Advanced Mathematical Physics Mod. A

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Abstract

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1 Fourier series and Fourier transform

1.1 Fourier series

Let us consider a periodic function $f : \mathbb{R} \to \mathbb{C}$, with period $L > 0$:

$$f(x + L) = f(x) \qquad \forall x \in \mathbb{R} \, . \tag{1.1}$$

An elementary example of such functions is the complex exponential, e^{ikx}, for $k \in \frac{2\pi}{L}\mathbb{Z}$. The goal of this section is to show that, under suitable regularity assumptions, periodic functions can be represented as linear combinations of such elementary periodic functions. This observation will be particularly useful when solving concrete partial differential equations.

Definition 1 (Fourier series.)**.** *Given an L-periodic function f, we define its Fourier series as:*

$$\sum_{k \in \frac{2\pi}{L}\mathbb{Z}} e^{ikx} c_k \, , \tag{1.2}$$

where the k-th Fourier coefficient is defined as:

$$c_k := \frac{1}{L} \int_0^L dx \, e^{-ikx} f(x) \, . \tag{1.3}$$

So far, the expression in (1.2) is purely formal: we do not know whether the series is convergent. As we shall see, whenever it is convergent, the Fourier series allows to reconstruct the function f. Let us start by discussing a sufficient criterion for convergence.

Theorem 1.1 (Convergence of the Fourier series for C^1 functions.)**.** *Let $f \in C^1(\mathbb{R})$, L-periodic. Let S_n be the partial Fourier series of f:*

$$S_n(x) := \sum_{\substack{k \in \frac{2\pi}{L}\mathbb{Z} \\ |k| \leqslant \frac{2\pi}{L} n}} e^{ikx} c_k \, . \tag{1.4}$$

Then, the following limit exists, uniformly in x:

$$f(x) = \lim_{n \to \infty} S_n(x) \, . \tag{1.5}$$

Remark 1.2. *The assumptions on the function f are by no means optimal. It is possible to show that the Fourier transform also converges for Hölder continuous function. Furthermore, almost-everywhere convergence of the Fourier transform is known to hold for square-summable functions f on $[0, L]$. We will not discuss such improvements, for which we refer the reader to e.g. [1].*

The proof of Theorem 1.1 relies on a number of simple but important ideas.

Scalar product. Given a complex vector space V, a scalar product $(\cdot, \cdot)$ is a bilinear map from $V \times V$ to $\mathbb{C}$ such that the following properties hold true:

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

(ii) $(g, \alpha f_1 + \beta f_2) = \alpha(g, f_1) + \beta(g, f_2)$ for all $\alpha, \beta \in \mathbb{C}$

(iii) $(f, f) \geqslant 0$ and $(f, f) = 0$ if and only if $f = 0$.

The first and the second property imply that $(\cdot,\cdot)$ is antilinear in the first entry:

$$(\alpha f_1 + \beta f_2, g) = \overline{\alpha}(f_1, g) + \overline{\beta}(f_2, g) \ . \tag{1.6}$$

Given a scalar product, we define its associated norm as:

$$\|f\| := \sqrt{(f,f)} \tag{1.7}$$

It is left to the reader to check that this operation really defines a norm (triangle inequality; homogeneity; positive definiteness). We say that V is a Hilbert space if it is complete with respect to the norm defined by the above scalar product. An example of Hilbert space is

$$L^2(A) := \left\{ f : A \to \mathbb{C} \mid \int_A dx\, |f(x)|^2 < \infty \right\} \tag{1.8}$$

with A a measurable subset of $\mathbb{R}$. The scalar product is the natural one,

$$(f,g) = \int_A dx\, \overline{f(x)} g(x) \ . \tag{1.9}$$

Approximation of continuous functions by trigonometric polynomials. Consider now as a vector space V the space of continuous L-periodic functions on $\mathbb{R}$:

$$C_{\text{per}}(\mathbb{R}) := \{ f \in C(\mathbb{R}) \mid f(x+L) = f(x) \quad \forall x \in \mathbb{R} \} \ . \tag{1.10}$$

On this vector space, let us define the scalar product:

$$(f,g) := \int_0^L dx\, \overline{f(x)} g(x) \ . \tag{1.11}$$

An orthonormal system with respect to this scalar product is provided by the plane waves e^{ikx}, appropriately normalized. Let:

$$e_k(x) := \frac{e^{ikx}}{\sqrt{L}} \ . \tag{1.12}$$

Then, one can easily check that:

$$(e_k, e_j) = \delta_{jk} \ . \tag{1.13}$$

with $\delta_{..}$ the Kronecker symbol. With this definition, we can rewrite the partial Fourier series of f as:

$$(S_n)(x) = \sum_{k : |k| \leqslant \frac{2\pi}{L} n} e_k(x)(e_k, f) \equiv \sum_{k : |k| \leqslant \frac{2\pi}{L} n} e_k(x) d_k \tag{1.14}$$

Comparing (1.14) with (1.4), we see that $c_k = L^{-1/2} d_k$. This rewriting shows that the partial Fourier transform is simply the orthogonal projection of the function f over the following finite dimensional vector space:

$$V_n = \text{span}\{e_k\}_{|k| \leqslant \frac{2\pi}{L} n} \ . \tag{1.15}$$

The elements of this vector space are called trigonometric polynomials:

$$P_n(x) = \sum_{k : |k| \leqslant \frac{2\pi}{L} n} a_k e^{ikx} \ , \qquad a_k \in \mathbb{C} \ . \tag{1.16}$$

Trigonometric polynomials can be used to approximate continuous periodic functions, to arbitrary precision. This is the content of the following theorem.

Theorem 1.3 (Weierstrass theorem.)**.** *Let f be continuous and L-periodic. For any $\varepsilon > 0$, there exists a trigonometric polynomial P_n of some order n such that:*

$$\sup_{x\in[0,L]} |f(x) - P_n(x)| \leqslant \varepsilon \, . \tag{1.17}$$

Proof. Consider the partial Fourier transform of f. We rewrite it in the following convenient way:

$$\begin{aligned} S_n(x) = \sum_{k\in\mathbb{Z}:|k|\leqslant n} c_k e^{i\frac{2\pi}{L}kx} &= \frac{1}{L}\int_0^L dy\, f(y) \sum_{k:|k|\leqslant n} e^{i\frac{2\pi}{L}k(x-y)} \\ &\equiv \int_0^L dy\, f(y) \frac{1}{L}\mathcal{D}_n((x-y)/L) \, . \end{aligned} \tag{1.18}$$

The function $\mathcal{D}_n(x-y)$ is called the Dirichlet kernel. A straightforward computation gives[1]:

$$\begin{aligned} \mathcal{D}_n(x-y) &= \sum_{k:|k|\leqslant n} e^{i2\pi k(x-y)} \\ &= \frac{\sin((2n+1)\pi(x-y))}{\sin(\pi(x-y))} \, . \end{aligned} \tag{1.20}$$

In general, $S_n(x)$ does not converge pointwise to f as $n \to \infty$, if only assume that f is continuous. We shall now find a better approximation of continuous functions in terms of trigonometric polynomials. Let us consider the Cesaro mean of the partial Fourier series:

$$\sigma_n(x) = \frac{1}{n}\sum_{k=0}^{n-1} S_n(x) \tag{1.21}$$

Using the expression (1.18), we rewrite it as:

$$\begin{aligned} \sigma_n(x) &= \int_0^L dy\, f(y) \frac{1}{L}\frac{1}{n}\sum_{k=0}^{n-1} \mathcal{D}_k((x-y)/L) \\ &\equiv \int_0^L dy\, f(y) \frac{1}{L}\mathcal{F}_n((x-y)/L) \end{aligned} \tag{1.22}$$

where $\mathcal{F}_n(x-y)$ is the Fejér kernel:

$$\mathcal{F}_n(x-y) = \frac{1}{n}\sum_{k=0}^{n-1} \mathcal{D}_k(x-y) \, . \tag{1.23}$$

A straightforward computation gives:

$$\mathcal{F}_n(x-y) = \frac{1}{n}\Big(\frac{\sin(\pi n(x-y))}{\sin\pi(x-y)}\Big)^2 \, . \tag{1.24}$$

The function $\sigma_n(x)$ is still a trigonometric polynomial, as manifest from (1.21), since S_n is a trigonometric polynomial. We claim that $\sigma_n(x)$ converges uniformly to $f(x)$ as $n \to \infty$. To prove this, we shall use the following two properties of the Fejér kernel:

[1] Use that:

$$\sum_{k=-n}^{n} e^{i2\pi k(x-y)} = e^{-i2\pi n(x-y)} \sum_{k=0}^{2n} e^{i2\pi k(x-y)} = e^{-i2\pi n(x-y)} \frac{1-e^{i2\pi(2n+1)(x-y)}}{1-e^{i2\pi(x-y)}} \, . \tag{1.19}$$

(i) $\int_0^1 dx\, \mathcal{F}_n(x) = 1$

(ii) $\int_\delta^{1-\delta} dx\, \mathcal{F}_n(x) \to 0$ as $n \to \infty$, for all $\delta > 0$.

The proof of the first property follows from:

$$\int_0^1 dx\, \mathcal{D}_n(x) = 1 \,. \tag{1.25}$$

The proof of the second property follows from the explicit expression (1.24), using that in the integral $\sin(\pi x)$ is bounded away from zero.

Let $\varepsilon > 0$, and let $\delta > 0$ such that:

$$|f(x) - f(y)| < \varepsilon/2 \qquad \forall y \in B_\delta(x) \,. \tag{1.26}$$

We write, using property (i):

$$\begin{aligned} f(x) - \sigma_n(x) &= \int_0^L dy\, (f(x) - f(y)) \frac{1}{L} \mathcal{F}_n((x-y)/L) \\ &= \int_{|x-y| \leqslant \delta/L} (\cdots) + \int_{|x-y| > \delta/L} (\cdots) \equiv \mathrm{I} + \mathrm{II} \,. \end{aligned} \tag{1.27}$$

Consider the first term. It is bounded as, using the positivity of the Fejér kernel and property (i):

$$|\mathrm{I}| \leqslant \frac{\varepsilon}{2} \int_0^L dy\, \frac{1}{L} \mathcal{F}_n((x-y)/L) = \frac{\varepsilon}{2} \,. \tag{1.28}$$

Consider the second term. Continuous periodic functions are in particular bounded. Hence:

$$\begin{aligned} |\mathrm{II}| &\leqslant C \int_{|x-y| > \delta/L} dy\, \frac{1}{L} \mathcal{F}_n((x-y)/L) \\ &\leqslant \varepsilon/2 \,, \end{aligned} \tag{1.29}$$

where the last inequality follows after taking n large enough, using property (ii) above. This concludes the proof. ∎

Convergence of the Fourier series. The above discussion allowed us to find an explicit approximation of continuous periodic functions in terms of trigonometric polynomials. We now turn to the problem of proving convergence of the Fourier series.

As discussed above, S_n can be viewed as the orthogonal projection of the function f over V_n. With this geometric interpretation at hand, the next lemma is not particularly surprising.

Lemma 1.4 (Bessel's inequality.)**.** *The following inequality holds true, for all L-periodic functions f, such that $\|f\| < \infty$:*

$$\|S_n\| \leqslant \|f\| \,. \tag{1.30}$$

Proof. By positivity of the norm, we have:

$$\|f - S_n\| \geqslant 0 \,. \tag{1.31}$$

Explicitly,

$$\begin{aligned}\|f-S_n\|^2 &= \Big(f-S_n\,,f-S_n\Big)\\ &= \Big(f-\sum_{k:|k|\leqslant\frac{2\pi}{L}n} e_k d_k\,,f-\sum_{j:|j|\leqslant\frac{2\pi}{L}n} e_j d_j\Big)\\ &= (f,f)+\sum_{k:|k|\leqslant\frac{2\pi}{L}n}\sum_{j:|j|\leqslant\frac{2\pi}{L}n}\overline{d_k}d_j(e_k,e_j)-\sum_{k:|k|\leqslant\frac{2\pi}{L}n}\overline{d_k}(e_k,f)-\sum_{j:|j|\leqslant\frac{2\pi}{L}n} d_j(f,e_j)\\ &= (f,f)+\sum_{j:|j|\leqslant\frac{2\pi}{L}n}|d_j|^2-\sum_{k:|k|\leqslant\frac{2\pi}{L}n}\overline{d_k}(e_k,f)-\sum_{j:|j|\leqslant\frac{2\pi}{L}n} d_j(f,e_j)\,,\end{aligned} \tag{1.32}$$

where in the last step we used the orthonormality of the plane waves. Finally, by definition of d_k's, we see that the sum of the last two terms is simply $-2\sum_{j:|j|\leqslant n}|d_j|^2$. Hence, we get:

$$0\leqslant(f,f)-\sum_{k:|k|\leqslant\frac{2\pi}{L}n}|d_k|^2\,, \tag{1.33}$$

which implies the claim. ∎

Corollary 1.1. *The following inequality holds true:*

$$\sum_k|d_k|^2\leqslant\|f\|^2\,. \tag{1.34}$$

Proof. The inequality immediately follows from (1.33), taking the limit $n\to\infty$. ∎

The partial Fourier series S_n is an element of the space of trigonometric polynomials V_n, defined in (1.15). It turns out that S_n provides the best approximation of f within V_n, in the L^2 sense.

Lemma 1.5. *Let $P_n(x)$ be a trigonometric polynomial, $P_n\in V_n$. Then, the following inequality holds true:*

$$\|f-S_n\|\leqslant\|f-P_n\|\,. \tag{1.35}$$

Proof. The starting point is the following identity:

$$(f-S_n,P_n)=0\,. \tag{1.36}$$

Next, we write:

$$\begin{aligned}\|f-P_n\|^2 &= \|f-S_n+S_n-P_n\|^2\\ &= \|f-S_n\|^2+\|S_n-P_n\|^2+2\mathrm{Re}(f-S_n,S_n-P_n)\,.\end{aligned} \tag{1.37}$$

The last term is zero, thanks to (1.36). Hence,

$$\|f-P_n\|^2\geqslant\|f-S_n\|^2\,, \tag{1.38}$$

and equality holds if and only if $\|S_n-P_n\|=0$. ∎

Remark 1.6. *(i) Lemma 1.5 combined with Theorem 1.3 prove the convergence of the Fourier series in the L^2 sense.*

(ii) Using that continuous functions are dense in L^2, and using that (e_k) is an orthonormal family, the above result also proves that (e_k) is an orthonormal basis for $L^2(S^1_L)$, with $S^1_L = \mathbb{R}/L\mathbb{Z}$ the circle of length L. The argument is as follows. Let $f \in L^2(S^1_L)$, and let $f_\varepsilon \in C(S^1_L)$ such that

$$\|f - f_\varepsilon\| < \varepsilon/3 \,. \tag{1.39}$$

Let $S_{n,\varepsilon}$ be the partial Fourier series of f_ε. By what we just proved:

$$\|f_\varepsilon - S_{n,\varepsilon}\| < \varepsilon/3 \tag{1.40}$$

for n large enough. Also, let S_n be the partial Fourier series of f. Then, by Bessel's inequality:

$$\|S_n - S_{n,\varepsilon}\| \leqslant \|f - f_\varepsilon\| < \varepsilon/3 \,. \tag{1.41}$$

Hence:

$$\|f - S_n\| \leqslant \|f - f_\varepsilon\| + \|f_\varepsilon - S_{n,\varepsilon}\| + \|S_{n,\varepsilon} - S_\varepsilon\| < \varepsilon \,. \tag{1.42}$$

This proves that any function $f \in L^2(S^1_L)$ can be approximated arbitrarily well, in the L^2-sense, by its orthogonal projection over V_n. In other words, (e_k) is an orthonormal basis for $L^2(S^1_L)$.

The next lemma plays the role of Pythagora's theorem, on an infinite dimensional vector space.

Lemma 1.7 (Parseval's identity)**.** *For any continuous, L-periodic function f, the following holds true:*

$$\sum_k |d_k|^2 = \|f\|^2 \,. \tag{1.43}$$

Proof. By Theorem 1.3, we know that for any $\varepsilon > 0$ there exists P_n of some order n such that:

$$\|f - P_n\| \leqslant \varepsilon \,. \tag{1.44}$$

Also, by (1.5):

$$\|f - S_n\| \leqslant \|f - P_n\| \leqslant \varepsilon \,. \tag{1.45}$$

Furthermore, from (1.32), (1.33) we have:

$$\left|(f,f) - \sum_{k:|k|\leqslant \frac{2\pi}{L}n} |d_k|^2\right| = \|f - S_n\|^2 \leqslant \varepsilon^2 \,. \tag{1.46}$$

By the arbitrariness of ε, this concludes the proof. ∎

Remark 1.8. *By the above mentioned density of continuous functions on $L^2(S^1_L)$, Parseval's theorem actually applies to all functions $f \in L^2(S^1_L)$.*

The following is an immediate corollary of Parseval's theorem.

Corollary 1.2. *Let f and g be two functions in $L^2(S^1_L)$. Suppose that their Fourier coefficients coincide. Then, $f = g$.*

Proof. The function $f - g$ is continuous and L-periodic, and has zero Fourier coefficients. Then, by Parseval's identity, $\|f - g\| = 0$ and hence $f - g = 0$. ∎

We are now ready to prove Theorem 1.1.

Proof of Theorem 1.1. [Pointwise convergence of the Fourier series.] We start by writing:

$$\begin{aligned} d_k &= \frac{1}{L^{1/2}} \int_0^L dx\, e^{-ikx} f(x) \\ &= \frac{1}{L^{1/2}} \int_0^L dx\, \frac{i}{k} (\partial_x e^{-ikx}) f(x) \\ &= -\frac{1}{L^{1/2}} \int_0^L dx\, \frac{i}{k} e^{-ikx} \partial_x f(x) \ , \end{aligned} \tag{1.47}$$

where the last identity follows integrating by parts (the boundary terms cancel thanks to the periodicity of the function). Therefore, we just proved that:

$$|d_k| \leqslant \frac{1}{k} |d'_k| \ , \tag{1.48}$$

where d'_k are the Fourier coefficients of $f'(x)$, a function in $C_{\rm per}(\mathbb{R})$. Therefore,

$$\sum_k \left| e^{ikx} c_k \right| \leqslant c_0 + \sum_{k\neq 0} \left| \frac{1}{k} c'_k \right| \leqslant c_0 + \Big(\sum_{k\neq 0} \frac{1}{k^2} \Big)^{\frac{1}{2}} \Big(\sum_k |c'_k|^2 \Big)^{\frac{1}{2}} \ , \tag{1.49}$$

and the last step follows from Cauchy-Schwarz inequality. Applying Parseval's theorem to the function f', we get:

$$\sum_k \left| e^{ikx} c_k \right| \leqslant c_0 + C \|f'\|^2 \ , \tag{1.50}$$

which proves absolute convergence of the Fourier series. Then, we notice that by construction the functions

$$f(x) \ , \qquad S(x) = \sum_k c_k e^{ikx} \tag{1.51}$$

have the same Fourier coefficients. Therefore, by Lemma 1.2 they coincide: $f(x) = S(x)$. Uniform convergence follows from:

$$|f(x) - S_n(x)| \leqslant \sum_{k:|k|\geqslant \frac{2\pi}{L} n} |c_k| \leqslant \Big(\sum_{k:|k|\geqslant \frac{2\pi}{L} n} \frac{1}{k^2} \Big)^{\frac{1}{2}} \Big(\sum_{k\geqslant \frac{2\pi}{L} n} |c'_k|^2 \Big)^{\frac{1}{2}} \tag{1.52}$$

which tends to zero as $N \to \infty$, uniformly in x. ∎

Before concluding this section, let us discuss some further properties of the Fourier series.

The Fourier series of real functions. Suppose that $f(x) \in \mathbb{R}$. Then,

$$\sum_k e^{ikx} c_k = \overline{\sum_k e^{ikx} c_k} = \sum_k e^{-ikx} \overline{c_k} = \sum_k e^{ikx} \overline{c_{-k}} \ . \tag{1.53}$$

Since the Fourier coefficients uniquely determine the function, we immediately get

$$c_k = \overline{c_{-k}} \ . \tag{1.54}$$

In particular, the coefficient c_0 is real. Real-valued periodic functions can be conveniently expanded in terms of sine and cosine:

$$\begin{aligned} f(x) &= \sum_k e^{ikx} c_k = c_0 + \sum_{k>0} (e^{ikx} c_k + e^{-ikx} c_{-k}) \\ &= c_0 + \sum_{k>0} (e^{ikx} c_k + e^{-ikx} \overline{c_k}) \\ &= \frac{a_0}{2} + \sum_{k>0} \cos(kx) a_k + \sin(kx) b_k \ , \end{aligned} \tag{1.55}$$

where we set:

$$a_k = c_k + \overline{c_k} \ , \qquad b_k = i(c_k - \overline{c_k}) \ . \tag{1.56}$$

Derivatives. The main application of the Fourier series to differential equations is that it allows to convert derivatives into multiplication operators. Let c'_n be the Fourier coefficients of f'. In the proof of Theorem 1.1 we have seen that:

$$\partial_x f(x) = \sum_k ike^{ikx} c_k \ . \tag{1.57}$$

More generally, provided the sum makes sense:

$$\partial_x^n f(x) = \sum_k (ik)^n e^{ikx} c_k \ . \tag{1.58}$$

These simple properties allow to turn differential equations for periodic functions into algebraic equations.

Higher dimensions. The previous discussion generalizes to periodic functions in $\mathbb{R}^d$:

$$f(x) = f(x + v_i n_i L) \ . \tag{1.59}$$

with v_i the standard basis of $\mathbb{R}^d$ and $n_i \in \mathbb{Z}$. The Fourier series of f is defined as:

$$\sum_{k \in \frac{2\pi}{L}\mathbb{Z}^d} e^{ik\cdot x} c_k \ , \tag{1.60}$$

with Fourier coefficients:

$$c_k = \frac{1}{L^d} \int_{[0,L]^d} dx \, e^{-ik\cdot x} f(x) \ . \tag{1.61}$$

All the results proved above for functions on $\mathbb{R}$ extends to functions on $\mathbb{R}^d$, and we leave the details to the reader.

Simple application. Before concluding the section, let us discuss a simple application of the Fourier series. Let $u(x,t)$ be the temperature profile of a conducting ring, of length L; $x \in S^1_L$ is the position on the ring, while t is time. Let $u(x)$ be the temperature distribution at the time $t = 0$. At later times, the evolution of the temperature profile satisfies the heat equation:

$$\partial_t u(x,t) = \partial_x^2 u(x,t) \ , \qquad u(x,0) = u(x) \ . \tag{1.62}$$

Later, we will discuss the heat equation in much greater generality. For the sake of the present discussion, let us show how to use the Fourier series to solve this PDE. Suppose that $u(x)$ is a smooth initial datum. We are looking for a smooth function $u(x,t)$, such that $u(x,t) = u(x+L,t)$ for all times, satisfying (1.62). It is convenient to represent the function in terms of its Fourier series:

$$u(x,t) = \sum_{k \in \frac{2\pi}{L}\mathbb{Z}} e^{ikx} c_k(t) \ . \tag{1.63}$$

By what we discussed above, the series converges pointwise. Also, being $u(x,t)$, the functions $\partial_t u(x,t)$ and $\partial_x^2 u(x,t)$ can also be represented in terms of the Fourier series. We have:

$$\partial_t u(x,t) = \sum_{k \in \frac{2\pi}{L}\mathbb{Z}} e^{ikx} \partial_t c_k(t) \ , \qquad \partial_x^2 u(x,t) = \sum_{k \in \frac{2\pi}{L}\mathbb{Z}} e^{ikx} (-k^2) c_k(t) \ . \tag{1.64}$$

The equation (1.62) reads:

$$0 = \sum_{k \in \frac{2\pi}{L}\mathbb{N}} e^{ikx} (\partial_t + k^2) c_k(t) \ . \tag{1.65}$$

By Plancherel's theorem, this equation holds if and only if the Fourier coefficients in the right-hand side are identically zero:

$$(\partial_t + k^2)c_k(t) = 0 \,, \qquad c_k(0) = \frac{1}{L}\int_0^L dx\, e^{-ikx}u(x) \,. \tag{1.66}$$

The solution to this ODE is simply:

$$c_k(t) = e^{-k^2 t}c_k(0) \,. \tag{1.67}$$

That is, the solution to the original PDE is:

$$u(x,t) = \sum_{k\in\frac{2\pi}{L}\mathbb{Z}} e^{ikx}e^{-k^2t}c_k(0) \,. \tag{1.68}$$

In particular, as $t \to \infty$, the solution converges pointwise to:

$$u_\infty(x) = c_0(0) = \frac{1}{L}\int_0^L dx\, u(x) \,. \tag{1.69}$$

Thus, the temperature gradient converges to the average initial temperature.

1.2 Fourier transform

As mentioned at the end of the previous section, the main application of the Fourier series to partial differential equations is that it allows to turn differential operators into multiplication operators. Not all interesting PDEs however involve unknown functions which are spatially periodic: we would like to have a similar tools for nonperiodic functions as well. Here we will introduce such tool, the Fourier transform; we will follow [2], Section 4.3.1.

In order to introduce the right functional setting for the Fourier transform, recall the definition of L^p spaces, for $0 < p < \infty$,

$$L^p(\mathbb{R}^d) := \left\{ f : \mathbb{R}^d \to \mathbb{C} \mid \int dx\, |f(x)|^p < \infty \right\} . \tag{1.70}$$

The definition of course applies to continuous functions, with $\int$ being the Riemann integral. More generally, it applied to measurable functions, in which case $\int$ has to be understood as the Lebesgue integral. The two notions coincide, whenever the f is continuous. We also define the L^∞ space as:

$$L^\infty(\mathbb{R}^d) := \left\{ f : \mathbb{R}^d \to \mathbb{C} \mid \sup_{x\in\mathbb{R}^d} |f(x)| < \infty \right\} . \tag{1.71}$$

The definition extends to measurable functions, and in that case the supremum is replaced by the essential supremum $\operatorname{ess\,sup}_{x\in\mathbb{R}^d}$. We refer to [6], Chapter 2, for an introduction to L^p spaces.

Definition 2 (Fourier transform of L^1 functions.)**.** *Let $f \in L^1(\mathbb{R}^d)$. We define the Fourier transform of f as:*

$$\hat{f}(k) = \int \frac{dx}{(2\pi)^{\frac{d}{2}}}\, e^{-ik\cdot x} f(x) \,. \tag{1.72}$$

Let us spell out some basic properties of the Fourier transform.

Basic properties.

(i) The function $\hat{f}(k)$ is bounded:

$$|\hat{f}(k)| \leqslant \frac{1}{(2\pi)^{\frac{d}{2}}}\int dx\, |f(x)| < \infty \tag{1.73}$$

due to the fact that the function f is in L^1.

(ii) The function $\hat{f}(k)$ is continuous:

$$\lim_{k\to q}\hat{f}(k)=\lim_{k\to q}\int\frac{dx}{(2\pi)^{\frac{d}{2}}}\,e^{-ik\cdot x}f(x)=\int\frac{dx}{(2\pi)^{\frac{d}{2}}}\,\lim_{k\to q}e^{-ik\cdot x}f(x)=\hat{f}(q)\;. \tag{1.74}$$

The second equality follows from dominated convergence theorem, which we can apply since the function $k\mapsto e^{-ik\cdot x}f(x)$ is continuous in k, and the function $x\mapsto e^{-ik\cdot x}f(x)$ is absolutely integrable, uniformly in k.

(iii) The function $\hat{f}(k)$ decays at infinity. At first, suppose that f is in $C^1\cap L^1$, such that $\partial_{x_j}f\in L^1$ Then:

$$k_j\hat{f}(k)=\int\frac{dx}{(2\pi)^{\frac{d}{2}}}\,k_je^{-ik\cdot x}f(x)=-i\int\frac{dx}{(2\pi)^{\frac{d}{2}}}\,e^{-ik\cdot x}\partial_{x_j}f(x)\;. \tag{1.75}$$

Therefore,

$$|k_j\hat{f}(k)|\leqslant\frac{1}{(2\pi)^d}\|\partial_{x_j}f\|_1\Rightarrow|\hat{f}(k)|\leqslant\frac{C}{|k_j|}\;. \tag{1.76}$$

Thus, $\lim_{k_j\to\infty}\hat{f}(k)=0$. The statement extends to functions with are just L^1. This follows from the fact smooth, compactly supported functions are dense in L^p with $1\leqslant p<\infty$. Let $(f_n)\subset C_c^\infty(\mathbb{R}^d)$, such that:

$$\lim_{n\to\infty}\|f-f_n\|_1=0\;. \tag{1.77}$$

Take $\varepsilon>0$. Write:

$$\hat{f}(k)=\hat{f}_n(k)+f(x)-f_n(x)\;. \tag{1.78}$$

For n large enough:

$$\Big|\int\frac{dx}{(2\pi)^{\frac{d}{2}}}\,e^{-ik\cdot x}(f(x)-f_n(x))\Big|\leqslant\frac{1}{(2\pi)^{\frac{d}{2}}}\|f-f_n\|_1\leqslant\frac{\varepsilon}{2}\;. \tag{1.79}$$

Also, for $|k|$ large enough:

$$|\hat{f}_n(k)|\leqslant\frac{\|\partial_{x_j}f_n\|_1}{|k_j|}\leqslant\frac{\varepsilon}{2}\;. \tag{1.80}$$

All in all, for $|k|$ large enough:

$$|\hat{f}(k)|\leqslant\varepsilon \tag{1.81}$$

that is $\hat{f}(k)\to 0$ as $|k|\to\infty$. This result takes the name of Riemann-Lebesgue lemma.

(iv) The Fourier transform turns convolutions into products. Let f and g be functions in $L^1\cap L^2$. Consider their convolution:

$$h(x):=f*g(x):=\int dy\,f(x-y)g(y)\;. \tag{1.82}$$

The requirement that f,g are in L^2 is needed in order to make sure that the convolution exists. Let us compute the Fourier transform of the convolution. We get:

$$\begin{aligned}\hat{h}(k)&=\int\frac{dz}{(2\pi)^{\frac{d}{2}}}\,e^{-ik\cdot z}h(z)\\&=\int\frac{dz}{(2\pi)^{\frac{d}{2}}}\int dy\,f(z-y)g(y)e^{-ik\cdot(z-y)}e^{-ik\cdot y}\\&=(2\pi)^{\frac{d}{2}}\int\frac{dy}{(2\pi)^{\frac{d}{2}}}\int\frac{dz}{(2\pi)^{\frac{d}{2}}}\,f(z)g(y)e^{-ik\cdot z}e^{-ik\cdot y}\equiv(2\pi)^{\frac{d}{2}}\hat{f}(k)\hat{g}(k)\;.\end{aligned} \tag{1.83}$$

The exchange of integrals in the third equality sign is allowed by Fubini's theorem, since both functions are in L^1.

(v) Rescalings. Let $f_\lambda(x) = f(\lambda x)$. Then:

$$\begin{aligned}(\hat{f_\lambda})(k) &= \int \frac{dx}{(2\pi)^{\frac{d}{2}}}\, e^{-ik\cdot x} f_\lambda(x) \\ &= \lambda^{-d} \int \frac{d\lambda x}{(2\pi)^{\frac{d}{2}}}\, e^{-i\lambda^{-1}k\cdot\lambda x} f(\lambda x) \\ &= \lambda^{-d}\hat{f}(k/\lambda)\ .\end{aligned} \tag{1.84}$$

(vi) Action on differential/multiplication operators. Let $\alpha = (\alpha_1, \dots, \alpha_d)$, $\beta = (\beta_1, \dots, \beta_d)$ be multi-indeces. Let us introduce the notation:

$$x^\alpha = \prod_{i=1}^d x_i^{\alpha_i}\ , \qquad D^\beta = \prod_{i=1}^d \partial_i^{\beta_i}\ . \tag{1.85}$$

Suppose that, for all $|\alpha| \leqslant k$, $|\beta| \leqslant j$:

$$x^\alpha D^\beta f \in L^1(\mathbb{R}^d)\ . \tag{1.86}$$

Then:

$$\begin{aligned}\widehat{x^\alpha D^\beta f}(k) &= \int \frac{dx}{(2\pi)^{\frac{d}{2}}}\, e^{-ik\cdot x} x^\alpha D^\beta f(x) \\ &= (iD)^\alpha \int \frac{dx}{(2\pi)^{\frac{d}{2}}}\, e^{-ik\cdot x} D^\beta f(x) \\ &= (iD)^\alpha \int \frac{dx}{(2\pi)^{\frac{d}{2}}}\, ((-D)^\beta e^{-ik\cdot x}) f(x) \\ &= (iD)^\alpha (ik)^\beta \hat{f}(k)\ .\end{aligned} \tag{1.87}$$

Thus, as for the Fourier series, the Fourier transform turns differential operators into multiplication operators (and viceversa). The importance of this is that it will allow to turn PDEs into algebraic equations.

