

# Basics of fluid mechanics

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ABSTRACT. This is an introduction to fluid mechanics, with emphasis on liquid dynamics. We first discuss the states of matter, with the standard theory of gases, then with a detailed explanation on what liquids precisely are, and with a look into plasma too. Then we discuss the general mathematics and physics of fluid dynamics, with the Euler equations, the Navier-Stokes equations, and other more specialized equations. Finally, we have a more detailed look into hydrodynamics, both theory and applications, and with some engineering included, followed by a similar look into aerodynamics.

## Preface

“Aerodynamically, the bumble bee shouldn’t be able to fly, but the bumble bee doesn’t know it, so it goes on flying anyway” - Mary Kay Ash. Although intended to be rather inspirational, this quote says it all about our knowledge of fluid dynamics too.

But you might know this already, just contemplating the waves at sea, or watching some cigarette smoke, suggests that what is going on there is no easy business, mathematically speaking. And if you are a bit familiar with computers, and what they can do, you will probably recognize here questions that are most likely beyond their reach, be them ordinary or super computers, and from the present or the foreseeable future.

This being said, a number of things can be done. To start with, water and other liquids are after all not that much complicated than a pile of snow or sand, so their dynamics should be governed by simple equations, basically coming from classical mechanics. Or, to be more precise, from “dirty” classical mechanics, with some friction allowed. And add to this the observation that, in the case of snow or sand at least, the individual particles can be labeled  $1, 2, 3, \dots, 1000$ , and their dynamics can be understood as a sort of spatial permutation of them, or diffeomorphism as mathematicians like to say, and we have here some basic mathematics going on, both of discrete and continuous nature, that can be very helpful, and that our computer friend can understand too.

As for the gases, and for plasma which is a fluid too, we can expect here to have some complications in our equations, coming from compressibility, but basically the same principles should apply, and we should end up with some simple equations.

Of course, solving these equations will be most likely a very difficult question, both for us and for our computer friend. But let’s be optimistic, after all if the bumble bee knows how to solve these equations, why shouldn’t we be able to come up with some engineering feats too, based on our fluid mechanics knowledge, developed along the above lines.

The present book is an introduction to this, basic equations of fluid mechanics, their mathematics and physics, and their basic applications too. The subject being quite difficult, we will juggle with mathematics, physics and engineering, typically by switching to mathematics or engineering, when the physics becomes too complicated, or by switching

to engineering and physics, when mathematics becomes too hard, or of course, cheap trick, switching to math and physics, when overwhelmed by numerics and engineering.

The book is organized in 4 parts, the plan being as follows:

I - We will first discuss the states of matter, with the theory of gases, then with a detailed explanation on what liquids precisely are, and with a look into plasma too.

II - Then we will discuss the general math and physics of fluid dynamics, with the Euler equations, the Navier-Stokes equations, and other more specialized equations.

III - Then, we will have a more detailed look into hydrodynamics, both theory and applications, and with some engineering discussion included.

IV - Finally, we will have a similar look into aerodynamics, this time more engineering oriented, with the aim of reaching higher and higher Mach speeds.

In the hope that you will find this book useful. The body of literature on fluid mechanics is actually remarkably wide, with countless possible good choices, depending on your precise motivations and goals, and with respect to this, the present book is rather aimed at readers having a bit of familiarity with basic mathematics, and with little to zero knowledge of physics and engineering, in the fluid mechanics area.

Many thanks to my PDE colleagues and friends, including my sister Valeria and her PDE gang, for various interesting discussions over the time. And with a tribute to the mechanics books of Vladimir Arnold too, for someone with a rather pure mathematics background as mine, these have always been a joy to browse. Finally, many thanks to my cats, usually they help when it comes to math and quantum physics, but here with Navier-Stokes they seem quite lost. But, as they say, no need to be a champion in swimming or flying, for catching and enjoying all sorts of aerodynamic beasts.

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Part I

Liquids, fluids

*Busted flat in Baton Rouge, waiting for a train  
When I was feeling near as faded as my jeans  
Bobby thumbed a diesel down, just before it rained  
And rode us all the way into New Orleans*

## CHAPTER 1

### Atoms, molecules

#### 1a. Atomic theory

We recall that light is an electromagnetic wave, depending on frequency and wavelength. The classification of light, in a rough form, is as follows:

Frequency	Type	Wavelength
	—	
$10^{18} - 10^{20}$	$\gamma$ rays	$10^{-12} - 10^{-10}$
$10^{16} - 10^{18}$	X – rays	$10^{-10} - 10^{-8}$
$10^{15} - 10^{16}$	UV	$10^{-8} - 10^{-7}$
	—	
$10^{14} - 10^{15}$	blue	$10^{-7} - 10^{-6}$
$10^{14} - 10^{15}$	yellow	$10^{-7} - 10^{-6}$
$10^{14} - 10^{15}$	red	$10^{-7} - 10^{-6}$
	—	
$10^{11} - 10^{14}$	IR	$10^{-6} - 10^{-3}$
$10^9 - 10^{11}$	microwave	$10^{-3} - 10^{-1}$
$1 - 10^9$	radio	$10^{-1} - 10^8$

Observe the tiny space occupied by the visible light, all the colors there, and the many more missing, being squeezed under the  $10^{14} - 10^{15}$  frequency banner. Here is a zoom on that part, with of course the remark that all this, colors, is something subjective:

Frequency THz = $10^{12}$ Hz	Color	Wavelength nm = $10^{-9}$ m
	—	
670 – 790	violet	380 – 450
620 – 670	blue	450 – 485
600 – 620	cyan	485 – 500
530 – 600	green	500 – 565
510 – 530	yellow	565 – 590
480 – 510	orange	590 – 625
400 – 480	red	625 – 750

Spectroscopy, a cheap and very useful technique, amounts in decomposing the light that an event has produced, by using a prism, recording the color components of that light, and trying to reconstruct that event, out of this data. This technique was key

to the beginnings of the atomic theory, There is a long story here, involving many discoveries, around 1890-1900, focusing on hydrogen H. We will present here things a bit retrospectively. First on our list is the following discovery, by Lyman in 1906:

FACT 1.1 (Lyman). *The hydrogen atom has spectral lines given by the formula*

$$\frac{1}{\lambda} = R \left( 1 - \frac{1}{n^2} \right)$$

where  $R \simeq 1.097 \times 10^7$  and  $n \geq 2$ , which are as follows,

$n$	Name	Wavelength	Color
—	—	—	—
2	$\alpha$	121.567	UV
3	$\beta$	102.572	UV
4	$\gamma$	97.254	UV
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\infty$	limit	91.175	UV

called *Lyman series of the hydrogen atom*.

Observe that all the Lyman series lies in UV, which is invisible to the naked eye. Due to this fact, this series, while theoretically being the most important, was discovered only second. The first discovery, which was the big one, and the breakthrough, was by Balmer, the founding father of all this, back in 1885, in the visible range, as follows:

FACT 1.2 (Balmer). *The hydrogen atom has spectral lines given by the formula*

$$\frac{1}{\lambda} = R \left( \frac{1}{4} - \frac{1}{n^2} \right)$$

where  $R \simeq 1.097 \times 10^7$  and  $n \geq 3$ , which are as follows,

$n$	Name	Wavelength	Color
—	—	—	—
3	$\alpha$	656.279	red
4	$\beta$	486.135	aqua
5	$\gamma$	434.047	blue
6	$\delta$	410.173	violet
7	$\varepsilon$	397.007	UV
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\infty$	limit	346.600	UV

called *Balmer series of the hydrogen atom*.

So, this was Balmer's original result, which started everything. As a third main result now, this time in IR, due to Paschen in 1908, we have:

FACT 1.3 (Paschen). *The hydrogen atom has spectral lines given by the formula*

$$\frac{1}{\lambda} = R \left( \frac{1}{9} - \frac{1}{n^2} \right)$$

where  $R \simeq 1.097 \times 10^7$  and  $n \geq 4$ , which are as follows,

$n$	Name	Wavelength	Color
—	—	—	—
4	$\alpha$	1875	IR
5	$\beta$	1282	IR
6	$\gamma$	1094	IR
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\infty$	limit	820.4	IR

called *Paschen series of the hydrogen atom*.

Observe the striking similarity between the above three results. In fact, we have here the following fundamental, grand result, due to Rydberg in 1888, based on the Balmer series, and with later contributions by Ritz in 1908, using the Lyman series as well:

CONCLUSION 1.4 (Rydberg, Ritz). *The spectral lines of the hydrogen atom are given by the Rydberg formula, depending on integer parameters  $n_1 < n_2$ ,*

$$\frac{1}{\lambda_{n_1 n_2}} = R \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

with  $R$  being the Rydberg constant for hydrogen, which is as follows:

$$R \simeq 1.096\,775\,83 \times 10^7$$

*These spectral lines combine according to the Ritz-Rydberg principle, as follows:*

$$\frac{1}{\lambda_{n_1 n_2}} + \frac{1}{\lambda_{n_2 n_3}} = \frac{1}{\lambda_{n_1 n_3}}$$

*Similar formulae hold for other atoms, with suitable fine-tunings of  $R$ .*

Here the first part, the Rydberg formula, generalizes the results of Lyman, Balmer, Paschen, which appear at  $n_1 = 1, 2, 3$ , at least retrospectively. The Rydberg formula predicts further spectral lines, appearing at  $n_1 = 4, 5, 6, \dots$ , and these were discovered later, by Brackett in 1922, Pfund in 1924, Humphreys in 1953, and others afterwards,

with all these extra lines being in far IR. The simplified complete table is as follows:

$n_1$	$n_2$	Series name	Wavelength $n_2 = \infty$	Color $n_2 = \infty$
		—	—	
1	$2 - \infty$	Lyman	91.13 nm	UV
2	$3 - \infty$	Balmer	364.51 nm	UV
3	$4 - \infty$	Paschen	820.14 nm	IR
		—	—	
4	$5 - \infty$	Brackett	1458.03 nm	far IR
5	$6 - \infty$	Pfund	2278.17 nm	far IR
6	$7 - \infty$	Humphreys	3280.56 nm	far IR
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Regarding the last assertion, concerning other elements, this is something conjectured and partly verified by Ritz, and fully verified and clarified later, via many experiments, the fine-tuning of  $R$  being basically  $R \rightarrow RZ^2$ , where  $Z$  is the atomic number.

From a theoretical physics viewpoint, the main result remains the middle assertion, called Ritz-Rydberg combination principle, which is something quite puzzling. But this combination principle reminds the formula  $e_{n_1 n_2} e_{n_2 n_3} = e_{n_1 n_3}$  for the usual matrix units  $e_{ij} : e_j \rightarrow e_i$ . Thus, we are in familiar territory here, and we can start dreaming of:

*THOUGHT 1.5. Observables in quantum mechanics should be some sort of infinite matrices, generalizing the Lyman, Balmer, Paschen lines of the hydrogen atom, and multiplying between them as the matrices do, as to produce further observables.*

We will see in a moment that this thought can be made into a theorem.

Now back to more concrete things, as a main problem that we would like to solve, we have the understanding the intimate structure of matter, at the atomic level. There is of course a long story here, regarding the intimate structure of matter, going back centuries and even millennia ago, and our presentation here will be quite simplified. As a starting point, since we need a starting point for all this, let us agree on:

*CLAIM 1.6. Ordinary matter is made of small particles called atoms, with each atom appearing as a mix of even smaller particles, namely protons +, neutrons 0 and electrons -, with the same number of protons + and electrons -.*

As a first observation, this is something which does not look obvious at all, with probably lots of work, by many people, being involved, as to lead to this claim. And so it is. The story goes back to the discovery of charges and electricity, which were attributed to a small particle, the electron -. Now since matter is by default neutral, this naturally leads to the consideration to the proton +, having the same charge as the electron.

But, as a natural question, why should be these electrons  $-$  and protons  $+$  that small? And also, what about the neutron  $0$ ? These are not easy questions, and the fact that it is so came from several clever experiments. Let us first recall that careful experiments with tiny particles are practically impossible. However, all sorts of brutal experiments, such as bombarding matter with other pieces of matter, accelerated to the extremes, or submitting it to huge electric and magnetic fields, do work. And it is such kind of experiments, due to Thomson, Rutherford and others, “peeling off” protons  $+$ , neutrons  $0$  and electrons  $-$  from matter, and observing them, that led to the conclusion that these small beasts  $+, 0, -$  exist indeed, in agreement with Claim 1.6.

So, taking now Claim 1.6 for granted, how are then the atoms organized, as mixtures of protons  $+$ , neutrons  $0$  and electrons  $-$ ? The answer here lies again in the above-mentioned “brutal” experiments of Thomson, Rutherford and others, which not only proved Claim 1.6, but led to an improved version of it, as follows:

CLAIM 1.7. *The atoms are formed by a core of protons  $+$  and neutrons  $0$ , surrounded by a cloud of electrons  $-$ , gravitating around the core.*

This is a considerable advance, because we are now into familiar territory, namely some kind of mechanics. And with this in mind, all the pieces of our puzzle start fitting together, and we are led to the following grand conclusion:

CLAIM 1.8 (Bohr and others). *The atoms are formed by a core of protons and neutrons, surrounded by a cloud of electrons, basically obeying to a modified version of electromagnetism. And with a fine mechanism involved, as follows:*

- (1) *The electrons are free to move only on certain specified elliptic orbits, labelled  $1, 2, 3, \dots$ , situated at certain specific heights.*
- (2) *The electrons can jump or fall between orbits  $n_1 < n_2$ , absorbing or emitting light and heat, that is, electromagnetic waves, as accelerating charges.*
- (3) *The energy of such a wave, coming from  $n_1 \rightarrow n_2$  or  $n_2 \rightarrow n_1$ , is given, via the Planck viewpoint, by the Rydberg formula, applied with  $n_1 < n_2$ .*
- (4) *The simplest such jumps are those observed by Lyman, Balmer, Paschen. And multiple jumps explain the Ritz-Rydberg formula.*

And isn’t this beautiful. Moreover, following now Heisenberg, the next claim is that the underlying mathematics in all the above can lead to a beautiful axiomatization of quantum mechanics, as a “matrix mechanics”, along the lines of Thought 1.5.

Before explaining what Heisenberg was saying, based on Lyman, Balmer, Paschen, namely developing some sort of “matrix mechanics”, let us hear as well the point of view of Schrödinger, which came a few years later. His idea was to forget about exact things, and try to investigate the hydrogen atom statistically. Let us start with:

QUESTION 1.9. *In the context of the hydrogen atom, assuming that the proton is fixed, what is the probability density  $\varphi_t(x)$  of the position of the electron  $e$ , at time  $t$ ,*

$$P_t(e \in V) = \int_V \varphi_t(x) dx$$

*as function of an initial probability density  $\varphi_0(x)$ ? Moreover, can the corresponding equation be solved, and will this prove the Bohr claims for hydrogen, statistically?*

In order to get familiar with this question, let us first look at examples coming from classical mechanics. In the context of a particle whose position at time  $t$  is given by  $x_0 + \gamma(t)$ , the evolution of the probability density will be given by:

$$\varphi_t(x) = \varphi_0(x) + \gamma(t)$$

However, such examples are somewhat trivial, of course not in relation with the computation of  $\gamma$ , usually a difficult question, but in relation with our questions, and do not apply to the electron. The point indeed is that, in what regards the electron, we have:

FACT 1.10. *In respect with various simple interference experiments:*

- (1) *The electron is definitely not a particle in the usual sense.*
- (2) *But in most situations it behaves exactly like a wave.*
- (3) *But in other situations it behaves like a particle.*

Getting back now to the Schrödinger question, all this suggests to use, as for the waves, an amplitude function  $\psi_t(x) \in \mathbb{C}$ , related to the density  $\varphi_t(x) > 0$  by the formula  $\varphi_t(x) = |\psi_t(x)|^2$ . Not that a big deal, you would say, because the two are related by simple formulae as follows, with  $\theta_t(x)$  being an arbitrary phase function:

$$\varphi_t(x) = |\psi_t(x)|^2 \quad , \quad \psi_t(x) = e^{i\theta_t(x)} \sqrt{\varphi_t(x)}$$

However, such manipulations can be crucial, raising for instance the possibility that the amplitude function satisfies some simple equation, while the density itself, maybe not. And this is what happens indeed. Schrödinger was led in this way to:

CLAIM 1.11 (Schrödinger). *In the context of the hydrogen atom, the amplitude function of the electron  $\psi = \psi_t(x)$  is subject to the Schrödinger equation*

$$ih\dot{\psi} = -\frac{h^2}{2m}\Delta\psi + V\psi$$

*$m$  being the mass,  $h = h_0/2\pi$  the reduced Planck constant, and  $V$  the Coulomb potential of the proton. The same holds for movements of the electron under any potential  $V$ .*

Observe the similarity with the wave equation  $\ddot{\varphi} = v^2\Delta\varphi$ , and with the heat equation  $\dot{\varphi} = \alpha\Delta\varphi$  too. Many things can be said here. Following now Heisenberg and Schrödinger, and then especially Dirac, who did the axiomatization work, we have:



DEFINITION 1.12. *In quantum mechanics the states of the system are vectors of a Hilbert space  $H$ , and the observables of the system are linear operators*

$$T : H \rightarrow H$$

*which can be densely defined, and are taken self-adjoint,  $T = T^*$ . The average value of such an observable  $T$ , evaluated on a state  $\xi \in H$ , is given by:*

$$\langle T \rangle = \langle T\xi, \xi \rangle$$

*In the context of the Schrödinger mechanics of the hydrogen atom, the Hilbert space is the space  $H = L^2(\mathbb{R}^3)$  where the wave function  $\psi$  lives, and we have*

$$\langle T \rangle = \int_{\mathbb{R}^3} T(\psi) \cdot \bar{\psi} dx$$

*which is called “sandwiching” formula, with the operators*

$$x \quad , \quad -\frac{i\hbar}{m}\nabla \quad , \quad -i\hbar\nabla \quad , \quad -\frac{\hbar^2\Delta}{2m} \quad , \quad -\frac{\hbar^2\Delta}{2m} + V$$

*representing the position, speed, momentum, kinetic energy, and total energy.*

In other words, we are doing here two things. First, we are declaring by axiom that various “sandwiching” formulae found before by Heisenberg, involving the operators at the end, that we will not get into in detail here, hold true. And second, we are raising the possibility for other quantum mechanical systems, more complicated, to be described as well by the mathematics of the operators on a certain Hilbert space  $H$ , as above.

