

# Introduction to modern physics

Teo Banica

DEPARTMENT OF MATHEMATICS, UNIVERSITY OF CERGY-PONTOISE, F-95000  
CERGY-PONTOISE, FRANCE. [teo.banica@gmail.com](mailto:teo.banica@gmail.com)

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ABSTRACT. This is an introduction to modern physics, assuming the basics of calculus known. We first review the foundations, namely classical mechanics, relativity theory, electromagnetism and thermodynamics. Then we make our way through quantum mechanics, starting with early thoughts, experiments and results, up to the standard basic formalism, still used nowadays, and with a look into quantum electrodynamics too.

## Preface

Einstein was not very happy with quantum mechanics, and he spent the whole last part of his career trying to fix it, or at least to contradict it, and without writing much. His point of view, which is something very natural, is still shared by loads of modern scientists, obviously passionate by quantum mechanics too, and not writing much about it either. You can usually find them in various areas surrounding quantum mechanics, such as pure mathematics, applied physics, chemistry, engineering and so on.

Moving ahead from these dark thoughts, quantum mechanics as we know it must be learned from somewhere, and there are many good books here. Standard choices for learning physics, and quantum mechanics in particular, all somewhat written with a Cold War touch, are the classical books by Feynman [33], [34], [35], [36], the equally classical books by Landau-Lifshitz [61], [62], [63], [64], the more modern books by Shankar [85], [86], [87], [88], the equally more modern books by Weinberg [92], [93], [94], [95], the modern and delightful books of Griffiths [42], [43], [44], [45], and beware of the cat, and the equally modern and delightful books of Huang [49], [50], [51], [52].

The present book is an introduction to theoretical physics, quantum mechanics oriented, and then to more advanced theory, such as quantum electrodynamics. It is not particularly aimed at mathematicians, or at physicists, or at other scientists, but rather at the people who would like to read it. To be more precise, here are the main ideas behind this book, and if you agree with them, this book might be for you:

(1) Physics is a whole, with all sorts of mechanics being related to each other, and with thermodynamics being the Queen, and all this must be learned at the same time, and the contents of the book will be half general physics, half quantum mechanics.

(2) Physics can be sometimes more complicated than mathematics, so if you want to read a physics book, like for instance the present one, please make sure that you love mathematics, at the bottom line, and that you master some of it, ideally.

(3) Basic quantum mechanics often insists on the dilemma between particles and waves, or between matrix and wave mechanics. Here we will adopt a simplified presentation, our favorite dilemma being the basic probabilistic one,  $P = 0$  for everything that happens.

(4) Advanced quantum mechanics often insists on the theory and behavior of a myriad small-lived particles, which are basically there to annoy us. We will insist here on electrons, protons, neutrons, and a few other selected particles, which are here to stay.

(5) Quantum mechanics in general is a wide discipline, with activities ranging from Einstein type thinking and silence, up to investing billions in machinery like the LHC. We will do here something in between, which means in practice rather philosophy.

(6) Most of quantum mechanics was developed around World War 2, and later during the Cold War, by people equally passionate by science and politics. So if you agree with 1-5 above, and in addition you're into action too, this book might be for you.

So, this will be the idea, and in what regards the contents, Part I deals with classical mechanics and relativity, Part II with electricity and heat, Part III with quantum mechanics, and Part IV with particle physics. As for notations and conventions:

- We use standard units (m, kg, s, C, K) everywhere, or almost, with all our formulae and constants being dimensionless. Our data will be at STP (0° C, 1 bar).

- We will try to use uniform notations all over classical mechanics, electromagnetism, thermodynamics, and quantum mechanics of all types, even if not standard.

- We use vectors for everything, denoted  $a, b, c, \dots, x, y, z$ . Our main tool for dealing with vectors will be the scalar products, denoted  $\langle x, y \rangle = \sum x_i \bar{y}_i$ .

The present book, besides written for being read by anyone interested, can serve as well as an academic textbook, for a 1-year course. I am myself a math professor, but every time I have the occasion I talk about physics, or even about other things like soccer, during my classes, and large parts of the present book have already been tested, in front of various audiences, all disciplines and all levels, and with students being happy.

I personally got into science, of quantum flavor, quite early in my life, after doing some experimental chemistry as a kid, highly exothermic reactions if my memories are good, with my buddy Alex S. that I would like to thank here. Many thanks go as well to my past and present students, in Toulouse and Cergy. Finally, many thanks go to my cats, for advice with a bit of everything, and some help with the computations.

*Cergy, July 2025*

*Teo Banica*

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## Part I

# Classical mechanics

*They're justified, and they're ancient  
And they drive an ice cream van  
They're justified, and they're ancient  
With still no master plan*

## CHAPTER 1

### Kepler and Newton

#### 1a. Observations, basic principles

Classical mechanics can be learned from many places, standard references here being Feynman [33], Kibble [57], Taylor [90] for an introduction, and Arnold [5], Goldstein [39], Landau and Lifshitz [61] for more advanced aspects. This chapter is an introduction to the subject, assuming that the fundamentals of calculus are known.

Before starting, we should mention that calculus was in fact invented by Newton for solving questions from classical mechanics, so what we are doing here is a bit upside down. But hey, some time has passed since Newton, and there might be young people out there who know calculus, and want to learn the physics this calculus comes from.

Getting started now, classical mechanics happens right in front of your eyes. Whenever an apple falls from a tree, this is because of gravitation which attracts the apple towards the Earth, or perhaps vice versa, and so the apple and Earth end up colliding.

It looks like we have a beginning of theory here, with gravitation acting between various bodies. However, it is quite hard to have something started, because of:

**FACT 1.1.** *Feathers fall slower than apples.*

So, how to solve this? The idea, which will be our first idea in this book, will be to divide the problem into 2 parts. Obviously the above fact has something to do with friction, with the surrounding air, which is higher for feathers than for apples, but getting into this looks quite complicated. So, we should proceed as follows:

(1) First, we will develop a theory without friction, with all bodies assumed, a bit in a mathematical and abstract way, to evolve in an ideal, void environment.

(2) And then, with all this understood, we will attack afterwards more complicated, real-life problems, involving air in between objects, and friction in general.

So, this will be our plan, and with the side remark that the scary word in the above is not “void”, but rather “ideal”, which in physics usually means “things here are complicated, time to do some tough mathematics, for solving their simplest instances”. Let us summarize the above discussion into a second fact, as follows:

FACT 1.2. *In classical mechanics, objects evolve in a void environment.*

Observe the careful wording here, with the words “classical mechanics”, referring to some abstract theory that we want to develop, added. These stand as a kind of disclaimer, with respect to things happening in real life, making Fact 1.1 and Fact 1.2 statements of different nature, the former being something true, and the latter being something more speculative. This will be the general convention, throughout this book, some “facts” being absolutely true, and some other not really, depending on the precise wording.

Moving ahead now, building a theory based on Fact 1.2 is quite problematic, because there is no void here on Earth, air, water droplets and so on, and friction everywhere, and so our intuition and observations won’t help that much. So, we should look instead at the skies, and at the gravitation acting between the various bodies out there.

We all know, since childhood, and with this being perhaps the one rock-solid thing, that we know well, that the Earth is obviously flat, and that the Sun moves around it, raising up from the East, and then traveling to the West, with a deviation towards the South, which is bigger during the Winter than during the Summer. How to axiomatize gravity, out of these observations? Obviously, no way, but the solution comes from:

FACT 1.3. *The Earth, as the other celestial objects, is round.*

With this new principle in hand, we can now understand what is going on, with the Sun moving around the Earth on some kind of circle, or perhaps ellipse, and with things being as simple as that. Observe that there is in fact still a mystery left here, concerning the difference between the Summer and Winter trajectories of the Sun. So, what to do with this? We will choose now to enjoy our recent findings, and leave this for later.

We have now all the needed ingredients for developing classical mechanics, based on astronomy, but before doing that, there is one more bug, to be discussed. Getting back to Earth, and to apples falling, as already said in the above, things there involve friction, and are more complicated, for later. However, in true honesty, if there is one basic observation to be derived from what happens with gravitation here on Earth, be that altered a bit by friction, this is that “objects subject to gravitation always end up colliding”, and with friction obviously having nothing to do with this. And this is in strong disagreement with what happens up in the skies, where things never collide, or almost.

Take a comet, for instance. That travels full-throttle towards the Sun, seemingly bound for guaranteed destruction, but then, by some kind of miracle, once it is really close to the Sun, and in this process getting at immense speed, it makes a kind of trick, and avoids the Sun, circling around it. And isn’t this fascinating, and totally opposite to what happens here on Earth. How in the world can we build a theory based on astronomy,

and in particular on the movements of comets, that will predict that apples want in fact to trick, and avoid collision with the Earth? This looks like total nonsense.

The answer to these issues involves more abstraction, as follows:

FACT 1.4. *In basic classical mechanics, all bodies are points.*

To be more precise here, it is all again about precise wording. We will first develop a basic classical mechanics theory, where all bodies are points, and with this solving the above apple-Earth collision problem, because when assuming that the Earth is a point, which is something quite bold, and contradicting our intuition, things after all might happen as up in the skies, with the apple, which is now a point too, being perhaps now free to trick like a comet, and avoid the Earth when falling.

Then, after all this understood, we will improve our theory into something dealing with round bodies, as in Fact 1.3 above, with collisions now allowed to happen. And finally, once this understood too, we will look at objects having different shapes, the idea here being that the point representing them is a certain special point inside them, called center of gravity, and that we can further model our object, if we want to, by a suitable sphere, centered there, and with the radius being the average radius of the object.

So, this will be our updated plan, and in the lack of other obvious bugs, we will stop here with the preliminaries. As a summary of the discussion made so far, we have:

FACT 1.5. *In basic classical mechanics, the bodies, also called “objects”, are points, moving through the void, and being subject to only the gravity forces between them.*

With all this understood, we can now start doing some work. Observing the night sky, and carefully adding some selected observations from what happens on Earth too, can only lead to a number of interesting conclusions regarding gravity.

In what regards the situation here on Earth, nothing that much interesting going on, first of course due to friction, but with this being not that much of a big problem, but then especially due to Fact 1.4 above, which needs the Earth to be a point in the theory that we want to develop. That is, when trying to interpret even very simple things, like an apple falling, we have now to think at bizarre questions of type “what would really happen to this apple falling, was the Earth a point”. So, no good all this, and as conclusions to various things that we can do, at best we could reach to the conclusion that the trajectories of objects acted upon by gravity are straight lines, or parabolas.

With astronomy, however, we can reach to a lot of interesting conclusions. First of all, the void is there as needed, or at least in the lack of observations of friction, passed the falling stars that we can blame the air surrounding the Earth for, we can just assume

that. Also, celestial bodies, including the Sun and the Moon, are fairly small, viewed from here, so we are in agreement with the point requirement for our bodies too.

The problem with astronomy, however, comes from the fact that, passed the Sun and the Moon, which move in nice orbits, reminding ellipses, around us, the rest of the planets and other nearby objects do not seem to obey any rule, and travel on all sorts of bizarre trajectories. So, we are in trouble here, but there is a solution to this, as follows:

**FACT 1.6.** *In celestial mechanics, stars are bigger than planets, and for understanding the math, best is to assume that the smaller object moves around the bigger object.*

Note the careful and a bit mysterious wording of this sentence, as if it was written in order to avoid the Inquisition. The problem indeed is that, as a consequence of this, it is not really the Sun moving around the Earth, but rather vice versa. So, when combining this with Fact 1.3 too, we are led to the conclusion that our beloved Earth, instead of being flat and fixed, is round and moving. Which is probably a bit too much.

But science is science, let's not be afraid, and keep going this way. The point indeed is that when using Fact 1.6, and so assuming that the Earth moves around the Sun, all the previously incomprehensible trajectories of the other planets simplify a lot, and start looking like gentle curves, basically ellipses. And isn't this magic.

The credit for working out the math, starting from these observations, at least in some rough form, goes to Kepler, whose discoveries can be summarized as follows:

**FACT 1.7** (Kepler laws). *The following happen:*

- (1) *The planetary orbits are elliptical, with the Sun at a focus.*
- (2) *The radius vector from the Sun to a planet sweeps equal areas in equal times.*
- (3) *The ratio of the square of the period of revolution and the cube of the ellipse semimajor axis is the same for all planets.*

Here the first law is the most important one, with the second and third laws being things which are more technical, and that we will not need at this point.

So, ellipses. This reminds right away the parabolas found when talking about experiments here on Earth, right after Fact 1.5 above. Indeed, it is known since the ancient Greeks that circles, ellipses and parabolas are part of the same family of curves, called conics, and which includes as well the hyperbolas. And guess what, when trying to go beyond what Kepler was saying in the above about planets, the next objects in our Solar system are asteroids and comets, which may well move on hyperbolas.

As a conclusion, with Kepler we are now very close to the solution. Gravity is most likely described by some simple equations, having as solutions the Greeks' conics.

In practice now, all this was in fact not obvious to find, among others due to the not very advanced status of mathematics, at that time. It was Newton who came up with a solution, some substantial time later, his theory being summarized as follows:

FACT 1.8 (Newton principles). *The force of attraction between two bodies of masses  $m_1, m_2$ , having distance  $d > 0$  between them, is given by the formula*

$$\|F\| = G \cdot \frac{m_1 m_2}{d^2}$$

*where  $G$  is a constant. This force alters the trajectory of one body with respect to another, and more specifically the position  $x$ , speed  $v$ , and acceleration  $a$ , via the formulae*

$$F = ma \quad , \quad a = \dot{v} \quad , \quad v = \dot{x}$$

*where the dot denotes the derivative with respect to time, with this meaning the infinitesimal rate of change of the given quantity, with respect to time.*

All this looks quite complicated to find, with bare hands, and so, just believe us. All the above formulae originate in years and years of astronomical observations, leading to piles and piles of data, and it was Newton, following the previous groundbreaking work of Kepler, who was able to put all this available data in the above concise form.

We will see later, when doing some math, how Fact 1.7 above, as well as many other things still missing from there, can be deduced from Fact 1.8, via calculus.

More in detail now, looking at Fact 1.8, some of the things there are in fact easy to establish. In order to understand what is going on, let us carefully look at the 4 formulae there. First we have the two formulae at the end, namely:

$$a = \dot{v} \quad , \quad v = \dot{x}$$

But these formulae have obviously nothing to do with gravity, and other complicated things. They are just the usual laws of motion, and with this coming from the magic of the dot, once you master a bit that dot, after some thinking. To be more precise, isn't the speed the infinitesimal rate of change of the position? Sure it is. What about acceleration, isn't it the infinitesimal rate of change of the speed? Sure it is, too. So, all in all, these two last formulae at the end of Fact 1.8 are just some trivialities.

As a side comment, however, observe that when combining the above two formulae we obtain the following formula, which all of the sudden is something less trivial:

$$a = \ddot{x}$$

To be more precise, in order to really “feel” this formula, you must be quite familiar with the notion of second derivative, and its mysteries, and this ain't no easy task. But, “shut up and compute”, as Dirac used to say, and you'll eventually get used to it.

By the way, along the same lines, for making things even more complicated, in the above context of the general movement of the bodies, we can also talk about the derivative of the acceleration, if we really want to. This is denoted  $j$ , and called the jerk:

$$j = \dot{a} = \ddot{v} = \dddot{x}$$

This looks like something a bit specialized, but you have certainly met this, in real life, too. Remember that bully friend of yours, who when driving with you or other friends onboard, was not only keeping accelerating his car, at a constant and frightening rate, but was also pushing the gas pedal down to the ground, for maximum fun, from times to times? That is the jerk. But let us not talk about the jerk here. More on this later.

Getting back now to Fact 1.8 above, we can formulate a simplified version of it, which is more advanced, taking into the account the above discussion, as follows:

FACT 1.9 (Newton, simplified). *The force of attraction between two bodies of masses  $m_1, m_2$ , having distance  $d > 0$  between them, is given by*

$$\|F\| = G \cdot \frac{m_1 m_2}{d^2}$$

where  $G$  is a constant. This force alters the trajectory of one body with respect to another according to the formula  $F = ma$ , with  $a$  being as usual the acceleration.

Are we done with our study? Not yet. The point indeed is that we have two formulae in the above, and it is the first formula which matters, because the second formula,  $F = ma$ , is once again something rather abstract, of “general motion of bodies” type. With the remark, however, that if you want to talk about  $F = ma$  in general, you need to find some other forces, different from gravity, to illustrate your general theory, and there are not some many choices here, with basically the thing to be done being that of getting into magnetism. This being said, let us agree however that  $F = ma$  is something trivial too, simply making the link between the first formula and  $a = \dot{v}$ ,  $v = \dot{x}$ .

Summarizing, everything in Fact 1.8 is more or less trivial, after some thinking, and mastering of the definition of the derivative, except for the first formula, namely:

$$\|F\| = G \cdot \frac{m_1 m_2}{d^2}$$

Regarding now this key formula, this is what basically comes from experiments, years and years of astronomy and then Kepler, and so in principle, nothing much to comment about it. A more careful looking, however, reveals a number of things. For instance, we can write this formula as follows, with  $\sim$  standing as usual for proportionality:

$$F \sim m_1 \quad , \quad F \sim m_2 \quad , \quad F \sim \frac{1}{d^2}$$



And here, again, we have a mixture of trivial and non-trivial things. To be more precise, the  $F \sim m$  formulae are both quite intuitive, so we can label them as obvious, and as a conclusion to this, it all comes down to the third formula, and we can state:

FACT 1.10 (Newton, advanced). *The force of gravity is subject to the formula*

$$F \sim \frac{1}{d^2}$$

*with  $d > 0$  being the distance between the two objects involved. Thus, we have*

$$||F|| = G \cdot \frac{m_1 m_2}{d^2}$$

*with  $m_1, m_2$  being the masses, and with  $G$  being a certain constant.*

Regarding now the constant  $G$ , which is the last thing to be discussed, things here are quite tricky. What is mass? What is distance? And also, what is force? There are not easy questions, and instead of discussing all this in detail, let us just formulate:

FACT 1.11. *The gravitation constant is given by*

$$G = 6.67430(15) \times 10^{-11}$$

*in standard units, with the 15 standing for the standard uncertainty.*

Obviously, some discussion would be needed here, and for simplifying, let us just say that “standard units” refers to what comes out of the big effort of mankind in regulating masses, lengths and so on, and which corresponds to the usual units that you are used to, as a scientist at least, namely meters and kilograms. As for the standard uncertainty, this is something of statistical nature, and let us not bother about that.

In practice, all this means that if you are an engineer who wants to build a high-rise building, or a bridge, by using the formulae in this book, then you can use the following value for the constant, and your building or bridge will stand, as required:

$$G = 6.674 \times 10^{-11}$$

By the way, be said in passing, this book is rather about theoretical physics, so if you want to build something concrete based on our formulae here, do it at your own risk.

Getting back now to our formalism, from Fact 1.10 above, we basically have there all that is needed in order to start some work. Indeed, we will be normally able to solve everything, or almost, just by computing derivatives, and solving equations. And this is what we will do, in the remainder of this chapter, and then in chapter 2 too.

### 1b. A word about relativity

Before getting started, however, we should be totally honest, and talk about some known bugs of Newton's theory, discovered later by Einstein, and to be discussed later on in this book, in chapter 4 below. It's all about time, the question being as follows:

QUESTION 1.12. *Does gravitation act instantly, or not?*

Imagine indeed, as in Fact 1.10 above, that we have two bodies of masses  $m_1, m_2$ , with a distance  $d \gg 0$  between them. Things fine so far, with the object  $m_2$  not seeing object  $m_1$ , but certainly feeling its attraction, and slowly moving towards it. But now let us imagine that object  $m_1$  suddenly disappears, or starts going to McDonald's and gets overweight, or to be more realistic, starts moving a bit, say to the right, under the influence of some other force. The question is, will  $m_2$  instantly feel this change of status of  $m_1$ , and instantly adjust its trajectory towards  $m_1$ , by going slower, or faster, or slightly to the right, and so on, depending on what exactly happened to  $m_1$ ?

This is not an easy question. Common sense would suggest that yes, gravitation happens instantly, but isn't this common sense something a bit too human, and to be more precise, a bit religious, assuming somehow that there is someone in this world, call him God, knowing in real time what happens everywhere in the universe, regardless of distances and so on, and then us, as humans and physicists, are here for understanding God's will, and to be more specific, his way of making things work in mechanics.

The point now, involving the above-mentioned discoveries of Einstein, is that gravitation is in fact not instantaneous, and with this being part of a more general philosophy, stating that nothing in this world, be it seemingly free-as-a-bird things like the propagation of light, or of any kind of information, is instantaneous. Call it good or bad, but that is the situation, everything in this world is subject to some slowness. Or to some divine slowness, if you prefer. And this is something quite complicated, that we will talk about later on, when discussing relativity, and other things like thermodynamics too.

Getting back now to our classical, Newtonian mechanics, what to do? No choice here, if we want to get started, we have to make an approximation, which as usual stands as a euphemism for "mistake", and complete our series of principles with:

FACT 1.13. *In basic classical mechanics, gravitation acts instantly.*

So, these will be our general principles for doing mechanics, or at least to get started, Fact 1.10 above, which is something rather reasonable, appearing as a careful and basically honest approximation of reality, leaving aside things that we left aside, knowing what we're doing, combined with Fact 1.13, which is again an approximation of reality, and of what mankind knows, but which is something a bit less honest, to put it this way.

Of course, do not worry about all this. It would be foolish to try to perfectly understand things, right from the beginning, and we will slowly make our way through this, by building first a solid, core theory, that we will gradually improve afterwards. And, in fact, we will be back to the above issues not long from now, just in chapter 4 below.

Finally, for being complete with our preliminaries, and perhaps by messing even more all this, let us point out that our criticism of Newton, following Question 1.12 above, is in fact quite shaky, with the criticism of our criticism coming from:

QUESTION 1.14. *In the context of an object  $m_2$  having to adapt its trajectory to changes in the status of an object  $m_1$ , what can really happen to  $m_1$ ?*

To be more precise, common sense dictates that  $m_1$  cannot just disappear, or suddenly shrink or grow like that, and the most plausible scenario is that  $m_1$  gets deviated by some other force, say by getting attracted by a third object  $m_3$ . But this new object  $m_3$  cannot appear just like that, either, out of nothing, and in case it was already there,  $m_2$  probably knew about it, via its gravity, and so was attracted by it too, and so we're in the end into a standard Newtonian 3-body problem, and there is no contradiction.

Unless, however, there is something beyond gravity, say magnetism, going on between  $m_1$  and  $m_3$ , with poor  $m_2$  made of clay, and unaware of all this. Who knows, and if such a thing was to happen,  $m_2$  would certainly be in trouble, on what to do.

But this is actually quite shaky too, because we decided in Fact 1.5 that we want to deal with gravity only, and avoid magnetism, and other demonic things that can happen. So, let us reproduce that Fact 1.5 again, as a matter of never ever forgetting it:

FACT 1.15 (again). *In basic classical mechanics, the bodies are points, moving through the void, and are subject to only the gravity forces between them.*

Welcome to theoretical physics. Following Einstein, such abstract pieces of thinking, called “Gedankenexperiments”, can be sometimes useful, but most often lead to troubles, and bad sleeping at night. So, better ignore them. And, in what concerns the above, just trust us, there are some bugs with the Newtonian mechanics that we are about to develop, but no worries, we will be back to this, and fix them, in chapter 4 below.

### 1c. Kepler and Newton, conics

With the basic phenomenology understood, we are now ready to do some mechanics, following Newton, then Lagrange and Hamilton. Our first and main objective will be that of understanding how Kepler's findings, from Fact 1.7 above, can be deduced from our axiomatization of classical mechanics, with mathematical proof. Needless to say, this mathematical proof will be not just for fun, or for annoying you if you're weak on calculus, but will stand as a doublecheck, or even supreme verification, of Kepler's findings.

In order to get started, recall from Fact 1.6 that for doing math it is better to assume that the small object moves around the big object. Thus, for best results, we have first to break the symmetry between  $m_1, m_2$ , in the Newton principles. So, assume that we have two objects of masses  $M, m$ , normally with  $M > m$ , or even  $M \gg m$ , but with the converse inequality being theoretically possible, too. We will assume that  $M$  is fixed, and get interested in  $m$  only, somewhat by placing ourselves there, riding on  $m$ .

Now since we don't care much about  $M$ , what matters for us is just its gravitational field. That is, we can even forget about the very existence of  $M$ , and simply say that we are at  $m$ , in the presence of a gravitational "field" which permeates the whole  $\mathbb{R}^3$ , and who really cares about where that field comes from. We are led in this way into:

FACT 1.16 (Newton). *In the 2-body problem, with an object of mass  $M$  fixed at the origin 0, the movement of the second object, of mass  $m$ , is governed by the field*

$$f = \frac{K}{d^2}$$

where  $d = ||x||$ , and  $K = GM$ , in the sense that  $m$  obeys to the usual rules of motion  $a = \dot{v}$ ,  $v = \dot{x}$ , by being continuously pulled towards 0, with acceleration  $f$ .

Let us do now the math, coming from this. We will be quite brief, and for further details on that follows, we refer to our standard books, [5], [33], [38], [57], [61], [90]. With the comment that, now with the basic phenomenology understood, and with calculus assumed to be known, the difference between undergraduate and graduate fades away, and you basically have the choice between US books [33], [38], [90], which are excellent, but a bit too verbose, and USSR books [5], [61], which are excellent too, but a bit not enough verbose. A good compromise here is the delightful English book by Kibble [57].

As a toy example for our theory, let us work out first the 1D case. We will be interested here in free falls, represented vertically, like those of the apples falling on Earth:

$$\begin{array}{c} \circ_m \\ \downarrow \end{array}$$

$$\bullet_M$$

The result here, which is something quite familiar, and that we can establish right from the Newton principles, with just a pinch of basic calculus, is as follows:

THEOREM 1.17. *In the context of a free fall from distance  $x_0 = R \gg 0$ , with initial velocity  $v_0 = 0$ , the equation of the trajectory is*

$$x \simeq R - \frac{gt^2}{2}$$

with the constant being  $g = GM/R^2$ , called gravity of  $M$ , at distance  $R$  from it.

PROOF. We must use the field equation from Fact 1.16 above, namely:

$$f = \frac{K}{d^2}$$

This equation, with  $d = ||x||$ , describes the magnitude  $f$  of the acceleration  $a$  of our moving object  $m$ . Now since  $a$  points towards 0, which is opposite to  $x$ , we have:

$$a = -\frac{K}{d^2} \cdot \frac{x}{||x||} = -\frac{Kx}{||x||^3}$$

Moreover, since the acceleration  $a$  is by definition the second derivative of the position vector  $x$ , the equation of motion of our object  $m$  is as follows:

$$\ddot{x} = -\frac{Kx}{||x||^3}$$

In one dimension now, things get simpler, and the equation of motion reads:

$$\ddot{x} = -\frac{K}{x^2}$$

Since we assumed  $R \gg 0$ , we must look for a solution of type  $x \simeq R + ct^2$ , with the lack of the  $t$  term coming from  $v_0 = 0$ . But with  $x \simeq R + ct^2$ , our equation reads:

$$2c \simeq -\frac{K}{R^2}$$

Now by multiplying by  $t^2/2$ , and adding  $R$ , we obtain as solution:

$$x \simeq R - \frac{Kt^2}{2R^2}$$

Thus, we have indeed  $x \simeq R - gt^2/2$ , with  $g$  being the following number:

$$g = \frac{K}{R^2} = \frac{GM}{R^2}$$

We are therefore led to the conclusion in the statement.  $\square$

As an illustration for the above 1D computation, let us do now a numeric check. The gravitational constant, the mass of the Earth, and the average radius of the Earth are as follows, expressed as usual in meters and kilograms:

$$G = 6.674 \times 10^{-11}$$

$$M = 5.972 \times 10^{24}$$

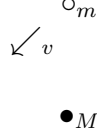
$$R = 6.371 \times 10^6$$

We obtain the following value for the number  $g$  computed above:

$$g = \frac{6.674 \times 5.972}{6.371 \times 6.371} \times 10 = 9.819$$

And this is quite decent, compared to the observed value  $g = 9.806$ .

As a second toy example now for our 3D gravitation theory, which is more advanced, lying somewhere between 1D and 2D, let us add an arbitrary initial speed  $v_0 = v$  to the above situation, which in addition is allowed to be a vector in  $\mathbb{R}^2$ , as follows:



We obtain in this way the following generalization of Theorem 1.17:

**THEOREM 1.18.** *In the context of a free fall from distance  $x_0 = R \gg 0$ , with initial plane velocity vector  $v_0 = v$ , the equation of the trajectory is*

$$x \simeq R + vt - \frac{gt^2}{2}$$

where  $g = GM/R^2$  as usual, and with the quantities  $R, g$  in the above being regarded now as vectors, pointing upwards. The approximate trajectory is a parabola.

**PROOF.** We have several assertions here, the idea being as follows:

(1) Let us first discuss the simpler case where we are still in 1D, as in Theorem 1.17 above, but with an initial velocity  $v_0 = v$  added. In order to find the equation of motion, we can just redo the computations from the proof of Theorem 1.17, with now looking for a general solution of type  $x \simeq R + vt + ct^2$ , and we get, as stated above:

$$x \simeq R + vt - \frac{gt^2}{2}$$

Alternatively, we can simply argue that, by linearity, what we have to do is to take the solution  $x \simeq R - gt^2/2$  found in Theorem 1.17, and add an extra  $vt$  term to it.

(2) In the general 2D case now, where the initial velocity  $v_0 = v$  is a vector in  $\mathbb{R}^2$ , the same arguments apply, either by redoing the computations from the proof of Theorem 1.17, or simply by arguing that by linearity we can just take the solution  $x \simeq R - gt^2/2$  found there, and add an extra  $vt$  term to it. Thus, we have our solution.

(3) Let us study now the solution that we found. In standard  $(x, y)$  coordinates, with  $v = (p, q)$ , and with  $R, g$  being now back scalars, our solution looks as follows:

$$\begin{aligned} x &= pt \\ y &\simeq R + qt - \frac{gt^2}{2} \end{aligned}$$

From the first equation we get  $t = x/p$ , and by substituting into the second:

$$y \simeq R + \frac{qx}{p} - \frac{gx^2}{2p^2}$$

We recognize here the approximate equation of a parabola, and we are done.  $\square$

Getting now to the real thing, 3D, in view of the Kepler findings from Fact 1.7, that we want to recover, we must first talk about conics. The result here, which goes back to the ancient Greeks, and is a must-know for any mathematician or physicist, is:

THEOREM 1.19. *The conics, which are plane curves of degree two,*

$$C = \left\{ (x, y) \in \mathbb{R}^2 \mid P(x, y) = 0, \deg P \leq 2 \right\}$$

*can be classified, modulo the degenerate cases, in three classes, as follows:*

- (1) *Ellipses.*
- (2) *Parabolas.*
- (3) *Hyperbolas.*

*Moreover, again modulo degeneration, these conics are exactly the curves which appear by cutting a two-sided cone in  $\mathbb{R}^3$  with a plane, thereby justifying their name.*

PROOF. We have two assertions here, the idea being as follows:

(1) The first assertion is standard, by doing suitable manipulations on the degree 2 polynomial  $P \in \mathbb{R}[x, y]$ , up to affine transformations of the curve, as to have it in some standard form, which standard form leads to the cases (1,2,3) in the statement.

(2) As for the second assertion, this can be proved either by doing some abstract algebra, proving that the cut must be indeed of degree 2, or directly, by computing the cut in the various cases that might appear, depending on the angle of the plane with respect to the cone, with this leading to the curves in (1,2,3) in the statement.

(3) Finally, there is a discussion to be made in relation with the degenerate cases, namely the lines, double lines, points, empty set, and  $\mathbb{R}^2$  itself. These basically appear when  $\deg P \leq 1$ , and also when cutting the cone in a “degenerate” way.  $\square$

The above statement is of course something quite simplified. Further discussion here includes the fact that the circles are particular cases of ellipses, that the parabolas can be regarded at the same time as being degenerate ellipses or hyperbolas, and so on. For more on all this, you can check any basic algebraic geometry book, a standard US choice here being the book of Harris [46], and with Shafarevich [84] for the USSR.

Going ahead now with physics, we can state and prove Newton’s main theorem, which comes as a verification and ultimate confirmation of Kepler’s findings, as follows:

THEOREM 1.20 (Kepler, Newton). *In the context of a 2-body problem,*

$$\begin{array}{ccc} & \nwarrow_v & \\ \bullet_M & \longleftarrow_F \circ_m & \end{array}$$

*the trajectory of  $m$  with respect to  $M$  lies in a plane, and is a conic.*

PROOF. Consider indeed two objects of masses  $M, m$ , and with the first object  $M$  being assumed to be fixed, at the origin of  $\mathbb{R}^3$ , as in Fact 1.16 above.

(1) We first want to understand why the trajectory of  $m$  will stay in a plane. But this is quite clear, because if at  $t = 0$  our object  $m$  has position  $x_0 \in \mathbb{R}^3$  and speed vector  $v_0 \in \mathbb{R}^3$ , then at any time  $t > 0$  our object  $m$  will be in the following plane:

$$E = \text{span}(x_0, v_0)$$

Indeed, the initial data being  $x_0, v_0 \in E$ , and the only force which acts upon  $m$  being the gravity, which pulls it towards the origin  $0 \in E$ , there is no reason why  $m$  should move upwards or downwards, with respect to  $E$ , and so we have, for any  $t > 0$ :

$$x_t, v_t \in E$$

So, done with this. It is of course possible to prove this abstractly too, by starting with the equation in Fact 1.16 and doing some math, involving a certain vector product which vanishes, but let us not bother here with proving obvious things.

(2) The next step is that of examining the trajectory of  $m$ , in this plane  $E$ . For this purpose, we can simply assume that our 2-body problem takes place in the standard plane  $E = \mathbb{R}^2$ . Now as explained in the beginning of the proof of Theorem 1.17 above, dealing with the general 3D case, the equation of motion in 3D is as follows:

$$\ddot{x} = -\frac{Kx}{||x||^3}$$

Since we are now in 2 dimensions, the most convenient is to use standard  $x, y$  coordinates, and to denote our point as  $z = (x, y)$ . The equation of motion becomes:

$$\ddot{z} = -\frac{Kz}{||z||^3}$$

In other words, in terms of the coordinates  $x, y$ , the equations are:

$$\ddot{x} = -\frac{Kx}{(x^2 + y^2)^{3/2}} \quad , \quad \ddot{y} = -\frac{Ky}{(x^2 + y^2)^{3/2}}$$

(3) Let us begin with a simple particular case, that of the circular solutions. To be more precise, we are interested in solutions of the following type:

$$x = r \cos \alpha t \quad , \quad y = r \sin \alpha t$$

In this case we have  $||z|| = r$ , so our equation of motion becomes:

$$\ddot{z} = -\frac{Kz}{r^3}$$

On the other hand, differentiating  $x, y$  leads to the following formula:

$$\ddot{z} = (\ddot{x}, \ddot{y}) = -\alpha^2(x, y) = -\alpha^2 z$$



Thus, we have a circular solution when the parameters  $r, \alpha$  satisfy:

$$r^3 \alpha^2 = K$$

(4) In the general case now, the problem can be solved via some calculus. Let us write indeed our vector  $z = (x, y)$  in polar coordinates, as follows:

$$x = r \cos \theta \quad , \quad y = r \sin \theta$$

We have then  $\|z\| = r$ , and our equation of motion becomes, as in (3) above:

$$\ddot{z} = -\frac{Kz}{r^3}$$

Let us differentiate now  $x, y$ . By using the standard calculus rules, we have:

$$\dot{x} = \dot{r} \cos \theta - r \sin \theta \cdot \dot{\theta}$$

$$\dot{y} = \dot{r} \sin \theta + r \cos \theta \cdot \dot{\theta}$$

Differentiating one more time gives the following formulae:

$$\ddot{x} = \ddot{r} \cos \theta - 2\dot{r} \sin \theta \cdot \dot{\theta} - r \cos \theta \cdot \dot{\theta}^2 - r \sin \theta \cdot \ddot{\theta}$$

$$\ddot{y} = \ddot{r} \sin \theta + 2\dot{r} \cos \theta \cdot \dot{\theta} - r \sin \theta \cdot \dot{\theta}^2 + r \cos \theta \cdot \ddot{\theta}$$

Consider now the following two quantities, appearing as coefficients in the above:

$$a = \ddot{r} - r\dot{\theta}^2 \quad , \quad b = 2\dot{r}\dot{\theta} + r\ddot{\theta}$$

In terms of these quantities, our second derivative formulae read:

$$\ddot{x} = a \cos \theta - b \sin \theta$$

$$\ddot{y} = a \sin \theta + b \cos \theta$$

(5) We can now solve the equation of motion, from (4) above. Indeed, with the formulae that we found for  $\ddot{x}, \ddot{y}$ , our equation of motion takes the following form:

$$a \cos \theta - b \sin \theta = -\frac{K}{r^2} \cos \theta$$

$$a \sin \theta + b \cos \theta = -\frac{K}{r^2} \sin \theta$$

But these two formulae can be written in the following way:

$$\left(a + \frac{K}{r^2}\right) \cos \theta = b \sin \theta$$

$$\left(a + \frac{K}{r^2}\right) \sin \theta = -b \cos \theta$$

By making now the product, and assuming that we are in a non-degenerate case, where the angle  $\theta$  varies indeed, we obtain by positivity that we must have:

$$a + \frac{K}{r^2} = b = 0$$

(6) We are almost there. Let us first examine the second equation,  $b = 0$ . Remembering who  $b$  is, from (4) above, this equation can be solved as follows:

$$\begin{aligned}
 b = 0 & \iff 2\dot{r}\dot{\theta} + r\ddot{\theta} = 0 \\
 & \iff \frac{\ddot{\theta}}{\dot{\theta}} = -2\frac{\dot{r}}{r} \\
 & \iff (\log \dot{\theta})' = (-2 \log r)' \\
 & \iff \log \dot{\theta} = -2 \log r + c \\
 & \iff \dot{\theta} = \frac{\lambda}{r^2}
 \end{aligned}$$

As for the first equation the we found, namely  $a + K/r^2 = 0$ , remembering from (4) that  $a$  was by definition given by  $a = \ddot{r} - r\dot{\theta}^2$ , this equation now becomes:

$$\ddot{r} - \frac{\lambda^2}{r^3} + \frac{K}{r^2} = 0$$

(7) As a conclusion to all this, in polar coordinates,  $x = r \cos \theta$ ,  $y = r \sin \theta$ , our equations of motion are as follows, with  $\lambda$  being a constant, not depending on  $t$ :

$$\ddot{r} = \frac{\lambda^2}{r^3} - \frac{K}{r^2} \quad , \quad \dot{\theta} = \frac{\lambda}{r^2}$$

Even better now, by writing  $K = \lambda^2/c$ , these equations read:

$$\ddot{r} = \frac{\lambda^2}{r^2} \left( \frac{1}{r} - \frac{1}{c} \right) \quad , \quad \dot{\theta} = \frac{\lambda}{r^2}$$

(8) As an illustration, let us quickly work out the case of a circular motion, where  $r$  is constant. Here  $\ddot{r} = 0$ , so the first equation gives  $c = r$ . Also we have  $\dot{\theta} = \alpha$ , with:

$$\alpha = \frac{\lambda}{r^2}$$

Assuming  $\theta = 0$  at  $t = 0$ , from  $\dot{\theta} = \alpha$  we obtain  $\theta = \alpha t$ , and so, as in (3) above:

$$x = r \cos \alpha t \quad , \quad y = r \sin \alpha t$$

Observe also that the condition found in (3) above is indeed satisfied:

$$r^3 \alpha^2 = \frac{\lambda^2}{r} = \frac{\lambda^2}{c} = K$$

(9) Back to the general case now, our claim is that we have the following formula, for the distance  $r = r(t)$  as function of the angle  $\theta = \theta(t)$ , for some  $\varepsilon, \delta \in \mathbb{R}$ :

$$r = \frac{c}{1 + \varepsilon \cos \theta + \delta \sin \theta}$$

Let us first check that this formula works indeed. With  $r$  being as above, and by using our second equation found before,  $\dot{\theta} = \lambda/r^2$ , we have the following computation:

$$\begin{aligned}\dot{r} &= \frac{c(\varepsilon \sin \theta - \delta \cos \theta)\dot{\theta}}{(1 + \varepsilon \cos \theta + \delta \sin \theta)^2} \\ &= \frac{\lambda c(\varepsilon \sin \theta - \delta \cos \theta)}{r^2(1 + \varepsilon \cos \theta + \delta \sin \theta)^2} \\ &= \frac{\lambda(\varepsilon \sin \theta - \delta \cos \theta)}{c}\end{aligned}$$

Thus, the second derivative of the above function  $r$  is given, as desired, by:

$$\begin{aligned}\ddot{r} &= \frac{\lambda(\varepsilon \cos \theta + \delta \sin \theta)\dot{\theta}}{c} \\ &= \frac{\lambda^2(\varepsilon \cos \theta + \delta \sin \theta)}{r^2 c} \\ &= \frac{\lambda^2}{r^2} \left( \frac{1}{r} - \frac{1}{c} \right)\end{aligned}$$

(10) The above check was something quite informal, and now we must prove that our formula is indeed the correct one. For this purpose, we use a trick. Let us write:

$$r(t) = \frac{1}{f(\theta(t))}$$

Abbreviated, and by always reminding that  $f$  takes  $\theta = \theta(t)$  as variable, this reads:

$$r = \frac{1}{f}$$

With the convention that dots mean as usual derivatives with respect to  $t$ , and that the primes will denote derivatives with respect to  $\theta = \theta(t)$ , we have:

$$\dot{r} = -\frac{f'\dot{\theta}}{f^2} = -\frac{f'}{f^2} \cdot \frac{\lambda}{r^2} = -\lambda f'$$

By differentiating one more time with respect to  $t$ , we obtain:

$$\ddot{r} = -\lambda f''\dot{\theta} = -\lambda f'' \cdot \frac{\lambda}{r^2} = -\frac{\lambda^2}{r^2} f''$$

On the other hand, our equation for  $\ddot{r}$  found in (7) above reads:

$$\ddot{r} = \frac{\lambda^2}{r^2} \left( \frac{1}{r} - \frac{1}{c} \right) = \frac{\lambda^2}{r^2} \left( f - \frac{1}{c} \right)$$

Thus, in terms of  $f = 1/r$  as above, our equation for  $\ddot{r}$  simply reads:

$$f'' + f = \frac{1}{c}$$

But this latter equation is elementary to solve. Indeed, both functions  $\cos t, \sin t$  satisfy  $g'' + g = 0$ , so any linear combination of them satisfies as well this equation. But the solutions of  $f'' + f = 1/c$  being those of  $g'' + g = 0$  shifted by  $1/c$ , we obtain:

$$f = \frac{1 + \varepsilon \cos \theta + \delta \sin \theta}{c}$$

Now by inverting, we obtain the formula announced in (9) above, namely:

$$r = \frac{c}{1 + \varepsilon \cos \theta + \delta \sin \theta}$$

(11) But this leads to the conclusion that the trajectory is a conic. Indeed, in terms of the parameter  $\theta$ , the formulae of the coordinates are:

$$x = \frac{c \cos \theta}{1 + \varepsilon \cos \theta + \delta \sin \theta}$$

$$y = \frac{c \sin \theta}{1 + \varepsilon \cos \theta + \delta \sin \theta}$$

But these are precisely the equations of conics in polar coordinates, as one can check by using various methods, based on the various viewpoints in Theorem 1.19 above.