It is useful to compute the Fourier transform of a Gaussian function.

Proposition 1.9 (Fourier transform of a Gaussian.)**.** *Let $g(x)$ be the Gaussian function,*

$$g(x) = e^{-|x|^2}\ . \tag{1.88}$$

Then,

$$\hat{g}(k) = 2^{-\frac{d}{2}} e^{-\frac{|k|^2}{4}}\ . \tag{1.89}$$

Proof. We write:

$$\begin{aligned}\hat{g}(k) &= \int \frac{dx}{(2\pi)^{\frac{d}{2}}}\, e^{-ik\cdot x} e^{-|x|^2} \\ &= \int \frac{dx}{(2\pi)^{\frac{d}{2}}}\, e^{-|x+ik/2|^2} e^{-|k|^2/4}\ .\end{aligned} \tag{1.90}$$

The integral can be written as:

$$\int \frac{dx}{(2\pi)^{\frac{d}{2}}}\, e^{-|x+ik/2|^2} = \prod_{j=1}^d \frac{1}{(2\pi)^{\frac{1}{2}}} \int da\, e^{-(a+ik_j)^2}\ . \tag{1.91}$$

A simple application of the residue theorem shows that the integral is actually independent of k_j. Hence:

$$\begin{aligned}\int \frac{dx}{(2\pi)^{\frac{d}{2}}}\, e^{-|x+ik/2|^2} &= \prod_{j=1}^{d} \frac{1}{(2\pi)^{\frac{1}{2}}} \int da\, e^{-a^2} \\ &= \frac{1}{2^{\frac{d}{2}}}\ .\end{aligned} \tag{1.92}$$

Plugging (1.92) into (1.90), we get the claim. ∎

It turns out that the Fourier transform can also be defined on $L^2(\mathbb{R}^d)$. The definition however cannot be the one given in (1.72), since the integral is in general divergent for L^2 functions. On this space, the Fourier transform will have the nice property defining an isometry. The starting point to define the Fourier transform in L^2 is the following theorem.

Theorem 1.10 (Plancherel.)**.** *Let $f \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$. Then, $\hat{f}$ is in $L^2(\mathbb{R}^d)$, and the following identity holds:*

$$\|f\|_2 = \|\hat{f}\|_2\ . \tag{1.93}$$

Proof. Let f, g in L^1. We start by noticing that:

$$\int dx\, f(x)\hat{g}(x) = \int dy\, \hat{f}(y) g(y)\ . \tag{1.94}$$

Let us now take g to be a rescaled Gaussian function:

$$g_\lambda(x) = e^{-\lambda|x|^2}\ . \tag{1.95}$$

As discussed in Proposition 1.9, the Fourier transform of this function is:

$$\hat{g}_\lambda(k) = \frac{1}{(2\lambda)^{\frac{d}{2}}} e^{-|k|^2/4\lambda}\ . \tag{1.96}$$

Eq. (1.94) reads:

$$\int dy\, f(y) \frac{1}{(2\lambda)^{\frac{d}{2}}} e^{-|k|^2/4\lambda} = \int dx\, \hat{f}(x) e^{-\lambda|x|^2}\ . \tag{1.97}$$

Now, take $f \in L^1 \cap L^2$, and define $h(x) = \overline{f(-x)}$. Let $w = h * f$. By property (iv) above,

$$\hat{w} = (2\pi)^{\frac{d}{2}} \hat{h}\hat{f} = (2\pi)^{\frac{d}{2}} |\hat{f}|^2\ . \tag{1.98}$$

The function w is continuous (exercise), and hence:

$$\lim_{\lambda\to 0} \int dx\, w(x)\hat{g}_\lambda(x) = (2\pi)^{\frac{d}{2}} w(0) = (2\pi)^{\frac{d}{2}} \|f\|_2^2\ . \tag{1.99}$$

On the other hand, by (1.94) the left-hand side of (1.99) is equal to:

$$\begin{aligned}\lim_{\lambda\to 0} \int dx\, \hat{w}(x) g_\lambda(x) &= \lim_{\lambda\to 0} \int dx\, \hat{w}(x) e^{-\lambda|x|^2} \\ &= \int dx\, \hat{w}(x) = (2\pi)^{\frac{d}{2}} \|\hat{f}\|_2^2\ .\end{aligned} \tag{1.100}$$

This concludes the proof of the theorem. ∎

Definition of the Fourier transform in L^2. Let $f \in L^2$, and let (f_n) be an approximating sequence in $L^1 \cap L^2$:

$$\lim_{n\to\infty} \|f - f_n\|_2 = 0 \,. \tag{1.101}$$

The existence of such sequence is guaranteed by the density of C_c^∞ in L^2. By Plancherel,

$$\|\hat{f}_n - \hat{f}_m\|_2 = \|f_n - f_m\|_2 \to 0 \qquad \text{as } n, m \to \infty. \tag{1.102}$$

Thus, $(\hat{f}_n)$ forms a Cauchy sequence in L^2. Being L^2 complete (all Cauchy sequences converge to a limit in L^2), there exists $\hat{f}$ such that:

$$\lim_{n\to\infty} \|\hat{f} - \hat{f}_n\|_2 = 0 \,. \tag{1.103}$$

We define $\hat{f}$ as the Fourier transform of f. To check that the definition is meaningful, let us verify that $\hat{f}$ does not depend on the choice of the approximating sequence. Let (g_n) be another sequence in $L^1 \cap L^2$ such that $g_n \to f$. Let $\hat{g}$ the Fourier transform constructed above. We have:

$$\|\hat{f} - \hat{g}\| = \lim_{n,m} \|\hat{f}_n - \hat{g}_m\| = \lim_{n,m} \|f_n - g_m\| \leqslant \lim_n \|f_n - f\| + \lim_m \|f - g_m\| = 0 \,. \tag{1.104}$$

One can check that the L^2 Fourier transform satisfies the properties (iv), (v) and (vi) above. Recall the definition of L^2-scalar product:

$$(f, g) = \int dx\, \overline{f(x)} g(x) \,. \tag{1.105}$$

The next property is a simple consequence of Plancherel's theorem.

Proposition 1.11. *Let f, g in L^2. Then:*

$$(f, g) = (\hat{f}, \hat{g}) \,. \tag{1.106}$$

Proof. For $f = g$, the identity is Plancherel theorem. More generally, we have:

$$\|f + \alpha g\|_2^2 = \|\hat{f} + \alpha \hat{g}\|_2^2 \,. \tag{1.107}$$

Expanding both sides and using Plancherel, we get:

$$\alpha(f, g) + \overline{\alpha}(g, f) = \alpha(\hat{f}, \hat{g}) + \overline{\alpha}(\hat{g}, \hat{f}) \,. \tag{1.108}$$

Let $\alpha = 1$. The identity reads:

$$\mathrm{Re}\,(f, g) = \mathrm{Re}\,(\hat{f}, \hat{g}) \,. \tag{1.109}$$

Instead, for $\alpha = i$ we get:

$$\mathrm{Im}\,(f, g) = \mathrm{Im}\,(\hat{f}, \hat{g}) \,. \tag{1.110}$$

Eq. (1.109) and (1.110) imply the claim. ∎

The above discussion shows that Fourier transform defined an isometry $\mathcal{F} : L^2 \to L^2$. To conclude, let us find the explicit form for the inverse Fourier transform. For $f \in L^1$, define:

$$\check{f}(k) = \hat{f}(-k) \,. \tag{1.111}$$

The $\check{\cdot}$ operation is then extended to L^2 as for the $\hat{\cdot}$ operation.

Proposition 1.12 (Inverse Fourier transform.)**.** *Let $f \in L^2$ and let $\mathcal{F}f := \hat{f}$. Then,*

$$\mathcal{F}^{-1} f(k) = \check{f}(k) \,. \tag{1.112}$$

Proof. Our goal is to show that $\check{\hat{f}} = f$. Recall that:

$$\int dx\, \check{f}(x) g(x) = \int dx\, f(x) \check{g}(x) \,. \tag{1.113}$$

Then,

$$\int dx\, \check{\hat{f}}(x) g(x) = \int dx\, \hat{f}(x) \check{g}(x) = \int dx\, \hat{f}(x) \overline{\hat{\overline{g}}}(x) \equiv (\hat{\overline{g}}, \hat{f}) \,. \tag{1.114}$$

By Eq. (1.106):

$$\int dx\, \check{\hat{f}}(x) g(x) = (\overline{g}, f) = \int dx\, f(x) g(x) \,. \tag{1.115}$$

Being (1.115) true for all $g \in L^2$, we get

$$\check{\hat{f}} = f \,, \tag{1.116}$$

and the proof is concluded. ∎

Simple application. Before concluding the section, let us discuss a simple application of the Fourier transform. As for the Fourier series, we shall consider again the heat equation, this time on the real line:

$$\partial_t u(x,t) = \partial_x^2 u(x,t) \,, \qquad u(x,0) = u(x) \,, \tag{1.117}$$

and we assume that $u(x)$ is smooth and such that all derivatives are in L^2. As we will discuss later in more detail, the above equation describes the evolution of a temperature gradient $u(x,t)$ of an infinite conducting bar. We look for a solution $u(x,t)$ which is smooth in both variables, and such that all derivatives are in L^2. Taking the Fourier transform of both sides of (1.117) we get:

$$\partial_t \hat{u}(k,t) = -k^2 \hat{u}(k,t) \,, \qquad \hat{u}(k,0) = \hat{u}(k) \,. \tag{1.118}$$

The solution is:

$$\hat{u}(k,t) = e^{-k^2 t} \hat{u}(k) \,. \tag{1.119}$$

This suggests the following expression for $u(x,t)$:

$$u(x,t) = \int \frac{dk}{(2\pi)^{\frac{1}{2}}}\, e^{ikx} e^{-k^2 t} \hat{u}(k) \,. \tag{1.120}$$

If $(1+k^2)\hat{u}(k) \in L^1$, one can easily check that this function is indeed a solution of the heat equation. In particular, the solution converges to, as $t \to \infty$:

$$u_\infty(x) = \lim_{t\to\infty} \int \frac{dk}{(2\pi)^{\frac{1}{2}}}\, e^{ikx} e^{-k^2 t} \hat{u}(k) = \int \frac{dk}{(2\pi)^{\frac{1}{2}}}\, e^{ikx} \lim_{t\to\infty} e^{-k^2 t} \hat{u}(k) = 0 \,. \tag{1.121}$$

The interchange of limit and integration is allowed by dominated convergence theorem. Physically, all the heat is dissipated at infinity.

2 Poisson equation

2.1 Motivations

The Poisson equation is a PDE describing the electrostatic potential generated by a fixed charge distribution. We shall discuss the mathematics of this equation, following [2], Section 2.2.

Let $f(x) : \mathbb{R}^3 \to \mathbb{R}$ be a charge distribution, and let $E(x) : \mathbb{R}^3 \to \mathbb{R}^3$ be the electric field generated by such distribution. The equations of electrostatics read:

$$\begin{aligned} \nabla \cdot E &= f \\ \nabla \times E &= 0 \, . \end{aligned} \tag{2.1}$$

Recall the significance of the electric field: $E(x)$ is the force per unit charge acting on a charged particle. The second equation in (2.1) encodes the fact that the electric force is conservative: the work performed by a charge moving in an electric field moving from a to b does not depend on the path connecting a and b. In order words, the work performed on a closed loop is exactly zero. In fact, considering a loop γ, encircling a region U:

$$\int_\gamma E \cdot d\ell = \int_U dx \, n(x) \cdot (\nabla \times E)(x) = 0 \tag{2.2}$$

where $n(x)$ is the normal vector at x, compatible with the orientation of the boundary γ. The first identity is Stokes' theorem, while the last follows from (2.1). Concerning the first equation (2.1), it encodes Gauss law, which states that, considering a region Ω of $\mathbb{R}^3$, the electric flux through $\partial\Omega$ is equal to the total charge contained in Ω. The total flux is equal to

$$\int_{\partial\Omega} E \cdot n \, dx = \int_\Omega \mathrm{div} E \, dx \, , \tag{2.3}$$

where the identity follows from the divergence theorem. Also, using the first equation of (2.1):

$$\int_\Omega \mathrm{div} E \, dx = \int_\Omega f(x) dx \, , \tag{2.4}$$

where the right-hand side has the meaning of total charge contained in Ω. This shows that the first of (2.1) is equivalent to Gauss' law.

Provided E is regular enough, the second equation of (2.1) is equivalent to:

$$E(x) = -\nabla u(x) \, , \tag{2.5}$$

for a function $u(x)$, called the electric potential. Therefore, the first equation of (2.1) then implies:

$$-\Delta u(x) = f \, , \tag{2.6}$$

which takes the name of Poisson equation. The solution to this equation describes the electric potential generated by the charge distribution f.

Eq. (2.6) is formulated in the whole space. It could be of relevance to consider the associated Dirichlet problem. Let $U \subset \mathbb{R}^d$, with U open. We define the Poisson equation with Dirichlet boundary conditions as:

$$\begin{aligned} -\Delta u(x) &= f(x) \qquad \text{for } x \in U \\ u(x) &= g(x) \qquad \text{for } x \in \partial U \, . \end{aligned} \tag{2.7}$$

The homogeneous version of the Poisson equation, obtained setting $f = 0$, is called Laplace equation. This equation describes the propagation of the electric field inside a region, conditioned to the value of the electrostatic potential at the boundary of the region. Functions satisfying the Laplace equation are called harmonic.

Definition 3 (Harmonic function.)**.** *Let $U \subseteq \mathbb{R}^d$, U open. Let $u : \overline{U} \to \mathbb{R}$ such that $u \in C^2(U)$ and*

$$\Delta u = 0 \qquad \text{in } U. \tag{2.8}$$

Then, we say that $u(x)$ is harmonic in U.

For $d = 1$, harmonic functions are linear, $u(x) = ax + b$. For $d \geqslant 2$, things become more complicated, as we will see below.

To conclude the introduction, let us stress that the Laplace/Poisson equation appears as mathematical description of many physical phenomena, that have nothing to do with electromagnetism. As we will see, it also describes stationary solutions of the heat equation, or stationary solutions of the wave equation. See [4], Chapter 12, for further examples.

2.2 Fundamental solution of the Laplace equation

To begin, let us look for solutions of the Laplace equation in $\mathbb{R}^d$. This equation always admits the trivial solution $u(x) = \text{const}$. In fact, from the theory of the Fourier transform, this is the only available solution, with const $= 0$, if we assume that $u \in L^2$ and $\Delta u \in L^2$. Taking the Fourier transform of the Laplace equation we get:

$$|k|^2 \hat{u}(k) = 0 \,, \tag{2.9}$$

which only admits $\hat{u}(k) = 0$ as solution. Thus, nontrivial solutions of the Laplace equation cannot be such that $u \in L^2$ and $\Delta u \in L^2$.

In order to find nontrivial solutions of the Laplace equation, we will not rely on the Fourier transform. To begin, we shall look for solutions respecting the symmetry properties of the equation.

Proposition 2.1 (Rotation invariance of the Laplace equation.)**.** *Let $u(x)$ be such that $\Delta u(x) = 0$. Then $v(x) = u(Rx)$ with $RR^T = R^T R = 1$ is such that $\Delta v(x) = 0$.*

Proof. By the chain rule:

$$\partial_i v(x) = \sum_j R_{ji} (\partial_j u)(Rx) \,. \tag{2.10}$$

Furthermore,

$$\partial_i^2 v(x) = \sum_{j,j'} R_{ji} R_{j'i} (\partial_{j,j'} u)(Rx) \,. \tag{2.11}$$

Hence:

$$\begin{aligned} \sum_i \partial_i^2 v(x) &= \sum_{i,j,j'} R_{ji} R_{j'i} (\partial_{j,j'} u)(Rx) \\ &= \sum_{j,j'} (RR^T)_{jj'} (\partial_{j,j'} u)(Rx) \\ &\sum_j (\partial_j^2 u)(Rx) \,, \end{aligned} \tag{2.12}$$

where in the last step we used that $(RR^T)_{j,j'} = \delta_{jj'}$. This concludes the proof. ∎

We will look for solutions of the Laplace equation that respect the symmetries of the equation. That is, we will look for $u(x)$ such that $u(x) = v(r)$, with $r = |x|$. Let us understand the action of the Laplacian on a radial function. We have:

$$\begin{aligned} \partial_{x_i} u(x) &= \partial_{x_i} v(|x|) = v'(|x|) \frac{x_i}{|x|} \\ \partial_i^2 u(x) &= v''(|x|) \left(\frac{x_i}{|x|} \right)^2 + v'(|x|) \left(\frac{1}{|x|} - \frac{x_i^2}{|x|^3} \right) . \end{aligned} \tag{2.13}$$

Therefore,

$$\sum_{i=1}^d \partial_i^2 u(x) = v''(r) \frac{r^2}{r^2} + v'(r) \left(\frac{n}{r} - \frac{r^2}{r^3} \right) \tag{2.14}$$

meaning that

$$\Delta u = 0 \iff v''(r) + v'(r)\frac{d-1}{r} = 0\ . \tag{2.15}$$

By defining $h(r) = v'(r)$, Eq. (2.15) becomes:

$$h'(r) + h(r)\frac{d-1}{r} = 0 \Rightarrow h(r) = \frac{a}{r^{d-1}}, \tag{2.16}$$

which gives:

$$v(r) = \int dr\, \frac{a}{r^{d-1}} = \begin{cases} b\log r + c & \text{if } d = 2, \\ \frac{b}{r^{d-2}} + c & \text{if } d \geqslant 3. \end{cases} \tag{2.17}$$

Definition 4 (Fundamental solution of the Laplace equation)**.** *Let $\alpha(d) = \frac{\pi^{d/2}}{\Gamma\left(\frac{d}{2}+1\right)}$ be the volume of the unit ball in $\mathbb{R}^d$, $\Gamma(z) = \int_0^\infty dx\, x^{z-1}e^{-x}$ for $\mathrm{Re}\, z > 0$. For $x \in \mathbb{R}^d\backslash\{0\}$, the function*

$$\Phi(x) = \begin{cases} -\frac{1}{2}|x| & \text{if } d = 1 \\ -\frac{1}{2\pi}\log|x| & \text{if } d = 2 \\ \frac{1}{d(d-2)\alpha(d)}\frac{1}{|x|^{d-2}} & \text{if } d \geqslant 3 \end{cases} \tag{2.18}$$

is called the fundamental solution of the Laplace equation*.*

Notice that the fundamental solution is defined only for $x \neq 0$. It is a solution of the following PDE:

$$\Delta u = 0 \qquad \text{in } \mathbb{R}^d\backslash\{0\}. \tag{2.19}$$

The function $x \mapsto \Phi(x-y)$ is harmonic in $x \neq y$, and so is the function $x \mapsto f(y)\Phi(x-y)$. We shall now be interested in considering linear combinations of such functions, namely:

$$u(x) = \int dy\, \Phi(x-y)f(y)\ . \tag{2.20}$$

Using that $\Phi(x-y)$ is harmonic in $x \neq y$, and using that in the integral the lack of harmonicity only involves a zero measure set, we would be temped to conclude that $u(x)$ is harmonic in x as well. The issue with this reasoning is that we cannot interchange the y integration with the Laplacian Δ_x. In fact,

$$\Delta_x \Phi(x-y) \sim \frac{1}{|x-y|^d}\ , \tag{2.21}$$

which is not integrable in d dimensions. As a consequence of this fact, the function $u(x)$ in (2.20) turns out to be not harmonic. Moreover, as the next theorem proves, the function $u(x)$ in (2.20) is a solution of the Poisson equation.

Theorem 2.2 (Solving the Poisson equation.)**.** *Suppose that $f \in C_c^2(\mathbb{R}^d)$. Let u be given by (2.20). Then, $u \in C^2(\mathbb{R}^d)$, and furthermore:*

$$-\Delta u = f \qquad \text{in } \mathbb{R}^d. \tag{2.22}$$

That is, f is a solution of the Poisson equation.

Proof. 1. We shall only discuss the cases $d \geqslant 2$, and we leave the case $d = 1$ as an exercise. Let

$$u(x) = \int_{\mathbb{R}^d} dy\, \Phi(x-y)f(y) = \int_{\mathbb{R}^d} dy\, \Phi(y)f(x-y), \tag{2.23}$$

by a simple change of variables. Let $v_1, \cdots, v_d$ be the standard basis of $\mathbb{R}^d$, and consider

$$\frac{u(x+hv_i)-u(x)}{h} = \int_{\mathbb{R}^d} dy\, \Phi(y) \frac{f(x+hv_i-y)-f(x-y)}{h}. \tag{2.24}$$

By assumption $f \in C_c^2$, which means that

$$\lim_{h\to 0} \frac{f(x+hv_i-y)-f(x-y)}{h} = f_{x_i}(x-y), \tag{2.25}$$

and the limit is reached uniformly in $x-y$. Therefore,

$$u_{x_i}(x) = \int_{\mathbb{R}^d} \Phi(y) f_{x_i}(x-y) dy. \tag{2.26}$$

Repeating the argument,

$$u_{x_i x_j} = \int_{\mathbb{R}^d} \Phi(y) f_{x_i x_j}(x-y) dy, \tag{2.27}$$

and using again that $f \in C_c^2$ we infer that $u_{x_i x_j}$ is continuous in x.

2. Let us now compute the integral. Let $\epsilon > 0$, and let us rewrite:

$$\Delta u(x) = \underbrace{\int_{B_\epsilon(0)} \Phi(y) \Delta_x f(x-y) dy}_{I_\epsilon} + \underbrace{\int_{\mathbb{R}^d \setminus B_\epsilon(0)} \Phi(y) \Delta_x f(x-y) dy}_{J_\epsilon}\ . \tag{2.28}$$

We will study the two integrals separately.

3. We have:

$$\begin{aligned} |I_\epsilon| &\leqslant \int_{B_\epsilon(0)} |\Phi(y)|\, |\Delta_x f(x-y)|\, dy \\ &\leqslant \sup_{y\in B_\epsilon(0)} |\Delta_x f(x-y)| \int_{B_\epsilon(0)} |\Phi(y)|\, dy \end{aligned} \tag{2.29}$$

Being $D^2 f$ continuous and compactly supported in $B_\epsilon(0)$, it is bounded by a constant. Hence:

$$(2.29) \leqslant C \int_{B_\epsilon(0)} |\Phi(y)|\, dy \leqslant C \begin{cases} \int_{B_\epsilon(0)} dy\, |\log|y|\,|, & \text{if } d=2, \\ \int_{B_\epsilon(0)} dy\, \frac{1}{|y|^{d-2}} & \text{if } d \geqslant 3. \end{cases} \tag{2.30}$$

Now we are left with bounding the integrals: let us first study the case $n=2$.

$$\begin{aligned} \int_{B_\epsilon(0)} d^2y\, |\log|y|\,| &= \left| \int_{B_\epsilon(0)} d^2y \log|y| \right| = c \left| \int_0^\epsilon dr r \log r \right| \\ &= c \left| \frac{r^2}{2} \log r \Big|_0^\epsilon - \int_0^\epsilon dr \frac{r^2}{2} \frac{1}{r} \right| \leqslant c\left(\epsilon^2 |\log\epsilon| + \epsilon^2\right) \end{aligned} \tag{2.31}$$

which vanishes as $\epsilon \to 0$. Suppose now $d \geqslant 3$. We have:

$$\int_{B_\epsilon(0)} dy\, \frac{1}{|y|^{d-2}} = c \int_0^\epsilon dr \frac{r^{d-1}}{r^{d-2}} \leqslant C\epsilon^2 \tag{2.32}$$

which vanishes as $\epsilon \to 0$. We then conclude that $I_\epsilon \to 0$ and $\epsilon \to 0$.

4. In order to study the integral J_ϵ, it is worth recalling that, by Gauss-Green theorem:

$$\int_U u_{x_i} dx = \int_{\partial U} u\nu_i ds \tag{2.33}$$

where ν is the outward normal of ∂U. Let $u(y) = \Phi(y)\partial_{y_i} f(x-y)$. We get:

$$\int_{B_\epsilon(0)} dy \left[\Phi(y)\partial^2_{y_i} f(x-y) + \partial_{y_i}\Phi(y)\partial_{y_i} f(x-y)\right] = \int_{\partial B_\epsilon(0)} \nu_i \Phi(y)\partial_{y_i} f(x-y) ds(y) \tag{2.34}$$

so that

$$J_\epsilon = \underbrace{\int_{\partial B_\epsilon(0)} ds(y)\, \Phi(y)\nu \cdot D_y f(x-y)}_{L_\epsilon} - \underbrace{\int_{\mathbb{R}^d \setminus B_\epsilon(0)} dy\, D\Phi(y) \cdot D_y f(x-y)}_{K_\epsilon}. \tag{2.35}$$

We will study the two terms separately. We have:

$$|L_\epsilon| \leqslant c \int_{\partial B_\epsilon(0)} ds(y)\ |\Phi(y)| = \begin{cases} c\epsilon |\log \epsilon| & \text{if } d = 2, \\ c\epsilon & \text{if } d \geqslant 3. \end{cases} \tag{2.36}$$

Therefore, $L_\epsilon \to 0$ as $\epsilon \to 0$. Consider now the term K_ϵ. Integrating again by parts:

$$\begin{aligned} K_\epsilon &= \underbrace{\int_{\mathbb{R}^d \setminus B_\epsilon(0)} dy\, \Delta\Phi(y) f(x-y)}_{=0} - \int_{\partial B_\epsilon(0)} ds(y)\, \nu \cdot D_y \Phi(y) f(x-y) \\ &= -\int_{\partial B_\epsilon(0)} ds(y)\, \nu \cdot D_y \Phi(y) f(x-y) \end{aligned} \tag{2.37}$$

where we used that $\Phi(y)$ is harmonic if $y \neq 0$. Next, we compute:

$$\begin{aligned} D\Phi(y) = D \begin{cases} -\frac{1}{2\pi} \log |y| & \text{if } d = 2 \\ \frac{1}{d(d-2)\alpha(d)} \frac{1}{|x|^{d-2}} & \text{if } d \geqslant 3 \end{cases} \\ = \begin{cases} -\frac{1}{2\pi} \frac{y}{|y|^2} & \text{if } d = 2, \\ -\frac{1}{d(d-2)\alpha(d)} (d-2) \frac{1}{|y|^{d-1}} \frac{y}{|y|} = -\frac{1}{d\alpha(d)} \frac{y}{|y|^d} & \text{if } d \geqslant 3, \end{cases} \end{aligned} \tag{2.38}$$

where we recall $\alpha(d) = \frac{\pi^{d/2}}{\Gamma(d/2+1)}$, and in particular $\alpha(2) = \pi$. Summarizing

$$D\Phi(y) = -\frac{1}{d\alpha(d)} \frac{y}{|y|^d}, \qquad \text{if } y \neq 0. \tag{2.39}$$

To compute the integral in (2.37) we use that, for $y \in \partial B_\epsilon(0)$:

$$\nu = -\frac{y}{|y|} = -\frac{y}{\epsilon} \Rightarrow \nu \cdot D\Phi(y) = \frac{1}{d\alpha(d)} \frac{|y|^2}{\epsilon^{d+1}} = \frac{1}{d\alpha(d)} \frac{1}{\epsilon^{d-1}}. \tag{2.40}$$

Hence

$$\begin{aligned} K_\epsilon &= -\int_{\partial B_\epsilon(0)} ds(y)\, \nu \cdot D_y \Phi(y) f(x-y) \\ &= -\frac{1}{\epsilon^{d-1} d\alpha(d)} \int_{\partial B_\epsilon(0)} ds(y)\, f(x-y) \end{aligned} \tag{2.41}$$

which converges to $-f(x)$ as $\epsilon \to 0$, by continuity of f. In conclusion, taking the limit $\epsilon \to 0$ we get

$$\Delta u(x) = -f(x). \tag{2.42}$$

■

Remark 2.3. *i) Even if the source term $f(x)$ is compactly supported, the solution $u(x)$ propagates over all $\mathbb{R}^d$.*

ii) It is obvious that the solution is not unique: if u solves the Poisson equation, so does $u + const$. As we shall see, the solution will be unique in an appropriate space of functions.

(iii) The above proof shows that $-\Delta_y \Phi(y-x) = \delta(y-x)$ in the sense of distributions. The symbol $\delta(y-x)$ denotes the Dirac delta distribution: it acts as

$$\int dy\, \delta(y-x) g(y) := g(x) \,, \qquad \text{for all } g \in C_c^\infty(\mathbb{R}^d). \tag{2.43}$$

Also, Δ denotes the distributional Laplacian, defined as:

$$\int dy\, \Delta_y \Phi(y-x) g(y) := \int dy\, \Phi(y-x) \Delta_y g(y) \,. \tag{2.44}$$

Thus, the above proof shows that the following identity holds:

$$\int dy (-\Delta_y \Phi(y-x)) g(y) = \int dy\, \delta(y-x) g(y) \qquad \text{for all } g \in C_c^\infty(\mathbb{R}^d) \,. \tag{2.45}$$

2.3 Properties of harmonic functions

Here we shall discuss some important properties of the Laplace equation. We start with the mean-value formula. Given a bounded set $U \subset \mathbb{R}^d$, we shall use the notation:

$$\fint_U ... = \frac{1}{|U|} \int_U ... \tag{2.46}$$

Unless otherwise specified, we shall assume that $U \subset \mathbb{R}^d$ is a bounded and open subset. Also, we will suppose that ∂U admits a continuous parametrization.

Theorem 2.4 (Mean-value theorem.)**.** *Suppose that $u(x)$ is harmonic in U, and let $B_r(x) \subset U$. Then:*

$$u(x) = \fint_{B_r(x)} dy\, u(y) = \fint_{\partial B_r(x)} ds(y)\, u(y) \,. \tag{2.47}$$

Proof. For $d = 1$ the theorem is trivial to check, since all harmonic functions are linear. For $d \geqslant 2$, the proof is an application of Gauss-Green theorem. Define

$$\phi(r) := \fint_{\partial B_r(x)} ds(y)\, u(y) = \fint_{\partial B_1(0)} ds(z)\, u(x + rz) \,. \tag{2.48}$$

We compute:

$$\begin{aligned} \phi'(r) &= \fint_{\partial B_1(0)} ds(z)\, Du(x+rz) \cdot z = \fint_{\partial B_1(0)} ds(y)\, Du(y) \cdot \frac{y-z}{r} \\ &= \frac{r}{d} \fint_{B_r(x)} \Delta u(y) dy = 0 \,, \end{aligned} \tag{2.49}$$

where the second identity follows from Gauss-Green theorem and the last from the fact that u is harmonic. This means that ϕ is constant, which implies:

$$\phi(r) = \lim_{t \to 0} \phi(t) = \lim_{t \to 0} \fint_{\partial B_t(x)} ds(y)\, u(y) = u(x). \tag{2.50}$$

To prove the equivalence with the average over the ball we write:

$$\begin{aligned}\int_{B_r(x)} u dy &= \int_0^r dt \left(\int_{\partial B_t(x)} ds(y)\, u(y) \right) = u(x) \int_0^r ds\, d\alpha(d) s^{d-1} = u(x)\alpha(d) t^d \\ &\equiv u(x)|B_r(x)| \,,\end{aligned} \tag{2.51}$$

which implies the desired claim. ∎

In $d = 1$, being harmonic functions linear, it is trivial that they attain their extremal values on the boundary of the interval in which they are defined. The analogous statement in more than one dimension is less trivial to prove, and it is the content of the next theorem.