In order to solve now the hydrogen atom, by using the Schrödinger equation, the idea will be that of reformulating this equation in spherical coordinates. We have:

THEOREM 1.13. *The time-independent Schrödinger equation in spherical coordinates separates, for solutions of type  $\phi = \rho(r)\alpha(s, t)$ , into two equations, as follows,*

$$\begin{aligned} \frac{d}{dr} \left( r^2 \cdot \frac{d\rho}{dr} \right) - \frac{2mr^2}{\hbar^2} (V - E)\rho &= K\rho \\ \sin s \cdot \frac{d}{ds} \left( \sin s \cdot \frac{d\alpha}{ds} \right) + \frac{d^2\alpha}{dt^2} &= -K \sin^2 s \cdot \alpha \end{aligned}$$

*with  $K$  being a constant, called radial equation, and angular equation.*

PROOF. We use the following well-known formula for the Laplace operator in spherical coordinates, whose proof can be found in any geometry or calculus book:

$$\Delta = \frac{1}{r^2} \cdot \frac{d}{dr} \left( r^2 \cdot \frac{d}{dr} \right) + \frac{1}{r^2 \sin s} \cdot \frac{d}{ds} \left( \sin s \cdot \frac{d}{ds} \right) + \frac{1}{r^2 \sin^2 s} \cdot \frac{d^2}{dt^2}$$

By using this formula, the time-independent Schrödinger equation reformulates in spherical coordinates as follows:

$$(V - E)\phi = \frac{\hbar^2}{2m} \left[ \frac{1}{r^2} \cdot \frac{d}{dr} \left( r^2 \cdot \frac{d\phi}{dr} \right) + \frac{1}{r^2 \sin s} \cdot \frac{d}{ds} \left( \sin s \cdot \frac{d\phi}{ds} \right) + \frac{1}{r^2 \sin^2 s} \cdot \frac{d^2\phi}{dt^2} \right]$$

Let us look now for separable solutions for this latter equation, consisting of a radial part and an angular part, as in the statement, namely:

$$\phi(r, s, t) = \rho(r)\alpha(s, t)$$

By plugging this function into our equation, we obtain:

$$(V - E)\rho\alpha = \frac{\hbar^2}{2m} \left[ \frac{\alpha}{r^2} \cdot \frac{d}{dr} \left( r^2 \cdot \frac{d\rho}{dr} \right) + \frac{\rho}{r^2 \sin s} \cdot \frac{d}{ds} \left( \sin s \cdot \frac{d\alpha}{ds} \right) + \frac{\rho}{r^2 \sin^2 s} \cdot \frac{d^2\alpha}{dt^2} \right]$$

By multiplying everything by  $2mr^2/(\hbar^2\rho\alpha)$ , and then moving the radial terms to the left, and the angular terms to the right, this latter equation can be written as follows:

$$\frac{2mr^2}{\hbar^2}(V - E) - \frac{1}{\rho} \cdot \frac{d}{dr} \left( r^2 \cdot \frac{d\rho}{dr} \right) = \frac{1}{\alpha \sin^2 s} \left[ \sin s \cdot \frac{d}{ds} \left( \sin s \cdot \frac{d\alpha}{ds} \right) + \frac{d^2\alpha}{dt^2} \right]$$

Since this latter equation is now separated between radial and angular variables, both sides must be equal to a certain constant  $-K$ , and this gives the result.  $\square$

Let us first study the angular equation. The result here is as follows:

**THEOREM 1.14.** *The separated solutions  $\alpha = \sigma(s)\theta(t)$  of the angular equation,*

$$\sin s \cdot \frac{d}{ds} \left( \sin s \cdot \frac{d\alpha}{ds} \right) + \frac{d^2\alpha}{dt^2} = -K \sin^2 s \cdot \alpha$$

are given by the following formulae, where  $l \in \mathbb{N}$  is such that  $K = l(l + 1)$ ,

$$\sigma(s) = P_l^m(\cos s) \quad , \quad \theta(t) = e^{imt}$$

and where  $m \in \mathbb{Z}$  is a constant, and with  $P_l^m$  being the Legendre function,

$$P_l^m(x) = (-1)^m (1 - x^2)^{m/2} \left( \frac{d}{dx} \right)^m P_l(x)$$

where  $P_l$  are the Legendre polynomials, given by the following formula:

$$P_l(x) = \frac{1}{2^l l!} \left( \frac{d}{dx} \right)^l (x^2 - 1)^l$$

These solutions  $\alpha = \sigma(s)\theta(t)$  are called spherical harmonics.

**PROOF.** This follows indeed from all the above, and with the comment that everything is taken up to linear combinations. We will normalize the wave function later.  $\square$

In order to finish our study, it remains to solve the radial equation, for the Coulomb potential  $V$  of the proton. Let us begin with some generalities, valid for any time-independent potential  $V$ . As a first manipulation on the radial equation, we have:

PROPOSITION 1.15. *The radial equation, written with  $K = l(l + 1)$ ,*

$$(r^2 \rho')' - \frac{2mr^2}{\hbar^2}(V - E)\rho = l(l + 1)\rho$$

takes with  $\rho = u/r$  the following form, called modified radial equation,

$$Eu = -\frac{\hbar^2}{2m} \cdot u'' + \left( V + \frac{\hbar^2 l(l + 1)}{2mr^2} \right) u$$

which is a time-independent 1D Schrödinger equation.

PROOF. With  $\rho = u/r$  as in the statement, we have:

$$\rho = \frac{u}{r} \quad , \quad \rho' = \frac{u'r - u}{r^2} \quad , \quad (r^2 \rho')' = u''r$$

By plugging this data into the radial equation, this becomes:

$$u''r - \frac{2mr}{\hbar^2}(V - E)u = \frac{l(l + 1)}{r} \cdot u$$

By multiplying everything by  $\hbar^2/(2mr)$ , this latter equation becomes:

$$\frac{\hbar^2}{2m} \cdot u'' - (V - E)u = \frac{\hbar^2 l(l + 1)}{2mr^2} \cdot u$$

But this gives the formula in the statement. As for the interpretation, as time-independent 1D Schrödinger equation, this is clear as well, and with the comment here that the term added to the potential  $V$  is some sort of centrifugal term.  $\square$

Getting back now to the Coulomb potential of the proton, we have here:

FACT 1.16. *The Coulomb potential of the hydrogen atom proton, acting on the electron by attraction, is given according to the Coulomb law by*

$$V = -\frac{Kep}{r}$$

where  $p$  is the charge of the proton, and  $K$  is the Coulomb constant. In practice however we have  $p \simeq e$  up to order  $10^{-7}$ , and so our formula can be written as

$$V \simeq -\frac{Ke^2}{r}$$

and we will use this latter formula, and with  $=$  sign, for simplifying.

It remains now to solve the modified radial equation, for this potential  $V$ . And we have here the following result, which proves the original claims by Bohr:

THEOREM 1.17 (Schrödinger). *In the case of the hydrogen atom, where  $V$  is the Coulomb potential of the proton, the modified radial equation, which reads*

$$Eu = -\frac{\hbar^2}{2m} \cdot u'' + \left( -\frac{Ke^2}{r} + \frac{\hbar^2 l(l+1)}{2mr^2} \right) u$$

leads to the Bohr formula for allowed energies,

$$E_n = -\frac{m}{2} \left( \frac{Ke^2}{\hbar} \right)^2 \cdot \frac{1}{n^2}$$

with  $n \in \mathbb{N}$ , the binding energy being

$$E_1 \simeq -2.177 \times 10^{-18}$$

with means  $E_1 \simeq -13.591$  eV.

PROOF. This is again something non-trivial, the idea being as follows:

(1) By dividing our modified radial equation by  $E$ , this becomes:

$$-\frac{\hbar^2}{2mE} \cdot u'' = \left( 1 + \frac{Ke^2}{Er} - \frac{\hbar^2 l(l+1)}{2mEr^2} \right) u$$

In terms of  $\alpha = \sqrt{-2mE}/\hbar$ , this equation takes the following form:

$$\frac{u''}{\alpha^2} = \left( 1 + \frac{Ke^2}{Er} + \frac{l(l+1)}{(\alpha r)^2} \right) u$$

In terms of the new variable  $p = \alpha r$ , this latter equation reads:

$$u'' = \left( 1 + \frac{\alpha Ke^2}{Ep} + \frac{l(l+1)}{p^2} \right) u$$

Now let us introduce a new constant  $S$  for our problem, as follows:

$$S = -\frac{\alpha Ke^2}{E}$$

In terms of this new constant, our equation reads:

$$u'' = \left( 1 - \frac{S}{p} + \frac{l(l+1)}{p^2} \right) u$$

(2) The idea will be that of looking for a solution written as a power series, but before that, we must “peel off” the asymptotic behavior. Which is something that can be done, of course, heuristically. With  $p \rightarrow \infty$  we are led to  $u'' = u$ , and ignoring the solution  $u = e^p$  which blows up, our approximate asymptotic solution is:

$$u \sim e^{-p}$$

Similarly, with  $p \rightarrow 0$  we are led to  $u'' = l(l+1)u/p^2$ , and ignoring the solution  $u = p^{-l}$  which blows up, our approximate asymptotic solution is:

$$u \sim p^{l+1}$$

(3) The above heuristic considerations suggest writing our function  $u$  as follows:

$$u = p^{l+1}e^{-p}v$$

So, let us do this. In terms of  $v$ , we have the following formula:

$$u' = p^l e^{-p} [(l+1-p)v + pv']$$

Differentiating a second time gives the following formula:

$$u'' = p^l e^{-p} \left[ \left( \frac{l(l+1)}{p} - 2l - 2 + p \right) v + 2(l+1-p)v' + pv'' \right]$$

Thus the radial equation, as modified in (1) above, reads:

$$pv'' + 2(l+1-p)v' + (S - 2(l+1))v = 0$$

(4) We will be looking for a solution  $v$  appearing as a power series:

$$v = \sum_{j=0}^{\infty} c_j p^j$$

But our equation leads to the following recurrence formula for the coefficients:

$$c_{j+1} = \frac{2(j+l+1) - S}{(j+1)(j+2l+2)} \cdot c_j$$

(5) We are in principle done, but we still must check that, with this choice for the coefficients  $c_j$ , our solution  $v$ , or rather our solution  $u$ , does not blow up. And the whole point is here. Indeed, at  $j \gg 0$  our recurrence formula reads, approximately:

$$c_{j+1} \simeq \frac{2c_j}{j}$$

But, surprisingly, this leads to  $v \simeq c_0 e^{2p}$ , and so to  $u \simeq c_0 p^{l+1} e^p$ , which blows up.

(6) As a conclusion, the only possibility for  $u$  not to blow up is that where the series defining  $v$  terminates at some point. Thus, we must have for a certain index  $j$ :

$$2(j+l+1) = S$$

In other words, we must have, for a certain integer  $n > l$ :

$$S = 2n$$

(7) We are almost there. Recall from (1) above that  $S$  was defined as follows:

$$S = -\frac{\alpha K e^2}{E} \quad : \quad \alpha = \frac{\sqrt{-2mE}}{h}$$

Thus, we have the following formula for the square of  $S$ :

$$S^2 = \frac{\alpha^2 K^2 e^4}{E^2} = -\frac{2mE}{h^2} \cdot \frac{K^2 e^4}{E^2} = -\frac{2mK^2 e^4}{h^2 E}$$

Now by using the formula  $S = 2n$  from (6), the energy  $E$  must be of the form:

$$E = -\frac{2mK^2 e^4}{h^2 S^2} = -\frac{mK^2 e^4}{2h^2 n^2}$$

Calling this energy  $E_n$ , depending on  $n \in \mathbb{N}$ , we have, as claimed:

$$E_n = -\frac{m}{2} \left( \frac{Ke^2}{h} \right)^2 \cdot \frac{1}{n^2}$$

(8) Thus, we proved the Bohr formula. Regarding numerics, the data is as follows:

$$\begin{aligned} K &= 8.988 \times 10^9 \quad , \quad e = 1.602 \times 10^{-19} \\ h &= 1.055 \times 10^{-34} \quad , \quad m = 9.109 \times 10^{-31} \end{aligned}$$

But this gives the formula of  $E_1$  in the statement. □

As a first remark, all this agrees with the Rydberg formula, due to:

**THEOREM 1.18.** *The Rydberg constant for hydrogen is given by*

$$R = -\frac{E_1}{h_0 c}$$

where  $E_1$  is the Bohr binding energy, and the Rydberg formula itself, namely

$$\frac{1}{\lambda_{n_1 n_2}} = R \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

simply reads, via the energy formula in Theorem 1.23,

$$\frac{1}{\lambda_{n_1 n_2}} = \frac{E_{n_2} - E_{n_1}}{h_0 c}$$

which is in agreement with the Planck formula  $E = h_0 c / \lambda$ .

**PROOF.** Here the first assertion is something numeric, coming from the fact that the formula in the statement gives, when evaluated, the Rydberg constant:

$$R = \frac{-E_1}{h_0 c} = \frac{2.177 \times 10^{-18}}{6.626 \times 10^{-34} \times 2.998 \times 10^8} = 1.096 \times 10^7$$

Regarding now the second assertion, by dividing  $R = -E_1/(h_0 c)$  by any number of type  $n^2$  we obtain, according to the energy convention in Theorem 1.17:

$$\frac{R}{n^2} = -\frac{E_n}{h_0 c}$$

But these are exactly the numbers which are subject to subtraction in the Rydberg formula, and so we are led to the conclusion in the statement. □

### 1b. Periodic table

In order to investigate heavier atoms, we need to know more about hydrogen. So, let us go back to our study of the Schrödinger equation for it. Our conclusions so far are:

**THEOREM 1.19.** *The wave functions of the hydrogen atom are the following functions, labelled by three quantum numbers,  $n, l, m$ ,*

$$\phi_{nlm}(r, s, t) = \rho_{nl}(r)\alpha_l^m(s, t)$$

where  $\rho_{nl}(r) = p^{l+1}e^{-p}v(p)/r$  with  $p = \alpha r$  as before, with the coefficients of  $v$  subject to

$$c_{j+1} = \frac{2(j+l+1-n)}{(j+1)(j+2l+2)} \cdot c_j$$

and  $\alpha_l^m(s, t)$  being the spherical harmonics found before.

**PROOF.** This follows indeed by putting together all the results obtained so far, and with the remark that everything is up to the normalization of the wave function.  $\square$

In what regards the main wave function, that of the ground state, we have:

**THEOREM 1.20.** *With the hydrogen atom in its ground state, the wave function is*

$$\phi_{100}(r, s, t) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$

where  $a = 1/\alpha$  is the inverse of the parameter appearing in our computations above,

$$\alpha = \frac{\sqrt{-2mE}}{h}$$

called Bohr radius of the hydrogen atom. This Bohr radius is given by

$$a = \frac{h^2}{mKe^2}$$

which numerically means  $a \simeq 5.291 \times 10^{-11}$ .

**PROOF.** There are several things going on here, as follows:

(1) According to our formulae above, the parameter  $\alpha$  there is given by:

$$\alpha = \frac{\sqrt{-2mE}}{h} = \frac{1}{h} \cdot m \cdot \frac{Ke^2}{h} = \frac{mKe^2}{h^2}$$

Thus, the inverse  $\alpha = 1/a$  is indeed given by the formula in the statement.

(2) Regarding the wave function, we know from the above that this consists of:

$$\rho_{10}(r) = \frac{2e^{-r/a}}{\sqrt{a^3}} \quad , \quad \alpha_0^0(s, t) = \frac{1}{2\sqrt{\pi}}$$

By making the product, we obtain the formula of  $\phi_{100}$  in the statement.

(3) But this formula of  $\phi_{100}$  shows in particular that the Bohr radius  $a$  is indeed the mean distance between the electron and the proton, in the ground state.

