need to assume that G is a Gaussian. We will only assume that $G \in L^2(\mathbb{R}^d)$ with $G(-x) = G(x)$ and $\|G\|_2 = 1$ (so that $\|F_{k,y}\|_2 = 1$ for all $k, y \in \mathbb{R}^d$).

For an arbitrary $\psi \in L^2(\mathbb{R}^d)$, we define the coherent state transform

$$\widetilde{\psi}(k,y) = \langle F_{k,y}, \psi \rangle = \int \overline{F_{k,y}(x)} \psi(x) dx = \int_{\mathbb{R}^d} e^{-ik\cdot x} \overline{G(x-y)} \psi(x) dx . \tag{8.35}$$

Since by Cauchy-Schwarz

$$\int |G(x-y)||\psi(x)| dx \leqslant \|G\| \|\psi\| \tag{8.36}$$

the transform $\widetilde{\psi}(k,y)$ is the Fourier transform of an L^1-function; hence $\widetilde{\psi}(k,y)$ is bounded. We denote by $\pi_{k,y}$ the orthogonal projection onto $F_{k,y}$, so that

$$(\pi_{k,y}\psi)(x) = F_{k,y}(x) \langle F_{k,y}, \psi \rangle = F_{k,y}(x) \widetilde{\psi}(k,y) . \tag{8.37}$$

The integral kernel of $\pi_{k,y}$ is given by $\pi_{k,y}(x; z) = F_{k,y}(x)\overline{F_{k,y}(z)}$.

Lemma 8.3. *Let $G \in L^2(\mathbb{R}^d)$ with $G(-x) = G(x)$ and $\|G\|_2 = 1$. Let $\psi \in L^2(\mathbb{R}^d)$. Then*

$$\begin{aligned} \frac{1}{(2\pi)^d} \int |\widetilde{\psi}(k,y)|^2 dk &= (|\psi|^2 * |G|^2)(y) \\ \frac{1}{(2\pi)^d} \int |\widetilde{\psi}(k,y)|^2 dy &= (|\widehat{\psi}|^2 * |\widehat{G}|^2)(k) \\ \frac{1}{(2\pi)^d} \int |\widetilde{\psi}(k,y)|^2 dy dk &= \|\psi\|_2^2 = \|\widehat{\psi}\|_2^2 . \end{aligned} \tag{8.38}$$

Moreover,

$$\widetilde{\psi}(k,y) = e^{-iky} \int \widehat{\psi}(q) e^{iqy} \overline{\widehat{G}(q-k)} dq . \tag{8.39}$$

Proof. Set $H(x,y) = |\psi(x)|^2 |G(x-y)|^2$. By Fubini:

$$\int \Big[\int H(x,y) dx \Big] dy = \int \Big[\int H(x,y) dy \Big] dx = \|\psi\|_2^2 < \infty . \tag{8.40}$$

Hence, the function $y \to \int H(x,y)dx = (|\psi|^2 * |G|^2)(y)$ is in $L^1(\mathbb{R}^d)$ and thus it is finite for a.e. $y \in \mathbb{R}^d$. This means that the function $x \to \psi(x)\overline{G(x-y)}$ is in $L^2(\mathbb{R}^d)$ for a.e. $y \in \mathbb{R}^d$. By Cauchy-Schwarz, this function is also in $L^1(\mathbb{R}^d)$, for all $y \in \mathbb{R}^d$, $\widetilde{\psi}(k,y)/(2\pi)^{d/2}$ is the Fourier transform of this function. Hence, by Plancherel,

$$\frac{1}{(2\pi)^d} \int |\widetilde{\psi}(k,y)|^2 dk = \int |\psi(x)|^2 |G(x-y)|^2 dx = (|G|^2 * |\psi|^2)(y) \tag{8.41}$$

and thus, by Fubini,

$$\frac{1}{(2\pi)^d}\int dy\Big[\int dk\,|\widetilde{\psi}(k,y)|^2\Big] = \int(|\psi|^2 * |G|^2)(y)dy = \int dx\int dy\,|\psi(x)|^2|G(x-y)|^2 = \|\psi\|_2^2\,. \tag{8.42}$$

The second formula can be proven similarly, Finally, we show (8.39). By Plancherel,

$$\widetilde{\psi}(k,y) = \langle F_{k,y},\psi\rangle = \langle \widehat{F}_{k,y},\widehat{\psi}\rangle\,. \tag{8.43}$$

Since $\widehat{F}_{k,y}(q) = e^{-iy\cdot k}\widehat{G}(q-k)$, this proves (8.39). ∎

Remark 8.4. *The relation:*

$$\|\psi\|^2 = \frac{1}{(2\pi)^d}\int|\widetilde{\psi}(k,y)|^2dkdy = \frac{1}{(2\pi)^d}\int\langle\psi,F_{k,y}\rangle\langle F_{k,y},\psi\rangle dkdy\,, \tag{8.44}$$

expresses the completeness of the coherent states $F_{y,k}$, i.e.

$$\frac{1}{(2\pi)^d}\int|F_{k,y}\rangle\langle F_{k,y}|\,dkdy = \mathbb{1}_{L^2(\mathbb{R}^d)}\,. \tag{8.45}$$

8.4.2 Proof of Theorem 8.2

We are now ready to prove the main result of this section, Theorem 8.2.

Proof. (of Theorem 8.2.) For $R>0$, we consider the domain $\widetilde{\Omega}(R) = \{x\in\Omega \mid \mathrm{dist}(x,\Omega^c) > R\}$. By definition of the boundary area $\mathcal{A}(\Omega)$, we have $|\widetilde{\Omega}(R)| \geqslant |\Omega| - 4R\mathcal{A}(\Omega)$, for $R>0$ small enough.

Let now $M(k,y)$ be a function on phase space, with $0\leqslant M(k,y)\leqslant 1$ for all k,y, with $\operatorname{supp} M(k,\cdot)\subset\widetilde{\Omega}(R)$ for all $k\in\mathbb{R}^d$, and with

$$\frac{1}{(2\pi)^d}\int dkdy\,M(k,y) = N+\varepsilon \tag{8.46}$$

for an arbitrary $\varepsilon>0$. We construct the operator K on $L^2(\mathbb{R}^d)$ by defining its integral kernel

$$K(x,z) = \frac{1}{(2\pi)^d}\int M(k,y)\pi_{k,y}(x,z)dkdy = \frac{1}{(2\pi)^d}\int M(k,y)F_{k,y}(x)\overline{F_{k,y}(z)}dkdy\,. \tag{8.47}$$

Here $F_{k,y}$ are the coherent states defined by

$$F_{k,y}(x) = e^{ik\cdot x}G_R(x-y)\,, \tag{8.48}$$

where $G_R(x) = R^{-d/2}G(x/R)$ and $G\in L^2(\mathbb{R}^d)$ is a non-negative smooth function with $G(x) = G(-x)$, $\|G\|_2 = 1$ and with $\operatorname{supp} G\subset B_1(0)$. This guarantees that G_R is non-negative, smooth, $G_R(-x) = G_R(x)$, $\|G_R\|_2 = 1$ for all $R>0$ and that $\operatorname{supp} G_R\subset B_R(0)$.

For any $f\in L^2(\mathbb{R}^d)$,

$$\begin{aligned} 0\leqslant\langle f,Kf\rangle &\leqslant \frac{1}{(2\pi)^d}\int M(k,y)\langle f,\pi_{k,y}f\rangle\,dkdy = \frac{1}{(2\pi)^d}\int M(k,y)|\langle f,F_{k,y}\rangle|^2dkdy \\ &\leqslant \frac{1}{(2\pi)^d}\int|\widetilde{f}(k,y)|^2\,dkdy = \|f\|_2^2 \end{aligned} \tag{8.49}$$

where we used Lemma 8.3. Hence, $0\leqslant K\leqslant 1$. Furthermore, we find

$$\int dx\,K(x,x) = N+\varepsilon\,. \tag{8.50}$$

In particular, this implies that K has discrete spectrum. We denote by:

$$\lambda_1\geqslant\lambda_2\geqslant\lambda_3\geqslant\ldots \tag{8.51}$$

the eigenvalues of K, and by $f_1, f_2, \ldots$ the corresponding normalized eigenvectors. Note that by the restriction on the support of M and of G, $\operatorname{supp} f_j \subset \Omega$, for all j. Note moreover, that $\sum_j \lambda_j = N + \varepsilon$. Hence, we can find an integer L large enough with

$$\sum_{j=1}^{L} \lambda_j > N \; . \tag{8.52}$$

We set $K_L = \sum_{j=1}^{L} \lambda_j |f_j\rangle\langle f_j|$. Then $K - K_L \geqslant 0$. Now we apply the generalized min-max principle, Eq. (7.117), with $\phi_j = \lambda_j^{1/2} f_j$, $j = 1, \ldots, L$. We are allowed to do so, because $\theta_{ij} = \langle \phi_i, \phi_j \rangle = \lambda_i \delta_{ij}$ and therefore $0 \leqslant \theta \leqslant 1$ and $\operatorname{Tr}\theta = \sum_{j=1}^{L} \lambda_j > N$. We conclude that:

$$\begin{aligned}\sum_{j=0}^{N-1} E_j &\leqslant \sum_{j=1}^{L} \varepsilon(\phi_j) = \sum_{j=1}^{L} \lambda_j \int |\nabla f_j(x)|^2 \, dx \\ &\leqslant \sum_{j=1}^{\infty} \lambda_j \int |\nabla f_j(x)|^2 \, dx = \int \nabla_x \nabla_z K(x,z) \,|_{z=x} \, dx \\ &= \frac{1}{(2\pi)^d} \int dk dy \, M(k,y) \int dx \, |\nabla F_{k,y}(x)|^2 \; . \end{aligned} \tag{8.53}$$

With:

$$\nabla F_{k,y}(x) = ike^{ik\cdot x} G_R(x-y) + e^{ik\cdot x} \nabla G_R(x-y) \; , \tag{8.54}$$

and noticing that

$$\int dx \, [\overline{G_R(x-y)} \nabla G_R(x-y) + G_R(x-y) \nabla \overline{G_R(x-y)}] = \int dx \, \nabla |G_R(x-y)|^2 = 0 \; , \tag{8.55}$$

we obtain:

$$\begin{aligned}\sum_{j=0}^{N-1} E_j &\leqslant \frac{1}{(2\pi)^d} \int k^2 M(k,y) \, dk dy + (N+\varepsilon) \|\nabla G_R\|^2 \\ &\leqslant \frac{1}{(2\pi)^d} \int k^2 M(k,y) \, dk dy + C R^{-2} (N+\varepsilon) \; , \end{aligned} \tag{8.56}$$

because, by definition of G_{R}, $\|\nabla G_R\|_2^2 = R^{-2} \|\nabla G\|_2^2 = C R^{-2}$.

This bounds hold for all choices of M with $0 \leqslant M(k,y) \leqslant 1$ for all k, y with $\operatorname{supp} M(k,\cdot) \subset \widetilde{\Omega}(R)$ for all $k \in \mathbb{R}^3$, and with

$$\frac{1}{(2\pi)^d} \int dk dy \, M(k,y) = N + \varepsilon \tag{8.57}$$

for an arbitrary $\varepsilon > 0$. To minimize the average of k^2, we choose

$$M(k,y) = \chi(y \in \widetilde{\Omega}(R)) \chi(|k| \leqslant \kappa) \tag{8.58}$$

where we fix $\kappa > 0$ such that

$$\frac{1}{(2\pi)^d} \int dk dy \, M(k,y) = \frac{1}{(2\pi)^d} |\widetilde{\Omega}(R)| \frac{|S_{d-1}|}{d} \kappa^d = N + \varepsilon \; . \tag{8.59}$$

Hence, $\kappa = (2\pi)(N+\varepsilon)^{1/d} (d/|S_{d-1}|)^{1/d} |\widetilde{\Omega}(R)|^{-1/d}$. With this choice of M, we compute

$$\begin{aligned}\frac{1}{(2\pi)^d} \int k^2 M(k,y) \, dk dy &= \frac{1}{(2\pi)^d} |\widetilde{\Omega}(R)| |S_{d-1}| \frac{\kappa^{d+2}}{d+2} \\ &= (2\pi)^2 (N+\varepsilon)^{1+2/d} |\widetilde{\Omega}(R)|^{-2/d} \frac{d}{d+2} \Big(\frac{|S_{d-1}|}{d} \Big)^{-2/d} . \end{aligned} \tag{8.60}$$

Since $|\widetilde{\Omega}(R)| \geqslant |\Omega| - 4R\mathcal{A}(\Omega)$, we can choose $R = N^{-\alpha}$, for a sufficiently small $\alpha > 0$. Letting $\varepsilon \to 0$, we conclude that

$$\sum_{j=0}^{N-1} E_j \leqslant (2\pi)^2 N^{1+2/d} |\Omega|^{-2/d} \frac{d}{d+2} \Big(\frac{|S_{d-1}|}{d} \Big)^{-2/d} + o(N^{1+2/d}) \tag{8.61}$$

which implies the theorem. ∎

8.5 General Schrödinger operators

To conclude, let us briefly discuss the extension of the previous result for Schrödinger operators of the form $H = -\Delta + V$ on $L^2(\mathbb{R}^d)$. Semiclassical analysis also give predictions for the sum of negative eigenvalues of such Hamiltonians, for potentials V decaying at infinity, corresponding to relatively compact perturbations of the Laplacian. By Weyl's theorem, the essential spectrum of the Hamiltonian is not affected by the potential: $\sigma_{\text{ess}}(H) = \sigma(-\Delta) = [0, \infty)$. However, the negative part of the potential $V_-(x) = -\min\{V(x), 0\}$ might generate negative eigenvalues.

Arguing semiclassically, that is associating a volume $(2\pi)^d$ in phase space for every quantum state, we can predict that the sum of all negative eigenvalues of H can be approximated by:

$$\begin{aligned}
\sum_j E_j &\simeq \frac{1}{(2\pi)^d}\int (p^2 - V_-(x))\chi(|p^2 - V_-(x)| < 0)dxdp \\
&= \frac{1}{(2\pi)^d}\int dx \int_{|p|\leqslant V_-^{1/2}(x)} p^2 dp - \frac{1}{(2\pi)^d}\int dx\, V_-(x)\int_{|p|\leqslant V_-^{1/2}(x)} dp \\
&= \frac{1}{(2\pi)^d}|S_{d-1}|\Big[\frac{1}{d+2} - \frac{1}{d}\Big]\int dx\, V_-(x)^{1+d/2} \\
&= -\frac{1}{(2\pi)^d}\frac{2|S_{d-1}|}{d(d+2)}\int dx\, V_-(x)^{1+d/2}\ . \qquad (8.62)
\end{aligned}$$

One can prove that this prediction is indeed correct in the *semiclassical limit*. In fact, in analogy with the Dirichlet Laplacian, we expect the prediction of semiclassical analysis to become more accurate after summming a large number of eigenvalues. Here, the number of negative eigenvalues is fixed by the choice of the potential V. In order to increase the number of negative eigenvalues, we perform the *semiclassical limit*: that is, instead of considering the Hamiltonian H, we consider:

$$H_\hbar = -\hbar^2\Delta + V\ , \qquad \hbar > 0\ . \qquad (8.63)$$

The parameter $\hbar$ plays the role of Planck constant in Physics. We shall be interested in the limit $\hbar \to 0^+$; in this limit, the number of negative eigenvalues of $H_\hbar$ diverges. This is clear after rewriting $H_\hbar = \hbar^2(-\Delta + \hbar^{-2}V(x))$, since the negative part of $\hbar^{-2}V$ becomes deeper in the semiclassical limit $\hbar \to 0^+$. Semiclassical analysis allows to prove that, as $\hbar \to 0^+$:

$$\sum_j E_j = -\frac{1}{(2\pi)^d}\frac{2|S_{d-1}|}{d(d+2)}\hbar^{-d}\int dx\, V_-(x)^{1+d/2} + o(\hbar^{-d})\ . \qquad (8.64)$$

Also, in analogy with the Li-Yau inequality, Theorem 8.1, one can prove that the semiclassical prediction gives a lower bound to the sum of the negative eigenvalues, for the initial Schrödinger operator H. This is encoded by the *Lieb-Thirring inequality*:

$$\sum_j E_j \geqslant C_{\text{LT}}\int dx\, V_-(x)^{1+d/2}\ , \qquad (8.65)$$

for a suitable constant $C_{\text{LT}} < C_{\text{sc}}$, where C_{sc} is the constant predicted by the semiclassical approximation, $C_{\text{sc}} = -\frac{1}{(2\pi)^d}\frac{2|S_{d-1}|}{d(d+2)}$. Proving that the inequality Eq. (8.65) holds with C_{LT} replaced by C_{sc} is a longstanding open problem in mathematical physics.

9 Many-body quantum mechanics

9.1 Bosons and fermions

In this Section we will consider quantum mechanical models for many particle systems. The wave function for a system of N quantum particles in $\mathbb{R}^d$ is described by a wave function $\psi_N(x_1, \ldots, x_N) \in L^2(\mathbb{R}^{dN})$, where x_i corresponds to the location of the i-th particle. More generally, one might want to include the presence of extra degrees of freedom for each particle, labelled by $\sigma_i = 1, \dots, M$; in that case, the wave function of the system is denote by $\psi_N(z_1, \dots z_M) \in L^2(\mathbb{R}^{dN}; \mathbb{C}^{MN})$. For instance, σ_i might denote the spin of the particle: in that case, $M = 2$. The scalar product in the presence of this extra degree of freedom is defined as:

$$\begin{aligned}\langle \psi_N, \phi_N \rangle &= \sum_{\sigma_1, \dots, \sigma_N} \int dx_1 \dots dx_N \, \overline{\psi_N(z_1, \dots, z_N)} \phi_N(z_1, \dots, z_N) \\ &\equiv \int dz_1 \dots dz_N \, \overline{\psi_N(z_1, \dots, z_N)} \phi_N(z_1, \dots, z_N) \,. \end{aligned} \tag{9.1}$$

We shall consider *identical* particles. These correspond to wave functions satisfying the property:

$$|\psi_N(\cdots z_i \cdots z_j \cdots)| = |\psi_N(\cdots z_j \cdots z_i \cdots)| \,. \tag{9.2}$$

That is, the probability density for finding the particles in a given configuration does not change is one exchanges two particles. It turns out that in Nature there exists only two type of particles: *bosons* and *fermions*. Bosonic wave functions are *symmetric* with respect to exchange of particles:

$$\psi_N(\cdots z_i \cdots z_j \cdots) = \psi_N(\cdots z_j \cdots z_i \cdots) \,. \tag{9.3}$$

We shall denote by $L^2_{\mathrm{sym}}(\mathbb{R}^{dN}; \mathbb{C}^{MN})$ the restriction of $L^2(\mathbb{R}^{dN}; \mathbb{C}^{MN})$ to functions such that Eq. (9.3) holds true. Example of bosonic particles are photons, the elementary constituents of light. Instead, *fermions* correspond to wave functions that are *antisymmetric* with respect to exchange of particles:

$$\psi_N(\cdots z_i \cdots z_j \cdots) = -\psi_N(\cdots z_j \cdots z_i \cdots) \,. \tag{9.4}$$

We shall denote by $L^2_{\mathrm{anti}}(\mathbb{R}^{dN}; \mathbb{C}^{MN})$ the restriction of $L^2(\mathbb{R}^{dN}; \mathbb{C}^{MN})$ to functions such that Eq. (9.4) holds. Example of fermionic particles are electrons, neutrons and protons, which form all elements in Nature. The antisymmetry of the wave function immediately implies Pauli exclusion principle: a fermionic wave function is vanishing whenever $x_i = x_j$, for any $i = j$. The probability density for finding two fermionic particles at the same location is zero.

As a matter of fact, there is a deep connection between the possible values of the spin of the particle and its bosonic or fermionic type: the spin-statistics theorem states that particles with an even number of spin states are fermions, while particles with an odd number of spin states are bosons. In the following, we shall neglect this fact, and keep the number of spin states arbitrary for both bosons and fermions. Also, for simplicity we shall often set $M = 1$.