Theorem 2.5 (Maximum principle.)**.** *Let $U \subset \mathbb{R}^d$ open and bounded, and let $u(x)$ be harmonic in U. Then:*

$$\max_{\overline{U}} u(x) = \max_{\partial U} u(x) \,. \tag{2.52}$$

Furthermore, if U is connected and there exists a point $x_0 \in U$ such that $\max_{\overline{U}} u(x) = u(x_0)$, then

$$u(x) = \textit{constant in } U \,. \tag{2.53}$$

The second statement is stronger than the first (it is also called strong maximum principle).

Remark 2.6. *Recall that a set U is called connected if it cannot be represented as the union of two or more disjoint and nonempty open sets. In $\mathbb{R}^d$ this notion is equivalent to path-connectedness. In particular, if U is open and connected, and $U = U_1 \cup U_2$ with U_1, U_2 open and disjoint, then either $U_1 = U$ and $U_2 = \varnothing$ or $U_2 = U$ and $U_1 = \varnothing$.*

Proof. We shall prove the second statement. The first follows from the second after possibly splitting the domain U in connected components. Suppose that there exists a point $x_0 \in U$ such that:

$$u(x_0) = \max_{x \in \bar{U}} u(x) \leqslant M \,. \tag{2.54}$$

Define:

$$V := \{ x \in U \,\big|\, u(x) = M \} \,. \tag{2.55}$$

Let now $0 < r < \mathrm{dist}(x_0, \partial U)$: by the mean value theorem we know that

$$M = u(x_0) = \fint_{B_r(x_0)} u(y) dy \leqslant M \tag{2.56}$$

The only way in which this can be true is by having:

$$u(y) = M \qquad \forall y \in B_r(x_0) \,. \tag{2.57}$$

In particular, this means that V is open. Let us rewrite:

$$U = V \cup (U \backslash V) \,, \tag{2.58}$$

where $U\backslash V = \big\{ x \in U \big| u(x) \neq M \big\}$. By continuity of u, this set is open as well. Clearly $U \cap (U\backslash V) = \varnothing$. Therefore, since U is open and connected:

$$\text{either } V = \{ x \in U \big| u(x) = M \} = \varnothing \text{ or } U\backslash V = \big\{ x \in U \big| u(x) \neq M \big\} = \varnothing. \tag{2.59}$$

However, by assumption $V \neq \varnothing$ since it contains the point x_0. Therefore $U\backslash V = \varnothing$, which means that $u(x)$ is constant in U. ∎

Remark 2.7. *Notice that the boundedness of U is only used to make sure that $M < \infty$. Thus, the same proof can be used to prove the maximum principle for bounded harmonic functions on unbounded sets U.*

Application: absence of stable equilibrium points in the vacuum. As an application of the maximum principle, we show that the electrostatic potential does not admit stable equilibrium points in the vacuum. Mathematically, these corresponds to strict local minima of the electrostatic potential $u(x)$. Suppose that x_0 is a strict local minimum of $u(x)$, and suppose that $x_0 \in U$ and that $\Delta u = 0$ in U. For r small enough, $B_r(x_0)$ is contained in U and x_0 is a global minimum of u in B_r. Equivalently, x_0 is a strict global maximum of $-u(x)$ in $B_r(x_0)$, which is also harmonic. By the strong maximum principle, Eq. (2.53), this is not possible. Another interesting application of the maximum principle is the uniqueness of solution of the Poisson equation.

Proposition 2.8 (Uniqueness of solutions of Poisson equation on bounded domains.)**.** *Let $U \subset \mathbb{R}^d$ be a bounded open set and suppose that u_1 and u_2 are two solutions of the Dirichlet boundary value problem:*

$$\begin{aligned} -\Delta u(x) &= f(x) \qquad \text{for } x \in U \\ u(x) &= g(x) \qquad \text{for } x \in \partial U. \end{aligned} \tag{2.60}$$

Then, $u_1 = u_2$.

Proof. Let $w = u_1 - u_2$. Then:

$$\begin{aligned} -\Delta w &= 0 \qquad \text{for } x \in U \\ w &= g \qquad \text{for } x \in \partial U. \end{aligned} \tag{2.61}$$

By the maximum principle, $w \leqslant 0$, that is $u_1 - u_2 \leqslant 0$. Reversing the roles of u_1 and u_2 the claim follows. ∎

Finally, the next theorem characterizes bounded harmonic functions on $\mathbb{R}^d$.

Theorem 2.9 (Liouville)**.** *Let u be bounded and harmonic in $\mathbb{R}^d$. Then,*

$$u(x) = \textit{constant.} \tag{2.62}$$

Proof. To begin, recall the mean-value formula:

$$u(x) = \fint_{B_r(x)} u(y) dy \tag{2.63}$$

which holds for any $r > 0$, since u is harmonic in $\mathbb{R}^d$. Changing variable,

$$u(x) = \frac{1}{|B_1(0)|} \int_{B_1(0)} dy\, u(x + ry)\ . \tag{2.64}$$

Taking the derivative with respect to x_i:

$$\begin{aligned} \partial_i u(x) &= \frac{1}{|B_1(0)|} \int_{B_1(0)} dy\, \partial_{x_i} u(x + ry) \\ &= \frac{1}{r|B_1(0)|} \int_{B_1(0)} dy\, \partial_{y_i} u(x + ry)\ . \end{aligned} \tag{2.65}$$

By Gauss-Green theorem:

$$\partial_i u(x) = \frac{1}{r|B_1(0)|} \int_{\partial B_1(0)} dS(y)\, \nu_i(y) u(x + ry) \,, \tag{2.66}$$

which gives the estimate:

$$|\partial_i u(x)| \leqslant \frac{|\partial B_1(0)|}{r|B_1(0)|} \|u\|_{L^\infty(\mathbb{R}^d)} \,. \tag{2.67}$$

Being r arbitrary and u bounded, the claim follows. ∎

To conclude, Liouville theorem can be used to prove the uniqueness of a bounded solution for the Poisson equation in $\mathbb{R}^d$, $d \geqslant 3$.

Proposition 2.10. *Let $d \geqslant 3$, and $f \in C_c^2(\mathbb{R}^d)$. Any bounded solution of $-\Delta u = f$ on $\mathbb{R}^d$ has the form:*

$$u(x) = \int_{\mathbb{R}^d} dy\, \Phi(x - y) f(y) + \textit{constant.} \tag{2.68}$$

Remark 2.11. *In $d = 1, 2$, the main term in the right-hand side of (2.68) is not bounded uniformly in x, due to the unboundedness of $\Phi(x)$.*

Proof. Let:

$$u_1(x) = \int_{\mathbb{R}^d} dy\, \Phi(x - y) f(y) \,. \tag{2.69}$$

In $d \geqslant 3$, the function $u_1(x)$ is bounded. Suppose that $u_2(x)$ is another bounded solution of the Poisson equation. Then, $w = u_1 - u_2$ is a bounded solution of the Laplace equation in $\mathbb{R}^d$. By Liouville theorem, $w =$ constant. This concludes the proof. ∎

2.4 Newton's theorem

In this section we shall have a closer look at the solution of the Poisson equation $-\Delta u = f$ in $\mathbb{R}^d$. In particular, we shall consider the case in which the source term $f(x)$ is radial, $f(x) = f(|x|)$. As for Theorem 2.2, we shall suppose that f is compactly supported, that is $f(x) = 0$ for $|x| > R$.

Theorem 2.12 (Newton's theorem.)**.** *Let $u(x)$ be given by (2.68), with $d \geqslant 1$. Then:*

$$u(x) = \int_{|y|<|x|} dy\, f(y)\Phi(x) + \int_{|y|\geqslant|x|} dy\, f(y)\Phi(y) \,. \tag{2.70}$$

Before discussing the proof, let us highlight some consequences of this remarkable identity. Suppose that $|x| > R$, that is we probe the electrostatic potential away from the support of f. Then, the second term in (2.70) is zero, and hence:

$$u(x) = \Phi(x) Q_f \,, \qquad Q_f := \int dy\, f(y) \,. \tag{2.71}$$

The constant Q_f physically corresponds to the total charge associated to the charge distribution f. Thus, $u(x)$ coincides with the electrostatic potential generated by a point-like charge at $x = 0$, with total charge given by Q_f. This is a very remarkable identity, of enormous importance both in electrostatics and in astrophysics (the gravitational potential behaves as the electrostatic potential, up to a minus sign).

Furthermore, suppose that $f(y) = 0$ for $|y| < R' \leqslant R$, and let $|x| < R'$. Thus, f describes the charge distribution of a spherically symmetric object with a cavity, and we are probing the

electrostatic field in the cavity. Then, the first term in (2.70) is identically zero. Eq. (2.70) reads:

$$u(x) = \int dy\, f(y)\Phi(y) \; . \tag{2.72}$$

The electrostatic field in the cavity is *constant*: no electrostatic force acts on a charge placed inside the cavity. This conclusion could have been anticipated by recalling that the electrostatic potential cannot have local maxima or minima inside the cavity, as we proved in the previous section. By the fact that $u(x)$ is radial, the reader can easily convince herself that $u(x)$ is constant.

Proof. We start by writing:

$$u(x) = \int_{|y|<|x|} dy\, f(y)\Phi(x-y) + \int_{|y|>|x|} dy\, f(y)\Phi(x-y) \; ; \tag{2.73}$$

the region $|y| = |x|$ can be omitted, since it is a zero measure set and since the function is integrable. Consider the first term. We have, using that $f(y)$ is radial:

$$\int_{|y|<|x|} dy\, f(y)\Phi(x-y) = \lim_{\varepsilon\to 0} \int_0^{|x|-\varepsilon} dr\, f(r) \int_{\partial B_r(0)} dS(y)\Phi(x-y) \; . \tag{2.74}$$

Since $|x| > r$ and $|y| = r$, the function $\Phi(x-y)$ is harmonic for $y \in B_r(0)$. Thus, by the mean-value formula:

$$\begin{aligned} \int_{|y|<|x|} dy\, f(y)\Phi(x-y) &= \lim_{\varepsilon\to 0} \int_0^{|x|-\varepsilon} dr\, f(r)|\partial B_r(0)|\Phi(x) \\ &\equiv \int_{|y|<|x|} dy\, f(y)\Phi(x) \; . \end{aligned} \tag{2.75}$$

Consider now the second term in (2.73). We write:

$$\int_{|y|>|x|} dy\, f(y)\Phi(x-y) = \lim_{\varepsilon\to 0} \int_{|x|+\varepsilon} dr\, f(r) \int_{\partial B_r(0)} dS(y)\, \Phi(x-y) \; . \tag{2.76}$$

Consider the function, for $|x| < r$:

$$g(x) = \int_{\partial B_r(0)} dS(y)\, \Phi(x-y) \; . \tag{2.77}$$

The function is radial. In fact, let R be a rotation matrix, describing rotations around the origin: $R \in SO(d)$, $RR^T = R^T R = 1$. Then,

$$\begin{aligned} g(Rx) &= \int_{\partial B_r(0)} dS(y)\, \Phi(Rx-y) \\ &= \int_{\partial B_r(0)} dS(y)\, \Phi(x-R^T y) \; , \end{aligned} \tag{2.78}$$

where in the second step we used that $\Phi(z)$ only depends on $|z|$, and furthermore that $|Rx-y| = |R(x-R^T y)| = |x-R^T y|$. Next, by a change of variable, and using that the integration domain is invariant under rotations,

$$g(Rx) = g(x) \iff g(x) \equiv g(|x|) \; . \tag{2.79}$$

In particular, $g(x)$ equals its spherical average:

$$\begin{aligned} g(x) &= \fint_{\partial B_{|x|}(0)} dS(z) g(z) \\ &= \fint_{\partial B_{|x|}(0)} dS(z) \int_{\partial B_r(0)} dS(y)\, \Phi(z-y) \ . \end{aligned} \tag{2.80}$$

Since $|x| < r$, we can interchange the integrations in y and z. We have:

$$g(x) = \int_{\partial B_r(0)} dS(y) \fint_{\partial B_{|x|}(0)} dS(z)\, \Phi(z-y) \ . \tag{2.81}$$

Now, the function $z \mapsto \Phi(z-y)$ is harmonic for $z \in B_{|x|}(0)$, since $|y| > |x|$. Therefore, by the mean-value theorem:

$$g(x) = \int_{\partial B_r(0)} dS(y) \Phi(y) \ . \tag{2.82}$$

Plugging this identity into (2.76), we get:

$$\begin{aligned} \int_{|y|>|x|} dy\, f(y) \Phi(x-y) &= \lim_{\varepsilon \to 0} \int_{|x|+\varepsilon} dr\, f(r) \int_{\partial B_r(0)} dS(y)\, \Phi(y) \\ &= \int_{|y|>|x|} dy\, f(y) \Phi(y) \ . \end{aligned} \tag{2.83}$$

Combined with (2.75), this concludes the proof. ∎

2.5 Green's function

Finding the solution of the Poisson equation on a general domain could be extremely hard, if not impossible. One can prove that such solution exists, for a large class of bounded domains U, under suitable regularity assumptions on the boundary; see *e.g.* [5]. Here we shall refrain from proving this general statement; instead, we will discuss a reformulation of the Poisson problem, that will allow to find explicit solutions in some special cases. The method is based on the notion of Green's function, that we shall introduce here. Roughly, the Green's function allows to understand the solution of the Laplace/Poisson equation as a suitable propagation of the boundary condition.

For $U \subset \mathbb{R}^d$ open, let us consider the Dirichlet boundary value problem:

$$\begin{aligned} -\Delta u &= f \qquad \text{in } U \\ u &= g \qquad \text{on } \partial U. \end{aligned} \tag{2.84}$$

For $x \notin \partial U$, let us define the function $y \mapsto \phi^x(y)$ as the solution of:

$$\begin{aligned} \Delta \phi^x &= 0 \qquad\qquad \text{in } U \\ \phi^x(y) &= \Phi(x-y) \qquad \text{on } \partial U. \end{aligned} \tag{2.85}$$

For reasons that will be clear in a moment, this function is called the corrector function.

Definition 5 (Green's function.)**.** *Let $x, y \in U$, $x \neq y$. The Green's function for the region U is defined as:*

$$G(x,y) := \Phi(y-x) - \phi^x(y) \ . \tag{2.86}$$

Remark 2.13. *As a function on y, the Green's function is harmonic in $U \backslash \{x\}$; moreover, it vanishes on the boundary of U. Physically, it corresponds to the electrostatic potential generated by a pointlike charge at x, under the constraint that it vanishes on the boundary of U.*

Theorem 2.14 (Representation formula for the solution of (2.84).)**.** *Suppose that $u \in C^2(\overline{U})$ solves the Poisson boundary value problem (2.84). Then, the following identity holds:*

$$u(x) = -\int_{\partial U} dS(y)\, g(y)\nu \cdot D_y G(x,y) + \int_U f(y)G(x,y)dy\ . \tag{2.87}$$

This result is quite remarkable: it provides an expression for a large class of boundary value problems, determined by f and g, provided one is able to find the Green's function G. This amounts to solving one specific boundary value problem, for the corrector function (2.85). Later, we will discuss how to find the Green function for two special cases, the sphere and the half-plane.

Proof. Let $x \in U$, and let $\varepsilon > 0$ be small enough so that $B_\varepsilon(x) \in U$. Let $V_\varepsilon = U \backslash B_\varepsilon(x)$. By Gauss-Green theorem:

$$\begin{aligned}\int_{V_\varepsilon} dy\, &[u(y)\Delta\Phi(y-x) - \Phi(y-x)\Delta u(y)] \\ &= \int_{\partial V_\varepsilon} dS(y)\left[u(y)\nu\cdot D\Phi(y-x) - \Phi(y-x)\nu\cdot Du(y)\right],\end{aligned} \tag{2.88}$$

with ν the outward normal on ∂V_ε. Rcall that $\Delta\Phi(y-x) = 0$ for $y \neq x$; thus, the left-hand side of (2.88) can be written as:

$$-\int_U dy\, \Phi(y-x)\Delta u(y) + o(1)\ , \tag{2.89}$$

where $o(1)$ denotes terms that vanish as $\varepsilon \to 0$. Consider now the right-hand side of (2.88). As we observed in the proof of Theorem 2.2:

$$\int_{\partial B_\varepsilon(x)} dS(y)\, \Phi(y-x)\nu\cdot D_y u(y) \to 0 \qquad \text{as } \varepsilon \to 0. \tag{2.90}$$

Furthermore, notice that, if ν is the *inward* normal of $\partial B_\varepsilon(x)$:

$$\begin{aligned}\int_{\partial B_\varepsilon(x)} dS(y)\, u(y)\nu\cdot D\Phi(y-x) &\equiv \int_{\partial B_\varepsilon(x)} dS(y)\, u(y)\nu\cdot D\Phi(y-x) \\ &= \frac{1}{|\partial B_\varepsilon(x)|}\int_{\partial B_\varepsilon(x)} dS(y)\, u(y)\ ,\end{aligned} \tag{2.91}$$

where in the last step we used that:

$$D_y\Phi(y-x) = -\frac{1}{d\alpha(d)}\frac{y-x}{|y-x|^d}\ , \tag{2.92}$$

with $\alpha(d)$ the volume of the unit ball, hence $d\alpha(d)$ the volume of the unit sphere, and $\nu = -(y-x)/|y-x|$. Therefore, by continuity of u:

$$\int_{\partial B_\varepsilon(x)} dS(y)\, u(y)\nu\cdot D\Phi(y-x) \to u(x) \qquad \text{as } \varepsilon \to 0. \tag{2.93}$$

Thus, the right-hand side of (2.88) can be written as:

$$u(x) + \int_{\partial U} dS(y)\left[u(y)\nu\cdot D\Phi(y-x) - \Phi(y-x)\nu\cdot Du(y)\right] + o(1)\ . \tag{2.94}$$

Hence, combining with (2.89), as $\varepsilon \to 0$, for $x \in U$:

$$\begin{aligned}u(x) &= -\int_U dy\, \Phi(y-x)\Delta u(y) + \int_{\partial U} dS(y)\left[\Phi(y-x)\nu\cdot Du(y) - u(y)\nu\cdot D\Phi(y-x)\right] \\ &\equiv \int_U dy\, \Phi(y-x)f(y) + \int_{\partial U} dS(y)\left[\Phi(y-x)\nu\cdot Du(y) - g(y)\nu\cdot D\Phi(y-x)\right].\end{aligned} \tag{2.95}$$

This identity almost provides a closed expression for the solution of the Poisson problem, provided we know the value of $\nu \cdot Du$ on ∂U. To solve this problem, let us now apply Gauss-Green theorem, to obtain:

$$-\int_U dy\, \phi^x(y)\Delta u(y) = \int_{\partial U} dS(y)\big[u(y)\nu \cdot D\phi^x(y) - \phi^x(y)\nu \cdot D_y u(y)\big]\,, \tag{2.96}$$

where we used that $\Delta\phi^x(y) = 0$ in U. Recalling the definition of corrector function (2.85), we rewrite (2.96) as:

$$0 = -\int_U dy\, \phi^x(y) f(y) + \int_{\partial U} dS(y)\big[g(y)\nu \cdot D\phi^x(y) - \Phi(y-x)\nu \cdot D_y u(y)\big]\,. \tag{2.97}$$

Therefore, adding this identity to (2.95) we get:

$$u(x) = \int_U dy\, G(y,x) f(y) - \int_{\partial U} dS(y)\, g(y)\nu \cdot D_y G(y,x)\,, \tag{2.98}$$

which proves the claim. ∎

Recalling Remark 2.3 (iii), the Green's function satisfies the following distributional equation, parametrized by $x \in U$:

$$\begin{aligned} -\Delta_y G(y,x) &= \delta(y-x) \qquad \text{in } U \\ G(y,x) &= 0 \qquad \text{on } \partial U. \end{aligned} \tag{2.99}$$

The solution describes the electrostatic potential generated by a charge at x, conditioned to vanish on ∂U. By linearity of the equation, this could be realized adding up to $\Phi(y-x)$ (the electrostatic potential of the charge at x) another electrostatic potential, generated by a charge *outside* U which *cancels* the potential generated by the charge at x on the region ∂U. This intuition is called the method of image charges, in electrostatics. We shall now discuss the computation of the Green's function in two special cases, in which the symmetry of the problem allows to use the method of images to find the solution.

2.5.1 Half-plane

Let $U = \mathbb{R}^d_+$, defined as

$$\mathbb{R}^d_+ = \{x \in \mathbb{R}^d \mid x_d > 0\}\,. \tag{2.100}$$

We look for a corrector function $\phi^x(y)$ such that: $\Phi(y-x) - \phi^x(y)$ is zero on $y_d = 0$ for all $x \in \mathbb{R}^d_+$; and $\phi^x(y)$ is harmonic for $y \in \mathbb{R}^n_+$. The natural choice is to consider

$$\phi^x(y) = \Phi(y - \tilde{x})\,, \qquad \tilde{x} = (x_1, \ldots, x_{d-1}, -x_d). \tag{2.101}$$

This function is singular at $y = \tilde{x}$, which however does not belong to $\mathbb{R}^d_+$, and it is harmonic for $y \in \mathbb{R}^d_+$. Also,

$$\Phi(y - \tilde{x}) = \Phi(y-x) \qquad \text{for all } y \in \partial\mathbb{R}^d_+. \tag{2.102}$$

This choice defines the Green's function on the half-plane.

2.5.2 Sphere

Let $U = B_1(0)$. We now look for a function $\phi^x(y)$ which is harmonic in $B_1(0)$, and which is such that, for all $x \in B_1(0)$:

$$\phi^x(y) = \Phi(y - x) \qquad \text{for all } y \in \partial B_1(0). \tag{2.103}$$

As for the half-plane we "reflected" the singularity by replacing x with $\tilde{x}$, here we consider the mapping

$$\tilde{x} = \frac{x}{|x|^2} \, . \tag{2.104}$$

For all $x \in B_1(0)$, the function $\Phi(y - \tilde{x})$ is harmonic for $y \in B_1(0)$. However, it is not true that $\Phi(y - \tilde{x}) = \Phi(y - x)$ for all $y \in \partial B_1(0)$. To adjust the situation, we consider

$$\phi^x(y) = \Phi(|x|(y - \tilde{x})) \, . \tag{2.105}$$

This function has the same harmonicity properties of $\Phi(y - \tilde{x})$. Moreover, we claim that $|x||y - \tilde{x}| = |y - x|$ for all $y \in \partial B_1(0)$. In fact, for $|y| = 1$:

$$\begin{aligned} |x|^2|y - \tilde{x}|^2 &= |x|^2\Big(1 - \frac{2y \cdot x}{|x|^2} + \frac{1}{|x|^2}\Big) \\ &= |x|^2 - 2y \cdot x + 1 \\ &= |x - y|^2 \, . \end{aligned} \tag{2.106}$$

Therefore, the choice (2.105) defines the Green's function for the Poisson problem in a ball.

3 The heat equation

3.1 Motivations

We are interested in describing the variation in time of a certain quantity, that cannot be created nor destroyed: no sources or sink are available. We shall denote by $u(x, t)$ the density of such quantity at a given point $x \in \mathbb{R}^d$, at the time $t \geqslant 0$. In our particular application, the quantity $u(x, t)$ will denote the heat density, which we shall also identity with the temperature (the two are related up to a proportionality constant).

Let $\Omega \subset \mathbb{R}^d$. We define the rate of variation of heat of Ω as:

$$\frac{\partial}{\partial t} \int_\Omega dx \, u(x, t) \, . \tag{3.1}$$

Since we are ruling out the presence of sink and sources, the body Ω is only able to exchange heat through its surface $\partial\Omega$. Thus, we expect:

$$\frac{\partial}{\partial t} \int_\Omega dx \, u(x, t) = - \int_{\partial\Omega} dS(x) \, h(x, t) \cdot \nu(x) \, , \tag{3.2}$$

with $\nu(x)$ the outward normal at x. The vector field $h(x, t)$ is called the heat flux. It describes the amount of heat that traverses the surface the infinitesimal surface element at x, at the time t. The minus sign in (3.2) is chosen so that the temperature decreases if the net heat flux through the surface is positive.

Experience suggests that the heat flux points from regions with higher temperature to regions with lower temperature. Thus, we postulate that:

$$h(x, t) = -\kappa \nabla u(x, t) \, , \qquad \kappa > 0 \, , \tag{3.3}$$

for a certain constant κ - the diffusion constant - that we shall fix to 1 from now on. Therefore, the equation (3.2) reads:

$$\frac{\partial}{\partial t}\int_\Omega dx\, u(x,t) = \int_{\partial\Omega} dS(x)\, \nu\cdot\nabla u(x,t)\ . \tag{3.4}$$

Applying Gauss-Green theorem, we have:

$$\frac{\partial}{\partial t}\int_\Omega dx\, u(x,t) = \int_{\Omega} dx\, \Delta u(x,t)\ . \tag{3.5}$$

Since the equation holds for all $\Omega\subset\mathbb{R}^d$, it is equivalent to:

$$\begin{aligned} \partial_t u(x,t) &= \Delta u(x,t) \\ u(x,0) &= g(x) \qquad \text{for all } x\in\mathbb{R}^d. \end{aligned} \tag{3.6}$$

Equation (3.6) is called the *heat equation*, and it will be the focus of the present section. It describes the evolution of an initial temperature profile $g(x)$.

Remark 3.1. *(i) Notice that steady state solutions of the heat equation, that is constant in time, are harmonic functions.*

(ii) The heat equation is ill posed for negative times. To see this, consider the heat equation on $S^1_{2\pi}$:

$$(\partial_t - \partial_{xx})u(x,t) = 0\ , \qquad u(x,0) = g(x) \tag{3.7}$$

with $u(x,t) = u(x+2\pi,t)$ for all t. As discussed in Section 1, the solution is:

$$u(x,t) = \sum_{n\in\mathbb{Z}} e^{-n^2t}e^{inx}\hat{g}_n\ . \tag{3.8}$$

Let us consider the following special initial datum:

$$\hat{g}_n = \delta_{|n|,j}e^{-|n|} \qquad \text{for } |n| = j. \tag{3.9}$$

Then, $g(x) = 2e^{-j}\cos(jx)$. The solution to the heat equation is:

$$u(x,t) = 2e^{-j^2t}e^{-j}\cos(jx)\ . \tag{3.10}$$

We notice that $g(x)\to 0$ pointwise, for $j\to\infty$, while $u(x,t)\to\infty$ as soon as $t<0$. This proves that the solution of the heat equation for negative times is not continuous in the initial datum.

(iii) The heat equation is not invariant under time reversal. Let $\tilde{u}(x,t) = u(x,-t)$. It satisfies the evolution equation $-\partial_t\tilde{u} = \Delta\tilde{u}$, the backwards heat equation, *which is different from the heat equation (3.6).*

3.2 Fundamental solution of the heat equation

As we have seen in Section 1.2, the heat equation can be solved by using the Fourier transform, for $g\in L^1(\mathbb{R}^d)$. Taking the Fourier transform of (3.6) we have:

$$\begin{aligned} \partial_t\hat{u}(k,t) &= -|k|^2\hat{u}(k,t) \\ \hat{u}(k,0) &= \hat{g}(k)\ . \end{aligned} \tag{3.11}$$

The solution is:

$$\hat{u}(k,t) = e^{-|k|^2t}\hat{g}(k)\ . \tag{3.12}$$

This function is L^1 in k, for $t > 0$. Taking the inverse Fourier transform, we obtain:

$$u(x,t) = \int \frac{dk}{(2\pi)^{\frac{d}{2}}} e^{-|k|^2 t} e^{ik\cdot x} \hat{g}(k) \ . \tag{3.13}$$

As one can easily check, this function is a solution of the heat equation (3.6). In fact:

$$\begin{aligned} (\partial_t - \Delta_x) u(x,t) &= \int \frac{dk}{(2\pi)^{\frac{d}{2}}} (\partial_t - \Delta_x) e^{-|k|^2 t} e^{ik\cdot x} \hat{g}(k) \\ &= \int \frac{dk}{(2\pi)^{\frac{d}{2}}} (-|k|^2 + |k|^2) e^{-|k|^2 t} e^{ik\cdot x} \hat{g}(k) = 0 \ . \end{aligned} \tag{3.14}$$

The exchange of integration and differentiation is justified, since the derivatives are L^1 functions in k. Next, we would like to represent the solution in terms of the inital datum $g(x)$, instead of $\hat{g}(k)$. To do this, we would like to apply the fact that, recall Eq. (1.83):

$$\widetilde{(fg)}(x) = (2\pi)^{-\frac{d}{2}} (\check{f} * \check{g})(x) \ . \tag{3.15}$$

In our case, $f \equiv \hat{f} = e^{-|k|^2 t}$ and $g \equiv \hat{g}(k)$. The formula (3.15) holds provided both functions $\hat{f}$, $\hat{g}$ are in $L^1 \cap L^2$. The Gaussian is in any L^p space, however the condition $g(x) \in L^1$ alone is not sufficient to ensure that $\hat{g} \in L^1 \cap L^2$. As discussed in Section 1.2, the integrability properties of $\hat{g}(k)$ are related to the regularity of $g(x)$. For the moment, we shall assume that $g(x)$ is regular enough, so that $\hat{g}(k) \in L^1 \cap L^2$. If so:

$$\begin{aligned} u(x,t) &= \int \frac{dk}{(2\pi)^{\frac{d}{2}}} e^{-|k|^2 t} e^{ik\cdot x} \hat{g}(k) \\ &= (2\pi)^{-\frac{d}{2}} \int dy \, \widetilde{e^{-|k|^2 t}}(x-y) g(y) \\ &= (2\pi)^{-\frac{d}{2}} 2^{-\frac{d}{2}} t^{-\frac{d}{2}} \int dy \, e^{-|x-y|^2/4t} g(y) \ , \end{aligned} \tag{3.16}$$

where we also used the behavior of the Fourier transform under rescalings (1.84).

Definition 6 (Fundamental solution of the heat equation.)**.** *The function:*

$$\Phi(x,t) := \frac{1}{(4\pi t)^{\frac{d}{2}}} e^{-|x-y|^2/4t} \ , \qquad (x,t) \in \mathbb{R}^d \times \mathbb{R}_+ \ , \tag{3.17}$$

is called the fundamental solution of the heat equation.

Remark 3.2. *(i) To see that $\Phi(x,t)$ solves the heat equation, simply write it in terms of its Fourier transform:*

$$\Phi(x,t) = \int \frac{dk}{(2\pi)^d} e^{-|k|^2 t} e^{ik\cdot x} \ . \tag{3.18}$$

(ii) Thus, the solution (3.16) can also be written as:

$$\begin{aligned} u(x,t) &= \int dy \, \Phi(y-x,t) g(y) \\ &\equiv (\Phi_t * g)(x) \qquad \Phi_t(y) \equiv \Phi(y,t) \ . \end{aligned} \tag{3.19}$$

The function $\Phi(y,t)$ is also called heat kernel.

To represent the solution of the heat equation as (3.19) we used a number of properties of the initial datum g. It turns out that the expression (3.19) provides a solution of the heat equation for a much larger class of initial data.

Theorem 3.3 (Solving the heat equation.)**.** *Assume that $g \in C(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$. Let:*

$$u(x,t) = \int dy\, \Phi(y-x,t) g(y) \,. \tag{3.20}$$

Then:

(i) $u \in C^\infty(\mathbb{R}^d \times \mathbb{R}_+)$,

(ii) $\partial_t u(x,t) = \Delta u(x,t)$ *for* $(x,t) \in \mathbb{R}^d \times \mathbb{R}_+$,

(iii) $\lim_{t\to 0^+} u(x,t) = g(x)$ *for all* $x \in \mathbb{R}^d$.

Remark 3.4. *The item (iii) in the above theorem implies that one can view the fundamental solution of the heat equation as the solution of the followind PDE, in the sense of distributions:*

$$\begin{aligned} (\partial_t - \Delta)\Phi_t(x) &= 0 \\ \lim_{t\to 0^+} \Phi_t(x) &= \delta(x) \,, \end{aligned} \tag{3.21}$$

with $\delta(x)$ the Dirac delta distribution at zero.