(4) Finally, in what regards the numerics, these are as follows:

$$a = \frac{1.055^2 \times 10^{-68}}{9.109 \times 10^{-31} \times 8.988 \times 10^9 \times 1.602^2 \times 10^{-38}} = 5.297 \times 10^{-11}$$

Thus, we are led to the conclusions in the statement.  $\square$

In order to improve our results, we will need the following standard fact:

PROPOSITION 1.21. *The polynomials  $v(p)$  are given by the formula*

$$v(p) = L_{n-l-1}^{2l+1}(p)$$

where the polynomials on the right, called associated Laguerre polynomials, are given by

$$L_q^p(x) = (-1)^p \left( \frac{d}{dx} \right)^p L_{p+q}(x)$$

with  $L_{p+q}$  being the Laguerre polynomials, given by the following formula:

$$L_q(x) = \frac{e^x}{q!} \left( \frac{d}{dx} \right)^q (e^{-x} x^q)$$

PROOF. The story here is very similar to that of the Legendre polynomials. Consider the Hilbert space  $H = L^2[0, \infty)$ , with the following scalar product on it:

$$\langle f, g \rangle = \int_0^\infty f(x)g(x)e^{-x} dx$$

The orthogonal basis obtained by applying Gram-Schmidt to the Weierstrass basis  $\{x^q\}$  is then formed by the Laguerre polynomials  $\{L_q\}$ , and this gives the results.  $\square$

With the above result in hand, we can now improve our main results, as follows:

THEOREM 1.22. *The wave functions of the hydrogen atom are given by*

$$\phi_{nlm}(r, s, t) = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n(n+l)!}} e^{-r/na} \left(\frac{2r}{na}\right)^l L_{n-l-1}^{2l+1} \left(\frac{2r}{na}\right) \alpha_l^m(s, t)$$

with  $\alpha_l^m(s, t)$  being the spherical harmonics found before.

PROOF. This follows indeed by putting together what we have, and then doing some remaining work, concerning the normalization of the wave function.  $\square$

Let us investigate now the case of arbitrary atoms. We will need some general theory for the many-particle systems in quantum mechanics. Let us start with:



DEFINITION 1.23. *The wave function of a system of electrons  $e_1, \dots, e_Z$ , given by*

$$P_t(e_1 \in V_1, \dots, e_Z \in V_Z) = \int_{V_1 \times \dots \times V_Z} |\psi_t(x_1, \dots, x_Z)|^2 dx$$

*is governed by the Schrödinger equation  $ih\dot{\psi} = \hat{H}\psi$ , with Hamiltonian as follows,*

$$\hat{H} = -\frac{\hbar}{2m} \sum_i \Delta_i + Ke^2 \sum_{i < j} \frac{1}{\|x_i - x_j\|} + V(x_1, \dots, x_Z)$$

*with the middle sum standing for the Coulomb repulsions between them.*

In general, and in fact at any  $Z > 1$ , and so even at  $Z = 2$ , the above Schrödinger equation is pretty much impossible to solve, due to the Coulomb repulsion term, which makes the mathematics extremely complicated. In fact, as an illustrating analogy here, managing that Coulomb repulsion term is more or less the same thing as solving the  $N$ -body problem in classical mechanics, for bodies with equal mass.

We will be interested here in the case of atoms, where  $V$  is the Coulomb attraction potential coming from a  $Ze$  charge. Here the problem to be solved is as follows:

PROBLEM 1.24. *Consider an atom of atomic number  $Z$ , meaning a fixed  $Ze$  charge, surrounded by electrons  $e_1, \dots, e_Z$ . The problem is to solve the Schrödinger equation*

$$ih\dot{\psi} = \hat{H}\psi$$

*with Hamiltonian as follows,*

$$\hat{H} = \sum_i \left( -\frac{\hbar}{2m} \Delta_i - \frac{KZe^2}{\|x_i\|} \right) + Ke^2 \sum_{i < j} \frac{1}{\|x_i - x_j\|}$$

*or at least to understand how  $e_1, \dots, e_Z$  manage to live together, in a stable way.*

A first idea would be of course that of ignoring the right term, Coulomb repulsion. In the simplest case, that of the helium atom, the situation is as follows:

FACT 1.25. *For the helium atom,  $Z = 2$ , ignoring the Coulomb repulsion between electrons leads, via separation of variables, to product wave functions*

$$\phi(x_1, x_2) = \phi'_{n_1 l_1 m_1}(x_1) \phi'_{n_2 l_2 m_2}(x_2)$$

*with the prime signs standing for the doubling  $e \rightarrow 2e$  of the central charge, with energies:*

$$E_{n_1 n_2} = 4(E_{n_1} + E_{n_2})$$

*This model predicts a ground state energy for helium given by*

$$E_0 = 8 \times (-13.6) = -109 \text{ eV}$$

*which is considerably smaller than the observed  $E_0 = -79 \text{ eV}$ .*

Moving ahead, let us focus on a more modest question, that at the end of Problem 1.24, namely understanding how the electrons  $e_1, \dots, e_Z$  manage to live together. Here our method of ignoring the Coulomb repulsion between electrons is not that bad, and for helium for instance, we are led in this way to some interesting conclusions. For instance the excited states of helium must appear as products as follows:

$$\phi_{100}(x_1)\phi_{nlm}(x_2) \quad , \quad \phi_{nlm}(x_1)\phi_{100}(x_2)$$

And this is actually quite close to reality, if we add the particle spin to our discussion. So, speaking now spin, this is indeed something that we ignored so far in the above. And spin is in fact a key component to our problem, because we have:

FACT 1.26 (Pauli exclusion principle). *Two electrons cannot occupy the same quantum numbers  $n, l, m$ , with same spin  $s = \pm 1/2$ .*

We have now all the ingredients for discussing the known atoms, or chemical elements,  $Z = 1, \dots, 118$ . These can be arranged in a table, called periodic table, as follows:

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
1	$\frac{\text{H}}{1}$																	$\frac{\text{He}}{2}$	
2	$\frac{\text{Li}}{3}$	$\frac{\text{Be}}{4}$											$\frac{\text{B}}{5}$	$\frac{\text{C}}{6}$	$\frac{\text{N}}{7}$	$\frac{\text{O}}{8}$	$\frac{\text{F}}{9}$	$\frac{\text{Ne}}{10}$	
3	$\frac{\text{Na}}{11}$	$\frac{\text{Mg}}{12}$											$\frac{\text{Al}}{13}$	$\frac{\text{Si}}{14}$	$\frac{\text{P}}{15}$	$\frac{\text{S}}{16}$	$\frac{\text{Cl}}{17}$	$\frac{\text{Ar}}{18}$	
4	$\frac{\text{K}}{19}$	$\frac{\text{Ca}}{20}$	$\frac{\text{Sc}}{21}$	$\frac{\text{Ti}}{22}$	$\frac{\text{V}}{23}$	$\frac{\text{Cr}}{24}$	$\frac{\text{Mn}}{25}$	$\frac{\text{Fe}}{26}$	$\frac{\text{Co}}{27}$	$\frac{\text{Ni}}{28}$	$\frac{\text{Cu}}{29}$	$\frac{\text{Zn}}{30}$	$\frac{\text{Ga}}{31}$	$\frac{\text{Ge}}{32}$	$\frac{\text{As}}{33}$	$\frac{\text{Se}}{34}$	$\frac{\text{Br}}{35}$	$\frac{\text{Kr}}{36}$	
5	$\frac{\text{Rb}}{37}$	$\frac{\text{Sr}}{38}$	$\frac{\text{Y}}{39}$	$\frac{\text{Zr}}{40}$	$\frac{\text{Nb}}{41}$	$\frac{\text{Mo}}{42}$	$\frac{\text{Tc}}{43}$	$\frac{\text{Ru}}{44}$	$\frac{\text{Rh}}{45}$	$\frac{\text{Pd}}{46}$	$\frac{\text{Ag}}{47}$	$\frac{\text{Cd}}{48}$	$\frac{\text{In}}{49}$	$\frac{\text{Sn}}{50}$	$\frac{\text{Sb}}{51}$	$\frac{\text{Te}}{52}$	$\frac{\text{I}}{53}$	$\frac{\text{Xe}}{54}$	
6	$\frac{\text{Cs}}{55}$	$\frac{\text{Ba}}{56}$	<i>l</i>	$\frac{\text{Lu}}{71}$	$\frac{\text{Hf}}{72}$	$\frac{\text{Ta}}{73}$	$\frac{\text{W}}{74}$	$\frac{\text{Re}}{75}$	$\frac{\text{Os}}{76}$	$\frac{\text{Ir}}{77}$	$\frac{\text{Pt}}{78}$	$\frac{\text{Au}}{79}$	$\frac{\text{Hg}}{80}$	$\frac{\text{Tl}}{81}$	$\frac{\text{Pb}}{82}$	$\frac{\text{Bi}}{83}$	$\frac{\text{Po}}{84}$	$\frac{\text{At}}{85}$	$\frac{\text{Rn}}{86}$
7	$\frac{\text{Fr}}{87}$	$\frac{\text{Ra}}{88}$	<i>a</i>	$\frac{\text{Lr}}{103}$	$\frac{\text{Rf}}{104}$	$\frac{\text{Db}}{105}$	$\frac{\text{Sg}}{106}$	$\frac{\text{Bh}}{107}$	$\frac{\text{Hs}}{108}$	$\frac{\text{Mt}}{109}$	$\frac{\text{Ds}}{110}$	$\frac{\text{Rg}}{111}$	$\frac{\text{Cn}}{112}$	$\frac{\text{Nh}}{113}$	$\frac{\text{Fl}}{114}$	$\frac{\text{Mc}}{115}$	$\frac{\text{Lv}}{116}$	$\frac{\text{Ts}}{117}$	$\frac{\text{Og}}{118}$
			<i>l</i> :	$\frac{\text{La}}{57}$	$\frac{\text{Ce}}{58}$	$\frac{\text{Pr}}{59}$	$\frac{\text{Nd}}{60}$	$\frac{\text{Pm}}{61}$	$\frac{\text{Sm}}{62}$	$\frac{\text{Eu}}{63}$	$\frac{\text{Gd}}{64}$	$\frac{\text{Tb}}{65}$	$\frac{\text{Dy}}{66}$	$\frac{\text{Ho}}{67}$	$\frac{\text{Er}}{68}$	$\frac{\text{Tm}}{69}$	$\frac{\text{Yb}}{70}$		
			<i>a</i> :	$\frac{\text{Ac}}{89}$	$\frac{\text{Th}}{90}$	$\frac{\text{Pa}}{91}$	$\frac{\text{U}}{92}$	$\frac{\text{Np}}{93}$	$\frac{\text{Pu}}{94}$	$\frac{\text{Am}}{95}$	$\frac{\text{Cm}}{96}$	$\frac{\text{Bk}}{97}$	$\frac{\text{Cf}}{98}$	$\frac{\text{Es}}{99}$	$\frac{\text{Fm}}{100}$	$\frac{\text{Md}}{101}$	$\frac{\text{No}}{102}$		

Here the horizontal parameter  $1, \dots, 18$  is called the group, and the vertical parameter  $1, \dots, 7$  is called the period. The two bottom rows consist of lanthanum  $_{57}\text{La}$  and its followers, called lanthanides, and of actinium  $_{89}\text{Ac}$  and its followers, called actinides.

Here are the elements up to krypton  ${}_{36}\text{Kr}$ , absolutely needed for everything:

DEFINITION 1.27. *The elements up to krypton  ${}_{36}\text{Kr}$  are as follows:*

- (1) *Hydrogen  ${}_{1}\text{H}$ , helium  ${}_{2}\text{He}$ .*
- (2) *Lithium  ${}_{3}\text{Li}$ , beryllium  ${}_{4}\text{Be}$ , boron  ${}_{5}\text{B}$ , carbon  ${}_{6}\text{C}$ , nitrogen  ${}_{7}\text{N}$ , oxygen  ${}_{8}\text{O}$ , fluorine  ${}_{9}\text{F}$ , neon  ${}_{10}\text{Ne}$ .*
- (3) *Sodium  ${}_{11}\text{Na}$ , magnesium  ${}_{12}\text{Mg}$ , aluminium  ${}_{13}\text{Al}$ , silicon  ${}_{14}\text{Si}$ , phosphorus  ${}_{15}\text{P}$ , sulfur  ${}_{16}\text{S}$ , chlorine  ${}_{17}\text{Cl}$ , argon  ${}_{18}\text{Ar}$ .*
- (4) *Potassium  ${}_{19}\text{K}$ , calcium  ${}_{20}\text{Ca}$ , scandium  ${}_{21}\text{Sc}$ , titanium  ${}_{22}\text{Ti}$ , vanadium  ${}_{23}\text{V}$ , chromium  ${}_{24}\text{Cr}$ , manganese  ${}_{25}\text{Mn}$ , iron  ${}_{26}\text{Fe}$ , cobalt  ${}_{27}\text{Co}$ .*
- (5) *Nickel  ${}_{28}\text{Ni}$ , copper  ${}_{29}\text{Cu}$ , zinc  ${}_{30}\text{Zn}$ , gallium  ${}_{31}\text{Ga}$ , germanium  ${}_{32}\text{Ge}$ , arsenic  ${}_{33}\text{As}$ , selenium  ${}_{34}\text{Se}$ , bromine  ${}_{35}\text{Br}$ , krypton  ${}_{36}\text{Kr}$ .*

In what regards the elements heavier than krypton  ${}_{36}\text{Kr}$ , it is heartbreaking to sort them out, but as a useful complement to the above list, we have:

FACT 1.28. *Remarkable elements heavier than krypton  ${}_{36}\text{Kr}$  include:*

- (1) *Noble gases: xenon  ${}_{54}\text{Xe}$ , radon  ${}_{86}\text{Rn}$ .*
- (2) *Noble metals: silver  ${}_{47}\text{Ag}$ , iridium  ${}_{77}\text{Ir}$ , platinum  ${}_{78}\text{Pt}$ , gold  ${}_{47}\text{Au}$ .*
- (3) *Heavy metals: mercury  ${}_{80}\text{Hg}$ , lead  ${}_{82}\text{Pb}$ .*
- (4) *Radioactive: polonium  ${}_{84}\text{Po}$ , radium  ${}_{88}\text{Ra}$ , uranium  ${}_{92}\text{U}$ , plutonium  ${}_{94}\text{Pu}$ .*
- (5) *Miscellaneous: rubidium  ${}_{37}\text{Rb}$ , strontium  ${}_{38}\text{Sr}$ , molybdenum  ${}_{42}\text{Mo}$ , technetium  ${}_{43}\text{Tc}$ , cadmium  ${}_{48}\text{Cd}$ , tin  ${}_{50}\text{Sn}$ , iodine  ${}_{53}\text{I}$ , caesium  ${}_{55}\text{Cs}$ , tungsten  ${}_{74}\text{Tu}$ , bismuth  ${}_{83}\text{Bi}$ , francium  ${}_{87}\text{Fr}$ , americium  ${}_{95}\text{Am}$ .*

Here the noble gases in (1) normally include oganesson  ${}_{118}\text{Og}$  as well. The noble metals in (2) are something subjective. There are of course plenty of other heavy metals (3), or radioactive elements (4). As for the list in (5), this is something subjective, basically a mixture of well-known metals used in engineering, and some well-known bad guys in the context of nuclear fallout. Technetium  ${}_{43}\text{Tc}$  is a bizarre element, human-made.

In relation with quantum mechanics, we have here:

FACT 1.29. *For the element having atomic number  $Z$ , the electrons will occupy successively the various positions with quantum numbers  $n, l, m \in \mathbb{N}$  and spin  $s = \pm 1/2$ , such as the total binding energy to be minimal. In practice, the period  $1, \dots, 7$  corresponds to the highest  $n$  occupied, and the group  $1, \dots, 18$  comes from  $l, m, s$ .*

This is of course something very basic, and there is a detailed analysis to be done afterwards, for  $Z = 1, \dots, 118$ . For the elements up to krypton  ${}_{36}\text{Kr}$ , the list of electron configurations can be found for instance in Feynman [33] or Griffiths [44].

### 1c. Isotopes, ionization

Isotopes, ionization.

**1d. Chemistry, molecules**

Chemistry, molecules.

**1e. Exercises**

Exercises:

EXERCISE 1.30.

EXERCISE 1.31.

EXERCISE 1.32.

EXERCISE 1.33.

EXERCISE 1.34.

EXERCISE 1.35.

EXERCISE 1.36.

EXERCISE 1.37.

Bonus exercise.

## CHAPTER 2

### States of matter

#### 2a. Ideal gases

In order to get started with states of matter, we must first talk about gases. Things however are quite tricky here, and leaving aside excessive rigor, which does not fit well with thermodynamics, let us start with the following basic fact, which was the beginning of everything, going back to work of Boyle, Charles, Avogadro, Gay-Lussac, Clapeyron and others from the 17th, 18th and 19th centuries, and with final touches from Maxwell, Boltzmann, Gibbs and others, in the late 19th and early 20th centuries:

FACT 2.1. *The ideal gases satisfy the equation  $PV = kT$ , where:*

- (1)  *$V$  is the volume of the gas, independently of the shape of the container used.*
- (2)  *$P$  is the pressure of the gas, measured with a manometer.*
- (3)  *$T$  is the temperature of the gas, measured with a thermometer.*
- (4)  *$k$  is a constant, depending on the gas.*

*That is,  $PV = kT$  basically tells us that “pressure and temperature are the same thing”.*

At the first glance, for instance if you are a mathematician not used to this, this looks more like a joke. Why not defining then  $P = T$  or vice-versa, you would say, and what is the point with that long list of distinguished gentlemen having worked hard on this.