A simple example of bosonic wave function $\psi_N \in L^2_{\mathrm{sym}}$ is given by:

$$\psi_N(z_1, \dots z_N) = f(z_1) \cdots f(z_N) \,, \tag{9.5}$$

for some $f \in L^2$. Instead, the simplest example of fermionic wave function is provided by a Slater determinant, defined as follows. Let $f_i(z_i)$, $i = 1, \dots, N$ be N orthonormal functions in $L^2(\mathbb{R}^d; \mathbb{C}^M)$. The N-particle wave function

$$\psi_N(z_1, \dots, z_N) = \frac{1}{\sqrt{N!}} \det(f_i(z_j))_{i,j=1}^N \tag{9.6}$$

is antisymmetric and normalized. It is called the Slater determinant associated to $f_1, \dots, f_N$. By Leibnitz formula, Eq. (9.6) can be rewritten as:

$$\psi_N(z_1, \dots, z_N) = \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} \mathrm{sgn}(\pi) f_{\pi(1)}(x_1) \cdots f_{\pi(N)}(x_N) \,, \tag{9.7}$$

where S_N is the set of all permutations π of $\{1, \dots, N\}$, with sign $\mathrm{sgn}(\pi) = \pm 1$. Notice that the Slater determinant vanishes if $f_i = f_j$ for some $i \neq j$, which is another instance of Pauli principle. If $(f_i)_{i=1}^\infty$ form a basis of L^2, it is not difficult to see that a basis for $L^2_{\mathrm{anti}}(\mathbb{R}^{dN}; \mathbb{C}^{NM})$ is given by the set of all Slater determinants that can be constructed choosing N functions among $(f_i)_{i=1}^\infty$.

9.2 Reduced density matrices

Given the wave function ψ_N of N identical particles, the k-particle reduced density matrix $\gamma^{(k)}_{\psi_N}$ is an operator on $L^2(\mathbb{R}^{dk})$ with integral kernel:

$$\begin{aligned}&\gamma^{(k)}_{\psi_N}(y_1,\ldots,y_k;x_1,\ldots,x_k) \\ &:= \binom{N}{k}\int dx_{k+1}\ldots dx_N\,\psi_N(x_1,\ldots,x_k,x_{k+1},\ldots,x_N)\overline{\psi_N(y_1,\ldots,y_k,x_{k+1},\ldots,x_N)}\,.\end{aligned} \tag{9.8}$$

Equivalently, one writes:

$$\gamma^{(k)}_{\psi_N} = \binom{N}{k}\mathrm{Tr}_{k+1,\ldots,N}|\psi_N\rangle\langle\psi_N|\,. \tag{9.9}$$

Notice that $\mathrm{Tr}_{L^2(\mathbb{R}^{dk})}\gamma^{(k)}_{\psi_N} = \binom{N}{k}$. Density matrices are interesting because they allow to compute averages of k-particle observables. For instance, consider:

$$O_N = \sum_i O^{(i)}\,, \qquad O_i = \mathbb{1}^{\otimes(i-1)}\otimes O\otimes \mathbb{1}^{\otimes(N-i)}\,, \tag{9.10}$$

with O acting on $L^2(\mathbb{R}^d)$. Then:

$$\begin{aligned}\langle\psi_N, O_N\psi_N\rangle &= \sum_i\langle\psi_N, O_i\psi_N\rangle \\ &= N\langle\psi_N, O_1\psi_N\rangle \\ &= \mathrm{Tr}_{L^2(\mathbb{R}^d)}O\gamma^{(1)}_{\psi_N}\,.\end{aligned} \tag{9.11}$$

In general, the k-particle density matrix allows to compute the average of observables of the type $\sum_{\{i_1,\ldots,i_k\}}O_{(i_1,\ldots,i_k)}$. In particular, let us consider the many-body Hamiltonian,

$$H_N = \sum_i h_i + \sum_{i<j}V_{ij}\,, \tag{9.12}$$

with $V_{ij} = V(x_i - x_j)$. One has:

$$\begin{aligned}\langle\psi_N, H_N\psi_N\rangle &= \mathrm{Tr}\,h\gamma^{(1)}_{\psi_N} + \binom{N}{2}\langle\psi_N, V_{12}\psi_N\rangle \\ &= \mathrm{Tr}\,h\gamma^{(1)}_{\psi_N} + \mathrm{Tr}\,V_{12}\gamma^{(2)}_{\psi_N}\,.\end{aligned} \tag{9.13}$$

Therefore, the many-body ground state energy is completely specified by $\gamma^{(1)}$ and $\gamma^{(2)}$. It is therefore important to know the mathematical properties of the density matrices. Being partial traces of a nonnegative operator, $\gamma^{(k)}_{\psi_N} \geqslant 0$. The next lemma will provide an important upper bound for the reduced one-particle density matrix of identical fermions.

Lemma 9.1. *Let $\psi_N \in L^2_{anti}(\mathbb{R}^{dN})$. Then:*

$$0 \leqslant \gamma^{(1)}_{\psi_N} \leqslant \mathbb{1}_{L^2(\mathbb{R}^d)}\,. \tag{9.14}$$

Remark 9.2. *Being a trace class operator, $\gamma^{(k)}_{\psi_N}$ can be approximated by finite rank operators. That is, $\gamma^{(k)}_{\psi_N} = \sum_{j=1}^\infty \lambda_j|f_j\rangle\langle f_j|$ with $\{f_j\}$ a ONB of $L^2(\mathbb{R}^d)$. The bounds in Eq. (9.14) imply that $0\leqslant\lambda_j\leqslant 1$.*

Proof. We shall use a Fock space formalism. We define the fermionic Fock space as:

$$\mathcal{F} = \mathbb{C}\oplus\bigoplus_n L^2_{\mathrm{anti}}(\mathbb{R}^{dn})\,. \tag{9.15}$$

That is, an element of $\mathcal{F}$ has the form $\psi = (\psi^{(0)},\psi^{(1)},\ldots,\psi^{(n)},\ldots)$ with $\psi^{(n)}\in L^2_{\mathrm{anti}}(\mathbb{R}^{dn})$. The space $\mathcal{F}$ becomes a Hilbert space if endowed with the standard scalar product

$$\langle\psi,\varphi\rangle_{\mathcal{F}} = \sum_{n\geqslant 0}\langle\psi^{(n)},\varphi^{(n)}\rangle_{L^2(\mathbb{R}^{dn})}\,. \tag{9.16}$$

Given $f \in L^2(\mathbb{R}^d)$, we define the creation and annihilation operators $a^*(f)$ and $a(f)$ as:

$$\begin{aligned}(a(f)\psi)^{(n)}(x_1,\ldots,x_n) &= \sqrt{(n+1)}\int dx\, \overline{f(x)}\psi^{(n+1)}(x,x_1,\ldots,x_n) \\ (a^*(f)\psi)^{(n)}(x_1,\ldots,x_n) &= \frac{1}{\sqrt{n}}\sum_{j=1}^{n}(-1)^j f(x_j)\psi^{(n-1)}(x_1,\ldots,x_{j-1},x_{j+1},\ldots,x_n)\,.\end{aligned} \tag{9.17}$$

It is not difficult to see that $a^*(f) = a(f)^*$. Physically, the operator $a(f)$ destroys a fermion with wave function f, while the operator $a^*(f)$ creates a fermion with wave function f. Let $\{A, B\}$ be the anticommutator of the operators A, B: $\{A, B\} = AB + BA$. It is a simple algebraic exercise to check that:

$$\{a(f), a^*(g)\} = \langle f, g\rangle_{L^2(\mathbb{R}^d)} \mathbb{1}_{\mathcal{F}}\,, \qquad \{a(f), a(g)\} = \{a^*(f), a^*(g)\} = 0\,. \tag{9.18}$$

The above relations are called the canonical anticommutation relations (CAR). An important consequence of the CAR is the boundedness of the fermionic operators:

$$\begin{aligned}\langle\psi, a^*(f)a(f)\psi\rangle &= \|f\|_2^2\|\psi\|_{\mathcal{F}}^2 - \langle\psi, a(f)a^*(f)\psi\rangle \\ &\leqslant \|f\|_2^2\|\psi\|_{\mathcal{F}}^2\,.\end{aligned} \tag{9.19}$$

We used that $\langle\psi, a(f)a^*(f)\psi\rangle = \|a^*(f)\psi\|^2 \geqslant 0$. As a consequence,

$$\|a(f)\| = \sup_{\psi\in\mathcal{F}}\frac{\|a(f)\psi\|}{\|\psi\|} \leqslant \|f\|_2\,. \tag{9.20}$$

This bound easily implies the desired statement for the one-particle density matrix. Let $\psi \in \mathcal{F}$ be an N-particle vector in the Fock space: $\psi = (0, 0, \ldots, 0, \psi^{(N)}, 0, \ldots, 0, \ldots)$, with $\psi^{(N)} = \psi_N$ a normalized fermionic wave function. A simple computation shows that:

$$\langle\psi, a^*(f)a(g)\psi\rangle = \langle(a(f)\psi)^{(N-1)}, (a(g)\psi)^{(N-1)}\rangle = \langle g, \gamma_\psi^{(1)} f\rangle_{L^2(\mathbb{R}^d)}\,. \tag{9.21}$$

Therefore:

$$\langle f, \gamma_\psi^{(1)} f\rangle = \langle\psi, a^*(f)a(f)\psi\rangle \leqslant \|f\|_2^2\,, \tag{9.22}$$

which implies that $\gamma_\psi^{(1)} \leqslant \mathbb{1}$. ∎

Remark 9.3. *The above upper bound is not true for bosons: there, $\gamma_\psi^{(1)} \leqslant N\mathbb{1}$. This suggests that bosonic one-particle density matrices might have large eigenvalues. One can check that for factorized states the reduced one-particle density matrix has one eigenvalue equal to N.*

To conclude, as an example let us compute the reduced one-particle density matrix of the simplest fermionic wave functions for N fermions, namely Slater determinants. Consider:

$$\psi_N = \frac{1}{\sqrt{N!}}\sum_\pi \mathrm{sgn}(\pi) f_{\pi(1)}(x_1)\cdots f_{\pi(N)}(x_N)\,, \tag{9.23}$$

with $\{f_i\}$ orthonormal. A simple computation shows:

$$\gamma_\psi^{(1)} = \sum_{i=1}^{N} |f_i\rangle\langle f_i|\,. \tag{9.24}$$

That is, $\gamma_\psi^{(1)}$ is a rank$-N$ orthogonal projector: $\gamma_\psi^{(1)} = \gamma_\psi^{(1)*} = \gamma_\psi^{(1)2}$, $\mathrm{Tr}\gamma_\psi^{(1)} = N$. In this case, the eigenvalues of the density matrix are either 0 or 1.

9.3 Atoms and molecules

In the following, we shall focus on a specific model in quantum mechanics, of great relevance for physics and chemistry. The model describes a system of N fermions (electrons) interacting with K fixed nuclei. For $K = 1$, this model describes an atom with N electrons, for $K > 1$ it describes a molecule. The Hamiltonian is:

$$H_{N,K}(\underline{Z},\underline{R}) = \sum_{i=1}^{N} -\Delta_i - \sum_{i=1}^{N}\sum_{j=1}^{K} \frac{Z_i}{|x_i - R_j|} + \sum_{i<j=1}^{N} \frac{1}{|x_i - x_j|} + \sum_{i<j=1}^{K} \frac{Z_i Z_j}{|R_i - R_j|}\ , \qquad (9.25)$$

on $L^2(\mathbb{R}^{3N};\mathbb{C}^{MN})$. Let us discuss the various terms. The first term describes the kinetic energy of the N particles; Δ_i is the Laplacian acting on the i-th particle,

$$(\Delta_i \psi_N)(z_1,\ldots,z_N) = \Delta_{x_i}\psi_N(z_1,\ldots,z_N)\ , \quad i = 1,\ldots,N\ . \qquad (9.26)$$

The second term takes into account the interaction between the electrons, with positions x_i, and the nuclei, located at R_j. Units are chosen so that the charge of the electron is -1, and the charge of the nuclei is $Z_j \in \mathbb{N}$. The sign of the Coulomb potential shows that the energy decreases when the particles and the nuclei are close: the interaction is attractive. The third term describes the electrostatic interaction among the electrons: the sign of the Coulomb potential shows that the energy increases when two electrons are close: the interaction is repulsive. Finally, the last term takes into account the Coulomb repulsion of the nuclei. Notice that x_i is a multiplication operator, while R_j is a fixed vector in $\mathbb{R}^3$: that is, the nuclei are treated as fixed in space. This is motivated by the fact that that, physically, the masses of the nuclei are much larger than the masses of the electrons (chosen to be equal to $1/2$ in our units). Later, we shall minimize over the positions of the nuclei, to find the optimal energy of the system.

At zero temperature, the state of the system coincides with the ground state of the Hamiltonian $H_{N,K}(\underline{Z},\underline{R})$. Since we are interested in describing a system of N electrons, and since electrons are fermions, we shall consider the fermionic ground state energy:

$$E_{N,K}(\underline{Z},\underline{R}) = \inf_{\substack{\psi_N \in L^2_{\mathrm{anti}}(\mathbb{R}^{3N};\mathbb{C}^{NM}) \\ \|\psi_N\|_2 = 1}} \langle \psi_N, H_{N,K}(\underline{Z},\underline{R})\psi_N\rangle \qquad (9.27)$$

These are the typical questions we shall study in the following.

1. Is the system stable? That is, $E_{N,K}(\underline{Z},\underline{R}) > -\infty$? If so, this is called *stability of matter of the first kind.* Stability is a purely quantum mechanical phenomenon: it is false in classical mechanics. We have seen that stability holds for $N = 1$, $K = 1$.

2. From experience, we know that the energy of a physical system scales linearly with the number of constituents. If not, this would imply a huge release or absorption of energy as two systems are merged together. Suppose for instance that $E_{N,K}(\underline{Z},\underline{R}) \sim -C(N+K)^2$. Then,

$$E_{2N,2K} = -4C(N+K)^2 \ll 2E_{N,K}\ . \qquad (9.28)$$

This means that it would be energetically much more convenient to merge together two systems composed by N particles and K nuclei, which is not what we observe. This gain is incompatible with the observation that matter is extensive (doubling the number of particles of a physical system corresponds to a macroscopic variation of the volume the system occupies). We say that *stability of matter of the second kind* occurs if:

$$E_{N,K}(\underline{Z},\underline{R}) \geqslant -C(\underline{Z},\underline{R})(N+K)\ . \qquad (9.29)$$

Of course, stability of matter of the second kind implies stability of matter of the first kind. Does stability of matter of the second kind occurs for the model in Eq. (9.25)?

3. In order for an atom or a molecule to be stable, the *ionization energy* to remove an electron must be positive. That is, if $E_{N+1,M} < E_{N,M}$: it is energetically more convenient for the system to attract one more electron. Under which conditions the ionization energy is positive? We know from experience that there are no atoms with $N > Z + 2$. This is intuitively clear: the ionization energy will be zero, when the total charge of the electrons compensates the total charge of the nucleus, so that the atoms looks neutral at large distances. Can one prove this mathematically?

4. As N increases, the model becomes quickly intractable from an analytic point of view. Can we say anything quantitative about, *e.g.*, the ground state energy of the system for N large?

In order to understand these questions, we shall first consider them in a simplified theory, the *Thomas-Fermi model.* Later, we shall discuss the rigorous connection between Thomas-Fermi theory and the original many-body problem.

9.4 Thomas-Fermi theory

Thomas-Fermi (TF) theory is an effective theory for many-body quantum mechanics, which takes as only input the density of the quantum system, defined as:

$$\rho(z) = N \int dz_2 \dots dz_N \, |\psi_N(z, z_2, \dots, z_N)|^2 \,, \tag{9.30}$$

where ψ_N is the many-body wave function of the system. Clearly, $\rho \geqslant 0$, $\int dz \, \rho(z) = N$. The quantity $\rho(z)/N$ describes the probability density for finding a particle at $z = (x, \sigma)$. Any wave function ψ_N determines uniquely a density ρ; clearly, the converse does not hold.

TF theory is much easier to study than the full many-body problem, due to the fact that it depends on much less degrees of freedom (the density is a function on $\mathbb{R}^3$, while the wave function is a function on $\mathbb{R}^{3N}$). Later, we will discuss the rigorous validity of this approximation, in the limit in which $N, Z \to \infty$.

The main approximation introduced in TF theory is the replacement of the kinetic energy of the system with a functional of ρ. In order to understand this approximation, let us first discuss a simple example.

9.4.1 The free Fermi gas

Consider a system of N spinless, noninteracting particles confined in a cubic box Λ, of side 1, with periodic boundary conditions: $\Lambda = \mathbb{T}^3$, with $\mathbb{T}^3$ the unit torus in three dimensions. Let us first start with $N = 1$. The Hamiltonian is $H = -\Delta$, on $L^2(\mathbb{T}^3)$. The eigenfunctions of the Hamiltonian are given by plane waves:

$$H f_p = |p|^2 f_p \,, \qquad f_p(x) = e^{-ip\cdot x} \,, \qquad p \in (2\pi)\mathbb{Z}^3 \,. \tag{9.31}$$

The vector p is called the momentum of the particle; the constraint $p \in (2\pi)\mathbb{Z}^3$ is due to the requirement of periodic boundary conditions. The energy of the quantum particle with momentum p is $|p|^2$. Consider now a system of $N > 1$ particles. The Hamiltonian is $H_N = \sum_{j=1}^N -\Delta_j$. Clearly, if (f_{p_i}) are eigenstates of the Laplacian, then their product $f_{p_1} \cdots f_{p_N}$ is an eigenstate of H_N with energy $\sum_{i=1}^N |p_i|^2$. Since we are interested in fermionic eigenstates, we shall consider antisymmetric combinations of products of plane waves, that is Slater determinants:

$$\frac{1}{\sqrt{N!}} \sum_\pi \mathrm{sgn}(\pi) f_{p_{\pi(1)}}(x_1) \cdots f_{p_{\pi(N)}}(x_N) \,. \tag{9.32}$$

Notice that as soon as $p_i = p_j$ for $i \neq j$, the Slater determinant vanishes (Pauli principle). The fermionic ground state of H_N is given by the Slater determinant with the smallest energy. To find such state, we have to minimize the quantity $\sum_{i=1}^N |p_i|^2$ under the constraints that $p_i \neq p_j$ for $i \neq j$, and $p_i \in (2\pi)\mathbb{Z}^3$. The solution to this problem is provided by "filling the Fermi ball": one considers the N momenta p_i with smallest modulus. In general, one has that $|p| \leqslant p_F$, where the Fermi momentum p_F scales as $p_F \sim cN^{1/3}$ for some constant $c > 0$. Notice that in general not all states with momenta such that $|p| \leqslant p_F$ will be occupied: the Fermi ball might be only partially filled, and the ground state might be degenerate.

Suppose, for the sake of simplicity, that the number of particles N is chosen so that the Fermi ball is completely filled. The ground state energy of the system is:

$$E_N = \sum_{\substack{p \in (2\pi)\mathbb{Z}^3 \\ |p| \leqslant cN^{1/3}}} |p|^2 = N \sum_{\substack{p \in (2\pi)\mathbb{Z}^3 \\ |p| \leqslant cN^{1/3}}} \frac{1}{N} |p|^2 \,. \tag{9.33}$$

Changing variable, one has:

$$E_N = N^{1+\frac{2}{3}} \sum_{\substack{p \in \frac{2\pi}{N^{1/3}}\mathbb{Z}^3 \\ |p| \leqslant c}} \frac{1}{N}|p|^2 \, . \tag{9.34}$$

As $N \to \infty$, the sum converges to an integral. One has:

$$E_N = N^{\frac{5}{3}} \int_{|p|\leqslant c} dp\, |p|^2 + o(N^{\frac{5}{3}}) = CN^{\frac{5}{3}} + o(N^{\frac{5}{3}}) \, . \tag{9.35}$$

Thus, the ground state energy of the system, which is purely kinetic, scales as $N^{5/3}$. More generally, in d-dimensions one would find $N^{1+\frac{2}{d}}$. This asymptotic behavior is in agreement with the Weyl law for the sum of the first N eigenvalues of the Dirichlet Laplacian, recall Theorem 8.2. In the present case, however, the domain Ω has no boundary, hence Theorem 8.2 does not apply directly. One can actually show that the constant C is equal to the constant appearing in the Weyl asymptotics. In the present example, the density $\rho(x)$ associated to the ground state is constant: $\rho(x) = \rho = N$. Thus, the kinetic energy of the confined system scales as $\rho^{5/3}$. This connection between kinetic energy and density turns out to be much more general, and it plays a crucial role in defining the Thomas-Fermi energy functional.