Before proving the theorem, notice the following fact:

$$\int dx\, \Phi(y-x,t) = 1 \,. \tag{3.22}$$

This follows from:

$$\int dx\, \Phi(y-x,t) = (2\pi)^{\frac{d}{2}} \hat{\Phi}(0,t) = 1 \,, \tag{3.23}$$

since $\hat{\Phi}(k,t) = (2\pi)^{-d/2} e^{-|k|^2 t}$, recall (3.18). More generally, let us denote denote the total heat of $u(x,t)$ as:

$$\int dx\, u(x,t) \,. \tag{3.24}$$

Then, if $g \in L^1$:

$$\int dx\, u(x,t) = \int dx \int dy\, \Phi(x-y,t) g(y) = \int dy \int dx\, \Phi(x-y,t) g(y) = \int dy\, g(y) \,, \tag{3.25}$$

where the exchange of integrals is justified by the fact that both Φ and g are L^1. Thus, the total heat of the solution $u(x,t)$ is a constant of motion, which is consistent with the fact that, when motivating the heat equation, we assumed that no sink or sources are present.

Proof of Theorem 3.3. The first item follows immediately from the fact that g is bounded, and from the integrability in y of all the space-time derivatives of $\Phi(x-y,t)$. The second item follows from the fact that $\Phi(x-y,t)$ solves the heat equation for positive times.

Let us now consider the third item. By continuity of g, for any $\varepsilon > 0$ there exists $\delta > 0$ such that for all $y \in B_\delta(x)$:

$$|g(x) - g(y)| < \varepsilon \,. \tag{3.26}$$

We rewrite, using the property (3.22):

$$\begin{aligned} u(x,t) - g(x) &= \int dy\, \Phi(y-x,t)(g(y) - g(x)) \\ &= \int_{B_\delta(x)} dy\, \Phi(y-x,t)(g(y) - g(x)) + \int_{B_\delta^{\mathrm{c}}(x)} dy\, \Phi(y-x,t)(g(y) - g(x)) \\ &\equiv \mathrm{I} + \mathrm{II} \,. \end{aligned} \tag{3.27}$$

Consider the first term. By continuity of g:

$$\begin{aligned} |\mathrm{I}| &\leqslant \int_{B_\delta(x)} dy\, \Phi(y-x,t)|g(y)-g(x)| \\ &\leqslant \varepsilon \int_{B_\delta(x)} dy\, \Phi(y-x,t) \\ &\leqslant \varepsilon\ . \end{aligned} \tag{3.28}$$

Next, consider the second term. We estimate it as:

$$\begin{aligned} |\mathrm{II}| &\leqslant 2\|g\|_\infty \int_{B^{\mathrm{c}}_\delta(x)} dy\, \Phi(x-y,t) \\ &= 2\|g\|_\infty \frac{1}{(4\pi t)^{\frac{d}{2}}} \int_{|y-x|\geqslant\delta} dy\, e^{-|x-y|^2/4t} \\ &\leqslant C \int_{|y|\geqslant\delta/\sqrt{t}} dy\, e^{-|y|^2/4} \end{aligned} \tag{3.29}$$

which vanishes as $t \to 0^+$. This concludes the proof. ∎

Remark 3.5. *The heat equation has infinite propagation speed: even if $g(x)$ has compact support, the time evolution $u(x,t)$ spreads over the whole $\mathbb{R}^d$. Physically, this is of course impossible: other effects, not taken into account by the heat equation, prevent this from happening. Mathematically, this is a consequence of the fact that time and space derivatives have different orders (first order for the time derivative, second order for the space derivative). For the wave equation, discussed in the next section, both derivatives are of second order and the propagation speed will be finite.*

3.3 Non-homogeneous heat equation

In this section we shall discuss the non-homogeneous heat equation in $\mathbb{R}^d \times \mathbb{R}_+$:

$$\begin{aligned} (\partial_t - \Delta)u(x,t) &= f(x,t) \\ u(x,0) &= g(x)\ , \end{aligned} \tag{3.30}$$

where $f(x,t)$ is a given source term. The reason for interpreting f as a source term is that the solution of the heat equation now satisfies the following integral equation (recall the discussion in Section 3.1):

$$\frac{\partial}{\partial t}\int_\Omega dx\, u(x,t) = \int_{\partial\Omega} dS(x)\, \nu\cdot\nabla u(x,t) + \int_\Omega dx\, f(x,t)\ , \qquad \Omega \subset \mathbb{R}^d\ . \tag{3.31}$$

Thus, the rate of variation of the heat in Ω is not only due to transmission through the boundary, but also to the bulk term appearing in the right-hand side of (3.31). In this section we shall discuss how to solve the non-homogeneous heat equation (3.30). The trick we shall use is called Duhamel principle, and it will be the content of this section.

As discussed in Section 1.2, the Fourier transform allows to convert differential operators into multiplication operators. That is, suppose that $f \in C^j(\mathbb{R}^d)$ and that $D^\alpha f \in L^1(\mathbb{R}^d)$, for all $|\alpha| \leqslant j$. Then:

$$(D^\alpha f)(x) = \int \frac{dk}{(2\pi)^{\frac{d}{2}}}\, e^{ik\cdot x}(ik)^\alpha \hat{f}(k)\ . \tag{3.32}$$

This identity suggests the following definition of *functions* of differential operators. For $F \in C(\mathbb{R}^d)$, and for f such that $F(ik)\hat{f}(k)$ is in $L^1(\mathbb{R}^d)$, we may define:

$$(F(D)f)(x) := \int \frac{dk}{(2\pi)^{\frac{d}{2}}} F(ik)\hat{f}(k)e^{ik\cdot x} \ . \tag{3.33}$$

Under the assumptions on f, the right-hand side makes sense, and it defines a bounded and continuous function. The identity (3.33) is an example of functional calculus, induced by the Fourier transform. Thus, consider:

$$(e^{\Delta t}f)(x) := \int \frac{dk}{(2\pi)^{\frac{d}{2}}} e^{-|k|^2 t}\hat{f}(k)e^{ik\cdot x} \ . \tag{3.34}$$

Notice that the right-hand side is well defined under rather mild assumptions on f. In particular, for the moment we can simply suppose that $f \in L^1(\mathbb{R}^d)$. Comparing Eq. (3.34) with Eq. (3.16), we see that the action of the heat kernel on the initial datum of the heat equation coincides with the action of the operator $\exp(\Delta t)$. In particular:

$$\partial_t e^{\Delta t}f = \Delta e^{\Delta t}f = e^{\Delta t}\Delta f \ , \tag{3.35}$$

where the last identity holds provided $\Delta f \in L^1$ as well. We shall use this representation of the heat kernel to find a solution of the non-homogeneous problem, under suitable regularity assumptions, and then later we will check that the obtained solutions makes sense for a large class of initial data and source terms.

Let $t > 0$ and $0 \leqslant s < t$. Let $u(x,s)$ be a solution of the non-homogeneous heat equation (3.30), and let $u^0(x,s)$ be a solution of the homogeneous heat equation ($f = 0$ in (3.30)). We define:

$$\tilde{u}(x,t;s) := (e^{\Delta(t-s)}u(\cdot,s))(x) \ . \tag{3.36}$$

According to the above definitions, this identity makes sense provided $u(\cdot,s) \in L^1$. Notice that:

$$\tilde{u}(x,t;t) = u(x,t) \ , \qquad \tilde{u}(x,t;0) = u^0(x,t) \ . \tag{3.37}$$

Thus, the function $s \mapsto u(x,t;s)$ allows to interpolate between what we know (the solution of the homogeneous problem), and what we would like to find (the solution of the non-homogeneous problem). We write:

$$\begin{aligned}
\tilde{u}(x,t;t) - \tilde{u}(x,t;0) &= \int_0^t ds\, \partial_s \tilde{u}(x,t;s) \\
&= \int_0^t ds \big[-(\Delta e^{\Delta(t-s)}u(\cdot,s))(x) + (e^{\Delta(t-s)}\partial_s u(\cdot,s))(x)\big] \\
&= \int_0^t ds \big[-(\Delta e^{\Delta(t-s)}u(\cdot,s))(x) + (e^{\Delta(t-s)}\Delta u(\cdot,s))(x) + (e^{\Delta(t-s)}f(\cdot,s))(x)\big] \ ,
\end{aligned} \tag{3.38}$$

where in the last step we used that $u(x,s)$ solves the non-homogeneous heat equation (3.30). Thus, assuming that: $\Delta u(x,s) \in L^1$, and $f(x,s) \in L^1$, we obtain:

$$u(x,t) = u^0(x,t) + \int_0^t ds\, (e^{\Delta(t-s)}f(\cdot,s))(x) \ , \tag{3.39}$$

or, more explicitly:

$$u(x,t) = \int dy\, \Phi(x-y,t)g(y) + \int_0^t ds \int dy\, \Phi(x-y,t-s)f(y,s) \ . \tag{3.40}$$

This way of solving the non-homogeneous problem, by interpolation with the solution of the homogeneous equation, is called Duhamel method. As the next result shows, the representation formula (3.38) holds for a much larger class of initial data and source terms.

Theorem 3.6 (Solution of the non-homogeneous heat equation)**.** *Suppose that* $g \in C(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ *and that* $f \in C_1^2(\mathbb{R}^d \times [0,\infty))$*, with* $f, \partial_t, Df, D^2 f$ *in* $L^\infty(\mathbb{R}^d \times [0,\infty))$*. Then:*

(i) $u \in C_1^2(\mathbb{R}^d \times (0,\infty))$

(ii) $(\partial_t - \Delta u)(x,t) = f(x,t)$ *for* $x \in \mathbb{R}^d$ *and* $t > 0$

(iii) $\lim_{t\to 0^+} u(x,t) = g(x)$ *for all* $x \in \mathbb{R}^d$*.*

Remark 3.7. *The notation* $f \in C_1^2(U)$ *means that* $f, Df, D^2 f, \partial_t f$ *are all continuous in* U*.*

Proof. As proven in Theorem 3.3, the first term in the right-hand side of (3.40) solves the homogeneous problem. Thus, we are left with checking that the second term in the right-hand side of (3.40) satisfies items $(i), (ii), (iii)$ above, with $g = 0$. From now on, we shall suppose that $g = 0$.

The function $\Phi(x-y, t-s)$ has a singularity at $(0,0)$, and we cannot exchange directly the integral and the derivatives ∂_t, Δ. To avoid this problem, we change variables in the integral, so that the derivatives only act on f:

$$u(x,t) = \int_0^t ds \int dy\, \Phi(x-y, t-s) f(y,s) = \int_0^t ds \int dy\, \Phi(y,s) f(x-s, t-s)\ . \tag{3.41}$$

Using that $f \in C_1^2(\mathbb{R}^n \times [0,\infty))$, we compute:

$$\partial_t u(x,t) = \int dy\, \Phi(y,t) f(x-y,0) + \int_0^t ds \int dy\, \Phi(y,s) \partial_t f(x-y, t-s)\ , \tag{3.42}$$

where the exchange of integrals and differentiation is allowed, since $f(\cdot,t)$, $\partial_t f(\cdot,t)$ are bounded, and hence the argument of the y-integrals are L^1 functions. Similarly,

$$\Delta u(x,t) = \int_0^t ds \int dy\, \Phi(y,s) \Delta f(x-y, t-s)\ . \tag{3.43}$$

Therefore, we write:

$$\begin{aligned} u_t - \Delta u &= \int dy\, \Phi(y,t) f(x-y,0) + \int_0^t ds \int dy\, \Phi(y,s) \big[\partial_t f(x-y,t-s) - \Delta f(x-y,t-s)\big] \\ &\equiv \int dy\, \Phi(y,t) f(x-y,0) + \int_0^t ds \int dy\, \Phi(y,s) \big[-\partial_s f(x-y,t-s) - \Delta f(x-y,t-s)\big]\ . \end{aligned} \tag{3.44}$$

Consider the second term. We rewrite it as:

$$\begin{aligned} &\int_0^t ds \int dy\, \Phi(y,s) \big[-\partial_s f(x-y,t-s) - \Delta f(x-y,t-s)\big] \\ &\quad = \int_0^\varepsilon ds \int dy\, \Phi(y,s) \big[-\partial_s f(x-y,t-s) - \Delta f(x-y,t-s)\big] \\ &\qquad + \int_\varepsilon^t ds \int dy\, \Phi(y,s) \big[-\partial_s f(x-y,t-s) - \Delta f(x-y,t-s)\big] \\ &\quad = \mathrm{I} + \mathrm{II}\ . \end{aligned} \tag{3.45}$$

Consider the first term. We have, using that $\int dy\, \Phi(y,s) = 1$:

$$\begin{aligned} |\mathrm{I}| &\leqslant \varepsilon \Big(\max_{s\in[0;\varepsilon]} \max_{y\in\mathbb{R}^d} |\partial_s f(x-y,t-s)| + \max_{s\in[0;\varepsilon]} \max_{y\in\mathbb{R}^d} |\Delta f(x-y,t-s)| \Big) \\ &= o(1)\ . \end{aligned} \tag{3.46}$$

Consider now the second term. Integrating by parts:

$$\begin{aligned} \mathrm{II} &= \int_\varepsilon^t ds \int dy\, (\partial_s - \Delta_y)\Phi(y,s) f(x-y,t-s) \\ &\quad - \int dy\, \Phi(y,t) f(x-y,0) + \int dy\, \Phi(y,\varepsilon) f(x-y,t-\varepsilon) \\ &= - \int dy\, \Phi(y,t) f(x-y,0) + \int dy\, \Phi(y,\varepsilon) f(x-y,t-\varepsilon)\ , \end{aligned} \tag{3.47}$$

where we used that $(\partial_s - \Delta_y)\Phi(y,s) = 0$. Combining this with (3.44), and taking the $\varepsilon \to 0$ limit, we get:

$$u_t - \Delta u = \lim_{\varepsilon \to 0^+} \int dy\, \Phi(y,\varepsilon) f(x-y,t-\varepsilon) = f(x,t)\ , \tag{3.48}$$

where we used the continuity of $f(x,t)$ in t. This proves item (ii). We are left with proving item (iii): in our setting, this means checking that $\lim_{t\to 0^+} u(x,t) = 0$. We have:

$$\begin{aligned} \|u(\cdot,t)\|_\infty &\leqslant \|f\|_\infty t \int dy\, \Phi(y,s) \\ &= \|f\|_\infty t \end{aligned} \tag{3.49}$$

which concludes the proof. ∎

3.4 Uniqueness

So far, we have not discussed the uniqueness of the solution of the heat equation in $\mathbb{R}^d$. Suppose that u_1 and u_2 are two solutions of the non-homogeneous heat equation:

$$\begin{aligned} (\partial_t - \Delta) u(x,t) &= f(x,t) \\ u(x,0) &= g(x)\ . \end{aligned} \tag{3.50}$$

Let $\omega = u_1 - u_2$. Then, ω solves the equation:

$$\begin{aligned} (\partial_t - \Delta) w(x,t) &= 0 \\ w(x,0) &= 0\ . \end{aligned} \tag{3.51}$$

Obviously, $w = 0$ is a solution of this equation. The problem is whether there are other solutions.

Theorem 3.8. *Let $T > 0$ and let $0 \leqslant t \leqslant T$. The function $w(x,t) = 0$ is the only solution of (3.51) such that, for some $A, a > 0$:*

$$|w(x,t)| \leqslant A e^{a|x|^2} \qquad \textit{for all } x \in \mathbb{R}^d \textit{ and for all } 0 \leqslant t \leqslant T. \tag{3.52}$$

The proof of this result follows from the maximum principle for the heat equation, that we shall not discuss; see [2]. It turns out that the growth condition is crucial: in general, it turns out that the heat equation (3.51) admits nontrivial solutions (Tychonov example).

We shall now turn to the problem on a bounded domain. To this end, we need to introduce some notation. Let U be an open and bounded subset of $\mathbb{R}^d$, with C^1 boundary ∂U. Let $T > 0$. We define the parabolic cylinder as:

$$U_T := U \times (0, T]\ . \tag{3.53}$$

Note that U_T includes the top $U \times \{t = T\}$, and does not include the bottom $U \times \{t = 0\}$. We also define the parabolic boundary of U_T as:

$$\Gamma_T := \overline{U}_T - U_T\ . \tag{3.54}$$

Notice that Γ_T includes the bottom $U \times \{t = 0\}$, but does not include the top $U \times \{t = T\}$. In also includes the time-translation of the space boundary, $\partial U \times \{t \in [0, T)\}$. We are interested in the following boundary value problem:

$$\begin{aligned} (\partial_t - \Delta)u &= f \qquad \text{in } U_T \\ u &= g \qquad \text{on } \Gamma_T. \end{aligned} \tag{3.55}$$

Notice that both g and f might depend nontrivially on time, $g \equiv g(x,t)$ and $f \equiv f(x,t)$. Finding a solution to (3.55) might be hard; however, the next result proves that, under mild assumptions on f and g, the solution is unique.

Theorem 3.9. *Let $f \in C(U_T)$ and $g \in C(\Gamma_T)$. Then, there exists at most one solution $u \in C_1^2(\overline{U}_T)$ of the initial/boundary value problem (3.55).*

Proof. The proof we shall give of this theorem is based on an energy argument. Suppose that u_1 and u_2 are two solutions, and let $w = u_1 - u_2$. Then, w solved the initial/boundary value problem (3.55) with $f = g = 0$. Let:

$$e(t) = \int_U w^2(x,t)dx \qquad 0 \leqslant t \leqslant T \; . \tag{3.56}$$

Clearly, $e(t) \geqslant 0$ and $e(t) = 0$ if and only if $w(x,t) = 0$. At $t = 0$, $e(0) = 0$. At later times, we compute the derivative:

$$\begin{aligned} \frac{d}{dt}e(t) &= 2\int_U dx\, w(x,t)w_t(x,t) \\ &= 2\int_U dx\, w(x,t)\Delta w(x,t) \; . \end{aligned} \tag{3.57}$$

Integrating by parts, and using that $w(x,t) = 0$ for $x \in \partial U$:

$$\frac{d}{dt}e(t) = -2\int_U |Dw(x,t)|^2 dx \leqslant 0 \; . \tag{3.58}$$

Therefore, $e(t) \leqslant e(0) = 0$. Since $e(t)$ is a nonnegative quantity, this implies that $w(x,t) = 0$. ∎

3.5 Green's function

As for the Poisson equation, also the heat equation admits a representation formula for its solution in terms of a suitable Green's function. Let U be open and bounded, with C^1 boundary. Consider the following boundary value/initial value problem:

$$\begin{aligned} \partial_t - \Delta u &= f \qquad \text{in } U_T \\ u &= g \qquad \text{on } \Gamma_T. \end{aligned} \tag{3.59}$$

Let us introduce the Green's function of the heat equation as the solution of the following PDE:

$$\begin{aligned} (\partial_t - \Delta_y)G(x,y,t) &= 0 \qquad \text{for } x, y \in U,\ t > 0 \\ G(x,y,t) &= 0 \qquad \text{for } y \in \partial U \text{ or } x \in \partial U,\ t > 0 \\ \lim_{t \to 0^+} G(x,y,t) &= \delta(x-y) \; . \end{aligned} \tag{3.60}$$

Let $u(x,t)$ be a solution of (3.59). We claim that:

$$\begin{aligned} u(x,t) = &\int_U dy \int_0^t ds\, f(y,s)G(x,y,t-s) + \int_U dy\, g(y,0)G(x,y,t) \\ &- \int_{\partial U} dS(y) \int_0^t ds\, g(y,s)\nu \cdot D_y G(x,y,t-s) \; , \end{aligned} \tag{3.61}$$

where ν is the outward normal of ∂U. To prove the statement, let us start from the following identity, which follows as a consequence of the fact that u and G solve the heat equation:

$$\begin{aligned}\int_U dy \int_0^{t-\varepsilon} ds\, \partial_s(u(y,s)G(x,y,t-s)) \\ = \int_U dy \int_0^{t-\varepsilon} ds\, [\Delta_y u(y,s)G(x,y,t-s) - u(y,s)\Delta_y G(x,y,t-s)] \\ + \int_U dy \int_0^{t-\varepsilon} ds\, f(y,s)G(x,y,t-s)\ .\end{aligned} \tag{3.62}$$

Consider the left-hand side. It is equal to:

$$\int_U dy \left[u(y,t-\varepsilon)G(x,y,\varepsilon) - u(y,0)G(x,y,t)\right]\ . \tag{3.63}$$

As $\varepsilon \to 0^+$, this expression converges to, using the last property in (3.60):

$$u(x,t) - \int_U dy\, g(y,0)G(x,y,t)\ . \tag{3.64}$$

Consider now the first term in the right-hand side in (3.62). By Gauss-Green theorem it is equal to:

$$\int_0^{t-\varepsilon} ds \int_{\partial U} dS(y)\, [\nu \cdot D_y u(y,s)G(x,y,t-s) - u(y,s)\nu \cdot D_y G(x,y,t-s)]\ . \tag{3.65}$$

Using that the Green's function vanishes for $y \in \partial U$, we get, as $\varepsilon \to 0^+$:

$$(3.65) = -\int_0^t ds \int_{\partial U} dS(y)\, g(y,s)\nu \cdot D_y G(x,y,t-s)\ . \tag{3.66}$$

Putting everything together, the claim (3.61) follows.

The representation formula (3.61) can be used to find solutions of the heat equation, in cases in which we can find the Green's function, under suitable regularity assumptions on f and on g. For instance, suppose that $U = \mathbb{R}^d_+$. As for the Laplace equation, the Green's function is obtained by the method of images. Let $\Phi(x,t)$ be the fundamental solution of the heat equation. Let $\tilde{y}$ be the reflection y across the boundary of $\mathbb{R}^d_+$: $\tilde{y}_i = y_i$ for $i \neq d$ and $\tilde{y}_d = -y_d$. Then, the Green's function for the heat equation on the half-plane is, for $x, y \in \mathbb{R}^d_+$:

$$G(x,y,t) = \Phi(x-y,t) - \Phi(x-\tilde{y},t)\ . \tag{3.67}$$

We leave to the reader the check that this function satisfies the properties (3.60).

4 The wave equation

4.1 Motivations

[...] This problem of explaining new phenomena in terms of old ones, when we know the laws of the old ones, is perhaps the greatest art of mathematical physics. The mathematical physicist has two problems: one is to find solutions, given the equations, and the other is to find the equations which describe a new phenomenon. (R. Feynman)

The wave equation is PDE of second order in time and space, that describes a wide class of phenomena, from sound propagation, to the oscillations of membranes, to the waves in the

sea. Here we shall heuristically discuss how the wave equation arises in the description of the propagation of sound in a one-dimensional medium. We will follow [3, Chapter 47].

We consider a thin, one-dimensional tube, filled with a gas initially at equilibrium. Let us denote by $\rho_0(x)$ the initial density of the gas, and by $P_0(x)$ the initial pressure. We postulate that the pressure is a local function of the density, $P_0(x) = f(\rho(x))$, for some f. At equilibrium, the density is constant $\rho_0(x) = \rho_0$. We are interested in discussing the evolution of the gas, once a variation of the density is introduced by an external perturbation.

We suppose that at time $t = 0$ a variation in the density is introduced, $\rho_0(x) \to \rho_0(x) + \rho_e(x)$. Correspondingly, the pressure at x also changes:

$$P_0(x) \to P_0(x) + P_e(x) = f(\rho_0(x) + \rho_e(x)) \simeq P_0(x) + \rho_e(x) f'(\rho_0(x)) \,. \tag{4.1}$$

Therefore,

$$P_e(x) \simeq \kappa \rho_e(x) \,, \qquad \kappa = f'(\rho_0(x)) \,. \tag{4.2}$$

At equilibrium, κ is a constant. A change in the pressure introduces a net force on a small portion of the gas, in the interval $[x, x + \Delta x]$. We are interested in finding as equation for this displacement. After a small time t, the interval $[x, \Delta x]$ will evolve as:

$$[x, x + \Delta x] \to [x + u(x,t), x + \Delta x + u(x + \Delta x, t)] \,, \tag{4.3}$$

for a small interval Δx. We are interested in finding an equation for $u(x,t)$. Ultimately, the gas is formed by molecules, that evolve following the laws of mechanics. Thus, we shall try to find an equation for $u(x,t)$ based on mechanical considerations. By mass conservation:

$$\rho_0 \Delta x \simeq \rho(x)[x + \Delta x + u(x + \Delta x, t) - x - u(x,t)] \,. \tag{4.4}$$

The left hand side is the total mass of the interval $[x, x + \Delta x]$, while the right-hand side is an approximation for the total mass in the evolved interval. The approximation is due to the fact that we are choosing the density ρ at the point x, while we should integrate $\rho(\cdot)$ in the evolved interval. This further approximation is motivated by the fact that Δx and $u(x,t)$ are small: we are studying a small displacement around x. Neglecting higher order corrections,

$$\rho_0 \simeq (\rho_0 + \rho_e(x))(1 + \partial_x u(x,t)) \Rightarrow \rho_e(x) \simeq -\rho_0 \partial_x u(x,t) \,. \tag{4.5}$$

The last relation in the above equation has the correct sign: if the size of the interval increases, the density has to decrease. To find an equation of motion for $u(x,t)$, we shall rely on Newton's second law. The acceleration of the particles inside the gas is given by $\partial_t^2 u(x,t)$, and the total mass of the interval is $\rho_0 \Delta x$. The net force acting on the interval is given by the pressure difference $P(x) - P(x + \Delta x)$. Therefore, for small times:

$$\rho_0 \Delta x \partial_t^2 u(x,t) = P(x) - P(x + \Delta x) \,. \tag{4.6}$$

Linearizing the right-hand side in Δx, and recalling the relation (4.2) for the pressure:

$$\rho_0 \partial_t^2 u(x,t) \simeq -\kappa \partial_x \rho_e(x) \simeq \kappa \rho_0 \partial_x^2 u(x,t) \,, \tag{4.7}$$

where in the last step we used (4.5). Therefore, we obtained the following evolution equation for $u(x,t)$:

$$\frac{1}{v_s^2} \partial_t^2 u(x,t) - \partial_x^2 u(x,t) = 0 \,, \tag{4.8}$$

with $v_s^2 := \kappa$ the speed of sound in the medium. Eq. (4.8) is the wave equation, in one spatial dimension. In higher dimension, the wave equation in $\mathbb{R}^d$ is the following initial value problem (we shall set $v_s = 1$ from now on):

$$\begin{aligned} \partial_t^2 u(x,t) - \Delta u(x,t) &= 0 \\ u(x,0) &= g(x) \\ \partial_t u(x,0) &= h(x) \,, \end{aligned} \tag{4.9}$$

where g and h specify the initial condition; notice that, being the equation second order in time, with respect to the heat equation we need an initial condition for the time-derivative as well.

4.2 Solution in $d = 1$: d'Alembert formula

To begin, we will discuss how to solve the wave equation in one space dimension. We consider the initial value problem:

$$\begin{aligned} (\partial_t^2 - \partial_x^2)u(x,t) &= 0 \\ u(x,0) &= g(x) \\ \partial_t u(x,0) &= h(x) \ . \end{aligned} \tag{4.10}$$

As usual, we shall suppose that a solution exists, and we shall find a representation formula for the solution. Then, we will have to check that the formula indeed provided a solution. It is convenient to rewrite the equation as:

$$(\partial_t + \partial_x)(\partial_t - \partial_x)u(x,t) = 0 \ . \tag{4.11}$$

Let us define $v(x,t) := (\partial_t - \partial_x)u(x,t)$. Then, the wave equation reduces to two coupled first order PDEs:

$$\begin{aligned} (\partial_t + \partial_x)v(x,t) &= 0 \\ (\partial_t - \partial_x)u(x,t) &= v(x,t) \ . \end{aligned} \tag{4.12}$$

We shall first solve the first, and then use it as a source term for the second. These two equations are a special case of the *transport equation*, which we now briefly discuss.

The transport equation. In $\mathbb{R}^d$, the transport equation is, for a fixed vector $b \in \mathbb{R}^d$:

$$\partial_t u(x,t) + b \cdot \nabla u(x,t) = 0 \ . \tag{4.13}$$

This equation described the evolution of the density of a rigid body; let us see why. Let $\Omega \subset \mathbb{R}^d$ be the volume occupied by a body, and let us define its translation along b as:

$$\Omega(t) := \{x \in \mathbb{R}^d \mid x - bt \in \Omega\} \ . \tag{4.14}$$

Let $u(x,t)$ be the mass density contained in $\Omega(t)$. Then, the total mass at time t is:

$$\int_{\Omega(t)} dx\, u(x,t) = \int_\Omega dx\, u(x+bt,t) \ . \tag{4.15}$$

The total mass is unchanged by the translation:

$$0 = \frac{d}{dt}\int_\Omega dx\, u(x+bt,t) = \int_\Omega dx\, (\partial_t u(x,t) + b \cdot \nabla u(x,t)) \ . \tag{4.16}$$

Being true for any $\Omega \subset \mathbb{R}^d$, we see that the density $u(x,t)$ satisfies the transport equation (4.13).

If $u(x,t)$ solves (4.13), the function $s \mapsto z(s) := u(x+sb, t+s)$ is constant in s. In particular,

$$z(0) = z(-t) \ , \tag{4.17}$$

which implies:

$$u(x,t) = u(x-bt,0) \ . \tag{4.18}$$

Therefore, the solution of the transport equation corresponds to a translation of the function $u(x,0)$. To conclude the discussion about the transport equation, let us consider the non-homogeneous case. We consider:

$$\begin{aligned} \partial_t u(x,t) + b \cdot \nabla u(x,t) &= f(x,t) \\ u(x,0) &= g(x) \ . \end{aligned} \tag{4.19}$$

Equivalently, we can reformulate the transport equation as:

$$\frac{d}{ds} z(s) = f(x+sb, t+s) \ . \tag{4.20}$$

Integrating:

$$\begin{aligned} z(0) - z(-t) &= \int_{-t}^{0} ds \, \frac{d}{ds} z(s) \\ &= \int_{-t}^{0} ds \, f(x+sb, t+s) \\ &= \int_{0}^{t} ds \, f(x+(s-t)b, s) \ . \end{aligned} \tag{4.21}$$

That is:

$$u(x,t) = g(x-tb) + \int_0^t ds \, f(x+(s-t)b, s) \ . \tag{4.22}$$

The formula (4.22) is useful in solving the wave equation in $d = 1$, (4.12). By the previous discussion, the solution of the first equation in (4.12) is:

$$v(x,t) = h(x-t) - (\partial_x g)(x-t) \ . \tag{4.23}$$

Let us now consider the second line, where now v acts as a source term. We have:

$$u(x,t) = g(x+t) + \int_0^t dx \, v(x-(s-t), s) \ ; \tag{4.24}$$

plugging the identity (4.23) in (4.24), after a few manipulations, we have:

$$u(x,t) = \frac{1}{2}(g(x+t) + g(x-t)) + \frac{1}{2} \int_{x-t}^{x+t} dy \, h(y) \ . \tag{4.25}$$

This is a representation formula for the solution of the one-dimensional wave equation, which takes the name of d'Alembert formula. It is not difficult to check that (4.25) solves the one-dimensional wave equation.

Theorem 4.1 (Solution of the wave equation in $d = 1$.)**.** *Let $g \in C^2(\mathbb{R})$, $h \in C^1(\mathbb{R})$. Let $u(x,t)$ be given by d'Alembert formula. Then:*

(i) $u \in C^2(\mathbb{R} \times [0, \infty))$

(ii) $u_{tt} - u_{xx} = 0$ *for* $(x,t) \in \mathbb{R} \times \mathbb{R}_+$

(iii) $\lim_{t \to 0} u(x,t) = g(x)$ *and* $\lim_{t \to 0} u_t(x,t) = h(x)$.