Error. The point indeed comes from the following:

EXPLANATION 2.2. *In the equation of state  $PV = kT$ , as formulated above, the pressure  $P$  and the temperature  $T$  appear more precisely as follows,*

- (1) *The manometer read comes from the gas molecules pushing a piston, so  $P$  is a statistical quantity, coming from the statistics of the molecular speeds,*
- (2) *The thermometer read is something even more complicated, and  $T$  is as well a statistical quantity, coming from the statistics of the molecular speeds,*

*so  $PV = kT$  is something non-trivial, telling us that the mathematical machinery producing  $P, T$ , via manometer and thermometer, out of the molecular speeds, is the same.*

Hope you got my point, and getting back now to historical details, Boyle, Charles, Avogadro, Gay-Lussac, Clapeyron, joined by Clausius, Carnot, Joule, Lord Kelvin and others, first observed  $PV = kT$ , and then reached to a good understanding of what this means, via an axiomatization of  $P$  and  $T$ . Later Maxwell started to look into the

molecular speeds and their statistics, then Boltzmann came with a tough mathematical computation, proving  $PV = kT$ , and then, even later, Gibbs and others further built on all this, by formalizing modern thermodynamics, in the form that is still used today.

But probably too much talking, let us get to work. As a first result now, dealing with pressure only, and for the gases without collisions between molecules, we have:

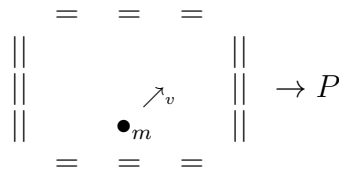
**THEOREM 2.3.** *The pressure  $P$ , volume  $V$  and total kinetic energy  $K$  of a gas, having point molecules, with no collisions between them, satisfy*

$$PV = \frac{2K}{d}$$

where  $d = 1, 2, 3$  is the dimensionality of the gas,  $d = 3$  for usual 3D gases.

**PROOF.** We can do this in several steps, as follows:

(1) Let us first assume that the gas is enclosed in a cubic volume,  $V = L^3$ . We want to compute the pressure  $P$  on the right wall. Since there are no collisions, we can assume by linearity that our gas has 1 molecule, having mass  $m$  and travelling at speed  $v$ . We must compute the pressure  $P$  exerted by this molecule on the right wall:



(2) We first look at a 1D gas. Our molecule hits the right wall at every  $\Delta t = 2L/v$  interval, with its change of momentum being  $\Delta p = 2mv$ . We obtain, as desired:

$$P = \frac{F}{L^2} = \frac{\Delta p}{L^2 \Delta t} = \frac{2mv}{L^2 \cdot 2L/v} = \frac{mv^2}{L^3} = \frac{2K}{V}$$

(3) In the case of a  $d$ -dimensional gas, exactly the same computation takes place, but this time with  $v$  being replaced by its horizontal component  $v_1$ . Thus, we have:

$$P = \frac{mv_1^2}{V}$$

But, we have the following formula, with the equality on the right being understood in a statistical sense, our molecule being assumed to follow a random direction:

$$\|v\|^2 = v_1^2 + \dots + v_d^2 = dv_1^2$$

Thus, the pressure in this case is given by the following formula, as desired:

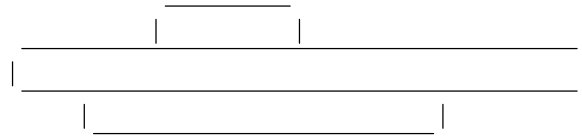
$$P = \frac{m\|v\|^2}{dV} = \frac{2K}{dV}$$

(4) It remains to extend our result to arbitrary volume shapes. For this purpose, let us first redo the above computations for a parallelepiped,  $V = L_1L_2L_3$ . Here the above 1D gas computation carries on, and gives the same result, as follows:

$$P = \frac{F}{L_2L_3} = \frac{\Delta p}{L_2L_3\Delta t} = \frac{2mv}{L_2L_3 \cdot 2L_1/v} = \frac{mv^2}{L_1L_2L_3} = \frac{2K}{V}$$

Thus the  $d$ -dimensional computation carries on too, and gives the result.

(5) In order now to reach to arbitrary shapes, the idea will be that of stacking thin parallelepipeds, best approximating the shape that we have in mind, as follows:



(6) But for this purpose it is better to drop our assumption that the gas has 1 molecule, and use  $N$  molecules instead. With  $\rho = N/V$  being the molecular density, and  $K_0$  being the kinetic energy of a single molecule, our computation in (4) for the parallelepiped, with now  $N$  molecules instead of 1, reformulates as follows:

$$P = \frac{2K}{dV} = \frac{2NK_0}{dV} = \frac{2\rho VK_0}{dV} = \frac{2\rho K_0}{d}$$

(7) But this latter formula shows that the pressure has nothing to do with the precise volume  $V$ , but just with the molecular density  $\rho = N/V$ . Thus, we can stack indeed parallelepipeds, with of course the assumption that  $\rho$  is constant over these parallelepipeds, and we obtain that the above formula holds for an arbitrary volume shape  $V$ :

$$P = \frac{2\rho K_0}{d}$$

Now by getting back to the volume  $V$ , we obtain the following formula:

$$P = \frac{2\rho K_0}{d} = \frac{2NK_0}{dV} = \frac{2K}{dV}$$

Thus, we are led to the conclusion in the statement.  $\square$

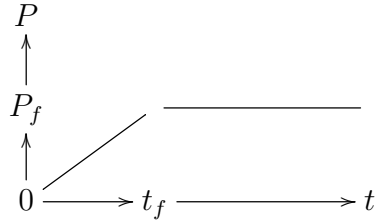
Observe that, when carefully looking at the above proof, and more specifically at step (3), we can see that pressure  $P$  is not something instantaneous, but rather something statistical. Which is of course in tune with our experience, from the real life.

In short, pressure reading is not instantaneous, and we have the following result:

**THEOREM 2.4.** *In the context of a gas consisting of point molecules, with no collisions between them, the correct time for reading the correct pressure is*

$$t_f = \frac{2\sqrt{d}V^{1/3}}{\|v\|} \quad : \quad P_f = \frac{2K}{dV}$$

with  $\|v\|$  being the average molecular speed, with the precise pressure reading being



and with this being taken in an approximate, statistical sense.

**PROOF.** We can do this in two steps, as follows:

(1) Let us first look at a 1D gas. We can assume that we are in a cubic container,  $V = L^3$ , and we know that each molecule  $i$  hits the right wall, where  $P$  is measured, at  $\Delta t_i = 2L/|v_i|$  intervals. But with this picture in hand, it is quite clear that, on average, the pressure reading process will be linear, starting from  $P = 0$ , up to time  $t_f = 2L/|v|$ , with  $|v|$  being the average molecular speed, where the correct pressure  $P_f = 2K/V$  will be read, and constant at  $P_f$  afterwards. Now since  $L = V^{1/3}$ , this gives, as desired:

$$t_f = \frac{2V^{1/3}}{|v|} \quad : \quad P_f = \frac{2K}{V}$$

(2) In the general case now, that of a  $d$ -dimensional gas, with  $d = 1, 2, 3$ , the same argument carries on, with the only change being that each molecular speed  $v_i \in \mathbb{R}^d$  is now replaced by its horizontal component  $v_{i1} \in \mathbb{R}$ , which by statistical reasons has squared magnitude as follows, as explained in the proof of Theorem 2.3:

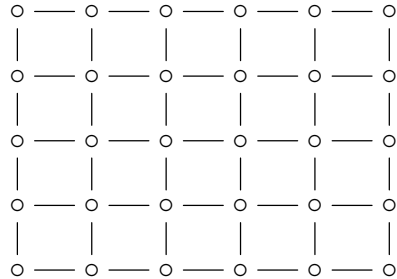
$$v_{i1}^2 = \|v_i\|^2/d$$

Thus, with respect to (1), the correct final pressure must be adjusted by a  $d$  factor, and becomes  $P_f = 2K/dV$ , as in Theorem 2.3. As for the correct reading time, this must be adjusted by a  $\sqrt{d}$  factor, and becomes  $t_f = 2\sqrt{d}V^{1/3}/\|v\|$ , as claimed.  $\square$

Getting back now to our lattice model questions, the above results, dealing with pressure  $P$  only, are quite interesting, and suggest doing a number of things. For instance,



we can focus on the piston surface, and model it with a square grid, as follows:



The point indeed is that what happens on the piston surface is some sort of “game” between the gas and the piston, reminding board games or arcade games, with the gas pushing here and there, with this or that speed, from time to time, and with the piston itself recording all these impulses, and converting them, via some mathematics, into pressure  $P$ . And this type of “game” can be obviously modelled on a grid, as above.

Along the same lines, a more complicated question is that of getting to 3D, with a lattice model for the whole gas, in the form of small 3D cubes constantly changing their status, depending on their neighbors. Note that this reminds a bit Conway’s Game of Life, and also, importantly, that we can model as well internal collisions, in this way.

Speaking collisions between the gas molecules, at a more advanced level now, dealing with the internal mechanism of the  $PV = kT$  formula, we have:

**THEOREM 2.5** (Maxwell, Boltzmann). *The molecular speeds  $v \in \mathbb{R}^3$  of a gas in thermal equilibrium are subject to the Maxwell-Boltzmann distribution formula*

$$P(v) = \left(\frac{m}{2\pi bT}\right)^{3/2} \exp\left(-\frac{m\|v\|^2}{2bT}\right)$$

with  $m$  being the mass of the molecules, and  $b$  being the Boltzmann constant.

**PROOF.** As before with other things, this is something in between fact and theorem. Maxwell came upon it as a fact, or perhaps as a sort of pseudo-theorem, and a bit later Boltzmann came with a proof. In what follows we will present the original argument of Maxwell, then briefly discuss Boltzmann’s proof. Here is Maxwell’s argument:

(1) We are looking for the precise probability distribution  $P$  of the molecular speeds  $v = (v_1, v_2, v_3)$  which makes the mechanics of gases work. Intuition tells us that  $P$  has no correlations between the  $x, y, z$  directions of space, and so we must have:

$$P(v) = f(v_1)g(v_2)h(v_3)$$

Moreover, by rotational symmetry the functions  $f, g, h$  must coincide, and so:

$$P(v) = f(v_1)f(v_2)f(v_3)$$

(2) Further thinking, again invoking rotational symmetry, leads to the conclusion that  $P(v)$  must depend only on the magnitude  $\|v\|$  of the velocity  $v \in \mathbb{R}^3$ , and not on the direction. Thus, we must have as well a formula of the following type:

$$P(v) = \varphi(\|v\|^2)$$

(3) Now by comparing the requirements in (1) and (2), we are led via some math to the conclusion that  $\varphi$  must be an exponential, which amounts in saying that:

$$P(v) = \lambda \exp(-C\|v\|^2)$$

(4) Obviously we must have  $C > 0$ , for things to be bounded, and then by integrating we can obtain  $\lambda$  as function of  $C$ , and our formula becomes:

$$P(v) = \left(\frac{C}{\pi}\right)^{3/2} \exp(-C\|v\|^2)$$

(5) It remains to find the value of  $C > 0$ . But for this purpose, observe that, now that we have our distribution, be that still depending on  $C > 0$ , we can compute everything that we want to, just by integrating. In particular, we find that on average:

$$v_1^2 = v_2^2 = v_3^2 = \frac{1}{2C}$$

Thus the average magnitude of the molecular speed is given by:

$$\|v\| = \frac{3}{2C}$$

It follows that the average kinetic energy of the molecules is:

$$K_0 = \frac{m\|v\|^2}{2} = \frac{3m}{4C}$$

(6) On the other hand, recall from our discussions above that one of the many equivalent formulations of  $PV = kT$ , using  $PV = 2K/3$ , was as follows:

$$\frac{2K_0}{3} = bT$$

Thus we obtain  $m/(2C) = bT$ , and so  $C = m/(2bT)$ , as desired.

(7) Observe that the above proof has in fact little physical content, with the whole thing being basically obtained by using  $PV = 2K/3$ , which is a mathematical theorem, then  $PV = kT$ , which is a crucial physics fact, and finally by invoking several times a number of clever symmetry arguments, and doing some calculus.

(8) However, Boltzmann came later with a more rigorous argument, fully establishing the above formula, via detailed computations in relation with the internal collisions.  $\square$

So long for basic thermodynamics. As before, an interesting question is that of coming up with a 3D lattice model for the gas, in the form of small 3D cubes constantly changing their status, depending on their neighbors, a bit like in Conway's Game of Life.

## 2b. Van der Waals gases

Going now towards more advanced thermodynamics, and states of matter, our scope will be quite broad, because we would like to talk about all sorts of matter, solid, liquid or gaseous, with a look into the extremes  $T \rightarrow 0$  and  $T \gg 0$  too, where other forms of matter appear, and finally with our matter being as 3D as possible, with this meaning occupying a precise body  $B \subset \mathbb{R}^3$ , instead of just a volume  $V = \text{vol}(B) \in \mathbb{R}$ .

In order to discuss this, we first need to talk about work, motivated by:

QUESTIONS 2.6. *What is the work done by a gas pushing a piston? What about the work done by a gas evolving on a path  $\gamma$ , in the state space  $f(P, V, T) = 0$ ?*

In order to answer this question, we will need some mathematics. Assume that we have a path in  $\mathbb{R}^3$ , which can be thought of as corresponding to a function as follows:

$$\gamma : [0, 1] \rightarrow \mathbb{R}^3$$

Observe that this function  $\gamma$  is not exactly the path itself, for instance because the functions  $r \rightarrow \gamma(r^2)$ , or  $r \rightarrow \gamma(1 - r)$ , and so on, produce the same path, parametrized differently. Our claim now is that we can talk about integrals as follows, with  $f, g, h : \mathbb{R}^3 \rightarrow \mathbb{R}$ , which are independent on the chosen parametrization of our path:

$$I = \int_{\gamma} f(x)dx_1 + g(x)dx_2 + h(x)dx_3$$

Indeed, by using the obvious symmetry between the coordinates  $x_1, x_2, x_3$ , in order to construct such integrals, we just need to construct integrals of the following type:

$$J = \int_{\gamma} f(x)dx_1$$

But here, by thinking infinitesimally, we can assume that our path  $\gamma = (\gamma_1, \gamma_2, \gamma_3)$  has the property that its first component  $\gamma_1 : [0, 1] \rightarrow \mathbb{R}$  is increasing, or decreasing, and so is bijective on its image  $\gamma_1[0, 1] = [a, b]$ . Thus, we can reparametrize our path in terms of the first coordinate  $x_1$ , with the help of some functions  $\varphi, \psi$ , as follows:

$$\gamma(x_1) = (x_1, \varphi(x_1), \psi(x_1))$$

And, with this convention made, we can define our contour integral, or rather its first component, as explained above, as a usual one-variable integral, as follows:

$$J = \int_a^b f(x_1, \varphi(x_1), \psi(x_1))dx_1$$

Thus, we have our definition for the contour integrals, and some easy mathematics does rest, such as filling the small gaps in the above construction, and also proving that these contour integrals do not depend on the choice of the parametrization  $\gamma$ .

More concretely now, let us temporarily forget about the paths  $\gamma$ , and have a look at the quantities which are to be integrated, namely:

$$\alpha = f(x)dx_1 + g(x)dx_2 + h(x)dx_3$$

Obviously, these are something rather mathematical, and many things can be said here. However, we can have some physical intuition on them. Assume indeed that we are given a function as follows, that you can think for instance as corresponding to an external force, with  $F(x) \in \mathbb{R}^3$  being the force vector applied at a given point  $x \in \mathbb{R}^3$ :

$$F : \mathbb{R}^3 \rightarrow \mathbb{R}^3$$

By writing  $F = (F_1, F_2, F_3)$ , we can then consider the following quantity, and when  $F : \mathbb{R}^3 \rightarrow \mathbb{R}^3$  varies, we obtain exactly the abstract quantities  $\alpha$  considered above:

$$\langle F(x), dx \rangle = F_1(x)dx_1 + F_2(x)dx_2 + F_3(x)dx_3$$

Thus, all in all, what we have done in the above with our construction of contour integrals, was to define quantities as follows, with  $\gamma$  being a path in  $\mathbb{R}^3$ , and with  $F : \mathbb{R}^3 \rightarrow \mathbb{R}^3$  being a certain function, that we can think of, if we want, as being a force:

$$I = \int_{\gamma} \langle F(x), dx \rangle$$

Which brings us into physics. Indeed, by assuming now that  $F : \mathbb{R}^3 \rightarrow \mathbb{R}^3$  does correspond to a force, we can formulate the following definition:

**DEFINITION 2.7.** *The work done by a force  $F = F(x)$  for moving a particle from point  $p \in \mathbb{R}^3$  to point  $q \in \mathbb{R}^3$  via a given path  $\gamma : p \rightarrow q$  is the following quantity:*

$$W(\gamma) = \int_{\gamma} \langle F(x), dx \rangle$$

*We say that  $F$  is conservative if this work quantity  $W(\gamma)$  does not depend on the chosen path  $\gamma : p \rightarrow q$ , and in this case we denote this quantity by  $W(p, q)$ .*

Now back to gases, we want to compute the work  $W$  done by a gas, pushing a piston. This work is quite easy to compute, and we are led to the following statement:

**PROPOSITION 2.8.** *The mechanical work done by a gas pushing a piston is*

$$W = \int_a^b PdV$$

*where  $[a, b]$  is the interval where the piston has travelled.*

PROOF. In order to compute mechanical work  $W$  done by the gas, observe that, infinitesimally, if we denote by  $dl$  the distance travelled by the piston in time  $dt$ , we have the following formula, with  $S$  being the area of the piston:

$$dW = Fdl = PSdl = Pd(Sl) = PdV$$

Here we have used the standard interpretation of the pressure  $P$ , as explained before. Now assuming that the piston has travelled from  $a$  to  $b$ , we obtain:

$$W = \int_a^b dW = \int_a^b PdV$$

Thus, we are led to the formula in the statement.  $\square$

Obviously what we have above is a general formula, which will hold in more general situations, not necessarily involving a container with a piston. So, let us formulate:

**THEOREM 2.9.** *The mechanical work done by a gas evolving on a path  $\gamma$ , in the state space  $f(P, V, T) = 0$ , is given by:*

$$W_\gamma = \int_\gamma PdV$$

When representing the transformation  $\gamma$  as a one-variable function  $P = \varphi(V)$ , with  $T$  being determined at each moment by  $f(P, V, T) = 0$ , this formula reads

$$W_\gamma = \int_{V_0}^{V_1} \varphi(V)dV$$

with  $V_0$  being the initial volume, and  $V_1$  being the final volume.