9.4.2 The Thomas-Fermi energy functional

In TF theory, the energy of the system is determined by the electron density via the following functional (we omit the spin of the system for simplicity):

$$\mathcal{E}_{\mathrm{TF}}(\rho) = c_{\mathrm{TF}} \int dx\, \rho(x)^{5/3} - \int dx\, \rho(x)V(x) + \frac{1}{2}\int dxdy\, \frac{\rho(x)\rho(y)}{|x-y|} + U \, , \tag{9.36}$$

where $V(x)$ is the electrostatic potential generated by the K fixed nuclei, and U is the electrostatic repulsion of the nuclei:

$$V(x) = \sum_{j=1}^{K} \frac{Z_j}{|x-R_j|} \, , \quad U = \sum_{i<j=1}^{K} \frac{Z_i Z_j}{|R_i - R_j|} \, . \tag{9.37}$$

The constant c_{TF} is positive, and later it will be suitably chosen, in order to connect with the original many-body problem. The following discussion will only use that $c_{\mathrm{TF}} > 0$.

The domain of the TF functional is given by the set of allowed densities:

$$\mathcal{F}_N = \{\rho : \mathbb{R}^3 \to \mathbb{R} \mid \rho(x) \geqslant 0 \, , \; \|\rho\|_1 = N \, , \; \rho \in L^{5/3}(\mathbb{R}^3)\} \, . \tag{9.38}$$

As we shall prove later, the TF functional is well-defined on this domain. The TF ground state energy is:

$$E_N^{\mathrm{TF}} = \inf_{\rho\in\mathcal{F}_N} \mathcal{E}_{\mathrm{TF}}(\rho) \, . \tag{9.39}$$

Before discussing the mathematical properties of the functional, let us discuss its physical origin. The first term in Eq. (9.36) takes into account the kinetic energy of the system. As we have seem for a homogeneous electron gas, Section 9.4.1, the kinetic energy of the system grows as $\rho^{5/3}$. For a general system, one cannot expect the density $\rho(x)$ associated to the ground state to be constant. Nevertheless, in general it will vary on a scale that is much smaller that the mean interparticle distance; to approximate the ground state, one fills a "local" Fermi ball, with radius $\rho(x)^{1/3}$, and integrates over space. This yields the $\int \rho(x)^{5/3}$ term in the TF energy functional. This approximation of the kinetic energy turns out to be rigorously justified, as we shall discuss later with the Lieb-Thirring kinetic energy inequality.

The second term describes the electrostatic interaction between the electrons and the nuclei. In the full many-body problem, this is given by:

$$\langle \psi_N, \sum_{i=1}^{N}\sum_{j=1}^{K} \frac{Z_j}{|x_i - R_j|} \psi_N \rangle \, . \tag{9.40}$$

We have:

$$\begin{aligned}
\langle \psi_N, \sum_{i=1}^N \sum_{j=1}^K \frac{Z_j}{|x_i - R_j|}\psi_N \rangle &= \sum_{i=1}^N \sum_{j=1}^K Z_j \int dx_1 \dots dx_N \, |\psi_N(x_1, \dots, x_N)|^2 \frac{1}{|x_i - R_j|} \\
&= N \sum_{j=1}^K Z_j \int dx_1 \dots dx_N \, |\psi_N(x_1, \dots, x_N)|^2 \frac{1}{|x_1 - R_j|} \\
&\equiv \int dx \, \rho(x) V(x) \,, \qquad (9.41)
\end{aligned}$$

where in the second step we used the (anti)symmetry of the wave function. The right-hand side reproduces exactly the second term in the TF energy functional: hence, no approximation is made here. Consider now the third term. This describes the electrostatic repulsion of the electrons: it appears as a classical electrostatic energy, generated by the charge density $\rho(x)$. In the full many-body problem, this terms corresponds to:

$$\langle \psi_N, \sum_{i<j=1}^N \frac{1}{|x_i - x_j|}\psi_N \rangle \,. \qquad (9.42)$$

Consider the electrons as classical point particles, with positions x_i; treat them as independent, identically distributed random variables, with probability distributions $\rho(x)/N$. The law of the large numbers implies:

$$\frac{1}{N} \sum_{j: j \neq j} \frac{1}{|x_i - x_j|} \simeq \int dx \, \frac{\rho(x)}{N} \frac{1}{|x_i - x|} \,. \qquad (9.43)$$

Under this approximation, we replace Eq. (9.42) by:

$$\begin{aligned}
\langle \psi_N, \sum_{i<j=1}^N \frac{1}{|x_i - x_j|}\psi_N \rangle &= \frac{1}{2} \langle \psi_N, \sum_{i \neq j}^N \frac{1}{|x_i - x_j|}\psi_N \rangle \\
&\simeq \frac{1}{2} \langle \psi_N, \sum_{i=1}^N w(x_i)\psi_N \rangle \,, \qquad (9.44)
\end{aligned}$$

with $w(x) = (\rho * |\cdot|^{-1})(x)$. The big conceptual simplification here is that we replaced a sum of two-body operators by a sum of one-body operators, exploiting an averaging principle. Then, we can repeat the computation in Eq. (9.41). We have:

$$\frac{1}{2} \langle \psi_N, \sum_{i=1}^N w(x_i)\psi_N \rangle = \frac{1}{2} \int dx dy \, \rho(x)\rho(y) \frac{1}{|x - y|} \,, \qquad (9.45)$$

which is precisely the third term appearing in the TF energy functional. Finally, the fourth term appearing in the TF functional is equal to the corresponding term appearing in the full many-body problem, hence no further approximation is introduced at this point.

The mathematical foundations of TF theory have been developed by Lieb and Simon in the seventies, see [2] for a review, fifty years after the introduction of the functional by Thomas and Fermi. It is a milestone in mathematical physics; its development played a crucial role in understanding the problem of stability of matter for large quantum systems. Here we shall discuss the mathematics of the TF energy functional, and in particular how to solve the problems **1.-4.** spelled out in Section 9.3 within the framework of TF theory. Later, we will show how the TF approximation can be rigorously justified starting from the original many-body problem.

Let us now prove that the TF energy functional is well-defined on its domain $\mathcal{F}_N$. The finiteness of the first term in Eq. (9.36) follows from $\rho \in L^{5/3}$. Consider the second term. We rewrite it as:

$$\int dx \, \rho(x) V(x) = \int dx \, \rho(x) V_<(x) + \int dx \, \rho(x) V_>(x) \,, \qquad (9.46)$$

where:

$$V_<(x) = \sum_{j=1}^{K} \frac{Z_j}{|x - R_j|}\chi(|x - R_k| \leqslant 1) \;, \quad V_>(x) = \sum_{j=1}^{K} \frac{Z_j}{|x - R_j|}\chi(|x - R_j| > 1) \;. \tag{9.47}$$

Consider the first term. By Hölder inequality, we have:

$$\int dx\, \rho(x)\frac{\chi(|x - R_j| \leqslant 1)}{|x - R_j|} \leqslant \|\rho\|_{5/3}\Big\|\frac{\chi(|\cdot| \leqslant 1)}{|\cdot|}\Big\|_{5/2} \tag{9.48}$$

which is finite, thanks to the fact that $\rho \in L^{5/3}$. The second term can be estimated immediately, using that:

$$\int dx\, \rho(x)\frac{\chi(|x - R_j| > 1)}{|x - R_j|} \leqslant \|\rho\|_1 = N \;. \tag{9.49}$$

All together:

$$\int dx\, \rho(x)V(x) \leqslant C\sum_{j=1} Z_j(\|\rho\|_1 + \|\rho\|_{5/3}) \;. \tag{9.50}$$

Finally, consider the third term in Eq. (9.36). This will be estimated using the Hardy-Littlewood-Sobolev inequality. Let $f \in L^p(\mathbb{R}^d)$ and $h \in L^r(\mathbb{R}^d)$. Then, for $\frac{1}{p} + \frac{1}{r} + \frac{\lambda}{d} = 2$:

$$\Big|\int dxdy\, f(x)h(y)\frac{1}{|x - y|^\lambda}\Big| \leqslant C(\lambda, d, p)\|f\|_p\|h\|_r \;. \tag{9.51}$$

See [3] for a proof. To apply this inequality to the TF functional, we choose $\lambda = 1$, $d = 3$, and $f = h = \rho$. Choosing $p = r$, one has $p = 6/5$; hence:

$$D(\rho, \rho) = \frac{1}{2}\int dxdy\, \rho(x)\rho(y)\frac{1}{|x - y|} \leqslant C\|\rho\|^2_{6/5} \;. \tag{9.52}$$

The right-hand side is finite, since by interpolation:

$$\|\rho\|_{6/5} \leqslant \|\rho\|_1^\lambda\|\rho\|_{5/3}^{1-\lambda} \;, \tag{9.53}$$

with $\lambda = 7/12$. This shows that $\mathcal{E}_{\mathrm{TF}}$ is well defined on $\mathcal{F}_N$.

9.4.3 Existence and uniqueness of the minimizer in $\mathcal{D}_N$

In this section we shall start the study of the variational problem associated to the TF functional. Before starting, let us comment about the fact that in general one does not expect the minimizer to exists for all values of N. In fact, one expects the system to be able to bind a finite number of electrons, dependent on the total nuclear charge $Z_{\mathrm{tot}} = \sum_{j=1}^K Z_j$. This is due to the fact that, for $N = Z_{\mathrm{tot}}$, the total charge of the electrons is equal to the total charge of the nuclei. Hence, at large distances, the system will look charge neutral, and will not be able to attract any further electron. This is confirmed by the fact that in nature one does not observe stable atoms with $N > Z_{\mathrm{tot}} + 2$.

Mathematically, one does not expect the minimizer to exists in $\mathcal{F}_N$, for any N. Calling ρ^* the minimizer, it might happen that:

$$\int dx\, \rho^*(x) < N \;, \tag{9.54}$$

which means that $\rho^* \notin \mathcal{F}_N$. Therefore, in order to avoid this problem for the moment, we will consider the functional on a larger domain,

$$\mathcal{D}_N = \Big\{\rho \in L^1 \cap L^{5/3} \mid \rho \geqslant 0,\; \int dx\, \rho(x) \leqslant N\Big\} \;. \tag{9.55}$$

This new space allows to take into account the "loss" of electrons at infinity. We will first prove the existence and uniqueness of the minimizer in this domain, and then later we will prove that, for suitable values of N, the minimizer actually belongs to $\mathcal{F}_N$ (particles are not lost at infinity).

Theorem 9.4 (Existence of minimizers in $\mathcal{D}_N$.)**.** *There exists $\rho_* \in \mathcal{D}_N$ such that the following is true:*

$$\inf_{\rho\in\mathcal{D}_N} \mathcal{E}_{TF}(\rho) = \mathcal{E}_{TF}(\rho_*) \; . \tag{9.56}$$

The proof will be based on the following auxiliary result.

Lemma 9.5. *Let ρ_1, ρ_2 in $\mathcal{D}_N$, and $\rho_j \to \rho_2$ weakly in L^p for all $p \in (1, 5/3]$. Then:*

$$\lim_{j\to\infty} D(\rho_1, \rho_j) = D(\rho_1, \rho_2) \; , \qquad D(\rho_1, \rho_2) \leqslant D(\rho_1, \rho_1)^{1/2} D(\rho_2, \rho_2)^{1/2} \; . \tag{9.57}$$

Proof. (of Lemma 9.5) Let us prove the first property. To this end, we rewrite:

$$D(\rho_1, \rho_j) = \frac{1}{2}\int dxdy\, \rho_1(y)\rho_j(x)\frac{1}{|x-y|} \equiv \int dx\, \rho_j(x) f(x) \; , \tag{9.58}$$

where $f(x) = (1/2)(\rho_1 * |\cdot|^{-1})(x)$. We decompose the function f as $f = f_< + f_>$, where:

$$f_<(x) = \frac{1}{2}\int dy\, \rho_1(y)\frac{\chi(|x-y| \leqslant 1)}{|x-y|} \; , \qquad f_>(x) = \frac{1}{2}\int dy\, \rho_1(y)\frac{\chi(|x-y| > 1)}{|x-y|} \tag{9.59}$$

Consider $f_<$. By Hölder inequality,

$$\|f_<\|_\infty \leqslant \|\rho_1\|_{5/3} \Big\| \frac{\chi(|\cdot| \leqslant 1)}{|\cdot|} \Big\|_{5/2} < \infty \tag{9.60}$$

and:

$$\|f_<\|_1 = \int dxdy\, \rho_1(x)\frac{\chi(|x-y| \leqslant 1)}{|x-y|} = C\|\rho_1\|_1 < \infty \; . \tag{9.61}$$

Therefore, by interpolation $f_< \in L^p(\mathbb{R}^3)$ for all $p \in [1, \infty)$. Hence, by weak convergence:

$$\lim_{j\to\infty} \int dx\, \rho_j(x) f_<(x) = \int dx\, \rho_*(x) f_<(x) \; . \tag{9.62}$$

Consider now $f_>(x)$. By Young's inequality for convolutions,

$$\|f_>\|_p \leqslant \|\rho_1\|_q \Big\| \frac{\chi(|\cdot| > 1)}{|\cdot|} \Big\|_r \tag{9.63}$$

with $\frac{1}{p} = \frac{1}{q} + \frac{1}{r} - 1 \leqslant \frac{1}{r} < \frac{1}{3}$. Therefore, $p > 3$. Using that L^p is equal to the dual of $L^{p'}$ with $p' \in (1, 3/2)$, by weak convergence:

$$\lim_{j\to\infty} \int dx\, \rho_j(x) f_>(x) = \int dx\, \rho_*(x) f_>(x) \; . \tag{9.64}$$

This together with Eq. (9.62) proves the first claim in Eq. (9.57). Consider now the second claim. To prove it, we proceed as follows. Let $h(x) = Ce^{-c|x|}$, and let $K(x) = (h * h)(x)$. Notice that K is a radial function: $K(x) = K(|x|)$. Let us choose the constant C such that:

$$\int_0^\infty dt\, K(t) = \frac{1}{2} \; . \tag{9.65}$$

In particular, by a change of variables:

$$\frac{1}{2|x-y|} = \int_0^\infty dt\, K(t|x-y|) \; . \tag{9.66}$$

We can further rewrite this as:

$$\frac{1}{2|x-y|} = \int_0^\infty dt\, t^3 \int dz\, h_t(x-z) h_t(y-z) \; , \qquad h_t(x-z) = h(t(x-z)) \; . \tag{9.67}$$

Therefore, using this decomposition of the Coulomb potential:

$$\begin{aligned} D(\rho_1,\rho_2) &= \int dxdy\,\rho_1(x)\rho_2(y)\int_0^\infty dt\,t^3\int dz\,h_t(x-z)h_t(y-z) \\ &= \int_0^\infty dt\,t^3\int dz\,(\rho_1 * h_t)(z)(\rho_2 * h_t)(z) \end{aligned} \tag{9.68}$$

where the exchange of integrations is allowed by Fubini's theorem. By Cauchy-Schwarz inequality:

$$\begin{aligned} D(\rho_1,\rho_2) &\leqslant \Big(\int_0^\infty dt\,t^3\int dz\,(\rho_1 * h_t)^2(z)\Big)^{1/2}\Big(\int_0^\infty dt\,t^3\int dz\,(\rho_2 * h_t)^2(z)\Big)^{1/2} \\ &= D(\rho_1,\rho_1)^{1/2}D(\rho_2,\rho_2)^{1/2}\;. \end{aligned} \tag{9.69}$$

This concludes the proof of the second of Eq. (9.57), and of the Lemma. ■

We are now ready to prove Theorem 9.4.

Proof. Let ρ_j be a minimizing sequence in $\mathcal{D}_N$. The bounds used to prove the wellposedness of the TF functional on $\mathcal{F}_N$ easily imply that:

$$\mathcal{E}_{TF}(\rho_j) \geqslant a\|\rho_j\|_{5/3}^{5/3} - bN\;. \tag{9.70}$$

Therefore, using that $|\mathcal{E}_{TF}(\rho_j)| \leqslant C$ (which follows from the finiteness of the $j\to\infty$ limit), the above estimate allows to prove an a priori bound on $\|\rho_j\|_{5/3}$:

$$\|\rho_j\|_{5/3} \leqslant K\;, \tag{9.71}$$

for some constant K independent of j. Since $\|\rho_j\|_1 \leqslant N$ for all j, by interpolation we get:

$$\|\rho_j\|_p \leqslant C\;,\qquad \forall p\in[1,5/3]\;. \tag{9.72}$$

By Banach-Alaoglu theorem, we know that, up to the extraction of a subsequence, $\rho_j \to \rho_*$ weakly in L^p, for $p\in(1,5/3]$ (one can actually prove that the limit is independent of p). Also, one can easily check that $\rho_*\in\mathcal{D}_N$. Let us first prove that $\rho_*\geqslant 0$. Suppose it is false. Then, there exists a bounded set $A\subset\mathbb{R}^3$ such that:

$$\int dx\,\rho_*(x)\chi_A(x) < 0\;. \tag{9.73}$$

However, since by weak convergence $\int dx\,\rho_*(x)\chi_A(x) = \lim_{j\to\infty}\int dx\,\rho_j(x)\chi_A(x)$, and $\rho_j\geqslant 0$, Eq. (9.73) would imply a contradiction. Thus, $\rho_*\geqslant 0$. In a similar way, one can prove that $\|\rho_*\|_1\leqslant N$. Suppose it is false. Then, there exists a bounded set A such that:

$$\int dx\,\rho_*(x)\chi_A(x) > N\;. \tag{9.74}$$

Repeating the same argument as before, this implies a contradiction. Thus, $\rho_*\in\mathcal{D}_N$. To prove the claim (9.56), we shall show that:

$$\mathcal{E}_{\rm TF}(\rho_*) \leqslant E_{\rm TF}\;. \tag{9.75}$$

Consider the kinetic energy contribution. By the lower semicontinuity of norms, one gets:

$$\liminf_j \|\rho_j\| \geqslant \|\rho_*\|_{5/3}\;. \tag{9.76}$$

Consider now the electrons-nuclei interaction. We claim that:

$$\lim_j \int dx\,\rho_j(x)V(x) = \int dx\,\rho_*(x)V(x)\;. \tag{9.77}$$

To prove this, we write:

$$V(x) = V_<(x) + V_>(x)\ , \tag{9.78}$$

with:

$$V_<(x) = \sum_{j=1}^{K} \frac{Z_j}{|x - R_j|}\chi(|x - R_j| \leqslant 1)\ , \qquad V_>(x) = \sum_{j=1}^{K} \frac{Z_j}{|x - R_j|}\chi(|x - R_j| > 1)\ . \tag{9.79}$$

Consider first $V_>$. This function belongs in L^p for $p > 3$, which is the dual of $L^{p'}$, for $p' \in (1, 3/2)$. Since $\rho_j \to \rho_*$ in L^p with $(1, 5/3]$ and $(1, 3/2) \subset (1, 5/3]$, we have:

$$\lim_{j\to\infty} \int dx\, \rho_j(x) V_>(x) = \int dx\, \rho_*(x) V_>(x)\ . \tag{9.80}$$

Consider now $V_<$. This function belongs to $L^{5/2}$, which is the dual of $L^{5/3}$. Thus, by weak convergence:

$$\lim_{j\to\infty} \int dx\, \rho_j(x) V_<(x) = \int dx\, \rho_*(x) V_<(x)\ . \tag{9.81}$$

Eqs. (9.80), (9.81) imply Eq. (9.77). Finally, we claim that:

$$\liminf_j D(\rho_j, \rho_j) \geqslant D(\rho_*, \rho_*)\ . \tag{9.82}$$

The proof of this inequality follows from Lemma 9.5. From

$$D(\rho_*, \rho_*) = \lim_{j\to\infty} D(\rho_*, \rho_j) \tag{9.83}$$

and:

$$D(\rho_*, \rho_j) \leqslant D(\rho_*, \rho_*)^{1/2} D(\rho_j, \rho_j)^{1/2}\ , \tag{9.84}$$

we get:

$$\liminf_j D(\rho_j, \rho_j)^{1/2} \geqslant D(\rho_*, \rho_*)^{1/2} \tag{9.85}$$

which proves Eq. (9.83). All in all,

$$\begin{aligned} E_{\mathrm{TF}} &= \lim_j \mathcal{E}_{\mathrm{TF}}(\rho_j) \geqslant \liminf_j c_{\mathrm{TF}} \|\rho_j\|_{5/3}^{5/3} - \lim_j \int dx\, V(x)\rho_j(x) + \liminf_j D(\rho_j, \rho_j) \\ &\geqslant \mathcal{E}_{\mathrm{TF}}(\rho_*)\ , \end{aligned} \tag{9.86}$$

which concludes the proof of the theorem. ■

To conclude, we will prove convexity of the TF energy functional, that will be important in establishing the uniqueness of the minimizer, and to understand the behavior in N of the TF ground state energy.