(12) To be more precise now, in order to find the precise equation of the conic, observe that the two functions  $x, y$  that we found above satisfy the following formula:

$$\begin{aligned} x^2 + y^2 &= \frac{c^2(\cos^2 \theta + \sin^2 \theta)}{(1 + \varepsilon \cos \theta + \delta \sin \theta)^2} \\ &= \frac{c^2}{(1 + \varepsilon \cos \theta + \delta \sin \theta)^2} \end{aligned}$$

On the other hand, these two functions satisfy as well the following formula:

$$\begin{aligned} (\varepsilon x + \delta y - c)^2 &= \frac{c^2(\varepsilon \cos \theta + \delta \sin \theta - (1 + \varepsilon \cos \theta + \delta \sin \theta))^2}{(1 + \varepsilon \cos \theta + \delta \sin \theta)^2} \\ &= \frac{c^2}{(1 + \varepsilon \cos \theta + \delta \sin \theta)^2} \end{aligned}$$

We conclude that our coordinates  $x, y$  satisfy the following equation:

$$x^2 + y^2 = (\varepsilon x + \delta y - c)^2$$

But what we have here is an equation of a conic, as claimed. □

Still with us? All the above was great, we have deduced Kepler's first law from the Newton principles of mechanics, by using nothing more than some standard calculus. It is possible of course to be more explicit in the above, by talking about explicit conics, and to deduce the second and third laws of Kepler as well, and more on this later.

As another comment, all the above was a brute-force computation, in the spirit of those done by Newton himself, a long time ago, in ancient times when people were strong, and used to computing. There are of course some more clever, modern proofs of all this, and we will discuss them later. As an example here, Theorem 1.19 above suggests solving the Kepler 2-body problem by suitably projecting on a plane the circular solution, which is something quite trivial, as seen in (3) in the above proof. More on this later.

### 1d. Parameters and orbits

Theorem 1.20 above remains something quite theoretical, more adapted for doing mathematics than applied physics or engineering, and we will perform now a more detailed study of the orbits. Let us start with a brief account of what we have, not from Theorem 1.20 itself, but rather from its proof, sort of “best of” the formulae found there:

**THEOREM 1.21** (Kepler, Newton). *In the context of a 2-body problem, with  $M$  fixed at 0, and  $m$  starting its movement from  $Ox$ , the equation of motion of  $m$ , namely*

$$\ddot{z} = -\frac{Kz}{||z||^3}$$

*with  $K = GM$ , and  $z = (x, y)$ , becomes in polar coordinates,  $x = r \cos \theta$ ,  $y = r \sin \theta$ ,*

$$\ddot{r} = \frac{\lambda^2}{r^2} \left( \frac{1}{r} - \frac{1}{c} \right) \quad , \quad \dot{\theta} = \frac{\lambda}{r^2}$$

*for some  $\lambda, c \in \mathbb{R}$ , related by  $\lambda^2 = Kc$ . The value of  $r$  in terms of  $\theta$  is given by*

$$r = \frac{c}{1 + \varepsilon \cos \theta + \delta \sin \theta}$$

*for some  $\varepsilon, \delta \in \mathbb{R}$ . At the level of the affine coordinates  $x, y$ , this means*

$$x = \frac{c \cos \theta}{1 + \varepsilon \cos \theta + \delta \sin \theta} \quad , \quad y = \frac{c \sin \theta}{1 + \varepsilon \cos \theta + \delta \sin \theta}$$

*with  $\theta = \theta(t)$  being subject to  $\dot{\theta} = \lambda^2/r$ , as above. Finally, we have*

$$x^2 + y^2 = (\varepsilon x + \delta y - c)^2$$

*which is a degree 2 equation, and so the resulting trajectory is a conic.*

**PROOF.** As already mentioned, this is a sort of “best of” the formulae found in the proof of Theorem 10.20. And in the hope of course that we have not forgotten anything. Finally, let us mention that the simplest illustration for this is the circular motion, and for details on this, not included in the above, we refer to the proof of Theorem 10.20.  $\square$

As a first question, we would like to understand how the various parameters appearing above, namely  $\lambda, c, \varepsilon, \delta$ , which via some basic math can only tell us more about the shape of the orbit, appear from the initial data. The formulae here are as follows:

PROPOSITION 1.22. *In the context of Theorem 1.21 above, and in polar coordinates,  $x = r \cos \theta$ ,  $y = r \sin \theta$ , the initial data is as follows, with  $R = r_0$ :*

$$\begin{aligned} r_0 &= \frac{c}{1 + \varepsilon} \quad , \quad \theta_0 = 0 \\ \dot{r}_0 &= -\frac{\delta\sqrt{K}}{\sqrt{c}} \quad , \quad \dot{\theta}_0 = \frac{\sqrt{Kc}}{R^2} \\ \ddot{r}_0 &= \frac{\varepsilon K}{R^2} \quad , \quad \ddot{\theta}_0 = \frac{4\delta K}{R^2} \end{aligned}$$

*The corresponding formulae for the affine coordinates  $x, y$  can be deduced from this. Also, the various motion parameters  $c, \varepsilon, \delta$  and  $\lambda = \sqrt{Kc}$  can be recovered from this data.*

PROOF. We have several assertions here, the idea being as follows:

(1) As mentioned in Theorem 1.21, the object  $m$  begins its movement on  $Ox$ . Thus we have  $\theta_0 = 0$ , and from this we get the formula of  $r_0$  in the statement.

(2) Regarding the initial speed now, the formula of  $\dot{\theta}_0$  follows from:

$$\dot{\theta} = \frac{\lambda}{r^2} = \frac{\sqrt{Kc}}{r^2}$$

Also, in what concerns the radial speed, the formula of  $\dot{r}_0$  follows from:

$$\begin{aligned} \dot{r} &= \frac{c(\varepsilon \sin \theta - \delta \cos \theta)\dot{\theta}}{(1 + \varepsilon \cos \theta + \delta \sin \theta)^2} \\ &= \frac{c(\varepsilon \sin \theta - \delta \cos \theta)}{c^2/r^2} \cdot \frac{\sqrt{Kc}}{r^2} \\ &= \frac{\sqrt{K}(\varepsilon \sin \theta - \delta \cos \theta)}{\sqrt{c}} \end{aligned}$$

(3) Regarding now the initial acceleration, by using  $\dot{\theta} = \sqrt{Kc}/r^2$  we find:

$$\ddot{\theta} = -2\sqrt{Kc} \cdot \frac{2r\dot{r}}{r^3} = -\frac{4\sqrt{Kc} \cdot \dot{r}}{r^2}$$

In particular at  $t = 0$  we obtain the formula in the statement, namely:

$$\ddot{\theta}_0 = -\frac{4\sqrt{Kc} \cdot \dot{r}_0}{R^2} = \frac{4\sqrt{Kc}}{R^2} \cdot \frac{\delta\sqrt{K}}{\sqrt{c}} = \frac{4\delta K}{R^2}$$

(4) Also regarding acceleration, with  $\lambda = \sqrt{Kc}$  our main motion formula reads:

$$\ddot{r} = \frac{Kc}{r^2} \left( \frac{1}{r} - \frac{1}{c} \right)$$

In particular at  $t = 0$  we obtain the formula in the statement, namely:

$$\ddot{r}_0 = \frac{Kc}{R^2} \left( \frac{1}{R} - \frac{1}{c} \right) = \frac{Kc}{R^2} \cdot \frac{\varepsilon}{c} = \frac{\varepsilon K}{R^2}$$

(5) Finally, the last assertion is clear, and since the formulae look better anyway in polar coordinates than in affine coordinates, we will not get into details here.  $\square$

With the above formulae in hand, which are a precious complement to Theorem 1.21, we can do some reverse engineering at the level of parameters, and work out how various initial speeds and accelerations lead to various types of conics. There are many things that can be said here, and we will discuss some of them later in this book.

### 1e. Exercises

As you might remember from high school, and more on this in this book too, in physics we have a concept of “work”, done by a force, which can be mechanical or of some other nature, which is something quite subtle. For instance a student trying to solve exercises counts as work, due to various chemical reactions in the brain, needed for neuronal activity. However, the same student sitting in class and carefully listening to what the professor has to say, perhaps quite surprisingly, does not count as work.

Be said in passing, the students are not the only bad guys in our system, and the same goes for professors. A professor preparing class, or teaching, or doing research, counts as work, while the same professor attending various meetings that we have in the academia, such as seminars, conferences, and campus committees, does not really count as work.

More concretely now, the saying goes that 10,000 hours of work are needed for being a high-level athlete, or craftsman, and so on, and the same goes for scientists. Usually the math for the latter is 1,000 hours spent during high school doing exercises, then 2,000-3,000 more during college, doing the same thing, and then 6,000-7,000 more during grad school, and afterwards as a young academic, writing 20-30 scientific papers or so.

So, exercises. Generally speaking, we recommend here our go-to mechanics books [5], [33], [38], [57], [61], [90], we won't attempt to compete with that, and with a recommendation for Goldman [38], Kibble [57] and Taylor [90], all Western books written in the 60s-70s, when work and exercises used to be a true Western value. There is of course the Eastern choice too, with Arnold [5] and Landau-Lifshitz [61], but you should know here that the Eastern system used to be quite different, with mathematicians, physicists, engineers, future teachers often having to attend dedicated universities, and with this, as a consequence, making many Eastern best-sellers, and especially their exercises, not always ideal for general-purpose use. As for Feynman [33], and its continuations [34], [35], these books were originally written without exercises, and there is a separate, blue volume with exercises, added later, but this system is not always very practical.

Back to our book now, our exercises here will be basically of Romanian flavor, with a French touch, and with admiration for the United States, Russia and China, and written by a mathematician rather than a physicist, whose inner self however is more that of a chemist and engineer. In any case, in the hope that they can help, and here they are:

EXERCISE 1.23. *Clarify the mathematics of the conics from Theorem 1.19, notably with the precise conditions on the degree 2 polynomial  $P \in \mathbb{R}[x, y]$ , or on the corresponding cone cut in  $\mathbb{R}^3$ , which produce the cases (1, 2, 3) there, or degenerations.*

EXERCISE 1.24. *Clarify as well the math of the conics coming from physics, as in Theorem 1.20, again by understanding which initial conditions produce which conics, and also by saying which of the degenerate conics can indeed appear in this way.*

EXERCISE 1.25. *Are the parabolas found in Theorem 1.18 particular cases of the conics found in Theorem 1.20? Justify, and if this is ever not the case, work out the math, by formulating an explanation for this phenomenon.*

EXERCISE 1.26. *Look up a more conceptual proof of Theorem 1.20, using whatever more advanced and clever arguments, and write down a brief account of that. For a bonus point, come up with two such proofs, instead of one.*

EXERCISE 1.27. *Prove the Kepler 2 and Kepler 3 laws by using the technology that we have so far, and notably the formula  $\dot{\theta} = \lambda/r^2$ . Also, try to formulate and prove such Kepler 2 and Kepler 3 laws in the parabolic and hyperbolic cases as well.*

EXERCISE 1.28. *Motivated by the parabolas found in Theorem 1.18, develop a full theory of gravity at distance  $R \gg 0$ , with some further results on what happens in that case. The more things that you find and write, the better.*

EXERCISE 1.29. *Do the math in connection with the end assertion in Proposition 1.22, by writing down formulae for  $x_0, \dot{x}_0, \ddot{x}_0$  and for  $y_0, \dot{y}_0, \ddot{y}_0$ , and also by recovering the motion parameters  $c, \varepsilon, \delta$  and  $\lambda = \sqrt{Kc}$  in terms of the initial data, affine or polar.*

EXERCISE 1.30. *Do as well the physics in connection with Proposition 1.22, by arguing that the initial angular acceleration should be  $\ddot{\theta}_0 = 0$ , and so that we should have  $\delta = 0$ , and rewrite the formulae in Theorem 1.21 by using this observation.*

For three bonus points, you can write a short, nice essay on phenomenology, based on whatever things about Einstein and others that you have heard of, clearly refuting Newton. Finally, in case you're stuck with some of the above exercises, do not worry. We will be back to them in this book, later on, at undisclosed locations.



## CHAPTER 2

### Energy, momentum

#### 2a. Collisions and rockets

We have seen so far the basics of classical mechanics, notably with Newton's derivation of the Kepler laws. There are many possible continuations of the above, because we can either stay with the 2-body problem, and do a more specialized study of it, or talk about the 3-body problem, covering our usual Sun-Earth-Moon system, or any other Sun-Earth-satellite system, or talk about the  $N$ -body problem, with  $N \in \mathbb{N}$  arbitrary, or why not with  $N \rightarrow \infty$ , by doing some probability, or talk about many other interesting classical mechanics systems, such as pendulums, balls moving inside wells, and so on.

Instead of stepping right away into this, let us rather develop some more general theory. The point indeed is that, technically speaking, we managed so far to prove the Kepler first law just by using the Newton principles, and basic calculus, but if we want to investigate more complicated questions, more theory would be welcome. As usual, we will be quite brief on all this, and for further details on that follows, we refer to our standard mechanics books, [5], [33], [38], [57], [61], [90]. And with a preference for Kibble [57] and Taylor [38], for intermediate classical mechanics, these are both good places.

Let us begin with a discussion of the usual motion, in the absence of forces. That is something very simple, with the motion being linear, the bodies traveling at constant speed, namely their initial speed. And there is no acceleration to worry about.

However, interesting things happen when such objects collide, and we have:

**FACT 2.1.** *In the context of general linear motion, in the case of a collision between two bodies,  $m_1, m_2$  traveling at speeds  $v_1, v_2$ , the total momentum of the system*

$$p = m_1 v_1 + m_2 v_2$$

*is conserved. The same happens of course without collision either, and also for systems of  $N$  bodies, with  $N \in \mathbb{N}$  arbitrary, with all sorts of collisions allowed between them.*

As a first comment, is this really physics, or just some abstraction? We know that gravity is everywhere, and that the very existence of  $m_1, m_2$  leads to their gravity, and so to the negation of the general linear motion setting above. However, two trains colliding is

certainly physics, and even scary physics, and this has nothing to do with gravity. Thus, what we have here is a true physics principle, dealing with real-life situations.

In order to understand now what is going on, consider two objects as in Fact 2.1, traveling first in 1D, for simplifying, and bound for collision:

$$\circ_{m_1} \rightarrow_{v_1} \quad \leftarrow_{v_2} \circ_{m_2}$$

We know from real life that two things can happen, in this situation. The first case is that of an inelastic, also called plastic collision, where  $m_1, m_2$  decide when meeting that they love each other, and pursue their journey as a couple,  $m = m_1 + m_2$ :

$$\bullet_m \rightarrow_v$$

Of course, who really knows what really happens during a plastic collision, at the microscopic level, but assuming somehow that no energy or something is dissipated, during that hot encounter, Fact 2.1 holds indeed, and allows us to do the math.

To be more precise, the math is quite simple, so let us upgrade right away our discussion, to the case where we have two bodies colliding, in arbitrary  $N$  dimensions:

$$\begin{array}{ccc} \circ_{m_1} & & \circ_{m_2} \\ & \searrow & \swarrow \\ & v_1 & v_2 \end{array}$$

As a result of our collision, we have a new body  $m = m_1 + m_2$ , with speed  $v$ :

$$\begin{array}{c} \bullet_m \\ \downarrow \\ v \end{array}$$

The math, coming from the conservation of momentum, is very simple, as follows:

**PROPOSITION 2.2.** *In the context of a plastic collision between two bodies,*

$$m = m_1 + m_2 \quad , \quad v = \frac{m_1 v_1 + m_2 v_2}{m_1 + m_2}$$

*are the mass and speed of the resulting body.*

**PROOF.** This follows straight from Fact 2.1, because the momentum of  $m = m_1 + m_2$  equals the sum of the initial momenta of  $m_1, m_2$ , and is therefore given by:

$$mv = m_1 v_1 + m_2 v_2$$

Thus, we are led to the speed formula in the statement. □

The second case now, that can happen as well, is that of an elastic collision. This is something more complicated, so let us go back to 1D, the situation being:

$$\circ_{m_1} \rightarrow_{v_1} \quad \leftarrow_{v_2} \circ_{m_2}$$

The elastic collision is then the case opposed to love, with our two bodies meeting, comparing their  $m_i, v_i$ , then exchanging some speed depending on that, via a few quick fists, and then either keeping travelling forward, but slower, or going backwards:

$$\begin{array}{ccc} \bullet_{m_1} \rightarrow_{v'_1} & & \circ_{m_2} \rightarrow_{v'_2} \\ \leftarrow_{v'_1} \circ_{m_1} & & \leftarrow_{v'_2} \bullet_{m_2} \\ \leftarrow_{v'_1} \circ_{m_1} & & \circ_{m_2} \rightarrow_{v'_2} \end{array}$$

In the above pictures, the winner, which was  $m_1$  in the first case, and  $m_2$  in the second case, was awarded a black belt. As for the third case, that is some sort of draw.

Getting back now to the conservation of momentum, from Fact 2.1, it is pretty much clear that what we have there won't allow us to do the math. To be more precise, we can get from there only 1 equation, which is not enough for computing the output data. Fortunately, in the case of elastic collisions, Fact 2.1 can be complemented with:

**FACT 2.3.** *In the context of general linear motion, in the case of an elastic collision between two bodies,  $m_1, m_2$  traveling at speeds  $v_1, v_2$ , the total energy of the system*

$$E = \frac{m_1 ||v_1||^2}{2} + \frac{m_2 ||v_2||^2}{2}$$

*is conserved. The same happens of course without collision either, and also for systems of  $N$  bodies, with  $N \in \mathbb{N}$  arbitrary, with multi-elastic collisions allowed between them.*

Again, as in the case of the plastic collisions, who really knows what really happens during an elastic collision, at the microscopic level, but again, assuming that no things are lost, during that event, Fact 2.3 holds indeed, and allows us to do the math.

As another comment, while the formula of the momentum  $p = mv$  from Fact 2.1 was something quite simple and intuitive, the above formula of the energy  $E = m||v||^2/2$  is obviously something more subtle. We will be back to this, later.

Going ahead now, let us first investigate, just out of curiosity, what happens to the energy during a plastic collision. The result here, contradicting our previous guess that the moment conservation comes somehow from “no energy lost”, is as follows:

**THEOREM 2.4.** *In the context of a plastic collision between two bodies, we have:*

$$E < E_1 + E_2$$

*That is, some of the initial energy gets dissipated during the collision.*

**PROOF.** We use the equations found in Proposition 2.2, namely:

$$m = m_1 + m_2 \quad , \quad v = \frac{m_1 v_1 + m_2 v_2}{m_1 + m_2}$$

According to our definition of energy, from Fact 2.3, the initial energy is:

$$E_1 + E_2 = \frac{m_1||v_1||^2 + m_2||v_2||^2}{2}$$

As for the final energy, this is given by the following formula:

$$E = \frac{m||v||^2}{2} = \frac{||m_1v_1 + m_2v_2||^2}{2(m_1 + m_2)}$$

So, let us compute now the difference between these two quantities. We obtain:

$$\begin{aligned} E_1 + E_2 - E &= \frac{(m_1 + m_2)(m_1||v_1||^2 + m_2||v_2||^2) - ||m_1v_1 + m_2v_2||^2}{2(m_1 + m_2)} \\ &= \frac{m_1m_2(||v_1||^2 + ||v_2||^2) - 2\langle m_1v_1, m_2v_2 \rangle}{2(m_1 + m_2)} \\ &= \frac{m_1m_2(||v_1||^2 + ||v_2||^2 - 2\langle v_1, v_2 \rangle)}{2(m_1 + m_2)} \end{aligned}$$

But the quantity on top right is subject to the following inequality, valid for any two vectors  $v_1, v_2 \in \mathbb{R}^N$ , and with the equality case happening precisely when  $v_1 = v_2$ :

$$||v_1||^2 + ||v_2||^2 \geq 2\langle v_1, v_2 \rangle$$

Thus  $E_1 + E_2 \geq E$ , and since a collision cannot happen when the initial speeds are the same,  $v_1 = v_2$ , the equality case cannot happen, and so  $E_1 + E_2 > E$ , as stated.  $\square$

As already mentioned, the above result might seem quite surprising, contradicting our previous guess that the moment conservation principle comes from something of type “no energy lost”. Let us record this finding in the form of an informal statement:

**CONCLUSION 2.5.** *Momentum ain't the same thing as energy.*

Moving ahead now, and back to the elastic collisions, the two conservation principles that we have, namely Fact 2.1 and Fact 2.3, allow us to do the math. Let us first work out the case of an elastic collision in 1D, the initial picture being as follows:

$$\circ_{m_1} \rightarrow_{v_1} \qquad \leftarrow_{v_2} \circ_{m_2}$$

Depending on the resulting fight, we can have either a win or  $m_1$  or  $m_2$ , or a draw. Abstractly however, we can simply say that we are in a draw situation, the picture being as follows, with the convention that we do not know yet the directions of  $v'_1, v'_2$ :

$$\leftarrow_{v'_1} \circ_{m_1} \qquad \circ_{m_2} \rightarrow_{v'_2}$$

With these conventions made, the precise 1D result is as follows:

PROPOSITION 2.6. *In the context of a 1D elastic collision between two bodies,*

$$v'_1 = \frac{(m_1 - m_2)v_1 + 2m_2v_2}{m_1 + m_2}$$

$$v'_2 = \frac{(m_2 - m_1)v_2 + 2m_1v_1}{m_1 + m_2}$$

*are the resulting speeds of the two bodies.*

PROOF. According to our momentum and energy conservation principles from Fact 2.1 and Fact 2.3, the resulting speeds  $v'_1, v'_2$  satisfy the following two equations:

$$m_1v_1 + m_2v_2 = m_1v'_1 + m_2v'_2$$

$$m_1v_1^2 + m_2v_2^2 = m_1v_1'^2 + m_2v_2'^2$$

Now observe that these equations can be written as follows:

$$m_1(v_1 - v'_1) = m_2(v'_2 - v_2)$$

$$m_1(v_1^2 - v_1'^2) = m_2(v_2'^2 - v_2^2)$$

By dividing the second equation by the first one, our system becomes:

$$m_1(v_1 - v'_1) = m_2(v'_2 - v_2)$$

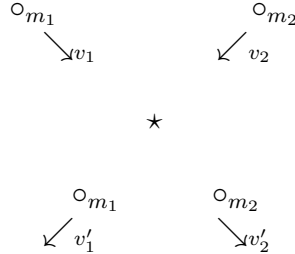
$$v_1 + v'_1 = v'_2 + v_2$$

And by doing now the math, we are led to the formulae in the statement.  $\square$

Getting now to arbitrary  $N$  dimensions, things here become more complicated, due to a number of reasons. As a first observation, which is actually very good news, we are in fact in 2 dimensions, and more specifically in the following plane:

$$E = \text{span}(v_1, v_2)$$

Thus we may assume  $E = \mathbb{R}^2$ , with the collision point being the origin  $0 \in \mathbb{R}^2$ , and do our computations here. Schematically, we can represent the collision as follows:



Let us quickly do the math. We have to compute two vectors  $v'_1, v'_2$ , accounting for a total of 4 numbers. But what we have is one vector equation, coming from momentum, and one scalar equation, coming from energy, so a total of 3 equations. Thus, we won't be able to do the math, unless we know something more on the collision mechanism.

To be more precise here, as already mentioned on numerous occasions, we don't really know what happens, at the microscopic level, when collisions take place, be them plastic or elastic, or of any other kind. And in the case of elastic collisions in  $N \geq 2$  dimensions, there are several possible mechanisms, which in practice each correspond to a different way in which the original angles of  $v_1, v_2$  get transformed into the output angles of  $v'_1, v'_2$ . More specifically, the extra parameter that we need is some sort of "scattering angle"  $\theta$ , coming from the precise mechanism of collision that we are investigating.

But this is something quite complicated, that we won't get into, at this stage. So long story short, and getting back now to math, in the absence of more data, and physical knowledge in general, our tools will be Fact 2.1 and Fact 2.3, and we will be able to solve the problem up to 1 degree of freedom. So, let us do this. The result is as follows:

**THEOREM 2.7.** *In the context of an elastic collision between two bodies, assumed without loss of generality to happen in  $\mathbb{R}^2$ , the output speeds are*

$$v'_1 = v_1 + \frac{q}{m_1} \quad , \quad v'_2 = v_2 - \frac{q}{m_2}$$

*with the vector parameter  $q \in \mathbb{R}^2$  being subject to the following equation:*

$$2 < v_2 - v_1, q > = \left( \frac{1}{m_1} + \frac{1}{m_2} \right) \|q\|^2$$

*Thus, the collision problem is solved, up to an angle  $\theta \in \mathbb{R}$ .*

**PROOF.** We can solve this by using Fact 2.1 and Fact 2.3, as follows:

(1) According to our general momentum and energy conservation principles, the output speeds  $v'_1, v'_2$  are subject to the following two equations:

$$\begin{aligned} m_1 v_1 + m_2 v_2 &= m_1 v'_1 + m_2 v'_2 \\ m_1 \|v_1\|^2 + m_2 \|v_2\|^2 &= m_1 \|v'_1\|^2 + m_2 \|v'_2\|^2 \end{aligned}$$

Let us first look at the first equation. This equation can be written as follows:

$$m_1(v'_1 - v_1) = m_2(v_2 - v'_2)$$

Now if we call  $q$  this quantity, which is the individual change of momentum, from the perspective of  $m_1$ , and from the opposite perspective of  $m_2$ , we have:

$$v'_1 = v_1 + \frac{q}{m_1} \quad , \quad v'_2 = v_2 - \frac{q}{m_2}$$

(2) Now let us plug these values into the second equation above. We obtain:

$$m_1 \|v_1\|^2 + m_2 \|v_2\|^2 = m_1 \left\| v_1 + \frac{q}{m_1} \right\|^2 + m_2 \left\| v_2 - \frac{q}{m_2} \right\|^2$$

By expanding the scalar products and then simplifying, we obtain:

$$\frac{\|q\|^2}{m_1} + \frac{\|q\|^2}{m_2} + 2 \langle v_1, q \rangle - 2 \langle v_2, q \rangle = 0$$

Thus, we are led to the formulae in the statement.

(3) As for the last assertion, this is something rather philosophical. To be more precise, we know that our parameter  $q \in \mathbb{R}^2$  is subject to an equation of the following type:

$$\langle v, q \rangle = \lambda \|q\|^2$$

Now if we denote by  $\theta \in \mathbb{R}$  the oriented angle between  $v, q$ , this equation reads:

$$\|v\| \cos \theta = \lambda \|q\|$$

Thus we can recover  $\|q\|$ , and so also  $q \in \mathbb{R}^2$  itself, out of this angle  $\theta \in \mathbb{R}$ , and this leads to the conclusion that our problem is indeed solved up to an angle  $\theta \in \mathbb{R}$ .  $\square$

As an illustration for Theorem 2.7, let us work out what happens in the case of a 1D collision. Here we already know the answer, from Proposition 2.6, but wait for it. So, let us get back to our usual 1D scheme, with  $m_1, m_2$  about to collide, on a line:

$$\circ_{m_1} \rightarrow_{v_1} \quad \leftarrow_{v_2} \circ_{m_2}$$

In the context of Theorem 2.7, the fact that we are now in 1D simply tells us that the speed vectors  $v_1, v_2 \in \mathbb{R}^2$  are proportional,  $v_1 = \lambda v_2$ . But this does not force in any way the vector  $q \in \mathbb{R}^2$  there to be aligned with  $v_1, v_2$ , or if you prefer, the angle  $\theta \in \mathbb{R}$  there to be 0. Thus, we are led to the peculiar conclusion that our general elastic collision formalism, leading to Theorem 2.7, theoretically allows escapes from 1D to 2D.

What to do? Modesty as usual, this is what we have, and it's after all not that bad. And for closing this 1D discussion, let us however formulate, as a consequence of our new knowledge from Theorem 2.7, a better formulation of Proposition 2.6, as follows:

**THEOREM 2.8.** *In the context of a 1D elastic collision between two bodies, staying as normal in 1D, the resulting speeds of the two bodies are*

$$v'_1 = v_1 + \frac{q}{m_1} \quad , \quad v'_2 = v_2 - \frac{q}{m_2}$$

where  $q \in \mathbb{R}$  is the individual change of momentum, given by

$$\left( \frac{1}{m_1} + \frac{1}{m_2} \right) q = 2(v_2 - v_1)$$

from the perspective of  $m_1$ , and from the opposite perspective of  $m_2$ .

PROOF. This follows either from Proposition 2.6, or from Theorem 2.7:

(1) From the perspective of Proposition 2.6, we have done some quick algebra there, without really knowing what we're doing, leading to the following formulae:

$$v'_1 = \frac{(m_1 - m_2)v_1 + 2m_2v_2}{m_1 + m_2} \quad , \quad v'_2 = \frac{(m_2 - m_1)v_2 + 2m_1v_1}{m_1 + m_2}$$

Now observe that these two formulae can be alternatively written as follows:

$$v'_1 = v_1 + \frac{2m_2(v_2 - v_1)}{m_1 + m_2} \quad , \quad v'_2 = v_2 + \frac{2m_1(v_1 - v_2)}{m_1 + m_2}$$

But this leads to the formulae in the statement, and to that conclusion about  $q$ .

(2) From the perspective of Theorem 2.7, we have indeed the formulae of  $v'_1, v'_2$  in the statement, and with  $q$  being the change of momentum, as stated. Thus, it remains to establish the precise formula of  $q$ . In the context of Theorem 2.7, the equation is:

$$2 < v_2 - v_1, q > = \left( \frac{1}{m_1} + \frac{1}{m_2} \right) \|q\|^2$$

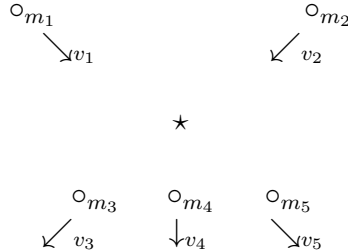
Now since everything happens, by assumption, in 1D, the vectors  $v_1, v_2, q$  are pairwise proportional. Thus the above scalar product becomes a usual product, and also the squared norm becomes a usual square, and so our equation simply reads:

$$2(v_2 - v_1)q = \left( \frac{1}{m_1} + \frac{1}{m_2} \right) q^2$$

But this gives the formula of  $q$  in the statement, and we are done.  $\square$

So long for elastic collisions. We will be back to them later on in this book, and to some related scattering questions too, once we'll decide what exact types of particles we are dealing with, as to be able to come up, via some more phenomenology and physics, with answers to some of the above questions, not to say weird mysteries.

Finally, again speaking generalities about collisions, remember that our first example was that of two trains colliding. But that type of collision, which is somewhat generic in real-life problems, is not elastic, neither plastic, but rather something in between, with the generic, 2D picture being something quite frightening, of the following type:





Again, this is something complicated, that we will not discuss at this stage. Let us point out, however, that the conservation of momentum, from Fact 2.1 above, does apply to such situations, and can be used in order to get information. More on this later.

As a main application now of the general theory developed above, and in relation with gravity as well, we can use momentum for beating gravity, as follows:

THEOREM 2.9. *We can build rockets, by ejecting mass from a body*

$$\dots\dots \bullet_M \rightarrow$$

*with the body moving in the opposite direction to the ejection direction.*

PROOF. The functioning principle of rockets is clear indeed from the conservation of the momentum principle, because ejecting mass to the left will move us to the right. As for the precise math of this, this can be worked out too, the idea being as follows:

(1) Let us first study the case of a single ejection. We begin with  $M$  at rest:

$$\bullet_M$$

Now let us eject to the left a mass  $m$ , with speed  $s$ . The situation becomes:

$$\leftarrow_s \circ_m \qquad \bullet_{M-m} \rightarrow_v$$

By conservation of momentum we have  $(M - m)v = ms$ , and so:

$$v = \frac{ms}{M - m}$$

(2) Let us study now a double ejection. At the first stage, we have as above, by labelling now the ejection data with a 1 index, standing for stage 1 of the ejection:

$$\leftarrow_{s_1} \circ_{m_1} \qquad \bullet_{M-m_1} \rightarrow_{v_1}$$

At the second stage now, that of ejecting a mass  $m_2$ , with speed  $s_2$ , with the observation that the ejection speed  $s_2$  is only relative to  $M$ , the situation becomes:

$$\leftarrow_{s_1} \circ_{m_1} \quad \leftarrow_{s_2-v_1} \circ_{m_2} \qquad \bullet_{M-m_1-m_2} \rightarrow_{v_2}$$

Neglecting the first ejection, the conservation of momentum tells us that:

$$(M - m_1 - m_2)v_2 - m_2(s_2 - v_1) = (M - m_1)v_1$$

But this equation can be written in the following way:

$$(M - m_1 - m_2)v_2 = (M - m_1 - m_2)v_1 + m_2s_2$$

By using now (1) for the value of  $v_1$ , the speed after the second ejection is given by:

$$\begin{aligned} v_2 &= v_1 + \frac{m_2s_2}{M - m_1 - m_2} \\ &= \frac{m_1s_1}{M - m_1} + \frac{m_2s_2}{M - m_1 - m_2} \end{aligned}$$

(3) In the general case now, that of a multiple ejection, of masses  $m_1, \dots, m_k$  with respective speeds  $s_1, \dots, s_k$ , the same idea applies, and gives as eventual speed:

$$v_k = \frac{m_1 s_1}{M - m_1} + \frac{m_2 s_2}{M - m_1 - m_2} + \dots + \frac{m_k s_k}{M - m_1 - \dots - m_k}$$

In the particular case where the ejection mass  $m$  is constant, we obtain:

$$v_k = \frac{m s_1}{M - m} + \frac{m s_2}{M - 2m} + \dots + \frac{m s_k}{M - km}$$

Also, in the particular case where the ejection speed  $s$  is constant, we obtain:

$$v_k = \left( \frac{m_1}{M - m_1} + \frac{m_2}{M - m_1 - m_2} + \dots + \frac{m_k}{M - m_1 - \dots - m_k} \right) s$$

And in the case where both the mass  $m$  and speed  $s$  are constant, we obtain:

$$v_k = \left( \frac{m}{M - m} + \frac{m}{M - 2m} + \dots + \frac{m}{M - km} \right) s$$

(4) Let us work out now the asymptotics. For simplifying we will assume that we are in the last case, that of a constant ejection mass  $m$  and speed  $s$ , although modifications of our argument will apply as well more generally. With  $m = \varepsilon M$ , we have:

$$v_k = \left( \frac{\varepsilon}{1 - \varepsilon} + \frac{\varepsilon}{1 - 2\varepsilon} + \dots + \frac{\varepsilon}{1 - k\varepsilon} \right) s$$

We will assume that  $\varepsilon$  is small, and that  $k \in \mathbb{N}$  is such that the total ejection mass, or rather the fraction  $k\varepsilon = r \in (0, 1)$  of this total ejection mass, compared to the initial mass  $M$  of our rocket, is fixed. Thus, we want to compute  $v_k$  in the following regime:

$$\varepsilon = \frac{r}{k} \quad , \quad k \rightarrow \infty$$

Now remember the definition of the integral, as the area below the graph of the function, which is approximable by the Riemann method by usual rectangles. In the particular case of the function  $1/x$ , this picture gives us the following formula:

$$\int_{1-r}^1 \frac{1}{x} \simeq \frac{1}{k} \left( \frac{1}{1 - \varepsilon} + \frac{1}{1 - 2\varepsilon} + \dots + \frac{1}{1 - k\varepsilon} \right)$$

Thus, the final velocity we are interested in is given by the following formula:

$$\begin{aligned} v &= \varepsilon s \left( \frac{1}{1 - \varepsilon} + \frac{1}{1 - 2\varepsilon} + \dots + \frac{1}{1 - k\varepsilon} \right) \\ &= \frac{rs}{k} \left( \frac{1}{1 - \varepsilon} + \frac{1}{1 - 2\varepsilon} + \dots + \frac{1}{1 - k\varepsilon} \right) \\ &\simeq rs \int_{1-r}^1 \frac{1}{x} \\ &= -r \log(1 - r)s \end{aligned}$$

(5) As an illustration here, assume that our rocket has shrunk, from a continuous ejection process at speed  $s$ , up to mass  $M/e$ , with  $e \simeq 2.718$  being the usual constant from analysis. In this case we have  $r = 1 - 1/e$ , and the velocity reached is given by:

$$v = - \left(1 - \frac{1}{e}\right) \log \left(\frac{1}{e}\right) s = \left(1 - \frac{1}{e}\right) s \simeq 0.632s$$

There are of course many other things that can be said here, and in particular we have some interesting questions related to the best strategy to be followed, in order to beat a given force  $F$ , such as gravity, or several such forces. More on this later.  $\square$

We did some good math in the above, and for future reference, let us record:

**THEOREM 2.10.** *For a rocket having initial mass  $M$ , and functioning by ejecting pieces of mass  $m$  at a constant speed  $s$ , the speed reached after  $k$  ejections is:*

$$v = \left( \frac{m}{M-m} + \frac{m}{M-2m} + \dots + \frac{m}{M-km} \right) s$$

*In the  $m = \varepsilon M$ ,  $k\varepsilon = r \in (0, 1)$  and  $k \rightarrow \infty$  regime we have*

$$v \simeq -r \log(1-r)s$$

*which represents the velocity after the rocket has shrunk to mass  $(1-r)M$ . Moreover, this latter conclusion holds under the sole assumption that  $s$  is constant.*

**PROOF.** Here the two formulae in the statement are our two main formulae, selected from the proof of Theorem 2.9. As for the last assertion, recall also from the proof of Theorem 2.9 that, assuming only that  $s$  is constant, the formula of the velocity is:

$$v = \left( \frac{m_1}{M-m_1} + \frac{m_2}{M-m_1-m_2} + \dots + \frac{m_k}{M-m_1-\dots-m_k} \right) s$$

The point now is that, assuming that the ejection pieces  $m_1, \dots, m_k$ , instead of being all equal to a certain  $m$ , are at least of comparable size, the Riemann integration arguments from the end of the proof of Theorem 2.9 will apply as well, and give the result.  $\square$

Let us record as well the continuous version of the above result:

**THEOREM 2.11.** *For a rocket with initial mass  $M$ , ejecting at speed  $s = s(x)$ , with  $x$  being the fraction of the already ejected mass, the speed reached at  $x = r$  is:*

$$v = r \int_{1-r}^1 \frac{s}{x} dx$$

*In particular, when the ejection speed is constant  $s \in \mathbb{R}$ , we have  $v = -r \log(1-r)s$ .*

PROOF. Again, this is something which follows from the above. To be more precise, the last assertion follows from Theorem 2.10, or from the first assertion. Regarding now the first assertion, recall from the proof of Theorem 2.9 that the discrete formula is:

$$v_k = \frac{ms_1}{M-m} + \frac{ms_2}{M-2m} + \dots + \frac{ms_k}{M-km}$$

We can now proceed as in the proof of Theorem 2.9, and with  $m = \varepsilon M$  as there, and then with  $k\varepsilon = r \in (0, 1)$  fixed and  $k \rightarrow \infty$  as there as well, we obtain:

$$\begin{aligned} v_k &= \varepsilon \left( \frac{s_1}{1-\varepsilon} + \frac{s_2}{1-2\varepsilon} + \dots + \frac{s_k}{1-k\varepsilon} \right) \\ &= \frac{r}{k} \left( \frac{s_1}{1-\varepsilon} + \frac{s_2}{1-2\varepsilon} + \dots + \frac{s_k}{1-k\varepsilon} \right) \\ &\simeq r \int_{1-r}^1 \frac{s}{x} dx \end{aligned}$$

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

As already mentioned, more on this later, when talking about gravity, and trying to beat it with such devices. In particular, we will be back to the above computations, and fine-tune the choice of the ejection method, depending on the problem to be solved.

Finally, let us mention that the above result remains a bit theoretical, because if you are a space engineer, one of your main concerns, besides of course beating gravity, is that of beating atmospheric drag too. More on this later, when talking about air and other fluids, corresponding drag, and all other kinds of friction.

## 2b. Angular momentum

Back to gravity now, in order to further advance on the Kepler problem, and on further problems, we would like to have more tools. So, a natural question appears: are there gravitational analogues of the principles of conservation of momentum, and energy?

Let us begin with some discussion. In what regards the principles of conservation of momentum, and of energy, we have met them in the general context of the linear motion of objects, in relation with collisions. So, as a preliminary, and perhaps naive question, are there actually collisions to be discussed, in the gravitational context? And the answer here is no, at least at the current stage of development of our theory, due to:

**FACT 2.12.** *In the context of basic classical mechanics, where bodies are points, acted upon by their gravitational attractions only, collisions happen with probability 0.*

As a first comment here, what kind of fact is this. Indeed, since basic classical mechanics was axiomatized via the Newton principles, that is math, and so the above fact is a “mathematical fact”. But why is it not a theorem, then? Well, because this is something

which, while being very plausible and intuitive, is quite hard to prove. We will however accept it as a fact. To be more precise, our facts so far in this book were things coming by observing Mother Nature, but why not including some things coming by observing mankind too, and more specifically the scientists, and what they know. So if they say it's right, it's probably right, and we can use this in the context of the present discussion.

Along the same lines, and less mathematically now, we have as well:

**FACT 2.13.** *In the context of basic celestial mechanics, where bodies are stars, acted upon by their gravitational attractions only, collisions almost never happen.*

Indeed, just take a look at the night sky, not many collisions going on there, right. Some falling stars of course, but these are not stars, just asteroids getting heated, usually up to destruction, by our atmosphere. Also, a supernova from time to time, but that is not something due to a collision, just an old star whose internal mechanism collapses.

There is of course some mathematics behind Fact 2.13 too, because what we call there stars are, gravitationally speaking, simply objects having small radius, when compared to the distances between them. Thus, Fact 2.13 can be regarded as being a difficult mathematical generalization of Fact 2.12. Which can be probably still be proved by mathematicians with their advanced tools, but let us not get here into that.

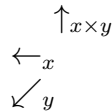
To summarize now, nothing going on with collisions, and in order to find gravitational principles of conservation of momentum and energy, we have to look somewhere else. And guess what, the answer here will be not that complicated, because such conservation principles can be found in fact in the context of the good old Kepler 2-body problem.