PROOF. This is quite clear from the previous discussion, involving the cylinder with a piston, the argument there carrying on to the general case without problems, and giving the first formula. As for the second formula, this follows from it, with again the case of the cylinder with a piston being a good illustration,  $\varphi$  being there linear.  $\square$

In order to discuss now examples, let us introduce as well the following notions:

**DEFINITION 2.10.** *A transformation of a gas is called:*

- (1) *Isobaric, if  $P$  is constant.*
- (2) *Isochoric, if  $V$  is constant.*
- (3) *Isothermal, if  $T$  is constant.*

Here all terminology comes from Greek, with isos meaning equal, baros meaning weight, chora meaning space, and therme meaning heat. In what regards the isochoric transformations, some authors, including Fermi [30], use the convention that this means  $W = 0$ , which is not the same as  $V$  being constant. Finally, there is as well a 4th class of transformations, the adiabatic ones, coming from the Greek adiabatos, meaning impassable. These latter transformations are the scary ones, and more on them later.

As an illustration for Theorem 2.9, for an ideal gas, we have the following result:

**THEOREM 2.11.** *For an ideal gas,  $PV = kT$ , isothermally expanding, we have*

$$W = T \log \frac{V_1}{V_0}$$

where  $V_0$  is the initial volume, and  $V_1$  is the final volume.

**PROOF.** This follows indeed from Theorem 2.8, in either formulation:

(1) With the first formula the work is readily computed, as follows:

$$W = \int_{\gamma} PdV = kT \int_{\gamma} \frac{dV}{V} = T \log \frac{V_1}{V_0}$$

(2) With the second formulation, since we have  $PV = kT$  by the equation of state, and  $T$  constant by assumption, the transformation is given by  $\varphi(V) = kT/V$ , and so:

$$W = \int_{V_0}^{V_1} \frac{kT}{V} dV = kT \int_{V_0}^{V_1} \frac{dV}{V} = T \log \frac{V_1}{V_0}$$

Thus, we are led to the conclusions in the statement. □

Finally, the first law of thermodynamics invites us to introduce, as a complement to the various elementary notions from Definition 2.10:

**DEFINITION 2.12.** *A transformation is called adiabatic if:*

$$Q = 0$$

*Equivalently, we must have the energy conservation law  $\Delta E = -W$ .*

Obviously, this is something a bit complicated. As basic examples here we have the transformations of the thermally insulated systems obeying to  $Q = C\Delta T$ , with  $C > 0$ . As an important result about adiabatics, regarding the ideal gases, we have:

**THEOREM 2.13.** *The adiabatic transformations of an ideal gas,  $PV = kT$ , satisfy*

$$TV^{K-1} = \text{constant}$$

where  $K$  is a modified version of  $k$ , appearing as follows:

$$K = \frac{C_P}{C_V} = 1 + \frac{k}{C_V}$$

Together with  $PV = kT$ , the above equation produces certain curves, called adiabatics.

**PROOF.** We use here the Joule formula  $C_V dT + PdV = dE$ . Since for an adiabatic transformation we have  $dE = 0$ , the Joule formula becomes:

$$C_V dT + PdV = 0$$

Now by using  $PV = kT$ , we successively obtain:

$$\begin{aligned}
 PV = kT &\implies C_V dT + \frac{kT}{V} dV = 0 \\
 &\implies \frac{dT}{T} + \frac{k}{C_V} \cdot \frac{dV}{V} = 0 \\
 &\implies \log T + \frac{k}{C_V} \log V = \text{constant} \\
 &\implies TV^{k/C_V} = \text{constant}
 \end{aligned}$$

Thus, we are led to the conclusion in the statement.  $\square$

All the above theory concerns the ideal gases, but in practice, things are more complicated than this. The key result here, due to Van der Waals, is as follows:

**THEOREM 2.14.** *Beyond the ideal gas setting, stating that we should have  $PV = kT$ , the gases are subject to the Van der Waals equation*

$$\left(P + \frac{\alpha}{V^2}\right)(V - \beta) = kT$$

depending on two parameters  $\alpha, \beta > 0$ .

**PROOF.** This is something quite tricky, with the correction parameters  $\alpha, \beta > 0$  appearing from a detailed study of the gas, from a kinetic viewpoint. It is possible of course to specify the parameters  $\alpha, \beta > 0$ , via various lists and tables, and even make some speculations on the precise meaning of these two parameters, using basic chemistry.  $\square$

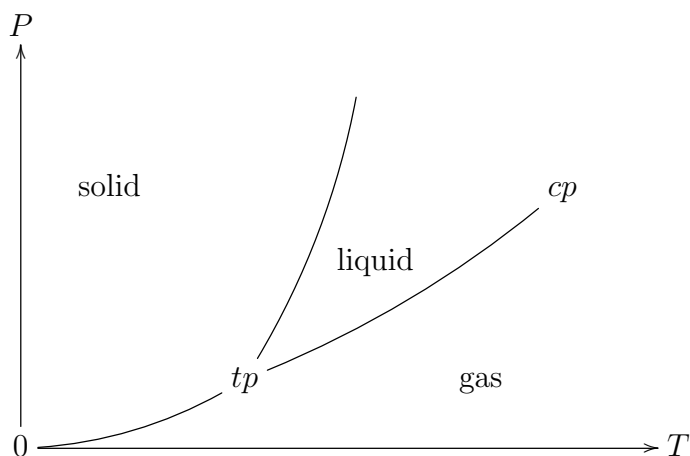
The above result is of key importance, and takes us into rethinking everything that we know about the ideal gases, which must be replaced with Van der Waals gases, at the advanced level. Among the main consequences of this replacement, the isobars, isochores, isothermals and adiabatics of the ideal gases, given by simple formulae, must be replaced by isobars, isochores, isothermals and adiabatics for the Van der Waals gases, which are no longer something trivial, with some interesting math being now involved.

Among others, the study of the Van der Waals gases makes appear some interesting points on the isothermals, called triple and critical points of the gas.

## 2c. States of matter

The results that we obtained so far about gases, via simple mathematics, make the connection with the general theory of matter, which can be summarized as follows:

FACT 2.15. *Ordinary matter appears in 3 forms, namely solid, liquid and gaseous, roughly appearing according to the following generic diagram*



*with  $tp, cp$  standing for the triple and critical points. Also, at low or high temperatures we have interesting phenomena like Bose-Einstein condensation, and plasma.*

All this is extremely interesting, and as already mentioned above, part of it simply comes by looking at the Van der Waals gases, with elementary mathematical tools.

## 2d. Solids and fluids

Solids and fluids.

### 2e. Exercises

Exercises:

EXERCISE 2.16.

EXERCISE 2.17.

EXERCISE 2.18.

EXERCISE 2.19.

EXERCISE 2.20.

EXERCISE 2.21.

EXERCISE 2.22.

EXERCISE 2.23.

Bonus exercise.



## CHAPTER 3

### Liquid state

#### 3a. Liquid state

3b.

3c.

3d.

#### 3e. Exercises

Exercises:

EXERCISE 3.1.

EXERCISE 3.2.

EXERCISE 3.3.

EXERCISE 3.4.

EXERCISE 3.5.

EXERCISE 3.6.

EXERCISE 3.7.

EXERCISE 3.8.

Bonus exercise.



## CHAPTER 4

### Static fluids

#### 4a. Static fluids

4b.

4c.

4d.

#### 4e. Exercises

Exercises:

EXERCISE 4.1.

EXERCISE 4.2.

EXERCISE 4.3.

EXERCISE 4.4.

EXERCISE 4.5.

EXERCISE 4.6.

EXERCISE 4.7.

EXERCISE 4.8.

Bonus exercise.



## Part II

# Math, equations

*No, I won't be afraid  
Oh, I won't be afraid  
Just as long as you stand  
Stand by me*

## CHAPTER 5

### Euler equations

#### 5a. Euler equations

Generally speaking, fluid mechanics is a complex science, which is organized by taking into account the two main properties that a fluid can have or not, which are:

- (1) Compressibility.
- (2) Viscosity.

Regarding compressibility, this is certainly a property of the gases, but not of most of the liquids, at least when idealized. We will often assume that our fluid is incompressible, which in practice means more or less that we are dealing with liquids, of rather “regular” type. However, this will be not the general rule, for instance because materials like sand, or snow, that we are also interested in, in view of their obvious strong link with classical mechanics, and with our modelling abilities so far, are incompressible too.

Regarding viscosity, this is something far more tricky. Intuitively, this comes from the mutual “friction” of the constituent molecules, when the fluid is moving, and with this being something quite difficult to model and understand, via precise mathematical equations. Without getting into details, for the moment, let us mention that, from this point of view, the fluids, or rather liquids, fall into 3 main classes, namely:

– Inviscid. This is intuitively the case of regular water, and other familiar liquids. However, this remains an idealization, with the true inviscid fluids, in the real life, being basically only the superfluids, met at very low temperatures.

– Newtonian. This is intuitively the case for most of the familiar visquous fluids, from the real life, whose viscosity is proportional to the applied stress, and with this proportionality being known as Newton’s law on viscosity.

– Non-Newtonian. These are visquous fluids which do not obey to Newton’s law on viscosity, and there are plenty of them, all very interesting, such as paint, toothpaste, ketchup and many more, not to forget basic things like snow or sand.

As a conclusion to all this, we can see that, even when looking at the simplest 2 possible things that can be said about a fluid, namely compressibility and viscosity, we end up with a whole menagerie of fluids, with each of them corresponding to its own branch of fluid mechanics. In what concerns us, let us first fix the following goal:

*GOAL 5.1. We will be first interested in the basic modelling of the incompressible fluids, which can be either inviscid, or non-Newtonian.*

Here our incompressibility assumption comes from our discussion above regarding compressibility, and is certainly something quite natural, and with this being the simplest situation anyway, mathematically speaking, that we would like to study first. As for our second assumption, “either inviscid or non-Newtonian”, this might sound a bit exotic, but the point here is that we want to avoid, at least in the beginning, the Newtonian, visquous case, whose basic mathematics is notoriously quite complicated.

Of course you might argue that non-Newtonian is more complicated than Newtonian, but my answer is that this is not exactly the case, with a pile of sand, and its mathematics, being probably something simpler than a visquous, Newtonian fluid flowing.

Speaking goals, let us discuss now as well the main PDE for the fluids, that we would like to recover, whenever possible, for the fluids that we are mainly interested in. As a first observation, which is of key importance in advanced fluid dynamics, we have:

*OBSERVATION 5.2. An incompressible fluid is right away something mathematical, whose dynamics is described by a diffeomorphism, evolving in time  $t > 0$ .*

Obviously, this is something very basic, coming from the very nature of the incompressibility property. To be more precise, assuming for instance that we have colored our fluid initially, say into tiny little cubes of red, yellow, green and so on, after some time  $t > 0$  we will obviously still have a mixture of red, yellow, green and so on, appearing in equal parts, and the function  $f : \mathbb{R}^3 \rightarrow \mathbb{R}^3$  mapping red to red, yellow to yellow, green to green, and so on, is what we call in mathematics a diffeomorphism.

In practice now, in order to reach from this to a PDE, let us assume that we are in the simplest case, where our fluid is inviscid, and also adiabatic, or with zero thermal conductivity. The dynamics of the diffeomorphisms  $f : \mathbb{R}^3 \rightarrow \mathbb{R}^3$  will be then, intuitively speaking, basically governed by the mechanics of the red, yellow, green and so on components, and we are led in this way to the Euler equations, which are as follows:

$$\dot{u} + \langle u, \nabla \rangle u = -\nabla w$$

$$\langle \nabla, u \rangle = 0$$



Here  $u$  is the vector velocity field, and  $w$  is the thermodynamic work, with the quantity on the right from the first equation being as follows,  $p$  being the pressure:

$$\nabla w = \frac{\nabla p}{\rho}$$

With this replacement made, the Euler equations become:

$$\begin{aligned} \dot{u} + \langle u, \nabla \rangle u &= -\frac{\nabla p}{\rho} \\ \langle \nabla, u \rangle &= 0 \end{aligned}$$

Here the first equation, which is the important one, is called the Euler momentum equation. This equation can be further complicated by adding an acceleration term  $+g$  on the right, accounting for exterior forces, gravitational, or magnetic or of some other kind. As for the second equation, this is the incompressibility constraint.

Although we will not really need this here, at least at this stage of our discussion, let us record as well what happens in the viscous case, by staying as before in the incompressible setting. Here the Euler momentum equation gets replaced by the Navier-Stokes equation, which is as follows, with  $v$  being the kinematic viscosity:

$$\dot{u} + \langle u, \nabla \rangle u = -\frac{\nabla p}{\rho} + v\Delta u$$

Summarizing, in relation with our modelling questions for the incompressible fluids, we will be mostly interested in the Euler equation, and its versions.

Getting now to modelling questions, let us begin by recalling, and we insist on this, the fact that fluid mechanics is something quite complicated, and so that what we will be doing here, of rather elementary nature, will be quite speculative. But, let's give this a go. We have several intuitive ways of modelling the incompressible fluids, as follows:

(1) With fluids modelled by little cubes, it is a bit unclear what we can get, because these cubes will obviously not slide exactly like fluids do. However, the little cubes will model well things like a pile of sand, because no friction is needed between our cubes for our pile to stand, as a pile of sand does stand, and this looks quite interesting.

(2) With little spheres, we are certainly close to reality, for somehow obvious reasons. However, at the mathematical level, things are quite tricky. In the static setting already, we are led to non-trivial questions, of sphere-packing flavor. And in the dynamic setting, which is the one that we are interested in, things can only be more complicated.

(3) In order to avoid the mathematics of the little cubes or little spheres, which obviously can be quite complicated, we can assume instead that we are dealing with

“random-shaped” little pieces of material. Which is in fact, when thinking well, not that far from what happens in the real life, with materials like sand.

There are many interesting questions here, coming as a continuation of the modelling work that we did before, and with phenomena like soil liquefaction confirming this. In fact, one interesting feature of what happens here concerns the liquid/solid mixtures.

For further fun, we can add magnetism to our incompressible fluids. However, in regards with discrete modelling questions, all this looks quite complicated.

**5b.**

**5c.**

**5d.**

**5e. Exercises**

Exercises:

EXERCISE 5.3.

EXERCISE 5.4.

EXERCISE 5.5.

EXERCISE 5.6.

EXERCISE 5.7.

EXERCISE 5.8.

EXERCISE 5.9.

EXERCISE 5.10.

Bonus exercise.

## CHAPTER 6

### Navier-Stokes

#### 6a. Navier-Stokes

6b.

6c.

6d.

#### 6e. Exercises

Exercises:

EXERCISE 6.1.

EXERCISE 6.2.

EXERCISE 6.3.

EXERCISE 6.4.

EXERCISE 6.5.

EXERCISE 6.6.

EXERCISE 6.7.

EXERCISE 6.8.

Bonus exercise.



## CHAPTER 7

### Exotic fluids

#### 7a. Exotic fluids

7b.

7c.

7d.

#### 7e. Exercises

Exercises:

EXERCISE 7.1.

EXERCISE 7.2.

EXERCISE 7.3.

EXERCISE 7.4.

EXERCISE 7.5.

EXERCISE 7.6.

EXERCISE 7.7.

EXERCISE 7.8.

Bonus exercise.



## CHAPTER 8

### Further equations

#### 8a. Further equations

8b.

8c.

8d.

#### 8e. Exercises

Exercises:

EXERCISE 8.1.

EXERCISE 8.2.

EXERCISE 8.3.

EXERCISE 8.4.

EXERCISE 8.5.

EXERCISE 8.6.

EXERCISE 8.7.

EXERCISE 8.8.

Bonus exercise.