Lemma 9.6 (Convexity of the TF functional.)**.** *The domain $\mathcal{D}_N$ is convex. Moreover, the TF functional is strictly convex: for any $\rho_1, \rho_2 \in \mathcal{D}_N$, $\rho_1 \neq \rho_2$ and $\lambda \in (0; 1)$:*

$$\mathcal{E}_{TF}(\lambda\rho_1 + (1 - \lambda)\rho_2) < \lambda \mathcal{E}_{TF}(\rho_1) + (1 - \lambda)\mathcal{E}_{TF}(\rho_2)\ . \tag{9.87}$$

Proof. The convexity of $\mathcal{D}_N$ is a simple exercise (if ρ_1 and ρ_2 belong to $\mathcal{D}_N$ then it is easy to check that the convex combination $\rho_\lambda = \lambda\rho_1 + (1 - \lambda)\rho_2$ belongs to $\mathcal{D}_N$). Next, let us prove the convexity of the TF functional. We shall study the different contributions separately.

Consider the kinetic energy term $c_{\mathrm{TF}} \int dx\, \rho(x)^{5/3}$. This term is strictly convex, thanks to the strict convexity of the function $s \mapsto s^{5/3}$, for $s \geqslant 0$.

Consider the electron-nuclei interaction, $\int dx\, \rho(x)V(x)$. Being linear in ρ, this term is trivially convext.

Finally, consider the electron-electron interaction, $D(\rho, \rho)$. We have:

$$D(\lambda\rho_1 + (1 - \lambda)\rho_2, \lambda\rho_1 + (1 - \lambda)\rho_2) = \lambda^2 D(\rho_1, \rho_1) + (1 - \lambda)^2 D(\rho_2, \rho_2) + 2\lambda(1 - \lambda)D(\rho_1, \rho_2) \tag{9.88}$$

By Lemma 9.5, $D(\rho_1, \rho_2) \leqslant D(\rho_1, \rho_1)^{1/2} D(\rho_2, \rho_2)^{1/2} \leqslant (1/2)(D(\rho_1, \rho_1) + D(\rho_2, \rho_2))$. Hence,

$$\begin{aligned} D(\lambda\rho_1 + (1-\lambda)\rho_2, \lambda\rho_1 + (1-\lambda)\rho_2) &\leqslant \lambda^2 D(\rho_1, \rho_1) + (1-\lambda)^2 D(\rho_2, \rho_2) \\ &\quad + \lambda(1-\lambda)\Big(D(\rho_1, \rho_1) + D(\rho_2, \rho_2)\Big) \\ &\leqslant \lambda D(\rho_1, \rho_1) + (1-\lambda) D(\rho_2, \rho_2) \ . \end{aligned} \tag{9.89}$$

This proves convexity of the electron-electron interaction, and concludes the proof of convexity of $\mathcal{E}_{\mathrm{TF}}(\rho)$. ∎

Uniqueness of the minimizer is an immediate consequence of strict convexity.

Corollary 9.7 (Uniqueness of the minimizer.)**.** *Let ρ_1, ρ_2 be two minimizers of $\mathcal{E}_{TF}(\rho)$ in $\mathcal{D}_N$. Then, $\rho_1 = \rho_2$.*

Proof. Suppose $\rho_1 \neq \rho_2$. By convexity of $\mathcal{D}_N$, $\rho_\lambda = \lambda\rho_1 + (1-\lambda)\rho_2 \in \mathcal{D}_N$, for $\lambda \in (0;1)$. By convexity of the TF functional:

$$\mathcal{E}_{\mathrm{TF}}(\rho_\lambda) < \lambda\mathcal{E}_{\mathrm{TF}}(\rho_1) + (1-\lambda)\mathcal{E}_{\mathrm{TF}}(\rho_2) = \lambda E_N^{\mathrm{TF}} + (1-\lambda)E_N^{\mathrm{TF}} \equiv E_N^{\mathrm{TF}} \ . \tag{9.90}$$

But this is absurd, since E_N^{TF} is the smallest energy that can be reached in $\mathcal{D}_N$. Hence $\rho_1 = \rho_2$. ∎

9.4.4 Ionization in TF theory

In this section we shall investigate the behavior of the TF energy as a function of the number of particles N. In particular, we would like to understand under which conditions the ionization energy is positive: $E_{N+1}^{\mathrm{TF}} < E_N^{\mathrm{TF}}$. As we shall see, the validity of this inequality is related to whether the minimizer in $\mathcal{D}_N$ is actually in $\mathcal{F}_N$. We will start from the following lower bound on the TF energy, that improves on (9.70). The bound shows that the energy cannot be arbitrarily negative as N increases.

Theorem 9.8. *There exists a universal constant $C > 0$ such that, for all $\rho \in \mathcal{D}_N$:*

$$\mathcal{E}_{TF}(\rho) \geqslant -C Z_{tot}^{5/3} \Big(\sum_{j=1}^{K} Z_j^2\Big)^{1/3} \ . \tag{9.91}$$

The proof of this theorem is based on the following important result, see [3] for a proof.

Theorem 9.9 (Newton's theorem)**.** *Let μ be a rotation invariant measure on $\mathbb{R}^3$. Then:*

$$\phi(x) := \int_{\mathbb{R}^3} \mu(dx) \frac{1}{|x-y|} = \frac{1}{|x|}\int_{|y|<|x|} \mu(dx) + \int_{|y|>|x|} \frac{1}{|y|}\mu(dx) \ . \tag{9.92}$$

If one thinks of μ as describing a charge distribution, the function $\phi(x)$ has the interpretation of electric potential generated by μ. As a consequence, this theorem shows that spherically symmetric charged objects are equivalent to pointlike charges. Another important consequence of this result is that the electric potential generated by a uniformly charged sphere is *constant* inside the sphere.

Proof. (of Theorem 9.8.) The N-dependence of the nonoptimal lower bound (9.70) came from a naive control of the tail of the Coulomb attraction between the nuclei and the electrons. Here, we will control the growth in N of this energetic contribution with the *positive* mutual Coulomb repulsion of the electrons.

To begin, we write:

$$V(x) = V_<(x) + V_>(x) \ , \tag{9.93}$$

where, for $R > 0$ to be chosen later:

$$V_>(x) = \sum_{j=1}^{K} Z_j \min\Big\{\frac{1}{|x-R_j|}, \frac{1}{R}\Big\} \ . \tag{9.94}$$

The function $V_>(x)$ captures the long range contribution to the electron-nuclei electrostatic interaction, while $V_<(x)$ takes into account the singularity. By Newton's theorem, $Z_j \min\left\{\frac{1}{|x-R_j|}, \frac{1}{R}\right\}$ is the electrostatic potential generated by a uniformly charged sphere, centered in R_j, with radius R:

$$Z_j \min\left\{\frac{1}{|x-R_j|}, \frac{1}{R}\right\} = \int \mu_j(dx)\, \frac{1}{|x-y|}\ , \quad \mu_j(x) = \frac{Z_j}{4\pi R^2}\delta(|x-R_j| - R)\ . \tag{9.95}$$

Therefore,

$$V_>(x) = \int \mu(dx)\, \frac{1}{|x-y|}\ , \qquad \mu(x) = \sum_{j=1}^{K} \mu_j(x)\ . \tag{9.96}$$

Hence:

$$\int dx\, V_>(x)\rho(x) = \int dxdy\, \mu(dy)\rho(x)\frac{1}{|x-y|} \equiv 2D(\mu,\rho)\ , \tag{9.97}$$

where, for two measures μ_1, μ_2, not necessarily absolutely continuous:

$$D(\mu_1,\mu_2) = \frac{1}{2}\int \mu_1(dx)\mu_2(dy)\, \frac{1}{|x-y|}\ . \tag{9.98}$$

We then rewrite the TF energy functional as:

$$\begin{aligned}
\mathcal{E}_{\mathrm{TF}}(\rho) &= c_{\mathrm{TF}}\|\rho\|_{5/3}^{5/3} - \int dx\, V_<(x)\rho(x) - 2D(\mu,\rho) + D(\rho,\rho) + U \\
&= c_{\mathrm{TF}}\|\rho\|_{5/3}^{5/3} - \int dx\, V_<(x)\rho(x) + D(\rho-\mu,\rho-\mu) - D(\mu,\mu) + U\ .
\end{aligned} \tag{9.99}$$

The next crucial remark is that $D(\rho-\mu,\rho-\mu)$, the electrostatic interaction of the net charge distribution $\rho-\mu$, is *positive*: $D(\rho-\mu,\rho-\mu) \geqslant 0$. The proof of this fact follows again from the representation of the Coulomb interaction as in Eq. (9.67). In fact, setting $\nu = \rho - \mu$:

$$\begin{aligned}
D(\nu,\nu) &= \frac{1}{2}\int \nu(dx)\nu(dy)\frac{1}{|x-y|} = \int \nu(dx)\nu(dy)\int_0^\infty dt\, t^3 \int dz\, h_t(x-z)h_t(y-z) \\
&= \int_0^\infty dt\, t^3 \int dz\, (\nu * h_t)(z)^2 \geqslant 0
\end{aligned} \tag{9.100}$$

where in the last step we exchanged integrations thanks to Fubini's theorem. Using this fact, we can bound from below the TF energy as:

$$\mathcal{E}_{\mathrm{TF}}(\rho) \geqslant c_{\mathrm{TF}}\|\rho\|_{5/3}^{5/3} - \int dx\, V_<(x)\rho(x) - D(\mu,\mu) + U\ . \tag{9.101}$$

Next, let us estimate the energetic contribution due to $V_<$. We have:

$$\begin{aligned}
V_<(x) = V(x) - V_>(x) &= \sum_{j=1}^{K} Z_j\Big(\frac{1}{|x-R_j|} - \min\Big\{\frac{1}{|x-R_j|}, \frac{1}{R}\Big\}\Big) \\
&= \sum_{j=1}^{K} Z_j\Big(\frac{1}{|x-R_j|} - \frac{1}{R}\Big)\chi(|x-R_j| \leqslant R)\ .
\end{aligned} \tag{9.102}$$

Therefore, by Hölder inequality:

$$\begin{aligned}
\int dx\, \rho(x)V_<(x) &\leqslant \sum_{j=1}^{K} Z_j \int dx\, \frac{1}{|x-R_j|}\rho(x)\chi(|x-R_j| \leqslant R) \\
&\leqslant \sum_j Z_j\|\rho\|_{5/3}\Big\|\frac{\chi(|\cdot| \leqslant 1)}{|\cdot|}\Big\|_{5/2} \leqslant CR^{1/5}\sum_j Z_j\|\rho\|_{5/3}\ .
\end{aligned} \tag{9.103}$$

Finally, let us consider the $D(\mu,\mu)$ term. We have:

$$
\begin{aligned}
D(\mu,\mu) &= \frac{1}{2}\int \mu(dx)\mu(dy)\,\frac{1}{|x-y|} \\
&= \frac{1}{2}\int \mu(dx)V_{>}(x) \\
&= \frac{1}{2}\int dx\,\sum_{j=1}^{K}\frac{Z_j}{4\pi R^2}\delta(|x-R_j|-R)\sum_{i=1}^{K}Z_i\min\Big\{\frac{1}{|x-R_i|},\frac{1}{R}\Big\} \\
&= \frac{1}{2}\sum_{i,j}\frac{Z_iZ_j}{4\pi R^2}\int dx\,\delta(|x|-R)\min\Big\{\frac{1}{|x-R_i+R_j|},\frac{1}{R}\Big\}\,. \qquad (9.104)
\end{aligned}
$$

Separating the $i=j$ terms from the $i\neq j$ terms:

$$
\begin{aligned}
D(\mu,\mu) &= \frac{1}{2}\sum_{i\neq j}\int dx\,\delta(|x|-R)\frac{1}{|x+R_i-R_j|}\frac{Z_iZ_j}{4\pi R^2} \\
&\quad+\frac{1}{2}\sum_{i}\int dx\,\delta(|x|-R)\frac{1}{|x|}\frac{Z_i^2}{4\pi R^2} \\
&\leqslant \sum_{i<j}\frac{Z_iZ_j}{|R_i-R_j|}+\frac{1}{2}\sum_i\frac{Z_i^2}{R}\equiv U+\frac{1}{2}\sum_i\frac{Z_i^2}{R}\,. \qquad (9.105)
\end{aligned}
$$

Eqs. (9.101), (9.103), (9.105) imply:

$$
\mathcal{E}_{\mathrm{TF}}(\rho)\geqslant c_{\mathrm{TF}}\|\rho\|_{5/3}^{5/3}-CZ_{\mathrm{tot}}\|\rho\|_{5/3}R^{1/5}-\frac{1}{2R}\sum_{i=1}^{K}Z_i^2\,. \qquad (9.106)
$$

The final statement, Eq. (9.91), follows optimizing over R (that is, choosing the $R>0$ that maximizes the right-hand side). ■

The next lemma is an immediate consequence of convexity and of the uniform lower bound.

Lemma 9.10. *The TF ground state energy E_N^{TF} is convex, nonincreasing and bounded below.*

Proof. Boundedness follows from Theorem 9.8. Let us prove convexity. Let ρ_1 be the minimizer in $\mathcal{D}_{N_1}$ and ρ_2 be the minimizer in $\mathcal{D}_{N_2}$. We have:

$$
\begin{aligned}
E^{\mathrm{TF}}_{\lambda N_1+(1-\lambda)N_2} &\leqslant \mathcal{E}_{\mathrm{TF}}(\lambda\rho_1+(1-\lambda)\rho_2) \qquad (9.107)\\
&\leqslant \lambda\mathcal{E}_{\mathrm{TF}}(\rho_1)+(1-\lambda)\mathcal{E}_{\mathrm{TF}}(\rho_2)=\lambda E^{\mathrm{TF}}_{N_1}+(1-\lambda)E^{\mathrm{TF}}_{N_2}\,,
\end{aligned}
$$

which proves convexity. To prove that the energy is nonincreasing in N, we simply notice that the set $\mathcal{D}_N$ grows with N, hence $\mathcal{D}_N$ can only decrease. ■

The previous result implies that the limit:

$$
\lim_{N\to\infty}E_N^{\mathrm{TF}}=E_\infty \qquad (9.108)
$$

exists. We define the critical number of particles N_{c} as:

$$
N_{\mathrm{c}}=\inf\Big\{N\mid E_N^{\mathrm{TF}}=E_\infty\Big\}\,. \qquad (9.109)
$$

Notice that we do not know yet whether $N_{\mathrm{c}}<\infty$. The next theorem characterizes the shape of E_N^{TF} as a function of N.

Theorem 9.11. *For $N\leqslant N_c$, there exists a unique minimizer on $\mathcal{E}_{TF}$ in $\mathcal{F}_N$. The function E_N^{TF} is strictly convex and decreasing in $[0,N_c]$. If $N_c<\infty$ and $N>N_c$, there is no minimizer in $\mathcal{F}_N$. The function ρ_{N_c} is the unique minimizer in $\mathcal{D}_N$. Moreover, E_N^{TF} is constant in $[N_c,\infty)$.*

Proof. Let $N \leqslant N_c$ and let ρ_* be the minimizer of $\mathcal{E}_{\mathrm{TF}}$ in $\mathcal{D}_N$. We claim that:

$$\int dx\, \rho_*(x) = N\ . \tag{9.110}$$

Suppose that $\int \rho_* = N' < N$. Then, $\rho_* \in \mathcal{D}_{N'}$, which implies that $E^{\mathrm{TF}}_{N'} = E^{\mathrm{TF}}_N$. Since E^{TF}_N is nonincreasing, $E^{\mathrm{TF}}_{\cdot}$ is constant in $[N', N]$. Also, by convexity $E^{\mathrm{TF}}_{\cdot}$ is constant for all $N'' \geqslant N'$, which implies that $N' \geqslant N_c$. This however contradicts $N' < N \leqslant N_c$. Hence, $N' = N$. The above argument also proves strict convexity.

Suppose now that $N_c < \infty$ and that $N > N_c$. Suppose that there is a minimizer in $\mathcal{F}_N$. Then, consider the trial state:

$$\frac{1}{2}\Big(\rho_{N_c} + \rho_N\Big) \tag{9.111}$$

which has $(N + N_c)/2$ particles. We have:

$$\begin{aligned} E^{\mathrm{TF}}_{N_c} = E\Big(\frac{1}{2}(N_c + N)\Big) \leqslant \mathcal{E}_{\mathrm{TF}}\Big(\frac{1}{2}(\rho_{N_c} + \rho_N)\Big) \quad &< \quad \frac{1}{2}\Big(\mathcal{E}_{\mathrm{TF}}(\rho_{N_c}) + \mathcal{E}_{\mathrm{TF}}(\rho_N)\Big) \\ &= \quad \frac{1}{2}(E^{\mathrm{TF}}_{N_c} + E^{\mathrm{TF}}_N) \\ &= \quad E^{\mathrm{TF}}_{N_c}\ . \end{aligned} \tag{9.112}$$

The first step follows from the (assumed) constant profile of E^{TF}_N for $N \geqslant N_c$; the second from the variational principle; the third from strict convexity (since $N_c < N$, $\rho_{N_c} \neq \rho_N$!); the fourth from the fact that ρ_N and ρ_{N_c} are minimizers; and the last from the fact that E^{TF}_N is constant for $N > N_c$. This gives a contradiction, and shows that there is no minimizer in $\mathcal{F}_N$ for $N > N_c$. ∎

All we are left to do is to determine the value of N_c. To do this, we shall use that the TF minimizer satisfies a self-consistent equation, called the TF equation.

Theorem 9.12. *Let $N \leqslant N_c$. Then, there exists $\mu \geqslant 0$ such that the unique minimizer $\rho_N \in \mathcal{F}_N$ satisfies the equation:*

$$\gamma \rho_N^{2/3}(x) = \Big(V(x) - \frac{1}{|\cdot|} * \rho_N(x) - \mu\Big)_+\ , \qquad (\gamma = \frac{5}{3}c_{TF})\ . \tag{9.113}$$

For $N = N_c$, $\mu = 0$.