Let us first discuss momentum. We will need here some math, as follows:

**DEFINITION 2.14.** *The vector product of two vectors in  $\mathbb{R}^3$  is given by*

$$x \times y = \|x\| \cdot \|y\| \cdot \sin \theta \cdot n$$

where  $n \in \mathbb{R}^3$  with  $n \perp x, y$  and  $\|n\| = 1$  is constructed using the right-hand rule:



Alternatively, in usual vertical linear algebra notation for all vectors,

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \times \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} x_2 y_3 - x_3 y_2 \\ x_3 y_1 - x_1 y_3 \\ x_1 y_2 - x_2 y_1 \end{pmatrix}$$

the rule being that of computing  $2 \times 2$  determinants, and adding a middle sign.

Obviously, this definition is something quite subtle, and also something very annoying, because you always need this, and always forget the formula. Here are my personal methods. With the first definition, what I always remember is that:

$$||x \times y|| \sim ||x||, ||y||$$

$$x \times x = 0$$

$$e_1 \times e_2 = e_3$$

So, here's how it works. We're looking for a vector  $x \times y$  whose length is proportional to those of  $x, y$ . But now the second formula tells us that the angle  $\theta$  between  $x, y$  must be involved via  $0 \rightarrow 0$ , and so the factor can only be  $\sin \theta$ . And with this we're almost there, it's just a matter of choosing the orientation, and this comes either from the right-hand rule (or perhaps left-hand rule, do I remember right?) or from  $e_1 \times e_2 = e_3$ .

As with the second definition, that I like the most, what I remember here is simply:

$$\begin{vmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{vmatrix} = ?$$

Indeed, when trying to compute this determinant, by developing over the first column, what you get as coefficients are the entries of  $x \times y$ . And with the good middle sign.

It is also good to know that  $x \times y$  exists only in 3 dimensions, with our only tool in  $N \neq 3$  dimensions being the usual  $\langle x, y \rangle$ . This is actually quite interesting for us, in relation with our conservation principles for gravity, but more on this later.

We are now ready to state our first conservation principle, the momentum one. This is something quite technical, at least at the first glance, as follows:

**THEOREM 2.15.** *In the gravitational 2-body problem, the angular momentum*

$$J = x \times p$$

*with  $p = mv$  being the usual momentum, is conserved.*

**PROOF.** There are several things to be said here, the idea being as follows:

(1) First of all the usual momentum,  $p = mv$ , is not conserved, because the simplest solution is the circular motion, where the moment gets turned around. But this suggests precisely that, in order to fix the lack of conservation of the momentum  $p$ , what we have to do is to make a vector product with the position  $x$ . Leading to  $J$ , as above.

(2) Another comment is that the conservation of  $J$  holds in fact in more general settings too, involving other kinds of mechanics, with the idea being that “the total torque of the system is 0”, which is something that you are probably familiar with. If not yet, try

changing a tyre on an old car. That tyre is probably stuck, and a lot of work there, and if you want to curse and blame somebody for that, blame the notion of torque.

(3) Regarding now the proof, consider indeed a particle  $m$  moving under the gravitational force of a particle  $M$ , assumed, as in chapter 1, to be fixed at 0. By using the fact that for two proportional vectors,  $p \sim q$ , we have  $p \times q = 0$ , we obtain:

$$\begin{aligned} \dot{J} &= \dot{x} \times p + x \times \dot{p} \\ &= v \times mv + x \times ma \\ &= m(v \times v + x \times a) \\ &= m(0 + 0) \\ &= 0 \end{aligned}$$

Now since the derivative of  $J$  vanishes, this quantity is constant, as stated.  $\square$

While the above principle looks like something quite trivial, the mathematics behind it is quite interesting, and has several notable consequences, as follows:

**THEOREM 2.16.** *In the context of a 2-body problem, the following happen:*

- (1) *The fact that the direction of  $J$  is fixed tells us that the trajectory of one body with respect to the other lies in a plane.*
- (2) *The fact that the magnitude of  $J$  is fixed tells us that the Kepler 2 law holds, namely that we have same areas swept by  $Ox$  over the same times.*

**PROOF.** This follows indeed from Theorem 2.15, as follows:

(1) We have by definition  $J = m(x \times v)$ , and since a vector product is orthogonal on both the vectors it comes from, we deduce from this that we have:

$$J \perp x, v$$

But this can be written as follows, with  $J^\perp$  standing for the plane orthogonal to  $J$ :

$$x, v \in J^\perp$$

Now since  $J$  is fixed by Theorem 2.15, we conclude that both  $x, v$ , and in particular the position  $x$ , and so the whole trajectory, lie in this fixed plane  $J^\perp$ , as claimed.

(2) Conversely now, forget about Theorem 2.15, and assume that the trajectory lies in a certain plane  $E$ . Thus  $x \in E$ , and by differentiating we have  $v \in E$  too, and so  $x, v \in E$ . Thus  $E = J^\perp$ , and so  $J = E^\perp$ , so the direction of  $J$  is fixed, as claimed.

(3) Regarding now the last assertion, we already know from chapter 1, or rather from the exercises there, if you worked hard on them, that Kepler 2 is more or less equivalent to  $\dot{\theta} = \lambda/r^2$ . However, the derivation of  $\dot{\theta} = \lambda/r^2$  was something tricky, and what we want to prove now is that this appears as a simple consequence of  $\|J\| = \text{constant}$ .

(4) In order to do so, let us compute  $J$ , according to its definition  $J = x \times p$ , but in polar coordinates, which will change everything. Since  $p = m\dot{x}$ , we have:

$$J = r \begin{pmatrix} \cos \theta \\ \sin \theta \\ 0 \end{pmatrix} \times m \begin{pmatrix} \dot{r} \cos \theta - r \sin \theta \cdot \dot{\theta} \\ \dot{r} \sin \theta + r \cos \theta \cdot \dot{\theta} \\ 0 \end{pmatrix}$$

Now recall from the definition of the vector product that we have:

$$\begin{pmatrix} a \\ b \\ 0 \end{pmatrix} \times \begin{pmatrix} c \\ d \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ ad - bc \end{pmatrix}$$

Thus  $J$  is a vector of the above form, with its last component being:

$$\begin{aligned} J_z &= rm \begin{vmatrix} \cos \theta & \dot{r} \cos \theta - r \sin \theta \cdot \dot{\theta} \\ \sin \theta & \dot{r} \sin \theta + r \cos \theta \cdot \dot{\theta} \end{vmatrix} \\ &= rm \cdot r(\cos^2 \theta + \sin^2 \theta)\dot{\theta} \\ &= r^2 m \cdot \dot{\theta} \end{aligned}$$

(5) Now with the above formula in hand, our claim is that the magnitude  $\|J\|$  is constant precisely when  $\dot{\theta} = \lambda/r^2$ , for some  $\lambda \in \mathbb{R}$ . Indeed, up to the obvious fact that the orientation of  $J$  is a binary parameter, who cannot just switch like that, let us just agree on this, knowing  $J$  is the same as knowing  $J_z$ , and is also the same as knowing  $\|J\|$ . Thus, our claim is proved, and this leads to the conclusion in the statement.  $\square$

This was for the basic theory of the angular momentum. There are many more things that can be said here, either of abstract nature, or in relation with all sorts of things happening in the real life, and for more on all this, we refer to a standard text, such as the book of Kibble [57], or the book of Taylor [90]. We also recommend coming for holidays and fun to France, where there are roundabouts all around the place, the thing being that, while  $p \gg 0$  is everywhere forbidden by law,  $J \gg 0$  is generally not.

## 2c. Potential energy

Let us go ahead now with our second task, namely finding and discussing the conservation of energy, in the gravitational context. This is something that you're very familiar with, because when you throw a rock up in the sky, the more energy you put into your throw, the higher the rock will get. And the higher the rock will get, the faster it will come back on your head. In other words, the kinetic energy  $T$  gets converted into height, and vice versa, so if we find a way of calling that height "potential" energy  $V$ , then our conservation principle will simply state that the total energy  $E = T + V$  is constant.

In technical terms now, following the material from chapter 1, what we did is more or less to solve the problem in the context of 1D gravity. So, let us do now the math.



Again following the discussion in chapter 1, the simplest situation is that of a free fall with initial velocity  $v_0 = 0$ , and our conservation principle here is as follows:

**PROPOSITION 2.17.** *In the context of a free fall from distance  $x_0 = R \gg 0$ , with initial velocity  $v_0 = 0$ , if we define the potential energy to be*

$$V = mgx$$

*then the total energy  $E = T + V$ , with  $T = mv^2/2$  as usual, is constant,  $E \simeq mgR$ .*

**PROOF.** We know that the equation of motion is as follows, with  $g = GM/R^2$ :

$$x \simeq R - \frac{gt^2}{2}$$

The kinetic energy, from now on to be denoted  $T$ , is then given by:

$$T \simeq \frac{mv^2}{2} = \frac{mg^2t^2}{2}$$

Thus with  $V = mgx$  as in the statement, and then with  $E = T + V$ , we have:

$$E = T + V \simeq mgR$$

But this is a constant, and so we have our conservation principle, as desired.  $\square$

At this point, we are rather inside math, and many questions arise. We know that  $E \simeq mgR$ , but by some kind of miracle, do we actually have  $E = mgR$ ? Also, what is the meaning of  $V$ ? What about the meaning of  $E$ ? What about adding a suitable constant to  $V$ , and so to  $E$  too, will that make these quantities easier to understand?

These questions will be answered in due time. For the moment, let us keep doing the math, that is always relaxing, and one solid lead. As a next result, we have:

**PROPOSITION 2.18.** *In the context of a free fall from distance  $x_0 = R \gg 0$ , with initial velocity vector  $v_0 \in \mathbb{R}^2$ , if we define the potential energy to be*

$$V = m \langle g, x \rangle$$

*with  $g = GM/R^2$  being regarded as usual as a vector pointing upwards, then*

$$E = T + V$$

*with  $T = m||v||^2/2$  as usual, is constant,  $E \simeq T_0 + mgR$ , with  $g$  now back scalar.*

**PROOF.** We can do this in two steps, first by adding an extra parameter to the computation in Proposition 2.17, and then by adding another extra parameter:

(1) Let us first examine the 1D case, where  $v_0 = s$  is a vector aligned to  $x$ , and so a number. Here the equation of motion is as follows, with  $g = GM/R^2$  as usual:

$$x \simeq R + st - \frac{gt^2}{2}$$

The speed being  $v \simeq s - gt$ , with  $V = mgx$  and  $E = T + V$  as above, we have:

$$\begin{aligned}
 E &= T + V \\
 &\simeq \frac{m(s - gt)^2}{2} + mg \left( R + st - \frac{gt^2}{2} \right) \\
 &= \frac{ms^2}{2} + mgR \\
 &= T_0 + mgR
 \end{aligned}$$

(2) In the general case now, with  $v_0 = s$ , the equation of motion is as before, with  $R, g$  being now vectors pointing upwards, and if we write  $s = (a, b)$ , then we have:

$$\begin{aligned}
 T &\simeq \frac{m||s - gt||^2}{2} \\
 &= \frac{m((a - gt)^2 + b^2)}{2} \\
 &= \frac{m(a^2 + b^2)}{2} - magt + \frac{mg^2t^2}{2} \\
 &= T_0 - mg \left( at - \frac{gt^2}{2} \right)
 \end{aligned}$$

With  $g$  vector pointing upwards, the last quantity is  $m < g, x - R >$ , so if we add  $V = m < g, x >$ , we obtain  $T_0 + mgR$ , with  $g, R$  being back scalars, as desired.  $\square$

With the above done, let us turn now to the real thing, 3D gravity. We are interested in the general 2-body problem, where  $M$  is fixed at 0, and  $m$  moves under the gravitational force of  $M$ . The above computations, coming from our “kinetic energy gets converted into height, and vice versa” principle, suggest defining the potential energy as:

$$V \sim ||x||$$

However, this is wrong, because in our formula  $V = mgx$  the quantity  $g = GM/R^2$  depends on the average height, which is the parameter  $R$ , no longer assumed to satisfy  $R \gg 0$ . In view of this, the correct formula for the potential energy should be:

$$V \sim \frac{1}{||x||}$$

In order now to find the constant, it is enough to rewrite  $V = mgx$  by getting rid of the parameter  $g = GM/R^2$ . We obtain in this way, with  $K = GM$  as usual:

$$V = mgx = \frac{mGMx}{R^2} \simeq \frac{mGM}{||x||} = \frac{Km}{||x||}$$

Thus, we have our formula for  $V$ , and the question now is if  $E = T + V$  is constant. And the answer here is unfortunately no, due to some bizarre reasons, with rather  $E = T - V$

appearing to be constant, or at least that's what computations tend to suggest. In short, stuck, and in the lack of valuable ideas, we will have to ask the cat. And cat says:

ADVICE 2.19. *In case your computation needs a  $-$  sign instead of a  $+$ , just change that sign, do the computation, and you'll understand later.*

So, following this precious advice, let us simply change the sign of  $V$ . We are led in this way to the following remarkable result, which not only says that  $E$  is approximately constant, as in our previous computations, but is actually a plain constant:

THEOREM 2.20. *In the context of the 2-body problem, with  $M$  fixed at 0 and with  $m$  moving, if we define the kinetic and potential energy of  $m$  to be*

$$T = \frac{m||v||^2}{2} \quad , \quad V = -\frac{Km}{||x||}$$

*with  $K = GM$  as usual, then the total energy  $E = T + V$  is constant.*

PROOF. The idea will be that of proving  $\dot{E} = 0$ . We can do this as follows:

(1) In what regards the derivative of  $T$ , the computation here is something very simple, coming straight from the formula  $||v||^2 = \langle v, v \rangle$ , as follows:

$$\begin{aligned} \dot{T} &= \frac{m(\langle v, \dot{v} \rangle + \langle \dot{v}, v \rangle)}{2} \\ &= m \langle v, \dot{v} \rangle \\ &= m \langle v, a \rangle \end{aligned}$$

(2) In order to compute now the derivative of  $V$ , let us first compute the derivative of the function  $f(x) = 1/||x||$ . Again by using  $||x||^2 = \langle x, x \rangle$ , we obtain:

$$\begin{aligned} \dot{f} &= -\frac{1}{2} \cdot \frac{\langle x, \dot{x} \rangle + \langle \dot{x}, x \rangle}{\langle x, x \rangle^{3/2}} \\ &= -\frac{\langle x, \dot{x} \rangle}{\langle x, x \rangle^{3/2}} \\ &= -\frac{\langle x, v \rangle}{||x||^3} \end{aligned}$$

(3) Thus, getting now to the potential energy  $V$ , we have the following formula:

$$\dot{V} = \frac{Km \langle x, v \rangle}{||x||^3}$$

In order to further process this, remember the equation of motion of  $m$ , namely:

$$a = -\frac{Kx}{||x||^3}$$

We will of course jump on this, as to get rid of  $\|x\|^3$ , and we finally obtain:

$$\dot{V} = -m \langle a, v \rangle$$

(4) We are ready now to prove our result. Indeed, we have:

$$\dot{E} = \dot{T} + \dot{V} = m \langle v, a \rangle - m \langle a, v \rangle = 0$$

Now since the derivative vanishes,  $E$  is constant, as claimed.  $\square$

Very good all this, but now we still have to understand the relation with Propositions 2.17 and 2.18, with that sign of  $V$  mysteriously switching. And we have here the following result, upgrading Propositions 2.17 and 2.18, and clarifying the whole thing:

**THEOREM 2.21.** *In the context of a free fall from distance  $x_0 = R \gg 0$ , with initial velocity  $v_0 = 0$ , if we define the kinetic and potential energy of  $m$  to be*

$$T = \frac{mv^2}{2} \quad , \quad V = -\frac{Km}{x}$$

*with  $K = GM$  as usual, then the total energy  $E = T + V$  is constant. Moreover,*

$$V \simeq mgx - 2mgR$$

*with  $g = GM/R^2$ , and so  $E' = T + mgx$  is approximately constant,  $E' \simeq mgR$ . The same happens for a free fall from  $x_0 = R \gg 0$ , with initial velocity vector  $v_0 \in \mathbb{R}^2$ .*

**PROOF.** The first assertion is something that we know, coming from Theorem 2.20. In order to clarify now the relation with Proposition 2.17, we first have:

$$V = -\frac{Km}{x} = -\frac{GMm}{x} = -\frac{mgR^2}{x}$$

Now by writing  $x = R(1 - \varepsilon)$ , we obtain the estimate in the statement, namely:

$$V = -\frac{mgR}{1 - \varepsilon} \simeq -mgR(1 + \varepsilon) = mgR[(1 - \varepsilon) - 2] = mgx - 2mgR$$

Thus with  $V' = mgx$  we have  $V \simeq V' - 2mgR$ , and so  $E' = T + V'$  satisfies:

$$E' \simeq E + 2mgR = E_0 + 2mgR = V_0 + 2mgR = mgR$$

Finally, the last assertion, which is a bit more general, follows in the same way.  $\square$

Observe how impressively Theorem 2.20 clarified our previous computations. However, that was a bit of a miracle, and the general philosophy “work out the asymptotics first, and get into the real problem afterwards”, also a cat advice, still stands, in general. Finally, cat also says that our wrong energy function  $L = T - V$  looks quite interesting to him, but sometimes you cannot really understand all that cats say. Maybe later.

## 2d. Conservative forces

We have seen that the momentum and energy conservation principles from the very basic, acceleration-free mechanics, have gravitational analogues, namely the conservation of the angular momentum  $J$ , and the conservation of the total energy  $E = T + V$ . Things have been quite tricky, both with  $J$  and  $E$ , but somehow trickier with  $E$ , and our purpose in what follows will be to develop some further general theory, in order to understand what the potential energy  $V$ , and then what the total energy  $E = T + V$ , truly are.

Getting back to Theorem 2.20 and its proof, everything there was based on two main formulae, both involving the potential energy  $V$ , which are as follows, the first one being our definition of  $V$ , and the second one coming from the equation of motion:

$$V = -\frac{Km}{\|x\|} \quad , \quad \dot{V} = -m < a, v >$$

The point now, which is something tricky, is that in order to fully understand the meaning of these formulae, and of  $V$  itself, we need a third formula, as follows:

**PROPOSITION 2.22.** *In the context of the 2-body problem, the force applied to  $m$  is*

$$F = -\nabla V$$

where  $V = -Km/\|x\|$  is as usual the potential energy of  $m$ .

**PROOF.** According to the Newton principles, and with  $K = GM$  as usual, the force applied to  $m$  by the object  $M$  positioned at 0 is given by:

$$F = -\|F\| \cdot \frac{x}{\|x\|} = -G \cdot \frac{mM}{\|x\|^2} \cdot \frac{x}{\|x\|} = -\frac{Kmx}{\|x\|^3}$$

Now let us compute the gradient  $\nabla V$ , pronounced “del  $V$ ” or “nabla  $V$ ” which is by definition the vector  $\nabla V \in \mathbb{R}^3$  formed by the 3 spatial derivatives of  $V$ . We have:

$$\begin{aligned} \frac{dV}{dx_i} &= -\frac{dKm/\sqrt{x_1^2 + x_2^2 + x_3^2}}{dx_i} \\ &= -Km \cdot \frac{d(x_1^2 + x_2^2 + x_3^2)^{-1/2}}{dx_i} \\ &= -Km \cdot \left(-\frac{1}{2}\right) \cdot \frac{2x_i}{(x_1^2 + x_2^2 + x_3^2)^{3/2}} \\ &= \frac{Kmx_i}{\|x\|^3} \end{aligned}$$

Thus we have  $\nabla V = Kmx/\|x\|^3$ , which by the above equals  $-F$ , as desired. □

The above result is interesting in connection with energy conservation problems, due to the following general fact, which is something going beyond gravitation:

THEOREM 2.23. *Assuming that an object of mass  $m$  moves under the influence of a force  $F$  which is conservative, in the sense that*

$$F = -\nabla V$$

*for a certain function  $V$ , then if we call this function  $V$  potential energy of  $m$ , and set*

$$E = T + V$$

*with  $T = m||v||^2/2$  being as usual the kinetic energy of  $m$ , then  $E$  is constant.*

PROOF. This statement looks a bit head-scratching, probably reminding some terribly abstract things that you had to endure, coming from your math professors. But please stay with us, we're doing physics here, not mathematics. We have:

$$\begin{aligned} \dot{T} &= \frac{m(<\dot{v}, v> + <v, \dot{v}>)}{2} \\ &= m <\dot{v}, v> \\ &= m <a, v> \\ &= <F, v> \\ &= - <\nabla V, v> \\ &= - \sum_i (\nabla V)_i v_i \\ &= - \sum_i \frac{dV}{dx_i} \cdot \frac{dx_i}{dt} \\ &= - \frac{dV}{dt} \\ &= -\dot{V} \end{aligned}$$

Thus we have  $\dot{E} = \dot{T} + \dot{V} = 0$ , and so the energy  $E$  is constant, as claimed.  $\square$

Observe that we have used in the above the chain rule, in order to differentiate the composite function  $V = V(x(t))$ . The chain rule in 1D, that you know well, is:

$$(f(g))' = f'(g)g'$$

In higher dimensions now, exactly the same happens, but with the derivative of a function  $f : \mathbb{R}^N \rightarrow \mathbb{R}^M$  at a point  $c \in \mathbb{R}^N$  being now the linear map  $f'(c) : \mathbb{R}^N \rightarrow \mathbb{R}^M$  which best approximates the function  $f$ , around that point  $c \in \mathbb{R}^N$ :

$$f(c+z) \simeq f(c) + f'(c)z$$

Moreover, by linear algebra this derivative  $f'(c) : \mathbb{R}^N \rightarrow \mathbb{R}^M$  can be regarded as a rectangular matrix,  $f'(c) \in M_{M \times N}(\mathbb{R})$ , acting on the vectors  $z \in \mathbb{R}^N$ , written as usual vertically,  $z \in M_{N \times 1}(\mathbb{R})$ , via the usual formula of matrix multiplication:

$$f'(c)z \in M_{M \times 1}(\mathbb{R}) = \mathbb{R}^M$$

In our context,  $V = V(x(t))$  appears by composing  $V : \mathbb{R}^3 \rightarrow \mathbb{R}$ , having as derivative the transpose of the gradient  $(\nabla V)^t \in M_{1 \times 3}(\mathbb{R})$ , with  $x : \mathbb{R} \rightarrow \mathbb{R}^3$ , having as derivative the vector  $\dot{x} \in M_{3 \times 1}(\mathbb{R})$ . Thus, the chain rule gives in this case the following number:

$$\dot{V} = (\nabla V)^t \dot{x} = \langle \nabla V, \dot{x} \rangle$$

All this might seem a bit complicated, but several variables means linear algebra, so it is. In practice, all this is best remembered as in the proof of Theorem 2.23, with that  $dx_i$  factors miraculously simplifying, and taking the  $\sum_i$  symbol with them.

Back to physics now, what we have in Theorem 2.23 above is quite conceptual. It is possible to say more about conservative forces, such as gravitation, but before that, let us restate and reprove Theorem 2.20, more conceptually, as follows:

**THEOREM 2.24.** *The gravitation force  $F$  is conservative,  $F = -\nabla V$ , coming from*

$$V = -\frac{Km}{\|x\|}$$

*and therefore the total energy  $E = T + V$ , with  $T = m\|v\|^2/2$  as usual, is constant.*

**PROOF.** Here the first assertion comes from Proposition 2.22, and the second assertion, that we already know from Theorem 2.20, comes now from Theorem 2.23.  $\square$

For more on all this, we refer to any mechanics book. Here, we will be back to this later, first in chapter 3 below, when further studying gravity, often regarded as a conservative force, and then also in chapters 5-6 below, when discussing magnetism.

This was for our basic presentation of basic classical mechanics. For more on all this, basic classical mechanics, we refer as usual to [5], [33], [38], [57], [61], [90]. We will be also back to this, on several occasions, in what follows, our plan being:

(1) In chapter 3 we will further build on all this, following Lagrange, then we will study rockets, ballistics and satellites. The questions there, more related to engineering, will bring us into several interesting topics, such as drag, fluids and friction.

(2) We also have the key topic of rotating bodies, including our good old Earth, with discoveries by Foucault, Coriolis and others. We will discuss this in chapter 4, in the context of inertial and non-inertial frames, as a prelude to Einstein's relativity theory.

(3) Many of the techniques developed above apply as well to other types of mechanics, such as electrodynamics, where the Coulomb law states that  $F \sim 1/d^2$ . Also, collisions are important in thermodynamics. We will discuss this in chapters 5-8 below.

(4) Finally, regarding more advanced aspects of classical mechanics, coming from the work of Hamilton, and also Noether, we will discuss them more in detail when doing quantum mechanics, in chapters 9-16, as a key ingredient for the theory there.

## 2e. Exercises

Time to do some weight lifting, and don't skip leg day. As usual, for good and exciting exercises, often having something to do with engineering, we recommend our go-to mechanics books [5], [33], [38], [57], [61], [90]. In what concerns us, we will be a bit theoretical, and here are a few exercises, in relation with the present chapter:

EXERCISE 2.25. *Write down the formulae for a simultaneous plastic collision between  $N$  bodies. Is there any difference between what you find, and what comes out by assuming that the bodies quickly collide in pairs, 1 with 2, then  $1 + 2$  with 3, and so on?*

EXERCISE 2.26. *Based on our rocket computations, develop a theory of destruction, mirroring and opposing the theory of plastic collisions, first in 1 dimension, and then in arbitrary  $N$  dimensions. Then, come back to rockets, and discuss taking turns.*

EXERCISE 2.27. *You have certainly heard about light entering a different medium, and getting on one hand reflected, and on the other hand refracted, at slightly different angles. Develop some math for this situation, regarded as a sort of collision.*

EXERCISE 2.28. *In relation with Fact 2.13, investigate what happens for the 2-body problem, with  $M, m$  being now assumed to be round objects, of size  $R, r$ , by computing the probability for a collision, under suitable random data. Use a computer if needed.*

EXERCISE 2.29. *Also in relation with Fact 2.13, but at a more advanced level, look up the notion of Roche limit, related to the tidal destruction of one body due to the gravitation of another, nearby body, and write down a brief account of what you learned.*

EXERCISE 2.30. *In the 2-body problem, the total angular momentum  $J = \sum x_i \times p_i$  is conserved when computed at both the initial positions of  $M, m$ . What about conservation at other points of  $\mathbb{R}^3$ ? What about  $N$ -body systems? What about higher dimensions?*

EXERCISE 2.31. *In the 2-body problem, the total energy  $E = \sum T_i + V_i$  is conserved when computed at both the initial positions of  $M, m$ . What about conservation at other points of  $\mathbb{R}^3$ ? What about  $N$ -body systems? What about higher dimensions?*

EXERCISE 2.32. *Learn some multivariable calculus, and notably the chain rule, and the formula  $\dot{V} = \langle \nabla V, \dot{x} \rangle$  used in the proof of Theorem 2.23, and write a brief account of what you learned. In case you know this well, upgrade to infinite dimensions.*

EXERCISE 2.33. *Look up the notion of conservative force, and the various properties of such forces, and in particular the fact that such forces must be of the form  $F = -\nabla V$ , for a certain potential  $V$ , and write down a brief account of what you learned.*

As usual, if you don't find answers to some of the above questions, even after working hard, don't worry. We will be back to some of these questions, later on.



## CHAPTER 3

### Lagrange and Hamilton

#### 3a. Some calculus

We have seen so far the foundations and main applications of classical mechanics. Our goal now will be to complete this discussion with an introduction to more advanced topics, belonging both to theoretical physics and applied physics, as follows:

(1) On one hand, we would like to further build on the general theory developed so far, following the work of Lagrange and Hamilton. Besides being very useful for all sorts of purposes, and particularly for us later on, when doing quantum mechanics, their formulation of classical mechanics is especially useful when dealing with 3-body problems, with in practice the bodies being usually the Earth, the Sun, and a satellite.

(2) On the other hand, we would like to systematically discuss certain concrete questions coming from engineering, in relation with rockets, ballistics and satellites. We will discuss such questions with and without drag, and at the theoretical level, this will lead us into a number of interesting versions and generalizations of classical mechanics, involving drag or friction, and also into the general topic of fluid mechanics.

Summarizing, many things to be done. As usual, we will be quite brief, and our standard references will be the classical mechanics books [5], [33], [38], [57], [61], [90]. For fluid mechanics, a standard reference is Batchelor [13], and Arnold-Khesin [7] for more advanced aspects. Finally, for differences between solids and fluids, a subtle question that we will get into as well, standard reads here are Ashcroft-Mermin [8], Chaikin-Lubensky [17], Goodstein [40], Harrison [47], Kittel [58], but only a quick look at them, because we will discuss this later in this book too, more in detail, in chapters 5-8 below.

Getting started now, we first need to clarify a bit the things discussed at the end of chapter 2. The discussion here, involving some non-trivial mathematics, will start erring on the upper undergraduate side of things, and a good, concise reference here is the opening chapter of Goldman's classical graduate textbook [38]. As for the detailed mathematics needed, this can be found in any multivariable calculus book.

In order to further clarify our concept of “conservative force”, which generalizes in an efficient and elegant way the usual gravity, the best is to start by talking about work. This

is certainly something that we already discussed, on the occasion of our various exercise sessions to far, but here is now the exact, physical definition of work:

DEFINITION 3.1. *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  $W(p, q)$ .*

We will see in a moment that this definition is compatible with our previous definition for the conservative forces. As a first comment now, assume that we have two paths  $\gamma : p \rightarrow q$  and  $\delta : p \rightarrow q$ . We can then consider the path  $\circ : p \rightarrow p$  obtained by going along  $\gamma : p \rightarrow q$ , and then along  $\delta$  reversed,  $\delta^{-1} : q \rightarrow p$ , and we have:

$$W(\circ) = W(\gamma) - W(\delta)$$

Thus  $F$  is conservative precisely when, for any loop  $\circ : p \rightarrow p$ , we have:

$$W(\circ) = 0$$

Intuitively, this means that  $F$  is some sort of “clean”, ideal force, with no dirty things like friction involved. As we will soon see, gravity is such a clean force, with a simple example coming from throwing a rock up in the sky. That rock will travel on a loop  $p \rightarrow q \rightarrow p$ , and will come back here to  $p$  unchanged, save for the fact that its speed vector is reversed. Thus, and assuming now that work has something to do with energy, which is intuitive, there has been no overall work of gravity on this loop,  $W(\circ) = 0$ .

An even better example, avoiding any reference to energy, is the movement of the Earth around the Sun. Every year that passes the Earth makes a loop, and with the Sun obviously not even noticing that, so the yearly work done by the Sun is  $W(\circ) = 0$ .

As a counterexample now, friction is not conservative. I would definitely prefer to make loops with my lawn mower in my garden, and say to myself, for motivation, that I’m doing  $-W(\circ) = 0$ , rather than taking that thing up to the North Pole, and back.

As a first result now, regarding the conservative forces, we have:

THEOREM 3.2. *The work done by a conservative force  $F$  on a mass  $m$  object is*

$$W(p, q) = T(q) - T(p)$$

*with  $T = m||v||^2/2$  standing as usual for the kinetic energy of the object.*

PROOF. Assuming that  $F$  is conservative, and acts via the usual formula  $F = ma$  on our object of mass  $m$ , we have the following computation, as desired:

$$\begin{aligned}
 W(p, q) &= \int_p^q \langle F(x), dx \rangle \\
 &= m \int_p^q \langle a(x), dx \rangle \\
 &= m \int_p^q \left\langle \frac{dv(x)}{dt}, v(x) dt \right\rangle \\
 &= \frac{m}{2} \int_p^q \frac{d \langle v(x), v(x) \rangle}{dt} dt \\
 &= \frac{m}{2} \int_p^q \frac{d \|v(x)\|^2}{dt} dt \\
 &= \frac{m}{2} (\|v(q)\|^2 - \|v(p)\|^2) \\
 &= T(q) - T(p)
 \end{aligned}$$

Here we have used in the middle the fact that the time derivative of a scalar product of functions  $\langle v, w \rangle$  consists of two terms, which are equal when  $v = w$ .  $\square$

Next, we have the following result, which uses some more advanced mathematics:

THEOREM 3.3. *A force  $F$  is conservative precisely when it is of the form*

$$F = -\nabla V$$

*for a certain function  $V$ , and in this case the work done by it is given by:*

$$W(p, q) = V(p) - V(q)$$

*Also, the gravitation force is conservative, coming from  $V = -Km/\|x\|$ .*

PROOF. This is something quite tricky, the idea being as follows:

(1) In one sense, assume that  $F$  is conservative. Since the work  $W(p, q) = W(\gamma)$  is independent of the chosen path  $\gamma : p \rightarrow q$ , we can find a function  $V$  such that:

$$W(p, q) = V(p) - V(q)$$

Observe that this function  $V$  is well-defined up to an additive constant. Now with this formula in hand, we further obtain, as desired:

$$\begin{aligned}
 W(p, q) = V(p) - V(q) &\implies \langle F, dx \rangle = -dV \\
 &\implies \langle F, x_i \rangle = -\frac{dV}{dx_i} \\
 &\implies F = -\nabla V
 \end{aligned}$$

(2) In the other sense now, assuming  $F = -\nabla V$ , we have the following computation, valid for any loop  $\circ : p \rightarrow p$ , which shows that  $F$  is indeed conservative:

$$W(\circ) = - \int_{\circ} \nabla V = 0$$

More generally, regarding the work done by such a force  $F = -\nabla V$ , along a path  $\gamma : p \rightarrow q$ , which is independent on this path  $\gamma$ , this is given by:

$$W(p, q) = - \int_p^q \nabla V = V(p) - V(q)$$

(3) Finally, the last assertion, regarding the gravitation, this is something that we know from chapter 2, coming via a quick gradient computation, done there.  $\square$

We can put now everything together, and we have the following result, which makes the link with the various conservation energy results from chapter 2, and to be more precise generalizes them, and fully clarifies the situation:

**THEOREM 3.4.** *Given a conservative force  $F$ , appearing as follows, with  $V$  being uniquely determined up to an additive constant,*

$$F = -\nabla V$$

*the movements of a particle under  $F$  preserve the total energy, given by*

$$E = T + V$$

*with  $T = m||v||^2/2$  being the kinetic energy, and with  $V$  being called potential energy.*

**PROOF.** This is something that we already know from chapter 2, established there by using a computation using the chain rule for derivatives, the idea being as follows:

$$\dot{T} = \langle F, v \rangle = - \langle \nabla V, v \rangle = -\dot{V}$$

However, we can now provide an alternative proof for this fact, based on the theory developed above, and more specifically on Theorem 3.2 and Theorem 3.3, which give:

$$W(p, q) = T(q) - T(p)$$

$$W(p, q) = V(p) - V(q)$$

Indeed, we obtain from these equalities the following formula:

$$T(p) + V(p) = T(q) + V(q)$$

Thus, the total energy  $E = T + V$  is conserved, as claimed.  $\square$

As a side remark here, observe that Theorem 3.4 completely closes the discussion about conservation of energy, at least linguistically, our conclusion being:

**CONCLUSION 3.5.** *Conservative forces conserve energy.*

So, this will be the general principle to remember. This being said, don't leave a fish out in the sun, it will not be conserved by gravity. Instead, use a refrigerator.

This was for the basic theory of conservative forces, and for more on all this, we refer as usual to [5], [33], [38], [57], [61], [90]. We will be back to such general forces, and to more theory about them later on, when talking about magnetism.

### 3b. Lagrange and Hamilton

Back now to gravity, and to the various questions that we would like to solve here, left open in the previous chapters, the point is that by using the above energy theory, we can reformulate the whole classical mechanics formalism and equations, in a far more efficient way. Discussing this, following Lagrange and Hamilton, will be our next task.

However, things are quite tricky here, and as we will see, involving some sort of unexpected discovery, of the type that you can only stumble upon when looking at various formulae coming from physics, with a good mathematical background.

In view of this, let us begin with some mathematics. The “good mathematical background” that we will need, and that Lagrange needed too, in order to find his discovery, is the following theorem, due to guess who, Euler and Lagrange himself:

**THEOREM 3.6.** *Given a function  $f : \mathbb{R}^N \times \mathbb{R}^N \rightarrow \mathbb{R}$ , the integral*

$$I = \int_{x_0}^{x_1} f(u, \dot{u}) dx$$

*is stationary, in the sense that it is left unchanged by small variations of  $u = u(x)$ , which vanish at the endpoints  $x_0, x_1$ , precisely when  $u = u(x)$  satisfies the equations*

$$\frac{df}{du_i} = \frac{d}{dx} \left( \frac{df}{d\dot{u}_i} \right)$$

*called Euler-Lagrange equations.*

**PROOF.** Let us just work out the case  $N = 1$ , the general case being similar. Consider a small variation  $\Delta u(x)$ , which vanishes at the endpoints  $x_0, x_1$ , as required above:

$$\Delta u(x_0) = \Delta u(x_1) = 0$$

The corresponding variation of  $f(u, \dot{u})$ , at first order, is then given by:

$$\Delta f = \frac{df}{du} \Delta u + \frac{df}{d\dot{u}} \Delta \dot{u}$$

Thus the corresponding variation of the integral in the statement is given by:

$$\begin{aligned}
\Delta I &= \int_{x_0}^{x_1} \frac{df}{du} \Delta u \, dx + \int_{x_0}^{x_1} \frac{df}{d\dot{u}} \Delta \dot{u} \, dx \\
&= \int_{x_0}^{x_1} \frac{df}{du} \Delta u \, dx + \int_{x_0}^{x_1} \frac{df}{d\dot{u}} \cdot \frac{d(\Delta u)}{dx} \, dx \\
&= \int_{x_0}^{x_1} \frac{df}{du} \Delta u \, dx + \left[ \frac{df}{d\dot{u}} \Delta u \right]_{x_0}^{x_1} - \int_{x_0}^{x_1} \frac{d}{dx} \left( \frac{df}{d\dot{u}} \right) \Delta u \, dx \\
&= \int_{x_0}^{x_1} \frac{df}{du} \Delta u \, dx - \int_{x_0}^{x_1} \frac{d}{dx} \left( \frac{df}{d\dot{u}} \right) \Delta u \, dx \\
&= \int_{x_0}^{x_1} \left( \frac{df}{du} - \frac{d}{dx} \left( \frac{df}{d\dot{u}} \right) \right) \Delta u \, dx
\end{aligned}$$

We conclude that  $I$  is stationary precisely when the following equation is satisfied:

$$\frac{df}{du} = \frac{d}{dx} \left( \frac{df}{d\dot{u}} \right)$$

But this is the Euler-Lagrange equation in the statement, as desired.  $\square$

The point now with the above is that, when looking at the usual motion equations of mechanics, but written in a somewhat bizarre way, we will get precisely into the Euler-Lagrange equations. So, remember our struggle from chapter 2 with the gravitational potential, and more specifically with  $E = T + V$  vs  $E = T - V$ . We had to ask at that time cat for help, and he said that  $E = T + V$  is the good formula, but that  $E = T - V$  looks like something quite interesting too. So, following now cat, let us formulate:

**DEFINITION 3.7.** *In the context of a conservative force  $F$  acting, the quantity*

$$L = T - V$$

*is called Lagrangian of the system.*

This is something quite tricky, but we will get more familiar with it when working out explicit examples, and with the reminder of course that we have already played a bit with  $T - V$ , in the simplest case, that of a 1D free fall, in chapter 2. In relation now with Theorem 3.6, the connection is very simple, called Hamilton principle, as follows:

**THEOREM 3.8.** *The following integral, called action integral, is stationary,*

$$I = \int_{t_0}^{t_1} L \, dt$$

*and the corresponding Euler-Lagrange equations are precisely the equations of motion.*

PROOF. According to Definition 3.7, the Lagrangian is given by the following formula, with  $V$  being the potential associated to our conservative force, via  $F = -\nabla V$ :

$$L = \frac{m}{2}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - V(x, y, z)$$

Thus, we are in the general framework of Theorem 3.6, with the function  $u$  there being played by the coordinates  $x, y, z$ . Now let us pick one of these coordinates,  $s = x, y, z$ , and compute the derivatives of  $L$  with respect to  $s, \dot{s}$ . By using  $F = -\nabla V$  we have:

$$\frac{dL}{ds} = -\frac{dV}{ds} = F_s$$

Also since the potential  $V$  is time-independent, we have:

$$\frac{dL}{d\dot{s}} = m\dot{s} = ma_s$$

Now consider the equation of motion, under the influence of the force  $F$ :

$$F = ma$$

This is a vector equation, with 3 components, and according to the above formulae its 3 components can be written as follows, in terms of the Lagrangian  $L$ :

$$\frac{dL}{ds} = \frac{d}{dt} \left( \frac{dL}{d\dot{s}} \right)$$

But these are precisely the Euler-Lagrange equations for the stationarity of the action integral  $I = \int L$ , and we are therefore led to the conclusions in the statement.  $\square$

The point now with the above result is that it leads right away into another result, which this time is something fundamental and powerful, as we will soon discover:

**THEOREM 3.9.** *The Euler-Lagrange equations for the action integral*

$$I = \int_{t_0}^{t_1} L dt$$

*hold in any system of coordinates  $(q_1, q_2, q_3)$ , and are as follows:*

$$\frac{dL}{dq} = \frac{d}{dt} \left( \frac{dL}{d\dot{q}} \right)$$

*These latter equations are called the Lagrange equations of motion.*

PROOF. We know from Theorem 3.8 that the action integral is stationary, with respect to the standard coordinates  $(x, y, z)$ . But this shows that the action integral is stationary with respect to any system of coordinates  $(q_1, q_2, q_3)$ , and so the corresponding Euler-Lagrange equations, which are the equations in the statement, hold indeed.  $\square$

All this might seem a bit complicated, but we will see examples in what follows. The idea every time will be the same, namely thinking a bit, than picking up a suitable system of coordinates  $(q_1, q_2, q_3)$  for our problem, and then instead of doing all sorts of computations for reformulating the equations of motion in terms of these coordinates  $(q_1, q_2, q_3)$ , simply writing the Lagrange equations, which are there for that.

As a basic illustration here, the Newton solution to the Kepler problem, discussed in chapter 1 above, was using polar coordinates, or rather cylindrical coordinates with  $z$  not mattering, to be fully correct. But the computations there can be heavily simplified by starting directly with the Lagrange equations in cylindrical coordinates.