Remark 4.2. *(i) In contrast to the heat equation, the solution of the wave equation does not get smoother.*

(ii) The solution has finite propagation speed. The solution u at the space time point (x,t) is determined by the functions $g(y)$ and $h(y)$ for values y such that $|x-y| \leqslant t$. In order words, perturbations of g and h for values of y such that $|y-x| > t$ do not affect the solution u at (x,t). Physically, the information carried by the propagation did not reach the space-time point (x,t).

(iii) The wave equation is time-reversal symmetric. Given a solution $u(x,t)$ with initial datum (g,h), we obtain another solution $\tilde{u}(x,t)$ by setting $\tilde{u}(x,t) = u(x,-t)$ and choosing initial datum $(\tilde{g},\tilde{h}) = (g,-h)$.

(iv) The solution of the one-dimensional wave equation can be rewritten as:

$$u(x,t) = F(x+t) + G(x-t) \tag{4.26}$$

with, for an arbitrary point x_0:

$$\begin{aligned} F(x+t) &= \frac{1}{2}g(x+t) + \frac{1}{2}\int_{x_0}^{x+t} dy\, h(y) \\ G(x-t) &= \frac{1}{2}g(x-t) + \frac{1}{2}\int_{x-t}^{x_0} dy\, h(y)\ . \end{aligned} \tag{4.27}$$

Thus, the solution can be viewed as the superposition of two travelling wavefronts, with opposite directions.

The wave equation on the half-line. Before concluding the section, let us discuss the solution of the wave equation on the half-line. This will be relevant for the content of next section as well. We consider:

$$\begin{aligned} u_{tt} - u_{xx} &= 0 \qquad \text{on } \mathbb{R}_+ \times \mathbb{R}_+ \\ u(x,0) &= g(x) \qquad \text{for } x \in \mathbb{R}_+ \\ u_t(x,0) &= h(x) \qquad \text{for } x \in \mathbb{R}_+ \\ u(0,t) &= 0 \qquad \text{for } t \in \mathbb{R}_+\ . \end{aligned} \tag{4.28}$$

Thus, for consistency $g(0) = h(0) = 0$. In order to solve (4.28), we shall use a reflection method. Suppose that $u(x,t)$ is a solution of (4.28). We extend this function to $x \in \mathbb{R}$ by defining:

$$\begin{aligned} \tilde{u}(x,t) &= u(x,t) \qquad x \geqslant 0 \\ \tilde{u}(x,t) &= -u(-x,t) \qquad x \leqslant 0\ . \end{aligned} \tag{4.29}$$

It is easy to check that $\tilde{u}(x,t)$ is continuous at $x=0$. Also, $\tilde{u}_x(x,t)$ is continuous at $x=0$. It order to have a C^2 solution on $\mathbb{R}$, we also have to assume that $g''(0) = 0$, as it will be clear in a moment. By construction, the function $\tilde{u}$ satisfies the wave equation on the real line:

$$\begin{aligned} \tilde{u}_{tt}(x,t) - \tilde{u}_{xx}(x,t) &= 0 \qquad \text{on } \mathbb{R} \times (0,\infty) \\ \tilde{u} &= \tilde{g} \qquad \text{on } \mathbb{R} \times \{t=0\} \\ \tilde{u}_t &= \tilde{h} \qquad \text{on } \mathbb{R} \times \{t=0\}\ . \end{aligned} \tag{4.30}$$

We can find the expression for $\tilde{u}$ by using d'Alembert formula. We get:

$$\tilde{u}(x,t) = \frac{1}{2}(\tilde{g}(x+t) + \tilde{g}(x-t)) + \frac{1}{2}\int_{x-t}^{x+t} dy\, \tilde{h}(y)\ . \tag{4.31}$$

Suppose $0 \leqslant x$, $x \geqslant t$. Then:

$$u(x,t) = \frac{1}{2}(g(x+t) + g(x-t)) + \frac{1}{2}\int_{x-t}^{x+t} dy\, h(y)\ . \tag{4.32}$$

Instead, if $0 \leqslant x < t$:

$$u(x,t) = \frac{1}{2}(g(x+t) - g(t-x)) + \frac{1}{2}\int_{t-x}^{x+t} dy\, h(y)\ . \tag{4.33}$$

These two branches of the solution can be joined in a C^2 way only if $g''(0) = 0$.

4.3 Solution in $d = 3$: Kirchhoff formula

In this section we shall discuss the wave equation in $d = 3$:

$$\begin{aligned} (\partial_t^2 - \Delta)u(x,t) &= 0 \qquad \text{on } \mathbb{R}^3 \times \mathbb{R}_+ \\ u(x,0) &= g(x) \qquad \text{on } \mathbb{R}^3 \\ u_t(x,0) &= h(x) \qquad \text{on } \mathbb{R}^3. \end{aligned} \tag{4.34}$$

The procedure we will follow to find the solution for this equation will rely on the $1d$ case on the half-line, discussed at the end of the previous section. Let us define the spherical averages:

$$\begin{aligned} U(x;r,t) &:= \fint u(y,t)dS(y) \\ G(x;r) &:= \fint g(y)dS(y) \\ H(x;r) &:= \fint h(y)dS(y)\ . \end{aligned} \tag{4.35}$$

By continuity, $\lim_{r\to 0^+} U(x;r,t) = u(x,t)$, and the same for H and G. Our strategy will be to find an equation in the (r,t) variables, at x fixed, for the spherical averages. The solution of the wave equation in $d = 3$ will be obtained as $r \to 0^+$ of the solution of this new equation.

Lemma 4.3 (Euler-Poisson-Darboux equation.)**.** *Suppose that $u \in C^m(\mathbb{R}^d \times \overline{\mathbb{R}_+})$ for $m \geqslant 2$ solves the wave equation. Then, $U \in C^m(\mathbb{R}_+ \times \overline{\mathbb{R}_+})$, and it solves the equation:*

$$\begin{aligned} U_{tt} - U_{rr} - \frac{d-1}{r}U_r &= 0 \qquad \textit{on } \mathbb{R}_+ \times \mathbb{R}_+ \\ U &= G \qquad \textit{on } \mathbb{R}_+ \times \{t = 0\} \\ U_t &= H \qquad \textit{on } \mathbb{R}_+ \times \{t = 0\}. \end{aligned} \tag{4.36}$$

Before proving this lemma, let us show how it allows to solve the wave equation in $d = 3$. To this end, let U be a solution of the EPD equation, and let:

$$\widetilde{U} = rU\ , \qquad \widetilde{G} = rG\ , \qquad \widetilde{H} = rH\ . \tag{4.37}$$

We claim that $\widetilde{U}$ solves the $1d$ wave equation on the half-line:

$$\begin{aligned} \widetilde{U}_{tt} - \widetilde{U}_{rr} &= 0 \qquad \text{on } \mathbb{R}_+ \times \mathbb{R}_+ \\ \widetilde{U} &= \widetilde{G} \qquad \text{on } \mathbb{R}_+ \times \{t = 0\} \\ \partial_t\widetilde{U} &= \widetilde{H} \qquad \text{on } \mathbb{R}_+ \times \{t = 0\} \\ \widetilde{U} &= 0 \qquad \text{on } \{r = 0\} \times \mathbb{R}_+. \end{aligned} \tag{4.38}$$

Also, $\widetilde{G}''(0) = 0$, as one might easily check. Let us check that (4.38) holds. From now on, we shall set $d = 3$. We have.

$$\widetilde{U}_{tt} = rU_{tt} = r\Big(U_{rr} + \frac{2}{r}U_r\Big) \tag{4.39}$$

where in the last step follows from the EPD equation. Therefore:

$$\widetilde{U}_{tt} = rU_{rr} + 2U_r = (U + rU_r)_r \ , \tag{4.40}$$

and the final claim follows after recognizing that $U + rU_r = \widetilde{U}_r$. Let us now use the explicit solution of the wave equation on the half-line, obtained at the end of the previous section, to determine $\widetilde{U}(x; r, t)$ for $0 \leqslant r \leqslant t$; this is the only range of parameters we are interested in, since we will eventually take the limit $r \to 0^+$. We have:

$$\widetilde{U}(x; r, t) = \frac{1}{2}\Big(\widetilde{G}(x; r + t) - \widetilde{G}(x; r - t)\Big) + \frac{1}{2}\int_{-r+t}^{r+t} dy\, \widetilde{H}(y) \ . \tag{4.41}$$

By continuity, $u(x, t) = \lim_{r\to 0^+} \widetilde{U}(x; r, t)/r$. Hence:

$$\begin{aligned} u(x, t) &= \lim_{r\to 0^+} \Big(\frac{\widetilde{G}(x; r + t) - \widetilde{G}(x; r - t)}{2r} + \frac{1}{2r}\int_{t-r}^{t+r} dy\, \widetilde{H}(y)\Big) \\ &= \partial_t \widetilde{G}(x; t) + \widetilde{H}(x; t) \ . \end{aligned} \tag{4.42}$$

Let us compute the first term. We have:

$$\begin{aligned} \partial_t \widetilde{G}(x; t) &= \frac{\partial}{\partial t}\Big(t \fint_{\partial B_t(x)} dS(y)\, g(y)\Big) \\ &= \frac{\partial}{\partial t}\Big(t \fint_{\partial B_1(0)} dS(z)\, g(x + tz)\Big) \\ &= \fint_{\partial B_1(0)} dS(z)\, g(x + tz) + \fint_{\partial B_1(0)} dS(z)\, tz \cdot Dg(x + tz) \\ &= \fint_{\partial B_t(x)} dS(y)\Big[g(y) + t\Big(\frac{y - x}{t}\Big) \cdot Dg(y)\Big] \ . \end{aligned} \tag{4.43}$$

Plugging this identity in (4.42), and recalling that $\widetilde{H}(x; t) = t \fint_{\partial B(x,t)} dS(y) h(y)$:

$$u(x, t) = \fint_{\partial B_t(x)} dS(y)\Big[g(y) + (y - x) \cdot Dg(y) + th(y)\Big] \ . \tag{4.44}$$

Eq. (4.44) is the explicit solution of the wave equation in $d = 3$. It is called Kirchhoff formula. Eq. (4.44) has been derived under the assumption that $u(x, t)$ is a solution. It is not difficult to check that Eq. (4.44) indeed provided a solution of the wave equation.

Theorem 4.4. *Suppose that $g \in C^3(\mathbb{R}^3)$ and $h \in C^2(\mathbb{R}^3)$. Let $u(x, t)$ be given by* (4.44)*. Then, $u(x, t)$ is a C^2 solution of the wave equation (4.34).*

Remark 4.5. *(i) Compared to the* 1*d case, we are requiring more regularity on g and h. In particular, the regularity of g is higher than the regularity of u.*

(ii) The solution has the finite propagation speed property. The value of u at (x, t) is determined by the values of g and h at y such that $|y - x| = t$. Equivalently, the value of g and h at a given y affect the solution u for all (x, t) such that $|x - y| = t$.

To conclude the discussion of the solution of the $d = 3$ wave equation, we have to show that if $u(x, t)$ is a solution then its spherical average satisfies the EPD equation (4.36).

Proof of Lemma 4.3. To begin, we compute:

$$\begin{aligned} U_r(x;r,t) &= \frac{\partial}{\partial r} \fint_{\partial B_r(x)} dS(y)\, u(y,t) \\ &= \frac{1}{r} \fint_{\partial B_1(0)} dS(y)\, y \cdot D_y u(x+ry,t) \ . \end{aligned} \tag{4.45}$$

By Gauss-Green theorem:

$$\begin{aligned} U_r(x;r,t) &= \frac{1}{r|\partial B_1(0)|} \int_{B_1(0)} dy\, \Delta_y u(x+ry,t) \\ &= \frac{r}{r|\partial B_1(0)|} \int_{B_1(0)} dy\, \Delta_x u(x+ry,t) \\ &= \frac{r}{d} \fint_{B_r(x)} dy\, \Delta u(y,t) \ , \end{aligned} \tag{4.46}$$

where we used that $|\partial B_1(0)| = d|B_1(0)|$. Hence,

$$\begin{aligned} r^{d-1} U_r(x;r,t) &= \frac{1}{d\alpha(d)} \int_{B_r(x)} dy\, \Delta u(y,t) \\ &= \frac{1}{d\alpha(d)} \int_{B_r(x)} dy\, u_{tt}(y,t) \end{aligned} \tag{4.47}$$

where we used that u solves the wave equation. Furthermore,

$$\begin{aligned} \big(r^{d-1} U_r(x;r,t)\big)_r &= \frac{1}{d\alpha(d)} \int_{\partial B_r(x)} dS(y)\, u_{tt}(y,t) \\ &= r^{d-1} \fint_{\partial B_r(x)} dS(y)\, u_{tt}(y,t) \ , \end{aligned} \tag{4.48}$$

which is equal to $r^{d-1} U_{tt}(x;r,t)$. Hence:

$$U_{tt}(x;r,t) - \frac{1}{r^{d-1}} \big(r^{d-1} U_r(x;r,t)\big)_r = 0 \tag{4.49}$$

which is equivalent to:

$$U_{tt}(x;r,t) - \frac{d-1}{r} U_r(x;r,t) - U_{rr}(x;r,t) = 0 \ . \tag{4.50}$$

This concludes the proof of Lemma 4.3. ∎

To conclude the section, let us briefly sketch the argument that one should follow to solve the wave equation in $d = 2$. Suppose that $u \in C^2(\mathbb{R}^2 \times \mathbb{R}_+)$ is a solution of the $2d$ wave equation. Define $\tilde{u} \in C^2(\mathbb{R}^3 \times \mathbb{R}_+)$ as:

$$\tilde{u}(x_1, x_2, x_3, t) = u(x_1, x_2, t\ .) \tag{4.51}$$

That is, the function $\tilde{u}$ is constant in x_3. Being u solution of the $2d$ wave equation, the function $\tilde{u}$ trivially solves the $3d$ wave equation. The solution of the $3d$ wave equation is given by Kirchhoff formula (4.44). In this expression, the argument of the integral is constant in y_3; thus, performing the y_3 integration we get, see [2] for details:

$$u(x,t) = \frac{1}{2} \fint_{B_t(x)} dy\, \frac{t g(y) + t^2 h(y) + t(y-x) \cdot Dg(y)}{|t^2 - |y-x|^2|^{1/2}} \ . \tag{4.52}$$

This expression takes the name of Poisson formula.

Remark 4.6. *Notice that the value of the solution at (x,t) is influenced by the values of g and h for y such that $|x-y| \leqslant t$, instead of $|x-y| = t$ as in the $3d$ case. Equivalently, after a time t, the initial datum at y influences the solution in a ball of radius t centered at y, while in the $3d$ case it influences the solution in a sphere of radius t centered at y. This phenomenon is called Huygens principle.*

4.4 Non-homogeneous wave equation

Let us now consider the wave equation in the presence of a source term:

$$\begin{aligned} (\partial_t^2 - \Delta)u(x,t) &= f(x,t) \qquad \text{on } \mathbb{R}^3 \times \mathbb{R}_+ \\ u(x,0) &= g(x) \qquad \text{on } \mathbb{R}^3 \\ u_t(x,0) &= h(x) \qquad \text{on } \mathbb{R}^3. \end{aligned} \tag{4.53}$$

The source term f describes an external force acting on the system. For instance, in the heuristic discussion of Section 4.1, it could take into account an external force acting on the gas confined in the thin tube, such as gravity, if the tube is tilted.

In this section we shall discuss how to solve (4.53). By linearity of the equation, we can represent the solution as $u = u_1 + u_2$, where u_1 is the solution of the non-homogeneous problem with $g = h = 0$, and u_2 is the solution of the homogeneous problem with $f = 0$. Thus, without loss of generality we shall suppose that $g = h = 0$.

Suppose for the moment that $u(x,t)$ is a solution, in $L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$, together with all its derivatives. Then, we can define the Fourier transform of u, which we can also invert. The Fourier transform of the solution of the wave equation satisfies the ODE:

$$\begin{aligned} &(\partial_t^2 + |k|^2)\hat{u}(k,t) = \hat{f}(k,t) \\ &\hat{u}(k,0) = \hat{u}_t(k,0) = 0 \, . \end{aligned} \tag{4.54}$$

In general, the solution of the homogeneous wave equation, with non-zero initial datum, is:

$$\hat{u}_0(k,t) = \cos(|k|t)\hat{g}(k) + \frac{\sin(|k|t)}{|k|}\hat{h}(k) \, . \tag{4.55}$$

By functional calculus, we could also represent the function $u_0(x,t)$ as:

$$u_0(x,t) = \cos(|\nabla|t)g(x,t) + \frac{\sin(|\nabla|t)}{|\nabla|}h(x,t) \, . \tag{4.56}$$

We shall apply Duhamel's method. We would like to define a function $\hat{u}(k,t;s)$ which allow to interpolate between the solution of the non-homogeneous equation and the solution of the homogeneous equation (for $g = h = 0$). To this end, it is natural to define:

$$\hat{u}(k,t;s) = \cos(|k|(t-s))\hat{u}(k,s) + \frac{\sin(|k|(t-s))}{|k|}\partial_s\hat{u}(k,s) \, , \tag{4.57}$$

with $\hat{u}(k,s)$ the solution of the non-homogeneous problem. We see that $\hat{u}(k,t;t) = \hat{u}(k,t)$ and $\hat{u}(k,t;0) = 0$. Hence:

$$\begin{aligned} \hat{u}(k,t) &= \int_0^t ds\, \partial_s\hat{u}(k,t;s) \\ &= \int_0^t ds \Big[|k| \sin(|k|(t-s))\hat{u}(k,s) + \cos(|k|(t-s))\partial_s\hat{u}(k,s) \\ &\qquad - \cos(|k|(t-s))\partial_s\hat{u}(k,s) + \frac{\sin(|k|(t-s))}{|k|}\partial_s^2\hat{u}(k,s) \Big] \, . \end{aligned} \tag{4.58}$$

Using that $\hat{u}$ solves the non-homogeneous problem, we have $\partial_s^2 \hat{u}(k,s) = -|k|^2 \hat{u}(k,s) + \hat{f}(k,s)$ and therefore:

$$\hat{u}(k,t) = \int_0^t ds \, \frac{\sin(|k|(t-s))}{|k|} \hat{f}(k,s) \; . \tag{4.59}$$

Notice that the argument of the integral is also the solution of the following homogeneous wave equation:

$$\begin{aligned} (\partial_{tt} + |k|^2)\hat{u}(k,t) = 0 \qquad & \text{for } t > s \\ \hat{u} = 0, \; \hat{u}_t = \hat{f}(\cdot, s) \qquad & \text{for } t = s. \end{aligned} \tag{4.60}$$

Thus, we found that the non-homogeneous wave equation with $g = h = 0$ is solved by:

$$u(x,t) = \int_0^t ds \, u_0(x,t;s) \; , \tag{4.61}$$

where $u_0(x,t;s)$ solves the homogeneous wave equation:

$$\begin{aligned} (\partial_{tt} - \Delta)u(x,t) = 0 \qquad & \text{for } t > s \\ u = 0, \; u_t = f(\cdot, s) \qquad & \text{for } t = s. \end{aligned} \tag{4.62}$$

We proved this by assuming suitable regularity properties of the solution. The next theorem proves that the expression we found, Eq. (4.62), holds on greater generality.

Theorem 4.7. *Let*[2] $f \in C^{[d/2]+1}(\mathbb{R}^d \times \mathbb{R}_+)$ *for* $d \geqslant 2$ *and* $f \in C^2(\mathbb{R} \times \mathbb{R}_+)$ *for* $d = 1$. *Then, the function* $u(x,t)$ *in (4.61) solves the non-homogeneous wave equation.*

Let $d = 3$. By Kirchhoff formula (4.44), the solution of the wave equation (4.62) is:

$$u_0(x,t;s) = (t-s) \fint_{\partial B_{t-s}(x)} dS(y) f(y;s) \; . \tag{4.63}$$

That is, plugging this expression in (4.61):

$$\begin{aligned} u(x,t) &= \int_0^t ds \, (t-s) \fint_{\partial B_{t-s}(x)} dS(y) \, f(y;s) \\ &= \frac{1}{4\pi} \int_0^t ds \int_{\partial B_{t-s}(x)} dS(y) \, \frac{f(y;s)}{t-s} \\ &\equiv \frac{1}{4\pi} \int_0^t ds \int_{\partial B_s(x)} dS(y) \, \frac{f(y;t-s)}{s} \; . \end{aligned} \tag{4.64}$$

Therefore, rewriting the expression in terms of an integral over a ball:

$$u(x,t) = \frac{1}{4\pi} \int_{B_t(x)} dy \, \frac{f(y;t-|y-x|)}{|y-x|} \; . \tag{4.65}$$

The integrand on the right-hand side is called a retarded potential.

[2] $[a]$ denotes the integer part of a.

4.5 Uniqueness

In this section we shall discuss the proof of uniqueness for the solution of the wave equation. We shall use energy methods, that allow to prove uniqueness of a bounded domain. The same method will allow us to reformulate the finite-speed of propagation property.

Let us consider the following initial value/boundary value problem:

$$\begin{aligned} u_{tt} - \Delta u &= f \ , \qquad \text{on } U_T \\ u &= g \ , \qquad \text{on } \Gamma_T \\ u_t &= h \ , \qquad \text{on } U \times \{t = 0\}. \end{aligned} \tag{4.66}$$

The set $U \subset \mathbb{R}^d$ is open and bounded, with C^1 boundary. See Section 3.4 for the definition of U_T and Γ_T.

Theorem 4.8 (Uniqueness for the wave equation.)**.** *There exists at most one function $u \in C^2(\overline{U}_T)$ solving (4.66).*

Proof. Suppose that u_1 and u_2 solve (4.66). Let $w = u_1 - u_2$. Then, $w(x,t)$ solves:

$$\begin{aligned} w_{tt} - \Delta w &= 0 \ , \qquad \text{on } U_T \\ w(x,t) &= 0 \ , \qquad \text{on } \Gamma_T \\ w_t(x,t) &= 0 \ , \qquad \text{on } U \times \{t = 0\}. \end{aligned} \tag{4.67}$$

Cleary, $w = 0$ is a solution of such PDE. We would like to know whether it is the unique solution. To this end, define the energy of $w(x,t)$ as:

$$E(t) := \frac{1}{2} \int_U ds \, [w_t(x,t)^2 + |Dw(x,t)|^2] \tag{4.68}$$

for $0 \leqslant t \leqslant T$. Trivially, $E(0) = 0$ and $E(t) \geqslant 0$. Suppose we know that $E(t) = 0$ for $0 \leqslant t \leqslant T$. This implies that $w_t(x,t) = 0$ and that $\partial_{x_i} w(x,t) = 0$ for $0 \leqslant t \leqslant T$. Since $w = 0$ on $U \times \{t = 0\}$, we find $w(x,t) = 0$ for $(x,t) \in U_T$.

Let us now prove that $E(t) = 0$ for $0 \leqslant t \leqslant T$. As for the heat equation, we compute the time derivative of the energy:

$$\frac{d}{dt} E(t) = \int_U dx \, [w_t(x,t) w_{tt}(x,t) + Dw(x,t) \cdot Dw_t(x,t)] \ . \tag{4.69}$$

Integrating by parts, using Gauss-Green theorem, we have:

$$\frac{d}{dt} E(t) = \int_U dx \, w_t(x,t)[w_{tt}(x,t) - \Delta w(x,t)] + \int_{\partial U} dS(x) \, Dw(x,t) \cdot \nu w_t(x,t) \ . \tag{4.70}$$

The boundary term is vanishing, due to the fact that $w(x,t) = 0$ for $(x,t) \in \partial U \times [0,T]$, and hence $w_t(x,t) = 0$ for $(x,t) \in \partial U \times [0,T]$. Also, the first term is vanishing, due to the fact that $w(x,t)$ solves the homogeneous wave equation. Therefore,

$$E(t) = E(0) \qquad \text{for all } 0 \leqslant t \leqslant T, \tag{4.71}$$

which proves that $w = 0$ is the only solution of (4.67), hence $u_1 = u_2$. ∎

Remark 4.9. *Notice that the above proof works also on unbounded domains, provided the energy of the solution is finite.*

To conclude the section, let us review the issue of the finite speed of propagation, using conservation of the energy. For the sake of the forthcoming discussion, U might be unbounded; e.g., it could be $U = \mathbb{R}^d$. Let us consider the following boundary value/initial value problem:

$$\begin{aligned} w_{tt} - \Delta w &= 0 \,, \qquad \text{on } U_T \\ w(x,t) &= g(x,t) \,, \qquad \text{on } \Gamma_T \\ w_t(x,t) &= h(x) \,, \qquad \text{on } U \times \{t=0\}. \end{aligned} \tag{4.72}$$

Let $x_0 \in U$, $T \geqslant t_0 > 0$. Suppose that $B_{t_0}(x_0) \subset U$. Let us define the *backwards wave cone* with apex (x_0, t_0) as:

$$K(x_0,t_0) := \{(x,t) \mid 0 \leqslant t \leqslant t_0 \,, \quad |x - x_0| \leqslant t_0 - t\} \,. \tag{4.73}$$

Notice that, due to the condition $B_{t_0}(x_0) \subset U$, $K(x_0,t_0) \subset U_{t_0}$. The following theorem generalizes the finite speed of propagation property, encountered in the previous discussion, when finding explicit solutions of the wave equation in $d = 1, 2, 3$.

Theorem 4.10 (Finite speed of propagation.)**.** *Let u be a solution of (4.72) in $C^2(\overline{U}_T)$. Suppose that $g(x,0) = h(x,0) = 0$ for $x \in B_{t_0}(x_0)$. Then, $u(x,t) = 0$ for all $(x,t) \in K(x_0,t_0)$.*

Remark 4.11. *This theorem easily implies that any perturbation of the initial datum away from $B_{t_0}(x_0)$ does not affect the shape of the solution inside the cone $K(x_0,t_0)$.*

Proof. For $0 \leqslant t \leqslant t_0 \leqslant T$, let us define the local energy:

$$e(t) := \frac{1}{2} \int_{B_{t_0-t}(x_0)} dx \, [u_t^2(x,t) + |Du(x,t)|^2] \,. \tag{4.74}$$

Clearly, $e(0) = 0$. To estimate $e(t)$ at later times, compute:

$$\frac{d}{dt} e(t) = \int_{B_{t_0-t}(x_0)} dx \, [u_t u_{tt} + Du \cdot Du_t] - \frac{1}{2} \int_{\partial B_{t_0-t}(x_0)} dS(y) \, [u_t^2 + |Du|^2] \,. \tag{4.75}$$

By Gauss-Green theorem:

$$\begin{aligned} \frac{d}{dt} e(t) = &\int_{B_{t_0-t}(x_0)} dx \, u_t (u_{tt} - \Delta u) + \int_{\partial B_{t_0-t}(x_0)} (\nu \cdot Du) u_t dS(y) \\ &- \frac{1}{2} \int_{\partial B_{t_0-t}(x_0)} dS(y) \, [u_t^2 + |Du|^2] \,. \end{aligned} \tag{4.76}$$

Using that u solves the homogeneous wave equation:

$$\frac{d}{dt} e(t) = \int_{\partial B_{t_0-t}(x_0)} (\nu \cdot Du) u_t dS(y) - \frac{1}{2} \int_{\partial B_{t_0-t}(x_0)} dS(y) \, [u_t^2 + |Du|^2] \,. \tag{4.77}$$

This is the point where we used that $B_{t_0}(x_0) \subset U$, which also implies $B_{t_0-t}(x_0) \subset U$. Next, by Cauchy-Schwarz inequality, recalling that $|\nu| = 1$:

$$\Big| (\nu \cdot Du) u_t \Big| \leqslant \frac{1}{2} |Du|^2 + \frac{1}{2} u_t^2 \,. \tag{4.78}$$

Inserting this inequality in (4.77), we get, for all $0 \leqslant t \leqslant t_0$:

$$\frac{d}{dt} e(t) \leqslant 0 \,. \tag{4.79}$$

Therefore, $0 \leqslant e(t) \leqslant e(0) = 0$, which means that

$$u_t(y,t) = 0 \quad \text{and} \quad \partial_i u(y,t) = 0 \quad \text{for all } x \in B_{t_0-t}(x_0) \text{ and for all } t \in [0,t_0]. \tag{4.80}$$

Since $u = 0$ on $B_{t_0}(x_0) \times \{t = 0\}$, the first condition in (4.80) implies that $u = 0$ in $K(x_0,t_0)$. This concludes the proof. ∎

5 Quantum mechanics

Quantum mechanics is the microscopic theory of nature that describes the properties of the microscopic world, on the scale of atoms and molecules. It is more fundamental than classical mechanics, in the sense that classical mechanics can be derived from quantum mechanics in a suitable limit. Evolution in quantum mechanics is defined by the Schrödinger equation, a linear PDE that will be introduced below. This section will be devoted to the study of the Schrödinger equation, in some special cases. Most of what will be discussed in this section can be found in the books [9, 8].

5.1 Postulates of quantum mechanics

States and observables. Let $\mathcal{H}$ be a vector space over $\mathbb{C}$, equipped with a scalar product $\langle \cdot, \cdot \rangle$. In the following, we shall denote by $\| \cdot \|$ the norm induced by the scalar product. If $\mathcal{H}$, equipped with this norm, is complete, then the pair $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ is called a Hilbert space. An important example is the space of square-integrable functions, $L^2(\mathbb{R}^d)$, equipped with the scalar product

$$\langle f, g \rangle = \int_{\mathbb{R}^d} dx \, \overline{f(x)} g(x) \, . \tag{5.1}$$

States in quantum mechanics correspond to vectors in a Hilbert space $\mathcal{H}$. The precise choice of the Hilbert space is dictated by the problem we want to study. Physically measurable quantities, called observables, correspond to self-adjoint operators on $\mathcal{H}$. Recall that a linear operator $O : \mathcal{H} \to \mathcal{H}$ is called self-adjoint if:

$$\langle f, Og \rangle = \langle Of, g \rangle \qquad \forall f, g \in \mathcal{H} \, . \tag{5.2}$$

The expected value of the observable O on the state ψ is defined as

$$\langle \psi, O\psi \rangle \, . \tag{5.3}$$

Being O self-adjoint, this quantity is real. Physically, this number is what one obtains after infinitely many measurements of the physical observable O.

Suppose for the moment that $\mathcal{H}$ is finite dimensional. By the spectral theorem for self-adjoint operators, we can represent O as:

$$O = \sum_j \lambda_j P_{\varphi_j} \, , \tag{5.4}$$

with λ_j the eigenvalues of O, and P_{φ_j} the orthogonal projector onto the eigenvector φ_j. That is:

$$P_{\varphi_j} \psi = \langle \varphi_j, \psi \rangle \varphi_j \, . \tag{5.5}$$

Then, we have:

$$\langle \psi, O\psi \rangle = \sum_j \lambda_j |\langle \psi, \varphi_j \rangle|^2 \, . \tag{5.6}$$

Notice that, by the completeness of the orthonormal basis generated by the eigenvectors of O,

$$\sum_j |\langle \psi, \varphi_j \rangle|^2 = 1 \, . \tag{5.7}$$

The interpretation of the identity (5.6) is the following. The eigenvalues λ_j are the possible values of the observable O, and $|\langle \psi, \varphi_j \rangle|^2$ is the probability that, if the system is in the state ψ, a measurement of O gives the value λ_j. If, for example, $\psi = \varphi_j$, then a measurement of O will produce the value λ_j with probability 1. In general, however, ψ will be a linear combination

of different eigenstates φ_j, hence a measurement of O will give different values with different probabilities. It makes sense, therefore, to introduce the variance of O in the state ψ by setting:

$$\Delta O_\psi := \langle \psi, (O - \langle \psi, O\psi \rangle)^2 \psi = \langle \psi, O^2 \psi \rangle - \langle \psi, O\psi \rangle^2 \ . \tag{5.8}$$

If, as before, $O = \sum_j \lambda_j P_{\varphi_j}$, then it is not difficult to see that:

$$\Delta O_\psi = \sum_j (\lambda_j - \langle \psi, O\psi \rangle)^2 |\langle \psi, \varphi_j \rangle|^2 \ . \tag{5.9}$$

An important property of quantum systems is that noncommuting observables cannot be measured simultaneously with arbitrary precision.