## Part III

### Into the waves

*When love takes over  
You know you can't deny  
When love takes over  
Cause something's here tonight*

## CHAPTER 9

### Wave equation

#### 9a. Laplace operator

Generally speaking, each major branch of physics is guided by its own “wave equation”, and with, coming a bit in advance, the truth about waves being as follows:

FACT 9.1. *Waves can be of many types, and basically fall into two classes:*

- (1) *Mechanical waves, such as the usual water waves, but also the sound waves, or the seismic waves. In all these cases, the wave propagates mechanically, via a certain medium, which can be solid, liquid or gaseous.*
- (2) *Electromagnetic waves, coming via a more complicated mechanism, namely an accelerating charge in the context of electromagnetism. These are the radio waves, microwaves, IR, visible light, UV, X-rays and  $\gamma$ -rays.*

Quite remarkably, the behavior of all the above waves is basically described by the same wave equation, which looks as follows, and details on this later:

$$\ddot{\varphi} = v^2 \Delta \varphi$$

Getting started for good now, some mathematics first. What is the Laplace operator  $\Delta$ , appearing in the above? The answer here is very simple, coming from:

PRINCIPLE 9.2. *The second derivative of a function  $\varphi : \mathbb{R}^N \rightarrow \mathbb{R}$ , making*

$$\varphi(x+h) \simeq \varphi(x) + \varphi'(x)h + \frac{\langle \varphi''(x)h, h \rangle}{2}$$

*work, is its Hessian matrix  $\varphi''(x) \in M_N(\mathbb{R})$ , given by the following formula:*

$$\varphi''(x) = \left( \frac{d^2 \varphi}{dx_i dx_j} \right)_{ij}$$

*However, when needing a number, as second derivative, the trace of  $\varphi''(x)$ , denoted*

$$\Delta \varphi = \sum_{i=1}^N \frac{d^2 \varphi}{dx_i^2}$$

*and called Laplacian of  $\varphi$ , usually does the job.*

So, let us try to understand this principle, to start with. In one variable, things are quite simple, and you certainly know them well. Given a function  $\varphi : \mathbb{R} \rightarrow \mathbb{R}$ , the first job is that of finding a quantity  $\varphi'(x) \in \mathbb{R}$  making the following formula work:

$$\varphi(x+h) \simeq \varphi(x) + \varphi'(x)h$$

But here, there are not so many choices, and the solution is that of defining the number  $\varphi'(x) \in \mathbb{R}$  by the following formula, provided that the limit converges indeed:

$$\varphi'(x) = \lim_{h \rightarrow 0} \frac{\varphi(x+h) - \varphi(x)}{h}$$

This number is called derivative of  $\varphi$  at the point  $x \in \mathbb{R}$ , and as you surely know, geometrically, we have  $\varphi'(x) = \tan \alpha$ , with  $\alpha$  being the slope of  $\varphi$  at the point  $x$ .

Still in one variable, we can talk as well about second derivatives, as follows:

**THEOREM 9.3.** *The second derivative of a function  $\varphi : \mathbb{R} \rightarrow \mathbb{R}$ , making*

$$\varphi(x+h) \simeq \varphi(x) + \varphi'(x)h + \frac{\varphi''(x)h^2}{2}$$

*work, is the derivative  $\varphi''$  of the derivative  $\varphi' : \mathbb{R} \rightarrow \mathbb{R}$ .*

**PROOF.** Assume indeed that  $\varphi$  is twice differentiable at  $x$ , and let us try to construct an approximation of  $\varphi$  around  $x$  by a quadratic function, as follows:

$$\varphi(x+h) \simeq a + bh + ch^2$$

We must have  $a = \varphi(x)$ , and we also know that  $b = \varphi'(x)$  is the correct choice for the coefficient of  $h$ . Thus, our approximation must be as follows:

$$\varphi(x+h) \simeq \varphi(x) + \varphi'(x)h + ch^2$$

In order to find the correct choice for  $c \in \mathbb{R}$ , observe that the function  $\psi(h) = \varphi(x+h)$  matches with  $P(h) = \varphi(x) + \varphi'(x)h + ch^2$  in what regards the value at  $h = 0$ , and also in what regards the value of the derivative at  $h = 0$ . Thus, the correct choice of  $c \in \mathbb{R}$  should be the one making match the second derivatives at  $h = 0$ , and this gives:

$$c = \frac{\varphi''(x)}{2}$$

We are therefore led to the formula in the statement. In order to prove this formula, we can use L'Hôpital's rule, which states that the  $0/0$  type limits are given by:

$$\frac{f(x)}{g(x)} \simeq \frac{f'(x)}{g'(x)}$$

Indeed, if we denote by  $\psi(h) \simeq P(h)$  the formula to be proved, we have:

$$\begin{aligned} \frac{\psi(h) - P(h)}{h^2} &\simeq \frac{\psi'(h) - P'(h)}{2h} \\ &\simeq \frac{\psi''(h) - P''(h)}{2} \\ &= \frac{\varphi''(h) - \varphi''(h)}{2} \\ &= 0 \end{aligned}$$

Thus, we are led to the conclusion in the statement.  $\square$

Many more things can be said, as a continuation of the above, and you surely know all this. Before leaving the subject, however, let us record the following statement, which is something a bit heuristic, which will play an important role, in what follows:

**PROPOSITION 9.4.** *Intuitively speaking, the second derivative  $\varphi''(x) \in \mathbb{R}$  computes how much different is  $\varphi(x)$ , compared to the average of  $\varphi(y)$ , with  $y \simeq x$ .*

**PROOF.** As already mentioned, this is something a bit heuristic, but which is good to know. Let us write the formula in Theorem 9.3, as such, and with  $h \rightarrow -h$  too:

$$\begin{aligned} \varphi(x+h) &\simeq \varphi(x) + \varphi'(x)h + \frac{\varphi''(x)}{2}h^2 \\ \varphi(x-h) &\simeq \varphi(x) - \varphi'(x)h + \frac{\varphi''(x)}{2}h^2 \end{aligned}$$

By making the average, we obtain the following formula:

$$\frac{\varphi(x+h) + \varphi(x-h)}{2} = \varphi(x) + \frac{\varphi''(x)}{2}h^2$$

Thus, thinking a bit, we are led to the conclusion in the statement. It is of course possible to say more here, but we will not really need all the details, in what follows.  $\square$

Moving now to several variables,  $N \geq 2$ , as a first job, given a function  $\varphi : \mathbb{R}^N \rightarrow \mathbb{R}$ , we would like to find a quantity  $\varphi'(x)$  making the following formula work:

$$\varphi(x+h) \simeq \varphi(x) + \varphi'(x)h$$

But here, again there are not so many choices, and the solution is that of defining  $\varphi'(x)$  as being the row vector formed by the partial derivatives at  $x$ :

$$\varphi'(x) = \left( \frac{d\varphi}{dx_1} \quad \cdots \quad \frac{d\varphi}{dx_N} \right)$$

To be more precise, with this value for  $\varphi'(x)$ , our approximation formula  $\varphi(x+h) \simeq \varphi(x) + \varphi'(x)h$  makes sense indeed, as an equality of real numbers, with  $\varphi'(x)h \in \mathbb{R}$  being obtained as the matrix multiplication of the row vector  $\varphi'(x)$ , and the column vector

$h$ . As for the fact that our formula holds indeed, this follows by putting together the approximation properties of each of the partial derivatives  $d\varphi/dx_i$ , which give:

$$\varphi(x+h) \simeq \varphi(x) + \sum_{i=1}^N \frac{d\varphi}{dx_i} \cdot h_i = \varphi(x) + \varphi'(x)h$$

Before moving forward, you might say, why bothering with horizontal vectors, when it is so simple and convenient to have all vectors vertical, by definition. Good point, and in answer, we can indeed talk about the gradient of  $\varphi$ , constructed as follows:

$$\nabla\varphi = \begin{pmatrix} \frac{d\varphi}{dx_1} \\ \vdots \\ \frac{d\varphi}{dx_N} \end{pmatrix}$$

With this convention,  $\nabla\varphi$  geometrically describes the slope of  $\varphi$  at the point  $x$ , in the obvious way. However, the approximation formula must be written as follows:

$$\varphi(x+h) \simeq \varphi(x) + \langle \nabla\varphi(x), h \rangle$$

In what follows we will use both  $\varphi'$  and  $\nabla\varphi$ , depending on the context. Moving now to second derivatives, the result here, generalizing Theorem 9.3, is as follows:

**THEOREM 9.5.** *The second derivative of a function  $\varphi : \mathbb{R}^N \rightarrow \mathbb{R}$ , making*

$$\varphi(x+h) \simeq \varphi(x) + \varphi'(x)h + \frac{\langle \varphi''(x)h, h \rangle}{2}$$

*work, is its Hessian matrix  $\varphi''(x) \in M_N(\mathbb{R})$ , given by the following formula:*

$$\varphi''(x) = \left( \frac{d^2\varphi}{dx_i dx_j} \right)_{ij}$$

*Moreover, this Hessian matrix is symmetric,  $\varphi''(x)_{ij} = \varphi''(x)_{ji}$ .*

**PROOF.** There are several things going on here, the idea being as follows:

(1) As a first observation, at  $N = 1$  the Hessian matrix constructed above is simply the  $1 \times 1$  matrix having as entry the second derivative  $\varphi''(x)$ , and the formula in the statement is something that we know well from Theorem 9.3, namely:

$$\varphi(x+h) \simeq \varphi(x) + \varphi'(x)h + \frac{\varphi''(x)h^2}{2}$$

(2) At  $N = 2$  now, we obviously need to differentiate  $\varphi$  twice, and the point is that we come in this way upon the following formula, called Clairaut formula:

$$\frac{d^2\varphi}{dx dy} = \frac{d^2\varphi}{dy dx}$$

But, is this formula correct or not? As an intuitive justification for it, let us consider a product of power functions,  $\varphi(z) = x^p y^q$ . We have then:

$$\frac{d^2 \varphi}{dx dy} = \frac{d}{dx} \left( \frac{dx^p y^q}{dy} \right) = \frac{d}{dx} (q x^p y^{q-1}) = p q x^{p-1} y^{q-1}$$

$$\frac{d^2 \varphi}{dy dx} = \frac{d}{dy} \left( \frac{dx^p y^q}{dx} \right) = \frac{d}{dy} (p x^{p-1} y^q) = p q x^{p-1} y^{q-1}$$

Next, let us consider a linear combination of power functions,  $\varphi(z) = \sum_{pq} c_{pq} x^p y^q$ , which can be finite or not. We have then, by using the above computation:

$$\frac{d^2 \varphi}{dx dy} = \frac{d^2 \varphi}{dy dx} = \sum_{pq} c_{pq} p q x^{p-1} y^{q-1}$$

Thus, we can see that our commutation formula for derivatives holds indeed, and this due to the fact that the functions in  $x$ , and in  $y$ , commute. Of course, all this does not prove our formula, in general. But exercise for you, to have this idea fully working, or to look up the standard proof of the Clairaut formula, using the mean value theorem.

(3) Moving now to  $N = 3$  and higher, we can use here the Clairaut formula with respect to any pair of coordinates, and we obtain the Schwarz formula, namely:

$$\frac{d^2 \varphi}{dx_i dx_j} = \frac{d^2 \varphi}{dx_j dx_i}$$

Thus, the second derivative, or Hessian matrix, is symmetric, as claimed.

(4) Getting now to the main topic, namely approximation formula in the statement, in arbitrary  $N$  dimensions, this is in fact something which does not need a new proof, because it follows from the one-variable formula in (1), applied to the restriction of  $\varphi$  to the following segment in  $\mathbb{R}^N$ , which can be regarded as being a one-variable interval:

$$I = [x, x + h]$$

To be more precise, let  $y \in \mathbb{R}^N$ , and consider the following function, with  $r \in \mathbb{R}$ :

$$f(r) = \varphi(x + ry)$$

We know from (1) that the Taylor formula for  $f$ , at the point  $r = 0$ , reads:

$$f(r) \simeq f(0) + f'(0)r + \frac{f''(0)r^2}{2}$$

And our claim is that, with  $h = ry$ , this is precisely the formula in the statement.

(5) So, let us see if our claim is correct. By using the chain rule, we have the following formula, with on the right, as usual, a row vector multiplied by a column vector:

$$f'(r) = \varphi'(x + ry) \cdot y$$

By using again the chain rule, we can compute the second derivative as well:

$$\begin{aligned}
 f''(r) &= (\varphi'(x + ry) \cdot y)' \\
 &= \left( \sum_i \frac{d\varphi}{dx_i}(x + ry) \cdot y_i \right)' \\
 &= \sum_i \sum_j \frac{d^2\varphi}{dx_i dx_j}(x + ry) \cdot \frac{d(x + ry)_j}{dr} \cdot y_i \\
 &= \sum_i \sum_j \frac{d^2\varphi}{dx_i dx_j}(x + ry) \cdot y_i y_j \\
 &= \langle \varphi''(x + ry)y, y \rangle
 \end{aligned}$$

(6) Time now to conclude. We know that we have  $f(r) = \varphi(x + ry)$ , and according to our various computations above, we have the following formulae:

$$f(0) = \varphi(x) \quad , \quad f'(0) = \varphi'(x) \quad , \quad f''(0) = \langle \varphi''(x)y, y \rangle$$

But with this data in hand, the usual Taylor formula for our one variable function  $f$ , at order 2, at the point  $r = 0$ , takes the following form, with  $h = ry$ :

$$\begin{aligned}
 \varphi(x + ry) &\simeq \varphi(x) + \varphi'(x)ry + \frac{\langle \varphi''(x)y, y \rangle r^2}{2} \\
 &= \varphi(x) + \varphi'(x)t + \frac{\langle \varphi''(x)h, h \rangle}{2}
 \end{aligned}$$

Thus, we have obtained the formula in the statement.  $\square$

As before in the one variable case, many more things can be said, as a continuation of the above. For instance the local minima and maxima of  $\varphi : \mathbb{R}^N \rightarrow \mathbb{R}$  appear at the points  $x \in \mathbb{R}^N$  where the derivative vanishes,  $\varphi'(x) = 0$ , and where the second derivative  $\varphi''(x) \in M_N(\mathbb{R})$  is positive, respectively negative. But, you surely know all this.

Getting back now to what we wanted to do, namely understand Principle 9.2, it remains to talk about the Laplace operator  $\Delta$ . Things are quite tricky here, basically requiring some physics that we still need to develop, but as something mathematical to start with, we have the following higher dimensional analogue of Proposition 9.4:

**PROPOSITION 9.6.** *Intuitively, the following quantity, called Laplacian of  $\varphi$ ,*

$$\Delta\varphi = \sum_{i=1}^N \frac{d^2\varphi}{dx_i^2}$$

*computes how much different is  $\varphi(x)$ , compared to the average of  $\varphi(y)$ , with  $y \simeq x$ .*



PROOF. As before with Proposition 9.4, this is something a bit heuristic, but good to know. Let us write the formula in Theorem 9.5, as such, and with  $h \rightarrow -h$  too:

$$\begin{aligned}\varphi(x+h) &\simeq \varphi(x) + \varphi'(x)h + \frac{\langle \varphi''(x)h, h \rangle}{2} \\ \varphi(x-h) &\simeq \varphi(x) - \varphi'(x)h + \frac{\langle \varphi''(x)h, h \rangle}{2}\end{aligned}$$

By making the average, we obtain the following formula:

$$\frac{\varphi(x+h) + \varphi(x-h)}{2} = \varphi(x) + \frac{\langle \varphi''(x)h, h \rangle}{2}$$

Thus, thinking a bit, we are led to the conclusion in the statement. It is of course possible to say more here, but we will not really need all the details, in what follows.  $\square$

With this understood, the problem is now, what can we say about the mathematics of  $\Delta$ ? As a first observation, which is a bit speculative, the Laplace operator appears by applying twice the gradient operator, in a somewhat formal sense, as follows:

$$\begin{aligned}\Delta\varphi &= \sum_{i=1}^N \frac{d^2\varphi}{dx_i^2} \\ &= \sum_{i=1}^N \frac{d}{dx_i} \cdot \frac{d\varphi}{dx_i} \\ &= \left\langle \begin{pmatrix} \frac{d}{dx_1} \\ \vdots \\ \frac{d}{dx_N} \end{pmatrix}, \begin{pmatrix} \frac{d\varphi}{dx_1} \\ \vdots \\ \frac{d\varphi}{dx_N} \end{pmatrix} \right\rangle \\ &= \langle \nabla, \nabla\varphi \rangle\end{aligned}$$

Thus, it is possible to write a formula of type  $\Delta = \nabla^2$ , with the convention that the square of the gradient  $\nabla$  is taken in a scalar product sense, as above. However, this can be a bit confusing, and in what follows, we will not use this notation.

Instead of further thinking at this, and at double derivatives in general, let us formulate a more straightforward question, inspired by linear algebra, as follows:

QUESTION 9.7. *The Laplace operator being linear,*

$$\Delta(a\varphi + b\psi) = a\Delta\varphi + b\Delta\psi$$

*what can we say about it, inspired by usual linear algebra?*

In answer now, the space of functions  $\varphi : \mathbb{R}^N \rightarrow \mathbb{R}$ , on which  $\Delta$  acts, being infinite dimensional, the usual tools from linear algebra do not apply as such, and we must be

extremely careful. For instance, we cannot really expect to diagonalize  $\Delta$ , via some sort of explicit formula, as we do for the usual matrices, and then end of the story.

Thinking some more, there is actually a real bug too with our problem, because at  $N = 1$  this problem becomes “what can we say about the second derivatives  $\varphi'' : \mathbb{R} \rightarrow \mathbb{R}$  of the functions  $\varphi : \mathbb{R} \rightarrow \mathbb{R}$ , inspired by linear algebra”, with answer “not much”.

And by thinking even more, still at  $N = 1$ , there is a second bug too, because if  $\varphi : \mathbb{R} \rightarrow \mathbb{R}$  is twice differentiable, nothing will guarantee that its second derivative  $\varphi'' : \mathbb{R} \rightarrow \mathbb{R}$  is twice differentiable too. Thus, we have some issues with the domain and range of  $\Delta$ , regarded as linear operator, and these problems will persist at higher  $N$ .