Moving ahead now, let us discuss some further interesting manipulations on the Lagrangian and the Lagrange equations, due to Hamilton. Let us start with:

DEFINITION 3.10. *Given a system of coordinates  $q_1, \dots, q_n$ , the quantities*

$$p_i = \frac{dL}{d\dot{q}_i}$$

*are called generalized momenta. In terms of them, the Lagrange equations read*

$$\frac{dL}{dq_i} = \dot{p}_i$$

*analogously to the usual motion equations  $F = \dot{p}$ .*

What are these new variables good for? Let us recall from Definition 3.7 above that the Lagrangian was by definition a function as follows:

$$L = L(q_1, \dots, q_n, \dot{q}_1, \dots, \dot{q}_n)$$

The point now, which is something quite subtle, and useful for all sorts of purposes, in classical mechanics, and especially in its versions and generalizations, is that we can get rid of the derivatives  $\dot{q}_1, \dots, \dot{q}_n$ , which are variables in the Lagrange formulation of mechanics, by replacing them by the generalized momenta  $p_1, \dots, p_n$  constructed above. In order to do so we need a clever new quantity  $H$ , replacing  $L$ , and we have here:

DEFINITION 3.11. *With  $q_1, \dots, q_n$  and  $p_1, \dots, p_n$  being as above, the quantity*

$$H(q, p) = \sum_i p_i \dot{q}_i - L$$

*is called Hamiltonian of the system.*

As we will soon see, for many simple systems  $H$  is in fact the total energy. Before that, however, let us explain how  $H$  replaces  $L$ , as a quantity which encapsulates as well what is going on, namely the equations of motion. The result here is as follows:



THEOREM 3.12. *The Hamiltonian  $H = H(q, p)$  is subject to the equations*

$$\frac{dH}{dp_i} = \dot{q}_i \quad , \quad \frac{dH}{dq_i} = -\dot{p}_i$$

*called Hamilton equations, which are equivalent to the usual equations of motion.*

PROOF. As a first observation, this statement reminds right away Theorem 3.9, namely the Lagrange formulation of mechanics, who was claiming the same type of thing. However, there are some differences. On one hand, the new variables  $q_1, \dots, q_n$  and  $p_1, \dots, p_n$  are certainly a bit more abstract than the old ones  $q_1, \dots, q_n$  and  $\dot{q}_1, \dots, \dot{q}_n$ . On the other hand, the new equations look great. Regarding now the proof, everything follows from the definition of the variables  $p_i$  and from the Lagrange equations, namely:

$$p_i = \frac{dL}{d\dot{q}_i} \quad , \quad \frac{dL}{dq_i} = \dot{p}_i$$

(1) By using the definition of the variables  $p_i$ , we obtain the following formula:

$$\begin{aligned} \frac{dH}{dp_i} &= \frac{d\left(\sum_j p_j \dot{q}_j - L\right)}{dp_i} \\ &= \dot{q}_i + \sum_j p_j \frac{d\dot{q}_j}{dp_i} - \sum_j \frac{dL}{d\dot{q}_j} \cdot \frac{d\dot{q}_j}{dp_i} \\ &= \dot{q}_i + \sum_j p_j \frac{d\dot{q}_j}{dp_i} - \sum_j p_j \frac{d\dot{q}_j}{dp_i} \\ &= \dot{q}_i \end{aligned}$$

(2) By using the Lagrange equations, we obtain the following formula:

$$\begin{aligned} \frac{dH}{dq_i} &= \frac{d\left(\sum_j p_j \dot{q}_j - L\right)}{dq_i} \\ &= -\frac{dL}{dq_i} + \sum_j p_j \frac{d\dot{q}_j}{dq_i} - \sum_j \frac{dL}{d\dot{q}_j} \cdot \frac{d\dot{q}_j}{dq_i} \\ &= -\dot{p}_i + \sum_j p_j \frac{d\dot{q}_j}{dq_i} - \sum_j p_j \frac{d\dot{q}_j}{dq_i} \\ &= -\dot{p}_i \end{aligned}$$

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

There are many other things that can be said about the Lagrangian  $L$  and the Hamiltonian  $H$ , and we will see some examples and general theory, in what follows.

### 3c. The N body problem

We have now in our bag all the standard tools of the classical mechanician. There are all sorts of problems that we can solve with them, and as usual here we refer to our standard books [5], [33], [38], [57], [61], [90]. In what follows we will focus on the generalizations of the Kepler 2-body problem, which is more or less the only serious problem that we have solved, so far. These generalizations follow into several classes:

- (1) 2-body problem with round bodies.
- (2) 2-body problem with atmospheric drag.
- (3) 2-body problem with one of the bodies rotating.
- (4) 3-body problem with 2 bodies being fixed.
- (5) 3-body problem with 1 big, distant body.
- (6) 3-body problem with 1 body being tiny.
- (7) Combinations of the above, and more.

All this screams for help, looks like we are in a complete jungle. And the problem is that (1-7) above are all serious questions, related to problems in the real life. Just throw a rock in front of you, and you're instantly into (1,2,3), taken altogether. Throw something more complicated, like a rocket with a satellite, and you'll have a taste of (4,5,6) too.

Can mathematics save us? We know so far how to solve the Kepler 2-body problem, and looking at the above list (1-7), and thinking underlying math, suggests that question (4) might be the easiest. Indeed, we should normally be able to replace our 2 fixed bodies with a single one, then solve the problem, and have our first 3-body theorem.

In order to discuss this, let us start with the following general notion:

**DEFINITION 3.13.** *Associated to a system of bodies  $M_1, \dots, M_k$ , located at positions  $c_1, \dots, c_k \in \mathbb{R}^3$  is their center of mass, located at the following position:*

$$c = \frac{\sum_i c_i M_i}{\sum_i M_i}$$

*A single body of mass  $\sum_i M_i$  located there, at the center of mass, and with  $M_1, \dots, M_k$  being erased, will be called average of the system formed by  $M_1, \dots, M_k$ .*

You are certainly a bit familiar with this, and we will work out the math in a moment. However, before doing that, let us see if this can help in connection with problem (4) above. When looking in real life for two fixed bodies  $M_1, M_2$  the first thing which comes to mind is a dumbbell. Which is however something quite small, so let us formulate:

**DEFINITION 3.14.** *The Devil's dumbbell is a system of two fixed objects*

$$\bullet_{M_1} \text{ --- } d \text{ --- } \bullet_{M_2}$$

*which can have arbitrary characteristics  $M_1 > 0$ ,  $M_2 > 0$ ,  $d > 0$ .*

As already mentioned, the simplest example is a usual dumbbell, which however at the galactic level is subject to  $M_i \simeq 0$  and  $d \simeq 0$ . Bigger examples exist in distant galaxies, with the giants there training with specially designed dumbbells,  $M_i$  being roughly the mass of an average planet, and  $d$  being accordingly large. As for the fully versatile dumbbell in Definition 3.14, that is a creation of the Devil, for annoying us physicists.

Getting back now to question (4), we would like to understand the motion of an object of mass  $m$  around a dumbbell of parameters  $M_1, M_2, d$ , as in Definition 3.14, by using the notion of center of mass of that dumbbell, constructed according to Definition 3.13:

$$\begin{array}{c} \circ_m \\ \bullet_{M_1} \text{ --- } \star_c \text{ --- } \bullet_{M_2} \end{array}$$

And the preliminary observations here are quite grim, as follows:

OBSERVATIONS 3.15. *In the context of a body of mass  $m$  moving around a dumbbell of parameters  $M_1, M_2, d$ , the following happen:*

- (1) *When  $m$  is at distance  $x \gg 0$  from the dumbbell, the gravitation force acting on it is  $F_1 + F_2 \simeq F_c$ , so  $m$  should travel on some sort of approximate conic.*
- (2) *However, when  $m$  is at distance  $x \simeq 0$  from the dumbbell, the physics and trajectory have nothing to do with the center of mass,  $F_1 + F_2 \not\simeq F_c$ .*

Here in what regards forces, (1) is something quite obvious and intuitive, and we will do the math in a moment, with a proof of  $F_1 + F_2 \simeq F_c$ , and a study of the correction term as well. As for (2), this is something obvious and intuitive too, because if you place  $m$  on the line joining  $M_1, M_2$ , bad things will happen, and the only possibility where  $c$  can be of help is when  $m$  was initially placed precisely on  $c$ , and with this, point on a line being at a prescribed location, being an event happening with probability 0.

As for the trajectory claim in (1), that is something sort of intuitive, but not really, because as you might know from observations with pendulums, balls rolling on various surfaces, and so on, involving equilibrium and non-equilibrium, there is no guarantee that the solution of a perturbed problem is a perturbation of the initial solution.

Getting back now to our list (1-7), it looks like the simplest question there, (4), while suggesting a quick solution using the center of mass, is something quite difficult. So what to do. As usual in such difficult situations, we will ask the cat. And cat says:

CAT 3.16. *Start with some basic math of the  $N$  body systems, but beware here of the center of mass, and of what certain physicists claim they can do with it.*

What cat says here is quite frightening. So not only we're into difficult questions, but in addition no one, including our standard mechanics books, can help us. Are all the formulae there, regarding conservation of momentum, angular momentum, energy and so on, all obtained by using an elegant use of the center of mass, correct or not?

To be seen. So let us start with the beginning, basic mathematics of the center of mass, as constructed in Definition 3.13 above. To be kept in mind first is:

**PROPOSITION 3.17.** *The center of mass is not a center of gravity, in the sense that the gravity there is not necessarily 0. For instance the center of mass of a dumbbell is*

$$\bullet_{M_1} \underbrace{\quad}_{\frac{M_2 d}{M_1 + M_2}} \star_{cm} \underbrace{\quad}_{\frac{M_1 d}{M_1 + M_2}} \circ_{M_2}$$

while the center of gravity, which is the unique point where the gravity is 0, is:

$$\bullet_{M_1} \underbrace{\quad}_{\frac{\sqrt{M_1} d}{\sqrt{M_1} + \sqrt{M_2}}} \star_{cg} \underbrace{\quad}_{\frac{\sqrt{M_2} d}{\sqrt{M_1} + \sqrt{M_2}}} \circ_{M_2}$$

The systems of  $k \geq 3$  bodies might have several centers of gravity, usually uncomputable.

**PROOF.** There are several assertions here, the idea being as follows:

(1) Regarding the dumbbell, pictured above with  $M_1 > M_2$ , the formula for the center of mass is clear from definitions. Regarding now the center of gravity, the formula there can be found by doing the math, and it works, because the acceleration there is:

$$a = -\frac{GM_1}{\left(\frac{\sqrt{M_1} d}{\sqrt{M_1} + \sqrt{M_2}}\right)^2} + \frac{GM_2}{\left(\frac{\sqrt{M_2} d}{\sqrt{M_1} + \sqrt{M_2}}\right)^2} = 0$$

(2) Getting now to systems  $M_1, \dots, M_k$  with  $k \geq 3$ , things here are quite complicated. With  $c_i$  being the position of  $M_i$ , a center of gravity  $x \in \mathbb{R}^3$  must satisfy:

$$\sum_i \frac{M_i(x - c_i)}{\|x - c_i\|^3} = 0$$

Equivalently, we are looking for solutions of the equation  $\nabla V = 0$ , where:

$$V = -\sum_i \frac{GmM_i}{\|x - c_i\|}$$

(3) Let us first examine the simplest case, that of 3 bodies on a line, at distinct positions. Here, by obvious reasons, we have 2 centers of gravity, as follows:

$$\bullet_{M_1} \text{ --- } \star_{x_1} \text{ --- } \bullet_{M_2} \text{ --- } \star_{x_2} \text{ --- } \bullet_{M_3}$$

More generally, again by obvious reasons, a system of aligned bodies  $M_1, \dots, M_k$  has  $k - 1$  centers of gravity, one in between each pair of consecutive bodies.

(4) In the 2D case now, and with  $k \geq 3$ , we are looking the the center of gravity of a triangle, with vertices weighted by masses  $M_1, M_2, M_3$ . The simplest possible situation is that of an equilateral triangle, with equal masses  $M, M, M$  at its vertices, and it is quite clear here that we will have 3 solutions, 1 lying on each of the 3 symmetry axes.

(5) This is of course quite bad news, because we have now 3 solutions, instead of the 2 ones found in one dimension, in (3). And for the disaster to be complete, let us attempt now to compute these solutions. Best is to use here complex numbers, with our triangle being  $1, w, w^2$  in the complex plane, with  $w = e^{2\pi i/3}$ . We will only look for the solution on the  $Ox$  axis, say  $r \in \mathbb{R}$ , the other solutions being  $wr, w^2r$ . The equation is:

$$\frac{r-1}{|r-1|^3} + \frac{r-w}{|r-w|^3} + \frac{r-w^2}{|r-w^2|^3} = 0$$

By simplifying at left and using  $1+w+w^2=0$  for the right terms, this reads:

$$\frac{2r+1}{|r-w|^3} = \frac{1}{(1-r)^2}$$

(6) And that is pretty much it, for computing  $r$  we must raise this to the square, which leads us into a degree 6 equation, and we will not do this. As a conclusion, things are hard for the equilateral triangle equally weighted, and can only be harder in general.

(7) As a final comment, however, and forgetting perhaps about exact numerics, this is a geometry problem. Indeed, the equations in (2) suggest looking at  $\mathbb{R}^3$  with a “hole” at each  $M_i$ , and the problem is that of understanding which points are in equilibrium. This is some sort of an Einstein idea, and we will be back to this later, in chapter 4.  $\square$

Moving ahead, and looking for an easier question, let us still examine the gravity of a rigid object, formed by fixed bodies  $M_1, \dots, M_k$ , but at a distance. We have here:

**THEOREM 3.18.** *Consider a rigid object, consisting of fixed bodies  $M_1, \dots, M_k$ , located at positions  $c_1, \dots, c_k \in \mathbb{R}^3$ . The corresponding gravitation force,  $F = -\nabla V$  with*

$$V = - \sum_i \frac{GmM_i}{||x - c_i||}$$

*can be approximated by the force coming from the center of mass,  $F_c = -\nabla V$  with*

$$V_c = - \frac{Gm \sum_i M_i}{||x - c||}$$

*at order zero, when  $x \gg c_i$ . The correction term can be computed as well.*

**PROOF.** We have several assertions here, the idea being as follows:

(1) The first assertion,  $F \simeq F_c$  when  $x \gg c_i$ , is something clear, and with this not even needing  $c$  to be the center of mass. Indeed, with  $V, V_c$  as above, we have:

$$V = - \sum_i \frac{GmM_i}{||x - c_i||} \simeq - \sum_i \frac{GmM_i}{||x - c||} = V_c$$

(2) Regarding now the correction term, the error to be estimated is:

$$\begin{aligned} V - V_c &= - \sum_i \frac{GmM_i}{\|x - c_i\|} + \frac{Gm \sum_i M_i}{\|x - c\|} \\ &= \sum_i GmM_i \left( \frac{1}{\|x - c\|} - \frac{1}{\|x - c_i\|} \right) \end{aligned}$$

(3) By translation we may assume  $c = 0$ . In order to evaluate the difference of inverses on the right, we use the following trick, valid for any two vectors  $x \gg d$ :

$$\begin{aligned} \frac{1}{\|x\|} - \frac{1}{\|x - d\|} &= \frac{\|x - d\| - \|x\|}{\|x\| \cdot \|x - d\|} \\ &= \frac{\|x - d\|^2 - \|x\|^2}{\|x\| \cdot \|x - d\| \cdot (\|x\| + \|x - d\|)} \\ &= \frac{\|d\|^2 - 2 \langle x, d \rangle}{\|x\| \cdot \|x - d\| \cdot (\|x\| + \|x - d\|)} \\ &\simeq - \frac{\langle x, d \rangle}{\|x\|^3} \end{aligned}$$

To be more precise, in the last step we have neglected upstairs the order 0 term  $\|d\|^2$ , and downstairs we have approximated all norms appearing there by  $\|x\|$ .

(4) Getting back now to the formula in (2), assuming  $c = 0$  by translation, as already mentioned above, and by using the trick in (3), we obtain:

$$\begin{aligned} V - V_c &= \sum_i GmM_i \left( \frac{1}{\|x\|} - \frac{1}{\|x - c_i\|} \right) \\ &\simeq - \sum_i GmM_i \frac{\langle x, c_i \rangle}{\|x\|^3} \\ &= - \frac{Gm}{\|x\|^3} \left\langle x, \sum_i M_i c_i \right\rangle \end{aligned}$$

(5) Let us think now at the meaning of the above formula. Normally this is the formula of the first order correction, but when  $c = 0$  is the center of mass, this means precisely that we have  $\sum_i M_i c_i = 0$ , so this correction that we computed vanishes. So, in short, on one hand good news, we are on the good way, with the center of mass  $c$  being the ideal location for the origin of the approximating potential  $V_c$ , but on the other hand, bad news, precisely due to this fact, we must fine-tune our tricks from (3) above, get a better inequality there, that we can use in order to compute the nonzero correction at  $c$ .

(6) So here we go again with estimates. Getting back to the end of the computation in (3), we need there an estimate for  $\|x - d\|$ , and this can be found as follows:

$$\begin{aligned}\|x - d\| &= \sqrt{\|x\|^2 + \|d\|^2 - 2\langle x, d \rangle} \\ &\simeq \sqrt{\|x\|^2 - 2\langle x, d \rangle} \\ &\simeq \|x\| - \langle x, d \rangle\end{aligned}$$

With this in hand, we can improve our master estimate in (3), as follows:

$$\begin{aligned}\frac{1}{\|x\|} - \frac{1}{\|x - d\|} &= \frac{\|d\|^2 - 2\langle x, d \rangle}{\|x\| \cdot \|x - d\| \cdot (\|x\| + \|x - d\|)} \\ &\simeq \frac{\|d\|^2 - 2\langle x, d \rangle}{\|x\| \cdot (\|x\| - \langle x, d \rangle) \cdot (2\|x\| - \langle x, d \rangle)} \\ &\simeq \frac{\|d\|^2 - 2\langle x, d \rangle}{\|x\| \cdot (2\|x\|^2 - 3\|x\| \langle x, d \rangle)} \\ &= \frac{\|d\|^2 - 2\langle x, d \rangle}{\|x\|^2 \cdot (2\|x\| - 3\langle x, d \rangle)}\end{aligned}$$

Now if we denote by  $\alpha$  the angle between  $x$  and  $d$ , this formula becomes:

$$\begin{aligned}\frac{1}{\|x\|} - \frac{1}{\|x - d\|} &\simeq \frac{\|d\|^2 - 2\|x\| \cdot \|d\| \cdot \cos \alpha}{\|x\|^2 \cdot (2\|x\| - 3\|x\| \cdot \|d\| \cdot \cos \alpha)} \\ &= \frac{\|d\|}{\|x\|^3} \cdot \frac{\|d\| - 2\|x\| \cdot \cos \alpha}{2 - 3\|d\| \cdot \cos \alpha}\end{aligned}$$

(7) Thus, we can improve the estimate found in (4), with the conclusion that at the center of mass, taken to be at the origin,  $c = 0$ , the error is as follows, with  $\alpha_i$  being the angles between our body  $m$ , and the components  $M_1, \dots, M_k$  of the rigid body:

$$\begin{aligned}V - V_c &= \sum_i GmM_i \left( \frac{1}{\|x\|} - \frac{1}{\|x - c_i\|} \right) \\ &\simeq \sum_i \frac{\|c_i\|}{\|x\|^3} \cdot \frac{\|c_i\| - 2\|x\| \cdot \cos \alpha_i}{2 - 3\|c_i\| \cdot \cos \alpha_i}\end{aligned}$$

(8) Assuming in addition that we are in a generic position, where  $\alpha_i \neq \pi/2$  for any  $i$ , the upper terms can be further estimated, and we obtain in this way:

$$\begin{aligned}V - V_c &\simeq - \sum_i \frac{\|c_i\|}{\|x\|^3} \cdot \frac{2\|x\| \cdot \cos \alpha_i}{2 - 3\|c_i\| \cdot \cos \alpha_i} \\ &= - \sum_i \frac{\|c_i\|}{\|x\|^2} \cdot \frac{2 \cos \alpha_i}{2 - 3\|c_i\| \cdot \cos \alpha_i}\end{aligned}$$

Summarizing, we have proved our result, and with a few bonus conclusions, namely that the center of mass  $c$  is indeed the ideal location for the approximate potential  $V_c$ , and that the computation of the error term there ultimately involves the angles  $\alpha_1, \dots, \alpha_k$  between our body  $m$ , and the components  $M_1, \dots, M_k$  of our rigid body.  $\square$

Before going ahead and leaving this subject, let us mention that an interesting generalization of the above comes when considering a “true” rigid body, made of matter arranged according to a certain density function  $\rho$  inside it. We will not go into details here, and instead let us just formulate a basic statement, as follows:

**THEOREM 3.19.** *Consider a rigid body, made of matter arranged according to a certain density function  $\rho$  inside it. Its gravitational force is then  $F = -\nabla V$  with*

$$V = - \int \frac{Gm\rho(z)}{\|x - z\|} dz$$

*and can be approximated by the force coming from the center of mass,  $F_c = -\nabla V$  with*

$$V_c = - \frac{Gm \int \rho(z) dz}{\|x - \int u\rho(u) du\|} dz$$

*at order zero, when  $m$  is far away. The correction term can be computed as well.*

**PROOF.** Here the formulae in the statement, which are perfectly similar to those in Theorem 3.18 above, can be obtained via the usual philosophy “replace sums by integrals”. Observe in particular the formula of the center of mass, producing  $V_c$ , namely:

$$c = \int u\rho(u) du$$

As for the last assertion, this can only hold too, by proceeding as in the proof of Theorem 3.18, and replacing everywhere at the end the sums by integrals.  $\square$

The above results, Theorem 3.18 and Theorem 3.19, are both quite interesting, and suggest a whole string of further questions, and potential generalizations. What happens in the context of Theorem 3.18 when the constituents  $M_1, \dots, M_k$  are allowed to move a bit, say by being confined by an external force? Then, what happens when the constituents  $M_1, \dots, M_k$  are allowed to freely move? Also, what about Theorem 3.19, if we allow there some kind of fluid movement inside the body? And so on. These are obviously all difficult questions, of general  $N$ -body problem type, so perhaps time to stop here.

Moving ahead now, and still in connection with the advice Cat 3.16, let us examine now various conservation questions. The simplest problematics here is most likely that of the angular momentum, but as we will soon discover, things are quite tricky here.

As a first question, we know from chapter 2 that when  $M_2$  moves around  $M_1$ , positioned at 0, its angular momentum  $J_2$  is constant. By symmetry, if we regard  $M_1$  moving around



$M_2$ , fixed at 0, its angular momentum  $J_1$  will be constant too. Thus in both cases  $J = J_1 + J_2$  is constant, which raises the question whether  $J$  is constant or not when computed at other points of  $\mathbb{R}^3$ . And here, we first have the following result:

**PROPOSITION 3.20.** *In the context of the 2-body problem, the following happen:*

- (1)  *$J$  is conserved when assuming that  $M_1$  or  $M_2$  is fixed at 0.*
- (2) *More generally,  $J$  is conserved at any  $\lambda_1 M_1 + \lambda_2 M_2$ , with  $\lambda_1 + \lambda_2 = 1$ .*
- (3) *In particular,  $J$  is conserved when computed at the center of mass.*
- (4) *However,  $J$  is not conserved when assuming that  $M_1$  or  $M_2$  is fixed at  $d \neq 0$ .*

**PROOF.** We have several assertions here, the idea being as follows:

(1) This is something that we know well, from chapter 2, as explained above.

(2) Assume first, as in (1), that  $M_1$  is fixed at 0, and that  $M_2$  moves around it, with position vector  $x \in \mathbb{R}^3$ . Given parameters  $\lambda_1, \lambda_2$  satisfying  $\lambda_1 + \lambda_2 = 1$ , let us set:

$$y = \lambda_1 \cdot 0 + \lambda_2 \cdot x = \lambda_2 x$$

We make now the convention that at  $t = 0$  this point was the origin, with coordinate axes parallel to our original coordinate axes, and that at any  $t > 0$  this is still the origin, with the directions of the coordinate axes being unchanged. Thus, we have a new frame, and the coordinates of our objects  $M_1, M_2$  with respect to this new frame are:

$$z_1 = -\lambda_1 x \quad , \quad z_2 = \lambda_2 x$$

But in this new frame the momenta of  $M_1, M_2$  are both proportional, by factors  $\lambda_1^2 M_2 / M_1$  and  $\lambda_2^2$ , to the original momentum of  $M_2$ , computed in (1), which was constant. Thus both these momenta  $J_1, J_2$  are constant, and so is their sum  $J = J_1 + J_2$ .

(3) This follows from (2), with  $\lambda_1 = M_2 / (M_1 + M_2)$  and  $\lambda_2 = M_1 / (M_1 + M_2)$ .

(4) Assuming that  $M_1$  is fixed at a given point  $d \neq 0$ , and that  $M_2$  travels around it, with position vector  $d + x$ , with  $x$  being as in (1), we still have  $J_1 = 0$ , and so:

$$\begin{aligned} J &= J_2 \\ &= (d + x) \times p \\ &= d \times p + x \times p \\ &= d \times p + \text{constant} \\ &\neq \text{constant} \end{aligned}$$

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

As a conclusion, the conservation of angular momentum depends on the “quality” of the frame that we are using. In a good frame, as in (1,2,3) above, the momentum will be conserved, while in a bad frame, as in (4), the momentum will be not conserved.

Generally speaking, we will be talking frames in chapter 4 below, before getting into relativity. In connection with our questions here we will be quite brief, and in order to keep moving, let us formulate the following informal definition, that will do:

DEFINITION 3.21. *An inertial frame is a frame where all basic formulae, namely*

$$||F|| = \frac{Gm_1m_2}{||x_1 - x_2||^2} \quad , \quad F = ma \quad , \quad a = \dot{v} \quad , \quad v = \dot{x} \quad , \quad F_{12} = -F_{21}$$

*hold, with the last formula standing for Newton's action-reaction principle.*

To be more precise here, the first 4 formulae are something that we have been heavily using, so far in this book. As for the last formula, also called Newton's third law, this expresses the fact that when an object 1 acts on an object 2, say via gravity, with force  $F_{12}$ , then object 2 acts as well on object 1, with force  $F_{21} = -F_{12}$ .

As already mentioned, we will discuss all this later, more in detail, in chapter 4 below. In relation with our present considerations, we have the following basic examples:

PROPOSITION 3.22. *In the context of the 2-body problem, the frames of type*

$$\lambda_1 M_1 + \lambda_2 M_2$$

*constructed above are all non-inertial, including the center of mass frame.*

PROOF. Since our definition of an inertial frame was something quite informal, so will be this proof. We want to check whether the forces between  $M_1, M_2$  satisfy:

$$F_{12} = -F_{21} = \frac{GM_1M_2(x_1 - x_2)}{||x_1 - x_2||^3}$$

(1) In the case of the frame centered at  $M_1$ , the formula  $F_{12} = -F_{21}$  certainly does not hold, because the acceleration of  $M_1$  is in this case  $\ddot{0} = 0$ , and so no force acting upon it, at least from our calculus viewpoint. The same holds for the frame centered at  $M_2$ .

(2) In general now, where we have parameters  $\lambda_1, \lambda_2$  satisfying  $\lambda_1 + \lambda_2 = 0$ , as in Proposition 3.20, as explained there, the positions of  $M_1, M_2$  are:

$$z_1 = -\lambda_1 x \quad , \quad z_2 = \lambda_2 x$$

Thus the forces acting upon  $M_1, M_2$ , computed according to calculus, are:

$$F_{21} = -M_1\lambda_1\ddot{x} \quad , \quad F_{12} = -M_2\lambda_2\ddot{x}$$

Thus, in order to have  $F_{12} = -F_{21}$ , the parameters  $\lambda_1, \lambda_2$  satisfy  $M_1\lambda_1 = M_2\lambda_2$ . But these are exactly the parameters of the center of mass.

(3) But the center of mass frame is not inertial either, because due to the fact that we performed a dilation, the magnitude of  $F_{12} = -F_{21}$  is not the correct one.  $\square$

Now back to momentum, we have the following extension of Proposition 3.20 (3):

THEOREM 3.23. *In an inertial frame, the total angular momentum*

$$J = \sum_i x_i \times p_i$$

*of a system of bodies  $M_1, \dots, M_k$  is conserved.*

PROOF. Our inertial frame assumption tells us that we can use at will all formulae in Definition 3.21, and by using them, and notably  $F_{12} = -F_{21}$ , we obtain:

$$\begin{aligned} \dot{J} &= \sum_i x_i \times \sum_{j \neq i} F_{ji} \\ &= \sum_{i < j} x_i \times F_{ji} + x_j \times F_{ij} \\ &= \sum_{i < j} x_i \times F_{ji} - x_j \times F_{ji} \\ &= \sum_{i < j} (x_i - x_j) \times F_{ji} \\ &= 0 \end{aligned}$$

Now since we have  $\dot{J} = 0$ , the angular momentum  $J$  is conserved, as claimed.  $\square$

Moving ahead now, our next problem will concern the conservation of energy. Here things are a bit similar with angular momentum, but more can be said, as follows:

THEOREM 3.24. *With a suitable potential formalism, the total energy*

$$E = \sum_i T_i + V_i$$

*of a system of bodies  $M_1, \dots, M_k$  is conserved. Also, the individual energy*

$$E' = T' + \sum_i V'_i$$

*of an extra body  $m$  added is conserved as well, again with a suitable formalism.*

PROOF. There are several questions here, the idea being as follows:

(1) In what regards  $T = \sum_i T_i$  we have, exactly as in the 2-body problem:

$$\begin{aligned} \dot{T} &= \sum_{i \neq j} \langle v_i, F_{ji} \rangle \\ &= \sum_{i \neq j} \langle v_i, -\nabla V_{ji} \rangle \\ &= - \sum_{i \neq j} \dot{V}_{ji} \end{aligned}$$

(2) With this in hand, we can group pairs of terms, as in the proof of Theorem 3.23, and we are led to the conclusion in the statement, and with the remark however that all the potentials appearing there are now time-dependent.

(3) In what regards now the second assertion, this is not exactly something of the same nature as the first assertion, because assuming that by some kind of miracle we would have a theory where all the bodies conserve their energy, the total energy of the system would be trivially conserved too, just by summing, and this does not look normal. So, getting now to the second assertion as formulated, we have, by computing as in (1) above:

$$\dot{T}' = - \sum_i \dot{V}'_i$$

(4) Thus, we are led to the conclusion in the statement, with the problem however that all the potentials appearing there are now time-dependent.  $\square$

### 3d. Satellites and ballistics

With the above questions discussed, let us go back now to our to-do list (1-7), from the beginning of the previous section. We have all sorts of difficult questions there, and we will focus first on (6), namely 3-body problem with one of the bodies being tiny.

Things here are quite complicated, technically speaking. Let us start with:

**DEFINITION 3.25.** *The 3-body problem is the general gravitational problem for three bodies  $M_1, M_2, M_3$ , with the corresponding equations of motion being as follows:*

$$\begin{aligned}\ddot{x}_1 &= -\frac{GM_2(x_1 - x_2)}{\|x_1 - x_2\|^3} - \frac{GM_3(x_1 - x_3)}{\|x_1 - x_3\|^3} \\ \ddot{x}_2 &= -\frac{GM_3(x_2 - x_3)}{\|x_2 - x_3\|^3} - \frac{GM_1(x_2 - x_1)}{\|x_2 - x_1\|^3} \\ \ddot{x}_3 &= -\frac{GM_1(x_3 - x_1)}{\|x_3 - x_1\|^3} - \frac{GM_2(x_3 - x_2)}{\|x_3 - x_2\|^3}\end{aligned}$$

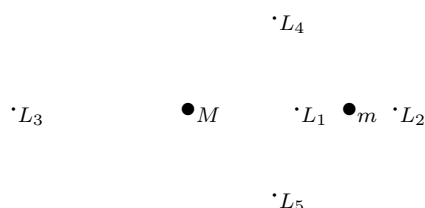
*The planar 3-body problem is this problem, in a plane. The restricted 3-body problem is also this problem, in the situation  $M_1, M_2 \gg M_3$ , and usually considered in a plane.*

The general 3-body problem has all sorts of weird solutions, and cannot be solved via exact mathematics. You would probably say no problem, just give it to a computer, but guess what, the computer cannot solve that either. The problem with computers is that, no matter how big and powerful they are, they can still only operate with a finite amount of data, and at a certain speed, and what happens, somehow, is that the 3 equations in Definition 3.25 can produce after some time  $t > 0$  all sorts of bizarre phenomena, going in all senses, and managing all this is impossible, even for a powerful computer.

The best here is to go on internet, and watch some animations. Just by looking at them, and how bizarre they can be, you will quickly realize that such things are beyond what you, what your professors, and even what a powerful computer, can do.

This being said, and in connection now with our satellite problem that we have in mind, question (6) on our to-do list, some mathematics is however possible, in certain simple cases, and we have the following remarkable result, due to Lagrange:

**THEOREM 3.26.** *The restricted 3-body problem has 5 distinguished solutions,*



*called Lagrange points L1-L5, whose positions with respect to  $M, m$  are as above.*

**PROOF.** This is certainly something quite complicated, using all sorts of advanced mathematics, further building on what has been developed in the above, and we won't get into details here. Instead, let us describe at least how each L1-L5 functions:

(1) L1 is the most intuitive solution, placed in between  $M$  and  $m$ , and closer to  $m$ , at that precise point where the gravitation of  $M$  equals in magnitude the gravitation of  $m$ . The math here for finding the distances is very simple, but recall however that  $m$  is supposed to move around  $M$ , on an ellipse. Thus, the picture is that an object  $\varepsilon$  placed at L1 moves as well around  $M$ , by staying aligned with  $m$ , on a smaller ellipse.

(2) One problem with L1 comes from the fact that it is unstable, in the sense that an object  $\varepsilon$  placed around there, but not exactly there, will not stay there. Indeed, was  $\varepsilon$  to be placed a tiny little bit towards  $M$ , it will start slowly moving towards  $M$ , and gone it will be. And the same can happen in the other sense, with  $m$  being able to capture it too, since L1 is some sort of no man's land between the gravities of  $M, m$ , which look equal from there. Thus, L1 looks like some sort of fake solution to the problem.

(3) However, all this is useful in practice, because with just a little bit of homemade acceleration, from time to time, in order to correct the trajectory and keep it on L1, a satellite can be placed there at L1, and will stay there. In fact, most of the scientific satellites are placed there at L1, first because its proximity to Earth, but also because there is no dirt like asteroids trapped there, due to the fact that L1 is unstable.

(4) Getting to L2 now, the functioning mechanism here is different, crucially relying on the fact that  $m$ , and so L2 too, does move around  $M$ , on an elliptic orbit. Indeed, what looks impossible in 1D, namely an object  $\varepsilon$  placed behind  $m$  not to be attracted by both  $M, m$ , and start going towards them, is now possible in the context of the 2D elliptical

movement, with the normal movement of  $\varepsilon$  with respect to  $M$  being slightly altered by the presence of  $m$ , which in practice tends to pull  $\varepsilon$  away from  $M$ ,  $m$ , and with the precise distance being that where equilibrium is achieved, in all this. As for L1, this point L2 is not far from Earth, and unstable, making it usable for satellites.

(5) In what regards now L3, yet another functioning mechanism going on here, which is this time something very simple, namely an object  $\varepsilon$  placed there at L3 will simply travel around  $M$ , in a standard elliptic way, basically on the same orbit as  $m$ , slightly adjusted as to take into account the gravity of  $m$  too. Again, this is an unstable point, suitable for satellites, but who would go up there to install one.

(6) Finally, regarding L4 and L5, these are two extra solutions, discovered later by Lagrange, located at the positions where they form, along with  $M$ ,  $m$ , equilateral triangles. An object  $\varepsilon$  say placed at L4 will stay there, or rather travel on an elliptical orbit around  $M$  passing through L4, keeping its L4 relative position with respect to  $M$ ,  $m$ , due to the fact that, due to the geometry of the equilateral triangle  $\varepsilon - m - M$ , the extra pull from  $m$  keeps it in tune with  $m$ , on that smaller orbit. And the same goes for L5.

(7) These two last points L4, L5 are stable, provided that the masses  $M$ ,  $m$  of the two big objects satisfy  $M/m > 24.96$ , which is the case for instance for the Sun-Earth system, and for the Earth-Moon system too. However, the stability makes them unsuitable for satellite use, due to the tons of space garbage accumulated there, over the years.  $\square$

So long for the  $N$ -body problem, and for the Lagrange points. Obviously there is some very interesting mathematics and physics going on here, which is relevant for anything in relation with the Solar System, be that natural or human-made. In fact, speaking astronomy, the Sun-Earth-Moon system is already something that you can spend your whole life of scientist on, because due to pure 3-body gravitation, and then also to various imperfections in the shape, density, and many other parameters of these objects, things in this system are continuously evolving, over the passing years, and with the very long term predictions on what will really happen being quite complicated to make.

Moving forward, now that we talked about satellites, do we really have the means of sending them in space? At the basic level, the situation here is as follows:

**THEOREM 3.27.** *The escape velocity from a body having mass  $M$  and radius  $r$  is*

$$v = \sqrt{2gr}$$

where  $g = GM/r^2$  is the surface gravitational acceleration.

**PROOF.** Many things can be said here, the idea being as follows:

(1) To start with, as we certainly know from chapter 2, a rock launched towards the sky, at various angles and speeds, will normally come back to Earth, on an approximate parabolic trajectory. However, we also know from chapter 2 that this phenomenon has

behind it the principle of energy conservation, and this viewpoint raises the possibility of launching the rock with an enormous speed, as to beat the Earth gravitation, and have no need to come back. This enormous speed is by definition the escape velocity.

(2) In practice now, the escape velocity can be computed via energy, as follows:

$$\begin{aligned} \frac{mv^2}{2} = \frac{GMm}{r} &\implies v^2 = \frac{2GM}{r} = 2gr \\ &\implies v = \sqrt{2gr} \end{aligned}$$

(3) Thus, we have the formula in the statement. However, in relation with applications, this is rather just a beginning, on one hand because we have to beat as well drag, and on the other hand because the Earth spins, which modifies the escape velocity as well.  $\square$

In practice now, in order to get an idea on what is going on, numerically, here is a table containing a few selected escape velocities, inside the Solar system:

Location	Beating	Escape velocity, km/s
—		
Sun	Sun gravity	617.5
Mercury	Mercury gravity	4.25
Mercury	Sun gravity	67.7
Earth	Earth gravity	11.18
Earth	Sun gravity	42.1
Moon	Moon gravity	2.38
Moon	Earth gravity	1.4
Neptune	Neptune gravity	23.56
Neptune	Sun gravity	7.7

Getting back now to our to-do list from the beginning of the previous section, let us focus now on question (2) there, namely the 2-body problem with atmospheric drag. This is something not discussed yet, and of crucial real-life importance, and for everything in relation with engineering, and which can bring us far, deep into fluid mechanics.

Mathematically, we have to go back to the Kepler 2-body problem, with the aim of doing some more study here, in the parabolic trajectory case, which is traditionally the field of ballistics. A well regulated militia being necessary to the security of a free state, we have here the following key fact, that you might find of interest:

FACT 3.28. *In the context of ballistics involving drag, the following happen,*

- (1) *At low speeds ( $R < 1$ ) the drag, called Stokes drag, is linear with  $v$ ,*
- (2) *At high speeds ( $R > 1000$ ) the drag, called Newton drag, is quadratic with  $v$ ,*

*with this being controlled by the Reynolds number  $R$ , which depends on the object speed and size, and density and dynamic viscosity of the medium.*

Obviously, many non-trivial things going on here, and with all this being called, and you guessed it right, fluid mechanics. And we will stop our study here, good physics that we learned in this chapter, but this remains, of course, just a beginning.

### 3e. Exercises

“An aircraft carrier is 100,000 tons of diplomacy” – H. Kissinger. Time to do some exercises, for getting stronger in order to support your cause, whatever that cause is, and here are some, in relation with the techniques developed in this chapter:

EXERCISE 3.29. *Write down the Lagrangian and Hamiltonian for the 2-body problem, and then solve this problem, by using both methods. Then try as well with 3 bodies or more, and see if you can say something quick in this way, about these questions.*

EXERCISE 3.30. *Go ahead and investigate the questions mentioned after Theorem 3.19 above, in relation with the various aspects of the rigid bodies, first taken discrete, then solid with a density  $\rho$ , the fluid with a density  $\rho$ , and report on what you found.*

EXERCISE 3.31. *Consider a usual 2-body problem under the influence of an external uniform field, which in practice amounts in having a 3-body problem, with one of the bodies being far away, and try solving it, using various methods developed in the above.*

EXERCISE 3.32. *Work out the formulae of the locations of the Lagrange points  $L_1$ ,  $L_2$ ,  $L_3$ , and also write down a proof for the functioning mechanism of  $L_4$ ,  $L_5$ , at the positions that we indicated above. What about stability, how would you investigate that?*

EXERCISE 3.33. *Study the pendulum, by using basic Newtonian mechanics, then Lagrangian mechanics, and then Hamiltonian mechanics, and with a look at equilibrium and stability questions. Then do the same for a ball moving inside a cup.*

EXERCISE 3.34. *Look up, or find by yourself, the mechanism of tides, along with some needed data on the water on the Earth surface, and then do some math, for the Earth-Moon system, and for the Sun-Earth system too. Which produces bigger tides?*

EXERCISE 3.35. *Learn some more fluid mechanics, in addition to the very few things that have been said in the above, and then examine the gravitational force of a big celestial body filled with a fluid of your choice, subject to some movement.*



## CHAPTER 4

### Einstein and relativity

#### 4a. Inertial frames

We have seen so far that classical mechanics, while from the outside strong, solid and successful, is more of a card castle, or rather a collection of old and clever homemade approximations, which must fixed every time you want to use it seriously. In addition, any application to the real life comes under some effects of drag and friction, which must be taken into account as well, and with this being something quite complicated, leading us into some delicate mathematics and physics of the solids and fluids.

Things here have been like this since ever, Newton and even before too, of course, and everything built on classical mechanics, namely mathematics, physics and engineering too, suffers from the same structural problems. There are of course many enthusiastic people working on this, but things are difficult, and in practice the saying goes that most of what mathematicians say and do is not interesting, and that most of what physicists say and do is wrong. As for engineers, they usually manage to do some decent work, although their buildings and bridges collapse every now and then, too.

In short, modesty, enjoy life and classical mechanics as they are, and don't be evil. With the latter meaning, for mathematicians and physicists, don't publish your formulae if you know that they are not interesting, or wrong. Remember there will be a Judgment Day, with a special evaluation committee for scientists, and their discoveries.

Getting to Einstein now, if there was ever a truly honest man in all this, math and physics alike, that was him. Motivated by some early work, on more advanced and casual topics, that he did by the way by avoiding academia and all the geniuses there, Einstein came upon the following principles, grossly contradicting classical mechanics:

FACT 4.1 (Einstein principles). *The following happen:*

- (1) *Light travels in vacuum at a finite speed,  $c < \infty$ .*
- (2) *This speed  $c$  is the same for all inertial observers.*
- (3) *In non-vacuum, the light speed is lower,  $v < c$ .*
- (4) *Nothing can travel faster than light,  $v \not> c$ .*

All this is a bit philosophical, and needs some explanations. First of all, we don't really know what light is, or at least we haven't met it yet, in our study of classical mechanics.

So let's just call it Beast. With this convention, all the above can be reformulated as follows: "There's a Beast traveling in vacuum at  $c > 0$ , and with this being the World Speed Record, and this number  $c > 0$  is the same for all inertial observers".