Remark 9.13. *Eq. (9.113) is called the Thomas-Fermi equation. One can actually prove that solutions of the TF equation in $L^1 \cap L^{5/3}$ are minimizers of the TF functional. The number of particles is determined by the chemical potential μ.*

Proof. Let ρ_N be the minimizer in $\mathcal{F}_N$. For any $\delta > 0$, for any bounded function f such that:

$$\int dx\, \chi(\rho_N(x) \geqslant \delta) f(x) = 0\ , \tag{9.114}$$

define:

$$\rho_\varepsilon = \rho_N + \varepsilon f(x) \chi(\rho_N(x) \geqslant \delta)\ . \tag{9.115}$$

For ε small enough (dependent of δ), $\rho_\varepsilon \geqslant 0$. Also, the assumption (9.114) implies that $\|\rho_\varepsilon\|_1 = \|\rho_N\|_1 = N$. Finally, since f is bounded and $\chi(\rho_N(x) \geqslant \delta)$ is supported on a bounded set, $\rho_\varepsilon \in L^{5/3}$. Hence, $\rho_\varepsilon \in \mathcal{F}_N$, and so:

$$\mathcal{E}_{\mathrm{TF}}(\rho_\varepsilon) \geqslant \mathcal{E}_{\mathrm{TF}}(\rho_N)\ . \tag{9.116}$$

Together with differentiability in a neighbourhood of $\varepsilon = 0$ (which can be easily proven), this implies:

$$0 = \frac{d}{d\varepsilon} \mathcal{E}_{\mathrm{TF}}(\rho_\varepsilon)\ |_{\varepsilon=0}\ . \tag{9.117}$$

Writing explicitly the right-hand side, one has:

$$0 = \int_{\rho_N \geqslant \delta} dx\, \Big(\gamma \rho_N^{5/3}(x) + (\rho_N * \frac{1}{|\cdot|})(x) - V(x)\Big) f(x) \tag{9.118}$$

for all bounded f such that $\int_{\rho_N(x)\geqslant\delta} dx\, f(x) = 0$. The arbitrariness of f in this class of functions implies that:

$$\gamma\rho_N^{2/3}(x) + \frac{1}{|\cdot|} * \rho_N(x) - V(x) = -\mu\;, \tag{9.119}$$

for some constant μ, and for all x such that $\rho_N(x) \geqslant \delta$. Being ρ_N nonnegative, this implies:

$$\gamma\rho_N^{2/3}(x) = \Big(V(x) - \frac{1}{|\cdot|} * \rho_N(x) - \mu\Big)_+ \tag{9.120}$$

for all x such that $\rho_N(x) > \delta$. Taking the $\delta \to 0$ limit, we found that $\rho_N(x)$ satisfies the TF equation for all x such that $\rho_N(x) > 0$. Let us now explore the region $\{x \mid \rho_N(x) = 0\}$. To this end, consider the function:

$$\rho_\varepsilon(x) = \rho_N(x) + \varepsilon f(x)\;, \tag{9.121}$$

for $\varepsilon \geqslant 0$, $f \in L^{5/3} \cap L^1$, $f \geqslant 0$ on $\{x \mid \rho_N(x) = 0\}$ and $\int dx\, f(x) = 0$. The function ρ_ε belongs to $\mathcal{F}_N$. Hence, $\mathcal{E}_{\mathrm{TF}}(\rho_\varepsilon) \geqslant \mathcal{E}_{\mathrm{TF}}(\rho_N)$ for $\varepsilon \geqslant 0$; taking the right derivative, one gets:

$$0 \leqslant \int \Big(\gamma\rho_N(x)^{2/3} - V(x) + \frac{1}{|\cdot|} * \rho_N(x)\Big) f(x)\, dx\;. \tag{9.122}$$

Next, we split the integral in the right-hand side as:

$$\int dx\,(\ldots) = \int_{\rho_N(x)=0} dx\,(\ldots) + \int_{\rho_N(x)>0} dx\,(\ldots)\;; \tag{9.123}$$

using the previous result for the region $\rho_N(x) > 0$, we have:

$$\begin{aligned} 0 \;&\leqslant\; \int_{\rho_N(x)=0} dx\,\Big(\gamma\rho_N(x)^{2/3} - V(x) + \frac{1}{|\cdot|} * \rho_N(x)\Big) f(x) - \mu \int_{\rho_N(x)>0} dx\, f(x) \\ &=\; \int_{\rho_N(x)=0} dx\,\Big(\gamma\rho_N(x)^{2/3} - V(x) + \frac{1}{|\cdot|} * \rho_N(x) + \mu\Big) f(x) \end{aligned} \tag{9.124}$$

where in the last step we used that $\int_{\rho_N(x)=0} dx\, f(x) = -\int_{\rho_N(x)>0} dx\, f(x)$. The arbitrariness of f implies that:

$$-\mu + V(x) - \frac{1}{|\cdot|}\rho_N(x) \leqslant 0 \qquad \text{on } x \text{ s.t. } \rho_N(x) = 0. \tag{9.125}$$

Taking the positive part:

$$0 = \Big(-\mu + V(x) - \frac{1}{|\cdot|}\rho_N(x)\Big)_+ \qquad \text{on } x \text{ s.t. } \rho_N(x) = 0. \tag{9.126}$$

Equivalently,

$$\gamma\rho_N^{2/3}(x) = \Big(-\mu + V(x) - \frac{1}{|\cdot|}\rho_N(x)\Big)_+ \qquad \text{on } x \text{ s.t. } \rho_N(x) = 0. \tag{9.127}$$

Eqs. (9.127), (9.120) give the TF equation for all values of x. To conclude, let us comment on the chemical potential μ. Since $\rho_N(x)$, $V(x)$ and $(\frac{1}{|\cdot|} * \rho_N)(x)$ decay at infinity, the TF equation implies that $\mu \geqslant 0$ (otherwise the right-hand side would be nonzero for $|x| \to \infty$, which would contradict decay for $\rho_N^{2/3}$). Let us prove that for $N = N_{\mathrm{c}}$ one as $\mu = 0$.

We repeat the trial state argument, with $\rho_\varepsilon = \rho_{N_{\mathrm{c}}} + \varepsilon f$. We only assume that $\varepsilon \geqslant 0$, $f \geqslant 0$ and that $f \in L^1 \cap L^{5/3}$. In this way, the number of particles is *not* N_{c}; this is however not important, since $\rho_{N_{\mathrm{c}}}$ is the density with the smallest energy. Hence, one has $\mathcal{E}_{\mathrm{TF}}(\rho_\varepsilon) \geqslant \mathcal{E}_{\mathrm{TF}}(\rho_{N_{\mathrm{c}}})$, for $\varepsilon \geqslant 0$. Taking the right derivative and proceeding as above:

$$\gamma\rho_{N_{\mathrm{c}}}^{2/3}(x) \geqslant \Big(V(x) - \rho * V(x)\Big)_+\;; \tag{9.128}$$

by the TF equation:

$$\Big(V(x) - \rho * V(x) - \mu\Big)_+ \geqslant \Big(V(x) - \rho * V(x)\Big)_+ \ . \tag{9.129}$$

Notice that the function $V(x) - |\cdot|^{-1} * \rho_{N_c}(x)$ has to be positive for some x, otherwise the TF equation would prove that $\rho_{N_c} = 0$. The assumption $\rho_{N_c} \in L^1 \cap L^{5/3}$ implies that $|\cdot| * \rho_{N_c}(x)$ is bounded, and $V(x) \to +\infty$ in proximity of the nuclei; hence $V(x) - |\cdot|^{-1} * \rho_{N_c}(x)$ is positive in a neighbourhood of the nuclei. For these values of x, Eq. (9.129) implies that $\mu = 0$. This concludes the proof of Theorem 9.12. ■

The function:

$$\phi(x) = V(x) - \frac{1}{|\cdot|} * \rho_N(x) \ , \tag{9.130}$$

is called the Thomas-Fermi potential. It describes the net electrostatic potential generated by the nuclei plus the electrons. In terms of this function the TF equation reads:

$$\gamma \rho_N^{2/3}(x) = \Big(\phi(x) - \mu\Big)_+ \ . \tag{9.131}$$

Therefore, the TF minimizer is supported for the values of x such that $\phi(x) \geqslant \mu$. This is certainly true if x is close enough to one of the nuclei, since $V(x) \to \infty$ there; hence, the TF equation is telling us that the electrons are localized close to the nuclei, as expected. The next proposition is an important property of the TF functional, that will be crucial to compute the critical number of particles N_c.

Proposition 9.14. *Let $N \leqslant N_c$. Then:*

$$\phi(x) \geqslant 0 \ . \tag{9.132}$$

Proof. Let Δ be the distributional Laplacian. Then:

$$\Delta \frac{1}{|\cdot|} = -\delta(\cdot) \ , \tag{9.133}$$

with $\delta(\cdot)$ the Dirac's delta. Hence, away from the nuclei:

$$\Delta\phi(x) = \rho_N(x) \ . \tag{9.134}$$

Now, using the TF equation we can rewrite the density as a function of ϕ as:

$$\rho_N = \Big(\gamma^{-1}\Big(V(x) - \frac{1}{|\cdot|} * \rho_N(x) - \mu\Big)_+\Big)^{3/2} \equiv \gamma^{-3/2}(\phi(x) - \mu)_+^{3/2} \ . \tag{9.135}$$

Therefore, the TF equation is equivalent to the following PDE:

$$\Delta\phi(x) = \gamma^{-3/2}(\phi(x) - \mu)_+^{3/2} \ . \tag{9.136}$$

Let us consider the set:

$$A = \{x \in \mathbb{R}^3 \mid \phi(x) < 0\} \ . \tag{9.137}$$

Notice that the nuclei do not belong to such set, since $V(x) \to \infty$ there and $\rho_N * |\cdot|^{-1}$ is bounded. Away from the nuclei, the function $\phi(x)$ is continuous, and hence A is open. By continuity the function $\phi(x)$ vanishes on the boundary of A. Notice that the set A need not be compact; nevertheless, the function $\phi(x)$ is also vanishing at infinity, since $|\cdot|^{-1} * \rho_N(x) \to 0$ as $|x| \to \infty$, see Chapter 2 of [3]. Hence, $\phi(x)$ vanishes on the boundary of A, and at infinity. In A, the function $-\phi$ is harmonic:

$$\Delta(-\phi)(x) = 0 \qquad \text{for all } x \in A. \tag{9.138}$$

By the maximum principle for harmonic functions [3, 1], the function $-\phi$ reaches its maximum on the boundary of A (or at infinity, if A is unbouded). (Strictly speaking, the maximum principle holds for open and connected domains; in case A is not connected, we split A into connected components, and we repeat the argument in each component.)

Hence $-\phi(x) \leqslant 0$ for all $x \in A$, which implies that $\phi(x) = 0$ in A. That is, A is the empty set. This proves that $\phi(x) \geqslant 0$ for all x. ■

To conclude the section, we compute the critical number of particles N_c.

Theorem 9.15. $N_c = Z_{tot}$.

Proof. The starting point is Newton's theorem, for a uniformly distributed charge on a sphere of radius r:

$$\frac{1}{4\pi r^2}\int_{|\omega|=r} d\omega\, \frac{1}{|\omega - y|} = \min\left\{\frac{1}{r}, \frac{1}{|y|}\right\} . \tag{9.139}$$

We then compute:

$$\begin{aligned}\frac{1}{4\pi r^2}\int_{|\omega|=r} d\omega\, \phi(\omega) &= \sum_{j=1}^{K} Z_j \frac{1}{4\pi r^2}\int_{|\omega|=r} d\omega\, \frac{1}{|\omega - R_j|} - \frac{1}{4\pi r^2}\int_{|\omega|=r} d\omega \left(\frac{1}{|\cdot|} * \rho_N\right)(\omega) \\ &= \sum_{j=1}^{K} Z_j \min\left\{\frac{1}{r}, \frac{1}{|R_j|}\right\} - \frac{1}{4\pi r^2}\int dy\, \rho_N(y) \min\left\{\frac{1}{|y|}, \frac{1}{r}\right\} \\ &\geqslant 0 . \end{aligned} \tag{9.140}$$

where the last inequality follows from Proposition 9.14. Taking $r \geqslant |R_j|$ for all j, we have:

$$\frac{Z_\mathrm{tot}}{r} - \int_{|y|\leqslant r} dy\, \min\left\{\frac{1}{r}, \frac{1}{|y|}\right\}\rho_N(y) \tag{9.141}$$

which implies:

$$Z_\mathrm{tot} \geqslant \int_{|y|\leqslant r} dy\, \rho_N(y) . \tag{9.142}$$

Taking the $r \to \infty$ limit:

$$Z_\mathrm{tot} \geqslant N \Rightarrow Z_\mathrm{tot} \geqslant N_\mathrm{c} . \tag{9.143}$$

To conclude the proof, suppose now that $Z_\mathrm{tot} > N_\mathrm{c}$. Let ρ_{N_c} be the minimizer with N_c particles. By the TF equation:

$$\begin{aligned}\gamma \rho_{N_\mathrm{c}}^{2/3}(x) &= \left(V(x) - \frac{1}{|\cdot|} * \rho_{N_\mathrm{c}}(x)\right)_+ \\ &= V(x) - \frac{1}{|\cdot|} * \rho_{N_\mathrm{c}}(x) \end{aligned} \tag{9.144}$$

where in the last step we used again the positivity of the TF potential. Averaging over a sphere of radius r we get:

$$\frac{\gamma}{4\pi r^2}\int_{|\omega|=r} d\omega\, \rho_{N_\mathrm{c}}^{2/3}(\omega) = \frac{1}{4\pi r^2}\int_{|\omega|=r} d\omega\, \phi(\omega) . \tag{9.145}$$

On one hand, by concavity of $s \mapsto s^{2/3}$:

$$\frac{1}{4\pi r^2}\int_{|\omega|=r} d\omega\, \rho_{N_\mathrm{c}}(\omega)^{2/3} \leqslant \left(\frac{1}{4\pi r^2}\int_{|\omega|=r} d\omega\, \rho_{N_\mathrm{c}}(\omega)\right)^{2/3} ; \tag{9.146}$$

on the other hand, by Newton's theorem, taking $r \geqslant |R_j|$ for all j:

$$\frac{1}{4\pi r^2}\int d\omega\, \phi(\omega) = \frac{Z_\mathrm{tot}}{r} - \int dy\, \min\left\{\frac{1}{r}, \frac{1}{|y|}\right\}\rho_{N_\mathrm{c}}(y) \geqslant \frac{Z_\mathrm{tot}}{r} - \int dy\, \frac{1}{r}\rho_{N_\mathrm{c}}(y) = \frac{Z_\mathrm{tot} - N_\mathrm{c}}{r} . \tag{9.147}$$

All together, for $r \geqslant |R_j|$:

$$\left(\frac{1}{4\pi r^2}\int_{|\omega|=r} d\omega\, \rho_{N_\mathrm{c}}(\omega)\right)^{2/3} \geqslant \frac{Z_\mathrm{tot} - N_\mathrm{c}}{\gamma r} \geqslant \frac{C}{r} \tag{9.148}$$

for some $C > 0$, since by assumption $Z_{\text{tot}} > N_{\text{c}}$. Now, let rewrite the number of particles N_{c} in spherical coordinates:

$$
\begin{aligned}
N_{\text{c}} = \int dx\, \rho_{N_{\text{c}}}(x) &= \int_0^\infty dr\, r^2 \int_{|\omega|=1} d\omega\, \rho_{N_{\text{c}}}(r\omega) \\
&= \int_0^\infty dr\, r^2 \frac{1}{r^2} \int_{|\omega|=r} d\omega\, \rho_{N_{\text{c}}}(\omega)
\end{aligned}
\tag{9.149}
$$

where in the last step we performed a change of variables. By the lower bound (9.148):

$$
N_{\text{c}} \geqslant \int_{\max\{|R_j|\}}^\infty dr\, r^2 \frac{C}{r^{3/2}} = +\infty \;, \tag{9.150}
$$

which contradicts $N_{\text{c}} < Z_{\text{tot}}$. Hence, $N_{\text{c}} = Z_{\text{tot}}$. ∎

9.4.5 Scaling properties of the TF energy

One of the advantages of TF theory is that it allows to obtain a very simple prediction for the energy of neutral atoms ($K = 1$, $Z = N$). As we shall see, this prediction becomes exact as $N \to \infty$.

Proposition 9.16. *Let $K = 1$. We have $\rho_Z(x) = \frac{Z^2}{\gamma^3}\overline{\rho}(Z^{1/3}x/\gamma)$, with $\overline{\rho}$ the minimizer of:*

$$
e_{TF}(\rho) = \frac{3}{5}\int dx\, \rho(x)^{5/3} - \int dx\, \rho(x)\frac{1}{|x|} + D(\rho,\rho) \tag{9.151}
$$

on $\mathcal{F}_1$. Oe has:

$$
E_Z^{TF} = (e_0/\gamma)Z^{7/3} \;, \tag{9.152}
$$

with e_0 the ground state energy of $e_{TF}(\rho)$ on $\mathcal{F}_1$. Numerically, $e_0 \simeq -3.678$.

Proof. For a given $\ell > 0$, let us define the corresponding function $\overline{\rho}$ as:

$$
\rho_Z(x) = Z\ell^3\overline{\rho}(Z^{1/3}\ell x) \;. \tag{9.153}
$$

Notice that $\overline{\rho} \in L^1 \cap L^{5/3}$, and $\|\overline{\rho}\|_1 = 1$. To find the correct value of ℓ, let us rewrite the energy of ρ_Z as:

$$
E_Z^{\text{TF}} = \gamma Z^{5/3}\ell^2 \frac{3}{5}\int dx\, \overline{\rho}(x)^{5/3} - Z^2\ell \int dx\, \overline{\rho}(x)\frac{1}{|x|} + Z^2\ell D(\overline{\rho},\overline{\rho}) \;. \tag{9.154}
$$

The final claim follows setting $\gamma Z^{5/3}\ell^2 = Z^2\ell$, that is $\ell = Z^{1/3}/\gamma$. ∎

Remark 9.17. *The above proposition shows that the TF density profile has amplitude $O(Z^2)$, and that it varies on scale $Z^{-1/3}$. In other words, TF theory shows that the TF minimizer is concentrated in a region of diameter $O(Z^{-1/3})$ around the position of the nucleus. The energy of a neutral atom takes a particularly simple form, Eq. (9.152); remarkably, in the $N \simeq Z \to \infty$ limit, this prediction becomes quantitatively correct.*

9.5 Stability of matter of the second kind via TF theory

9.5.1 The no-binding theorem

One of the limitations of TF theory is that it does not predict the existence of molecules: this is the content of the *no-binding theorem*, due to Teller in '62 and proven by Lieb and Simon in '77.

Suppose we are given a system of nuclei. Let us partition them in two sets, A and B. We define the electrostatic potential of the nuclei in the set $\sharp = A, B$ as:

$$
V_\sharp(x) = \sum_{j\in\sharp}\frac{Z_j}{|x-R_j|} = \int d\mu_\sharp(y)\frac{1}{|x-y|} \;. \tag{9.155}
$$

The TF energy of the system corresponding to the nuclei in $\sharp$ is:

$$\mathcal{E}^{\mathrm{TF}}_{\sharp}(\rho) = c_{\mathrm{TF}} \int dx\, \rho(x)^{5/3} - \int dx\, V_{\sharp}(x)\rho(x) + D(\rho,\rho) + \sum_{\substack{k<j\\ k,j\in\sharp}} \frac{Z_k Z_j}{|R_i - R_j|} \,. \tag{9.156}$$

We denote by $E^{\mathrm{TF}}_{\sharp,N}$ the corresponding ground state energy: $E^{\mathrm{TF}}_{\sharp,N} = \inf_{\rho\in\mathcal{D}_N} \mathcal{E}^{\mathrm{TF}}_{\sharp,N}(\rho)$.

Theorem 9.18 (No binding theorem.)**.** *Suppose $N \leqslant Z_{tot} = \sum_{j=1}^{K} Z_j$. Then:*

$$\min\{E^{TF}_{A,N_1} + E^{TF}_{B,N_2} \mid N_1 + N_2 = N\} \leqslant E^{TF}_{N} \,. \tag{9.157}$$

We can think of $E^{\mathrm{TF}}_{A,N_1} + E^{\mathrm{TF}}_{B,N_2}$ as the energy of the system after the sets A and B have been pushed infinitely far away from each other, so that their mutual interaction is negligible. Consider the configuration of N_1 and N_2 particles in the sets A and B such that the sum of the two energies is minimal. The theorem is telling us that there is no energetic gain in bringing the two systems close together. Of course, the argument can be iterated for A and B separately, and so on.

The conclusion is that the energetic gain due to the formation of a molecule (a stable system composed by more than one nucleus) is missed by TF theory. As we shall see later, this limitation of TF theory will be used in a positive way, to give a very simple proof of stability of matter of the second kind. But first, let us prove the no binding theorem.

A crucial role in the proof we shall present is due to the following lemma, due to Baxter.

Lemma 9.19. *Let $\rho \geqslant 0$, $\rho \in L^1(\mathbb{R}^3) \cap L^p(\mathbb{R}^3)$, with $p > 3/2$. There exists g such that $0 \leqslant g \leqslant \rho$ such that:*

$$(\frac{1}{|\cdot|} * g)(x) = V_A(x) \qquad \textit{if } \rho(x) > g(x) \geqslant 0. \tag{9.158}$$

Moreover,

$$(\frac{1}{|\cdot|} * g)(x) \leqslant V_A(x) \qquad \textit{if } \rho(x) = g(x). \tag{9.159}$$

Proof. The proof is based on calculus of variations. Let us define the functional:

$$I(g) = D(g,g) - \int dxdy\, g(x) \frac{\mu_A(y)}{|x-y|} \,. \tag{9.160}$$

The functional is well defined on $\mathcal{D}_\rho = \{g \mid 0 \leqslant g \leqslant \rho\}$, and it is bounded below. Let $\{g_j\}$ be a minimizing sequence in $\mathcal{D}_\rho$. Then, $\|g_j\|_p \leqslant \|\rho\|_p \leqslant C$ for $p > 3/2$. This means that there exists a weakly convergent subsequence $g \in \mathcal{D}_\rho$ in L^p, that we shall still denote by g_j with a slight abuse of notation. We claim that:

$$\liminf_j I(g_j) \geqslant I(g) \,. \tag{9.161}$$

This shows that g is a minimizer of I. The proof of (9.161) follows from $\liminf_j D(g_j, g_j) \geqslant D(g,g)$, Eq. (9.83), and from $\lim_j D(g_j, \mu_A) = D(g, \mu_A)$, Eq. (9.77).