Theorem 5.1 (Heisenberg's uncertainly principle.)**.** *Let A, B be two self-adjoint operators on $\mathcal{H}$. Then, we have:*

$$\Delta A_\psi \Delta B_\psi \geqslant \frac{1}{4} |\langle \psi, [A, B]\psi \rangle|^2 \ , \tag{5.10}$$

where $[A, B] = AB - BA$ is the commutator of A and B.

Proof. Without loss of generality, suppose that $\langle \psi, A\psi \rangle = \langle \psi, B\psi \rangle = 0$. If not, we redefine A and B by subtracting them their respective averages on ψ. Then:

$$\langle \psi, [A, B]\psi \rangle = \langle \psi, AB\psi \rangle - \langle \psi, BA\psi \rangle = 2i \mathrm{Im} \langle \psi, AB\psi \rangle \ . \tag{5.11}$$

Therefore,

$$|\langle \psi, [A, B]\psi \rangle| \leqslant 2\langle \psi, AB\psi \rangle = 2|\langle A\psi, B\psi \rangle| \leqslant 2\|A\psi\|\|B\psi\| = 2\Delta A_\psi^{1/2} \Delta B_\psi^{1/2} \ , \tag{5.12}$$

which proves the claim. ∎

Many applications of quantum mechanics rely on infinite dimensional Hilbert spaces, such as $L^2(\mathbb{R}^d)$. In these cases, self-adjoint operators might have continuous spectrum as well. Also, the operator O might be unbounded, which means that $O\varphi$ makes sense only for φ in a dense domain $D(O)$ of $\mathcal{H}$:

$$D(O) = \{\psi \in \mathcal{H} \mid O\psi \in \mathcal{H}\} \ . \tag{5.13}$$

For an infinite dimensional Hilbert space, the spectral resolution of O takes the more general form, for all $\varphi \in D(O)$

$$\langle \varphi, O\varphi \rangle = \int_{\mathbb{R}} \mu_\varphi(d\lambda) \lambda \ , \tag{5.14}$$

where $\mu_\varphi(\cdot)$ is a Borel measure. Physically, this Borel measure describes the probability measure for the outcomes λ, which might form a continuum.

Theorem 5.1 also holds for unbounded operators, provided the vector ψ is chosen in the appropriate (dense) subspace of $\mathcal{H}$.

Time evolution. Time-evolution in quantum mechanics is generated by a self-adjoint operator H on $\mathcal{H}$, called the Hamiltonian. The precise form of the Hamiltonian depends on the physical problem we are interested in. Given a Hamiltonian H and a state ψ, the expected value $\langle \psi, H\psi \rangle$ has the significance of average energy of the systems.

Once a Hamiltonian is given, the time evolution is given by the Schrödinger equation:

$$i\partial_t \psi(t) = H\psi(t) \ , \qquad \psi(0) = \psi \ , \tag{5.15}$$

with $\psi(t) \in \mathcal{H}$. A key feature of this evolution equation is that it preserves the norm of $\psi(t)$:

$$\begin{aligned} \frac{d}{dt}\|\psi(t)\|^2 &= \frac{d}{dt}\langle\psi(t),\psi(t)\rangle \\ &= i[\langle i\partial_t\psi(t),\psi(t)\rangle - \langle\psi(t),i\partial_t\psi(t)\rangle] \\ &= i[\langle H\psi(t),\psi(t)\rangle - \langle\psi(t),H\psi(t)\rangle] \\ &= 0\ , \end{aligned} \tag{5.16}$$

since H is self-adjoint. If H is a bounded operator on H, the solution of the Schödinger equation is given by:

$$\psi(t) = e^{-iHt}\psi(0)\ , \tag{5.17}$$

where the exponential e^{-iHt} is defined through the absolutely convergent series:

$$e^{-iHt} = \sum_{\ell\geqslant 0} \frac{(-itH)^\ell}{\ell!}\ . \tag{5.18}$$

In particular, if H has the spectral decomposition $H = \sum_j \lambda_j P_{\varphi_j}$, the exponential map is given by:

$$e^{-iHt} = \sum_j e^{-i\lambda_j t} P_{\varphi_j}\ . \tag{5.19}$$

In particular, the solution of the Schrödinger equation associated with initial data $\psi(0) = \varphi_j$ is:

$$\psi(t) = e^{-i\lambda_j t}\varphi_j\ . \tag{5.20}$$

In other words, the time-dependence of the state reduces to a phase, which has no physical significance. In fact, the expectation value of an arbitrary self-adjoint operator is:

$$\langle\psi(t), A\psi(t)\rangle = \langle\varphi_j, A\varphi_j\rangle\ , \tag{5.21}$$

and does not depend on t. Thus, the vectors $\psi(t)$ and φ_j describe the same quantum state. For this reason, we say that eigenvectors of $\mathcal{H}$ describe stationary states.

The uniqueness of the solution of the Schrödinger equation for bounded operators follows from the definition of the exponential map. For unbounded operators, the series in (5.18) does not make sense; the existence and uniqueness of the solution of the Schrödinger equation, on the domain of H, is proved using the spectral theorem for unbounded operators. Later, we will focus on special choices of the Hamiltonian H, and we will not make use of this general result.

Measurements. What happens to the state $\psi \in \mathcal{H}$ of a quantum system when we perform a measurement of an observable O (a self-adjoint operator on $\mathcal{H}$)? Measurements in quantum mechanics correspond to interactions with classical devices. For example, to measure the position of an electron we let it interact with a detector. We do not want to describe the detector as part of the quantum system; we want to consider it instead as a classical device, obeying the rules of classical mechanics. As a consequence, we cannot describe the measurement process through the Schrödinger equation. We need to establish new rules to describe what happens to the quantum system when it undergoes a measurement. This is still a highly debated subject in quantum mechanics (the problem of foundations of quantum mechanics). The most common interpretation of the measurement process, called Copenhagen interpretation, is as follows. Suppose that a quantum system is described by a normalized vector ψ in a Hilbert space $\mathcal{H}$. We perform a measurement of an observable associated with the self-adjoint operator O. For simplicity, let us assume that O has the spectral representation $O = \sum_j \lambda_j P_{\varphi_j}$, where λ_j are the eigenvalues and φ_j the corresponding normalized eigenvectors of O. As explained above a measurement of O produces the outcome λ_j with probability $|\langle\psi,\varphi_j\rangle|^2$. If the measurement of O produces the

outcome λ_j, then, after the measurement, the system is described by the eigenvector φ_j. More precisely, as a result of the measurement, the vector ψ collapses into the vector $P_j\psi/\|P_j\psi\|$, where P_j denotes the orthogonal projection onto the eigenspace associated with the eigenvalue λ_j. In particular, if the eigenvalue is nondegenerate, we have $P_j\psi/\|P_j\psi\| = \varphi_j$.

Canonical quantization. From now on, we shall assume that $\mathcal{H} = L^2(\mathbb{R}^d)$. This choice is relevant for describing the motion of one quantum particle on $\mathbb{R}^d$. The wave function of a particle is a function $\psi \in L^2(\mathbb{R}^d)$. The position operator $\hat{x}$ is the multiplication operator acting as:

$$(\hat{x}\psi)(x) = x\psi(x) \; . \tag{5.22}$$

The expectation value of the i-th component of the position operator is:

$$\langle \psi, \hat{x}_i \psi \rangle = \int_{\mathbb{R}^d} dx \, x_i |\psi(x)|^2 \; . \tag{5.23}$$

In particular, $|\psi(x)|^2$ has the interpretation of probability distribution for finding the particle at x. That is, the probability for finding the particle in $A \subset \mathbb{R}^d$ is defined as:

$$\mathbb{P}_\psi(A) := \int_A dx \, |\psi(x)|^2 \; . \tag{5.24}$$

By the normalization of the wave function, $\mathbb{P}_\psi(\mathbb{R}^d) = 1$.

The momentum operator $\hat{p}$ is a differential operator acting as:

$$(\hat{p}\psi)(x) = -i\nabla\psi(x) \; , \tag{5.25}$$

where the $-i$ factor makes it self-adjoint on a suitable dense domain. Let $\hat{\psi}$ be the L^2-Fourier transform of ψ. The expectation value of the i-th component of the momentum operator is:

$$\langle \psi, \hat{p}_i \psi \rangle = \int_{\mathbb{R}^d} dk \, k_i |\hat{\psi}(k)|^2 \; , \tag{5.26}$$

where we used Plancherel's theorem. Thus, the momentum operator $\hat{p}_i$ acts as a multiplication operator, in Fourier space. Later, after discussing the solution of the free Schrödinger equation, we will motivate the definition of momentum operator as given above. Notice that position and momentum operator correspond to two non-commuting operators on $\mathcal{H}$. In particular, by Heisenberg's uncertainty principle, Theorem 5.1, we have:

$$\Delta(P_k)_\psi \Delta(X_j)_\psi \geqslant \frac{\delta_{k,j}}{4} \|\psi\|_2^2 \; . \tag{5.27}$$

Informally, this means that a localized state in position space has to be delocalized in momentum space, and viceversa. This fact, which has no counterpart in classical mechanics, plays a crucial role in the stability of matter, as we will see later.

The classical Hamiltonian for a non-relativistic, pointlike particle in $\mathbb{R}^d$, subject to an external potential $V(x)$, is:

$$H(x,p) = \frac{p^2}{2m} + V(x) \; . \tag{5.28}$$

This is a function on the phase space, $\mathbb{R}^d \times \mathbb{R}^d$, which generates the classical evolution from Hamilton's equation of motion:

$$\frac{d}{dt} \begin{pmatrix} x(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} \nabla_p H(x(t), p(t)) \\ -\nabla_x H(x(t), p(t)) \end{pmatrix} \; . \tag{5.29}$$

The quantum counterpart of this equation of motion is given by the Schrödinger equation (5.15), where the Hamiltonian H is an operator on $L^2(\mathbb{R}^d)$ defined as:

$$\begin{aligned} H &= \frac{\hat{p}^2}{2m} + V(\hat{x}) \\ &\equiv -\frac{\Delta}{2m} + V(\hat{x}) \ , \end{aligned} \tag{5.30}$$

with Δ the Laplacian on $\mathbb{R}^d$, and $V(\hat{x})$ a multiplication operator:

$$(V(\hat{x})\psi)(x) = V(x)\psi(x) \ . \tag{5.31}$$

Notice that H is now an *unbounded operator* on L^2. For a wide class of external potentials V, such as those we will consider, it turns out to be a self-adjoint operator, on a dense domain $D(H)$. What makes the problem of studying the quantum evolution generated by (5.30) particularly interesting is that the operators p^2 and $V(\hat{x})$ do not commute, in general.

5.2 The free Schrödinger equation

To begin, we will consider the free Schödinger equation, that is:

$$i\partial_t\psi(t) = -\Delta\psi(t) \ , \qquad \psi(0) = \psi \in L^2(\mathbb{R}^d) \ . \tag{5.32}$$

We will restrict our attention to a nice enough class of initial data, that will allow us to find a strong solution of the equation. Notice that we set $m = 1/2$, for convenience.

Definition 7 (Schwartz functions.)**.** *For any two multi-indices α, β, define:*

$$\|f\|_{\alpha,\beta} = \|x^\alpha D^\beta f\|_\infty \ . \tag{5.33}$$

We define the space of Schwartz function as:

$$\mathcal{S}(\mathbb{R}^d) := \{f \in C^\infty(\mathbb{R}^d) \mid \|f\|_{\alpha,\beta} < \infty \text{ for all multi-indices } \alpha, \beta.\} \tag{5.34}$$

It is not difficult to check that $\mathcal{S}(\mathbb{R}^d) \subset L^p(\mathbb{R}^d)$, for all p. Also, $\mathcal{S}(\mathbb{R}^d)$ is dense in $L^2(\mathbb{R}^d)$. Another nice aspect of the Schwartz space is that it is left invariant by the Fourier transform.

Lemma 5.2. *Let $f \in \mathcal{S}(\mathbb{R}^d)$. Then, $\hat{f} \in \mathcal{S}(\mathbb{R}^d)$.*

Proof. Recall the properties of the Fourier transform, in particular Property (vi) in Section 1.2. We have:

$$\begin{aligned} \|\hat{f}\|_{\alpha,\beta} &= \|k^\alpha D^\beta \hat{f}\|_\infty \\ &= \|\widehat{D^\alpha x^\beta f}\|_\infty \end{aligned} \tag{5.35}$$

where in the last identity we omitted the i factors, since they do not affect the norm. Then, we estimate:

$$\begin{aligned} \|\widehat{D^\alpha x^\beta f}\|_\infty &\leqslant \frac{1}{(2\pi)^d}\|D^\alpha x^\beta f\|_1 \\ &= \frac{1}{(2\pi)^d}\left\|\frac{1}{1+|x|^{d+1}}(1+|x|^{d+1})D^\alpha x^\beta f\right\|_1 \\ &\leqslant \frac{1}{(2\pi)^d}\left\|\frac{1}{1+|x|^{d+1}}\right\|_1\left\|(1+|x|^{d+1})D^\alpha x^\beta f\right\|_\infty \\ &\leqslant C\left\|(1+|x|^{d+1})D^\alpha x^\beta f\right\|_\infty \ . \end{aligned} \tag{5.36}$$

The last term can be written in terms of a finite combination of the $\|\cdot\|_{\tilde{\alpha},\tilde{\beta}}$ norms, which are all finite since f is Schwartz. ∎

Remark 5.3. *In particular, since the Schwartz space is in L^2, the Fourier transform defines a bijection on $\mathcal{S}(\mathbb{R}^d)$.*

We shall consider the Schrödinger equation on the Schwartz space.

Proposition 5.4 (Solution of the free Schrödinger equation.)**.** *The free Schrödinger equation (5.32) has a unique solution $\psi \in C^\infty(\mathbb{R}, \mathcal{S}(\mathbb{R}^d))$. It is given by, for all $t \in \mathbb{R}$ and $x \in \mathbb{R}^d$:*

$$\psi(t,x) = \frac{1}{(4\pi i t)^{d/2}} \int_{\mathbb{R}^d} dy\, e^{-i|x-y|^2/4t} \psi(y) \ . \tag{5.37}$$

Moreover,

$$\|\psi(t,\cdot)\|_2 = \|\psi(0,\cdot)\|_2 \ . \tag{5.38}$$

Remark 5.5. *Notice that $\psi(t,x)$ is equal to the solution of the heat equation, Eq. (3.19), after replacing t by it.*

Proof. Since $\psi(t,\cdot) \in \mathcal{S}(\mathbb{R}^d)$, rewrite the Schrödinger equation in Fourier space:

$$i\partial_t \hat{\psi}(t,k) = |k|^2 \hat{\psi}(t,k) \ . \tag{5.39}$$

The solution is:

$$\hat{\psi}(t,k) = e^{-i|k|^2 t} \hat{\psi}(k) \ . \tag{5.40}$$

The conservation of the L^2 norm immediately follows from this expression, combined with Plancherel's theorem. To conclude, let us prove the formula (5.37), for the solution in configuration space. Notice that (5.37) is a convolution; one would be tempted to say that (5.37) holds because it is the Fourier transform of a product $e^{-i|k|^2 t}\hat{\psi}(k)$, recall Property (iv) of the Fourier transform. However, this is not a valid proof, since the inverse Fourier transform of the function $e^{-i|k|^2 t}$ is not defined. We have:

$$\begin{aligned}
\psi(t,x) &= \int \frac{dk}{(2\pi)^{d/2}}\, e^{ik\cdot x} e^{-i|k|^2 t} \hat{\psi}(k) \\
&= \lim_{R\to\infty} \int_{|k_i|\leqslant R} \frac{dk}{(2\pi)^{d/2}}\, e^{ik\cdot x} e^{-i|k|^2 t} \hat{\psi}(k) \\
&= \lim_{R\to\infty} \int_{|k_i|\leqslant R} \frac{dk}{(2\pi)^{d/2}}\, e^{ik\cdot x} e^{-i|k|^2 t} \int \frac{dy}{(2\pi)^{d/2}} e^{-ik\cdot y} \psi(y) \\
&= \lim_{R\to\infty} \int \frac{dy}{(2\pi)^d}\, \psi(y) \int_{|k_i|\leqslant R} dk\, e^{ik\cdot(x-y)} e^{-i|k|^2 t} \ .
\end{aligned} \tag{5.41}$$

Let us now compute the innermost integral. Completing the square, we have:

$$\begin{aligned}
\int_{|k_i|\leqslant R} dk\, e^{ik\cdot(x-y)} e^{-i|k|^2 t} &= e^{-i|x-y|^2/4t} \int_{|k_i|\leqslant R} dk\, e^{-it|k-(x-y)/2t|^2} \\
\int_{|k_i|\leqslant R} dk\, e^{ik\cdot(x-y)} e^{-i|k|^2 t} &= e^{-i|x-y|^2/4t} \int_{|k_i+(x-y)_i/2t|\leqslant R} dk\, e^{-it|k|^2} \\
&\equiv e^{-i|x-y|^2/4t} \prod_{j=1}^{d} \int_{-R-(x-y)_j/2t}^{R-(x-y)_j/2t} dk_j\, e^{-itk_j^2}
\end{aligned} \tag{5.42}$$

Therefore, the problem reduces to computing:

$$\int_{-R-a}^{R-a} dx\, e^{-itx^2} = \int_0^{R-a} dx\, e^{-itx^2} + \int_{-R-a}^{0} dx\, e^{-itx^2} \ . \tag{5.43}$$

Consider the first term in the right-hand side, the other will be studied in the same way. The function e^{-itz^2} is entire in $\mathbb{C}$. Let $\mathcal{C}$ be the closed complex path:

$$0 \to R-a \to (R-a)-i(R-a) \to 0 \,, \tag{5.44}$$

where all arrows correspond to straight paths. Correspondingly, by Cauchy theorem:

$$\int_0^{R-a} dx\, e^{-itx^2} = -\int_{(R-a)-i(R-a)\to 0} dz\, e^{-itz^2} - \int_{R-a\to(R-a)-i(R-a)} dz\, e^{-itz^2} \,. \tag{5.45}$$

Consider the first term. Writing $z = e^{-i\pi/4}y$ with $y \in [0, R-a]$, we have:

$$\int_{(R-a)-i(R-a)\to 0} dz\, e^{-itz^2} = e^{-i\pi/4}\int_0^{R-a} dy\, e^{-ty^2} = \sqrt{-i}\Big[\int_0^{\infty} dy\, e^{-ty^2} + \varepsilon_1(R)\Big] \tag{5.46}$$

with $\varepsilon_1(R) \to 0$ as $R \to \infty$. Consider the second term in the right-hand side of (5.45). We have, writing $z = R-a-iy$:

$$\begin{aligned}\int_{R-a\to(R-a)-i(R-a)} dz\, e^{-itz^2} &= \int_0^{R-a} dy\, e^{-it(R-a-iy)^2} \\ &= e^{-itR^2}\int_0^{R-a} dy\, e^{ity^2-2t(R-a)y} =: \varepsilon_2(R) \,,\end{aligned} \tag{5.47}$$

with $\varepsilon_2(R) \to 0$ as $R \to \infty$. A similar analysis can be performed for the second term in (5.43). All together:

$$\begin{aligned}\int_{-R-a}^{R-a} dx\, e^{-itx^2} &= \sqrt{-i}\int_{-\infty}^{\infty} dy\, e^{-ty^2} + \varepsilon(R) \\ &= \sqrt{\frac{\pi}{it}} + \varepsilon(R) \,,\end{aligned} \tag{5.48}$$

with $\varepsilon(R) \to 0$ as $R \to \infty$. Thus, coming back to (5.42):

$$\int_{|k_i|\leqslant R} dk\, e^{ik\cdot(x-y)}e^{-i|k|^2t} = \Big(\frac{\pi}{it}\Big)^{d/2} e^{-i|x-y|^2/4t} + \varepsilon_d(R) \,, \tag{5.49}$$

with $\varepsilon_d(R) \to 0$ as $R \to \infty$. Plugging this result in (5.41) we easily get:

$$\psi(t,x) = \frac{1}{(2\pi)^d}\Big(\frac{\pi}{it}\Big)^{d/2}\int dy\, \psi(y) e^{-i|x-y|^2/4t} \,. \tag{5.50}$$

which gives the claim (5.37) ∎

From this expression, we immediately get that:

$$\|\psi(t,\cdot)\|_\infty \leqslant \frac{1}{(4\pi t)^{d/2}}\|\psi\|_1 \to 0 \qquad \text{as } t \to \infty. \tag{5.51}$$

This bound is called *dispersive inequality*. Let $A \subset \mathbb{R}$, and recall the definition of probability for finding the particle in the set A at the time t:

$$\mathbb{P}_{\psi_t}(A) = \int_A dx\, |\psi(t,x)|^2 \,. \tag{5.52}$$

In particular, for a bounded set A:

$$\mathbb{P}_{\psi_t}(A) \leqslant |A| \frac{\|\psi\|_{L^1}}{(4\pi t)^{d/2}} \to 0 \qquad \text{as } t \to \infty. \tag{5.53}$$

That is, as time goes to infinity, the probability for finding the particle in any bounded subset of $\mathbb{R}^d$ is zero: the particle escapes at infinity. At this stage, it is useful to compare the behavior of the solution of the free Schrödinger equation with the one corresponding to the solution of the heat equation, Eq. (3.19). The estimate (5.51) also holds for the solution of the heat equation. However, the heat equation preserves the L^1 norm of the solution, while the Schrödinger equation preserves the L^2 norm of the solution.

The dispersive estimate (5.51), combined with the conservation of the L^2 norm, can be used to prove a bound for the L^p norms of $\psi(t,\cdot)$, for $p > 2$. We have:

$$\begin{aligned} \|\psi(t,\cdot)\|_p^p &\leqslant \int dx\, |\psi(t,x)|^p \\ &\leqslant \|\psi(t,\cdot)\|_\infty^{p-2} \|\psi(t,\cdot)\|_2^2 \\ &\leqslant C t^{-\frac{d}{2}(p-2)} \|\psi\|_1^{p-2} \|\psi\|_2^2 \,, \end{aligned} \tag{5.54}$$

that is:

$$\|\psi(t,\cdot)\|_p \leqslant C t^{-\frac{d}{2}(1-2/p)} \|\psi\|_1^{1-2/p} \|\psi\|_2^{2/p} \,. \tag{5.55}$$

One can prove an even stronger bound, as stated in the next theorem, which we will not prove.

Theorem 5.6 (L^p to L^q estimate.)**.** *Let $\psi(t,x)$ be the solution of the free Schrödinger equation. Then, the following bound holds, for all $p \in [2,\infty]$ and q such that $1/p + 1/q = 1$:*

$$\|\psi(t,\cdot)\|_p \leqslant C t^{-\frac{d}{2}(1-2/p)} \|\psi\|_q \,. \tag{5.56}$$

This bound is stronger than (5.55), due to the fact that by interpolation, $\|\psi\|_q \leqslant \|\psi\|_1^{1-2/p} \|\psi\|_2^{2/p}$ for $q \in [1,2]$ and $1/p + 1/q = 1$.

Asymptotics of the momentum operator. Recall the expression for finding the particle in the region $A \subset \mathbb{R}^d$:

$$\mathbb{P}(X(t) \in A) = \int_A |\psi(t,x)|^2 \, dx \,. \tag{5.57}$$

Next, we want to determine the "asymptotic momentum distribution" of the quantum particle. Recall that we have set $m = 1/2$. Consider:

$$\lim_{t\to\infty} \mathbb{P}\Big(\frac{(1/2)X(t)}{t} \in A \Big) = \lim_{t\to\infty} \mathbb{P}(X(t) \in 2tA) = \lim_{t\to\infty} \int_{2tA} |\psi(t,x)|^2 \, dx \,. \tag{5.58}$$

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

$$\psi(t,x) = \frac{e^{i\frac{x^2}{4t}}}{(2it)^{d/2}} \hat{\psi}_0(x/2t) + r(t,x) \,, \tag{5.59}$$

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

Proof. We have, by Eq. (5.37):

$$\begin{aligned}\psi(t,x) &= \frac{e^{i\frac{x^2}{4t}}}{(2it)^{d/2}}\frac{1}{(2\pi)^{d/2}}\int e^{-i\frac{x}{2t}y}\Big(e^{i\frac{y^2}{4t}}+1-1\Big)\psi_0(y)\,dy \\ &= \frac{e^{i\frac{x^2}{4t}}}{(2it)^{d/2}}\Big(\hat{\psi}_0(x/2t)+\frac{1}{(2\pi)^{d/2}}\int e^{-i\frac{x}{2t}y}\Big(e^{i\frac{y^2}{4t}}-1\Big)\psi_0(y)\,dy\Big) \\ &= \frac{e^{i\frac{x^2}{4t}}}{(2it)^{d/2}}\Big(\hat{\psi}_0(x/2t)+\hat{h}(t,x/2t)\Big)\,, \end{aligned} \tag{5.60}$$

with $h(t,y)=\big(e^{i\frac{y^2}{4t}}-1\big)\psi_0(y)$. We set:

$$r(t,x)=\frac{e^{i\frac{x^2}{4t}}}{(2it)^{d/2}}\hat{h}(t,x/2t)\,. \tag{5.61}$$

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

$$\|r(t,\cdot)\|_{L^2}^2=\int|r(t,x)|^2\,dx=\frac{1}{(2t)^d}\int|\hat{h}(t,x/2t)|^2\,dx=\int|\hat{h}(t,y)|^2dy=\int|h(t,y)|^2dy\,. \tag{5.62}$$

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:

$$\lim_{t\to\infty}\int|h(t,x)|^2dx=0\,. \tag{5.63}$$

This concludes the proof. ∎

Theorem 5.8. *Let $\psi(t,x)$ be a solution of the free Schrödinger equation and let $A\subset\mathbb{R}^d$. Then:*

$$\lim_{t\to\infty}\mathbb{P}\Big(\frac{(1/2)X(t)}{t}\in A\Big)=\int_A|\hat{\psi}_0(p)|^2dp\,. \tag{5.64}$$

Proof. By Lemma 5.7, we have:

$$\int_{2tA}|\psi(t,x)|^2dx=\frac{1}{(2t)^d}\int_{2tA}|\hat{\psi}_0(x/2t)|^2dx+R(t)=\int_A|\hat{\psi}_0(p)|^2dp+R(t)\,, \tag{5.65}$$

where, following the proof of the Lemma:

$$\begin{aligned}\lim_{t\to\infty}R(t) &= \lim_{t\to\infty}\int_{2tA}|r(t,x)|^2\,dx+\lim_{t\to\infty}2\mathrm{Re}\Big(\frac{1}{(2t)^d}\int_{2tA}\overline{\hat{\psi}_0(x/2t)}\hat{h}(t,x/2t)dx\Big) \\ &= \lim_{t\to\infty}2\mathrm{Re}\Big(\int_A\overline{\hat{\psi}_0(p)}\hat{h}(t,p)\Big)\,. \end{aligned} \tag{5.66}$$

By the Cauchy-Schwarz inequality we have:

$$\lim_{t\to\infty}\Big|\int_A\overline{\hat{\psi}_0(p)}\hat{h}(t,p)dp\Big|\leqslant\lim_{t\to\infty}\|\hat{\psi}_0\|_{L^2}\|\hat{h}(t)\|_{L^2}=0\,, \tag{5.67}$$

where in the last step we used (5.63). ∎

The above result elucidates why the operator $\hat{p} := -i\nabla$ has the interpretation of momentum operator. Its expectation value is:

$$\langle \psi_t, \hat{p}\psi_t \rangle = \int_{\mathbb{R}^d} \overline{\psi(t,x)}(\hat{p}\psi)(t,x)dx = \int_{\mathbb{R}^d} \overline{\hat{\psi}(t,k)}k\hat{\psi}(t,k)dk = \int_{\mathbb{R}^d} k|\hat{\psi}(0,k)|^2 dk \ , \tag{5.68}$$

where we used that $|\hat{\psi}(t,p)| = |\hat{\psi}(0,p)|$. By (5.64), we interpret $|\hat{\psi}(0,k)|^2$ as the probability distribution of the values of the asymptotic momentum operator. Thus, Eq. (5.68) corresponds to the expectation value of the asymptotic momentum, which is consistent with the interpretation of $\hat{p}$ as momentum operator.

L^2 solutions. To conclude the section about the free Schrödinger equation, let us comment about a more general notion of solvability of (5.32). Let us define the m-th Sobolev space as:

$$H^m(\mathbb{R}^d) := \left\{ \psi \in L^2(\mathbb{R}^d) \mid (1+|k|^2)^{m/2}\hat{\psi}(k) \in L^2(\mathbb{R}^d) \right\} . \tag{5.69}$$

In particular, if $\psi \in H^2(\mathbb{R}^d)$, we define the L^2-Laplacian as the inverse Fourier transform of $|k|^2\hat{\psi}(k)$. Thus, $-\Delta\psi \in L^2(\mathbb{R}^d)$; the space $H^2(\mathbb{R}^d)$ is called the domain of the Laplacian. Let us now introduce the notion of L^2-solution of the free Schrödinger equation.

Given $\psi_0 \in H^2(\mathbb{R}^d)$, let $\hat{\psi}_0$ be its Fourier transform, and consider the function:

$$\hat{\psi}(t,k) = e^{-i|k|^2 t}\hat{\psi}_0(k) \ . \tag{5.70}$$

One can check that $t \mapsto \hat{\psi}(t,k)$ is continuous in the L^2 sense: we have:

$$\|\hat{\psi}(t,k) - \hat{\psi}(t_0,k)\|_2 \to 0 \qquad \text{as } t \to t_0 \tag{5.71}$$

by dominated convergence. Also, the function $\hat{\psi}(t,k)$ is differentiable in time in the L^2-sense, and its derivative equals $|k|^2\hat{\psi}(k,t)$. In fact:

$$\left\| \frac{\hat{\psi}(t,k) - \hat{\psi}(t_0,k)}{t-t_0} - |k|^2\hat{\psi}(t,k) \right\|_2 = \int dk \left| \frac{1}{t-t_0}\left(e^{-i|k|^2 t} - e^{-i|k|^2 t_0} \right) - |k|^2 \right|^2 |\hat{\psi}(k,t)|^2 \ . \tag{5.72}$$

As $t \to t_0$, the argument of the first absolute value converges to 0, and for all t it is estimated by $2|k|^2$. Since $|k|^4|\hat{\psi}(k)|^2$ is integrable, by dominated convergence we conclude that:

$$\left\| \frac{\hat{\psi}(t,k) - \hat{\psi}(t_0,k)}{t-t_0} - |k|^2\hat{\psi}(t,k) \right\|_2 \to 0 \qquad \text{for } t \to t_0. \tag{5.73}$$

That is, the sequence of L^2 functions given by $\frac{\hat{\psi}(t,k)-\hat{\psi}(t_0,k)}{t-t_0}$ converges in L^2 to $|k|^2\hat{\psi}(t,k)$. In this sense, the function $\hat{\psi}(t,k)$ satisfies:

$$i\partial_t\hat{\psi}(t,k) = |k|^2\hat{\psi}(t,k) \ . \tag{5.74}$$

Or, taking the anti-Fourier transform:

$$i\partial_t\psi(t) = -\Delta\psi(t) \ . \tag{5.75}$$

Notice that this notion of solvability does not rely on pointwise differentiability.