Where is the contradiction with classical mechanics? In the last part, concerning the fact that  $c > 0$  is constant for all inertial observers. Indeed, assuming that Beast starts running on the top of a train moving itself at a constant speed  $v$ , his speed should be  $c + v > c$ , contradiction. Equivalently, with Beast jogging as usual, on a sunny morning, on the ground, an observer from a train traveling in the opposite direction at constant speed  $v$  would see Beast running at speed  $c + v > c$ , contradiction again.

So, what do to. Doublecheck your discoveries of course, but (1-4) in the above, which by the way are not all due to Einstein himself, with Einstein's main contribution being the really bad thing, namely (2), are strongly supported by all sorts of experiments.

And so again, what to do. Fixing classical mechanics, of course. Mathematically speaking, we must deal here with something of type  $c + v = c$ , and if there's a number made for that, that is  $c = \infty$ . But (1) clearly says that  $c < \infty$ , so no good. We must come up with something more complicated, and thinking and thinking about all this, which is what Einstein did, following his discovery, leads to the following conclusion:

CONCLUSION 4.2 (Einstein). *Things in classical mechanics are a bit curved at the  $v = \infty$  end, leading to  $v < c$ . In order to fix classical mechanics, we must add a bit of curvature in all formulae, allowing at the same time for  $c + v = c$ , and  $c < \infty$ .*

We will go on this path, following Einstein, in a moment, and we will discover that the curvature of the world that we're living in coming from speed, at the  $v = \infty$  end, forces in fact many other familiar things, such as the distances  $d$ , masses  $m$ , energies  $E$ , and even the time  $t$  itself, to be curved as well. And with this being no longer something speculative, but just truths, coming from basic mathematics, based on Fact 4.1.

Excited about this? In short, we will be embarking on a total destruction process, dealing with the  $\infty$  end of everything that we know, and always took for granted. Let us mention that other familiar things like the temperature  $T$  will not be spared either, and we will talk about this later, when doing thermodynamics.

Importantly, all these things that we've been talking about, namely speed  $v$ , distance  $d$ , mass  $m$ , time  $t$ , energy  $E$  and temperature  $T$ , and perhaps some other too, will turn to be curved at their 0 end as well, due to all sorts of other phenomena, which are of more complicated, quantum mechanical nature. So, anticipating a bit, and including a number of things that we don't know yet, let us upgrade Conclusion 4.2 into:

FACT 4.3. *Everything in life is a bit curved at the  $\infty$  end, and at the 0 end too.*

With this being more than enough as a philosophical conclusion, normally guaranteeing a good place in an asylum, let us get now back to work. We know from the above that the contradiction inside classical mechanics basically comes from Fact 4.1 (2), dealing with inertial observers. So back to our good old friends the inertial frames, that we get to meet in chapter 3 above, and we have now to further build on that material, which was for the least a bit unclear. As in chapter 3, our starting point will be:

DEFINITION 4.4. *An inertial frame is a frame where all basic formulae, namely*

$$||F|| = \frac{Gm_1m_2}{||x_1 - x_2||^2} \quad , \quad F = ma \quad , \quad a = \dot{v} \quad , \quad v = \dot{x} \quad , \quad F_{12} = -F_{21}$$

*hold, with the last formula standing for Newton's action-reaction principle.*

To be more precise here, the first 4 formulae are something that we have been heavily using, so far in this book. As for the last formula, also called Newton's third law, this expresses the fact that when an object 1 acts on an object 2, say via gravity, with force  $F_{12}$ , then object 2 acts as well on object 1, with force  $F_{21} = -F_{12}$ . Which is something that we have used only at selected places in this book, when really needed.

The above definition is of course something a bit informal, somewhat at an advanced level, but aren't we here already knowing how to solve the Kepler problem, with calculus, ellipses and everything, and having learned many other things as well. For a more axiomatic treatment we refer to our standard undergraduate mechanics books, namely Feynman [33], Kibble [57] or Taylor [90], or to any introductory book to relativity, some good references here being the good old book of French [37] on special relativity, or the modern book of Carroll [16], dealing with both special and general relativity.

Let us also recall a few things that we know about inertial frames, from chapter 3:

PROPOSITION 4.5. *The following hold, regarding the inertial frames:*

- (1) *In the context of the 2-body problem, the standard frames used for computations, with  $M_1$  or  $M_2$  fixed, are not inertial.*
- (2) *In fact, the linear combination frames of type  $\lambda_1 M_1 + \lambda_2 M_2$ , including the center of mass frame, are all non-inertial.*
- (3) *The total angular momentum of a system of bodies  $M_1, \dots, M_k$  is conserved, when computed with respect to an inertial frame.*
- (4) *However, this is not the end of the story with angular momentum, because at  $k = 2$ , this is conserved as well in the frames of type  $\lambda_1 M_1 + \lambda_2 M_2$ .*

PROOF. These are all things that we know from chapter 3, with (1) and (2) being trivial, (3) coming trivially from  $F_{12} = -F_{21}$ , and (4) being something trivial too.  $\square$

All in all, the conclusion would be that inertial frames are a rare asset, and also that the conservation of angular momentum, although not proving that the frame is inertial, is a good test for inertiality. Quite modest all this, but not bad, as a starting point.

So, let us start hunting for inertial frames. And also discuss what exactly, and to what precise extent, is wrong with the various non-inertial frames that we might meet on the way. A simple idea here is to start with a familiar problem, such as the 2-body one, written in some standard non-inertial frame that is well-adapted for computations, and then try to transform that non-inertial frame into an inertial one. And regarding now transformations, there are several things that we can do, according to:

**PROPOSITION 4.6.** *Any frame can be obtained from another frame, by performing the following operations, which are independent of each other:*

- (1) *Changing the origin,  $x \rightarrow x - d$ .*
- (2) *Rescaling the coordinates,  $x \rightarrow r \cdot x$ .*
- (3) *Rotating the coordinates,  $x \rightarrow Ux$  with  $U \in O_3$ .*

**PROOF.** This is something obvious, written perhaps in a somewhat fancy way. To be more precise, (1) amounts in moving the origin 0 at an arbitrary location  $d \in \mathbb{R}^3$ , (2) amounts in rescaling the coordinates by  $r_1, r_2, r_3 \in \mathbb{R}$  respectively, and (3) amounts in rotating the frame, with  $O_3$  standing for the group of rotations in 3 dimensions. But these three operations clearly allow passing from one frame to another, as claimed.  $\square$

Let us first examine the 2-body problem. Here we know from chapter 3 that the center of mass frame, obtained via (1), is the best one that we have, so the problem is whether we can make it inertial using (2). And here, we have the following result:

**THEOREM 4.7.** *In the standard context of the 2-body problem, by moving the origin at the center of mass, and then rescaling all three coordinates by  $r = r(t) \in \mathbb{R}$  given by*

$$(rx)'' = -\frac{GM_1(M_1 + M_2)(rx)}{\|(rx)^3\|}$$

*with this meaning that  $y = rx$  must be the trajectory of a body of mass  $M_1$  travelling around a body of mass  $M_1 + M_2$ , the resulting frame is inertial.*

**PROOF.** We will be actually looking at all the inertial frames that can be obtained via the operations (1) and (2) in Proposition 4.6, and only at the end we will particularize to the frame discussed in the statement. Our study goes as follows:

(1) Assume that  $M_1$  is fixed at 0, and that  $M_2$  moves around it, with position vector  $x \in \mathbb{R}^3$ . By changing the origin at  $d \in \mathbb{R}^3$ , then rescaling the coordinates by  $r \in \mathbb{R}^3$ , as in Proposition 4.6 (1,2), the new coordinates of  $M_1, M_2$  are as follows:

$$z_1 = -r \cdot d \quad , \quad , z_2 = r \cdot (x - d)$$

We want to check whether the forces between  $M_1, M_2$  satisfy the following formula:

$$M_1 \ddot{z}_1 = -M_2 \ddot{z}_2 = \frac{GM_1 M_2 (z_2 - z_1)}{\|z_2 - z_1\|^3}$$

By using the above formulae of  $z_1, z_2$ , this formula to be checked reads:

$$-M_1(r \cdot d)'' = -M_2(r \cdot x)'' + M_2(r \cdot d)'' = \frac{GM_1 M_2 (r \cdot x)}{\|r \cdot x\|^3}$$

(2) This looks complicated, so let us look for a uniform solution,  $r = (r, r, r)$ . In this case the componentwise dot product is a usual product, and our equation becomes:

$$-M_1(rd)'' = -M_2(rx)'' + M_2(rd)'' = \frac{GM_1 M_2 x}{r^2 \|x\|^3}$$

By using now the formula of gravity in the initial frame, this equation becomes:

$$-M_1(rd)'' = -M_2(rx)'' + M_2(rd)'' = -M_1 \cdot \frac{x''}{r^2}$$

But this formula can be written, more conveniently, as follows:

$$(rd)'' = \frac{M_2}{M_1 + M_2} (rx)'' = \frac{x''}{r^2}$$

Thus, we have our equations, which look good, and we can now solve for  $r$  on the right, and then solve for  $d$  on the left, as to get our inertial frame.

(3) Let us first solve for  $r$  on the right. It is convenient here to replace  $x''$  by the Newtonian gravitation formula it came from, and our equation becomes:

$$\frac{M_2}{M_1 + M_2} (rx)'' = -\frac{GM_1 M_2 x}{r^2 \|x\|^3}$$

But this equation can be written in the following more convenient way:

$$(rx)'' = -\frac{GM_1(M_1 + M_2)(rx)}{\|(rx)^3\|}$$

We conclude that  $y = rx$  must be the trajectory of a body of mass  $M_1$  travelling around a body of mass  $M_1 + M_2$ , with arbitrary initial data  $y_0, w_0$ .

(4) Let us solve now for  $d$  on the left, in the equations found in (2) above. Here the situation is very simple, the solutions  $rd$  being as follows, with  $a, b \in \mathbb{R}^3$ :

$$rd = \frac{M_2}{M_1 + M_2} rx + at + b$$

Thus, with  $r$  being as in (3) above, the solutions are as follows, with  $a, b \in \mathbb{R}^3$ :

$$d = \frac{M_2}{M_1 + M_2} x + \frac{at + b}{r}$$

Thus with  $c$  being the center of mass, the formula is as follows, with  $a, b \in \mathbb{R}^3$ :

$$d = c + \frac{at + b}{r}$$

Now by taking  $a = b = 0$ , we are led to the conclusion in the statement.  $\square$

As a comment now, the above computation was certainly successful, but its technical details raise grim perspectives about the  $k$ -body case, with  $k \geq 3$ . Indeed, the equations of motion will be far more complicated, and we will not be able to perform even the simplest algebraic manipulations done in the above. As a second issue, we cannot hope for a simple answer, via a uniform rescaling  $r = (r, r, \dots, r)$ , simply because the parameter  $M_1(M_1 + M_2)$  appearing in Theorem 4.7 has no  $k$ -analogue, when  $k \geq 3$ . And finally, above everything, at  $k \geq 3$  we have no solution to the problem that we can rely upon when needed. Thus, overall bad news, and time to stop this discussion here.

Regarding now the conservation of the angular momentum, we have here the following result, which improves our previous knowledge of the subject:

**THEOREM 4.8.** *In the context of the 2-body problem, by moving the origin at  $d \in \mathbb{R}^3$ , then uniformly rescaling by  $r \in \mathbb{R}$ , the angular momentum is conserved when:*

$$M_2(x \times (rd)'' + d \times (rx)'' - x \times (rx)'') = (M_1 + M_2) \cdot d \times (rd)''$$

*In the particular case where  $d = \lambda x$ , with  $\lambda$  being constant, these equations reduce to*

$$(rx)'' \sim x$$

*and  $r$  constant, as well as the inertial frame in Theorem 4.7, provide solutions.*

**PROOF.** As before with the study in Theorem 4.7, we will do things slowly, by looking for explicit solutions only at the end. Our study goes as follows:

(1) Assume that  $M_1$  is fixed at 0, and that  $M_2$  moves around it, with position vector  $x \in \mathbb{R}^3$ . By changing the origin at  $d \in \mathbb{R}^3$ , then uniformly rescaling the coordinates by  $r \in \mathbb{R}$ , the new coordinates of  $M_1, M_2$  are as follows:

$$z_1 = -rd \quad , \quad , z_2 = r(x - d)$$

Thus, the derivative of the total angular momentum is given by:

$$\begin{aligned} J' &= J'_1 + J'_2 \\ &= M_1 \cdot (-rd) \times (-(rd)'') + M_2 \cdot (rx - rd) \times ((rx)'' - (rd)'') \\ &= r(M_1 + M_2) \cdot d \times (rd)'' - rM_2(x \times (rd)'' + d \times (rx)'' - x \times (rx)'') \end{aligned}$$

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

(2) In the particular case  $d = \lambda x$ , with  $\lambda$  constant, the above formula of  $J'$  reads:

$$\begin{aligned} J' &= r(M_1 + M_2)\lambda^2 \cdot x \times (rx)'' - rM_2(2\lambda x \times (rx)'' - x \times (rx)'') \\ &= r((M_1 + M_2)\lambda^2 + M_2(1 - 2\lambda)) \cdot x \times (rx)'' \\ &= r((M_1 + M_2)\lambda^2 - 2M_2\lambda + M_2) \cdot x \times (rx)'' \end{aligned}$$

The discriminant on the left being  $\Delta = -4M_1M_2 < 0$ , our only hope is  $x \times (rx)'' = 0$ , which amounts in saying that we must have  $(rx)'' \sim x$ , as stated.

(3) Finally, in what regards the explicit solutions mentioned at the end, we already know from the above that the conservation of  $J$  holds for them. But these are now all particular cases of the present result. Indeed,  $r$  constant gives  $(rx)'' \sim x$ , and at  $r = 1$  we obtain the frames of type  $\lambda_1 M_1 + \lambda_2 M_2$ , studied before. Also, with  $d = c$  being the center of mass, and with  $r$  being as in Theorem 4.7, we have  $(rx)'' \sim rx \sim x$ , and the frame here coincides with the inertial one constructed in Theorem 4.7, as desired.  $\square$

As before with Theorem 4.7, the above computation was something successful in the 2-body case, unifying things that we knew so far. But also as before with Theorem 4.7, the details of the proof raise grim perspectives on what will happen for  $k$  bodies, with  $k \geq 3$ . Indeed, the only non-inertial frames that we can start with are the center of mass frame, or the frame centered at the smallest, or the biggest body, assuming that this smallest or biggest body is tiny, or huge, with respect to the others. But here, again as it was the case with Theorem 4.7, many forces, things too complex, and so on.

Before leaving the subject, however, and getting back now to given inertial frames, we know from chapter 3 that the angular momentum is conserved in this case, and with this coming from a trivial computation. Here is a useful complement to that result:

**THEOREM 4.9.** *Given bodies  $M_1, \dots, M_k$  moving in an inertial frame, with coordinates  $x_1, \dots, x_k$ , their total angular momentum, which is constant, is given by*

$$J = \sum_i M_i \cdot c \times \dot{c} + \sum_i M_i \cdot y_i \times \dot{y}_i$$

where  $y_i = x_i - c$  are the relative coordinates with respect to the center of mass  $c$ . Thus  $J$  is the momentum of the average system, plus the momentum computed at  $c$ .

**PROOF.** The fact that  $J$  is constant is something that we know, coming from:

$$\begin{aligned} \dot{J} &= \sum_{i < j} x_i \times F_{ji} + x_j \times F_{ij} \\ &= \sum_{i < j} (x_i - x_j) \times F_{ji} \\ &= 0 \end{aligned}$$

Regarding now the second assertion, consider the center of mass  $c$ , and write the coordinates of  $M_1, \dots, M_k$  in the form  $x_i = c + y_i$ . We have then:

$$\begin{aligned} J &= \sum_i M_i \cdot x_i \times \dot{x}_i \\ &= \sum_i M_i \cdot (c + y_i) \times (\dot{c} + \dot{y}_i) \\ &= \sum_i M_i \cdot c \times \dot{c} + \sum_i M_i y_i \times \dot{c} + c \times \sum_i M_i \dot{y}_i + \sum_i M_i \cdot y_i \times \dot{y}_i \end{aligned}$$

Now since  $c$  is the center of mass we have  $\sum_i M_i y_i = 0$ , and we are left with:

$$J = \sum_i M_i \cdot c \times \dot{c} + \sum_i M_i \cdot y_i \times \dot{y}_i$$

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

As a last general topic regarding frames, let us examine now the rotations of frames, and what can be done with them, a subject that we have not got into, so far. With the remark that this question is of particular interest for us humans, living on Earth, which rotates. There are many things that can be said here, and we first have:

**THEOREM 4.10.** *Assume that a 3D body rotates along an axis, with angular speed  $w$ . For a fixed point of the body, with position vector  $x$ , the usual 3D speed is*

$$v = \omega \times x$$

where  $\omega = wn$ , with  $n$  unit vector pointing North. When the point moves on the body

$$V = \dot{x} + \omega \times x$$

is its speed computed by an inertial observer  $O$  on the rotation axis.

**PROOF.** We have two assertions here, both requiring some 3D thinking, as follows:

(1) Assuming that the point is fixed, the magnitude of  $\omega \times x$  is the good one, due to the following computation, with  $r$  being the distance from the point to the axis:

$$\|\omega \times x\| = w\|x\|\sin t = wr = \|v\|$$

As for the orientation of  $\omega \times x$ , this is the good one as well, because the North pole rule used above amounts in applying the right-hand rule for finding  $n$ , and so  $\omega$ , and this right-hand rule was precisely the one used in defining the vector products  $\times$ .



(2) Next, when the point moves on the body, the inertial observer  $O$  can compute its speed by using a frame  $(u_1, u_2, u_3)$  which rotates with the body, as follows:

$$\begin{aligned} V &= \dot{x}_1 u_1 + \dot{x}_2 u_2 + \dot{x}_3 u_3 + x_1 \dot{u}_1 + x_2 \dot{u}_2 + x_3 \dot{u}_3 \\ &= \dot{x} + (x_1 \cdot \omega \times u_1 + x_2 \cdot \omega \times u_2 + x_3 \cdot \omega \times u_3) \\ &= \dot{x} + \omega \times (x_1 u_1 + x_2 u_2 + x_3 u_3) \\ &= \dot{x} + \omega \times x \end{aligned}$$

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

In what regards now the acceleration, the result, which is famous, is as follows:

**THEOREM 4.11.** *Assuming as before that a 3D body rotates along an axis, the acceleration of a moving point on the body, computed by  $O$  as before, is given by*

$$A = a + 2\omega \times v + \omega \times (\omega \times x)$$

*with  $\omega = \omega n$  being as before. In this formula the second term is called Coriolis acceleration, and the third term is called centripetal acceleration.*

**PROOF.** This comes by using twice the formulae in Theorem 4.10, as follows:

$$\begin{aligned} A &= \dot{V} + \omega \times V \\ &= (\ddot{x} + \dot{\omega} \times x + \omega \times \dot{x}) + (\omega \times \dot{x} + \omega \times (\omega \times x)) \\ &= \ddot{x} + \omega \times \dot{x} + \omega \times \dot{x} + \omega \times (\omega \times x) \\ &= a + 2\omega \times v + \omega \times (\omega \times x) \end{aligned}$$

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

The truly famous result is actually the one regarding forces, obtained by multiplying everything by a mass  $m$ , and writing things the other way around, as follows:

$$ma = m\ddot{x} = m\ddot{x} - 2m\omega \times v - m\omega \times (\omega \times x)$$

Here the second term is called Coriolis force, and the third term is called centrifugal force. These forces are both called apparent, or fictitious, because they do not exist in the inertial frame, but they exist however in the non-inertial frame of reference, as explained above. And with of course the terms centrifugal and centripetal not to be messed up.

In fact, even more famous is the terrestrial application of all this, as follows:

**THEOREM 4.12.** *The acceleration of an object  $m$  subject to a force  $F$  is given by*

$$ma = F - mg - 2m\omega \times v - m\omega \times (\omega \times x)$$

*with  $g$  pointing upwards, and with the last terms being the Coriolis and centrifugal forces.*

**PROOF.** This follows indeed from the above discussion, by assuming that the acceleration  $A$  there comes from the combined effect of a force  $F$ , and of the usual  $g$ .  $\square$

We refer to any standard undergraduate mechanics book, such as Feynman [33], Kibble [57] or Taylor [90] for more on the above, including various numerics on what happens here on Earth, the Foucault pendulum, history of all this, and many other things. Let us just mention here, as a basic illustration, that a rock dropped from 100m deviates about 1cm from its intended target, due to the formula in Theorem 4.12.

All this is quite interesting, but it's getting late, time to stop our hunting for inertial frames, get back home, and grill a steak bought at the supermarket. The day has been long, and our first discovery was that the inertial frames do not really exist, mathematically speaking. That is, given a concrete math question, formulated in a non-inertial frame, you cannot really prove via math that an inertial frame for it exists.

As for our second discovery, this was the fact that the inertial frames do not really exist in the real life either. There is rotation everywhere, and a myriad other problems, and there might be an inertial frame suspended somewhere, out there in the universe, in the void, but we will certainly not be able to find it, with our technology.

What about Einstein and relativity, then? Looking back at Fact 4.1, it is not very clear what the key point there, namely (2), really says. From our knowledge so far of the inertial frames, these are rather theoretical objects, approximating what is going on, and whose existence is quite uncertain. So (2) there should be rather reformulated as “the speed of light in vacuum is approximately  $c$ , for all well-intentioned observers”. With well-intentioned meaning scientists who did the physics, did the math, and carefully fixed various bugs of their frames, as to make them as inertial as possible.

This sounds quite reasonable, but in practice now, again by getting back to Fact 4.1, it is better to leave it as it is, because a revolution as we are planning to develop, following Einstein, can only come from simple new principles like that. So, all in all, things fine, and not that some disaster has struck, but we're however a bit in an uncomfortable situation with respect to Fact 4.1, and so time to ask the cat. Who cat is unfortunately in a bad mood today, and instead of coming as usual with a gentle piece of advice, says:

CAT 4.13. *Finding inertial frames is not your business, shut up and compute, and leave it to experimentalists to observe speed at  $v > c$ .*

Damn cat. I was expecting such rude things only later, when doing quantum mechanics. But he's probably right. Sometimes it helps remembering what your job is.

#### 4b. Light, trains, clocks

With the notion of inertial frame understood, we can now go back to Fact 4.1, regarding the speed of light  $c$ , and then develop the Einstein theory, as to fix the  $c + v = c$  bug of classical mechanics, as outlined in Conclusion 4.2, and then in Fact 4.3 as well.

There is however still a bit of discussion left, regarding the light itself. Whatever that light is, does it really belong to classical mechanics? And the answer here is yes, with several celestial observations, and experiments here on Earth, having shown that light has mass  $m > 0$ , and with mass being the only requirement for being part of this big circus which is classical mechanics. And finally, for being complete, let us also remind:

FACT 4.14. *The speed of light in vacuum is  $c = 299\,792\,458$  m/s.*

This is a figure which comes out of experiments, and with  $c \simeq 3 \times 10^9$  m/s being actually something quite old. As an interesting feature, the above formula is exact, due to the well-known mess with regulating meters, seconds and other units. To be more precise, there is a rock-solid definition for the second, based on atomic clocks, but not for the meter, and by a recent decision the above formula was declared exact, and any further changes in the observed value of  $c$  will be blamed on the meter.

Be said in passing, would such a wise decision have been taken much earlier, the speed of light would be  $c = 3 \times 10^9$  m/s, exactly. But now it is too late. Finally, all these issues do not bother much theoretical physicists, who use tailored units depending on the precise problems they are working on, with around 50 orders of magnitude on the menu, and who usually, when dealing often with  $c$ , arrange things as to take  $c = 1$ .

As a final piece of ingredient, let us formulate as well a clear objective:

PROBLEM 4.15. *How to fix the  $c + v = c$  bug of classical mechanics?*

Following Einstein, we will do this in two steps. The first step, called special relativity, consists in forgetting gravity, and fixing the basic laws of motion of mechanics. Indeed,  $c + v = c$  is something about speeds, and not accelerations or gravity, so all the basic laws of motion must be fixed, by introducing a bit of curvature in them, as to make  $c$  to play somehow the role of  $\infty$ . And this will be actually not that hard, with just a little bit of algebra involved, and we will explain this in this section.

As for the question coming afterwards, that of including gravity into this new theory of motion, the special relativity, this is something more complicated, called general relativity, and using some serious geometry, and we will discuss this in the next section.

As usual, we will be quite brief. An excellent introduction to special relativity is the good old book of French [37], and to general relativity, the book of Carroll [16]. You can also go with all sorts of other books, since basically any book of physics, be that an academic textbook or something more popular, needs and contains some sort of introduction to relativity. Particularly enjoyable reads here are the books of Griffiths [45] and Huang [52]. And also, don't forget about Feynman [33], if there's someone who managed to find a nice way to explain  $E = mc^2$  to everyone, that is him.

Getting started now,  $c + v = c$  is obviously about adding speeds, so this topic, adding speeds, will be the first one that we will discuss. In the classical case, we have:

THEOREM 4.16. *The classical speeds add according to the Galileo formula*

$$v_{AC} = v_{AB} + v_{BC}$$

where  $v_{AB}$  denotes the relative speed of  $A$  with respect to  $B$ .

PROOF. This is clear indeed from the definition of speed, and very intuitive.  $\square$

In order to find the fix, we will first discuss the 1D case, and leave the 3D case, which is a bit more complicated, for later. We will use two tricks. First, let us forget about absolute speeds, with respect to a given frame, and talk about relative speeds only. In this case we are allowed to sum only quantities of type  $v_{AB}$ ,  $v_{BC}$ , and we denote by  $v_{AB} +_g v_{BC}$  the corresponding sum  $v_{AC}$ . With this convention, the Galileo formula becomes:

$$u +_g v = u + v$$

As a second trick now, observe that this Galileo formula holds in any system of units. In order now to deal with our problems, basically involving high speeds, it is convenient to change the system of units, as to have  $c = 1$ . With this convention our  $c + v = c$  problem becomes  $1 + v = 1$ , and the solution to it is quite obvious, as follows:

PROPOSITION 4.17. *If we define the Einstein sum  $+_e$  of relative speeds by*

$$u +_e v = \frac{u + v}{1 + uv}$$

*in  $c = 1$  units, then we have the formula  $1 +_e v = 1$ , valid for any  $v$ .*

PROOF. This is clear indeed from our definition of  $+_e$ , because if we plug in  $u = 1$  in the above formula, we obtain as result  $(1 + v)/(1 + v) = 1$ .  $\square$

Summarizing, we have solved our problem. In order now to formulate a final result, we must do some reverse engineering, by waiving the above two tricks. First, by getting back to usual units,  $v \rightarrow v/c$ , our new addition formula becomes:

$$\frac{u}{c} +_e \frac{v}{c} = \frac{\frac{u}{c} + \frac{v}{c}}{1 + \frac{u}{c} \cdot \frac{v}{c}}$$

By multiplying by  $c$ , we can write this formula in a better way, as follows:

$$u +_e v = \frac{u + v}{1 + uv/c^2}$$

In order now to finish, it remains to get back to absolute speeds, as in Theorem 4.16 above. And by doing so, we are led to the following result:

THEOREM 4.18. *If we sum the speeds according to the Einstein formula*

$$v_{AC} = \frac{v_{AB} + v_{BC}}{1 + v_{AB}v_{BC}/c^2}$$

*then the Galileo formula still holds, approximately, for low speeds*

$$v_{AC} \simeq v_{AB} + v_{BC}$$

*and if we have  $v_{AB} = c$  or  $v_{BC} = c$ , the resulting sum is  $v_{AC} = c$ .*

PROOF. We have two assertions here, which are both clear, as follows:

(1) Regarding the first assertion, if we are at low speeds,  $v_{AB}, v_{BC} \ll c$ , the correction term  $v_{AB}v_{BC}/c^2$  disappears, and we are left with the Galileo formula, as claimed.

(2) As for the second assertion, this follows from the above discussion, but let us doublecheck this, to make sure that we have made no mistake. With  $v_{AB} = c$  we get:

$$v_{AC} = \frac{c + v_{BC}}{1 + v_{BC}/c} = c$$

Similarly, with  $v_{BC} = c$  we get  $v_{AC} = c$  too, and so no mistakes, and we're done.  $\square$

As a conclusion, we have solved the problem, mathematically. All this is very nice, and fits with the Einstein principles from Fact 4.1, and to be more precise, fixes the laws of motion, as to make them fit with that Fact 4.1. But the problem is now, does all this math really correspond to physics? And the answer here is fortunately yes, due to:

FACT 4.19. *The Einstein addition formula is correct.*

This is of course a physics fact, based on several things. First we have the Galileo formula, thought before to be exact,  $v_{AC} = v_{AB} + v_{BC}$ , and some numerics were to be done here, in order to convince the audience that this formula might well be  $v_{AC} \simeq v_{AB} + v_{BC}$ , due to the inevitable tiny errors in our speed measuring machinery, and with the correction term which might well be the Einstein one,  $v_{AB}v_{BC}/c^2$  as above. This of course does not prove the Einstein formula, but shows that it is compatible with the Galileo formula.

As a second piece of evidence now, which is considerably more serious, the Einstein formula is compatible with Fact 4.1, which itself is a physics fact. Thus, we're here at the point where the Einstein formula is a "beautiful mathematical fix, compatible with everything known before, namely Fact 4.1 and the Galileo formula".

Finally, as a third and ultimate piece of evidence, various observations and experiments at very high speeds,  $v_{AC} \simeq c$ , which needless to say, were as usual subject to some tolerances in our speed measuring machinery, confirmed the Einstein formula.

So this was for the story, a bit oversimplified because the real story involved in fact the 3D generalization of Theorem 4.18 and of Fact 4.19, that we have chosen here in this

book to discuss later. The credit for the key experiment goes to Michelson and Morley, and the credit for the fix, and for putting everything together, goes to Einstein. For more on all this, we refer as usual to any standard relativity book, such as French [37].

Getting back now to the Einstein summation formula from Theorem 4.18, or rather to its more compact formulation from Proposition 4.17, that formula, while looking very simple, is in fact quite subtle, and must be handled with care. Indeed, we have:

PROPOSITION 4.20. *The Einstein speed summation, written in  $c = 1$  units as*

$$u +_e v = \frac{u + v}{1 + uv}$$

*has the following properties:*

- (1)  $u, v < 1$  implies  $u +_e v < 1$ .
- (2)  $u +_e v = v +_e u$ .
- (3)  $(u +_e v) +_e w = u +_e (v +_e w)$ .
- (4) *However,  $\lambda u +_e \lambda v = \lambda(u +_e v)$  fails.*

PROOF. All these assertions are elementary, as follows:

- (1) This follows from the following formula, valid for any speeds  $u, v$ :

$$1 - u +_e v = 1 - \frac{u + v}{1 + uv} = \frac{(1 - u)(1 - v)}{1 + uv}$$

- (2) This is clear too, coming from the following computation:

$$u +_e v = \frac{u + v}{1 + uv} = \frac{v + u}{1 + vu} = v +_e u$$

- (3) We have indeed the following computation:

$$(u +_e v) +_e w = u +_e (v +_e w) = \frac{u + v + w + uvw}{1 + uv + uw + vw}$$

- (4) This is clear too, with the remark however that the formula  $\lambda u +_e \lambda v = \lambda(u +_e v)$  works at  $\lambda = -1, 0, 1$ , or when  $u = 0$ ,  $v = 0$ , or  $u + v = 0$ .  $\square$

Going ahead now with the fix of classical mechanics, speed is distance/time, so we must now fix as well distance, or time, or both. Fortunately the solution to the problem, involving a Gedankenexperiment using a train and a clock, is unique, as follows:

THEOREM 4.21. *Time and length are subject to the Lorentz dilation and contraction*

$$t \rightarrow \gamma t \quad , \quad L \rightarrow L/\gamma$$

*where the number  $\gamma \geq 1$ , called Lorentz factor, is given by the formula*

$$\gamma = \frac{1}{\sqrt{1 - v^2/c^2}}$$

*with  $v$  being the moving speed, at which time and length are measured.*

PROOF. Armed with a train and a clock, along with some useful extra material, namely a light bulb, a mirror and a calculator, the proof goes as follows:

(1) Assume that the train moves to the right with speed  $v$ . In order to compute the height  $h$  of the train, the passenger switches on the ceiling light bulb, measures the time  $t$  that the light needs to hit the floor, and concludes that the train height is:

$$h = ct$$

On the other hand, an observer on the ground sees a right triangle here, with on the vertical the height of the train  $h$ , on the horizontal the distance  $vT$  that the train has traveled, and on the hypotenuse the distance  $cT$  that light has traveled, with  $T$  being the duration of the event, according to his watch. Now by Pythagoras we have:

$$(cT)^2 = h^2 + (vT)^2$$

It follows that the two times  $t$  and  $T$  are indeed not equal, and related by:

$$T = \sqrt{\frac{h^2}{c^2 - v^2}} = \sqrt{\frac{t^2}{1 - v^2/c^2}} = \gamma t$$

(2) Regarding now distances, still in the same train traveling at speed  $v$ , the passenger wants to measure the length  $L$  of the car. For this purpose he switches on the light bulb, now at the rear of the car, and measures the time  $t$  needed for the light to reach the front of the car, and get reflected back by a mirror installed there. He concludes that:

$$L = \frac{ct}{2}$$

Viewed from the ground, the duration of the event is  $T = T_1 + T_2$ , where  $T_1 > T_2$  are respectively the time needed for the light to travel forward, among others for beating  $v$ , and the time for the light to travel back, helped this time by  $v$ . More precisely, if  $l$  denotes the length of the train car viewed from the ground, the formula of  $T$  is:

$$T = T_1 + T_2 = \frac{l}{c - v} + \frac{l}{c + v} = \frac{2lc}{c^2 - v^2}$$

With this data, the formula  $T = \gamma t$  of time dilation established in (1) reads:

$$\frac{2lc}{c^2 - v^2} = \frac{2\gamma L}{c}$$

Thus, the two lengths  $L$  and  $l$  are indeed not equal, and related by:

$$l = \frac{\gamma L(c^2 - v^2)}{c^2} = \frac{\gamma L}{\gamma^2} = \frac{L}{\gamma}$$

(3) So this was for the proof, which is standard, with the remark however that the speeds  $c \pm v$  used in (2) are something rather formal. Moreover, the same Gedankenexperiments performed with a “slow bulb”, emitting at  $d < c$ , or with an angle  $\alpha \in \mathbb{R}$  added in (1) or (2), or with both, lead to all sorts of complicated formulae and thinking.  $\square$

As a first comment, the above result is of course due to Einstein, as all the math in this section. The occurrence of Lorentz, who previously discovered similar phenomena in the context of electromagnetism, is something very interesting, ultimately standing as a heavy and final piece of support for Einstein’s theory, the idea being that “among Newton and Maxwell, the latter was right, and Einstein proved it”. More on this later.

As another comment, at this point we are starting a bit to be into abstract things, and a deluge of examples, illustrations and exercises will probably not hurt. Up to you to decide if you want to stay with us, our plan being rather to further build on all this, or take a break and consult some other book, for examples and everything. Nothing here beats Feynman [33], but if looking for old Cadillacs traveling at  $c/2$ , or for thieves escaping from cops using tricks based on  $c$ , illustrated, pick any of Griffiths’ books [42], [43], [44], [45] and check the relativity chapter there, you won’t be deceived.

Back to work now, for things to be complete, we still have to discuss mass and energy. Things here are quite tricky, and as a first objective we would like to fix the momentum conservation equations for the plastic collisions, from chapter 2 above, namely:

$$m = m_1 + m_2$$

$$mv = m_1v_1 + m_2v_2$$

This cannot really be done with bare hands, and by this meaning with mathematics only, but with some help from experiments, the conclusion is as follows:

**FACT 4.22.** *When defining the relativistic mass of an object of rest mass  $m > 0$ , moving at speed  $v$ , by the formula*

$$M = \gamma m \quad : \quad \gamma = \frac{1}{\sqrt{1 - v^2/c^2}}$$

*this relativistic mass  $M$ , and the corresponding relativistic momentum  $P = Mv$ , are both conserved during collisions.*

In other words, the situation here is a bit similar to that of the Galileo addition vs Einstein addition for speeds. The collision equations given above are in fact low-speed approximations of the correct, relativistic equations, which are as follows:

$$M = M_1 + M_2$$

$$Mv = M_1v_1 + M_2v_2$$

Again, for the full story here, we recommend a solid special relativity book.



Finally, it remains to discuss kinetic energy. You have certainly heard of the formula  $E = mc^2$ , which might actually well be on your T-shirt, now as you read this book, and in this case here is the explanation for it, in relation with the above:

**THEOREM 4.23.** *The relativistic energy of an object of rest mass  $m > 0$ ,*

$$\mathcal{E} = Mc^2 \quad : \quad M = \gamma m$$

*which is conserved, as being a multiple of  $M$ , can be written as  $\mathcal{E} = E + T$ , with*

$$E = mc^2$$

*being its  $v = 0$  component, called rest energy of  $m$ , and with*

$$T = (1 - \gamma)mc^2 \simeq \frac{mv^2}{2}$$

*being called relativistic kinetic energy of  $m$ .*

**PROOF.** All this is a bit abstract, coming from Fact 4.22, as follows:

(1) Given an object of rest mass  $m > 0$ , consider its relativistic mass  $M = \gamma m$ , as appearing in Fact 4.22, and then consider the following quantity:

$$\mathcal{E} = Mc^2$$

We know from Fact 4.22 that the relativistic mass  $M$  is conserved, so  $\mathcal{E} = Mc^2$  is conserved too. In view of this, it makes somehow sense to call  $\mathcal{E}$  energy. There is of course no clear reason for doing that, but let's just do it, and we'll understand later.

(2) Let us compute  $\mathcal{E}$ . This quantity is by definition given by:

$$\mathcal{E} = Mc^2 = \gamma mc^2 = \frac{mc^2}{\sqrt{1 - v^2/c^2}}$$

Since  $1/\sqrt{1-x} \simeq 1 + x/2$  for  $x$  small, by calculus, we obtain, for  $v$  small:

$$\mathcal{E} \simeq mc^2 \left(1 + \frac{v^2}{2c^2}\right) = mc^2 + \frac{mv^2}{2}$$

And, good news here, we recognize at right the kinetic energy of  $m$ .

(3) But this leads to the conclusions in the statement. Indeed, we are certainly dealing with some sort of energies here, and so calling the above quantity  $\mathcal{E}$  relativistic energy is legitimate, and calling  $E = mc^2$  rest energy is legitimate too. Finally, the difference between these two energies  $T = \mathcal{E} - E$  follows to be given by:

$$T = (1 - \gamma)mc^2 \simeq \frac{mv^2}{2}$$

Thus, calling  $T$  relativistic kinetic energy is legitimate too, and we are done.  $\square$

This was for the basics of Einstein's relativity theory, in 1D. Of course the last result, Theorem 4.23 dealing with energy, remains a bit unclear, but haven't we been struggling with energy since the beginning of this book, and this even in dumb situations, like dumb rock falling on Earth. So, modesty here, and we'll enjoy Theorem 4.23 as it is.

By the way, the above formula  $E = mc^2$  is quite frightening when thinking a bit numerics, to the point that you might now start fearing a calm glass of water, knowing how much energy is stored in it, and what will happen if that was to explode. Fortunately, water does not spontaneously explode, however other more specialized materials do, and we will discuss all this, with numerics and details, at the end of the present chapter.

#### 4c. Mathematics, cosmology

Let us discuss now the 3D extension of all the above. Basically there is just some math to be done here, because in all what we've been talking about, the object in question is just subject to a speed  $v$ , so if we change our system of coordinates  $xyz$  such that  $x$  is parallel to  $v$ , all the previous 1D results apply, with  $y, z$  being irrelevant.

In fact, for most of the formulae to be extended, considering the 2D case is enough, because adding quantities like speeds or momenta in 3D is in fact a 2D problem, and the extra irrelevant dimension is often something cumbersome. On the other hand, as seen in chapters 1-3, it is often better to switch directly to  $\mathbb{R}^3$ , as to take advantage of the magic vector product  $\times$ , which is defined only there. We will follow this latter path.

Let us start our discussion with a look at the non-relativistic case. Assuming that the object moves with speed  $v$  in the  $x$  direction, the frame change is given by:

$$\begin{aligned}x' &= x - vt \\y' &= y \\z' &= z \\t' &= t\end{aligned}$$

To be more precise, here the first 3 equations come from the law of motion, and  $t' = t$  is the old  $t' = t$ . In the relativistic setting now, the result is more tricky, as follows:

**THEOREM 4.24.** *In the context of an object moving with speed  $v$  along the  $x$  axis, the frame change is given by the Lorentz transformation*

$$\begin{aligned}x' &= \gamma(x - vt) \\y' &= y \\z' &= z \\t' &= \gamma(t - vx/c^2)\end{aligned}$$

where  $\gamma = 1/\sqrt{1 - v^2/c^2}$  is as usual the Lorentz factor.

PROOF. We know that, with respect to the non-relativistic formulae,  $x$  is subject to the Lorentz dilation by  $\gamma$ , and we obtain as desired  $x' = \gamma(x - vt)$ . Regarding  $y, z$ , these are obviously unchanged. Finally, regarding  $t$ , a naive thought would suggest that this is subject to a Lorentz contraction by  $1/\gamma$ , but this is not true, and more thinking leads to the conclusion that we must use the reverse Lorentz transformation, given by:

$$x = \gamma(x' + vt')$$

$$y = y'$$

$$z = z'$$

By using the formula of  $x'$  we can compute  $t'$ , and we obtain:

$$t' = \frac{x - \gamma x'}{\gamma v} = \frac{x - \gamma^2(x - vt)}{\gamma v} = \frac{\gamma^2 vt + (1 - \gamma^2)x}{\gamma v}$$

On the other hand, we have the following computation:

$$\gamma^2 = \frac{c^2}{c^2 - v^2} \implies \gamma^2(c^2 - v^2) = c^2 \implies (\gamma^2 - 1)c^2 = \gamma^2 v^2$$

Thus we can finish the computation of  $t'$  as follows:

$$t' = \frac{\gamma^2 vt + (1 - \gamma^2)x}{\gamma v} = \frac{\gamma^2 vt - \gamma^2 v^2 x / c^2}{\gamma v} = \gamma \left( t - \frac{vx}{c^2} \right)$$

We are therefore led to the conclusion in the statement.  $\square$

The Lorentz transformation being linear, time to do some math. Since  $y, z$  are irrelevant, we will put them at the end, and put the time  $t$  first, as to be close to  $x$ . By multiplying as well the time equation by  $c$ , our system looks better, as follows:

$$ct' = \gamma(ct - vx/c)$$

$$x' = \gamma(x - vt)$$

$$y' = y$$

$$z' = z$$

In linear algebra terms, the result is as follows:

THEOREM 4.25. *The Lorentz transformation is given by*

$$\begin{pmatrix} \gamma & -\beta\gamma & 0 & 0 \\ -\beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} ct' \\ x' \\ y' \\ z' \end{pmatrix}$$

where  $\gamma = 1/\sqrt{1 - v^2/c^2}$  as usual, and where  $\beta = v/c$ .