To prove Eqs. (9.158), (9.159) we shall use a trial state argument. Let us first explore the region $x : 0 < g(x) < \rho(x)$. Consider:

$$g_\varepsilon(x) = g(x) + \varepsilon f(x) \chi(\delta \leqslant g(x) \leqslant \rho(x) - \delta) \,, \tag{9.162}$$

with f bounded and $\delta > 0$. Clearly, $g_\varepsilon \in \mathcal{D}_\rho$ for $|\varepsilon|$ small enough. Hence,

$$I(g_\varepsilon) \geqslant I(g) \,. \tag{9.163}$$

Taking the derivative with respect to ε (it can be proven that the function is differentiable):

$$0 = \frac{d}{d\varepsilon} I(g_\varepsilon) \mid_{\varepsilon=0} \Rightarrow 0 = \int_{\delta \leqslant g(x) \leqslant \rho(x)-\delta} dx\, f(x) \Big((\frac{1}{|\cdot|} * g)(x) - V_A(x) \Big) \,. \tag{9.164}$$

By arbitrariness of f, taking the $\delta \to 0^+$ limit:

$$(\frac{1}{|\cdot|} * g)(x) = V_A(x) \qquad \text{if } 0 < g(x) < \rho(x). \tag{9.165}$$

Let us now explore the region $g(x) = \rho(x)$. Consider the trial state:

$$g_\varepsilon(x) = g(x) + \varepsilon f(x)\chi(\max\{\rho(x) - \delta, \delta\} \leqslant g(x) \leqslant \rho(x)) \ , \tag{9.166}$$

for $\varepsilon \leqslant 0$, $f \geqslant 0$. Taking the left derivative:

$$0 \geqslant \int_{\max\{\rho(x)-\delta,\delta\}\leqslant g(x)\leqslant\rho(x)} dx\, f(x)\Big((\frac{1}{|\cdot|} * g)(x) - V_A(x)\Big) \ . \tag{9.167}$$

Again by arbitrariness of f, for $\delta \to 0^+$:

$$(\frac{1}{|\cdot|} * g)(x) \leqslant V_A(x) \qquad \text{if } g(x) = \rho(x). \tag{9.168}$$

Finally, let us consider the region $g(x) = 0$. Let us introduce the trial state:

$$g_\varepsilon(x) = g(x) + \varepsilon f(x)\chi(0 \leqslant g(x) \leqslant \min\{\delta, \rho(x) - \delta\}) \ , \tag{9.169}$$

for $\varepsilon \geqslant 0$, $f \geqslant 0$. Taking the right derivative:

$$0 \leqslant \int_{0\leqslant g(x)\leqslant\min\{\delta,\rho(x)-\delta\}} dx\, f(x)\Big((\frac{1}{|\cdot|} * g)(x) - V_A(x)\Big) \tag{9.170}$$

which implies, as $\delta \to 0^+$:

$$(\frac{1}{|\cdot|} * g)(x) \geqslant V_A(x) \qquad \text{if } g(x) = 0. \tag{9.171}$$

We are left with excluding the case $(\frac{1}{|\cdot|} * g)(x) > V_A(x)$. To this end, consider the set:

$$P = \Big\{x \mid (\frac{1}{|\cdot|} * g)(x) \geqslant V_A(x)\Big\} \ . \tag{9.172}$$

Clearly, $P \subset \{x \mid g(x) = 0\}$. Notice that the points R_j, the center of the nuclei, do not belong to P: this is due to the fact that $V_A(x) = +\infty$ there, and $\frac{1}{|\cdot|} * g)(x)$ is bounded. Away from these points, the function

$$(\frac{1}{|\cdot|} * g)(x) - V_A(x) \tag{9.173}$$

is continuous. Hence, the set P is open, and $(\frac{1}{|\cdot|} * g)(x) - V_A(x) = 0$ on ∂P. Moreover,

$$\Delta_x\Big((\frac{1}{|\cdot|} * g)(x) - V_A(x)\Big) = -g(x) + \mu_A(x) = 0 \qquad \forall x \in P \ , \tag{9.174}$$

since $x \neq R_j$ and $P \subset \{x \mid g(x) = 0\}$. Therefore, function $(\frac{1}{|\cdot|} * g)(x) - V_A(x)$ is harmonic in P. By the maximum principle, $(\frac{1}{|\cdot|} * g)(x) - V_A(x) = 0$, which proves that P is empty. ∎

We are now ready to prove the no-binding theorem, Theorem 9.18.

Proof. (of Theorem 9.18.) Let $\rho \equiv \rho_N$ be the minimizer of $\mathcal{E}^{\mathrm{TF}}$ in $\mathcal{F}_N$, for $N \leqslant Z_{\mathrm{tot}}$. To prove the theorem, it is enough to show that there exists g, h such that $0 \leqslant g, h \leqslant \rho$ such that $g + h = \rho$ and:

$$\mathcal{E}_A^{\mathrm{TF}}(g) + \mathcal{E}_B^{\mathrm{TF}}(h) \leqslant \mathcal{E}^{\mathrm{TF}}(\rho) \ . \tag{9.175}$$

Consider the kinetic energies. Since $(a + b)^{5/3} \geqslant a^{5/3} + b^{5/3}$ for all $a, b \geqslant 0$, we immediately get:

$$\int dx\, g(x)^{5/3} + \int dx\, h(x)^{5/3} \leqslant \int dx\, (g(x) + h(x))^{5/3} \ . \tag{9.176}$$

Let us now study the interaction. In view of Eq. (9.176), to conclude the proof it is enough to show that:

$$\begin{aligned}
&-2D(g,\mu_A) + D(g,g) + \sum_{\substack{k<j\\ k,j\in A}} \frac{Z_j Z_k}{|R_j - R_k|} \\
&\qquad -2D(h,\mu_B) + D(h,h) + \sum_{\substack{k<j\\ k,j\in B}} \frac{Z_j Z_k}{|R_j - R_k|} \\
&\leqslant -2D(g+h,\mu_A+\mu_B) + D(g+h,g+h) + \sum_{k<j} \frac{Z_k Z_j}{|R_j - R_k|}\ . \qquad (9.177)
\end{aligned}$$

The inequality (9.177) can be rewritten as:

$$\begin{aligned}
0 &\leqslant -2D(g,\mu_B) - 2D(h,\mu_A) + 2D(g,h) + \sum_{\substack{k<j\\ k\in A, j\in B}} \frac{Z_k Z_j}{|R_k - R_j|} \\
&= -2D(g,\mu_B) - 2D(h,\mu_A) + 2D(g,h) + 2D(\mu_A,\mu_B) \\
&= 2D(g-\mu_A, h-\mu_B)\ . \qquad (9.178)
\end{aligned}$$

Let now now choose g, ρ to be as in Lemma 9.19. We rewrite $D(g-\mu_A, h-\mu_B)$ as:

$$\begin{aligned}
D(g-\mu_A, h-\mu_B) &= \int_{x: g(x)=\rho(x)} dx\, (h(x) - \mu_B(x)) * \Big((\frac{1}{|\cdot|} * g)(x) - V_A(x) \Big) \\
&\quad + \int_{x: g(x)<\rho(x)} dx\, (h(x) - \mu_B(x)) * \Big((\frac{1}{|\cdot|} * g)(x) - V_A(x) \Big) \\
&\equiv -\int_{x: g(x)=\rho(x)} dx\, \mu_B(x) * \Big((\frac{1}{|\cdot|} * g)(x) - V_A(x) \Big) \qquad (9.179)
\end{aligned}$$

where we used that $h(x) = 0$ if $g(x) = \rho(x)$ and that $(\frac{1}{|\cdot|} * g)(x) - V_A(x) = 0$ if $g(x) < \rho(x)$, by Lemma 9.19. Also, the same lemma implies that $(\frac{1}{|\cdot|} * g)(x) - V_A(x) \leqslant 0$ for $g(x) = \rho(x)$, hence $D(g-\mu_A, h-\mu_B) \geqslant 0$, which proves Eq. (9.177). This concludes the proof of Theorem 9.18. ∎

The next result is a simple corollary of the no-binding theorem, that will play a crucial role in the proof of stability of matter of the second kind for the many-body problem.

Corollary 9.20. *For any $\rho \in L^1 \cap L^{5/3}$, $\rho \geqslant 0$, for any $\gamma > 0$:*

$$\mathcal{E}_{TF}(\rho) \geqslant -\frac{3.678}{\gamma} \sum_{j=1}^{K} Z_j^{7/3}\ . \qquad (9.180)$$

Proof. Consider a collection of K nuclei, and separate one, say the one in R_1 with charge Z_1, from the rest: $A = \{R_1\}$ and $B = \{R_j\}_{j=2}^{K}$. By the no-binding theorem, using that $E^{\mathrm{TF}}_{\sharp,N} \geqslant E^{\mathrm{TF}}_{\sharp,Z_{\mathrm{tot}}}$:

$$\begin{aligned}
\mathcal{E}_{\mathrm{TF}}(\rho) &\geqslant E^{\mathrm{TF}}_{A,Z_1} + \inf\{\mathcal{E}^{\mathrm{TF}}_{Z_2,\ldots,Z_k}(\rho) \mid \rho \in \mathcal{F}_{Z_2+\ldots Z_K}\} \\
&= -\frac{3.678}{\gamma} Z_1^{7/3} + \inf\{\mathcal{E}^{\mathrm{TF}}_{Z_2,\ldots,Z_k}(\rho) \mid \rho \in \mathcal{F}_{Z_2+\ldots Z_K}\}\ , \qquad (9.181)
\end{aligned}$$

where in the last step we used Proposition 9.16. Iterating the argument $K-1$ times, the claim follows. ∎

9.5.2 Proof of stability of matter

As we shall see in this section, the no binding theorem of Thomas-Fermi theory can be used to proved stability of matter of the second kind for the full many-body probblem, described by the Hamiltonian $H_{N,K}(\underline{Z}, \underline{R})$ on $L^2_{\mathrm{anti}}(\mathbb{R}^{3N})$. We shall prove the following theorem.

Theorem 9.21 (Stability of matter of the second kind.). *There exists a constant $C(\underline{Z}) > 0$ such that, for all $\psi_N \in H^1_{anti}(\mathbb{R}^{3N})$, $\|\psi_N\|_2 = 1$:*

$$\langle \psi_N, H_{N,K}(\underline{Z}, \underline{R})\psi_N \rangle \geqslant -C(\underline{Z})(N + K) \; . \tag{9.182}$$

This lower bound is compatible with the fact that the ground state energy of the initial many-body problem grows linearly with the number of particles. If not, matter could not be extensive (recall the discussion in Section 9.3): splitting the system into subsystems could produce an enormous increase/decrease of the energy. The first proof of stability of matter was given by Dyson and Lenard in '67. Here we shall discuss the proof of Lieb and Thirring '77, much simpler than the original one, based on Thomas-Fermi theory and on the Lieb-Thirring kinetic energy inequality.

Theorem 9.22 (LT kinetic energy inequality.). *There exists $K > 0$ such that for any $\psi_N \in L^2_{anti}(\mathbb{R}^{3N})$:*

$$\langle \psi_N, \sum_{j=1}^{N} -\Delta_j \psi_N \rangle \geqslant K \int dx \, \rho_\psi(x)^{\frac{5}{3}} \; , \tag{9.183}$$

where $\psi_\psi(x) = N \int dx_2 \ldots dx_N \, |\psi_N(x, x_2, \ldots, x_N)|^2$ is the density associated to ψ_N.

This inequality is a consequence of another important result in quantum mechanics, the *Lieb-Thirring inequality* for sums of negative eigenvalues. Let $H = -\Delta + V$ on $L^2(\mathbb{R}^d)$ be a self-adjoint Schrödinger operator, with $V \in L^{1+d/2}(\mathbb{R}^d)$, and V satisfying the assumptions in Section 7.4 needed in order to define the eigenvalues with the min-max principles. Let E_j be the eigenvalues of H (which can be defined as in Section 7.4). Then, the Lieb-Thirring inequality states that:

$$\sum_{j: E_j \leqslant 0} |E_j| \leqslant L_d \int dx \, V(x)^{1+d/2} \; , \tag{9.184}$$

for some explicit $L_d > 0$ (see [3] for generalizations). This inequality is compatible with the semiclassical approximation for the sum of negative eigenvalues, recall the discussion of Section 8.5. Let us show how Eq. (9.184) implies the kinetic energy inequality (9.183).

Proof. (of Theorem 9.22) Let $\gamma^{(1)}_\psi$ be the reduced one-particle density matrix of ψ_N, and consider a class of Schrödinger operators $H = -\Delta + V$ with V such that (9.184) holds true. Let $H_N = \sum_i H^{(i)}$. By the definition of density matrix:

$$\langle \psi_N, H_N \psi_N \rangle = \operatorname{Tr} H \gamma^{(1)}_\psi \; . \tag{9.185}$$

Being $\gamma^{(1)}_\psi$ a nonnegative, trace-class operator, it can be written as $\gamma^{(1)}_\psi = \sum_j \lambda_j |f_j\rangle\langle f_j|$, for some orthonormal $f_j \in L^2(\mathbb{R}^d)$ and $0 \leqslant \lambda_j \leqslant 1$, due to the fact that $0 \leqslant \gamma^{(1)}_\psi \leqslant \mathbb{1}$, recall Section 9.2. Therefore:

$$\langle \psi_N, H_N \psi_N \rangle = \sum_j \lambda_j \operatorname{Tr} H P_j = \sum_{j=1}^{\infty} \lambda_j \langle f_j, H f_j \rangle \; . \tag{9.186}$$

Clearly, $\langle f_0, H f_0 \rangle \geqslant E_0$, the ground state of H. Hence:

$$\langle \psi_N, H_N \psi_N \rangle \geqslant E_0 + \sum_{j=2}^{\infty} \lambda_j \langle f_j, H f_j \rangle \; . \tag{9.187}$$

Being f_1 orthogonal to f_0, $\langle f_1, H f_1 \rangle \geqslant E_1$, the first excited state of H. The argument can be iterated for all negative eigenvalues; we have:

$$\langle \psi_N, H_N \psi_N \rangle \geqslant \sum_{j: E_j \leqslant 0} E_j + \sum_{j}^{*} \lambda_j \langle f_j, H f_j \rangle \tag{9.188}$$

where the asterisk denotes that f_j are orthogonal to all eigenfunctions ϕ_i of the negative eigenvalues. Therefore, by the variational characterization of eigenvalues, $\langle f_j, Hf_j\rangle \geqslant 0$, which gives:

$$\langle\psi_N, H_N\psi_N\rangle \geqslant \sum_{j:E_j\leqslant 0} E_j \geqslant -C\int dx\, V_-(x)^{1+\frac{d}{2}}\ , \tag{9.189}$$

where the last step follows from Eq. (9.184). Now, let us choose:

$$V(x) = -c\rho_\psi(x)^{\frac{2}{d}}\ . \tag{9.190}$$

Since $\rho_\psi \in L^1$, $V(x) \in L^{d/2}$. For this choice of V, Eq. (9.189) implies:

$$\begin{aligned}\langle\psi_N, \sum_{j=1}^N -\Delta_j\psi_N\rangle &\geqslant -Cc^{1+2/d}\int dx\,\rho_\psi(x)^{1+2/d} - \langle\psi_N, \sum_{j=1}^N V(x_j)\psi_N\rangle \\ &= -Cc^{1+2/d}\int dx\,\rho_\psi(x)^{1+2/d} + c\int dx\,\rho_\psi(x)^{1+2/d}\ . \end{aligned}\tag{9.191}$$

The claim follows after optimizing over $c > 0$. ■

We are now ready to prove Theorem 9.21.

Proof. By the Lieb-Thirring kinetic energy inequality:

$$\langle\psi_N, H_{N,K}\psi_N\rangle \geqslant K\int dx\,\psi_\psi(x)^{5/3} - \sum_{j=1}^K Z_j\int dx\,\rho_\psi(x)\frac{1}{|x-R_j|} + \langle\psi_N, \sum_{i<j}\frac{1}{|x_i-x_j|}\psi_N\rangle + U\ . \tag{9.192}$$

Let us now find a useful lower bound for the many-body interaction, in terms of the TF interaction. Let us apply Corollary 9.20 for $Z_j = 1$, $R_j = x_j$ and $K = N$. In this setting, $U = \sum_{i<j}\frac{1}{|x_i-x_j|}$. The bound (9.180) implies the following lower bound:

$$\sum_{i<j}^N \frac{1}{|x_i-x_j|} \geqslant -\frac{3.678}{\gamma}N - \frac{3}{5}\gamma\int dx\,\rho(x)^{5/3} + \sum_{j=1}^N\int dx\,\rho(x)\frac{1}{|x-x_j|} - D(\rho,\rho) \tag{9.193}$$

for any $\gamma > 0$ and for any $\rho \in L^1 \cap L^{5/3}$, $\rho \geqslant 0$. Choose $\rho \equiv \rho_{\psi_N}$, Then, plugging the bound (9.193) in (9.192) we get:

$$\begin{aligned}\langle\psi_N, H_{N,K}\psi_N\rangle &\geqslant (K - \frac{3}{5}\gamma)\int dx\,\rho_\psi(x)^{5/3} - \sum_{j=1}^K Z_j\int dx\,\rho_\psi(x)\frac{1}{|x-R_j|} \\ &\quad + \sum_{j=1}^N\int dx\,\rho(x)\langle\psi_N, \frac{1}{|x-x_j|}\psi_N\rangle - D(\rho_\psi,\rho_\psi) + U - \frac{3.678}{\gamma}N \\ &\equiv (K - \frac{3}{5}\gamma)\int dx\,\rho_\psi(x)^{5/3} - \sum_{j=1}^K Z_j\int dx\,\rho_\psi(x)\frac{1}{|x-R_j|} + D(\rho_\psi,\rho_\psi) + U \\ &\quad - \frac{3.678}{\gamma}N\ . \end{aligned}\tag{9.194}$$

The first line reconstructs the TF energy functional, with a new constant c_{TF} (positive, choosing the old γ small enough). Therefore, the final claim follows from Corollary 9.20. ■

9.6 TF theory as the $N \to \infty$ limit of quantum mechanics

In this section we shall give a rigorous derivation of TF theory starting from many-body quantum mechanics. As we shall see, TF theory becomes *exact* once the number of particles goes to infinity. We shall prove a theorem that provides a rigorous bound for the energy difference of large quantum systems and the TF approximation.

The result will hold in a suitable scaling regime, that we shall describe here. Let $N^0 \in \mathbb{N}$, and let $Q_N = N/N^0$. Also, let $\underline{Z}^0 \in \mathbb{N}^K$, and let $\underline{Z} = Q_N \underline{Z}^0$. Finally, let $\underline{R}^0 \in \mathbb{R}^{3K}$, and let $\underline{R} = Q_N^{-1/3} \underline{R}^0$. It is not difficult to see that:

$$E_N^{\mathrm{TF}}(\underline{Z}, \underline{R}) = Q_N^{7/3} E_{N^0}^{\mathrm{TF}}(\underline{Z}^0, \underline{R}^0) \,. \tag{9.195}$$

That is, as $N \to \infty$, every contribution to the TF ground state energy scales as $Q_N^{7/3}$. We shall suppose that $N^0 \leqslant Z_{\mathrm{tot}}^0$, to make sure that the TF minimizer has N_0 particles. We will prove the following theorem.

Theorem 9.23. *Let $\gamma = (6\pi^2)^{2/3}$. Then, there exists $\delta > 0$ independent of N such that:*

$$|E_N^{\mathrm{Q}}(\underline{Z}, \underline{R}) - Q_N^{7/3} E_{N_0}^{TF}(\underline{Z}^0, \underline{R}^0)| \leqslant C N^{7/3-\delta} \,. \tag{9.196}$$

Therefore, the theorem proves that Thomas-Fermi theory becomes *exact* in the $N \to \infty$, for the ground state energy:

$$\lim_{N\to\infty} \frac{E_N^{\mathrm{Q}}(\underline{Z}, \underline{R})}{Q_N^{7/3} E_{N_0}^{\mathrm{TF}}(\underline{Z}^0, \underline{R}^0)} = 1 \,. \tag{9.197}$$

The proof of the theorem will be based on matching upper and lower bounds for the ground state energy.