So, shall we trash Question 9.7? Not so quick, because, very remarkably, some magic comes at  $N = 2$  and higher in relation with complex analysis, and we have:

PRINCIPLE 9.8. *The functions  $\varphi : \mathbb{R}^N \rightarrow \mathbb{R}$  which are 0-eigenvectors of  $\Delta$ ,*

$$\Delta\varphi = 0$$

*called harmonic functions, have the following properties:*

- (1) *At  $N = 1$ , nothing spectacular, these are just the linear functions.*
- (2) *At  $N = 2$ , these are, locally, the real parts of holomorphic functions.*
- (3) *At  $N \geq 3$ , these still share many properties with the holomorphic functions.*

In order to understand this, or at least get introduced to it, let us first look at the case  $N = 2$ . Here, any function  $\varphi : \mathbb{R}^2 \rightarrow \mathbb{R}$  can be regarded as function  $\varphi : \mathbb{C} \rightarrow \mathbb{R}$ , depending on  $z = x + iy$ . But, in view of this, it is natural to enlarge to attention to the functions  $\varphi : \mathbb{C} \rightarrow \mathbb{C}$ , and ask which of these functions are harmonic,  $\Delta\varphi = 0$ . And here, we have the following remarkable result, making the link with complex analysis:

THEOREM 9.9. *Any holomorphic function  $\varphi : \mathbb{C} \rightarrow \mathbb{C}$ , when regarded as function*

$$\varphi : \mathbb{R}^2 \rightarrow \mathbb{C}$$

*is harmonic. Moreover, the conjugates  $\bar{\varphi}$  of holomorphic functions are harmonic too.*

PROOF. The first assertion comes from the following computation, with  $z = x + iy$ :

$$\begin{aligned} \Delta z^n &= \frac{d^2 z^n}{dx^2} + \frac{d^2 z^n}{dy^2} \\ &= \frac{d(nz^{n-1})}{dx} + \frac{d(inz^{n-1})}{dy} \\ &= n(n-1)z^{n-2} - n(n-1)z^{n-2} \\ &= 0 \end{aligned}$$

As for the second assertion, this follows from  $\Delta\bar{\varphi} = \overline{\Delta\varphi}$ , which is clear from definitions, and which shows that if  $\varphi$  is harmonic, then so is its conjugate  $\bar{\varphi}$ .  $\square$



Now let us send an impulse, and see how the balls will be moving. For this purpose, we zoom on one ball. The situation here is as follows,  $l$  being the spring length:

$$\cdots \cdots \bullet_{\varphi(x-l)} \times \times \times \bullet_{\varphi(x)} \times \times \times \bullet_{\varphi(x+l)} \cdots \cdots$$

We have two forces acting at  $x$ . First is the Newton motion force, mass times acceleration, which is as follows, with  $m$  being the mass of each ball:

$$F_n = m \cdot \ddot{\varphi}(x)$$

And second is the Hooke force, displacement of the spring, times spring constant. Since we have two springs at  $x$ , this is as follows,  $k$  being the spring constant:

$$\begin{aligned} F_h &= F_h^r - F_h^l \\ &= k(\varphi(x+l) - \varphi(x)) - k(\varphi(x) - \varphi(x-l)) \\ &= k(\varphi(x+l) - 2\varphi(x) + \varphi(x-l)) \end{aligned}$$

We conclude that the equation of motion, in our model, is as follows:

$$m \cdot \ddot{\varphi}(x) = k(\varphi(x+l) - 2\varphi(x) + \varphi(x-l))$$

(2) Now let us take the limit of our model, as to reach to continuum. For this purpose we will assume that our system consists of  $B \gg 0$  balls, having a total mass  $M$ , and spanning a total distance  $L$ . Thus, our previous infinitesimal parameters are as follows, with  $K$  being the spring constant of the total system, which is of course lower than  $k$ :

$$m = \frac{M}{B} \quad , \quad k = KB \quad , \quad l = \frac{L}{B}$$

With these changes, our equation of motion found in (1) reads:

$$\ddot{\varphi}(x) = \frac{KB^2}{M}(\varphi(x+l) - 2\varphi(x) + \varphi(x-l))$$

Now observe that this equation can be written, more conveniently, as follows:

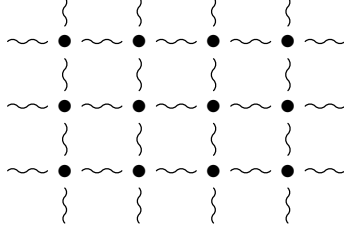
$$\ddot{\varphi}(x) = \frac{KL^2}{M} \cdot \frac{\varphi(x+l) - 2\varphi(x) + \varphi(x-l)}{l^2}$$

With  $N \rightarrow \infty$ , and therefore  $l \rightarrow 0$ , we obtain in this way:

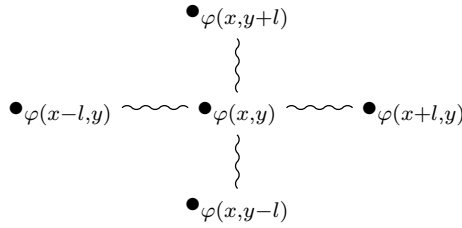
$$\ddot{\varphi}(x) = \frac{KL^2}{M} \cdot \frac{d^2\varphi}{dx^2}(x)$$

We are therefore led to the wave equation in the statement, which is  $\ddot{\varphi} = v^2\varphi''$  in our present  $N = 1$  dimensional case, the propagation speed being  $v = \sqrt{K/M} \cdot L$ .

(3) In 2 dimensions now, the same argument carries on. Indeed, we can use here a lattice model as follows, with all the edges standing for small springs:



As before in one dimension, we send an impulse, and we zoom on one ball. The situation here is as follows, with  $l$  being the spring length:



We have two forces acting at  $(x, y)$ . First is the Newton motion force, mass times acceleration, which is as follows, with  $m$  being the mass of each ball:

$$F_n = m \cdot \ddot{\varphi}(x, y)$$

And second is the Hooke force, displacement of the spring, times spring constant. Since we have four springs at  $(x, y)$ , this is as follows,  $k$  being the spring constant:

$$\begin{aligned} F_h &= F_h^r - F_h^l + F_h^u - F_h^d \\ &= k(\varphi(x+l, y) - \varphi(x, y)) - k(\varphi(x, y) - \varphi(x-l, y)) \\ &\quad + k(\varphi(x, y+l) - \varphi(x, y)) - k(\varphi(x, y) - \varphi(x, y-l)) \\ &= k(\varphi(x+l, y) - 2\varphi(x, y) + \varphi(x-l, y)) \\ &\quad + k(\varphi(x, y+l) - 2\varphi(x, y) + \varphi(x, y-l)) \end{aligned}$$

We conclude that the equation of motion, in our model, is as follows:

$$\begin{aligned} m \cdot \ddot{\varphi}(x, y) &= k(\varphi(x+l, y) - 2\varphi(x, y) + \varphi(x-l, y)) \\ &\quad + k(\varphi(x, y+l) - 2\varphi(x, y) + \varphi(x, y-l)) \end{aligned}$$

(4) Now let us take the limit of our model, as to reach to continuum. For this purpose we will assume that our system consists of  $B^2 \gg 0$  balls, having a total mass  $M$ , and spanning a total area  $L^2$ . Thus, our previous infinitesimal parameters are as follows, with

$K$  being the spring constant of the total system, taken to be equal to  $k$ :

$$m = \frac{M}{B^2} \quad , \quad k = K \quad , \quad l = \frac{L}{B}$$

With these changes, our equation of motion found in (3) reads:

$$\begin{aligned} \ddot{\varphi}(x, y) &= \frac{KB^2}{M} (\varphi(x+l, y) - 2\varphi(x, y) + \varphi(x-l, y)) \\ &+ \frac{KB^2}{M} (\varphi(x, y+l) - 2\varphi(x, y) + \varphi(x, y-l)) \end{aligned}$$

Now observe that this equation can be written, more conveniently, as follows:

$$\begin{aligned} \ddot{\varphi}(x, y) &= \frac{KL^2}{M} \times \frac{\varphi(x+l, y) - 2\varphi(x, y) + \varphi(x-l, y)}{l^2} \\ &+ \frac{KL^2}{M} \times \frac{\varphi(x, y+l) - 2\varphi(x, y) + \varphi(x, y-l)}{l^2} \end{aligned}$$

With  $N \rightarrow \infty$ , and therefore  $l \rightarrow 0$ , we obtain in this way:

$$\ddot{\varphi}(x, y) = \frac{KL^2}{M} \left( \frac{d^2\varphi}{dx^2} + \frac{d^2\varphi}{dy^2} \right) (x, y)$$

Thus, we are led in this way to the following wave equation in two dimensions, with  $v = \sqrt{K/M} \cdot L$  being the propagation speed of our wave:

$$\ddot{\varphi}(x, y) = v^2 \left( \frac{d^2\varphi}{dx^2} + \frac{d^2\varphi}{dy^2} \right) (x, y)$$

But we recognize at right the Laplace operator, and we are done. As before in 1D, there is of course some discussion to be made here, arguing that our spring model in (3) is indeed the correct one. But do not worry, experiments confirm our findings.

(5) In 3 dimensions now, which is the case of the main interest, corresponding to our real-life world, the same argument carries over, and the wave equation is as follows:

$$\ddot{\varphi}(x, y, z) = v^2 \left( \frac{d^2\varphi}{dx^2} + \frac{d^2\varphi}{dy^2} + \frac{d^2\varphi}{dz^2} \right) (x, y, z)$$

(6) Finally, the same argument, namely a lattice model, carries on in arbitrary  $N$  dimensions, and the wave equation here is as follows:

$$\ddot{\varphi}(x_1, \dots, x_N) = v^2 \sum_{i=1}^N \frac{d^2\varphi}{dx_i^2} (x_1, \dots, x_N)$$

Thus, we are led to the conclusion in the statement. □

Observe that there are some subtleties in the above, with the convention for the total spring constant  $K$ , which varies with the dimension  $N$ . We will be back to this.

As another comment, once we are in  $N \geq 2$  dimensions, modifying the springs in our lattice model, as to allow a dissymmetry between horizontal and vertical, either at the level of spring lengths, or spring constants, leads to different results.

In order to reach to some further insight into our spring models above, we must get deeper into elasticity. Indeed, the Hooke law that we used has behind it some non-trivial elasticity, of “linear” type, and understanding all this, and further modifying our models, according to what elasticity theory says, is certainly an interesting question.

Observe that all this can only lead us too into a better understanding of the fact that the propagation speed is finite,  $v < c$ . Indeed, the Hooke law is something static, and for better understanding what happens dynamically, we must go into elasticity.

As a starting point for all this, we have the following result:

**THEOREM 9.12.** *The wave equation can be understood as well directly, as a wave propagating through a linear elastic medium, via stress.*

**PROOF.** This is indeed something very standard, with the  $N = 1$  picture involving a pulse propagating through a bar, and with at  $N \geq 2$  something of a similar type:

(1) In the 1D case, assume that we have a bar of length  $L$ , made of linear elastic material. The stiffness of the bar is then the following quantity, with  $A$  being the cross-sectional area, and with  $E$  being the Young modulus of the material:

$$K = \frac{EA}{L}$$

Now when sending a pulse, this propagates as follows,  $M$  being the total mass:

$$\ddot{\varphi} = \frac{EAL}{M} \cdot \varphi''(x)$$

But since  $V = AL$  is the volume, with  $\rho = M/V$  being the density, we have:

$$\ddot{\varphi} = \frac{E}{\rho} \cdot \varphi''(x)$$

Thus, as a conclusion, the wave propagates with speed  $v = \sqrt{E/\rho}$ .

(2) In two or more dimensions, the study, and final result, are similar. □

### 9c. Basic solutions

We have seen so far that the mechanical waves propagate according to the wave equation, which is as follows, with  $\Delta$  being the Laplace operator:

$$\ddot{\varphi} = v^2 \Delta \varphi$$

In what regards this wave equation, in 1D, we first have:

**THEOREM 9.13.** *The 1D wave equation, with speed  $v$ , namely*

$$\ddot{\varphi} = v^2 \frac{d^2 \varphi}{dx^2}$$

*has as basic solutions the following functions,*

$$\varphi(x) = A \cos(kx - wt + \delta)$$

*with  $A$  being called amplitude,  $kx - wt + \delta$  being called the phase,  $k$  being the wave number,  $w$  being the angular frequency, and  $\delta$  being the phase constant. We have*

$$\lambda = \frac{2\pi}{k} \quad , \quad T = \frac{2\pi}{kv} \quad , \quad \nu = \frac{1}{T} \quad , \quad w = 2\pi\nu$$

*relating the wavelength  $\lambda$ , period  $T$ , frequency  $\nu$ , and angular frequency  $w$ . Moreover, any linear combination of such basic solutions is a solution of the wave equation.*

**PROOF.** There are several things going on here, the idea being as follows:

(1) Our first claim is that the function  $\varphi$  in the statement satisfies indeed the wave equation, with speed  $v = w/k$ . For this purpose, observe that we have:

$$\ddot{\varphi} = -w^2 \varphi \quad , \quad \frac{d^2 \varphi}{dx^2} = -k^2 \varphi$$

Thus, the wave equation is indeed satisfied, with speed  $v = w/k$ :

$$\ddot{\varphi} = \left(\frac{w}{k}\right)^2 \frac{d^2 \varphi}{dx^2} = v^2 \frac{d^2 \varphi}{dx^2}$$

(2) Regarding now the other things in the statement, all this is basically terminology, which is very natural, when thinking how  $\varphi(x) = A \cos(kx - wt + \delta)$  propagates.

(3) Finally, the last assertion is clear. We will see later in this book, using Fourier analysis, that any solution of the 1D wave equation appears in fact in this way.  $\square$

As a first observation, the above result invites the use of complex numbers. Indeed, we can write the solutions that we found in a more convenient way, as follows:

$$\varphi(x) = \operatorname{Re} [A e^{i(kx - wt + \delta)}]$$

And we can in fact do even better, by absorbing the quantity  $e^{i\delta}$  into the amplitude  $A$ , which becomes now a complex number, and writing our formula as:

$$\varphi = \operatorname{Re}(\tilde{\varphi}) \quad , \quad \tilde{\varphi} = \tilde{A} e^{i(kx - wt)}$$



In fact, with a bit more work, we can fully solve the 1D wave equation. In order to explain this, we will need a standard calculus result, as follows:

PROPOSITION 9.14. *The derivative of a function of type*

$$\varphi(x) = \int_{g(x)}^{h(x)} f(s) ds$$

is given by the formula  $\varphi'(x) = f(h(x))h'(x) - f(g(x))g'(x)$ .

PROOF. Consider a primitive of the function that we integrate,  $F' = f$ . We have:

$$\begin{aligned} \varphi(x) &= \int_{g(x)}^{h(x)} f(s) ds \\ &= \int_{g(x)}^{h(x)} F'(s) ds \\ &= F(h(x)) - F(g(x)) \end{aligned}$$

By using now the chain rule for derivatives, we obtain from this:

$$\begin{aligned} \varphi'(x) &= F'(h(x))h'(x) - F'(g(x))g'(x) \\ &= f(h(x))h'(x) - f(g(x))g'(x) \end{aligned}$$

Thus, we are led to the formula in the statement.  $\square$

Now back to the 1D waves, the general result here, due to d'Alembert, along with a little more, in relation with our lattice models above, is as follows:

THEOREM 9.15. *The solution of the 1D wave equation with initial value conditions  $\varphi(x, 0) = f(x)$  and  $\dot{\varphi}(x, 0) = g(x)$  is given by the d'Alembert formula, namely:*

$$\varphi(x, t) = \frac{f(x - vt) + f(x + vt)}{2} + \frac{1}{2v} \int_{x-vt}^{x+vt} g(s) ds$$

*In the context of our lattice model discretizations, what happens is more or less that the above d'Alembert integral gets computed via Riemann sums.*

PROOF. There are several things going on here, the idea being as follows:

(1) Let us first check that the d'Alembert solution is indeed a solution of the wave equation  $\ddot{\varphi} = v^2 \varphi''$ . The first time derivative is computed as follows:

$$\dot{\varphi}(x, t) = \frac{-vf'(x - vt) + vf'(x + vt)}{2} + \frac{1}{2v}(vg(x + vt) + vg(x - vt))$$

The second time derivative is computed as follows:

$$\ddot{\varphi}(x, t) = \frac{v^2 f''(x - vt) + v^2 f''(x + vt)}{2} + \frac{vg'(x + vt) - vg'(x - vt)}{2}$$

Regarding now space derivatives, the first one is computed as follows:

$$\varphi'(x, t) = \frac{f'(x - vt) + f'(x + vt)}{2} + \frac{1}{2v}(g'(x + vt) - g'(x - vt))$$

As for the second space derivative, this is computed as follows:

$$\varphi''(x, t) = \frac{f''(x - vt) + f''(x + vt)}{2} + \frac{g''(x + vt) - g''(x - vt)}{2v}$$

Thus we have indeed  $\ddot{\varphi} = v^2\varphi''$ . As for the initial conditions,  $\varphi(x, 0) = f(x)$  is clear from our definition of  $\varphi$ , and  $\dot{\varphi}(x, 0) = g(x)$  is clear from our above formula of  $\dot{\varphi}$ .