PROOF. In terms of  $\beta = v/c$ , replacing  $v$ , the system looks as follows:

$$ct' = \gamma(ct - \beta x)$$

$$x' = \gamma(x - \beta ct)$$

$$y' = y$$

$$z' = z$$

But this gives the formula in the statement.  $\square$

As an illustration, let us verify that the inverse Lorentz transformation is indeed given by reversing the speed,  $v \rightarrow -v$ . With notations as in Theorem 4.24, the result is:

PROPOSITION 4.26. *The inverse of the Lorentz transformation is given by  $v \rightarrow -v$ ,*

$$x = \gamma(x' + vt')$$

$$y = y'$$

$$z = z'$$

$$t = \gamma(t' + vx'/c^2)$$

where  $\gamma = 1/\sqrt{1 - v^2/c^2}$  is as usual the Lorentz factor, identical for  $v$  and  $-v$ .

PROOF. In terms of the formalism in Theorem 4.25, reversing the speed  $v \rightarrow -v$  amounts in reversing the  $\beta = v/c$  parameter there,  $\beta \rightarrow -\beta$ , and what we have to prove is that by doing so, we obtain the inverse of the matrix appearing there. But here we can restrict attention to the upper left corner, where we have, as desired:

$$\begin{pmatrix} \gamma & -\beta\gamma \\ -\beta\gamma & \gamma \end{pmatrix} \begin{pmatrix} \gamma & \beta\gamma \\ \beta\gamma & \gamma \end{pmatrix} = \begin{pmatrix} \gamma^2(1 - \beta^2) & 0 \\ 0 & \gamma^2(1 - \beta^2) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Now by getting back to notations as in Theorem 4.24, we obtain the result.  $\square$

Getting back now to physics, let us try to understand how space  $\mathbb{R}^3$  and time  $\mathbb{R}$  are exactly intricated. In non-relativistic physics two events are separated by space  $\Delta x$  and time  $\Delta t$ , with these two separation variables being independent. In relativistic physics this is no longer true, and the correct analogue of this comes from:

THEOREM 4.27. *The following quantity, called relativistic spacetime separation,*

$$\Delta s^2 = c^2 \Delta t^2 - (\Delta x^2 + \Delta y^2 + \Delta z^2)$$

*is invariant under relativistic frame changes.*

PROOF. We must prove that the quantity  $K = c^2t^2 - x^2 - y^2 - z^2$  is invariant under Lorentz transformations. For this purpose, observe that we have:

$$K = \left\langle \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix}, \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix} \right\rangle$$

Thus, if we denote by  $L$  the matrix of the Lorentz transformation, from Theorem 4.25, and by  $E$  the above matrix, we must prove that for any vector  $\xi$  we have:

$$\langle E\xi, \xi \rangle = \langle EL\xi, L\xi \rangle$$

Since  $L$  is symmetric we have  $\langle EL\xi, L\xi \rangle = \langle LEL\xi, \xi \rangle$ , so we must prove:

$$E = LEL$$

But this is the same as proving  $L^{-1}E = EL$ , and by using the fact that  $L \rightarrow L^{-1}$  is given by  $\beta \rightarrow -\beta$ , what we eventually want to prove is that:

$$L_{-\beta}E = EL_{\beta}$$

So, let us prove this. As usual we can restrict the attention to the upper left corner, call that NW corner, and here we have the following computations:

$$\begin{aligned} (L_{-\beta}E)_{NW} &= \begin{pmatrix} \gamma & \beta\gamma \\ \beta\gamma & \gamma \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} \gamma & -\beta\gamma \\ \beta\gamma & -\gamma \end{pmatrix} \\ (EL_{\beta})_{NW} &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \gamma & -\beta\gamma \\ -\beta\gamma & \gamma \end{pmatrix} = \begin{pmatrix} \gamma & -\beta\gamma \\ \beta\gamma & -\gamma \end{pmatrix} \end{aligned}$$

The matrices on the right being equal, this gives the result.  $\square$

There are many things that can be said about the spacetime separation variable in Theorem 4.27, and generally speaking, the understanding of relativistic spacetime consists in further building on the above results, and particularly on Theorem 4.27. As usual, we refer here to the literature, as for instance French [37], or Carroll [16].

As a final comment here, in relation with special relativity in general, when looking for “examples” for all this, namely particles traveling at very high speeds, the most obvious candidate is the usual electron, traveling as electricity. We will see later, in chapters 5-6 below, that the general equations there, called Maxwell equations, which were found well before Einstein, without any kind of relativity idea in mind, are in fact compatible by definition with the Lorentz transformation. And with this being a very interesting fact, fully confirming Einstein’s relativity theory. More on this later.

Time to get back now to gravity. Still following Einstein, we have here:

**THEOREM 4.28** (Einstein). *The theory of gravity can be suitably modified, and merged with relativity, into a theory called general relativity.*

**PROOF.** All this is a bit complicated, involving some geometry, as follows:

(1) Before anything, we have seen that in the relativistic context, mass  $m$  must be replaced by relativistic mass  $M = \gamma m$ , and momentum  $p = mv$  must be replaced by relativistic momentum  $P = Mv$ . Thus, as with Galileo and many other things, such as the conservation of mass and of momentum, seen above, there's a bug with the Newton formula  $F = \dot{p}$ , which must be replaced by something of type  $F = \dot{P}$ .

(2) In practice now, as a starting point, let us go back to the formula  $F = -\Delta V$ , that we know well. Geometrically, this suggests looking at the gravitational field of  $k$  bodies  $M_1, \dots, M_k$  as being represented by  $\mathbb{R}^3$  having  $k$  holes in it, and with the heavier the  $M_i$ , the bigger the hole, and with poor  $m \simeq 0$  having to roll on all this.

(3) Of course we are here in 4D, for the full picture, that of the potential  $V$ , or rather of its graph, and in order to better understand this, it is of help to first consider the question where our bodies  $M_1, \dots, M_k$  lie in a plane  $\mathbb{R}^2$ .

(4) Still staying inside classical mechanics, it is possible to further build on the above picture in (2), which was something rather intuitive, now with some precise math formulae, relating the geometry of  $V$  to the motion of  $m$  under its influence.

(5) The point now is that, with (4) done, the passage to relativity can be understood as well, by modifying a bit the geometry there, as to fit with relativistic spacetime, and by having the  $F = \dot{P}$  idea from (1) in mind too. That is the main idea behind general relativity, and in practice, all this needs a bit of technical geometry and formulae.  $\square$

So, this is it, a bit complicated, and of course feel welcome to get into this, with what you learned from here, you're on the good path. In what concerns us, in this book, we will be back to this only later, towards the end, with a few words there on the comparison of gravity with other forces that we will meet, electromagnetism and other.

#### 4d. Atomic bombs and black holes

With this done, relativity theory, let us get back now towards real life, and applications. Perhaps a bit surprisingly, these applications fall into two main classes, as follows:

(1) First we have applications to real life at the microscopic level, which, and with apologies for the offense, is our everyday life, here on Earth. The point indeed is that everything surrounding us is made of atoms, or rather of subatomic particles forming these atoms, such as electrons, protons and neutrons, and the usual movement of these subatomic particles is at speeds  $v \simeq c$ , which makes relativity theory mandatory for their study and understanding. Thus, in a certain sense, and going up now through the hierarchy, atoms and then ordinary matter, everything comes from certain things governed

by relativity theory. But this is something that we will discuss only later in this book, starting from chapter 5 below, when knowing more about such particles.

(2) At the opposite end, that of the macroscopic level, or perhaps normal level of Nature, and sorry again for the offense, we have all sorts of phenomena involving very high or very low parameters, such as speed  $v$ , time  $t$ , temperature  $T$ , mass  $m$ , density  $\rho$ , and so on. These too belong to relativity, and more specifically either to special relativity, due to all sorts of particles travelling at  $v \simeq c$ , but also to general relativity, due to all sorts of celestial objects of truly enormous mass,  $m \gg 0$ , which can only be understood in the framework of general relativity. We will discuss this a bit, in what follows.

Summarizing, we want to get now into  $m \gg 0$  astronomy. But if there is something to be discussed here, as an urgent matter, these are the most common objects appearing, namely the stars, their formation, mechanisms and main properties.

Obviously, and just by thinking for instance at the free heating coming from our Sun during the Summer, when compared to our individual energy bills in the Winter, stars have something to do with high energy. And this becomes even more obvious when reminding that the default temperature for our universe is set to  $T \simeq 0$ , in Kelvin.

So, let us go back first to the main energy formula that we have so far,  $E = mc^2$ , and try to understand its numerics, and consequences. At the terrestrial level, we have:

**THEOREM 4.29.** *An atomic bomb based on a glass of water releasing all its  $E = mc^2$  energy is equivalent to the Giza Pyramid hitting you at 30 km/s.*

**PROOF.** When converting  $E = mc^2$  into kinetic energy of a body  $M$ , the formula is:

$$mc^2 = \frac{Mv^2}{2} \implies v = \sqrt{\frac{2m}{M}} c$$

In our case the glass of water  $m$ , glass included, is about 300 grams, and the Giza Pyramid  $M$  is about 6 million tons. Thus the impact speed is:

$$v = \sqrt{\frac{2 \times 3 \times 10^{-1}}{6 \times 10^9}} c = \frac{c}{10^5} = 30,000 \text{ m/s}$$

As already mentioned before, do not worry about this. We will see however later on, when doing quantum mechanics, that certain atomic bombs, based on other materials, can however be constructed. As for the glass of water, as long as it stays far away from a big source of energy, of stellar or atomic type, it will certainly not explode.  $\square$

Getting now to stars, many things to be said, with most actually needing things that we haven't talked about yet in this book, such as quantum mechanics, and we will be quite brief here. Good introductions to astrophysics include the classical books of Choudhuri

[19], Clayton [20], Ryden-Peterson [76], Weinberg [94], and for cosmology you can do with Dodelson [28], or with Ryden [75] or Weinberg [95] again.

The idea here, at least vaguely and in relation with gravity, is as follows:

FACT 4.30. *The stars fall into several classes, as follows:*

- (1) *Main sequence stars, and their versions.*
- (2) *Dwarfs, of various types.*
- (3) *Neutron stars, of various types.*
- (4) *Black holes, of various types.*

To be more precise here, (1) are the “usual” stars, whose functioning mechanisms, following Bethe and others, can be understood via some quantum mechanics. Then (2) and (3) are also of quantum mechanical nature, and we will be back to all these objects later. As for (4), these are quite interesting for us, with our present knowledge. Indeed, while being of course real and observed, black holes are somehow purely mathematical objects, that can be studied by using the geometry tools discussed in the above.

#### 4e. Exercises

En hommage to Einstein, all our exercises here will be Gedankenexperiments, or thought experiments. For full credit please present the experiment, then examine all possible criticisms, coming from the possible weaknesses of your experiment, and present as well the criticism of these criticisms. And for two bonus points, prepare as well a counterargumentation against the criticism directed to your second wave of opinions.

Here are these Gedankenexperiments, or rather the themes for them, with the first one building on a quite unclear discussion started in chapter 1 above:

GEDANKENEXPERIMENT 4.31. *Is gravity instantaneous or not.*

GEDANKENEXPERIMENT 4.32. *What is the best system of units.*

GEDANKENEXPERIMENT 4.33. *Do inertial frames really exist.*

GEDANKENEXPERIMENT 4.34. *How to compute the mass of light.*

GEDANKENEXPERIMENT 4.35. *Can you trick aging using relativity.*

GEDANKENEXPERIMENT 4.36. *Are there lower or upper bounds on time.*

GEDANKENEXPERIMENT 4.37. *Changing  $c$  or other constants of physics.*

GEDANKENEXPERIMENT 4.38. *Changing  $\pi$  or other constants of mathematics.*

In case you find all this exciting, take a look too at mathematical logic, or rather keep in mind that idea, for later. Einstein, during the last years of his career, was having long walks with his Princeton colleague Gödel, a logician, discussing such things.



## Part II

# Electricity and heat

*Design a rhyme I just won't fear  
Back to react, enough is enough  
Let me ask you a question:  
What time is love?*

## CHAPTER 5

### Electrostatics

#### 5a. Charges, Coulomb law

In this chapter and in the next one we discuss electrodynamics. This is something which, at least at its beginnings, is quite similar to classical mechanics, with the masses  $m > 0$  being now replaced by charges  $q \in \mathbb{R}$ , and with Newton's law  $F \sim 1/d^2$  being replaced by Coulomb's law, which states exactly the same thing,  $F \sim 1/d^2$ .

However, passed some basic theory for the fixed charges, the analogy between classical mechanics and electrodynamics stops short when these charges  $q \in \mathbb{R}$  are allowed to move, even a tiny little bit. In classical mechanics, when a mass  $m > 0$  moves a bit, nothing spectacular happens. In electrodynamics, however, a small displacement of a charge  $q \in \mathbb{R}$  produces magnetism, whose equations are quite complicated, coming on top of Coulomb's law, and the problem comes from this. The ultimate conclusion is that the correct analogue of Newton's gravitation law are the complete equations for electromagnetism, called Maxwell equations, and finding these equations will be in fact our main goal here. Finally, in what regards Einstein's relativity, good news here, no need for a fix, the Maxwell equations being compatible with it by definition.

So, this is what we intend to talk about, in this chapter and in the next one. Many things to be discussed, and as usual, we will be quite brief. The standard references for electrodynamics include the classical books of Feynman [34], Griffiths [42], Purcell [72], Schwartz [79], Shankar [86] at the undergraduate level, and Jackson [54], Landau-Lifshitz [62], Panofsky-Phillips [68], Schwinger [82] at the graduate level. We will be mostly following Feynman [34] and Griffiths [42], for our presentation here.

Getting started now, what is a charge? Not an easy question. The first thought goes to a magnet, or perhaps battery, but these have  $+$  and  $-$  ends, and so are something more complicated. The second thought goes to something like electricity, but that is rather moving charges, electrons – traveling, and as explained above, too complicated, for later. As a third thought now, why not an electron – itself? But if we agree on this, we need a positive buddy for our electron, in our theory, and that can only be the proton  $+$ , and the thing now is that this couple electron/proton is exactly the hydrogen atom, rather belonging to quantum mechanics, and too complicated, again for later.

So, in the lack of anything simple, we have to start at a somewhat advanced level, physically speaking, but also very down-to-earth, just speaking like this, as follows:

**FACT 5.1.** *Ordinary matter is made of electrons  $-$ , protons  $+$  and neutrons  $0$ , with the number of  $+$  and  $-$  being rigorously equal, up to tiny tolerances. When the number of  $-$  is greater than the number of  $+$ , or vice versa, we say that we have a charge.*

This is something quite interesting already, with the “tiny tolerances” mentioned above being, perhaps quite suprisingly, of the order of less than  $10^{-10}$ . So when you touch a Van de Graaff generator, even after cranking well, please be sure that you won’t be a Terminator afterwards, but still well within that modest  $10^{-10}$  tolerance. At  $> 10^{-10}$  things violently explode, as bit as masses can explode too, due to  $E = mc^2$ .

In order to axiomatize our theory, we will proceed a bit like for gravity, in chapter 1. We will assume that charges  $q = \#p - \#e$  as in Fact 5.1 are no longer quantized,  $q \in \mathbb{R}$ , that they are points, and that they live in the void. Thus, we are led to:

**DEFINITION 5.2.** *An electrostatic charge is a point  $x \in \mathbb{R}^3$  having associated to it a certain number  $q \in \mathbb{R}$ , called charge of that point, and living in the void.*

Here the last part, referring to the void, is something quite subtle, corresponding to a phenomenon not appearing in gravitation. In gravitation we know well about friction and drag, the two bad guys, but these affect the object itself, or rather its movement, and not the gravitation force which produces this movement. Things are not like this in electrodynamics, where matter in between objects affects the magnitude of the attraction or repulsion force, even before it comes to movement, and with the explanation of this coming somehow from the picture of matter from Fact 5.1. Thus, we need void.

We have now all the needed ingredients for getting started, with:

**FACT 5.3 (Coulomb law).** *Any pair of charges  $q_1, q_2 \in \mathbb{R}$  is subject to a force as follows, which is attractive if  $q_1 q_2 < 0$  and repulsive if  $q_1 q_2 > 0$ ,*

$$||F|| = K \cdot \frac{|q_1 q_2|}{d^2}$$

*where  $d > 0$  is the distance between the charges, and  $K > 0$  is a certain constant.*

Observe the amazing similarity with the Newton law for gravity. However, as explained in the above, passed a few simple facts, things will be more complicated here.

As in the gravity case, the force  $F$  appearing above is understood to be parallel to the vector  $x_2 - x_1 \in \mathbb{R}^3$  joining as  $x_1 \rightarrow x_2$  the locations  $x_1, x_2 \in \mathbb{R}^3$  of our charges, and by taking into account the attraction/repulsion rules above, we have:

PROPOSITION 5.4. *The Coulomb force of  $q_1$  at  $x_1$  acting on  $q_2$  at  $x_2$  is*

$$F = K \cdot \frac{q_1 q_2 (x_2 - x_1)}{\|x_2 - x_1\|^3}$$

with  $K > 0$  being the Coulomb constant, as above.

PROOF. We have indeed the following computation:

$$\begin{aligned} F &= \operatorname{sgn}(q_1 q_2) \cdot \|F\| \cdot \frac{x_2 - x_1}{\|x_2 - x_1\|} \\ &= \operatorname{sgn}(q_1 q_2) \cdot K \cdot \frac{|q_1 q_2|}{\|x_2 - x_1\|^2} \cdot \frac{x_2 - x_1}{\|x_2 - x_1\|} \\ &= K \cdot \frac{q_1 q_2 (x_2 - x_1)}{\|x_2 - x_1\|^3} \end{aligned}$$

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

In relation now with the value of the constant  $K$  appearing in the above, called Coulomb constant, things here are a bit tricky, as follows:

FACT 5.5. *The Coulomb constant  $K$  is given by the formula*

$$K = 8.987\,551\,7923(14) \times 10^9$$

in standard units, with the charges being measured in coulombs  $C$ , given by

$$1C \simeq 6.241\,509 \times 10^{18} e$$

where  $e$  is the elementary charge, namely minus that of an electron.

There are in fact several interesting things going on here. First, at the end you would say why not simply saying that  $e$  is the charge of the proton, but the thing is that the proton and the electron do not have in fact the same exact charge, with sign switched, and the electron was preferred, as always, over the proton for formulating things.

Which takes us into the question of why the charge of the electron is  $-$ , instead of  $+$ . And there is a long story here, involving debates among the 18th century greats, and with a little bit of confusion being involved too, because the electrons  $-$  are attracted by positive charges  $q > 0$ , and so observed around these positive charges  $q > 0$ , which might lead to the idea that they might have themselves a positive charge  $+$ , contributing to  $q > 0$ . Benjamin Franklin is generally credited for the  $-$  convention.

Things were later restored in the early 20th century, with the atomic theory of Bohr and others, where electrons  $-$  spin around a proton and neutron core  $q > 0$ , and with this picture, including the signs, looking like something very reasonable.

Passed all this, another peculiarity of Fact 5.5 comes in relation with the definition of the coulomb, which is in fact given by definition by an exact formula, namely:

$$1C = \frac{5 \times 10^{18}}{0.801\,088\,317} e$$

This in practice gives the following more precise formula for the coulomb, which shows that a charge of  $1C$  is something fractionary, that cannot be realized in real life:

$$1C = 6241\,509\,074\,460\,762\,607.776 e$$

The problem comes from the following alternative definition of the coulomb, in terms of the ampere, which is something more complicated, that we will talk about later:

$$1C = 1A \cdot 1s$$

Hang on, we are not done yet. Adding to the confusion, the Coulomb constant is usually denoted  $K$ , but also  $k$ , or most often  $k_e$ , but in fact the most often is written in the following form, with  $\varepsilon_0$  being the so-called permittivity of free space:

$$K = \frac{1}{4\pi\varepsilon_0}$$

And the story is not over here, because  $\varepsilon_0$  itself is given by the following formula, with  $\mu_0$  being the magnetic permeability of free space, and  $c$  being the speed of light:

$$\varepsilon_0 = \frac{1}{\mu_0 c^2}$$

And we are surely still not done, because all the above discussion assumes that the other units that are used are standard, namely meter and second, and this is not always standard, due to the about 50 orders of magnitude physics has to deal with.

In any case, let us end this interesting discussion about units with something concrete, useful, and very illustrating, in relation with gravity, as follows:

**THEOREM 5.6.** *The electrical repulsion between two electrons is about*

$$R = 10^{42}$$

*times bigger than their gravitational attraction.*

**PROOF.** Consider indeed two electrons, having masses  $m, m$  and charges  $-e, -e$ . The magnitudes of the electric repulsion  $F_e$  and gravity attraction  $F_g$  are given by:

$$||F_e|| = \frac{Ke^2}{d^2} \quad , \quad ||F_g|| = \frac{Gm^2}{d^2}$$

Thus the ratio of forces  $R$  that we want to measure is given by:

$$R = \frac{||F_e||}{||F_g||} = \frac{Ke^2}{Gm^2}$$

Regarding now the data, this is as follows, with  $m$  at rest, and in standard units, namely meters and seconds, also kilograms, and including now coulombs too:

$$\begin{aligned} K &= 8.897 \times 10^9 \\ G &= 6.674 \times 10^{-11} \\ e &= 1.602 \times 10^{-19} \\ m &= 9.109 \times 10^{-31} \end{aligned}$$

We obtain the following approximation for the ratio  $R$  considered above:

$$\begin{aligned} R &= \frac{8.897 \times 1.602^2}{6.674 \times 9.109^2} \times \frac{10^9 \times 10^{-38}}{10^{-11} \times 10^{-62}} \\ &= (4.123 \times 10^{-2}) \times 10^{44} \\ &\simeq 10^{42} \end{aligned}$$

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

For adding to the picture, and in order to fully understand what that  $R = 10^{42}$  number that we found truly means, let us complement the above result with:

PROPOSITION 5.7. *The universe, or at least the known universe, is about*

$$r = 10^{37}$$

*bigger than a hydrogen atom, with this ratio being 10,000 smaller than  $R$ .*

PROOF. The radius of the hydrogen atom can be anywhere between 25 – 120 pm, with 1 pm =  $10^{-12}$  m, depending on the convention used, with a commonly accepted figure being 53 pm, representing the mean distance between the proton and the electron. As for the radius of the known universe, again there is a story here, with a commonly accepted figure being  $4.4 \times 10^{26}$  m. Thus the ratio that we are interested in is:

$$r = \frac{4.4 \times 10^{26}}{53 \times 10^{-12}} \simeq 10^{37}$$

And this is 10,000 smaller than  $10^{42}$ , as claimed.  $\square$

As a side comment, however, when speaking masses instead of sizes, the number  $R = 10^{42}$  pales when compared to the mass of the known universe, counting ordinary mass only, accounting for 4.9%, divided by the mass of a hydrogen atom, which is:

$$\mathfrak{R} = \frac{1.5 \times 10^{53}}{1.8 \times 10^{-30}} \simeq 10^{83}$$

Getting back now to Theorem 5.6 as it is, let us point out that this is something not at all anecdotal, even in the context of the most abstract theoretical physics that you can ever imagine, not to say pure mathematics, because of the following rule of thumb, which is something widely agreed upon, by most of the scientists:

**RULE 5.8.** *Don't ever expect the mathematics and physics to be the same, over 10 orders of magnitude or so.*

In other words, with this in hand, Theorem 5.6 tells us a very interesting thing, namely that the mathematics and physics of the Coulomb force  $F_e \sim 1/d^2$  will be in fact very different from the mathematics and physics of the Newton force  $F_g \sim 1/d^2$ . We will see in what follows that indeed it is so, but it is of course far better to be warned in advance of the potential difficulties on the way. So, Theorem 5.6 is something very smart.

As a final comment, as already mentioned, Rule 5.8 is something widely agreed upon, by applied mathematicians and physicists, chemists and engineers, and with that 10 orders of magnitude being usually replaced by something far sharper, of type 2-3. In theoretical physics and pure mathematics however, things can be quite wild, with quantum gravity research for instance trying to unify things which are about 50 orders of magnitude apart, no less than that. We will talk a bit about this at the end of this book.

### 5b. The Gauss law

In this section and in the next one we develop the basic math needed for electrostatics, and with this being actually a quite easy task, due to all sorts of mathematics and physics that we have already learned, in chapters 1-4, when studying gravity.

As usual, we will be quite brief. Standard introductions to all this, with many pictures, examples and exercises, and also with far more material that we will discuss here, include the classical books of Feynman [34], Griffiths [42], Purcell [72] and Shankar [86].

In analogy with our study of gravity, let us start with:

**DEFINITION 5.9.** *Given charges  $q_1, \dots, q_k \in \mathbb{R}$  located at positions  $x_1, \dots, x_k \in \mathbb{R}^3$ , we define their electric field to be the vector function*

$$E(x) = K \sum_i \frac{q_i(x - x_i)}{\|x - x_i\|^3}$$

*so that their force applied to a charge  $Q \in \mathbb{R}$  positioned at  $x \in \mathbb{R}^3$  is given by  $F = QE$ .*

Observe the analogy with gravity, save for the fact that instead of masses  $m > 0$  we have now charges  $q \in \mathbb{R}$ , and that at the level of constants,  $G$  gets replaced by  $K$ .

More generally, we will be interested in electric fields of various non-discrete configurations of charges, such as charged curves, surfaces and solid bodies. We have already talked about such things in chapter 3 above, in the gravitational context, but the discussion there, involving the gravitational force of a solid body having non-trivial shape or density, was something rather specialized. In the electricity context, however, things



like wires or metal sheets or solid bodies coming in all sorts of shapes, tailored for their purpose, play a key role, so this extension is essential. So, let us go ahead with:

DEFINITION 5.10. *The electric field of a charge configuration  $L \subset \mathbb{R}^3$ , with charge density function  $\rho : L \rightarrow \mathbb{R}$ , is the vector function*

$$E(x) = K \int_L \frac{\rho(z)(x - z)}{\|x - z\|^3} dz$$

so that the force of  $L$  applied to a charge  $Q$  positioned at  $x$  is given by  $F = QE$ .

With the above definitions in hand, it is most convenient now to forget about the charges, and focus on the study of the corresponding electric fields  $E$ .

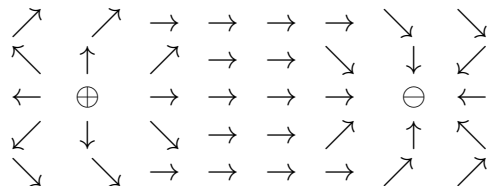
These fields are by definition vector functions  $E : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ , with the convention that they take  $\pm\infty$  values at the places where the charges are located, and intuitively, are best represented by their field lines, which are constructed as follows:

DEFINITION 5.11. *The field lines of an electric field  $E : \mathbb{R}^3 \rightarrow \mathbb{R}^3$  are the oriented curves  $\gamma \subset \mathbb{R}^3$  pointing at every point  $x \in \mathbb{R}^3$  at the direction of the field,  $E(x) \in \mathbb{R}^3$ .*

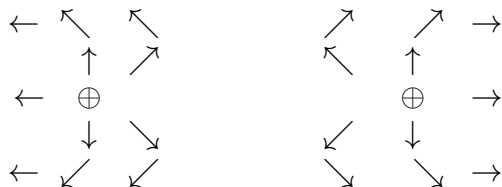
As a basic example here, for one charge the field lines are the half-lines emanating from its position, oriented according to the sign of the charge:



For two charges now, if these are of opposite signs,  $+$  and  $-$ , you get a picture that you are very familiar with, namely that of the field lines of a bar magnet:



If the charges are  $+, +$  or  $-, -$ , you get something of similar type, but repulsive this time, with the field lines emanating from the charges being no longer shared:



These pictures, and notably the last one, with  $+, +$  charges, are quite interesting, because the repulsion situation does not appear in the context of gravity. Thus, we can only expect our geometry here to be far more complicated than that of gravity.

In general now, the first thing that can be said about the field lines is that, by definition, they do not cross. Thus, what we have here is some sort of oriented 1D foliation of  $\mathbb{R}^3$ , in the sense that  $\mathbb{R}^3$  is smoothly decomposed into oriented curves  $\gamma \subset \mathbb{R}^3$ .

The field lines, as constructed in Definition 5.11, obviously do not encapsulate the whole information about the field, with the direction of each vector  $E(x) \in \mathbb{R}^3$  being there, but with the magnitude  $\|E(x)\| \geq 0$  of this vector missing. However, say when drawing, when picking up uniformly radially spaced field lines around each charge, and with the number of these lines proportional to the magnitude of the charge, and then completing the picture, the density of the field lines around each point  $x \in \mathbb{R}$  will give you then the magnitude  $\|E(x)\| \geq 0$  of the field there, up to a scalar.

Let us summarize these observations as follows:

**PROPOSITION 5.12.** *Given an electric field  $E : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ , the knowledge of its field lines is the same as the knowledge of the composition*

$$nE : \mathbb{R}^3 \rightarrow \mathbb{R}^3 \rightarrow S$$

where  $S \subset \mathbb{R}^3$  is the unit sphere, and  $n : \mathbb{R}^3 \rightarrow S$  is the rescaling map, namely:

$$n(x) = \frac{x}{\|x\|}$$

However, in practice, when the field lines are accurately drawn, the density of the field lines gives you the magnitude of the field, up to a scalar.

**PROOF.** We have two assertions here, the idea being as follows:

(1) The first assertion is clear from definitions, with of course our usual convention that the electric field and its problematics take place outside the locations of the charges, which makes everything in the statement to be indeed well-defined.

(2) Regarding now the last assertion, which is of course a bit informal, this follows from the above discussion. It is possible to be a bit more mathematical here, with a definition, formula and everything, but we will not need this, in what follows.  $\square$

Let us introduce now a key definition, as follows:

**DEFINITION 5.13.** *The flux of an electric field  $E : \mathbb{R}^3 \rightarrow \mathbb{R}^3$  through a surface  $S \subset \mathbb{R}^3$ , assumed to be oriented, is the quantity*

$$\Phi_E(S) = \int_S \langle E(x), n(x) \rangle dx$$

with  $n(x)$  being unit vectors orthogonal to  $S$ , following the orientation of  $S$ . Intuitively, the flux measures the signed number of field lines crossing  $S$ .

Here by orientation of  $S$  we mean precisely the choice of unit vectors  $n(x)$  as above, orthogonal to  $S$ , which must vary continuously with  $x$ . For instance a sphere has two possible orientations, one with all these vectors  $n(x)$  pointing inside, and one with all these vectors  $n(x)$  pointing outside. More generally, any surface has locally two possible orientations, so if it is connected, it has two possible orientations. In what follows the convention is that the closed surfaces are oriented with each  $n(x)$  pointing outside.

Regarding the last sentence of Definition 5.13, this is of course something informal, meant to help, coming from the interpretation of the field lines from Proposition 5.12. However, we will see later that this simple interpretation can be of great use.

As a first observation, we could have done of course the same thing with gravity in chapters 1-4, but these notions of field lines and flux are less interesting, in that context. In the present setting, however, electric fields passing through metal sheets are a common occurrence, and all the above is important, for any application.

As a first illustration, let us do a basic computation, as follows:

PROPOSITION 5.14. *For a point charge  $q \in \mathbb{R}$  at the center of a sphere  $S$ ,*

$$\Phi_E(S) = \frac{q}{\varepsilon_0}$$

*where the constant is  $\varepsilon_0 = 1/(4\pi K)$ , independently of the radius of  $S$ .*

PROOF. Assuming that  $S$  has radius  $r$ , we have the following computation:

$$\begin{aligned} \Phi_E(S) &= \int_S \langle E(x), n(x) \rangle dx \\ &= \int_S \left\langle \frac{Kqx}{r^3}, \frac{x}{r} \right\rangle dx \\ &= \int_S \frac{Kq}{r^2} dx \\ &= \frac{Kq}{r^2} \times 4\pi r^2 \\ &= 4\pi Kq \end{aligned}$$

Thus with  $\varepsilon_0 = 1/(4\pi K)$  as above, we obtain the result.  $\square$

As a comment here, the constant  $\varepsilon_0 = 1/(4\pi K)$  which appears in the above is the permittivity of free space constant that we talked about before, when discussing units. In what follows we will use this new constant instead of the Coulomb constant  $K$ .

More generally now, we have the following result:

THEOREM 5.15. *The flux of a field  $E$  through a sphere  $S$  is given by*

$$\Phi_E(S) = \frac{Q_{enc}}{\varepsilon_0}$$

where  $Q_{enc}$  is the total charge enclosed by  $S$ , and  $\varepsilon_0 = 1/(4\pi K)$ .

PROOF. This can be done in several steps, as follows:

(1) Before jumping into computations, let us do some manipulations. First, by discretizing the problem, we can assume that we are dealing with a system of point charges. Moreover, by additivity, we can assume that we are dealing with a single charge. And if we denote by  $q \in \mathbb{R}$  this charge, located at  $v \in \mathbb{R}^3$ , we want to prove that we have the following formula, where  $B \subset \mathbb{R}^3$  denotes the ball enclosed by  $S$ :

$$\Phi_E(S) = \frac{q}{\varepsilon_0} \delta_{v \in B}$$

(2) By linearity we can assume that we are dealing with the unit sphere  $S$ . Moreover, by rotating we can assume that our charge  $q$  lies on the  $Ox$  axis, that is, that we have  $v = (r, 0, 0)$  with  $r \geq 0$ ,  $r \neq 1$ . The formula that we want to prove becomes:

$$\Phi_E(S) = \frac{q}{\varepsilon_0} \delta_{r < 1}$$

(3) Let us start now the computation. With  $u = (x, y, z)$ , we have:

$$\begin{aligned} \Phi_E(S) &= \int_S \langle E(u), u \rangle du \\ &= \int_S \left\langle \frac{Kq(u-v)}{\|u-v\|^3}, u \right\rangle du \\ &= Kq \int_S \frac{\langle u-v, u \rangle}{\|u-v\|^3} du \\ &= Kq \int_S \frac{1 - \langle v, u \rangle}{\|u-v\|^3} du \\ &= Kq \int_S \frac{1 - rx}{(1 - 2xr + r^2)^{3/2}} du \end{aligned}$$

(4) In order to compute the above integral, we will use spherical coordinates for the unit sphere  $S$ , which are as follows, with  $s \in [0, \pi]$  and  $t \in [0, 2\pi]$ :

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

The corresponding Jacobian is readily computed, as follows:

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

(5) With the above change of coordinates, our integral from (3) becomes:

$$\begin{aligned}
 \Phi_E(S) &= Kq \int_S \frac{1 - rx}{(1 - 2xr + r^2)^{3/2}} du \\
 &= Kq \int_0^{2\pi} \int_0^\pi \frac{1 - r \cos s}{(1 - 2r \cos s + r^2)^{3/2}} \cdot \sin s \, ds \, dt \\
 &= 2\pi Kq \int_0^\pi \frac{(1 - r \cos s) \sin s}{(1 - 2r \cos s + r^2)^{3/2}} ds \\
 &= \frac{q}{2\varepsilon_0} \int_0^\pi \frac{(1 - r \cos s) \sin s}{(1 - 2r \cos s + r^2)^{3/2}} ds
 \end{aligned}$$

(6) The point now is that the integral on the right can be computed with the change of variables  $x = \cos s$ . Indeed, we have  $dx = -\sin s \, ds$ , and we obtain:

$$\begin{aligned}
 \int_0^\pi \frac{(1 - r \cos s) \sin s}{(1 - 2r \cos s + r^2)^{3/2}} ds &= \int_{-1}^1 \frac{1 - rx}{(1 - 2rx + r^2)^{3/2}} dx \\
 &= \left[ \frac{x - r}{\sqrt{1 - 2rx + r^2}} \right]_{-1}^1 \\
 &= \frac{1 - r}{\sqrt{1 - 2r + r^2}} - \frac{-1 - r}{\sqrt{1 + 2r + r^2}} \\
 &= \frac{1 - r}{|1 - r|} + 1 \\
 &= 2\delta_{r < 1}
 \end{aligned}$$

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

As a technical comment here, at  $r = 1$ , which is normally avoided by our problematics, the integral  $I_r$  computed in (6) above converges too, and can be evaluated as follows:

$$I_1 = \left[ \frac{x-1}{\sqrt{2-2x}} \right]_{-1}^1 = \left[ -\sqrt{\frac{1-x}{2}} \right]_{-1}^1 = 1$$

Thus, we have the correct middle step between the 0, 2 values of the integral  $I_r$ , and getting back now to the flux, at  $r = 1$  we formally have  $\Phi_E(S) = q/(2\varepsilon_0)$ , which again is the correct middle step between the 0,  $q/\varepsilon_0$  values of the flux.

Even more generally now, we have the following result, due to Gauss, which is the foundation of advanced electrostatics, and of everything following from it, namely electrodynamics, and then quantum mechanics, and particle physics:

**THEOREM 5.16 (Gauss law).** *The flux of a field  $E$  through a surface  $S$  is given by*

$$\Phi_E(S) = \frac{Q_{enc}}{\varepsilon_0}$$

where  $Q_{enc}$  is the total charge enclosed by  $S$ , and  $\varepsilon_0 = 1/(4\pi K)$ .

**PROOF.** This basically follows from Theorem 5.15, or even from Proposition 5.14, by adding to the results there a number of new ingredients, as follows:

(1) Our first claim is that given a closed surface  $S$ , with no charges inside, the flux through it of any choice of external charges vanishes:

$$\Phi_E(S) = 0$$

This claim is indeed supported by the intuitive interpretation of the flux, as corresponding to the signed number of field lines crossing  $S$ . Indeed, any field line entering as  $+$  must exit somewhere as  $-$ , and vice versa, so when summing we get 0.

(2) In practice now, in order to prove this rigorously, there are several ways. A first argument, which is quite elementary, is the one used by Feynman in [34], based on the fact that, due to  $F \sim 1/d^2$ , local deformations of  $S$  will leave invariant the flux, and so in the end we are left with a rotationally invariant surface, where the result is clear.

(3) A second argument, which basically uses the same idea, but is perhaps a bit more robust, is by redoing the computations in the proof of Theorem 5.15, by assuming this time that the integration takes place on an arbitrary surface as follows:

$$S_\lambda = \left\{ \lambda(u)u \mid u \in S \right\}$$

To be more precise, here  $\lambda : S \rightarrow (0, \infty)$  is a certain function, defining the surface, whose derivatives will appear both in the construction of the normal vectors  $n(x)$  with  $x = \lambda(u)u$ , and in the Jacobian of the change of variables  $x \rightarrow u$ , and in the end, when integrating over  $S$  as in the proof of Theorem 5.15, this function  $\lambda$  disappears.

(4) A third argument, used by basically all electrodynamics books at the graduate level, and by some undergraduate books too, is by using heavy calculus, namely partial integration in 3D, and we will discuss this later, more in detail, in the next section.

(5) A fourth argument is by following the nice idea in (1), namely carefully axiomatizing the field lines, and their relation with the field, and then obtaining  $\Phi_E(S) = 0$  by using the in-and-out trick in (1), as explained for instance by Griffiths in [42], or by Shankar in [86]. However, when looking for full rigor here, in practice this is something quite complicated, amounting more or less in proving the heavy 3D calculus results mentioned in (4) above via foliation methods, and we will not get here into this.

(6) To summarize, we are led to the conclusion that given a closed surface  $S$ , with no charges inside, the flux through it of any choice of external charges vanishes:

$$\Phi_E(S) = 0$$

(7) The point now is that, with this and Proposition 5.14 in hand, we can finish by using a standard math trick. Let us assume indeed, by discretizing, that our system of charges is discrete, consisting of enclosed charges  $q_1, \dots, q_k \in \mathbb{R}$ , and an exterior total charge  $Q_{ext}$ . We can surround each of  $q_1, \dots, q_k$  by small disjoint spheres  $U_1, \dots, U_k$ , chosen such that their interiors do not touch  $S$ , and we have:

$$\begin{aligned} \Phi_E(S) &= \Phi_E(S - \cup U_i) + \Phi_E(\cup U_i) \\ &= 0 + \Phi_E(\cup U_i) \\ &= \sum_i \Phi_E(U_i) \\ &= \sum_i \frac{q_i}{\varepsilon_0} \\ &= \frac{Q_{enc}}{\varepsilon_0} \end{aligned}$$

(8) To be more precise, in the above the union  $\cup U_i$  is a usual disjoint union, and the flux is of course additive over components. As for the difference  $S - \cup U_i$ , this is by definition the disjoint union of  $S$  with the disjoint union  $\cup(-U_i)$ , with each  $-U_i$  standing for  $U_i$  with orientation reversed, and since this difference has no enclosed charges, the flux through it vanishes by (6). Finally, the end makes use of Proposition 5.14.  $\square$

So long for the Gauss law. We will talk about it more in the next chapter, by exploring some new proofs for it, first by using some heavy 3D calculus, which is actually based on integration theorems due to Gauss himself, and which considerably simplifies the proof, and then by doing something even more conceptual, namely using potentials as in chapter 3, and killing again the problem with advanced 3D calculus.

As already mentioned, having all this discussion is essential, the Gauss law being at the origin of many things, namely the Maxwell equations, and then the hydrogen atom, quantum mechanics, and particle physics too. So, fully understanding the Gauss law, and its various proofs, and the relation between these proofs, is a kind of initiation ritual, for any physicist having to deal with phenomena coming from electrons.

### 5c. Poisson and Laplace

We have seen that the study of electrostatics leads us into some serious 3D geometry. So, time to review and improve our math tools, for dealing with all this. To be more precise, we would like to extend our basic 1D calculus tools to 3D.

It is convenient to keep the discussion, when possible, in  $N$  dimensions, among others for covering at the same time 1D, 2D, 3D, and also 4D needed for relativity. Regarding the derivative, this is something that we already met in chapter 3, as follows:

**PROPOSITION 5.17.** *The derivative of a function  $f : \mathbb{R}^N \rightarrow \mathbb{R}^M$  at a point  $c \in \mathbb{R}^N$  is the linear map  $f'(c) : \mathbb{R}^N \rightarrow \mathbb{R}^M$  which best approximates  $f$  around  $c$ ,*

$$f(c + z) \simeq f(c) + f'(c)z$$

*regarded as a rectangular matrix,  $f'(c) \in M_{M \times N}(\mathbb{R})$ , acting on the vectors  $z \in \mathbb{R}^N$ , written vertically. With these conventions, the chain rule for derivatives holds,*

$$(f \circ g)'(c) = f'(g(c)) \cdot g'(c)$$

*in the sense that the matrix on the left is the product of the matrices on the right.*

**PROOF.** This is something that we are very familiar with, since our computations in chapter 3. The proof can be found in any multivariable calculus book.  $\square$

Next in line, we have the formula of change of variables. Here the result, that we already used in the proof of the Gauss law for the sphere, is as follows:

**THEOREM 5.18.** *Given a function  $f : E \rightarrow \mathbb{R}$ , with  $E \subset \mathbb{R}^N$ , and a transformation in  $N$  variables,  $\varphi = (\varphi_1, \dots, \varphi_N)$ , we have the change of variable formula,*

$$\int_E f(x)dx = \int_{\varphi^{-1}(E)} f(\varphi(y))|J_\varphi(y)|dy$$

*with the  $J_\varphi$  quantity on the right, called Jacobian of  $\varphi$ , being given by:*

$$J_\varphi(y) = \det \left[ \left( \frac{d\varphi_i}{dx_j}(y) \right)_{ij} \right]$$

*For spherical coordinates, the Jacobian is  $J_\varphi = r^{N-1}$  times a product of sines.*



PROOF. Again, this is something that you are familiar with, as follows:

(1) When performing a change of variables  $\varphi : \mathbb{R}^N \rightarrow \mathbb{R}^N$ , the coefficient that appears when integrating is the “inflation coefficient” of  $\varphi$ , around the given point  $y \in \mathbb{R}^N$ . In 1D this is just the number  $\varphi(y)$ , or rather its absolute value  $|\varphi(y)|$ , when putting the bounds as above. In  $N$  dimensions, however,  $\varphi(y)$  is no longer a number, so what to do.