9.6.1 Upper bound

Let us start by proving an upper bound for the ground state energy, that gives the TF energy at leading order in N. To do this, we shall use *Hartree-Fock theory.*

Consider a Slater determinant:

$$\psi_N = \frac{1}{\sqrt{N!}} \sum_\pi \mathrm{sgn}(\pi) f_{\pi(1)}(x_1) \cdots f_{\pi(N)}(x_N) \,, \tag{9.198}$$

with reduced one-particle density matrix given by:

$$\omega = \sum_{j=1}^N |f_j\rangle\langle f_j| \,. \tag{9.199}$$

As we have seen in Section 9.2, the energy of a fermionic wave function is expressed in terms of the one- and two-particle density matrices. For the special case of Slater determinants, it turns out that the energy is a functional of the one-particle density matrix only. Consider a many-body Hamiltonian of the form:

$$H_N = \sum_i h_i + \sum_{i<j} V_(x_i - x_j) \,. \tag{9.200}$$

Then:

$$\langle \psi_N, H_N \psi_N \rangle = \mathcal{E}_{\mathrm{HF}}(\omega) \,, \tag{9.201}$$

where $\mathcal{E}_{\mathrm{HF}}$ is the Hartree-Fock energy functional:

$$\mathcal{E}_{\mathrm{HF}}(\omega) = \mathrm{Tr} h\omega + \frac{1}{2} \int dx dy\, V(x-y)(\omega(x;x)\omega(y;y) - |\omega(x;y)|^2) \,. \tag{9.202}$$

The last term describes the many-body interaction in HF theory. It is given by a sum of two terms: the first is called the direct term, the second is called the exchange term. Notice that for a positive potential, the exchange term is negative.

We define the HF ground state energy as the smallest energy of a Slater determinant. Due to the one-to-one correspondence between Slater determinants and rank$-N$ orthogonal projections, the HF ground state energy is:

$$E_N^{\mathrm{HF}} = \inf_{\omega \in \mathcal{P}_N} \mathcal{E}_{\mathrm{HF}}(\omega) \,, \tag{9.203}$$

where $\mathcal{P}_N := \{\omega : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3) \mid \omega^2 = \omega^* = \omega,\ \mathrm{Tr}\omega = N\}$. Since Slater determiants form a subset of $L^2_{\mathrm{a}}(\mathbb{R}^{3N})$, we trivially have:

$$E_N^{\mathrm{Q}} = \inf_{\psi_N \in L^2_{\mathrm{a}}(\mathbb{R}^{3N})} \frac{\langle \psi_N, H_N \psi \rangle}{\langle \psi_N, \psi_N \rangle} \leqslant E_N^{\mathrm{HF}} . \tag{9.204}$$

The idea will be to come up with a good trial state for the HF energy functional, that reproduces E_N^{TF} at leading order in N. To do that, we shall rely on the next Theorem.

Theorem 9.24. *Suppose that $V \geqslant 0$. Let $K : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ be an admissible one-particle density matrix: $0 \leqslant K \leqslant \mathbb{1}$, $\mathrm{Tr}\, K = N$. Then, there exists a Slater determinant ψ_N such that:*

$$\langle \psi_N, H_N \psi \rangle \leqslant \mathcal{E}_{HF}(K) . \tag{9.205}$$

This theorem immediately implies the *Lieb's variational principle:*

$$E_N^{\mathrm{TF}} = \inf_{K \text{ admissible}} \mathcal{E}_{\mathrm{HF}}(K) . \tag{9.206}$$

Hence, it gives us the freedom to look for a larger class of trial states:

$$E_N^{\mathrm{Q}} \leqslant E_N^{\mathrm{HF}} \leqslant \mathcal{E}_{\mathrm{HF}}(K) \qquad \text{for any admissible } K. \tag{9.207}$$

Proof. (of Theorem 9.24.) We shall prove the theorem in the case K is finite rank: $K = \sum_{i=1}^{M} \lambda_i |f_i\rangle\langle f_i|$, with $0 \leqslant \lambda_i \leqslant 1$. The general case follows from an approximation argument, that we leave as an exercise. Define:

$$h^{(k)} = \langle f_k, h f_k \rangle , \qquad V^{(k\ell)} = \langle f_k \wedge f_\ell, V f_k \wedge f_\ell \rangle , \tag{9.208}$$

where $f_k \wedge f_\ell = \frac{1}{\sqrt{2}}(f_k \otimes f_\ell - f_\ell \otimes f_k)$. Then, a simple computation gives:

$$\mathcal{E}_{\mathrm{HF}}(K) = \sum_k \lambda_k h^{(k)} + \frac{1}{2} \sum_{k,\ell} \lambda_k \lambda_\ell V^{(k\ell)} . \tag{9.209}$$

Suppose $M > N$. If not, $M = N$ and there is nothing to prove. Then, there exists at least two eigenvalues λ_p and λ_q such that $0 < \lambda_p, \lambda_q < 1$. Without loss of generaily, we assume that:

$$h^{(q)} + \sum_k \lambda_k V^{(kq)} \leqslant h^{(p)} + \sum_k \lambda_k V^{(kp)} . \tag{9.210}$$

Let $\delta = \min\{\lambda_p, 1 - \lambda_1\}$. Clearly, $\delta > 0$. Define:

$$\begin{aligned} \overline{K} &= \sum_{k \notin \{p,q\}} \lambda_k |f_k\rangle\langle f_k| + (\lambda_p - \delta)|f_p\rangle\langle f_p| + (\lambda_q + \delta)|f_p\rangle\langle f_p| \\ &\equiv \sum_k \overline{\lambda}_k |f_k\rangle\langle f_k| . \end{aligned} \tag{9.211}$$

Obviously, $\overline{K}$ is admissible. Notice that if $\delta = \lambda_p$ then $\overline{\lambda}_p = 0$, and if $\delta = 1 - \lambda_q$ then $\overline{\lambda}_q = 1$. Hence, the number of eigenvalues of K that are neither 0 or 1 is strictly smaller than the same quantity for K. After iterating the above procedure at most M times, we will be left with a density matrix with eigenvalues equal to either 0 or 1, *i.e.* the reduced one-particle density matrix of a Slater determinant. To conclude the proof, we have to make sure that the energy does not increase in the process:

$$\mathcal{E}_{\mathrm{HF}}(\overline{K}) \leqslant \mathcal{E}_{\mathrm{HF}}(K) . \tag{9.212}$$

To do this, we compute, recalling Eq. (9.209):

$$\mathcal{E}_{\mathrm{HF}}(K) - \mathcal{E}_{\mathrm{HF}}(\overline{K}) = \delta\Big(h^{(p)} + \sum_\ell V^{(p\ell)}\lambda_\ell - h^{(q)} - \sum_\ell V^{(q\ell)}\lambda_\ell\Big) - \delta^2 V_{qp} , \tag{9.213}$$

where the term in parenthesis is $\geqslant 0$, by Eq. (9.210), and $V_{qp} \geqslant 0$, as a consequence of $V \geqslant 0$. This implies Eq. (9.212), and concludes the proof. ■

Legitimated by Lieb's variational principle, we will choose a trial state K for the HF functional that is not a projetcion. Since TF theory is a semiclassical approximation of quantum mechanics, it makes sense to use coherent states. We define:

$$K = \frac{1}{(2\pi)^3}\int dpdq\, M(p,q)\pi_{pq}\;, \qquad \pi_{pq} = |F_{pq}\rangle\langle F_{pq}|\;, \qquad F_{pq}(x) = e^{ipx}G(x-q)\;. \quad (9.214)$$

We shall assume that $0 \leqslant M(p,q) \leqslant 1$, and that $\frac{1}{(2\pi)^3}\int dpdq\, M(p,q) = N$. This implies that K is admissible. The idea is to try to choose $M(p,q)$ so to make the energy as small as possible. A good ansatz is:

$$M(p,q) = \chi(p^2 - \phi_{\rm TF}(q) \leqslant -\mu)\;, \quad (9.215)$$

with $\phi_{\rm TF}$ the Thomas-Fermi potential and $\mu \geqslant 0$ chosen so that K is admissible. Using the TF equation, Eq. (9.215) can be rewritten as:

$$M(p,q) = \chi(p^2 \leqslant (\phi_{\rm TF}(q) - \mu)_+) = \chi(p^2 \leqslant \gamma\rho(q)^{2/3})\;, \quad (9.216)$$

with ρ the N-particle TF minimizer. Notice that:

$$\mathrm{Tr}K = \frac{1}{(2\pi)^3}\int dpdq\, M(p,q) = \frac{4\pi}{(2\pi)^3}\frac{\gamma^{3/2}}{3}\int dq\, \rho(q) = N\;, \quad (9.217)$$

provided $\gamma = (6\pi^2)^{2/3}$. Also:

$$\begin{aligned} \mathrm{Tr} - \Delta K &= \frac{1}{(2\pi)^3}\int dqdp\, M(p,q)(p^2 + \|\nabla G\|_2^2) \\ &= \frac{3}{5}\gamma\int dq\, \rho(q)^{5/3} + N\|\nabla G\|_2^2\;. \end{aligned} \quad (9.218)$$

Hence, we get, using that the exchange term is nonpositive:

$$\begin{aligned} \mathcal{E}_{\rm HF}(K) \;\leqslant\;& \frac{3}{5}\gamma\int dx\, \rho(x)^{5/3} - \int dx\, V(x)K(x,x) + \frac{1}{2}\int dxdy\, \frac{1}{|x-y|}K(x;x)K(y;y) \\ &+ U + CN\|\nabla G\|_2^2\;. \end{aligned} \quad (9.219)$$

The first line looks very much like the TF functional, except that $K(x,x)$ appears instead of $\rho(x)$. We compute:

$$K(x;x) = \frac{1}{(2\pi)^3}\int dpdq\, M(p,q)|G(x-q)|^2 = \int dq\, \rho(q)|G(x-q)|^2 \equiv (\rho * |G|^2)(x)\;. \quad (9.220)$$

Consider the density-density interaction. We rewrite it as:

$$D(\rho * |G|^2, \rho * |G|^2) = \frac{1}{2}\int dx\, (\rho * |G|^2)(x)(\rho * |G|^2 * \frac{1}{|\cdot|})(x)\;, \quad (9.221)$$

that is as a L^2 scalar product. Rewriting it in Fourier space, and using that the Fourier transform of the convolution is the product of the Fourier transforms:

$$D(\rho * |G|^2, \rho * |G|^2) = \frac{1}{2}\int dp\, |\hat{\rho}(p)|^2 |\widehat{|G|^2}(p)|^2 \frac{1}{p^2} \leqslant D(\rho,\rho)\;, \quad (9.222)$$

where we used that:

$$|\widehat{|G|^2}(p)| \leqslant \|\widehat{|G|^2}\|_\infty \leqslant \||G|^2\|_1 = 1\;. \quad (9.223)$$

Thus, the bound (9.222) reproduces the TF density-density interaction. To conclude, consider the electron-nuclei interaction. We rewrite it as:

$$-\int dx\, V(x)K(x;x) = -\int dx\, V(x)\rho(x) + \int dx\, V(x)(\rho(x) - K(x;x))\;. \quad (9.224)$$

The last term is an error term, that we have to estimate. We rewrite it as:

$$\int dx\, V(x)(\rho(x) - K(x;x)) = \sum_{j=1}^{K} Z_j \int dx\, \rho(x)\Big(\frac{1}{|x-R_j|} - |G|^2 * \frac{1}{|\cdot - R_j|}(x)\Big)\,. \tag{9.225}$$

Let us suppose that:

$$G(x) = R^{-3/2} G_0(x/R)\,, \qquad G_0(x) \equiv G_0(|x|)\,, \tag{9.226}$$

with G_0 compactly supported for $|x| \leqslant 1$ and $\|G_0\|_2 = 1$, $\|\nabla G_0\|_2 \leqslant C$. With this choice,

$$\|\nabla G\|_2^2 = R^{-2}\|\nabla G_0\|_2^2\,. \tag{9.227}$$

Thus, $|G(x)|^2$ is a spherically symmetric charge distribution, with total charge 1: by Newton's theorem,

$$|G|^2 * \frac{1}{|\cdot - R_j|}(x) = \frac{1}{|x-R_j|}\,, \qquad \text{for } |x-R_j| > R. \tag{9.228}$$

Hence, we can rewrite Eq. (9.225) as:

$$\begin{aligned}\int dx\, V(x)(\rho(x) - K(x;x)) &= \sum_{j=1}^{K} Z_j \int_{|x-R_j|\leqslant R} dx\, \rho(x)\Big(\frac{1}{|x-R_j|} - |G|^2 * \frac{1}{|\cdot - R_j|}(x)\Big) \\ &\leqslant \sum_{j=1}^{K} Z_j \int_{|x-R_j|\leqslant R} dx\, \rho(x)\frac{1}{|x-R_j|}\,. \end{aligned} \tag{9.229}$$

Now, from the TF equation for the minimizer:

$$\begin{aligned}\gamma\rho(x)^{2/3} &= \Big(\sum_{j=1}^{K}\frac{Z_j}{|x-R_j|} - \rho * \frac{1}{|\cdot|}(x) - \mu\Big)_+ \\ &\leqslant \sum_{j=1}^{K}\frac{Z_j}{|x-R_j|}\,. \end{aligned} \tag{9.230}$$

Assuming that $R \ll |R_i - R_j|$ for $i \neq j$, we get:

$$\rho(x) \leqslant C\frac{Z_{\max}^{3/2}}{|x-R_j|^{3/2}}\,. \tag{9.231}$$

Hence, plugging this bound in Eq. (9.229) we get:

$$\int dx\, V(x)(\rho(x) - K(x;x)) \leqslant C Z_{\max}^{5/2}\int_{|x|\leqslant R} dx\, \frac{1}{|x|^{5/2}} \leqslant C N^{5/2} R^{1/2}\,. \tag{9.232}$$

All in all, plugging the bounds (9.222), (9.232) in Eq. (9.219) we find:

$$\mathcal{E}_{\mathrm{HF}}(K) \leqslant E_N^{\mathrm{TF}} + CNR^{-2} + CN^{5/2}R^{1/2}\,. \tag{9.233}$$

The optimal value of R is $R = CN^{-3/5}$, which is indeed such that $R \ll |R_i - R_j|$ for $i \neq j$ (recall that, by assumption, the internuclear distance is order $N^{-1/3}$). With this choice:

$$E_N^{\mathrm{Q}} \leqslant \mathcal{E}_{\mathrm{HF}}(K) \leqslant E_N^{\mathrm{TF}} + CN^{11/5}\,. \tag{9.234}$$

Since $E_N^{\mathrm{TF}} \sim N^{7/3}$, the error term is subleading as $N \to \infty$. This concludes the proof of the upper bound.

9.6.2 Lower bound

To conclude the proof of Theorem 9.23, we need a lower bound on the ground state energy that agrees with TF at leading order.

A Properties of Sobolev spaces

Here we shall collect some basic properties of Sobolev spaces. We refer the reader to [3, 1] for more details. Given an open set $U \subseteq \mathbb{R}^d$, recall the definition of Sobolev space $W^{k,p}(U)$:

$$W^{k,p}(U) = \{u : U \to \mathbb{C} \mid \partial^\alpha u \in L^p(U) \text{ for all } \alpha \text{ s.t. } |\alpha| \leqslant k\} \ . \tag{A.1}$$

The norm $\|\cdot\|_{W^{k,p}(U)}$ is defined as:

$$\|u\|^p_{W^{k,p}(U)} = \sum_{\alpha : |\alpha| \leqslant k} \|\partial^\alpha u\|^p_{L^p(U)} \ . \tag{A.2}$$

A special role in quantum mechanics is played by $H^1(U) := W^{1,2}(U)$. More generally, we define $H^k(U) = W^{k,2}(U)$. We shall also denote by $W^{k,p}_0(U)$ the space of functions in $W^{k,p}(U)$ which are vanishing on the boundary of U.

A.1 Sobolev inequality

The Sobolev inequality allows to bound from below L^p norms of Du with L^q norms of u. As we shall see, this cannot be true for all p, q. Let $u \in C^\infty_c(\mathbb{R}^d)$, $u \neq 0$, $u_\lambda(x) := u(\lambda x)$. Suppose that there exists $C > 0$, *independent of* λ, such that:

$$\|u_\lambda\|_{L^q(\mathbb{R}^d)} \leqslant C \|\nabla u_\lambda\|_{L^p(\mathbb{R}^d)} \ . \tag{A.3}$$

By a change of variables,

$$\begin{aligned} \|u_\lambda\|_{L^q(\mathbb{R}^d)} &= \left(\int dx |u_\lambda(x)|^q \right)^{\frac{1}{q}} = \left(\frac{1}{\lambda^d} \right)^{\frac{1}{q}} \|u\|_{L^q(\mathbb{R}^d)}, \\ \|\nabla u_\lambda\|_{L^p(\mathbb{R}^d)} &= \left(\int dx |\nabla u_\lambda(x)|^p \right)^{\frac{1}{p}} = \left(\frac{\lambda}{\lambda^{\frac{d}{p}}} \right) \|\nabla u\|_{L^p(\mathbb{R}^d)} \ . \end{aligned} \tag{A.4}$$

Therefore, Eq. (A.3) implies:

$$\|u\|_{L^q(\mathbb{R}^d)} \leqslant C \lambda^{1 - \frac{d}{p} + \frac{d}{q}} \|\nabla u\|_{L^p(\mathbb{R}^d)}. \tag{A.5}$$

Thus, *if* $1 - \frac{d}{p} + \frac{d}{q} \neq 0$, by taking either $\lambda \to 0$ or $\lambda \to \infty$, Eq. (A.5) would imply $\|u\|_{L^p(\mathbb{R}^d)} \leqslant 0$, that is $u = 0$, which is a contradiction.

Therefore, we might only hope to prove Eq. (A.3) for:

$$1 + \frac{d}{q} - \frac{d}{p} = 0 \Rightarrow \frac{1}{q} = \frac{1}{p} - \frac{1}{d}. \tag{A.6}$$

Let $1 \leqslant p < d$. We define the *Sobolev conjugate* of p as the number $q \equiv p^*$ for which Eq. (A.6) holds true:

$$p^* := \frac{dp}{d - p} \ . \tag{A.7}$$

Notice that $p^* > p$.