5.3 Confinement in presence of an external potential

In this section we shall consider quantum Hamiltonians of the following type:

$$H = -\Delta + V(\hat{x}) \,, \tag{5.76}$$

under suitable assumptions on V, to be specified. In classical mechanics, the dynamics associated to the Hamiltonian $H = p^2/2m + V(x)$ depends strongly on the shape of the potential V. In particular, suppose that x_* is a local minimum of V. Let $E = H(p_0, x_0)$ be the energy of the initial datum, which is conserved under the Hamilton flow: $E = H(p(t), x(t))$. Suppose that $E - V(x_*)$ is small enough, so that the equation $E = H(0, x)$ has two and only two solutions in a suitably small neighbourhood of x_*: $x \equiv x_\pm(E)$. Then, by energy conservation the motion $t \mapsto x(t) \in [x_-, x_+]$ for all times, and the motion is periodic, with period:

$$T = 2 \int_{x_-}^{x_+} dx \, \frac{1}{\sqrt{(2/m)(E - V(x))}} \tag{5.77}$$

For special choices of the potential V, one can actually determine the trajectory $t \mapsto x(t)$. A paradigmatic example is the harmonic oscillator, for which $V(x) = (k/2)|x|^2$. There:

$$x(t) = A \sin(\omega t - B) \,, \qquad \omega = \sqrt{k/m} \tag{5.78}$$

In this section we would like to understand how to formulate confinement, in a quantum setting. To this end, let us make the simplifying assumption that:

$$c|x - x_*|^\alpha \leqslant V(x) \leqslant C|x - x_*|^\beta \tag{5.79}$$

for some positive constants c, C, α, β. Under these assumptions, the potential is confining at x_* in a classical sense, and also $\mathcal{S}(\mathbb{R}^d)$ belongs to the domain of the quantum Hamiltonian $H = -\Delta + V$.

As we have seen, in quantum mechanics there is no notion of position of the quantum particle. Instead, the state of the system is specified by the wave function $\psi \in L^2(\mathbb{R}^d)$, and $|\psi(x)|^2$ describes the *probability distribution* for finding the particle at x. Thus, the question we would like to address is: what is the probability for finding the particle "far" from x_*? By our classical intuition, we expect that being very far from x_* should not be convenient from an energetic viewpoint. This intuition relies on the notion of energy conservation, that we shall prove in the next proposition.

Proposition 5.9 (Energy conservation)**.** *Let $\psi \in \mathcal{S}(\mathbb{R}^d)$, $\|\psi\|_2 = 1$. Let us define the energy of ψ as:*

$$E_\psi := \langle \psi, H\psi \rangle \,. \tag{5.80}$$

Let $\psi(t)$ be the solution of the Schrödinger equation:

$$i\partial_t \psi(t) = H\psi(t) \,, \qquad \psi(0) = \psi \,. \tag{5.81}$$

Then,

$$\langle \psi(t), H\psi(t) \rangle = \langle \psi(0), H\psi(0) \rangle \,. \tag{5.82}$$

Remark 5.10. *Strictly speaking, we are only considering potentials satisfying (5.79). However, the proof below applies to self-adjoint Hamiltonians H, provided the initial datum ψ is chosen in the domain $D(H)$.*

Proof. We compute:

$$\begin{aligned}\frac{d}{dt}\langle\psi(t),H\psi(t)\rangle &= \langle\partial_t\psi(t),H\psi(t)\rangle+\langle\psi(t),H\partial_t\psi(t)\rangle\\ &= (-i)\langle H\psi(t),H\psi(t)\rangle+i\langle\psi(t),HH\psi(t)\rangle\\ &= (-i)\langle H\psi(t),H\psi(t)\rangle+i\langle H\psi(t),H\psi(t)\rangle\\ &= 0\,.\end{aligned} \tag{5.83}$$

where the third step follows thanks to the self-adjointness of H. ∎

Then, the next proposition gives a first instance of confinement, for a quantum particle.

Proposition 5.11. *Suppose that (5.79) holds true. Let $\psi\in\mathcal{S}(\mathbb{R}^d)$. Consider:*

$$\mathbb{P}\big(X(t)\notin B_{2L}(x_*)\big) := \int dx\,|\psi(t,x)|^2\chi\big(B^c_{2L}(x_*)\big)\,. \tag{5.84}$$

where $\chi(A)$ is the characteristic function of the set $A\subset\mathbb{R}^d$. Then:

$$\mathbb{P}\big(X(t)\notin B_{2L}(x_*)\big)\leqslant\frac{C}{L^\alpha}\,, \tag{5.85}$$

uniformly in $t\in\mathbb{R}$.

Remark 5.12. *(i) This result proves that the probability for finding the particle away from x_* is arbitrarily small, provided one looks away enough from x_*. The important point here is that the bound is uniform in time. In fact, using that $\psi(t)\in L^2$ for all times, it trivially follows that $\mathbb{P}\big(X(t)\notin B_{2L}(x_*)\big)\leqslant\varepsilon$ for all $\varepsilon>0$ provided L is taken large enough, however possibly not uniformly in t.*

(ii) The bound (5.85) is false if $V=0$, by the dispersive inequality:

$$\begin{aligned}\mathbb{P}\big(X(t)\notin B_{2L}(x_*)\big) &= 1-\mathbb{P}\big(X(t)\in B_{2L}(x_*)\big)\\ &\geqslant 1-\varepsilon\end{aligned} \tag{5.86}$$

where the last step follows from (5.53), for all $L>0$ and for t large enough.

Proof. A moment of thought shows that:

$$\chi\big(B^c_{2L}(x_*)\big)\leqslant\frac{|x-x_*|^\alpha}{L^\alpha}\,. \tag{5.87}$$

Therefore,

$$\mathbb{P}\big(X(t)\notin B_{2L}(x_*)\big)\leqslant\frac{1}{L^\alpha}\int dx\,|\psi(t,x)|^2|x-x_*|^\alpha\,. \tag{5.88}$$

By the assumption (5.79), we also have:

$$\begin{aligned}\mathbb{P}\big(X(t)\notin B_{2L}(x_*)\big) &\leqslant\frac{1}{cL^\alpha}\int dx\,|\psi(t,x)|^2V(x)\\ &= \frac{1}{cL^\alpha}\langle\psi(t),V(\hat{x})\psi(t)\rangle\,.\end{aligned} \tag{5.89}$$

Finally, by the positivity of the kinetic energy, which follows from $\langle\psi,-\Delta\psi\rangle=\int dk\,|\hat{\psi}(k)|^2|k|^2$, we have:

$$\begin{aligned}\mathbb{P}\big(X(t)\notin B_{2L}(x_*)\big) &\leqslant\frac{1}{cL^\alpha}\langle\psi(t),H\psi(t)\rangle\\ &\leqslant\frac{1}{cL^\alpha}\langle\psi(0),H\psi(0)\rangle\,,\end{aligned} \tag{5.90}$$

where the last step follows from the conservation of energy. Thanks to the finiteness of the energy of ψ, the claim follows. ∎

Remark 5.13. *(i) The estimate (5.85) holds under the assumption that V is confining, in the sense of the lower bound in (5.79). More generally, a similar bound holds for the eigenstates of H, that is for L^2 solutions of:*

$$H\psi = E\psi \ . \tag{5.91}$$

These are stationary states of the Schrödinger equation, in the sense that the evolution is simply $\psi(t) = e^{-iEt}\psi$. Thus, one immediately has:

$$\begin{aligned} \mathbb{P}\big(X(t) \notin B_{2L}(x_*)\big) &= \mathbb{P}\big(X(0) \notin B_{2L}(x_*)\big) \\ &\leqslant \varepsilon \end{aligned} \tag{5.92}$$

for all $\varepsilon > 0$ and for L large enough.

(ii) The bound (5.85) can actually be used to prove that the spectrum of H is pure point if V is confining (as an application of the RAGE theorem, see e.g. [8]).

(iii) For explicit choices of V, much more can be said. In the next section, we will consider the quantum counterpart of the harmonic oscillator.

5.4 The harmonic oscillator

Here we shall describe the prototype of the exactly solvable model in quantum mechanics: the harmonic oscillator. The Hamiltonian is:

$$H = -\Delta + |x|^2 \ , \tag{5.93}$$

and for the moment we shall consider this operator as acting on $\mathcal{S}(\mathbb{R}^d)$. Also, for simplicity we shall set $d = 1$. The importance of the harmonic oscillator in physics is that it allows to describe the low-energy behavior of Hamiltonians $H = -\Delta + V(x)$, for a large class of potentials. In fact, suppose that x_* is a global minimum of V. Then, by Taylor expansion:

$$V(x) = V(x_*) + \frac{1}{2}V''(x_*)(x - x_*)^2 + O(|x - x_*|^3) \ . \tag{5.94}$$

Informally speaking, if $V''(x_*) \neq 0$, it is reasonable to expect that, on states with low enough energy, the dynamics generated by the Hamiltonian H can be approximated by the one of the harmonic oscillator, for a certain time scale.

The goal of this section will be to solve the eigenvalue problem in $L^2(\mathbb{R})$:

$$H\psi = E\psi \ . \tag{5.95}$$

As already discussed, eigenstates of H correspond to stationary states of the dynamics. We will start by solving this equation on the Schwartz space $\mathcal{S}(\mathbb{R})$, and then later we will discuss how to extend the analysis to the whole $L^2(\mathbb{R})$. In particular, we will prove that the solutions of (5.95) form an orthonormal basis for L^2. This will allow to study the dynamics generated by H of any initial datum $\psi \in D(H)$. To begin, we will introduce the notion of creation and annihilation operators (or rasing and lowering operators).

Creation and annihilation operators. Let us define the following operators, on $\mathcal{S}(R)$:

$$A_\pm := \frac{1}{\sqrt{2}}\Big(x \mp \frac{d}{dx}\Big) \ . \tag{5.96}$$

Integration by parts shows that the adjoint of A_+ on $\mathcal{S}(R)$ is A_-: $A_+^* = A_-$. The operators $A_\pm$ satisfy a number of useful algebraic properties, which we will now discuss. To begin, we claim that:

$$[A_-, A_+] = 1 \ , \tag{5.97}$$

understood as the identity on $\mathcal{S}(\mathbb{R})$. In fact:

$$\begin{aligned} [A_-, A_+]\psi(x) &= \frac{1}{2}\Big[x + \frac{d}{dx}\,, x - \frac{d}{dx}\Big]\psi(x) \\ &= \Big[\frac{d}{dx}, x\Big]\psi(x) \\ &= \psi(x) \ . \end{aligned} \tag{5.98}$$

Next, we notice that the Hamiltonian H can be rewritten in terms of $A_\pm$. To this end, define the number operator as:

$$\mathcal{N} = A_+ A_- \ . \tag{5.99}$$

Then,

$$\begin{aligned} 2\mathcal{N} + 1 &= \Big(x - \frac{d}{dx}\Big)\Big(x + \frac{d}{dx}\Big) + 1 \\ &= x^2 - \frac{d^2}{dx^2} - \Big[\frac{d}{dx}, x\Big] + 1 \\ &= H \ , \end{aligned} \tag{5.100}$$

since $\Big[\frac{d}{dx}, x\Big] = 1$. Thus, there is a one-to-one correspondence between the eigenvalues of $\mathcal{N}$ and the eigenvalues of H:

$$\mathcal{N}\psi = n\psi \iff H\psi = (2n+1)\psi \ . \tag{5.101}$$

The motivation for the names "creation operator" and "annihilation operator" is that they "raise" or "lower" eigenvalues of $\mathcal{N}$. Suppose that $\psi \in \mathcal{S}(\mathbb{R})$ is an eigenvector of $\mathcal{N}$, $\mathcal{N}\psi = n\psi$. Consider the new state $A_\pm\psi$, which is also in the Schwartz space. Then,

$$\begin{aligned} \mathcal{N}A_\pm\psi &= A_\pm\mathcal{N}\psi + [\mathcal{N}, A_\pm]\psi \\ &= nA_\pm\psi + [\mathcal{N}, A_\pm]\psi \ . \end{aligned} \tag{5.102}$$

Furthermore,

$$\begin{aligned} [\mathcal{N}, A_\pm] &= A_+[A_-, A_\pm] + [A_+, A_\pm]A_- \\ &= \pm A_\pm \ . \end{aligned} \tag{5.103}$$

where we used (5.97), together with the trivial identities $[A_-, A_-] = [A_+, A_+] = 0$. Therefore, we obtain:

$$\mathcal{N}A_\pm\psi = (n \pm 1)A_\pm\psi \ . \tag{5.104}$$

Thus, $A_+\psi$ and $A_-\psi$ are eigenvectors of $\mathcal{N}$ with eigenvalues $n+1$ and $n-1$, respectively. This observation can be used to generate infinitely many eigenvectors for $\mathcal{N}$ in $\mathcal{S}(\mathbb{R})$, if we only know one.

Eigenvalues of $\mathcal{N}$ on $\mathcal{S}(\mathbb{R})$. To begin, we claim that if n is an eigenvalue of $\mathcal{N}$, then $n \geqslant 0$. In fact:

$$\mathcal{N}\psi = n\psi \iff \langle\psi, \mathcal{N}\psi\rangle = n\langle\psi, \psi\rangle \ . \tag{5.105}$$

The claim follows from the observation that $\langle \psi, \mathcal{N}\psi \rangle = \|A_-\psi\|_2^2 \geqslant 0$. Then, we claim that the value $n = 0$ is attained by a unique function in $\mathcal{S}(\mathbb{R})$. To see this, notice that:

$$\mathcal{N}\psi = 0 \iff A_-\psi = 0 \, . \tag{5.106}$$

One implication is trivial. To prove the other one, suppose that $\mathcal{N}\psi = 0$. We claim that $A_-\psi = 0$. We shall proceed by contradiction. Suppose that $A_-\psi \neq 0$. Then, by (5.104):

$$\mathcal{N}A_-\psi = (-1)A_-\psi \, . \tag{5.107}$$

Thus, $A_-\psi$ is an eigenvector of $\mathcal{N}$ with eigenvalue -1, which is impossible since we just proved that $n \geqslant 0$.

Hence, to find the eigenvectors of $\mathcal{N}$ with eigenvalue $n = 0$ we have to solve $A_-\psi = 0$, that is:

$$\frac{d}{dx}\psi(x) = -x\psi(x) \, . \tag{5.108}$$

The solution to this ODE is, up to a multiplicative constant,

$$\psi(x) = Ce^{-x^2/2} \, . \tag{5.109}$$

Choosing the constant C so that $\|\psi\|_2 = 1$, we find:

$$\psi(x) = \pi^{-\frac{1}{4}} e^{-x^2/2} \equiv \psi_0(x) \, . \tag{5.110}$$

In particular, $H\psi_0 = \psi_0$. We shall call ψ_0 the *ground state* of the harmonic oscillator. Now that we know one eigenstate of H, we can construct infinitely many others acting with A_+^k. We define:

$$\psi_k := \frac{A_+^k \psi_0}{\|A_+^k \psi_0\|_2} \, . \tag{5.111}$$

These functions satisfy $\mathcal{N}\psi_k = k\psi_k$, or equivalently $H\psi_k = (2k+1)\psi_k$. By the uniqueness of the solution of the ODE (5.108), the ground state ψ_0 is unique. Also, one can show that the excited states ψ_k are also unique. Suppose that $\varphi_k \in \mathcal{S}(\mathbb{R})$ is a solution of $\mathcal{N}\varphi_k = k\varphi_k$ with $k \in \mathbb{N}$. Consider

$$\xi_k = A_-^k \varphi_k \, . \tag{5.112}$$

We claim that ξ_k is equal to ψ_0, up to a proportionality constant. This follows from the fact that:

$$\mathcal{N}\xi_k = A_-^k(\mathcal{N} - k)\varphi_k = 0 \, . \tag{5.113}$$

By uniqueness of the ground state, $\xi_k = (\text{const.})\psi_0$. Next, we claim that $\varphi_k = (\text{const.})A_+^k\psi_0$. In fact, as a consequence of what we just proved:

$$(\text{const.})A_+^k\psi_0 = A_+^k A_-^k \varphi_k \, . \tag{5.114}$$

Also,

$$\begin{aligned} A_+^k A_-^k \varphi_k &= A_+^{k-1} \mathcal{N} A_-^{k-1} \varphi_k \\ &= A_+^{k-1} A_-^{k-1} (\mathcal{N} - (k-1))\varphi_k \\ &= \mathcal{N}(\mathcal{N}-1)\cdots(\mathcal{N}-(k-1))\varphi_k \\ &= k!\varphi_k \, . \end{aligned} \tag{5.115}$$

Therefore, we proved that $\varphi_k = CA_+^k\psi_0$. Choosing the constant so that $\|\varphi_k\|_2 = 1$, we get $\varphi_k = \psi_k$. To conclude the discussion about the spectrum of $\mathcal{N}$ on $\mathcal{S}(\mathbb{R})$, we show that the only eigenvalues are $k \in \mathbb{N}$. To this end, suppose that $\psi_\alpha \in \mathcal{S}(\mathbb{R})$ is such that $\mathcal{N}\psi_\alpha = \alpha\psi_\alpha$ with $\alpha \notin \mathbb{N}$.

Consider $A_-\psi_\alpha$; this is an eigenvector of $\mathcal{N}$, with eigenvalue $\alpha - 1$, which is $\neq 0$ since $\alpha \notin \mathbb{N}$. Thus, $A_-\psi_\alpha \neq \psi_0$, which means that $A_-^2\psi_0 \neq 0$. Iterating this argument, $A_-^k\psi_0 \neq 0$; these are eigenstates of $\mathcal{N}$ with eigenvalues $\alpha - k$, which can be arbitrarily negative. This contradicts the property $n \geqslant 0$, proved after (5.107). In conclusion, all the solutions of $\mathcal{N}\psi = n\psi$ in $\mathcal{S}(\mathbb{R})$ have $n \in \mathbb{N}$.

To summarize, we proved that all the solutions of $H\psi = E\psi$ in $\mathcal{S}(\mathbb{R})$ are:

$$(\psi, E) = (\psi_k, E_k) \qquad k = 0, 1, 2, \dots \tag{5.116}$$

with $E_k = (2k + 1)$ and $\psi_k = C_k A_+^k \psi_0$, where the normalization constant C_k is (exercise):

$$\frac{1}{C_k} = \|A_+^k\psi_0\|_2 = \sqrt{k!}\ . \tag{5.117}$$

Notice that eigenstates corresponding to different eigenvectors are orthogonal. In fact, for $k \neq j$:

$$\begin{aligned} \langle \psi_k, \psi_j \rangle &= \frac{1}{k-j}\big[\langle k\psi_k, \psi_j\rangle - \langle \psi_k, j\psi_j\rangle\big] \\ &= \frac{1}{k-j}\big[\langle \mathcal{N}\psi_k, \psi_j\rangle - \langle \psi_k, \mathcal{N}\psi_j\rangle\big] \\ &= 0\ , \end{aligned} \tag{5.118}$$

since $\langle \mathcal{N}\psi_k, \psi_j\rangle = \langle \psi_k, \mathcal{N}\psi_j\rangle = \langle A_-\psi_k, A_-\psi_j\rangle$. Finally, we point out that the functions ψ_k can be written explicitly in terms of *Hermite polynomials:*

$$\psi_k(x) = \frac{1}{\sqrt{2^k k!}} H_k(x)\psi_0(x)\ , \tag{5.119}$$

where $H_k(x)$ is a polynomial of degree k, that is determined by the following recursion:

$$H_k(x) = -\frac{d}{dx}H_{k-1}(x) + 2xH_{k-1}(x) \qquad H_0(x) = 1\ . \tag{5.120}$$

Explicitly, one has:

$$H_k(x) = \sum_{j=0}^{[k/2]} (-1)^j \frac{k!}{(k-2k)!j!}(2x)^{k-2j}\ , \tag{5.121}$$

where $[k/2]$ is the largest integer less or equal than $k/2$.

Minimal energy. The eigenstates of H on $\mathcal{S}(\mathbb{R})$ have strictly positive energy, $2n + 1 \geqslant 1$. As we will see, the energy of any (normalized) state $\psi \in D(H)$ is bounded below by 1. This is in contrast with what happens in classical mechanics, in which the lowest energy configuration of the harmonic oscillator is the one associated to $(p, x) = (0, 0)$. Informally, this configuration is not allowed in quantum mechanics, because it would imply infinite localization in position and in momentum, which violates Heisenberg's uncertainly principle. To see this more precisely, let $\psi \in D(H)$. This implies, in particular, that

$$\langle \psi, -\Delta\psi\rangle = \|\hat{p}\psi\|_2^2 < \infty \qquad \langle \psi, x^2\psi\rangle = \|x\psi\|_2^2 < \infty\ . \tag{5.122}$$

For general $\psi \in D(H)$, derivatives have to be understood in the L^2-sense, recall the discussion at the end of Section 5.32. The energy of ψ is:

$$\langle \psi, H\psi\rangle = \Big\|\frac{d}{dx}\psi\Big\|_2^2 + \Big\|x\psi\Big\|_2^2\ . \tag{5.123}$$

From $a^2 + b^2 \geqslant 2ab$, we have:

$$\langle \psi, H\psi \rangle \geqslant 2 \Big\| \frac{d}{dx}\psi \Big\|_2 \|x\psi\|_2 \geqslant 2 \Big| \Big\langle \frac{d}{dx}\psi, x\psi \Big\rangle \Big| \tag{5.124}$$

where the last inequality is Cauchy-Schwarz inequality. On the other hand, we have:

$$\begin{aligned} \Big| \Big\langle \frac{d}{dx}\psi, x\psi \Big\rangle \Big|^2 &= \Big(\mathrm{Re} \Big\langle \frac{d}{dx}\psi, x\psi \Big\rangle \Big)^2 + \Big(\mathrm{Im} \Big\langle \frac{d}{dx}\psi, x\psi \Big\rangle \Big)^2 \\ &\geqslant \Big(\mathrm{Re} \Big\langle \frac{d}{dx}\psi, x\psi \Big\rangle \Big)^2 . \end{aligned} \tag{5.125}$$

We have:

$$\begin{aligned} \Big(\mathrm{Re} \Big\langle \frac{d}{dx}\psi, x\psi \Big\rangle \Big) &= \frac{1}{2} \Big(\Big\langle \frac{d}{dx}\psi, x\psi \Big\rangle + \Big\langle x\psi, \frac{d}{dx}\psi \Big\rangle \Big) \\ &= \frac{1}{2} \Big\langle \psi, \Big[x, \frac{d}{dx} \Big] \psi \Big\rangle \\ &= \frac{1}{2} \|\psi\|_2^2 . \end{aligned} \tag{5.126}$$

In conclusion,

$$\langle \psi, H\psi \rangle \geqslant \|\psi\|_2^2 = 1 , \tag{5.127}$$

as claimed.

Uncertainty principle. Let us rewrite the position and the momentum operator as:

$$\hat{x} = \frac{1}{\sqrt{2}}(A_+ + A_-) , \qquad \hat{p} = -i\frac{d}{dx} = \frac{i}{\sqrt{2}}(A_+ - A_-) . \tag{5.128}$$

Recall that $\langle A_+^k \psi_0, A_+^j \psi_0 \rangle = 0$ for $k \neq j$. This, together with (5.128) immediately implies:

$$\langle \psi_k, \hat{x}\psi_k \rangle = \langle \psi_k, \hat{p}\psi_k \rangle = 0 . \tag{5.129}$$

That is, the position and the momentum operators have zero average on the eigenstates ψ_k. Let us now consider the variance of the position and of the momentum. Let us start from the ground state ψ_0. We have:

$$\begin{aligned} \langle \psi_0, x^2 \psi_0 \rangle &= \frac{1}{2} \langle \psi_0, (A_+ + A_-)(A_+ + A_-)\psi_0 \rangle \\ &= \frac{1}{2} \langle \psi_0, A_- A_+ \psi_0 \rangle = \frac{1}{2} . \end{aligned} \tag{5.130}$$

Similarly,

$$\begin{aligned} \langle \psi_0, p^2 \psi_0 \rangle &= -\frac{1}{2} \langle \psi_0, (A_+ - A_-)(A_+ - A_-)\psi_0 \rangle \\ &= \frac{1}{2} \langle \psi_0, A_- A_+ \psi_0 \rangle = \frac{1}{2} . \end{aligned} \tag{5.131}$$

Thus, recalling that the averages of x and p are zero:

$$\Delta X_{\psi_0} \Delta P_{\psi_0} = \frac{1}{4} . \tag{5.132}$$

This shows that the ground state ψ_0 saturates the uncertainly principle. Similarly (using that the averages on ψ_k of A_+^2 and of A_-^2 are zero)

$$\begin{aligned} \langle \psi_k, x^2 \psi_k \rangle &= \frac{1}{2} \langle \psi_k, (A_+ A_- + A_- A_+)\psi_k \rangle \\ &= \frac{1}{2} \langle \psi_k, (2\mathcal{N} + 1)\psi_k \rangle = k + \frac{1}{2} . \end{aligned} \tag{5.133}$$

Also,

$$\begin{aligned}\langle\psi_k, p^2\psi_k\rangle &= -\frac{1}{2}\langle\psi_k, (-A_+A_- - A_-A_+)\psi_k\rangle \\ &= k + \frac{1}{2}\,.\end{aligned} \tag{5.134}$$

That is:

$$\Delta X_{\psi_k}\Delta P_{\psi_k} = \left(k + \frac{1}{2}\right)^2\,. \tag{5.135}$$

One can actually prove that the uncertainly principle is saturated if and only if the state is a Gaussian.

Lemma 5.1 (Minimizers of the uncertainly principle are Gaussians.)**.** *Let $\psi \in L^2(\mathbb{R})$, $\|\psi\|_2 = 1$. Let:*

$$a := \langle\psi, x\psi\rangle\,, \qquad b := \langle\psi, \hat{p}\psi\rangle\,. \tag{5.136}$$

Then:

$$\Delta X_\psi \Delta P_\psi = \frac{1}{4} \iff \psi(x) = e^{ixb}\psi_0(x-a) \tag{5.137}$$

Proof. To begin, let us prove that $\psi(x) = e^{ixb}\psi_0(x-a)$ has minimal uncertainly. Notice that:

$$\begin{aligned}\Delta X_\psi &= \langle\psi, x^2\psi\rangle - \langle\psi, x\psi\rangle^2 \\ &= \langle\psi_0, (x+a)^2\psi_0\rangle - \langle\psi_0, (x+a)\psi_0\rangle^2 \\ &= \langle\psi_0, x^2\psi_0\rangle \equiv \Delta X_{\psi_0}\,.\end{aligned} \tag{5.138}$$

Similarly, one can verify that:

$$\Delta P_\psi = \Delta P_{\psi_0}\,. \tag{5.139}$$

Thus, ψ saturates the uncertainly principle because ψ_0 does, as we have seen in (5.132). Let us now prove the converse implication. Suppose that ψ saturates the uncertainly principle. Let:

$$\varphi(x) := e^{-ixb}\psi(x+a)\,. \tag{5.140}$$

Then, one easily checks that

$$\Delta X_\psi = \langle\varphi, x^2\varphi\rangle\,, \qquad \Delta P_\psi = \langle\varphi, p^2\varphi\rangle\,. \tag{5.141}$$

Therefore, the function φ satisfies:

$$\|p\varphi\|_2^2\|x\varphi\|_2^2 = \frac{1}{4}\,. \tag{5.142}$$

From (5.124), (5.125), we see that (5.142) holds if and only if

$$\left\|\frac{d}{dx}\varphi\right\|_2\|x\varphi\|_2 = \left|\left\langle\frac{d}{dx}\varphi, x\varphi\right\rangle\right|\,, \qquad \mathrm{Im}\left\langle\frac{d}{dx}\varphi, x\varphi\right\rangle = 0\,. \tag{5.143}$$

The first condition holds provided:

$$\frac{d}{dx}\varphi = \lambda x\varphi \qquad \text{for } |\lambda| = 1. \tag{5.144}$$

The second condition holds provided:

$$\mathrm{Im}\,\lambda\|x\varphi\|_2^2 = 0 \Rightarrow \lambda \in \mathbb{R}\,. \tag{5.145}$$

Therefore, the minimizer satisfies the equation:

$$\frac{d}{dx}\varphi = \pm x\varphi \ . \tag{5.146}$$

The solution of this ODE is:

$$\varphi(x) = Ce^{\pm x^2/2} \ ; \tag{5.147}$$

hence, in order to have an L^2 solution we are forced to choose $\lambda = -1$, which implies that $\varphi = \psi_0$ (choosing the constant C to enforce the L^2 normalization). All in all:

$$\psi_0(x) = e^{-ixb}\psi(x+a) \Rightarrow \psi(x) = e^{ixb}\psi_0(x-a) \ , \tag{5.148}$$

which concludes the proof of the lemma. ∎

Remark 5.14 (Coherent states)**.** *Thus, the minimizers of the uncertainty principle coincide with the functions:*

$$\psi(x) = e^{ixb}\psi_0(x-a) \ . \tag{5.149}$$

These are called coherent states, *and will play a role in the following discussion.*

Eigenstates on $L^2(\mathbb{R})$. So far, we have found infinitely many eigenstates of H on the Schwartz space. We are now interested in understanding whether it is possible to have other solutions of $H\psi = E\psi$. To answer this question, we shall restrict the attention to the following class of coherent states:

$$\psi^{(a)}(x) = \pi^{-\frac{1}{4}}e^{-(x-a)^2/2} \ , \qquad a \in \mathbb{R} \ . \tag{5.150}$$

That is, $\psi^{(a)}$ is simply a translation of the ground state ψ_0. Let us discuss how to represent these coherent states in terms of the Schwartz eigenstates of H. As we have seen in the previous paragraph, these states saturate the uncertainty principle. In terms of the Fourier transform,

$$\begin{aligned} \psi^{(a)}(x) &\equiv \psi_0(x-a) \\ &= \int \frac{dk}{(2\pi)^{1/2}}\, e^{ikx}e^{ika}\hat{\psi}_0(x) \\ &\equiv e^{i\hat{p}a}\psi_0(x) \ . \end{aligned} \tag{5.151}$$

As we have seen, $\hat{p}$ can be represented in terms of $A_\pm$ as:

$$\hat{p} = \frac{i}{\sqrt{2}}(A_+ - A_-) \ . \tag{5.152}$$

Therefore, the coherent state $\psi^{(a)}$ can be represented as:

$$\psi^{(a)} = e^{-(a/\sqrt{2})(A_+ - A_-)}\psi_0 \ . \tag{5.153}$$

Formally, by expanding the exponential, we have:

$$\psi^{(a)} = \sum_{k \geqslant 0} c_k \psi_k \ , \tag{5.154}$$

for some coefficients $c_k \geqslant 0$. We claim that the series is convergent in L^2; let us sketch the proof of this statement. Consider the estimate for the k-th term in the Taylor series of the exponential:

$$\frac{|a|^k}{k!2^{k/2}}\|(A_+ - A_-)^k\psi_0\|_2 \ . \tag{5.155}$$

The norm is estimated by the sum of 2^k terms, all of the form:

$$\|A_{\varepsilon_1} \cdots A_{\varepsilon_k} \psi_0\|_2 \, . \tag{5.156}$$

We claim that:

$$\|A_\varepsilon \varphi\|_2^2 \leqslant \langle \varphi, (\mathcal{N}+1)\varphi \rangle =: \|(\mathcal{N}+1)^{1/2}\varphi\|_2^2 \, . \tag{5.157}$$

If $\varepsilon = -$, $\|A_\varepsilon \varphi\|_2^2 = \langle \varphi, \mathcal{N}\varphi \rangle$ and the claim is trivially true. If $\varepsilon = +$, we have $\|A_\varepsilon \varphi\|_2^2 = \langle \varphi, (\mathcal{N}+1)\varphi \rangle$, where we used the commutation relation of $A_\pm$. Therefore, we estimate:

$$\|A_{\varepsilon_1} \cdots A_{\varepsilon_k} \psi_0\|_2 \leqslant \|(\mathcal{N}+1)^{1/2} A_{\varepsilon_2} \cdots A_{\varepsilon_k} \psi_0\|_2 = \sqrt{k} \|A_{\varepsilon_2} \cdots A_{\varepsilon_k} \psi_0\|_2 \, . \tag{5.158}$$

Repeating the argument, we have:

$$\|A_{\varepsilon_1} \cdots A_{\varepsilon_k} \psi_0\|_2 \leqslant \sqrt{k!} \|\psi_0\| = \sqrt{k!} \, , \tag{5.159}$$

which gives:

$$\frac{|a|^k}{k! 2^{k/2}} \|(A_+ - A_-)^k \psi_0\|_2 \leqslant \frac{|a|^k 2^k \sqrt{k!}}{k! 2^{k/2}} \, , \tag{5.160}$$

which is summable in k. Thus, the sum in (5.154) is convergent, and defines a function in L^2. One could actually compute the coefficients c_k; we have, omitting the details,

$$c_k = e^{-a^2/4} \frac{a^k}{\sqrt{2^k k!}} \, . \tag{5.161}$$

Thus, we found that the coherent states can be approximated in terms of the Schwartz eigenstates ψ_k. Our ultimate goal will be to show that *all* functions in L^2 can be approximated by ψ_k's, that is they form a orthonormal basis of L^2. To see this, let us consider the set of all linear combinations of coherent states:

$$\mathcal{G} := \left\{ \psi \in L^2(\mathbb{R}) \,\middle|\, \psi = \sum_{k=0}^{N} \alpha_k \psi^{(a_k)} \right\} \, . \tag{5.162}$$

Proposition 5.15. *$\mathcal{G}$ is dense in $L^2(\mathbb{R})$.*

Proof. That is, for all $\phi \in L^2$ and for all $\varepsilon > 0$ there exists $\psi_\varepsilon \in \mathcal{G}$ such that

$$\|\phi - \psi_\varepsilon\|_2 < \varepsilon \, . \tag{5.163}$$

Equivalently, by unitarity of the Fourier transform $\mathcal{F} : L^2 \to L^2$:

$$\|\hat{\phi} - \hat{\psi}_\varepsilon\|_2 < \varepsilon \, . \tag{5.164}$$

We will find it convenient to show that $\mathcal{F}\mathcal{G}$ (the unitary conjugation of $\mathcal{G}$ with the Fourier transform) is dense in L^2. To this end, recall the Fourier transform of a given coherent state:

$$\hat{\psi}^{(a)}(k) = \pi^{-\frac{1}{4}} e^{ika} e^{-k^2/2} \, . \tag{5.165}$$

In order to show that the linear combinations of such functions are dense in L^2 we shall use that a linear subspace $\mathcal{A}$ of L^2 is dense in L^2 if and only if for all $\phi \in L^2$:

$$\langle \psi, \phi \rangle = 0 \quad \forall \psi \in \mathcal{A} \Rightarrow \phi = 0 \, . \tag{5.166}$$

We plan to apply this criterion with $\mathcal{A} = \mathcal{F}\mathcal{G}$. In fact, it will be enough to check that the condition (5.166) holds for a subset of $\mathcal{F}\mathcal{G}$. Also, it will be enough to check the condition (5.166) for vectors ϕ in a dense subset of L^2; in our case, we shall take $\phi \in L^2(\mathbb{R}) \cap C_c(\mathbb{R})$.