(2) In order to solve the problem, the first remark is that, according to Proposition 5.17, the function  $\varphi$  is best approximated around  $y$  by its derivative, as follows:

$$\varphi(y + u) = \varphi(y) + \varphi'(y)u$$

Moreover, by linear algebra, this derivative is a square matrix, given by:

$$\varphi'(y) = \left( \frac{d\varphi_i}{dx_j}(y) \right)_{ij}$$

(3) Now recall that the determinant of a square matrix  $A$  having column vectors  $v_1, \dots, v_N \in \mathbb{R}^N$  is the signed volume of the parallelepiped formed by these vectors:

$$\det(v_1 \dots v_N) = \pm \text{vol} \langle v_1, \dots, v_N \rangle$$

Thus, the inflation coefficient of  $A$  is the number  $|\det A| \geq 0$ , and getting back now to our problem,  $|J_\varphi(y)| = |\det \varphi'(y)|$  is the number that must be added, as claimed.

(4) Finally, in what regards spherical coordinates, these are as follows:

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

We are already familiar with this in 2D, 3D. In  $N$  dimensions now, the Jacobian can be computed exactly as in 2D, 3D, and is given by the following formula:

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

(5) So, this was for the idea, and the detailed proof of all the above, except for (4) which is easy, to be best done by yourself, can be found in any calculus book.  $\square$

Moving ahead now, if there is one thing missing from our picture, this is the scary one, namely partial integration. Things here are quite tricky in  $N$  dimensions, but in the cases where we are mainly interested in,  $N = 2, 3$ , we have several useful results. Let us start with a standard definition, immersing us into 3D problematics, as follows:

DEFINITION 5.19. Given a function  $f : \mathbb{R}^3 \rightarrow \mathbb{R}$ , its usual derivative  $f'(u) \in \mathbb{R}^3$  can be written as  $f'(u) = \nabla f(u)$ , where the gradient operator  $\nabla$  is given by:

$$\nabla = \begin{pmatrix} \frac{d}{dx} \\ \frac{d}{dy} \\ \frac{d}{dz} \end{pmatrix}$$

By using  $\nabla$ , we can talk about the divergence of a function  $\varphi : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ , as being

$$\langle \nabla, \varphi \rangle = \left\langle \begin{pmatrix} \frac{d}{dx} \\ \frac{d}{dy} \\ \frac{d}{dz} \end{pmatrix}, \begin{pmatrix} \varphi_x \\ \varphi_y \\ \varphi_z \end{pmatrix} \right\rangle = \frac{d\varphi_x}{dx} + \frac{d\varphi_y}{dy} + \frac{d\varphi_z}{dz}$$

as well as about the curl of the same function  $\varphi : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ , as being

$$\nabla \times \varphi = \begin{vmatrix} u_x & \frac{d}{dx} & \varphi_x \\ u_y & \frac{d}{dy} & \varphi_y \\ u_z & \frac{d}{dz} & \varphi_z \end{vmatrix} = \begin{pmatrix} \frac{d\varphi_z}{dy} - \frac{d\varphi_y}{dz} \\ \frac{d\varphi_x}{dz} - \frac{d\varphi_z}{dx} \\ \frac{d\varphi_y}{dx} - \frac{d\varphi_x}{dy} \end{pmatrix}$$

where  $u_x, u_y, u_z$  are the unit vectors along the coordinate directions  $x, y, z$ .

All this might seem a bit abstract, but is in fact very intuitive. The gradient  $\nabla f$  points in the direction of the maximal increase of  $f$ , with  $|\nabla f|$  giving you the rate of increase of  $f$ , in that direction. As for the divergence and curl, these measure the divergence and curl of the vectors  $\varphi(u + v)$  around a given point  $u \in \mathbb{R}^3$ , in a usual, real-life sense.

Getting back now to calculus tools, what was missing from our picture was the higher dimensional analogue of the fundamental theorem of calculus, and more generally of the partial integration formula. In 3 dimensions, we have the following result:

THEOREM 5.20. The following results hold, in 3 dimensions:

- (1) Fundamental theorem for gradients, namely

$$\int_a^b \langle \nabla f, dx \rangle = f(b) - f(a)$$

- (2) Fundamental theorem for divergences, or Gauss or Green formula,

$$\int_B \langle \nabla, \varphi \rangle = \int_S \langle \varphi(x), n(x) \rangle dx$$

- (3) Fundamental theorem for curls, or Stokes formula,

$$\int_A \langle (\nabla \times \varphi)(x), n(x) \rangle dx = \int_P \langle \varphi(x), dx \rangle$$

where  $S$  is the boundary of the body  $B$ , and  $P$  is the boundary of the area  $A$ .

PROOF. This is a mixture of trivial and non-trivial results, as follows:

(1) This is something that we know well in 1D, namely the fundamental theorem of calculus, and the general,  $N$ -dimensional formula follows from that.

(2) This is something more subtle, and we had a taste of it when dealing with the Gauss law, and its various proofs. In general, the proof is similar, by using the various ideas from the proof of the Gauss law, and this can be found in any calculus book.

(3) This is again something subtle, and again with a flavor of things that we know, from the proof of the Gauss law, and which can be found in any calculus book.  $\square$

All the above was of course quite short, and at this point of reading this book, we can only recommend if needed a short break, for a brief calculus Navy Seals training camp. Such facilities are provided by basically any undergraduate electrodynamics book, in the opening chapter, and a particularly enjoyable read here is Griffiths [42].

As for further details on all this, including mathematical proofs, generalizations, and more, go first to Lax' books [65], [66] for good linear algebra, then to Rudin [73], [74] for advanced calculus, and then to do Carmo [26], [27] for differential geometry.

Getting back now to electrostatics, as a first application of the above, we have the following new point of view on the Gauss formula, which is more conceptual:

THEOREM 5.21 (Gauss). *Given an electric potential  $E$ , its divergence is given by*

$$\langle \nabla, E \rangle = \frac{\rho}{\varepsilon_0}$$

where  $\rho$  denotes as usual the charge distribution. Also, we have

$$\nabla \times E = 0$$

meaning that the curl of  $E$  vanishes.

PROOF. We have several assertions here, the idea being as follows:

(1) The first formula, called Gauss law in differential form, follows from:

$$\begin{aligned} \int_B \langle \nabla, E \rangle &= \int_S \langle E(x), n(x) \rangle dx \\ &= \Phi_E(S) \\ &= \frac{Q_{enc}}{\varepsilon_0} \\ &= \int_B \frac{\rho}{\varepsilon_0} \end{aligned}$$

Now since this must hold for any  $B$ , this gives the formula in the statement.

(2) As a side remark, the Gauss law in differential form can be established as well directly, with the computation, involving a Dirac mass, being as follows:

$$\begin{aligned}
 \langle \nabla, E \rangle(x) &= \left\langle \nabla, K \int_{\mathbb{R}^3} \frac{\rho(z)(x-z)}{\|x-z\|^3} dz \right\rangle \\
 &= K \int_{\mathbb{R}^3} \left\langle \nabla, \frac{x-z}{\|x-z\|^3} \right\rangle \rho(z) dz \\
 &= K \int_{\mathbb{R}^3} 4\pi \delta_x \cdot \rho(z) dz \\
 &= 4\pi K \int_{\mathbb{R}^3} \delta_x \rho(z) dz \\
 &= \frac{\rho(x)}{\varepsilon_0}
 \end{aligned}$$

And with this in hand, we have via (1) a new proof of the usual Gauss law.

(3) Regarding the curl, by discretizing and linearity we can assume that we are dealing with a single charge  $q$ , positioned at 0. We have, by using spherical coordinates  $r, s, t$ :

$$\begin{aligned}
 \int_a^b \langle E(x), dx \rangle &= \int_a^b \left\langle \frac{Kqx}{\|x\|^3}, dx \right\rangle \\
 &= \int_a^b \left\langle \frac{Kq}{r^2} \cdot \frac{x}{\|x\|}, dx \right\rangle \\
 &= \int_a^b \frac{Kq}{r^2} dr \\
 &= \left[ -\frac{Kq}{r} \right]_a^b \\
 &= Kq \left( \frac{1}{r_a} - \frac{1}{r_b} \right)
 \end{aligned}$$

In particular the integral of  $E$  over any closed loop vanishes, and by using now Stokes' theorem, we conclude that the curl of  $E$  vanishes, as stated.

(4) Finally, as a side remark, both the formula of the divergence and the vanishing of the curl are somewhat clear by looking at the field lines of  $E$ . However, as all the above mathematics shows, there is certainly something to be understood, in all this.  $\square$

With this done, let us discuss now energy and potentials. Recall from chapter 3 the tricky formula  $F = -\nabla V$  there, which was moving us to the “next level”, in the context of gravity? The same holds in the present setting, and we first have:

THEOREM 5.22. *Consider an electric field, given as usual by:*

$$E(x) = K \int_L \frac{\rho(z)(x - z)}{\|x - z\|^3} dz$$

*We have then  $E = -\nabla V$ , with the corresponding potential  $V$  being given by*

$$V = K \int_L \frac{\rho(z)}{\|x - z\|} dz$$

*and the usual work and energy considerations for conservative forces hold.*

PROOF. Generally speaking, all this is something that we know well from chapter 3, in the general context of the conservative forces discussed there. However, there are a few notable differences with respect to gravity, as follows:

(1) First of all, as said time and again, strange things happen when allowing charges to move, and we don't know yet about that, so such energy considerations remain something quite formal, and we won't insist here. We will be back to this later, in the next chapter, after having the full equations of electrodynamics, namely the Maxwell equations.

(2) This being said, the notion of potential and the formula  $E = -\nabla V$  are extremely useful, for all sorts of considerations, as we will soon see. In what regards the formula for  $V$  in the statement, this is the usual formula for gravity, with masses replaced by charges, and with  $G$  replaced by  $K$ , and then with two other changes, as follows.

(3) First, the previous  $-$  sign from gravity has dissappeared, because in the gravitational context  $m_1 m_2 > 0$ , always true, corresponds to an attractive force, while in our setting  $q_1 q_2 > 0$  corresponds to a repulsive force. Thus, we must change the sign.

(4) And second, as already mentioned in (1), things here are a bit formal, so we have chosen to divide  $V$ , previously in gravity thought as being potential energy, by the receiving charge, as for this  $V$  to be a feature of the electric field  $E$  only.  $\square$

Moving ahead now, the question appears, what happens to the Gauss equations for the electric field  $E$ , as formulated in Theorem 5.12, when written in terms of the associated potential  $V$ . And the answer here, which is remarkable, is as follows:

THEOREM 5.23 (Poisson). *In terms of the electric potential  $V$ , the Gauss formula becomes the Poisson equation, namely*

$$\Delta V = -\frac{\rho}{\varepsilon_0}$$

*with  $\Delta = \langle \nabla, \nabla \rangle$  being the Laplace operator, given by the formula*

$$\Delta f = \sum_i \frac{d^2 f}{dx_i^2}$$

*and the curl equation dissappears, being automatic for gradients.*

PROOF. Here both the assertions are elementary, as follows:

(1) With  $E = -\nabla V$  the Gauss equation  $\langle \nabla, E \rangle = \rho/\varepsilon_0$  becomes:

$$\langle \nabla, \nabla V \rangle = -\frac{\rho}{\varepsilon_0}$$

Thus we must have  $\Delta V = -\rho/\varepsilon_0$ , with the operator  $\Delta$  being given by:

$$\begin{aligned} \Delta f &= \langle \nabla, \nabla f \rangle \\ &= \left\langle \begin{pmatrix} \frac{d}{dx} \\ \frac{d}{dy} \\ \frac{d}{dz} \end{pmatrix}, \begin{pmatrix} \frac{df}{dx} \\ \frac{df}{dy} \\ \frac{df}{dz} \end{pmatrix} \right\rangle \\ &= \frac{d^2 f}{dx^2} + \frac{d^2 f}{dy^2} + \frac{d^2 f}{dz^2} \end{aligned}$$

Thus, we are led to the Poisson equation in the statement.

(2) Regarding now the curl, our claim is that the equation  $\nabla \times E = 0$  simply disappears, this type of vanishing being automatic for gradients. Indeed, for any  $f$  we have:

$$\begin{aligned} \nabla \times \nabla f &= \begin{vmatrix} u_x & \frac{d}{dx} & \frac{df}{dx} \\ u_y & \frac{d}{dy} & \frac{df}{dy} \\ u_z & \frac{d}{dz} & \frac{df}{dz} \end{vmatrix} \\ &= \begin{pmatrix} \frac{d^2 f}{dydz} - \frac{d^2 f}{dzdy} \\ \frac{d^2 f}{dzdx} - \frac{d^2 f}{dxdz} \\ \frac{d^2 f}{dxdy} - \frac{d^2 f}{dydx} \end{pmatrix} \\ &= \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \end{aligned}$$

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

As an interesting feature of the potential approach, the Poisson equation makes sense, and is in fact very interesting, even when no charge is present, and we have here:

**THEOREM 5.24 (Laplace).** *In the case where no charges are present, the Poisson equation, and so the Gauss and even Coulomb laws too, in a certain sense, become*

$$\Delta V = 0$$

*called Laplace equation, whose solutions are called harmonic functions. These functions have an interesting mathematics, reminding that of the holomorphic functions in  $2D$ .*

PROOF. There are many things that can be said here, as follows:

(1) First of all, the Laplace equation and its physical meaning come from the Poisson equation, and from the various potential considerations in the above.

(2) Mathematically now, the idea is that various remarkable results about the holomorphic functions in 2D, such as the mean formula, extend to the harmonic functions.

(3) There is as well some more advanced theory to be developed here, involving for instance soap films, which are harmonic functions in the above sense.

(4) Summarizing, too many things to be discussed, and we refer to Rudin [74] for the mathematics of harmonic functions, and to Griffiths [42] for their physics.  $\square$

### 5d. The Faraday cage

As a main application of all this, let us discuss the Faraday cage. You have probably heard of it, and maybe thought a bit at its validity too, when stuck during a huge rain-storm, in your metal car, in the hope that the Faraday cage principle will indeed work. We will see now, with proof, that the Faraday cage principle always works:

**THEOREM 5.25** (Faraday cage). *In a cavity surrounded by a conductor, the electric field is 0. Moreover, the same principle holds when the cavity is not exactly perfect.*

PROOF. This is based on some more physics, the idea being as follows:

(1) There are all sorts of materials, but these basically fall into two classes. First we have the insulators, like plastic or glass, where the electrons are not free to move. And then we have the conductors, like metals, where there are electrons which can freely move. Conductors include as well other materials, at specific conditions and so on, but in what follows we will be interested in the “perfect conductors”, those having an unlimited supply of free electrons, and metals at normal conditions are close to this status.

(2) Let us first try to understand what happens when putting a charge  $q > 0$  near a conductor  $C$ . Since electrons are free to move, they will tend to go to the side of  $C$  which is close to  $q$ , making that side a charge  $-$ . And on the opposite side, we will have a lack of electrons, accounting for a charge  $+$ , the picture being as follows:

$$\begin{array}{c} \ominus \oplus \\ \oplus_q \quad \ominus C \oplus \\ \ominus \oplus \end{array}$$

(3) The point now is that, for the above to happen, an induced charge on  $C$ , we don't really need a charge  $q > 0$ , but just an electric field  $E$ . To be more precise, when putting  $C$  in no matter which electric field  $E$ , what will happen is that the electrons inside  $C$  will start moving, as to eventually produce a charge at the surface of  $C$ , producing itself a field  $-E$  inside the conductor, countering the external field  $E$ .

(4) In particular, when putting a conductor  $C$  in the path of an electric field  $E$ , no matter what surface phenomena will happen, as explained above, and which of course are in direct relation with the magnitude of  $E$ , the field inside the conductor will be always  $E + (-E) = 0$ . Thus, you are safe in a cavity inside  $C$ , as stated.  $\square$

As a conclusion to the general theory developed in this chapter, you won't be electrocuted when inside a Faraday cage. Note however that you might get cooked.

### 5e. Exercises

We have been extremely brief in the above, and it's a pity, but business is business, next chapter we'll go directly into magnetism and the Maxwell equations, and then we still have thermodynamics to be discussed. We will be back however to all this, at the theoretical level, later on, on several occasions, when doing quantum mechanics. The simplest 2-charge system that you can ever imagine is formed by a proton  $+$  and an electron  $-$ , and that is the hydrogen atom, the basic object of quantum mechanics.

For complements on the above, electrostatics, including far more theory, examples and exercises, we refer to our standard undergraduate books, namely Feynman [34], Griffiths [42], Purcell [72], Schwartz [79] and Shankar [86]. A look at related math books, on topics such as advanced calculus or differential geometry, is worth too, with well-known authors here including Rudin [73], [74], Lax [65], [66] and do Carmo [26], [27].

And here are now our exercises on the subject, all a bit vague and time-consuming:

EXERCISE 5.26. *Write down formulae for the electric fields of various metal wires, plates and solid bodies, coming in increasingly complicated shapes.*

EXERCISE 5.27. *Clarify all the possible proofs for the Gauss law, in its various formulations, and then for the Poisson law too, and the relation between them.*

EXERCISE 5.28. *In relation with potentials, learn some of the theory of the multipole expansion, and write down a brief account of what you learned.*

EXERCISE 5.29. *Learn more about capacitors and their properties, and write down a brief account of what you learned.*

EXERCISE 5.30. *Learn as well about materials and polarization, and write down a brief account of what you learned.*

As usual, if you don't find answers to some of the questions above, do not worry. You can keep reading this book instead, and always come back to them later, for relaxing.



## CHAPTER 6

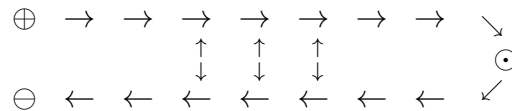
### The Maxwell equations

#### 6a. Motors and magnets

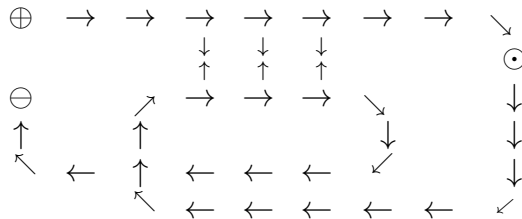
Magnetism, eventually. Who has not played with magnets as a kid, wishing to use them later at work, as an engineer, or at least understand them later, as a scientist. If you're reading now this book, magnets have probably something to do with it.

Unfortunately magnets are quite complicated things, and we will have to start our discussion with motors. And not even with cool gas engines, but with vulgar, electric motors. Yes, you heard me right, electric motors. So, let us do this, and we'll come back to magnets short after, that's promised. As for gas engines and Mad Max, we will come back to them too, in the next chapter, when discussing thermodynamics.

In order to understand the functioning of an electric motor, we don't need an actual motor, to start with, but just a battery feeding a light bulb. As a first observation, in a normal configuration of our device, the feeding cables will repel each other:



This is already quite surprising, and things are not over here. Indeed, when twisting a bit the cables, as to see what happens to parallel currents when moving in the same direction too, the conclusion is that in this case, we have attraction:

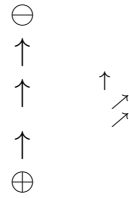


Summarizing, just by feeding a light bulb with a battery, and looking at the cables, and playing a bit with them, we are led to the following interesting conclusion:

**FACT 6.1.** *Parallel electric currents in opposite directions repel, and parallel electric currents in the same direction attract.*

We can in fact say even more, by further playing with the cables, armed this time with a compass. The conclusion is that each cable produces some kind of “magnetic field” around it, which interestingly, is not oriented in the direction of the current, but orthogonal to it, given by the right-hand rule, as follows:

FACT 6.2 (Right-hand rule). *An electric current produces a magnetic field  $B$  which is orthogonal to it, whose direction is given by the right-hand rule,*



*namely wrap your right hand around the cable, with the thumb pointing towards the direction of the current, and the movement of your wrist will give you the direction of  $B$ .*

This is something even more interesting than Fact 6.1. Indeed, not only moving charges produce something new, that we’ll have to investigate, but they know well about 3D, and more specifically about orientation there, left and right, even if living in 1D.

And isn’t this amazing. Let us summarize this discussion with:

FACT 6.3. *Charges are smart, they know about 3D, and about left and right.*

This invites to some philosophy, before moving ahead with some further physics, and then math. What is smartness? Not an easy question, but with our physics knowledge so far, we have at least two answers to it, as follows:

(1) Human smartness comes from chemical reactions in the brain, which reactions come from certain electrons taking certain decisions. But these electrons are exactly our charges, so human smartness ultimately comes from the charge smartness in Fact 6.3.

(2) Which leads us into the question whether masses are smart too. Not clear, but is there’s something to be said here, you have to agree that a tiny mass  $m$  exploding next to you, and releasing all its  $E = mc^2$  energy, was probably smarter than you.

With this discussed, let us go ahead and investigate the charge smartness, and more specifically the magnetic fields discovered above.

In order to evaluate the properties of the magnetic fields  $B$  coming from electric currents, as in Fact 6.2, the simplest way is that of making them act on exterior charges  $Q$ . And we have here the following formula, to start with, due to Lorentz:

FACT 6.4 (Lorentz force law). *The magnetic force on a charge  $Q$ , moving with velocity  $v$  in a magnetic field  $B$ , is as follows, with  $\times$  being a vector product:*

$$F_m = (v \times B)Q$$

*In the presence of both electric and magnetic fields, the total force on  $Q$  is*

$$F = (E + v \times B)Q$$

*where  $E$  is the electric field.*

Here the occurrence of the vector product  $\times$  is not surprising, due to the fact that the right-hand rule appears both in Fact 6.2, and in the definition of  $\times$ . In fact, the Lorentz force law is just a fancy mathematical reformulation of Fact 6.2, telling us that, once the magnetic fields  $B$  duly axiomatized, and with this being a remaining big problem, their action on exterior charges  $Q$  will be proportional to the charge,  $F_m \sim Q$ , and with the orientation and magnitude coming from the 3D of the right-hand rule in Fact 6.2.

As a side comment here, speaking various right-hand rules, we have met one in the context of gravity too, in chapter 4 above, when talking about rotating frames. So, which of these right-hand rules that we know is the main one? And answer here, for a true physicist at least, that's the one in Fact 6.2, mother of all right-hand rules.

As an interesting application of the Lorentz force law, we have:

THEOREM 6.5. *Magnetic forces do not work.*

PROOF. This might seem quite surprising, but the math is there, as follows:

$$\begin{aligned} dW_m &= \langle F_m, dx \rangle \\ &= \langle (v \times B)Q, v dt \rangle \\ &= Q \langle v \times B, v \rangle dt \\ &= 0 \end{aligned}$$

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

Moving ahead now, let us talk axiomatization of electric currents, including units. We have here the following definition, clarifying our previous discussion about coulombs:

DEFINITION 6.6. *The electric currents  $I$  are measured in amperes, given by:*

$$1A = 1C/s$$

*As a consequence, the coulomb is given by  $1C = 1A \times 1s$ .*

With this notion in hand, let us keep building the math and physics of magnetism. So, assume that we are dealing with an electric current  $I$ , producing a magnetic field  $B$ . In this context, the Lorentz force law from Fact 6.4 takes the following form:

$$F_m = \int (dx \times B)I$$

The current being typically constant along the wire, this reads:

$$F_m = I \int dx \times B$$

We can deduce from this the following result:

THEOREM 6.7. *The volume current density  $J$  satisfies*

$$\langle \nabla, J \rangle = -\dot{\rho}$$

*called continuity equation.*

PROOF. We have indeed the following computation, for any surface  $S$  enclosing a volume  $V$ , based on the Lorentz force law, and on the overall charge conservation:

$$\begin{aligned} \int_V \langle \nabla, J \rangle &= \int_S \langle J, n(x) \rangle dx \\ &= -\frac{d}{dt} \int_V \rho \\ &= -\int_V \dot{\rho} \end{aligned}$$

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

Moving ahead now, let us formulate the following definition:

DEFINITION 6.8. *The realm of magnetostatics is that of the steady currents,*

$$\dot{\rho} = 0 \quad , \quad \dot{J} = 0$$

*in analogy with electrostatics, dealing with fixed charges.*

As a first observation, for steady currents the continuity equation reads:

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

We have here a bit of analogy between electrostatics and magnetostatics, and with this in mind, let us look for equations for the magnetic field  $B$ . We have:

FACT 6.9 (Biot-Savart law). *The magnetic field of a steady line current is given by*

$$B = \frac{\mu_0}{4\pi} \int \frac{I \times x}{||x||^3}$$

*where  $\mu_0$  is a certain constant, called the magnetic permeability of free space.*

This law not only gives us all we need, for studying steady currents, and we will talk about this in a moment, with math and everything, but also makes an amazing link with the Coulomb force law, due to the following fact, which is also part of it:

FACT 6.10 (Biot-Savart, continued). *The electric permittivity of free space  $\varepsilon_0$  and the magnetic permeability of free space  $\mu_0$  are related by the formula*

$$\varepsilon_0\mu_0 = \frac{1}{c^2}$$

where  $c$  is as usual the speed of light.

This is something truly remarkable, and very deep, that will have numerous consequences, in what follows, be that for investigating phenomena like radiation, or for making the link with Einstein's relativity theory, both crucially involving  $c$ .

But, first of all, this is certainly an invitation to rediscuss units and constants, as a continuation of our discussion from chapter 5. In what regards the units, we won't be impressed by the ampere, and keep using the coulomb, as a main unit:

CONVENTIONS 6.11. *We keep using standard units, namely meters, kilograms, seconds, along with the coulomb, defined by the following exact formula*

$$1C = \frac{5 \times 10^{18}}{0.801\,088\,317} e$$

with  $e$  being minus the charge of the electron, which in practice means:

$$1C \simeq 6.241 \times 10^{18} e$$

We will also use the ampere, defined as  $1A = 1C/s$ , for measuring currents.

In what regards constants, however, time to do some cleanup. We have been boycotting for some time already the Coulomb constant  $K$ , and using instead  $\varepsilon_0 = 1/(4\pi K)$ , due to the ubiquitous  $4\pi$  factor, first appearing as the area of the unit sphere,  $A = 4\pi$ , in the computation for the Gauss law for the unit sphere. Together with Fact 6.10, this suggests using the numbers  $\varepsilon_0, \mu_0$  as our new constants, by always keeping in mind  $\varepsilon_0\mu_0 = 1/c^2$ , and by having of course  $c$  as constant too, and we are led in this way into:

CONVENTIONS 6.12. *We use from now on as constants the electric permittivity of free space  $\varepsilon_0$  and the magnetic permeability of free space  $\mu_0$ , given by*

$$\varepsilon_0 = 8.854\,187\,8128(13) \times 10^{-12}$$

$$\mu_0 = 1.256\,637\,062\,12(19) \times 10^{-6}$$

as well as the speed of light, given by the following exact formula,

$$c = 299\,792\,458$$

which are related by  $\varepsilon_0\mu_0 = 1/c^2$ , and with the Coulomb constant being  $K = 1/(4\pi\varepsilon_0)$ .

Observe in passing that we are not messing up our figures, which can be quite often the case in this type of situation, because according to our data, and by truncating instead of rounding, as busy theoretical physicists usually do, we have:

$$\varepsilon_0 \mu_0 c^2 = 8.854 \times 1.256 \times 2.997^2 \times 10^{16-12-6} = 0.998$$

We will be back to numerics later on, when rediscussing as well the relation between electricity and gravitation, following a discussion from chapter 5, but this time with magnetism added. As an obvious comment, however, observe how the above figures show that magnetic forces are far weaker than electric forces. More on this later.

Getting back now to theory and math, the Biot-Savart law has as consequence:

THEOREM 6.13. *We have the following formula:*

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

PROOF. We recall that the Biot-Savart law tells us that the magnetic field  $B$  of a steady line current  $I$  is given by the following formula:

$$B = \frac{\mu_0}{4\pi} \int \frac{I \times x}{||x||^3}$$

By applying the divergence operator to this formula, we obtain:

$$\begin{aligned} \langle \nabla, B \rangle &= \frac{\mu_0}{4\pi} \int \left\langle \nabla, \frac{I \times x}{||x||^3} \right\rangle \\ &= \frac{\mu_0}{4\pi} \int \left\langle \nabla \times J, \frac{x}{||x||^3} \right\rangle - \left\langle \nabla \times \frac{x}{||x||^3}, J \right\rangle \\ &= \frac{\mu_0}{4\pi} \int \left\langle 0, \frac{x}{||x||^3} \right\rangle - \langle 0, J \rangle \\ &= 0 \end{aligned}$$

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

Regarding now the curl, we have here a similar result, as follows:

THEOREM 6.14 (Ampère law). *We have the following formula:*

$$\nabla \times B = \mu_0 J$$

PROOF. Again, we use the Biot-Savart law, telling us that the magnetic field  $B$  of a steady line current  $I$  is given by the following formula:

$$B = \frac{\mu_0}{4\pi} \int \frac{I \times x}{||x||^3}$$

By applying the curl operator to this formula, we obtain:

$$\begin{aligned}
 \nabla \times B &= \frac{\mu_0}{4\pi} \int \nabla \times \frac{I \times x}{||x||^3} \\
 &= \frac{\mu_0}{4\pi} \int \left\langle \nabla, \frac{x}{||x||^3} \right\rangle J - \langle \nabla, J \rangle \frac{x}{||x||^3} \\
 &= \frac{\mu_0}{4\pi} \int 4\pi \delta_x \cdot J - \frac{\mu_0}{4\pi} \cdot 0 \\
 &= \mu_0 \int \delta_x \cdot J \\
 &= \mu_0 J
 \end{aligned}$$

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

As a conclusion to all this, the equations of magnetostatics are as follows:

**THEOREM 6.15.** *The equations of magnetostatics are*

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

$$\nabla \times B = \mu_0 J$$

*with the second equation being the Ampère law.*

**PROOF.** This follows indeed from the above discussion, and more specifically from Theorem 6.13 and Theorem 6.14, which both follow from the Biot-Savart law. □

Observe the obvious analogy with the Gauss equations of electrostatics, namely:

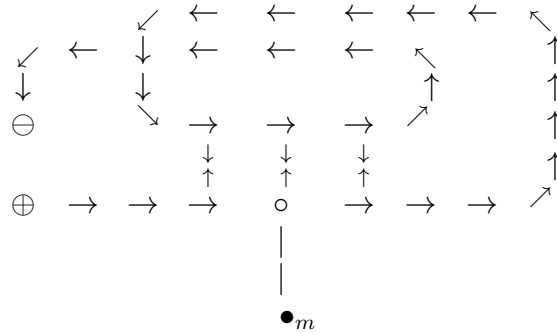
$$\langle \nabla, E \rangle = \frac{\rho}{\varepsilon_0}$$

$$\nabla \times E = 0$$

As a conclusion to all this, looks like someone has played here with basic 3D math, vectors, products and so on, and messed them up, as for electrostatics to become magnetostatics, and vice versa. More on this later, when talking about unification.

As an application of all this, let us discuss motors. The simplest idea of an electromagnetic motor comes from the attracting cables in Fact 6.1, but unfortunately, when doing the engineering and building such a motor, we are led to:

**THEOREM 6.16.** *A basic electromagnetic motor, pulling a weight  $m$  by using the attraction of two parallel currents, traveling in the same direction,*



*will not work.*

**PROOF.** Want it or not, this comes from the math in Theorem 6.5, telling us that magnetic forces do not work. And you can't beat such simple math. We will see however, later, that functioning and reliable electromagnetic motors can be built, by tricking the 3D in Theorem 6.5, the idea being that of replacing straight wires by coils.  $\square$

As a side comment here, when talking later about gas engines, in chapter 7 below, the situation will be pretty much similar. Our math there will lead us into some wonderful, ideal engines, called "Carnot engines", that are in fact so slow, due to being fantastically fuel-saving, that even your grandma won't buy a car fit with a Carnot engine.

Getting back now to work, and to serious engineering, for being complete, and also for keeping our promises, made at the beginning of this chapter, it remains to discuss magnets. But let us do this slowly. In view of the clear analogy between electrostatics and magnetostatics, it makes sense to investigate first the problem for electrostatics, and then for magnetostatics. And here, we first have, in the context of electrostatics:

**FACT 6.17.** *When exposed to small electric fields, non-conductors are subject to polarization, coming from small electric rearrangements inside their atoms or molecules.*

To be more precise here, in order to have some discussion started, let us recall from our study of the Faraday cage, from chapter 5, that materials basically fall into two classes, insulators and conductors, and with the conductors being subject to a surface phenomenon of induced charge, when exposed to an electric field.

In the case of insulators, or non-conductors in general, this surface phenomenon of induced charge does not appear, since electrons are strongly bound to their respective atoms or molecules. Of course, when the electric field is very strong, it can blow away electrons, and the material gets ionized. But for lower intensity fields, in the lack of ionization or of an induced surface charge phenomenon, the only thing that can happen is some small rearrangement inside the atoms or molecules, known as polarization.



At the atomic level, the polarization can be understood as being a modification of the electron cloud, or rather of the density of the electron cloud, in the direction of the field. Here is for illustration a picture of polarized boron  ${}_5\text{B}$ , exaggerated of course:



For molecules things are far more complicated, because due to the complex geometry of such molecules, the polarization can appear in various 3D directions with respect to the orientation of the field, including the direction orthogonal to it.

This was for the basics of polarization. For more, we refer as usual to any of our standard undergraduate books, such as Griffiths [42]. In what concerns us we will be back to this only later on, when talking about polarized light.

Moving ahead now with magnetism, we have here:

**FACT 6.18.** *When exposed to small magnetic fields, materials are subject to magnetization, similarly to polarization. However, certain special materials like iron  ${}_{26}\text{Fe}$  can conserve their magnetization, even after the original magnetizing field is gone.*

In what regards the basics of magnetization, these are a bit similar to the basics of polarization, with some physics and geometry going on there, and with the magnetized materials being roughly classified into paramagnets, whose magnetization appears along the field, and diamagnets, whose magnetization appears against the field.

Regarding however the permanent magnets, those which keep their magnetization after the magnetizing field is gone, and which are called ferromagnets, the story here is far more complicated. The general idea is that such materials, including the iron  ${}_{26}\text{Fe}$ , have the remarkable property of being permanently damaged by a magnetic field, due to a number of quite complicated reasons. In addition, temperature has something to do with all this too, with high temperatures, above the so-called Curie point of the material, which is  $T = 770^\circ \text{C}$  for iron, turning ferromagnets into paramagnets.

Again, for more on all this, we refer here as usual to any of our standard undergraduate books, such as Griffiths [42]. More on metals can be learned by doing some survival-type metallurgy, and using the Curie point when cooking, or of course by listening to Metallica. There are also several dedicated books on metals, such as the one by Abrikosov [1].

As a conclusion, we have now a full theory of magnetostatics, complementing the theory of electrostatics. We will see in a moment that these theories can be unified.

### 6b. The Maxwell equations

In the context of moving charges, some of the laws that we know well from electrostatics and from magnetostatics must be altered. But let us first begin with the basics, by forgetting the ideal void that we are used to, and which will be back in a moment, no worries for that. A first question is that of understanding the current density  $J$  flowing through a given material, and the answer here is given by Ohm's law, as follows:

FACT 6.19 (Ohm's law). *The current density  $J$  is given by*

$$J = \sigma E$$

*where  $\sigma$  is a constant, called conductivity of the material.*

We are already a bit familiar with this, with our notion of ideal conductor corresponding to  $\sigma = \infty$ , and our notion of ideal insulator corresponding to  $\sigma = 0$ . In real life, however, we have of course  $\sigma \in (0, \infty)$ . Here are 3 + 3 + 3 basic examples, at 20° C and 1 atm, consisting of 3 conductors, 3 semiconductors and 3 insulators, and with  $\sigma$  being replaced by its inverse  $\rho = 1/\sigma$ , called resistivity, more employed in engineering:

Silver	:	$1.59 \times 10^{-8}$
Iron	:	$9.61 \times 10^{-8}$
Graphite	:	$1.6 \times 10^{-5}$
—		
Seawater	:	0.2
Diamond	:	2.7
Silicon	:	2500
—		
Water	:	8300
Glass	:	$10^9 - 10^{14}$
Teflon	:	$10^{22} - 10^{24}$

Getting back now to Ohm's law, a more familiar version of it is as follows, expressing the total current flowing from one electrode to the other in terms of the potential difference between them, or rather vice versa, and with  $R \sim \rho$  being the resistance, which depends, besides on  $\rho$ , on the precise configuration of the resistor to be crossed:

$$V = IR$$

With this second formulation of the Ohm law in hand, we can now formulate as well, following Joule, a formula in regards with energy, as follows:

FACT 6.20 (Joule heating law). *The work done by the electric force is*

$$P = VI = I^2 R$$

*with this being understood as corresponding to heating the resistor.*

As usual, we refer to our standard undergraduate books, such as Griffiths [42], for more on all this, and to an engineering book for even more. In what concerns us, we will be back to Joule and his heating law in chapter 7 below, when doing thermodynamics, after properly explaining what heating is, and what temperature is.

Let us go back now to the void, with the aim of suitably fixing and unifying the equations of electrostatics and magnetostatics that we have, in the dynamic setting. The normal path here is via a continuation of the Joule law, by observing this time quantities like work and energy, in connection with moving charges, and with the experiments arranged as for the resistance of the various materials met not to be revelant, or at least to be extractable via the Ohm and Joule laws, and their refinements and generalizations.

However, and here comes the interesting point, there is in fact simpler than that, with no need of going through such things as resistors and heating. We have indeed:

FACT 6.21 (Faraday laws). *The following happen:*

- (1) *Moving a wire loop  $\gamma$  through a magnetic field  $B$  produces a current through  $\gamma$ .*
- (2) *Keeping  $\gamma$  fixed, but changing the strength of  $B$ , produces too current through  $\gamma$ .*

These laws are truly amazing facts of nature, relating electricity, magnetism and motion, and can be used both for generating current from motion, and for generating motion from current. We will explain them more in detail in the next section, when talking electromechanics, and in particular, eventually building our first electric motor.

In relation now with the mathematics and physics of electrodynamics, happening abstractly in the void, these two Faraday laws are of immense help too. To be more precise, such considerations led Faraday to the following beautiful conclusion:

FACT 6.22 (Faraday). *In the context of moving chages, the electrostatics law*

$$\nabla \times E = 0$$

*must be replaced by the following equation,*

$$\nabla \times E = -\dot{B}$$

*called Faraday law.*

Along the same lines, and following now Maxwell, there is a correction as well to be made to the main law of magnetostatics, namely the Ampère law, as follows:

FACT 6.23 (Maxwell). *In the context of moving chages, the Ampère law*

$$\nabla \times B = \mu_0 J$$

*must be replaced by the following equation,*

$$\nabla \times B = \mu_0 (J + \varepsilon_0 \dot{E})$$

*called Ampère law with Maxwell correction term.*

Now by putting everything together, and perhaps after doublechecking as well, with all sorts of experiments, that the remaining electrostatics and magnetostatics laws, that we have not modified, work indeed fine in the dynamic setting, we obtain:

THEOREM 6.24 (Maxwell). *Electrodynamics is governed by the formulae*

$$\langle \nabla, E \rangle = \frac{\rho}{\varepsilon_0}$$

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

$$\nabla \times E = -\dot{B}$$

$$\nabla \times B = \mu_0 J + \mu_0 \varepsilon_0 \dot{E}$$

*called Maxwell equations.*

PROOF. This follows indeed from the above, the details being as follows:

- (1) The first equation is the Gauss law, that we know well from chapter 5.
- (2) The second equation is something anonymous, that we know well too.
- (3) The third equation is a previously anonymous law, modified into Faraday's law.
- (4) And the fourth equation is the Ampère law, as modified by Maxwell.  $\square$

So, these are the famous Maxwell equations. With this in hand, you can now escape from time to time from consulting, as a complement to the material here, our standard undergraduate books, namely Feynman [34], Griffiths [42], Purcell [72], Schwartz [79] and Shankar [86], and have an escapade with graduate books, such as Jackson [54], Landau-Lifshitz [62], Panofsky-Phillips [68], or Schwinger [82].

As an example here, Schwinger starts [82] with chapter 1, the Maxwell equations. Which is in fact, forgetting now about level, fully legitimate from an honest scientific point of view, because honest physics should start with the honest laws of the phenomena that you are investigating, and in our case, these are the Maxwell equations.

But not everyone is Schwinger. By the way it should be mentioned that the book [82] is available to us thanks to the efforts of his students DeRaad, Milton and Tsai, who after his death made his old lecture notes on electrodynamics into a book. And with a similar story for Schwinger's quantum mechanics book [83], but more on that later.

At the level of general theory now, there are many things that can be said, as a continuation of the above. In what concerns us, we will be mostly theoretical. As a first key result, making the connection with Einstein's relativity theory, we have:

THEOREM 6.25. *The Maxwell equations are invariant under Lorentz transformations*

$$x' = \gamma(x - vt)$$

$$y' = y$$

$$z' = z$$

$$t' = \gamma(t - vx/c^2)$$

with  $\gamma = 1/\sqrt{1 - v^2/c^2}$  being as usual the Lorentz factor.

PROOF. This is something a bit complicated, the idea being as follows:

(1) As a first comment, this result, due to Lorentz himself, working on electromagnetism, was established some time before Einstein's relativity theory, and with this clarifying the various comments that we made in chapter 4, when talking relativity.

(2) As for the proof, this follows by doing some computations, and with the speed of light  $c > 0$  having something to do with all this coming from the formula  $\varepsilon_0\mu_0 = 1/c^2$ , which was part of the Biot-Savart law, as explained in Fact 6.10.