Theorem A.1 (Gagliardo-Nirenberg-Sobolev inequality)**.** *Let $1 \leqslant p < d$. There exists a constant $C \equiv C(d, p)$ such that*

$$\|u\|_{L^{p^*}(\mathbb{R}^d)} \leqslant C \|\nabla u\|_{L^p(\mathbb{R}^d)}, \qquad \forall u \in C^1_c(\mathbb{R}^d). \tag{A.8}$$

The proof will be based on the generalized Hölder inequality:

$$\int_U \Big| \prod_{i=1}^m u_i \Big| dx \leqslant \prod_{i=1}^m \|u_i\|_{L^{p_i}(U)}, \qquad \sum_{i=1}^m \frac{1}{p_i} = 1. \tag{A.9}$$

Remark A.2. *The proof crucially relies on the fact that u is compactly supported: the inequality is trivially false if $u = 1$. However, the constant C does not depend on the support of u.*

Proof. Let us start with the case $p = 1$. Using the compact support of u,

$$u(x) = \int_{-\infty}^{x_i} dy_i u_{x_i}(x_1, \cdots, x_{i-1}, y_i, x_{i+1}, \cdots, x_d) \tag{A.10}$$

thus

$$|u(x)| \leqslant \int_{-\infty}^{\infty} dy_i |\nabla u(x_1, \cdots, y_i, \cdots, x_d)|. \tag{A.11}$$

For $p = 1$ the Sobolev conjugate of p is $p^* = \frac{d}{d-1}$. Therefore, it is natural to consider:

$$|u(x)|^{\frac{d}{d-1}} \leqslant \prod_{i=1}^{d} \left(\int_{-\infty}^{\infty} dy_i |\nabla u(x_1, \cdots, y_i, \cdots, x_d)| \right)^{\frac{1}{d-1}}. \tag{A.12}$$

We have:

$$\begin{aligned}
\int_{-\infty}^{\infty} dx_1 |u(x)|^{\frac{d}{d-1}} &\leqslant \int_{-\infty}^{\infty} dx_1 \prod_{i=1}^{d} \left(\int_{-\infty}^{\infty} dy_i |\nabla u(x_1, \cdots, y_i, \cdots)| \right)^{\frac{1}{d-1}} = \qquad (A.13)\\
&= \int_{-\infty}^{\infty} dx_1 \left(\int_{-\infty}^{\infty} dy_1 |\nabla u(y_1, \cdots)| \right)^{\frac{1}{d-1}} \prod_{i=2}^{n} \left(\int_{-\infty}^{\infty} dy_i |\nabla u(x_1, \cdots, y_i, \cdots)| \right)^{\frac{1}{d-1}}\\
&= \left(\int_{-\infty}^{\infty} dy_1 |Du(y_1, \cdots)| \right)^{\frac{1}{d-1}} \int_{-\infty}^{\infty} dx_1 \prod_{i=2}^{d} \left(\int_{-\infty}^{\infty} dy_i |Du(x_1, \cdots, y_i, \cdots)| \right)^{\frac{1}{d-1}}.
\end{aligned}$$

Let us now apply the generalized Hölder inequality, with $p_i = d - 1$. We have

$$\int_{-\infty}^{\infty} dx_1 |u(x)|^{\frac{d}{d-1}} \leqslant \left(\int_{-\infty}^{\infty} dy_1 |\nabla u(y_1, \cdots)| \right)^{\frac{1}{d-1}} \prod_{i=2}^{n} \left(\int_{-\infty}^{\infty} dx_1 dy_i |\nabla u(x_1, \cdots, y_i, \cdots)| \right)^{\frac{1}{d-1}}. \tag{A.14}$$

Next, let us integrate over x_2. We get:

$$\begin{aligned}
&\int_{-\infty}^{\infty} dx_1 dx_2 |u(x)|^{\frac{d}{d-1}}\\
&\leqslant \int dx_2 \left(\int_{-\infty}^{\infty} dy_1 |\nabla u(y_1, \cdots)| \right)^{\frac{1}{d-1}} \prod_{i=2}^{d} \left(\int_{-\infty}^{\infty} dx_1 dy_i |\nabla u(x_1, \cdots, y_i, \cdots)| \right)^{\frac{1}{d-1}}\\
&= \left(\int_{-\infty}^{\infty} dx_1 dy_2 |\nabla u(x_1, y_2 \cdots)| \right)^{\frac{1}{d-1}} \int dx_2 \left(\int_{-\infty}^{\infty} dy_1 |\nabla u(y_1, x_2, \cdots)| \right)^{\frac{1}{d-1}} \cdot\\
&\quad \cdot \prod_{i=3}^{d} \left(\int_{-\infty}^{\infty} dx_1 dy_i |\nabla u(x_1, x_2, \cdots, y_i, \cdots)| \right)^{\frac{1}{d-1}}.
\end{aligned} \tag{A.15}$$

Using again the generalized Hölder inequality for the x_2 integration, choosing $p_i = d - 1$, we have

$$\begin{aligned}
(A.15) &\leqslant \left(\int_{-\infty}^{\infty} dx_1 dx_2 |\nabla u(x_1, x_2 \cdots)| \right)^{\frac{2}{d-1}} \cdot\\
&\quad \cdot \prod_{i=3}^{n} \left(\int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dx_1 dy_i |\nabla u(x_1, \cdots, y_i, \cdots, x_d)| \right)^{\frac{1}{d-1}}.
\end{aligned} \tag{A.16}$$

Iterating the same procedure n times (*i.e.* integrating again over $dx_3, \cdots, dx_d$) we finally get

$$\int dx_1 \cdots dx_d |u(x)|^{\frac{d}{d-1}} \leqslant \left(\int dx_1 \cdots dx_d |\nabla u(x_1, \cdots, x_d)| \right)^{\frac{d}{d-1}}, \tag{A.17}$$

which proves the inequality for $p = 1$.

Let us now consider $1 < p < d$. Let $v := |u|^\gamma$, $\gamma > 1$ to be chosen later. By Eq. (A.17), we have

$$\left(\int |u|^{\frac{\gamma d}{d-1}} dx\right)^{\frac{d-1}{d}} \leqslant \int |\nabla |u|^\gamma| dx = \gamma \int |u|^{\gamma-1} |\nabla u| dx \leqslant \gamma \left(\int |u|^{(\gamma-1)\frac{p}{p-1}} dx\right)^{\frac{p-1}{p}} \left(\int |\nabla u|^p\right)^{\frac{1}{p}}, \tag{A.18}$$

where in the last step we used the Hölder with $q = p/(p-1)$. Now let us choose γ such that $\frac{\gamma d}{d-1} = (\gamma - 1)\frac{p}{p-1}$. That is,

$$\gamma\left(\frac{d}{d-1} - \frac{p}{p-1}\right) = -\frac{p}{p-1} \Rightarrow \gamma\left(\frac{p-d}{(d-1)(p-1)}\right) = -\frac{p}{p-1}, \tag{A.19}$$

i.e. $\gamma = p(d-1)/(d-p) > 1$. Plugging this choice into Eq. (A.18) we get:

$$\left(\int |u|^{\frac{\gamma d}{d-1}}\right)^{\frac{d-1}{d}} \left(\int |u|^{\frac{\gamma d}{d-1}}\right)^{-\frac{p-1}{p}} \leqslant \gamma \left(\int |Du|^p\right)^{\frac{1}{p}}, \tag{A.20}$$

with

$$\frac{d-1}{d} - \frac{p-1}{p} = \frac{p(d-1) - d(p-1)}{dp} = \frac{d-p}{dp} \equiv \frac{1}{p^*}, \tag{A.21}$$

and hence

$$\frac{\gamma d}{d-1} = \frac{pd}{d-p} = p^* . \tag{A.22}$$

We conclude that:

$$\left(\int dx |u|^{p^*}\right)^{\frac{1}{p^*}} \leqslant \gamma \left(\int dx |\nabla u|^p\right)^{\frac{1}{p}}, \qquad 1 < p < d\,, \tag{A.23}$$

which is what we wanted to prove. ■

This inequality can be used to prove that, in some cases, Sobolev spaces are *embedded* in L^q spaces.

Theorem A.3 (Sobolev embedding). *Let $U \subset \mathbb{R}^d$ open and bounded. Let $u \in W_0^{1,p}(U)$, $1 \leqslant p < d$. Then*

$$\|u\|_{L^q(U)} \leqslant C \|\nabla u\|_{L^p(U)}, \qquad \forall q \in [1, p^*], \tag{A.24}$$

with $C \equiv C(p, q, U)$.

Remark A.4. *i) In particular, $q = p$ is allowed, since $p^* > p$. We have:*

$$\|u\|_{L^p(U)} \leqslant C \|\nabla u\|_{L^p(U)}, \tag{A.25}$$

which takes the name of Poincaré inequality.

ii) The Poincaré inequality allows us to prove that on $H_0^p(U)$, the norms $\|\nabla u\|_{L^p(U)}$ and $\|u\|_{H^p(U)}$ are equivalent. In fact, one trivially has:

$$\|\nabla u\|_{L^p(U)} \leqslant \|u\|_{H^p(U)} \tag{A.26}$$

and, by Poincaré inequality:

$$\|u\|_{H^p(U)} \leqslant \left(\|u\|^p_{L^p(U)} + \|\nabla u\|^p_{L^p(U)}\right)^{\frac{1}{p}} \leqslant C \|\nabla u\|_{L^p(U)} . \tag{A.27}$$

iii) Theorem A.3 is telling us that

$$u \in H_0^p(U) \Rightarrow u \in L^q(U), \qquad \forall q \in [1, p^*]. \tag{A.28}$$

We stress that the smallest such $L^q(U)$ space is $L^{p^*}(U)$. Indeed, by Hölder:

$$\|u\|_q = \left(\int_U dx |u(x)|^q\right)^{\frac{1}{q}} \leqslant \left(\int_U dx |u(x)|^{qp}\right)^{\frac{1}{qp}} \left(\int_U dx\right)^{\frac{1}{p'}} \leqslant C \|u\|_{p^*}, \tag{A.29}$$

where $\frac{1}{p'} + \frac{1}{p} = 1$ and $p = \frac{p^*}{q} > 1$. We say that the space $H_0^p(U)$ is embedded in $L^{p^*}(U)$, $p^* = \frac{dp}{d-p}, 1 \leqslant p < n$.

iv) Finally, the Sobolev inequality (A.24) can be extended to functions in $H^p(U)$, under the assumption that the boundary of U is of class C^1.

Proof. Let $u \in W_0^{1,p}(U)$. Then, there exists $\{u_m\}_{m\in\mathbb{N}}$, $u_m \in C_c^\infty(U)$ such that $u_m \to u$ in $W^{1,p}(U)$. Let us extend u_m to $\mathbb{R}^d$, setting $u_m = 0$ on $\mathbb{R}^d\backslash U$. By the GNS inequality,

$$\|u_m - u_l\|_{p*} \leqslant C\|D(u_m - u_l)\|_p \to 0 \quad \text{as } m, l \to \infty. \tag{A.30}$$

Thus, $\{u_m\}$ is a Cauchy sequence in $L^{p^*}(U)$, and hence $u_m \to \tilde{u}$ in $L^{p^*}(U)$. Being U bounded, $\tilde{u} \in L^q(U)$, $\forall q : 1 \leqslant q \leqslant p^*$. In particular, $\tilde{u} \in L^p(U)$, which shows that $u = \tilde{u}$, and therefore that $u \in L^q$ for all $q \in [1, p^*]$.

By the GNS inequality:

$$\|u_m\|_{L^{p*}(U)} \leqslant C\|\nabla u_m\|_{L^p(U)} \,. \tag{A.31}$$

Then, by convergence in $W^{1,p}(U)$:

$$\|\nabla u_m\|_{L^p(U)} = \|\nabla(u_m - u + u)\|_{L^p(U)} \to \|\nabla u\|_{L^p(U)} \quad \text{as } m \to \infty. \tag{A.32}$$

Also,

$$\|u_m\|_{L^{p*}(U)} \geqslant C\|u_m\|_{L^q(U)}, \qquad \forall 1 \leqslant q \leqslant p^*, \tag{A.33}$$

and

$$\|u_m\|_{L^q(U)} = \|u_m - u + u\|_{L^q(U)} \to \|u\|_{L^q(U)} \quad \text{as } m \to \infty. \tag{A.34}$$

by convergence in $L^{p^*}(U)$. All in all:

$$\|u\|_{L^q(U)} \leqslant C\|\nabla u\|_{L^p(U)}, \tag{A.35}$$

for some $C \equiv C(U, d, p)$. ■

A.2 Weak to strong convergence

Here we shall use the result of the previous section to prove the following result.

Theorem A.5 (Weak to strong convergence)**.** *Suppose that $\psi_j \to \psi$ weakly in $H^1(\mathbb{R}^d)$. Let $A \subset \mathbb{R}^d$ be any set of finite measure and let χ_A be its characteristic function. Then:*

$$\chi_A\psi_j \to \chi_A\psi \qquad \textit{strongly in } L^p(\mathbb{R}^d) \tag{A.36}$$

for every $1 \leqslant p < 2d/(d-2)$ when $d \geqslant 3$, every $p < \infty$ when $d = 2$ and every $p \leqslant \infty$ when $d = 1$. In fact, for $d = 1$ the convergence is pointwise and uniform.

Proof. The proof is based on an approximation argument via the heat kernel $e^{\Delta t}$. We claim that for any $\psi \in H^1(\mathbb{R}^d)$:

$$\|\psi - e^{\Delta t}\psi\|_2 \leqslant \|\nabla\psi\|_2\sqrt{t} \,, \tag{A.37}$$

where:

$$(e^{\Delta t}\psi)(x) = \frac{1}{(4\pi t)^{d/2}}\int_{\mathbb{R}^d} \exp\{-|x-y|^2/4t\}\psi(y)dy \,. \tag{A.38}$$

The estimate (A.37) follows from Plancherel theorem:

$$\begin{aligned} \|\psi - e^{\Delta t}\psi\|_2^2 &= \int_{\mathbb{R}^d} |\hat{\psi}(k)|^2(1 - \exp\{-|k|^2 t\})^2 dk \\ &\leqslant \int_{\mathbb{R}^d} |\hat{\psi}(k)|^2|k|^2 t \equiv \|\nabla\psi\|_2^2 t \,, \end{aligned} \tag{A.39}$$

where we used that $(1 - \exp\{-|k|^2 t\} \leqslant \min\{1, |k|^2 t\}$. By the uniform boundedness principle, see Theorem 2.12 of [3], the weak convergence $\psi_j \to \psi$ in $H^1(\mathbb{R}^d)$ implies that $\|\nabla\psi_j\|_2 \leqslant C$ uniformly in j. Therefore,

$$\|\psi_j - e^{\Delta t}\psi_j\|_2 \leqslant \sqrt{t}C \,. \tag{A.40}$$

Now, let $\phi_j = e^{\Delta t}\psi_j$. Assuming for the moment that ϕ_j converges strongly in $L^2(\mathbb{R}^d)$ to $\phi = e^{\Delta t}\psi$, we shall prove that $\chi_A\psi^j$ converges strongly to $\chi_A\psi$. Simply note that:

$$\|\chi_A(\psi_j - \psi)\|_2 \leqslant \|\chi_A(\psi_j - \phi_j)\|_2 + \|\chi_A(\phi_j - \phi)\|_2 + \|\chi_A(\phi - \psi)\|_2 \ . \tag{A.41}$$

The first and the last term can be bounded using that:

$$\begin{aligned} \|\chi_A\psi_j - \phi_j\|_2 &\leqslant \|\psi_j - \phi_j\|_2 \leqslant \sqrt{t}\|\nabla\psi_j\|_2 \\ \|\chi_A(\phi - \psi)\|_2 &\leqslant \|\phi - \psi\|_2 \leqslant \sqrt{t}\|\nabla\psi\|_2 \end{aligned} \tag{A.42}$$

Again by the uniform boundedness principle, $\|\nabla\psi_j\|_2 \leqslant C$. Also, by the lower semicontinuity of norms, Theorem 2.11 of [3],

$$\|\nabla\psi\|_2 \leqslant \liminf_{j\to\infty} \|\nabla\psi_j\| \leqslant C \tag{A.43}$$

we see that the sum of the first and of the last term in Eq. (A.41) is estimated by $2C\sqrt{t}$. Therefore, under the assumption that ϕ_j converges strongly to ϕ, for any $\varepsilon > 0$ we can find t and j such that:

$$\|\chi_A(\psi_j - \psi)\|_2 \leqslant 2C\sqrt{t} + \|\chi_A(\phi_j - \phi)\|_2 \leqslant \varepsilon \ . \tag{A.44}$$

This proves the claim Eq. (A.36) for $p = 2$. It remains to prove that $\chi_A\phi_j \to \chi_A\phi$ strongly in $L^2(\mathbb{R}^d)$. To see this, note that by (A.38) and Hölder inequality:

$$\chi_A(x)|\phi_j(x)| \leqslant (4\pi t)^{-d/2}\Big(\int \exp\{-2x^2/4t\}dx\Big)^{1/2}\|\psi_j\|_2\chi_A(x) \ . \tag{A.45}$$

By the uniform boundedness principle, $\|\psi_j\|_2 \leqslant \|\psi_j\|_{H_1} \leqslant C$. Therefore, ϕ_j is bounded uniformly in j. On the other hand, $\phi_j(x) \to \phi(x)$ pointwise, since $\psi_j \to \psi$ weakly in H^1 and for every fixed x the function $y \mapsto \exp\{-|x-y|^2/4t\}$ is in the dual of H^1. Therefore, pointwise convergence follows from dominated convergence. This concludes the proof of (A.36) for $p = 2$.

Let us now prove Eq. (A.36) for all p such that $1 \leqslant p < 2d/(d-2)$. Consider first $1 \leqslant p \leqslant 2$. By Hölder inequality:

$$\|\chi_A(\psi - \psi_j)\|_p \leqslant \|\chi_A\|_r\|\chi_A(\psi - \psi_j)\|_2 \ , \tag{A.46}$$

with $1/p = 1/r + 1/2$. Using that $\chi_A \in L^r$ for all r, this proves the theorem for $1 \leqslant p < 2$. Finally, consider $p > 2$. Again by Hölder:

$$\|\chi_A(\psi - \psi_j)\|_p \leqslant \|\chi_A(\psi - \psi_j)\|_2^{\alpha}\|\chi_A(\psi - \psi_j)\|_q^{1-\alpha} \tag{A.47}$$

with $\alpha = (1/p - 1/q)(1/2 - 1/q)$, which is strictly positive if $p < q$. Then, by the Sobolev inequality:

$$\|\chi_A(\psi - \psi_j)\|_{L^q(\mathbb{R}^d)} = \|\psi - \psi_j\|_{L^q(A)} \leqslant C(\|\nabla\psi\|_{L^2(\mathbb{R}^d)} + \|\nabla\psi\|_{L^2(A)}) \leqslant C' \ , \tag{A.48}$$

where we used again the uniform boundedness principle and the lower semicontinuity of the norm. ∎

B Bathtub principle

In this appendix we shall briefly discuss the bathtub principle, used for instance in Section 8.2. We refer the reader to [3] for a more extensive discussion. Let μ be a Borel measure, and let f be a real valued function, such that $\mu(x : f(x) < t)$ is bounded for all t. Consider the functional

$$I(g) = \int d\mu(x)\, f(x)g(x) \ , \tag{B.1}$$

defined on $g(x)$ such that $0 \leqslant g(x) \leqslant 1$ and $\int d\mu(x)\, g(x) = G$. We are interested in minimizing $I(g)$ over all such functions. We claim that:

$$\inf I(g) = I(g_*) \ , \qquad g_*(x) = \chi(f(x) < s) + c\chi(f(x) = s) \ , \tag{B.2}$$

where the numbers s and c are defined as:

$$s = \sup\{t \mid \mu(x : f(x) < t) \leqslant G\} \,, \qquad c\mu(x : f(x) = s) = G - \mu(x : f(x) < s) \,. \tag{B.3}$$

Notice that $\int d\mu(x) g_*(x) = G$. First of all, let us prove that $c \leqslant 1$. Suppose that $\mu(f(x) = s) \neq 0$; otherwise, c is undetermined. Suppose that $c > 1$. Then:

$$\int d\mu(x)\, \chi(f(x) \leqslant s) < \int d\mu(x)\, g_*(x) = G \,. \tag{B.4}$$

Moreover,

$$\begin{aligned} \mu(f(x) \leqslant s) &= \int d\mu(x)\, \chi(f(x) \leqslant s) \\ &= \int d\mu(x)\, \lim_{n\to\infty} \chi(f(x) < s + 1/n) \\ &= \lim_{n\to\infty} \mu(f(x) < s + 1/n) \,, \end{aligned} \tag{B.5}$$

where the last step follows from monotone convergence theorem: the function $\chi(f(x) < s+1/n)$ is nonincreasing in n, and its integral is bounded uniformly in n, by the assumptions on f. Therefore:

$$\lim_{n\to\infty} \mu(f(x) < s + 1/n) < G \tag{B.6}$$

which means that there exists N large enough such that:

$$\mu(f(x) < s + 1/N) < G \,. \tag{B.7}$$

This however contradicts the definition of s in Eq. (B.3), hence $c \leqslant 1$.

To prove that g_* is a minimizer, it is enough to show that given any h such that $0 \leqslant h(x) \leqslant 1$ and $\int d\mu(x)\, h(x) = G$, one has $I(g_* - h) \leqslant 0$. Let us check this. We write:

$$\begin{aligned} I(g_* - h) &= \int_{f<s} d\mu(x) f(x)(g_*(x) - h(x)) + \int_{f>s} d\mu(x) f(x)(g_*(x) - h(x)) \\ &\quad + \int_{f=s} d\mu(x) f(x)(g_*(x) - h(x)) \\ &\leqslant s \int_{f<s} d\mu(x)(g_*(x) - h(x)) + \int_{f>s} d\mu(x) f(x)(-h(x)) \\ &\quad + s\int_{f=s} d\mu(x)(g_*(x) - h(x)) \\ &\leqslant s \int_{f<s} d\mu(x)(g_*(x) - h(x)) + s\int_{f>s} d\mu(x)(-h(x)) \\ &\quad + s\int_{f=s} d\mu(x)(g_*(x) - h(x)) \\ &= s\Big(\int_{f<s} d\mu(x)(g_*(x) - h(x)) + \int_{f>s} d\mu(x)(g_*(x) - h(x)) \\ &\quad + \int_{f=s} d\mu(x)(g_*(x) - h(x))\Big) \end{aligned} \tag{B.8}$$

where in the first inequality we used that $g_*(x) = 1$ is $f(x) < s$, and in the second inequality that $g_*(x) = 0$ if $f(x) > s$. Therefore,

$$I(g_* - h) \leqslant s \int d\mu(x)(g_*(x) - h(x)) = s(G - G) = 0 \,, \tag{B.9}$$

which concludes the proof of the claim.

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