(2) Conversely now, we must show that our solution is unique, but instead of going here into abstract arguments, we will simply solve our equation, which among others will doublecheck out computations in (1). Let us make the following change of variables:

$$\xi = x - vt \quad , \quad \eta = x + vt$$

With this change of variables, which is quite tricky, mixing space and time variables, our wave equation  $\ddot{\varphi} = v^2\varphi''$  reformulates in a very simple way, as follows:

$$\frac{d^2\varphi}{d\xi d\eta} = 0$$

But this latter equation tells us that our new  $\xi, \eta$  variables get separated, and we conclude from this that the solution must be of the following special form:

$$\varphi(x, t) = F(\xi) + G(\eta) = F(x - vt) + G(x + vt)$$

Now by taking into account the initial conditions  $\varphi(x, 0) = f(x)$  and  $\dot{\varphi}(x, 0) = g(x)$ , and then integrating, we are led to the d'Alembert formula in the statement.

(3) In regards now with our discretization questions, by using a 1D lattice model with balls and springs as before, what happens to all the above is more or less that the above d'Alembert integral gets computed via Riemann sums, in our model, as stated.  $\square$

In  $N \geq 2$  dimensions things are more complicated. We will be back to this.

### 9d. Spherical coordinates

Let us start with something well-known, namely:

PROPOSITION 9.16. *We have polar coordinates in 2 dimensions,*

$$\begin{cases} x = r \cos t \\ y = r \sin t \end{cases}$$

*the corresponding Jacobian being  $J = r$ .*

PROOF. This is elementary, the Jacobian being:

$$\begin{aligned}
 J &= \begin{vmatrix} \frac{d(r \cos t)}{dr} & \frac{d(r \cos t)}{dt} \\ \frac{d(r \sin t)}{dr} & \frac{d(r \sin t)}{dt} \end{vmatrix} \\
 &= \begin{vmatrix} \cos t & -r \sin t \\ \sin t & r \cos t \end{vmatrix} \\
 &= r \cos^2 t + r \sin^2 t \\
 &= r
 \end{aligned}$$

Thus, we have indeed the formula in the statement.  $\square$

Moving now to 3 dimensions, we have here the following result:

PROPOSITION 9.17. *We have spherical coordinates in 3 dimensions,*

$$\begin{cases} x = r \cos s \\ y = r \sin s \cos t \\ z = r \sin s \sin t \end{cases}$$

*the corresponding Jacobian being  $J(r, s, t) = r^2 \sin s$ .*

PROOF. The fact that we have indeed spherical coordinates is clear. Regarding now the Jacobian, this is given by the following formula:

$$\begin{aligned}
 &J(r, s, t) \\
 &= \begin{vmatrix} \cos s & -r \sin s & 0 \\ \sin s \cos t & r \cos s \cos t & -r \sin s \sin t \\ \sin s \sin t & r \cos s \sin t & r \sin s \cos t \end{vmatrix} \\
 &= r^2 \sin s \sin t \begin{vmatrix} \cos s & -r \sin s \\ \sin s \sin t & r \cos s \sin t \end{vmatrix} + r \sin s \cos t \begin{vmatrix} \cos s & -r \sin s \\ \sin s \cos t & r \cos s \cos t \end{vmatrix} \\
 &= r \sin s \sin^2 t \begin{vmatrix} \cos s & -r \sin s \\ \sin s & r \cos s \end{vmatrix} + r \sin s \cos^2 t \begin{vmatrix} \cos s & -r \sin s \\ \sin s & r \cos s \end{vmatrix} \\
 &= r \sin s (\sin^2 t + \cos^2 t) \begin{vmatrix} \cos s & -r \sin s \\ \sin s & r \cos s \end{vmatrix} \\
 &= r \sin s \times 1 \times r \\
 &= r^2 \sin s
 \end{aligned}$$

Thus, we have indeed the formula in the statement.  $\square$

Let us work out as well the general spherical coordinate formula, in arbitrary  $N$  dimensions. The formula here, which generalizes those at  $N = 2, 3$ , is as follows:

THEOREM 9.18. *We have spherical coordinates in  $N$  dimensions,*

$$\begin{cases} x_1 &= r \cos t_1 \\ x_2 &= r \sin t_1 \cos t_2 \\ \vdots & \\ x_{N-1} &= r \sin t_1 \sin t_2 \dots \sin t_{N-2} \cos t_{N-1} \\ x_N &= r \sin t_1 \sin t_2 \dots \sin t_{N-2} \sin t_{N-1} \end{cases}$$

*the corresponding Jacobian being given by the following formula,*

$$J(r, t) = r^{N-1} \sin^{N-2} t_1 \sin^{N-3} t_2 \dots \sin^2 t_{N-3} \sin t_{N-2}$$

*and with this generalizing the known formulae at  $N = 2, 3$ .*

PROOF. As before, the fact that we have spherical coordinates is clear. Regarding now the Jacobian, also as before, by developing over the last column, we have:

$$\begin{aligned} J_N &= r \sin t_1 \dots \sin t_{N-2} \sin t_{N-1} \times \sin t_{N-1} J_{N-1} \\ &+ r \sin t_1 \dots \sin t_{N-2} \cos t_{N-1} \times \cos t_{N-1} J_{N-1} \\ &= r \sin t_1 \dots \sin t_{N-2} (\sin^2 t_{N-1} + \cos^2 t_{N-1}) J_{N-1} \\ &= r \sin t_1 \dots \sin t_{N-2} J_{N-1} \end{aligned}$$

Thus, we obtain the formula in the statement, by recurrence. □

In order to reformulate our equations in spherical coordinates, we will need:

THEOREM 9.19. *The Laplace operator in spherical coordinates is*

$$\Delta = \frac{1}{r^2} \cdot \frac{d}{dr} \left( r^2 \cdot \frac{d}{dr} \right) + \frac{1}{r^2 \sin s} \cdot \frac{d}{ds} \left( \sin s \cdot \frac{d}{ds} \right) + \frac{1}{r^2 \sin^2 s} \cdot \frac{d^2}{dt^2}$$

*with our standard conventions for these coordinates, in 3D.*

PROOF. There are several proofs here, a short, elementary one being as follows:

(1) Let us first see how  $\Delta$  behaves under a change of coordinates  $\{x_i\} \rightarrow \{y_i\}$ , in arbitrary  $N$  dimensions. Our starting point is the chain rule for derivatives:

$$\frac{d}{dx_i} = \sum_j \frac{d}{dy_j} \cdot \frac{dy_j}{dx_i}$$

By using this rule, then Leibnitz for products, then again this rule, we obtain:

$$\begin{aligned}
\frac{d^2 f}{dx_i^2} &= \sum_j \frac{d}{dx_i} \left( \frac{df}{dy_j} \cdot \frac{dy_j}{dx_i} \right) \\
&= \sum_j \frac{d}{dx_i} \left( \frac{df}{dy_j} \right) \cdot \frac{dy_j}{dx_i} + \frac{df}{dy_j} \cdot \frac{d}{dx_i} \left( \frac{dy_j}{dx_i} \right) \\
&= \sum_j \left( \sum_k \frac{d}{dy_k} \cdot \frac{dy_k}{dx_i} \right) \left( \frac{df}{dy_j} \right) \cdot \frac{dy_j}{dx_i} + \frac{df}{dy_j} \cdot \frac{d^2 y_j}{dx_i^2} \\
&= \sum_{jk} \frac{d^2 f}{dy_k dy_j} \cdot \frac{dy_k}{dx_i} \cdot \frac{dy_j}{dx_i} + \sum_j \frac{df}{dy_j} \cdot \frac{d^2 y_j}{dx_i^2}
\end{aligned}$$

(2) Now by summing over  $i$ , we obtain the following formula, with  $A$  being the derivative of  $x \rightarrow y$ , that is to say, the matrix of partial derivatives  $dy_i/dx_j$ :

$$\begin{aligned}
\Delta f &= \sum_{ijk} \frac{d^2 f}{dy_k dy_j} \cdot \frac{dy_k}{dx_i} \cdot \frac{dy_j}{dx_i} + \sum_{ij} \frac{df}{dy_j} \cdot \frac{d^2 y_j}{dx_i^2} \\
&= \sum_{ijk} A_{ki} A_{ji} \frac{d^2 f}{dy_k dy_j} + \sum_{ij} \frac{d^2 y_j}{dx_i^2} \cdot \frac{df}{dy_j} \\
&= \sum_{jk} (AA^t)_{jk} \frac{d^2 f}{dy_k dy_j} + \sum_j \Delta(y_j) \frac{df}{dy_j}
\end{aligned}$$

(3) So, this will be the formula that we will need. Observe that this formula can be further compacted as follows, with all the notations being self-explanatory:

$$\Delta f = Tr(AA^t H_y(f)) + \langle \Delta(y), \nabla_y(f) \rangle$$

(4) Getting now to spherical coordinates,  $(x, y, z) \rightarrow (r, s, t)$ , the derivative of the inverse, obtained by differentiating  $x, y, z$  with respect to  $r, s, t$ , is given by:

$$A^{-1} = \begin{pmatrix} \cos s & -r \sin s & 0 \\ \sin s \cos t & r \cos s \cos t & -r \sin s \sin t \\ \sin s \sin t & r \cos s \sin t & r \sin s \cos t \end{pmatrix}$$

The product  $(A^{-1})^t A^{-1}$  of the transpose of this matrix with itself is then:

$$\begin{pmatrix} \cos s & \sin s \cos t & \sin s \sin t \\ -r \sin s & r \cos s \cos t & r \cos s \sin t \\ 0 & -r \sin s \sin t & r \sin s \cos t \end{pmatrix} \begin{pmatrix} \cos s & -r \sin s & 0 \\ \sin s \cos t & r \cos s \cos t & -r \sin s \sin t \\ \sin s \sin t & r \cos s \sin t & r \sin s \cos t \end{pmatrix}$$

But everything simplifies here, and we have the following remarkable formula, which by the way is something very useful, worth to be memorized:

$$(A^{-1})^t A^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & r^2 \sin^2 s \end{pmatrix}$$

Now by inverting, we obtain the following formula, in relation with the above:

$$AA^t = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/r^2 & 0 \\ 0 & 0 & 1/(r^2 \sin^2 s) \end{pmatrix}$$

(5) Let us compute now the Laplacian of  $r, s, t$ . We first have the following formula, that we will use many times in what follows, and is worth to be memorized:

$$\begin{aligned} \frac{dr}{dx} &= \frac{d}{dx} \sqrt{x^2 + y^2 + z^2} \\ &= \frac{1}{2} \cdot \frac{2x}{\sqrt{x^2 + y^2 + z^2}} \\ &= \frac{x}{r} \end{aligned}$$

Of course the same computation works for  $y, z$  too, and we therefore have:

$$\frac{dr}{dx} = \frac{x}{r} \quad , \quad \frac{dr}{dy} = \frac{y}{r} \quad , \quad \frac{dr}{dz} = \frac{z}{r}$$

(6) By using the above formulae, twice, we can compute the Laplacian of  $r$ :

$$\begin{aligned} \Delta(r) &= \Delta\left(\sqrt{x^2 + y^2 + z^2}\right) \\ &= \frac{d}{dx} \left(\frac{x}{r}\right) + \frac{d}{dy} \left(\frac{y}{r}\right) + \frac{d}{dz} \left(\frac{z}{r}\right) \\ &= \frac{r^2 - x^2}{r^3} + \frac{r^2 - y^2}{r^3} + \frac{r^2 - z^2}{r^3} \\ &= \frac{2}{r} \end{aligned}$$

(7) In what regards now  $s$ , the computation here goes as follows:

$$\begin{aligned}
\Delta(s) &= \Delta\left(\arccos\left(\frac{x}{r}\right)\right) \\
&= \frac{d}{dx}\left(-\frac{\sqrt{r^2-x^2}}{r^2}\right) + \frac{d}{dy}\left(\frac{xy}{r^2\sqrt{r^2-x^2}}\right) + \frac{d}{dz}\left(\frac{xz}{r^2\sqrt{r^2-x^2}}\right) \\
&= \frac{2x\sqrt{r^2-x^2}}{r^4} + \frac{r^2(z^2-2y^2)+2x^2y^2}{r^4\sqrt{r^2-x^2}} + \frac{r^2(y^2-2z^2)+2x^2z^2}{r^4\sqrt{r^2-x^2}} \\
&= \frac{2x\sqrt{r^2-x^2}}{r^4} + \frac{x(2x^2-r^2)}{r^4\sqrt{r^2-x^2}} \\
&= \frac{x}{r^2\sqrt{r^2-x^2}} \\
&= \frac{\cos s}{r^2 \sin s}
\end{aligned}$$

(8) Finally, in what regards  $t$ , the computation here goes as follows:

$$\begin{aligned}
\Delta(t) &= \Delta\left(\arctan\left(\frac{z}{y}\right)\right) \\
&= \frac{d}{dx}(0) + \frac{d}{dy}\left(-\frac{z}{y^2+z^2}\right) + \frac{d}{dz}\left(\frac{y}{y^2+z^2}\right) \\
&= 0 - \frac{2yz}{(y^2+z^2)^2} + \frac{2yz}{(y^2+z^2)^2} \\
&= 0
\end{aligned}$$

(9) We can now plug the data from (4) and (6,7,8) in the general formula that we found in (2) above, and we obtain in this way:

$$\begin{aligned}
\Delta f &= \frac{d^2 f}{dr^2} + \frac{1}{r^2} \cdot \frac{d^2 f}{ds^2} + \frac{1}{r^2 \sin^2 s} \cdot \frac{d^2 f}{dt^2} + \frac{2}{r} \cdot \frac{df}{dr} + \frac{\cos s}{r^2 \sin s} \cdot \frac{df}{ds} \\
&= \frac{2}{r} \cdot \frac{df}{dr} + \frac{d^2 f}{dr^2} + \frac{\cos s}{r^2 \sin s} \cdot \frac{df}{ds} + \frac{1}{r^2} \cdot \frac{d^2 f}{ds^2} + \frac{1}{r^2 \sin^2 s} \cdot \frac{d^2 f}{dt^2} \\
&= \frac{1}{r^2} \cdot \frac{d}{dr} \left( r^2 \cdot \frac{df}{dr} \right) + \frac{1}{r^2 \sin s} \cdot \frac{d}{ds} \left( \sin s \cdot \frac{df}{ds} \right) + \frac{1}{r^2 \sin^2 s} \cdot \frac{d^2 f}{dt^2}
\end{aligned}$$

Thus, we are led to the formula in the statement.  $\square$

With the above result in hand, we can do now some advanced study of the wave equation, by using spherical coordinates, going beyond what we know in 1D.

The mathematics here is, and no surprise, quite complicated.

**9e. Exercises**

Exercises:

EXERCISE 9.20.

EXERCISE 9.21.

EXERCISE 9.22.

EXERCISE 9.23.

EXERCISE 9.24.

EXERCISE 9.25.

EXERCISE 9.26.

EXERCISE 9.27.

Bonus exercise.



CHAPTER 10

**Laminar flow**

**10a.**

**10b.**

**10c.**

**10d.**

**10e. Exercises**

Exercises:

EXERCISE 10.1.

EXERCISE 10.2.

EXERCISE 10.3.

EXERCISE 10.4.

EXERCISE 10.5.

EXERCISE 10.6.

EXERCISE 10.7.

EXERCISE 10.8.

Bonus exercise.



CHAPTER 11

**Turbulent flow**

**11a.**

**11b.**

**11c.**

**11d.**

**11e. Exercises**

Exercises:

EXERCISE 11.1.

EXERCISE 11.2.

EXERCISE 11.3.

EXERCISE 11.4.

EXERCISE 11.5.

EXERCISE 11.6.

EXERCISE 11.7.

EXERCISE 11.8.

Bonus exercise.



## CHAPTER 12

### About solitons

**12a.**

**12b.**

**12c.**

**12d.**

**12e. Exercises**

Exercises:

EXERCISE 12.1.

EXERCISE 12.2.

EXERCISE 12.3.

EXERCISE 12.4.

EXERCISE 12.5.

EXERCISE 12.6.

EXERCISE 12.7.

EXERCISE 12.8.

Bonus exercise.



## Part IV

# Learning to fly

*All we are saying  
Is give peace a chance  
All we are saying  
Is give peace a chance*



CHAPTER 13

**Turbulence, again**

**13a.**

**13b.**

**13c.**

**13d.**

**13e. Exercises**

Exercises:

EXERCISE 13.1.

EXERCISE 13.2.

EXERCISE 13.3.

EXERCISE 13.4.

EXERCISE 13.5.

EXERCISE 13.6.

EXERCISE 13.7.

EXERCISE 13.8.

Bonus exercise.



CHAPTER 14

**Aeroplane wings**

14a.

14b.

14c.

14d.

14e. Exercises

Exercises:

EXERCISE 14.1.

EXERCISE 14.2.

EXERCISE 14.3.

EXERCISE 14.4.

EXERCISE 14.5.

EXERCISE 14.6.

EXERCISE 14.7.

EXERCISE 14.8.

Bonus exercise.



CHAPTER 15

**Going supersonic**

**15a.**

**15b.**

**15c.**

**15d.**

**15e. Exercises**

Exercises:

EXERCISE 15.1.

EXERCISE 15.2.

EXERCISE 15.3.

EXERCISE 15.4.

EXERCISE 15.5.

EXERCISE 15.6.

EXERCISE 15.7.

EXERCISE 15.8.

Bonus exercise.



CHAPTER 16

**Rockets, capsules**

**16a.**

**16b.**

**16c.**

**16d.**

**16e. Exercises**

Congratulations for having read this book, and no exercises for this final chapter.





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