Consider:

$$\begin{aligned}\langle\hat{\psi}^{(a)},\phi\rangle &= \int dk\,\overline{\hat{\psi}^{(a)}(k)}\phi(k)\\ &= \int dk\,\pi^{-\frac{1}{4}}e^{-ika}e^{-k^2/2}\phi(k)\ .\end{aligned} \tag{5.167}$$

Suppose that $\langle\hat{\psi}^{(a)},\phi\rangle = 0$ for all $a\in\mathbb{R}$. Then, the previous identity implies that

$$\mathcal{F}\big(e^{-k^2/2}\phi(k)\big)(a) = 0 \qquad \forall a\in\mathbb{R}\ . \tag{5.168}$$

That is, being the Fourier transform unitary, this implies that:

$$e^{-k^2/2}\phi(k) = 0\ , \tag{5.169}$$

which can only hold if $\phi = 0$, since $e^{-k^2/2} > 0$. This shows that the only vector $\phi\in L^2(\mathbb{R})\cap C_c(\mathbb{R})$ orthogonal to all $\psi^{(a)}$ is $\phi = 0$; in particular, the only vector $\phi\in L^2(\mathbb{R})\cap C_c(\mathbb{R})$ orthogonal to all vectors in $\mathcal{FG}$ is $\phi = 0$. Thus, $\mathcal{FG}$ is dense in $L^2(\mathbb{R})\cap C_c(\mathbb{R})$. Being $L^2(\mathbb{R})\cap C_c(\mathbb{R})$ dense in $L^2(\mathbb{R})$, the claim follows. ∎

The next proposition shows that the ψ_k are the only eigenstates of H on L^2. Let:

$$\mathcal{D} = \{\psi\in L^2(\mathbb{R})\,\Big|\,\psi = \sum_{k=0}^{N}\beta_k\psi_k\}\ , \tag{5.170}$$

and let us denote by $\overline{\mathcal{D}}$ the closure in L^2 of $\mathcal{D}$.

Proposition 5.16. $\overline{\mathcal{D}} = L^2(\mathbb{R})$.

Proof. By the formula (5.154), one easily finds $\mathcal{G}\subset\overline{\mathcal{D}}$. Also, by the previous proposition, $\overline{\mathcal{G}} = L^2(\mathbb{R})$. Therefore, since $\overline{G}\subseteq\overline{\mathcal{D}}\subseteq L^2(\mathbb{R})$ we get $\overline{\mathcal{D}} = L^2(\mathbb{R})$. ∎

Remark 5.17. *This result proves that any vector $\psi\in L^2(\mathbb{R})$ can be represented as $\psi = \sum_{k\geqslant 0}\beta_k\psi_k$, for suitable coefficients β_k. Also, the vectors ψ_k are orthonormal; therefore, (ψ_k) is an orthonormal basis of $L^2(\mathbb{R})$.*

The next is an immediate corollary of Proposition 5.16.

Corollary 5.1. *Suppose that ψ is an L^2-solution of $H\psi = E\psi$. Then, $\psi = \psi_k$ for some $k\in\mathbb{N}$.*

Proof. Suppose that $\psi\in L^2(\mathbb{R})$ solves $H\psi = E\psi$ for $E\notin 2\mathbb{N}+1$. Then, $\langle\psi,\psi_k\rangle = 0$ for all k, since ψ and ψ_k are eigenvectors of H with different eigenvalues. Being (ψ_k) an orthonormal basis of L^2, this implies that $\psi = 0$.

Next, suppose that $\psi\in L^2(\mathbb{R})$ solves $H\psi = E\psi$ for $E = 2n+1$ and $n\in\mathbb{N}$. Without loss of generality, suppose that $\|\psi\|_2 = 1$. We represent ψ as:

$$\psi = \sum_k\beta_k\psi_k\ , \tag{5.171}$$

where we used that ψ_k form an ONB of L^2. Taking the scalar product with ψ_n we have, using the orthonormality:

$$1 = \langle\psi,\psi\rangle = \beta_n\langle\psi,\psi_n\rangle\ . \tag{5.172}$$

Since $\|\psi\|^2 = \sum_n|\beta_n|^2$, we known that $|\beta_n|\leqslant 1$. Also, $|\langle\psi,\psi_n\rangle|\leqslant 1$. Thus, the only way to satisfy (5.172) is by having $\beta_n = 1$ and $|\langle\psi,\psi_n\rangle| = 1$. In particular, the normalization of ψ implies that $\beta_k = 0$ for all $k\neq n$. This shows that $\psi = \psi_n$, and it concludes the proof of the corollary. ∎

Periodicity of dynamics. In conclusion, we have shown that the spectrum of H, as an operator on L^2, is given by:

$$\sigma(H) = \left\{ 2n+1 \,\middle|\, n \in \mathbb{N} \right\} , \tag{5.173}$$

and that the eigenvectors are given by $\psi_n = \sqrt{n!}^{-1} A_+^n \psi_0$. In particular, the spectrum of H is discrete. Instead, the spectrum of the Laplacian is continuous, and it coincides with $\mathbb{R}_+ = [0, \infty)$. This is a consequence of the fact that $-\Delta$ is unitarily equivalent to the multiplication operator $|k|^2$, via the Fourier transform. The discreteness vs. continuity of the spectrum of the model has important consequences on the dynamics of the system. The general connection between the spectral properties of H and the qualitative properties of motion is provided by the RAGE theorem [8]. We shall not discuss such result; instead, we shall limit ourselves to the following remarks. As we have seen, the free Schrödinger equation is dispersive: the particle escapes at infinity. Instead, the dynamics generated by the harmonic oscillator gives rise to a periodic motion. To see this, let $\psi \in D(H)$, and let us represent it in the basis of the eigenstates of H:

$$\psi = \sum_k c_k \psi_k \, . \tag{5.174}$$

The solution of the Schrödinger equation with initial datum $\psi(0) = \psi$ is given by:

$$\psi(t) = \sum_k c_k e^{-i(2k+1)t} \psi_k \tag{5.175}$$

(since $e^{-i(2k+1)t}\psi_k$ is the stationary state associated with the initial datum ψ_k). Thus, from the expression (5.175) it is clear that:

$$\psi(t) = \psi(t + 2\pi) \, , \tag{5.176}$$

which shows periodicity of the dynamics.

Dynamics of coherent states. It is natural to understand whether the quantum evolution resembles the classical one, at least for a special class of quantum states. Here we shall consider the dynamics of coherent states; since they minimize uncertainly, the evolution of these states is close to the classical one, in a suitable sense. Recall Hamilton's equation of motion for the harmonic oscillator, with Hamiltonian $H(x,p) = p^2/2m + kx^2/2$:

$$\frac{d}{dt} x(t) = p(t)/m \, , \qquad \frac{d}{dt} p(t) = -kx(t) \, . \tag{5.177}$$

Thus, the solution is given by:

$$x(t) = A \cos(\omega t) + B \sin(\omega t) \qquad \omega = \sqrt{k/m} \, , \tag{5.178}$$

with A and B determined by the initial datum:

$$x_0 = A \, , \qquad p_0 = B\omega \, . \tag{5.179}$$

In quantum mechanics, position and momentum corresponds to operators acting on the wave function. Given $\varphi, \psi \in \mathcal{S}(\mathbb{R})$, we can define the evolution of the position and of the momentum operator as:

$$\langle \varphi, \hat{x}(t)\psi \rangle := \langle \varphi(t), x\psi(t) \rangle \, , \qquad \langle \varphi, \hat{p}(t)\psi \rangle := \langle \varphi(t), \hat{p}\psi(t) \rangle \, , \tag{5.180}$$

with $\psi(t)$ and $\varphi(t)$ the solutions of the Schrödinger equation with initial data given by ψ and φ, $\psi(t) = e^{-iHt}\psi$, $\varphi(t) = e^{-iHt}\varphi$. That is,

$$\hat{x}(t) = e^{iHt} \hat{x} e^{-iHt} \, , \qquad \hat{p}(t) = e^{iHt} \hat{p} e^{-iHt} \, . \tag{5.181}$$

We are interested in finding the evolution equations for such operators. We have:

$$\begin{aligned}\frac{d}{dt}\langle\varphi,\hat{x}(t)\psi\rangle &= \Big\langle\frac{d}{dt}\varphi(t),\hat{x}\psi(t)\Big\rangle+\Big\langle\varphi(t),\hat{p}\frac{d}{dt}\psi(t)\Big\rangle\\ &= i\langle H\varphi(t),\hat{x}\psi(t)\rangle - i\langle\varphi(t),\hat{x}H\psi(t)\rangle\\ &= -i\langle\varphi(t),[\hat{x},H]\psi(t)\rangle\,.\end{aligned} \tag{5.182}$$

Since $H=\hat{p}^2+\hat{x}^2$, the commutator is given by:

$$[\hat{x},p^2]=2i\hat{p}\,. \tag{5.183}$$

Therefore,

$$\frac{d}{dt}\langle\varphi,\hat{x}(t)\psi\rangle = 2\langle\varphi(t),\hat{p}\psi(t)\rangle\,. \tag{5.184}$$

Similarly, one has:

$$\frac{d}{dt}\langle\varphi,\hat{p}(t)\psi\rangle = -2\langle\varphi(t),\hat{x}\psi(t)\rangle\,. \tag{5.185}$$

That is:

$$\frac{1}{2}\frac{d}{dt}\hat{x}(t)=\hat{p}(t)\,,\qquad \frac{d}{dt}p(t)=-2\hat{x}(t)\,. \tag{5.186}$$

If the Hamiltonian has the more general form $H=\hat{p}^2/2m+k\hat{x}^2/2$, the $1/2$ factor is replaced by m, while the -2 factor is replaced by $-k$. Solving the differential equation, we get:

$$\hat{x}(t)=\sin(2t)\hat{p}+\cos(2t)\hat{x}\,,\qquad \hat{p}(t)=\cos(2t)\hat{p}-\sin(2t)\hat{x}\,. \tag{5.187}$$

Let us consider the evolution of a coherent state,

$$\psi^{(a)}(x)=\psi_0(x-a)\equiv e^{i\hat{p}a}\psi_0(x)\,. \tag{5.188}$$

Then, the solution of the Schrödinger equation with initial datum given by $\psi^{(a)}(x)$ is:

$$\begin{aligned}e^{-iHt}\psi^{(a)}(x) &= e^{-iHt}e^{i\hat{p}a}e^{iHt}e^{-iHt}\psi_0(x)\\ &= e^{-it}e^{i\hat{p}(-t)a}\psi_0(x)\,.\end{aligned} \tag{5.189}$$

where we used the fact that ψ_0 is a stationary state of H, and where $\hat{p}(t)=e^{iHt}\hat{p}e^{-iHt}$. Therefore, from (5.187):

$$e^{-iHt}\psi^{(a)}(x)=e^{-it}e^{i(\cos(2t)\hat{p}+\sin(2t)\hat{x})}\psi^{(a)}(x)\,. \tag{5.190}$$

Notice that, due to the fact that $\hat{p}$ and $\hat{x}$ do not commute,

$$e^{i(\cos(2t)\hat{p}+\sin(2t)\hat{x})}\neq e^{i\cos(2t)\hat{p}}e^{i\sin(2t)\hat{x}}\,. \tag{5.191}$$

The correct factorization property is provided by the next result.

Proposition 5.18 (Weyl relations.)**.** *For all $\alpha,\beta\in\mathbb{R}$, the following is true:*

$$e^{i(\alpha\hat{p}+\beta\hat{x})}=e^{i\alpha\hat{p}}e^{i\beta\hat{x}}e^{i\alpha\beta}=e^{i\beta\hat{x}}e^{i\alpha\hat{p}}e^{-i\alpha\beta}\,. \tag{5.192}$$

Proof. Let us define $A=\alpha\hat{p}$ and $B=\beta\hat{x}$. Let us define the unitary operator:

$$F(t):=e^{i(A+B)t}e^{-iAt}e^{-iBt}\,. \tag{5.193}$$

Clearly, $F(0)=1$. Let us compute the time derivative. We have:

$$\begin{aligned}\frac{d}{dt}F(t) &= ie^{i(A+B)t}Be^{-iAt}e^{-iBt}-ie^{i(A+B)t}e^{-iAt}Be^{-iBt}\\ &= ie^{i(A+B)t}\Big[B,e^{-iAt}\Big]e^{-Bt}\,.\end{aligned} \tag{5.194}$$

To compute the commutator, we rewrite it as:

$$\begin{aligned}\left[B, e^{-iAt}\right] &= \int_0^t ds\, \frac{d}{ds} e^{-iA(t-s)} B e^{-iAs} \\ &= -i \int_0^t ds\, e^{-iA(t-s)} [B, A] e^{-iAs} \\ &= t\alpha\beta e^{-iAt} \,,\end{aligned} \tag{5.195}$$

where we used that $[B, A] = \alpha\beta i$, which commutes with all operators. That is:

$$\frac{d}{dt} F(t) = it\alpha\beta F(t) \,, \tag{5.196}$$

which gives $F(t) = e^{i\alpha\beta t^2/2}$. Therefore, $F(1) = e^{i(A+B)} e^{-iA} e^{-iB} = e^{i\alpha\beta/2}$, which gives:

$$e^{i(A+B)} = e^{iB} e^{iA} e^{i\alpha\beta/2} \,; \tag{5.197}$$

recalling the definition of A and B, this proves the claim. ∎

As an application of the Weyl relations, we can determine the time evolution of coherent states, under the dynamics generated by the harmonic oscillator. We get:

$$e^{-iHt} \psi^{(a)}(x) = e^{-it - i\sin(2t)\cos(2t)} e^{i\sin(2t)\hat{x}} e^{i\cos(2t)\hat{p}} \psi^{(a)}(x) \,. \tag{5.198}$$

Thus, up to an irrelevant phase, the time evolution of a coherent state is again a coherent state, with time-dependent position and momentum given by the solution of the classical equation of motion (5.177).

5.5 The hydrogen atom and stability of matter

The classical Hamiltonian for a pointlike negative charge $e = -1$ interacting with a fixed positive charge $Z > 0$ at the location $R = 0$ is:

$$H(p, x) = \frac{p^2}{2m} - \frac{Z}{|x|} \,. \tag{5.199}$$

The same Hamiltonian plays an important role in the description of gravitational motion; in that case, the charges are replaced by the masses of the planets. The assumption that the particle/planet at with charge/mass Z is fixed at $R = 0$ is reasonable if we assume that the mass of this particle is much larger than the mass of the particle at x. It is obvious that this Hamiltonian is unbounded from below: the configuration $(x, p) = (0, 0)$ has energy equal to $-\infty$. Classically, the system is *unstable,* as it is an unbounded source of energy.

In gravitational physics, what prevents the system from collapsing is the conservation of angular momentum. Both the energy of the initial datum and the modulus angular momentum are conserved quantities along the Hamiltonian flow. From the solution of the two-body problem, we know that $|x(t)| \geqslant \rho_-$, where:

$$\rho_- = \frac{Z}{|E|} - \sqrt{\frac{Z^2}{E^2} - \frac{A^2}{2Em}} \,, \tag{5.200}$$

with $E = H(p_0, x_0)$ is the energy of the initial datum, while A is the modulus of the angular momentum:

$$A = |x(t) \times \dot{x}(t)| = |x_0 \times \dot{x}_0| \,. \tag{5.201}$$

Thus, the minimal distance of the particle from the fixed charge vanishes as $A \to 0$. The same mechanism could be applied to the electrostatic problem. This however would not be enough to rule out instability: a more complete description of the system should also take into account the energy radiated by the fact that the charge $e = -1$ is *accelerating* around the nucleus. The Larmor formula predicts that the energy of the system should decrease, which eventually would imply the collapse of the electron on the nucleus.

Let us now consider the quantum mechanical counterpart of this problem. The *hydrogen atom* is the simplest element of the periodic table of elements. It consists of one proton and one electron; since the mass of the proton is much larger than the mass of the electron, it is reasonable to describe the system by the quantization of the Hamiltonian (5.199):

$$H = -\frac{1}{2m}\Delta - \frac{Z}{|\hat{x}|} , \tag{5.202}$$

on a suitable dense domain $D(H) \subset L^2(\mathbb{R}^3)$. For $Z = 1$, the system is charge neutral. For general $Z > 0$, we shall talk about hydrogenic systems. The ground state of the system is defined as the smallest energy attained by $\psi \in L^2(\mathbb{R}^3)$; we have:

$$E_0 = \inf_{\psi \in D(H)} \frac{\langle \psi, H\psi \rangle}{\|\psi\|_2^2} . \tag{5.203}$$

A first question, which is already nontrivial, is whether this quantity is finite or not. From a classical viewpoint, this object should be $-\infty$. This would correspond to the configuration in which the electron collapses on the nucleus: classical mechanics is not able to prove the existence of a stable hydrogen atom, and more generally of stable atoms and molecules.

This is of course in contrast with the fact that matter exists and it is extensive. One of the major triumphs of quantum mechanics is the explanation for this observation, whose importance cannot be overemphasized. Intuitively, the reason for stability is the uncertainly principle: infinite localization in both position and velocity is not allowed. How can we quantify this? From the uncertainly principle, we obtain:

$$\Delta X_i \Delta P_i \geqslant \frac{1}{4} , \tag{5.204}$$

that is, supposing that ψ is such that $\langle \psi, \hat{x}\psi \rangle = \langle \psi, \hat{p}\psi \rangle = 0$,

$$\langle \psi, p^2 \psi \rangle \geqslant \frac{9}{4\langle \psi, x^2 \psi \rangle} . \tag{5.205}$$

This inequality unfortunately does not tell us anything about the finiteness of E_0; we would like to have a bound that allows to related kinetic and potential energy in (5.202). Before proving such estimate, let us try to develop an intuition by considering the energy variation for a state $\psi \in \mathcal{S}(\mathbb{R}^d)$, after a space rescaling. Consider, for $\lambda \geqslant 1$:

$$\psi_\lambda(x) = \lambda^{\frac{3}{2}} \psi(\lambda x) . \tag{5.206}$$

Clearly, $\|\psi_\lambda\|_2$ is independent of λ. Let us consider the energy of ψ_λ. We have:

$$\begin{aligned} \langle \psi_\lambda, H\psi_\lambda \rangle &= \langle \psi_\lambda, -\frac{1}{2m}\Delta\psi_\lambda \rangle - \langle \psi_\lambda, \frac{Z}{|x|}\psi_\lambda \rangle \\ &= \lambda^2 \langle \psi, -\frac{1}{2m}\Delta\psi \rangle - \lambda \langle \psi, \frac{Z}{|x|}\psi \rangle . \end{aligned} \tag{5.207}$$

In particular, this shows that the energy diverges to $+\infty$ as $\lambda \to \infty$: space localization is not energetically convenient! Highly localized states have very high kinetic energy, which eventually dominates the potential energy. This discussion suggests that collapse is avoided by the growth of kinetic energy, but of course it does not prove it. Stability follows from the next result.

Lemma 5.19 (Coulomb uncertainty principle.)**.** *Let $H \in H^1(\mathbb{R}^3)$. Then:*

$$\int dx \, \frac{1}{|x|} |\psi(x)|^2 \leqslant \|\nabla\psi\|_{L^2(\mathbb{R}^3)} \|\psi\|_{L^2(\mathbb{R}^3)} \, . \tag{5.208}$$

Before discussing the proof, let us use this lemma to prove the stability of the hydrogenic atom.

Proposition 5.20. *Let $\psi \in H^2(\mathbb{R}^d)$, $E_\psi = \langle \psi, H\psi \rangle$. Then, the following inequality holds true:*

$$E_\psi \geqslant -\frac{Z^2}{4} \|\psi\|_2^2 \, . \tag{5.209}$$

Equality is reached for $\psi = Ke^{-(Z/4)|x|}$.

Proof. (of Proposition 5.20.) Suppose that $\|\psi\|_2 = 1$. By Lemma 5.19, we have:

$$E_\psi \geqslant \|\nabla\psi\|_2^2 - Z\|\nabla\psi\|_2 \geqslant -\frac{Z^2}{4} \, , \tag{5.210}$$

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 5.19.

Proof. (of Lemma 5.19.) The starting point is the following identity:

$$2\langle \psi, \frac{1}{|x|} \psi \rangle = \sum_{j=1,2,3} \langle \psi, [\partial_{x_j}, \frac{x_j}{|x|}] \psi \rangle \, , \tag{5.211}$$

where we used that:

$$\Big[\partial_{x_j}, \frac{x_j}{|x|} \Big] = \frac{1}{|x|} - \frac{x_j^2}{|x|^3} \, . \tag{5.212}$$

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:

$$\begin{aligned} 2\langle \psi, \frac{1}{|x|} \psi \rangle &\leqslant 2 \sum_j \|\partial_{x_j}\psi\|_{L^2} \Big\| \frac{x_j}{|x|}\psi \Big\|_{L^2} \\ &\leqslant 2 \Big(\sum_j \|\partial_{x_j}\psi\|_{L^2}^2 \Big)^{1/2} \Big(\sum_j \Big\| \frac{x_j}{|x|}\psi \Big\|_{L^2}^2 \Big)^{1/2} \\ &\leqslant 2\|\nabla\psi\|_{L^2} \|\psi\|_{L^2} \, . \end{aligned} \tag{5.213}$$

This concludes the proof. ∎

Since $H^2(\mathbb{R}^3) \subset H^1(\mathbb{R}^3)$, the above result proves that the hydrogen atom, on its natural domain $D(H) = H^2$, has bounded ground state energy. In particular, since $e^{-(Z/4)|x|}$ is in the domain, the ground state energy is:

$$E_0 = -\frac{Z^2}{4} \,. \tag{5.214}$$

Remark 5.21. *The mass of the particle can be reintroduced recalling the scaling (5.207). Given $\psi \in D(H)$, consider the unitary transformation:*

$$\widetilde{\psi}(x) = \Big(\frac{1}{\sqrt{2m}}\Big)^{3/2} \psi\Big(\frac{x}{\sqrt{2m}}\Big) \,. \tag{5.215}$$

It turns out that:

$$\langle \widetilde{\psi}, H\widetilde{\psi}\rangle = \Big\langle \psi, -\frac{1}{2m}\Delta\psi\Big\rangle - \frac{Z}{\sqrt{2m}}\Big\langle \psi, \frac{1}{|x|}\psi\Big\rangle \tag{5.216}$$

This shows that the ground state energy of the system with mass $1/2$ and nuclear charge Z is equal to the ground state energy of the system with mass m and nuclear charge $Z/\sqrt{2m}$. In particular, the ground state energy of the system with mass m and nuclear charge Z is:

$$E_0 = -\frac{mZ^2}{2} \,. \tag{5.217}$$

The ground state wave function is:

$$\psi(x) = Ce^{-\sqrt{2m}(Z/4)|x|} \tag{5.218}$$

So far, we have only discussed systems involving one particle at the time. This, in particular, does not allow to consider any other element in the periodic table: except for the hydrogen atom, all elements in the periodic table involve more than one electron. For instance, the helium atom is formed by a nucleus of two neutrons and two protons, interacting with two electrons. To properly discuss such system, one has to be able to take into account the repulsion between the negatively charged electrons.

For an N-particle system, the many-body wave function is:

$$\psi_N \equiv \psi_N(x_1, \sigma_1; \ldots; x_N, \sigma_N) \,, \tag{5.219}$$

where x_i denotes the position of the i-th particle, and σ_i is the spin of the particle. The spin variable σ_i takes integer values. The probability distribution for finding the particles in the positions $x_1, \ldots, x_N$ and spin states $\sigma_1, \ldots, \sigma_N$ is:

$$|\psi_N(x_1, \sigma_1; \ldots; x_N, \sigma_N)|^2 \,. \tag{5.220}$$

Thus, the natural space for such wave functions is $L^2((\mathbb{R}^3 \times \mathbb{C})^N)$. The normalization of probability corresponds to the requirement:

$$1 = \|\psi_N\|_2^2 := \sum_{\underline{\sigma}} \int dx_1 \ldots dx_N \, |\psi_N(z_1, \ldots, z_N)|^2 \tag{5.221}$$

with $z_i = (x_i, \sigma_i)$. For *identical particles*, the N-particle probability distribution is invariant under permutation of the particle labels $1, \ldots, N$:

$$|\psi_N(z_1, \ldots, z_N)| = |\psi_N(z_{\pi(1)}, \ldots, z_{\pi(N)})| \,. \tag{5.222}$$

In nature, there are two kind of identical particles: bosons and fermions. *Bosons* correspond to symmetric wave functions:

$$\psi_N(z_1, \ldots, z_N) = \psi_N(z_{\pi(1)}, \ldots, z_{\pi(N)}) \,. \tag{5.223}$$

Example of bosons are photons, the Higgs boson, Helium atoms etc.. *Fermions*, instead, correspond to antisymmetric wave functions:

$$\psi_N(z_1,\dots,z_N) = \mathrm{sgn}(\pi)\psi_N(z_{\pi(1)},\dots,z_{\pi(N)}) \ . \tag{5.224}$$

In particular, fermionic wave functions vanish whenever two particles have same coordinates. Examples of fermions are electrons, protons, neutrons etc. Ordinary matter is made of fermions, and it is therefore of utter importance to understand their properties. By the spin-statistics theorem, which is proved using relativistic quantum mechanics, fermions correspond to particles with an even number of possible spin values, while bosons correspond to wave functions with an odd number of possible spin values.

Many-particle Hamiltonians are self-adjoint operators acting on $L^2((\mathbb{R}^3\times\mathbb{C})^N)$. The Hamiltonian for a molecule formed by M fixed nuclei and N electrons is:

$$H_{N,M}(\underline{Z},\underline{R}) = \sum_{j=1}^N \Big(-\frac{1}{2m_j}\Delta_{x_j} - \sum_{i=1}^M \frac{Z_i}{|x_j-R_i|}\Big) + \sum_{i<j}^N \frac{1}{|x_i-x_j|} + \sum_{i<j}^M \frac{Z_iZ_j}{|R_i-R_j|} \ . \tag{5.225}$$

The fermionic ground state energy of the system is defined as:

$$E_{N,M}(\underline{Z},\underline{R}) := \inf_{\psi_N\in L^2_a((\mathbb{R}^3\times\mathbb{C})^N)} \frac{\langle\psi_N, H_{N,M}(\underline{Z},\underline{R})\psi_N\rangle}{\|\psi_N\|_2^2} \ , \tag{5.226}$$

where $L^2_a((\mathbb{R}^3\times\mathbb{C})^N)$ is the space of antisymmetric, or fermionic, wave functions. A first question to address is the extension of what we discussed before: is the ground state energy bounded below? A natural attempt to attack this problem is to estimate:

$$\begin{aligned}\langle\psi_N, H_{N,M}(\underline{Z},\underline{R})\psi_N\rangle &\geqslant \Big\langle\psi_N, \sum_{j=1}^N \Big(-\frac{1}{2m_j}\Delta_{x_j} - \sum_{i=1}^M \frac{Z_i}{|x_j-R_i|}\Big)\psi_N\Big\rangle \\ &= \sum_{j=1}^N\sum_{i=1}^M \langle\psi_N, \Big(-\frac{1}{2m_jM}\Delta_{x_j} - \frac{Z_i}{|x_j-R_i|}\Big)\psi_N\rangle\end{aligned} \tag{5.227}$$

where we used the fact that the Coulomb repulsion is positive. Each term in the sum corresponds to the Hamiltonian of a hydrogenic atom, with electron mass m_jM, and with nucleus at position R_j and with charge Z_j. This suggest that the ground state energy of the system is bounded below by the sum of the ground state energies of these individual problems. To prove this, one can repeat the argument of the proof of Lemma 5.19, using the identity (we can get rid of the nuclear coordinates by a change of variables):

$$2\langle\psi_N, \frac{1}{|x_k|}\psi_N\rangle = \sum_{j=1,2,3} \Big\langle\psi_N, \Big[\partial_{x_{k,j}}, \frac{x_{k,j}}{|x_k|}\Big]\psi_N\Big\rangle \tag{5.228}$$

where x_k is the position of the k-th particle, $x_k = (x_{k,1}, x_{k,2}, x_{k,3})$. We then have:

$$E_{N,M}(\underline{Z},\underline{R}) \geqslant -\sum_{j=1}^N\sum_{i=1}^M \frac{m_jMZ_i^2}{2} > -\infty \ . \tag{5.229}$$

This bound proves *stability of matter of the first kind*: the ground state energy of the system is finite, for any finite value of N and M. This is nice, but however not very useful from a practical viewpoint. What we actually would like to prove is that the energy per particle is bounded below uniformly in N and M. Equivalently, we would like to have a lower bound for the ground state energy of the form:

$$E_{N,M}(\underline{Z},\underline{R}) \geqslant -C(N+M) \ . \tag{5.230}$$

This estimate is called *stability of matter of the second kind*. This bound is compatible with a bounded energy per particle. Physically, this is what one expects: the energy of a system with $N_1 + N_2$ electrons and $M_1 + M_2$ protons should be of the same order of the energy of two separate systems of (N_1, M_1) and (N_2, M_2) particles. If the energy did not depend linearly on the number of constituents, one could extract a huge amount of energy simply by merging or splitting systems. This would ultimately rule out the existence of matter as we see it.

It turns out that the bound (5.230) only holds for fermions, and it is false for bosons. The proof of stability of matter of the second kind is much more involved, and it relies on two key ingredients:

(i) The antisymmetry of the wave function (or Pauli principle),

(ii) A partial cancellation between the positive Coulomb repulsion between the electrons, and the negative Coulomb attraction between electrons and nuclei.

The proof of this statement is a major achievement of mathematical physics, and it goes far beyond the scope of the present course. We refer the reader to [7] for a review of this topic and of its modern extensions.

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