(3) To be more precise, consider an electromagnetic field  $(E, B)$ . This is altered by a Lorentz transformation into a field  $(E', B')$ , the equations for  $E'$  being as follows:

$$E'_x = E_x$$

$$E'_y = \gamma(E_y - vB_z)$$

$$E'_z = \gamma(E_z + vB_y)$$

As for the equations of  $B'$ , these are quite similar, as follows:

$$B'_x = B_x$$

$$B'_y = \gamma\left(B_y + \frac{v}{c^2} E_z\right)$$

$$B'_z = \gamma\left(B_z - \frac{v}{c^2} E_y\right)$$

(4) In order to do the math, consider the following matrices, with  $\beta = v/c$  as usual:

$$D = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \gamma & 0 \\ 0 & 0 & \gamma \end{pmatrix}, \quad M = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\beta\gamma \\ 0 & \beta\gamma & 0 \end{pmatrix}$$

In terms of these matrices, the formulae for the new field  $(E', B')$  read:

$$E' = DE + cMB$$

$$B' = DB - \frac{M}{c}E$$

(5) But this is already not that bad, and starting from these formulae, it is possible to prove that  $(E', B')$  satisfies as well the Maxwell equations, as desired.

(6) In practice, however, the best is to learn some more geometry, and further reformulate the equations in (4) on one hand, and the Maxwell equations on the other hand, and why not the Lorentz transformation itself too, on the other other hand, and with the conclusion being, of course, that the invariance is trivial, at least to connoisseurs.  $\square$

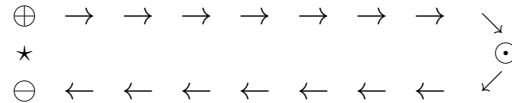
There are many other things that can be said here, in relation with Einstein's relativity, which are all very interesting. In fact, the discussion here is quite endless. We will come back to this later in this book, first at the end of the present chapter, when talking radiation and waves, and then later on, towards the end, when talking QED.

In fact, when talking QED (quantum electrodynamics) we will see as well a more conceptual explanation for the Maxwell equations, which, we must admit, arise so far as a bizarre collection of math computations and experimental facts.

### 6c. Electromechanics

In this section we discuss the relation between electromagnetism and mechanics, or at least we attempt to discuss it, at the beginner level which is presently ours. We will see that this is a fascinating theme, which is extremely wide, ranging from everyday appliances and engineering to fairly crazy things, such as modern physicists doing quantum gravity, or the magnetism of all sorts of celestial bodies, standard or more crazy.

In order to get started, let us get back to the work of Faraday, and his principles from Fact 6.21. In order to understand what is going on there, let us start with the simplest electric loop that we know, namely a battery feeding a light bulb:



Here the star stands for the fact that we don't really know what happens inside the battery, typically a complicated chemical process. Nor we will actually worry about the bulb, let us simply assume that this bulb does not exist at all. We will be interested in the force driving the current around the loop, and we have here:

PROPOSITION 6.26. *When writing the force driving the current through a loop  $\gamma$  as*

$$F = F_{\star} + F_e$$

*with  $F_{\star}$  coming from the source, and  $F_e$  coming from the loop, the quantity*

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

*called electromotive force, or emf of the loop, is simply obtained by integrating  $F_{\star}$ .*

PROOF. We have indeed the following computation, based on the fact that  $F_e$  being an electrostatic force, its integral over the loop vanishes:

$$\begin{aligned}
 \mathcal{E} &= \int_{\gamma} \langle F(x), dx \rangle \\
 &= \int_{\gamma} \langle F_{\star}(x), dx \rangle + \int_{\gamma} \langle F_e(x), dx \rangle \\
 &= \int_{\gamma} \langle F_{\star}(x), dx \rangle + 0 \\
 &= \int_{\gamma} \langle F_{\star}(x), dx \rangle
 \end{aligned}$$

Thus, we have our result, and with the remark of course that the emf  $\mathcal{E} \in \mathbb{R}$  is not really a force, but this is the standard terminology, and we will use it.  $\square$

In relation now with the Faraday principles from Fact 6.21, these can be fine-tuned, and reformulated in terms of the emf, in the following way:

FACT 6.27 (Faraday). *The emf of a loop  $\gamma$  moving through a magnetic field  $B$  is*

$$\mathcal{E} = -\dot{\Phi}$$

where  $\Phi$  is the flux of the field  $B$  through the loop  $\gamma$ , given by:

$$\Phi = \int_{\gamma} \langle B(x), dx \rangle$$

As for the emf of a fixed loop  $\gamma$  in a changing magnetic field  $B$ , this is

$$\mathcal{E} = - \int_{\gamma} \langle \dot{B}(x), dx \rangle$$

which by Stokes is equivalent to the Faraday law  $\Delta \times E = -\dot{B}$ .

Summarizing, not only we have understood how the Faraday principles from Fact 6.21 eventually got transformed into his law from Fact 6.22, destined to be the 3rd of the Maxwell equations, with the full story involving the emf and Stokes, but we have now all needed tools for constructing generators and motors, and working out their numerics.

Forgetting about generators, the best method for producing energy being  $E = mc^2$  anyway, we can now build functioning electric motors, as follows:

THEOREM 6.28. *Functioning and reliable electric motors can be build by using the basic principles of electromagnetism, by using coils of wire.*

PROOF. This is something which improves our previous attempt of building such a motor, reported in Theorem 6.16. To be more precise, that attempt failed due to the math in Theorem 6.5, telling us that magnetic forces do not work. But now we know from Fact 6.27 how to trick Theorem 6.5, by replacing straight wires by loops, or even better, by coils of wire. As for the math and numerics of these motors, these can be worked out too, once again by using the Faraday formulae from Fact 6.27.  $\square$

There are of course tons of other things that can be said about electromechanics, and we refer here to any of our standard undergraduate books on electrodynamics, such as Griffiths [42]. And with the remark however that, for serious applications, you are in need afterwards of a solid engineering book, centered on electromechanics.

Let us keep discussing the relation between electromagnetism and mechanics. An obvious question is about unifying gravity and electromagnetism, and we have here:

THEOREM 6.29. *The theory of the Newton-Coulomb quadratic force between charged masses  $(m, q)$ , which is attractive with the convention*

$$F = \frac{Gm_1m_2 - Kq_1q_2}{d^2}$$

*can be refined into a theory of a quadratic force between bodies  $(p, n, e)$  formed of protons, neutrons and electrons. However, it is not clear what happens in the dynamic setting.*

PROOF. As the statement tends to indicate, things are quite complicated here, and this will be rather an introduction to some open questions. The idea is as follows:

(1) First, we will be playing here, at a very elementary level, with classical field theory, and a good reference for this, and for much more, are the books of Landau-Lifshitz [61], [62], and their continuations [63], [64], and afterwards. By the way, be said in passing, these Landau-Lifshitz books, while quite hard to read to start with, are a true delight at the advanced level, with many formulae there, when it comes to really complicated things, beating by their beauty and elegance everything else on the market.

(2) Still talking Landau-Lifshitz, and as an irony now, the fourth book in the series [64], on quantum electrodynamics, was originally written based on an old version of QED, now obsolete, and had to be rewritten later by Berestetskii, Lifshitz and Pitaevskii, with Lev Landau being no longer among the authors. Beware of theoretical physics.

(3) Getting now to our unification questions, the formula of the Newton-Coulomb force  $F = F_n + F_c$  is indeed the one in the statement, with the  $-$  sign on the charges term coming from our convention that this unified force  $F$  is attractive.

(4) The point now is that, at least in the real life surrounding us, the objects are rather triples  $a = (p, n, e)$ , with the parameters  $p, n, e \in \mathbb{N}$  counting respectively the number of



protons, neutrons and electrons. The conversion formulae are as follows:

$$m = pm_p + nm_n + em_e$$

$$q = pq_p + nq_n + eq_e$$

(5) It is most convenient at this point to regard our bodies  $a = (p, n, e)$  as being vertical vectors,  $a \in \mathbb{R}^3$ , and also to forget that they are quantized and positive,  $a \in \mathbb{N}^3$ . With this convention, the above conversion formulae become as follows, with  $\mu, \gamma \in \mathbb{R}^3$  collecting the mass and charge figures for protons, neutrons and electrons:

$$m = \langle a, \mu \rangle \quad , \quad q = \langle a, \gamma \rangle$$

Also with this convention, the Newton-Coulomb force is given by:

$$\begin{aligned} F_{ab} &= \frac{G \langle a, \mu \rangle \langle b, \mu \rangle - K \langle a, \gamma \rangle \langle b, \gamma \rangle}{d^2} \\ &= \frac{\sum_{ij} a_i b_j (G \mu_i \mu_j - K \gamma_i \gamma_j)}{d^2} \end{aligned}$$

We can write this formula in a more compact form, as follows:

$$F_{ab} = \frac{\langle Ma, b \rangle}{d^2} \quad : \quad M = \left[ G \mu_i \mu_j - K \gamma_i \gamma_j \right]_{ij}$$

(6) Regarding now the data for elementary particles, this is as follows, and with the comment that things are in fact quite complicated for the charge vector  $\gamma$ , because  $-\gamma_3 > \gamma_1$  starting at order  $10^{-7}$ , and  $\gamma_2 = 0$  is only known up to order  $10^{-22}$ :

$$\mu = \begin{pmatrix} 1.672 \times 10^{-27} \\ 1.674 \times 10^{-27} \\ 9.109 \times 10^{-31} \end{pmatrix} \quad , \quad \gamma = \begin{pmatrix} 1.602 \times 10^{-19} \\ 0 \\ -1.602 \times 10^{-19} \end{pmatrix}$$

(7) As another important remark, as already mentioned in chapter 5 above, in what regards the bodies  $a$ , these are known to satisfy  $a_1 = a_3$  up to order  $10^{-10}$ , and with  $a_2$ , the number of neutrons, being by basic atomic physics close to these numbers. Thus, we have some data regarding our bodies as well, quite restrictive, of the following type:

$$a \simeq \begin{pmatrix} n \\ \alpha n \\ n \end{pmatrix} \quad , \quad \alpha \simeq 1 - 2$$

However, we will not use this extra piece of data, because most of the matter in the universe is hydrogen, then helium and so on, and for such small atoms isotopes or ionization bring serious issues to our general approximation formula above.

(8) To be more precise, let us look for instance at hydrogen, the most abundant element. This is usually met as protium  $^1\text{H}$ , consisting of a proton and an electron, but

the isotopes deuterium  ${}^2\text{H}$  and tritium  ${}^3\text{H}$  exist too, and so do the hydron  $\text{H}^+$  and hydride  $\text{H}^-$  ions, with all these versions being as follows, clearly messing up our algebra:

$${}^1\text{H} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad {}^2\text{H} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad {}^3\text{H} = \begin{pmatrix} 1 \\ 2 \\ 1 \end{pmatrix}, \quad \text{H}^+ = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \text{H}^- = \begin{pmatrix} 1 \\ 0 \\ 2 \end{pmatrix}$$

(9) Summarizing, we will still assume in what follows that our bodies  $a$  are arbitrary, not quantized, and not subject to some estimate either,  $a \in \mathbb{R}^3$ . Thus, we are left with studying the matrix  $M$  from (5) above, by using the data from (6) above. Let us recall now as well, as the other needed piece of data, that the constants  $G, K$  are:

$$G = 6.674 \times 10^{-11}$$

$$K = 8.897 \times 10^9$$

And problem here, we cannot use this data, because  $K$  is so much bigger than  $G$ . To be more precise,  $K$  is given by an exact formula, and we can have as many decimals for it, as we want to. In what regards  $G$ , however, which is the small and problematic constant, this is known only up to order  $10^{-5}$ , the precise figure being as follows:

$$G = 6.67430(15) \times 10^{-11}$$

Thus, thinking a bit at our data, decimals, approximations, and what we want to do, the conclusion is that in regards with the problem that we want to solve, namely estimating the matrix  $M$  from (5) above, the only data that we have about  $G$  is:

$$G \simeq 0$$

(10) As a conclusion to all this, the only thing to be done is to keep both bodies  $a$  and constants  $G, K$  abstract, and use only the data in (6). Before doing so, however, let us rescale everything, as to not have to deal with all these powers of 10. Let us introduce new mass and charge vectors  $\mu', \gamma'$ , according to the following formulae:

$$\mu' = \mu \times 10^{30}, \quad \gamma' = \gamma \times 10^{19}$$

Numerically, our data from (6) becomes as follows:

$$\mu' = \begin{pmatrix} 1.672 \times 10^3 \\ 1.674 \times 10^3 \\ 0.910 \end{pmatrix}, \quad \gamma' = \begin{pmatrix} 1.602 \\ 0 \\ -1.602 \end{pmatrix}$$

As for the constants, let us introduce as well new constants  $\mathcal{G}, \mathcal{K}$  as follows:

$$\mathcal{G} = G \times 10^{-60} = 6.674 \times 10^{-71}$$

$$\mathcal{K} = K \times 10^{-38} = 8.897 \times 10^{-29}$$

Here the exponents 60, 38 come from the exponents 30, 19 used before, and so there is no correction to the formula of  $F$ , which stays the same, namely:

$$F_{ab} = \frac{\langle Ma, b \rangle}{d^2} \quad : \quad M = \left[ \mathcal{G} \mu'_i \mu'_j - \mathcal{K} \gamma'_i \gamma'_j \right]_{ij}$$

Observe by the way that we have the following formula relating our new constants, in agreement with some previous numeric computations, from chapter 5:

$$\mathcal{K} \simeq \mathcal{G} \times 10^{42}$$

(11) What's next? Not very clear, the problem being that of coming up with something clever, based on the obvious special features of the vectors  $\mu', \gamma'$  given above, as to simplify the math. And perhaps by reconsidering too our previous decision to leave our bodies  $a \in \mathbb{R}^3$  not quantized and arbitrary, ignoring the information about them from (7) above. However, things are quite unclear here, suggesting leaving this problem like this.

(12) Let us not get discouraged, however. The point indeed is that quarks can come rescue us. These quarks are surely reputed to be quite complicated things, but in relation with our considerations, the algebra is very simple, a proton being made of 2 up quarks and 1 down quark, and a neutron being made of 1 up quark and 2 down quarks:

$$p = 2u + 1d$$

$$n = 1u + 2d$$

This suggests replacing our old bodies  $a = (p, n, e)$  with new bodies  $a = (u, d, e)$ , according to the above formulae. To be more precise, in terms of the quark mass and charge vectors  $\mu'', \gamma''$ , the quadratic force formula will stay the same, namely:

$$F_{ab} = \frac{\langle Ma, b \rangle}{d^2} \quad : \quad M = \left[ \mathcal{G} \mu''_i \mu''_j - \mathcal{K} \gamma''_i \gamma''_j \right]_{ij}$$

(13) So, let us compute the new data. Regarding charges, things are quickly settled by using the formulae in (12) above, the new charge vector being by linear algebra as follows, and with this being in agreement with the real-life data for quarks:

$$\gamma'' = \begin{pmatrix} 2/3 & -1/3 & 0 \\ -1/3 & 2/3 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1.602 \\ 0 \\ -1.602 \end{pmatrix} = \begin{pmatrix} 1.068 \\ -0.534 \\ -1.602 \end{pmatrix}$$

In what regards masses, however, things are complicated, the real-life data for the up and down quarks being relativistic, as follows, with  $1\text{Mev}/c^2 \simeq 1.782 \times 10^{-30}$ :

$$m_u = 2.2^{+0.5}_{-0.4} \text{ MeV}/c^2 \quad , \quad m_d = 4.7^{+0.5}_{-0.3} \text{ MeV}/c^2$$

What to do? Let us better ignore these latter formulae, and their potentially complicated meaning, and abstractly declare that the quark mass vector should be given by

simple linear algebra, as the charge vector was. We obtain, in this way:

$$\mu'' = \begin{pmatrix} 2/3 & -1/3 & 0 \\ -1/3 & 2/3 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1.672 \times 10^3 \\ 1.674 \times 10^3 \\ 0.910 \end{pmatrix} = \begin{pmatrix} 5.566 \times 10^2 \\ 5.586 \times 10^2 \\ 0.910 \end{pmatrix}$$

(14) All this looks nice, but at the end of the day the problem remains the same, as explained in (11) above, with our  $1/3 - 2/3$  quark tricks not really helping the algebra. Plus, in addition, we got here into some serious troubles in regards with masses, taking us into the question on whether we should be relativistic or not.

(15) Importantly now, all the above, be it abstract or numeric, was about the statics of the quadratic force  $F = F_n + F_c$ , but the big problem now is that of working out the dynamics, which amounts in using the Maxwell equations instead of  $F_c$ . But this latter fact brings us into the Lorentz transformation invariance, and so suggests to use the Einstein general relativity as well instead of  $F_n$ . And so, as a conclusion, we are left with unifying general relativity with the Maxwell equations.

(16) And there is even worse, because the various particles that we met above, namely protons, neutrons and electrons, and then quarks at a more advanced level, are subject to two supplementary forces, call weak and strong, which are no longer quadratic, with the weak force acting at  $10^{-18}$  range, and with the strong force acting at  $10^{-15}$  range. Thus, as a truly final conclusion, we would like to have here some kind of “quantum gravity” theory, unifying, both dynamically and relativistically, these 4 forces of nature.  $\square$

To summarize, all this looks quite complicated, well beyond what we can do, and with even our simplest static numerics failing, due to the fact that the rescaled gravitational and Coulomb constants,  $\mathcal{G} = G \times 10^{-60}$  and  $\mathcal{K} = K \times 10^{-38}$ , are subject to:

$$\mathcal{K} \simeq \mathcal{G} \times 10^{42}$$

So time perhaps to ask the cat, that we actually haven’t met in a while, since chapter 4, when talking about Einstein and relativity. And cat says:

CAT 6.30. *As a mathematician, you should respect numbers, and in particular  $10^{42}$ . Better look into fluid dynamics, that’s more reasonable, and useful.*

This sounds wise, as usual, but I must admit that, for one time, I do not fully agree with cat. Look for instance at the Einstein energy formula, which is as follows, with the first and second terms differing, at low speeds, by a factor of type  $c^2 \simeq 10^{19}$ :

$$\mathcal{E} = mc^2 + \frac{mv^2}{2} + \dots$$

So, would have Einstein followed his cat’s advice, with cats being of course like electrons, having nearly identical knowledge, and respected the number  $10^{19}$ , he would have not worked towards his discovery, and we will be nowadays still without  $E = mc^2$ .

This being said, in the lack of any valuable idea, let us leave quantum gravity for later, towards the end of the present book, and follow now the advice of cat, what else can we do. So, as a last topic of our discussion here, let us discuss the unification of electromagnetism with fluid dynamics, known as magnetohydrodynamics:

THEOREM 6.31. *Electromagnetism and fluid dynamics can be successfully unified as Magnetohydrodynamics by merging the Euler equations with the Maxwell equations.*

PROOF. There are many things that can be said here, as follows:

(1) First of all, magnetohydrodynamics deals with the behavior of a fluid body which is at the same time a conductor, which means typically a hot metal, but which can be something more complicated too, as a plasma. Our beloved Earth falls into this category, its core being molten metal, mostly iron–nickel, boiling at about 5,700 K.

(2) So, let us talk about the Earth first. Its magnetism comes from this metal core, which moves because of the rotation of the Earth, and therefore produces a magnetic field. This field is of course very weak, but for other celestial bodies, which can be subject to far higher rotation movements, with angular speed of the same order of magnitude as  $c$  being not an unknown phenomenon in the universe, it can be quite strong too.

(3) Importantly, the magnetic field, be it weak or strong, is always ever-changing, with the changes coming on one hand from small external stimuli on the celestial body, such as small variations in the rotation speed, gravity from other objects which varies across an elliptic orbit, tides and so on, and on the other hand, importantly, from the fluid itself, which changes its shape due to the combined effect of fluid dynamics and magnetism.

(4) In practice now, in order to get started, the first thing to be done is to include into the basic equations of fluid dynamics, which are the Euler equations, the Maxwell equations for electromagnetism, and then further build on this, on one hand with developing the math, and on the other hand with fine-tuning the Euler equations.

(5) But this can be done indeed, leading to some very interesting mathematics and physics, with the math being basically related to all sorts of fashionable mathematics you have ever heard of, from the 80s and onwards, and with the physics having all sorts of applications, to things ranging from celestial bodies to plasmas. In short, we are here into beautiful science, hot as we love it. For more on all this, we recommend the math book of Arnold-Khesin [7], and the physics book of Davidson [23].  $\square$

## 6d. Radiation and waves

Things have been quite crowded in this chapter, but we still have to discuss radiation and waves. This is a very important topic, making the link with a flurry of real-life things,

such as light, coming in all colors and flavors, radio waves, infrared, microwaves, and then scary things like X-rays and  $\gamma$ -rays, not to forget nuclear fallout.

We will be quite brief here, with a modest introduction to the subject, and defer the rest of the discussion to the end of chapter 8 below, when discussing radiation of black bodies, following Max Planck, right before getting into quantum mechanics. As usual, for more, you can check any physics book, such as Feynman [34] or Griffiths [42].

So, what is a wave? We certainly all know that, just go the beach, watch the ocean, and these are your waves. However, watching the ocean reveals too the fact that the math of the waves is probably terribly complicated. How do these waves exactly merge, when they meet? That's a collision, sure, but what are the exact equations? Also, what about monster waves reported by fishermen, on a calm water, can small waves really add up to such beasts? Or are rather terrifying sea monsters responsible for them?

Let us start with some math. We have here the following result:

THEOREM 6.32. *The wave equation is*

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

where  $\Delta$  is as usual the Laplace operator.

PROOF. There are several proofs here, a nice one, by discretizing, being as follows:

(1) Let us first consider the 1D case. In order to understand the propagation of waves, we will model  $\mathbb{R}$  as a network of balls, with springs between them, as follows:

$$\cdots \times \times \times \bullet \times \times \times \bullet \times \times \times \bullet \times \times \times \bullet \times \times \times \bullet \times \times \times \cdots$$

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

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

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  $N \gg 0$  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  $k$ :

$$m = \frac{M}{N} \quad , \quad k = KN \quad , \quad l = \frac{L}{N}$$

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

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

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:

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

(3) In arbitrary  $N$  dimensions now, the same argument carries on, and we are led to the following equation, with  $v = \sqrt{K/M} \cdot L$  being the propagation speed:

$$\ddot{\varphi}(x) = v^2 \sum_i \frac{d^2\varphi}{dx_i^2}(x)$$

But we recognize at right the Laplace operator, and we are done. There is of course some more discussion to be made here, arguing that our spring model in (1) is indeed the correct one, for modeling such wave propagation questions. But hey, we're doing theoretical physics here. And don't worry, experiments confirm our findings.  $\square$

With this done, let us go back to electromagnetism. The point here is that we have:

**THEOREM 6.33.** *In regions of space where there is no charge or current, both the electric field  $E$  and the magnetic field  $B$  are subject to the wave equation*

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

*with  $c$  being as usual the speed of light.*

**PROOF.** Under the circumstances in the statement, namely no charge or current present, the Maxwell equations simply read, taking into account  $\mu_0 \epsilon_0 = 1/c^2$ :

$$\langle \nabla, E \rangle = \langle \nabla, B \rangle = 0$$

$$\nabla \times E = -\dot{B}$$

$$\nabla \times B = \dot{E}/c^2$$

By applying the curl operator to the last two equations, we obtain:

$$\nabla \times (\nabla \times E) = -\nabla \times \dot{B} = -(\nabla \times B)' = -\ddot{E}/c^2$$

$$\nabla \times (\nabla \times B) = \nabla \times \dot{E}/c^2 = (\nabla \times E)'/c^2 = -\ddot{B}/c^2$$

But the double curl operator is subject to the following formula:

$$\nabla \times (\nabla \times \varphi) = \nabla < \nabla, \varphi > - \Delta \varphi$$

Now by using the first two equations, we are led to the conclusion in the statement.  $\square$

The above result opens a whole new perspective on electromagnetism, with the possibility of 3D electromagnetic waves travelling at the speed of light  $c$  appearing. We will discuss this later on, more in detail, in chapter 8 below, in connection with the work of Max Planck too, but in order now to finish our discussion here, let us just mention that such electromagnetic waves exist indeed, and are very familiar objects, as follows:

Frequency	Wave type	Wavelength
	—	
$10^{21}$	$\gamma$ rays	$10^{-12}$
$10^{18}$	X — rays	$10^{-9}$
$10^{16}$	UV	$10^{-7}$
	—	
$10^{15}$	blue	$10^{-6}$
$10^{15}$	yellow	$10^{-6}$
$10^{15}$	red	$10^{-6}$
	—	
$10^{14}$	IR	$10^{-5}$
$10^{10}$	microwave	$10^{-1}$
$10^6$	AM	$10^3$

This looks very interesting, and more on this later, in chapter 8 below.

### 6e. Exercises

Things have been crowded in this chapter, and as unique exercise, we have:

EXERCISE 6.34. *Read a book on electromagnetism, of your choice.*

As usual, we recommend Feynman [34] or Griffiths [42], both amazing books.



## CHAPTER 7

### Thermodynamics

#### 7a. Principles and demons

We have been dealing so far with “clean” physics, clear forces acting on clear objects, given by exact formulae, or at least by exact equations. Of course, we have met a few dirty phenomena too, such as friction and drag in the context of gravity, or resistors opposed to flow, and even heating, in the context of electricity. But we have usually waived such phenomena with equations of the following type, with  $\lambda \in (0, 1)$  being a constant:

$$F_{real} = \lambda F_{abstract}$$

Time to get now into dirty, real-life physics, in connection with nature surrounding us. Obviously what happens around us is not the effect of a single force, or of a handful of such forces. At work are millions and millions of tiny little forces, acting between the various small particles that we are made of, and what makes things rolling is the resulting “force”, which appears as an average of these tiny little forces, over time  $t > 0$ :

$$F_{real} = \int_{time} \int_{space} F_{tiny}$$

As a first comment, such kind of average is obviously not a force in the usual sense. It is rather “something”, corresponding to a transformation of a complex system, over a perceptible period of time  $t > 0$ . So, as a conclusion, we will have to abandon our beloved concept of force, and look for more realistic physical quantities to deal with.

A first such quantity, that you are very familiar with, is temperature. But, are you really that familiar with it. Here is my question, in all honesty, from me to you:

QUESTION 7.1. *What is temperature?*

You would answer well, temperature is what comes out when reading a thermometer. This is certainly a good idea, so let’s go for it, and understand how a thermometer works. That thermometer is made of colored alcohol in a glass bulb, and when you move it to a warmer room, the environment manages to interact with the alcohol, despite the glass in between, and dilates that alcohol, leading to a higher reading on the scale.

The same goes of course in the other sense, with a colder room leading to a contraction of that same alcohol, and a lower reading on the scale. Thus, what we have here is a reliable scientific device, measuring temperature based on the exchange of heat.

By going now a bit abstract, alcohol is not really needed in all this, and the same thermometer can function as well with mercury, or more generally with any liquid, or even gas, and even solid, of your choice. Needless to say, nor is the glass bulb really needed. And finally, the scale is not needed either, we just need a volume measuring device, for recording the dilation or contraction of our material.

Summarizing, we have now an answer to our question, or at least some sort of engineering method, building on your previous answer, as follows:

*METHOD 7.2. Temperature measures the heat present in the environnement, and can be computed by exposing various materials, which can be solids, liquids or gases, to the environnement, and measuring their volume, based on the following facts:*

- (1) *Heat dilates the material, and cold contracts the material.*
- (2) *Heat flows from warm to cold, aiming at equalizing temperature.*
- (3) *That heat flow needs some perceptible time  $t > 0$ , to fully happen.*
- (4) *Temperature can be regulated, as to be independent of the material used.*

All this looks quite reasonable, save perhaps for (1) which certainly does not apply to things like freezing water, then for the flow direction in (2), which is opposite to the direction where the wind goes, but this will be the least of our concerns, for the moment, and then for the mysterious time  $t > 0$  needed in (3), and finally for some engineering concerns in relation with (4) which again, will be the least of our concerns.

This being said, the above does not really solve our question, because we still need to know what exactly is heat. Or, to put it squarely, we still need to know what exactly is temperature, which measures that heat. So, getting to experiments now, we have:

*FACT 7.3. Increases in overall heat, and so in temperature, are produced by:*

- (1) *Friction or drag, acting on a moving object.*
- (2) *Letting electricity fight with a resistor, via the Joule law.*
- (3) *Lighting gas, or doing other chemical reactions which release heat.*
- (4) *Microbes and viruses in your body, producing illness and fever.*

Here (1,2) are something that we already know, from previous chapters, while (3,4), taking us into chemistry and biology, which means chemistry for short, are new.

So, what to do. Obviously we are in an impasse here, and we need some kind of model for our problem, in order to be able to intelligibly answer Question 7.1.

Fortunately, there is an answer here, coming from gases. So gases are materials that we have been boycotting so far, when doing mechanics and electrodynamics, due to their ability to slip around various forces proposed to them. But in our context, heat and temperature, these are in fact the simplest materials, and in any case, far simpler than liquids or solids. To be more precise, based on our usual life knowledge, we have:

**GUESS 7.4.** *The pressure, volume and temperature of a given amount of gas should be related, at least approximately, by a formula of type*

$$PV \sim T$$

*with the proportionality constant related to the nature of the gas, the precise amount of gas, and also the shape of that amount of gas.*

This is surely something intuitive, coming from the fact that heating the gas in a given volume increases the pressure, that compressing the gas at constant temperature increases the pressure too, and so on. What is really amazing is that, upon measuring, all these changing quantities vary linearly with each other, and we have indeed:

**FACT 7.5.** *The formula guessed above holds indeed, under the circumstances there,*

$$PV \sim T$$

*with  $P$  being measured by usual means, and with  $T$  being measured by Method 7.2.*

To be more precise here, in order to measure the pressure  $P$ , we can put the gas in a container with a piston, and measure the pressure exerted by the gas on that piston:

$$\begin{array}{ccccccc} & = & = & = & = & = & = \\ || & \circ & \circ & \circ & | & & \\ || & \circ & \circ & \circ & | & \rightarrow & P \\ || & \circ & \circ & \circ & | & & \\ & = & = & = & = & = & = \end{array}$$

This is already quite nice, and as an answer now to Question 7.1, we can formulate:

**ANSWER 7.6.** *The temperature of gases is given by the following formula, adjusted for different gases by constants found by using Method 7.2,*

$$T \sim PV$$

*and the temperature of various liquids and solids can be afterwards computed too, based on these gas standards, again by using Method 7.2.*

So far so good, but there is still a bit of mystery in all this. What is the pressure  $P$  on that piston due to? Or, more simply put, what is the reason for gas pressure? And also, importantly, why the phenomena (1,2,3,4) in Method 7.2 hold indeed for gases?

Obviously, we are here into some kind of mechanics, with all the above questions requiring, more specifically, some basic understanding of the mechanics of gases. And here, fortunately, a look through a good microscope reveals:

*FACT 7.7. Gases are formed of free molecules, moving around with certain speeds, and colliding from time to time. This movement produces the pressure  $P$  of the gas, say as mechanical force on a measuring piston, and so the temperature  $T$  too, via:*

$$T \sim PV$$

*Moreover, both the pressure  $P$  and the temperature  $T$  are proportional to the average molecular speed  $v$ , and so temperature can be defined equivalently as*

$$T \sim v$$

*with of course all these formulae being approximate, and subject to certain rescaling factors, coming from the nature, amount and shape of the gas.*

This certainly looks simple, good and quite final, so time now to put everything together, and nicely answer Question 7.1. By putting together our findings from Method 7.2, Answer 7.6 and Fact 7.7, and then making a bit of cleanup, first by forgetting about liquids and solids, to be discussed later, and also by forgetting the formula  $T \sim PV$ , which is certainly lower technology than  $T \sim v$ , we are led to the following answer:

*ANSWER 7.8. Temperature  $T$  of a gas is its average molecular speed  $v$ , up to a scaling factor, which corresponds to the amount of heat present in the gas. Moreover:*

- (1) Heat dilates the gas, and cold contracts it.*
- (2) Heat flows from warm to cold, aiming at equalizing temperature.*
- (3) That heat flow needs some perceptible time  $t > 0$ , to fully happen.*
- (4) Temperature can be regulated, as to be independent of the gas used.*

Armed with this answer, let us get now into the underlying math and physics, trying to understand how  $v$  and  $T$  exactly work, for gases as above. We are particularly interested in knowing more about (2,3) above, which look quite mysterious, so as a first piece of work, let us separate these two items from the rest, by formulating:

*PRINCIPLE 7.9. Heats flows from warm to cold, aiming at equalizing temperature, and with the flow needing some perceptible time  $t > 0$ , in order to fully happen.*

Note in passing that, in view of Method 7.2 above, which was a correct statement too, but not fully satisfactory as answer to Question 7.1, this principle holds for liquids and solids as well. Thus, we have here a general principle of thermodynamics, that we have to understand, first for the gases, and then for other materials like liquids or solids.

Generally speaking, Principle 7.9 is something quite intuitive for gases. Imagine indeed a box containing two gases, or two samples of the same gas, with a separation between

them, with the gas on the left being hotter than the gas on the right:



Obviously the pressure is higher on the left, so when removing the separation, there will be a warm wind from left to right, in agreement with Principle 7.9. And also, this warm wind will take some time  $t > 0$  to happen, because each fast particle  $\oplus$  is just a free particle, not knowing about the separation, and the other gas, consisting of slower moving particles  $\ominus$ , and it will take this particle  $\oplus$  some time, in order to discover all this, and perhaps decide to join the warm wind. As predicted, again, by Principle 7.9.

So far so good, we have a beginning of theory here. This being said, there is still a bit of a bug with Principle 7.9, because that is something of statistical nature. Imagine for instance that our two gases in a box, as above, consist of one molecule each:



In this case, what Principle 7.9 says will obviously not work, and who really knows that will happen. And there is even worse, along these lines, as follows:

FACT 7.10 (Maxwell demon). *There might be a demon  $\star$  out there, who one day will start playing with our nice, uniformly arranged gases*



*by staying somewhere in the middle, and sorting out fast and slow molecules, as to rearrange everything into a hot gas and a cold gas, as follows,*



*thereby violating Principle 7.9, and pushing our whole universe on a path of destruction.*

As a first observation, the Maxwell demon exists indeed, because for a gas made of 2 molecules there are 50% chances for things to evolve exactly as the demon wants, and this even without the demon having to move a single finger:



As for the remaining 50%, these are obviously not any good either. What can happen here is either the demon to intervene, making things as above, or the demon not to intervene, in which case the gas will be separated again into hot and cold, as follows, not exactly in the sense desired by the demon, but still violating Principle 7.9:



Welcome to probability. In real life such things never happen, because gases are made of tons of molecules, say 1 billion for having a figure, and the probability for things to happen like the demon wants, with the fate of each single molecule sealed, is:

$$P = \frac{1}{2^{1,000,000,000}} = 0$$

This being said, let us record however, as a complement to Principle 7.9, coming from this discussion, and for the sake of correct science, the following:

WARNING 7.11 (Demon's advice). *Principle 7.9 is something of statistical nature, but shall we really trust statistics.*

Of course, we are a bit into personal things here, and you might agree with all this or not. What if things happening with probability 0 will indeed happen? But wait, isn't everything that happens, happening with probability 0? And so on.

Usually the solution to such things, and in particular to the possible existence of the Maxwell demon, is to have a good meal, or some drinks, or go to a party, lift some weights, cut some wood, and so on. Sometimes science can be quite abstract, temporarily taking you away from reality, but it does not take much to get back to real life, and realize, time and again, that this world was certainly not built with bad intentions.

Excuse me for interrupting, but cat is here, meowing for something, so let's ask him too, what he thinks about all this. And cat says:

FACT 7.12 (Cat's take). *I ate the Maxwell demon.*

Wow, that's quite something. It surely arranges our physics, and surely sounds plausible too. Knowing the fate of small birds and other mice, when meeting cat when in shape, I can hardly imagine how a small demon like Maxwell's could have escaped from his claws. So no more demon, and we will now develop our physics with optimism.

So, getting back now to serious physics, our theory above starts taking shape, but there are still a number of mysteries in regards with temperature, as follows:

QUESTIONS 7.13. *Regarding the temperature  $T$ , as defined above, besides fixing all the theory, with details, constants, and correction terms where needed:*

- (1) *Is  $T$  quantized?*
- (2) *Is  $T$  bounded from above?*
- (3) *Is  $T$  bounded from below?*
- (4) *Does measuring  $T$  affect  $T$ ?*

These are all difficult questions, that we will discuss later on, once the basic theory of  $T$  clarified. To be more precise, anticipating a bit, the situation is as follows:

(1) Things like this were a bit of a joke in the context of gravity and electromagnetism, at least at the beginner level, but the interesting thing is that, in the context of thermodynamics, passed the basics, the next interesting problem to be solved is that of determining the radiation of a black body. And here, surprise, not only we will reach to the conclusion that  $T$  is quantized, but also that any theory with  $T$  non-quantized spectacularly fails. We will discuss this at the end of chapter 8, following Max Planck and others.

(2) This is a bit of a philosophical question, because at the  $T \gg 0$  end things are no longer solid, liquid or gaseous, but rather plasma, or worse, and it takes some skill in order to talk about the temperature of such things, and to measure it. We will talk a bit about this, the idea being that there should be indeed an upper bound.

(3) This is, quite surprisingly, the easiest question in the list, as opposed to the difficulties of bounding other things like time  $t \in \mathbb{R}$  or distance  $d > 0$  from below. We will see that, with suitable conventions, we have  $T > 0$ , as a theorem.

(4) This is another philosophical question, coming by looking carefully at Method 7.2, and also at the method used for measuring the pressure  $P$ , and so on. We will not investigate it here, obviously such things being way too philosophic, but keep however this observation in mind for later, when doing quantum mechanics.

## 7b. Energy and heat, Joule

Things have been a bit messy so far, and fixing all this mess will take us the full remainder of this chapter, and next chapter too. We will do this in two parts:

(1) In the present chapter we will discuss thermodynamics, based on Principle 7.9, and on the handful of other things that we know about temperature and heat. The discussion here will be a bit low-tech of course, but truly lovely. Among others, we will get familiar with the geometry of the parameters  $(P, V, T)$  for gases, which is one good thing to know, which will tend to disappear afterwards, killed by probability computations.

(2) And then in the next chapter we will go for heavier theory, involving collisions and their math, known as statistical mechanics, with a full explanation for pressure, temperature and everything. But, again, with the remark that this is actually not everything, but just the advanced side of things, one goal of the advanced probability theory in the area being precisely that of recovering the geometry in (1), initially lost.

Getting started now, we already know a bit about temperature and heat, but time now to take things seriously, and formulate some precise definitions. As usual when starting a new physical theory, as it was already the case with classical mechanics and electromagnetism, we must approximate a bit what we know, take some things for granted, and be modest in general. So, let us start with something modest, as follows:

DEFINITION 7.14. *We are interested in gases, described by their equation of state*

$$f(P, V, T) = 0$$

*relating their pressure  $P$ , volume  $V$  and temperature  $T$ .*

Here the parameters  $P, V, T$  should be taken in an intuitive sense, at least to start with. The pressure  $P > 0$  is measured by using a cylinder with a piston, as explained in the previous section. The volume  $V > 0$  is the usual 3D volume, and with the remark here that our theory, as formulated above, neglects the precise shape of this volume. As for the temperature  $T \in \mathbb{R}$ , this is measured by using a thermometer, as explained in Method 7.2, with this thermometer being for the moment arbitrarily calibrated, meaning that  $T$  is well-determined up to  $T \rightarrow aT + b$ , but that we chose some  $a, b \in \mathbb{R}$ , as to be able to talk about  $T \in \mathbb{R}$ , and write our equation of state  $f(P, V, T) = 0$ .

Regarding the equation of state  $f(P, V, T) = 0$  itself, we already know that  $PV = kT$  with  $k \in \mathbb{R}$  is something quite reasonable, to start with, but we will not make this assumption. First because our thermometer is for the moment arbitrarily calibrated, but then also because we will need later, when talking corrections to it, some of the general theory to be developed right next. Let us record however, for future reference:

DEFINITION 7.15. *An ideal gas is described by the equation of state*

$$PV = kT$$

*or rather  $PV = k(T + e)$ , our thermometer being so far arbitrarily calibrated.*

This is, of course, something quite theoretical, and we will be using such gases in what follows, for illustrations for our computations. Later on, after calibrating our thermometer, we will back to them, explaining who these ideal gases are, and what their constants  $k$  are, with numerics and everything. And we will talk about corrections too.

So, getting back now to Definition 7.14, our equation of state  $f(P, V, T) = 0$  there is for the moment assumed to be arbitrary. Geometrically, this means that we are on a certain surface in  $\mathbb{R}^3$ , defined by the equation  $f(P, V, T) = 0$ , with the parameters  $P, V, T$  being of course the coordinates. We will also tacitly assume that the equation of state  $f(P, V, T) = 0$  is something non-degenerate, say appearing as a perturbation of  $PV = kT$ , allowing us to recover any of the parameters  $P, V, T$ , once two of them are given.

As an important observation, note the radical change with respect to mechanics, where the 3D coordinates  $x, y, z$  used to refer to the ambient space. Gone all that, the 3D space from now on will be for us that of all possible  $(P, V, T)$  points, with  $P, V, T \in \mathbb{R}$ , and with of course the regions  $P < 0$  and  $V < 0$  being excluded by obvious reasons.



As a first piece of math now, let us take a look at  $P$ , measured with a piston:

$$\begin{array}{ccccccc} = & = & = & = & = & = & \\ || & \circ & \circ & \circ & | & & \\ || & \circ & \circ & \circ & | & \rightarrow P & \\ || & \circ & \circ & \circ & | & & \\ = & = & = & = & = & = & \end{array}$$

When performing this measurement, the gas does some mechanical work  $W$ . In order to compute  $W$ , observe that, infinitesimally, if we denote by  $dl$  the distance traveled by the piston in time  $dt$ , we have the following formula,  $S$  being the area of the piston:

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

Now assuming that the piston has traveled from  $a$  to  $b$ , we obtain:

$$W = \int_a^b PdV$$

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

**THEOREM 7.16.** *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 above 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, and with again the case of the cylinder with a piston being a good illustration,  $\varphi$  being there linear.  $\square$

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

**DEFINITION 7.17.** *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 [32], 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 7.16, for an ideal gas, we have the following result:

PROPOSITION 7.18. *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 7.16, in either formulation:

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

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

(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:

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

(3) Finally, there is a discussion to be made too in connection with the calibration of the thermometer. As explained in Definition 7.15, in the lack of a precise calibration, the equation of state of ideal gases is rather  $PV = k(T + e)$ , with  $k, e \in \mathbb{R}$ . But this leads to exactly the same final answer, with  $T$  being now replaced by  $T + e$ .  $\square$

We know from classical mechanics that work is intimately related to energy. So, let us discuss now energy, in the context of thermodynamics. In analogy with what happens in classical mechanics, we will have two guiding principles, as follows:

PRINCIPLES 7.19. *In the context of thermodynamics:*

- (1) *Energy  $E$  comes in two flavors, namely work  $W$  and heat  $Q$ .*
- (2) *We will talk about variations  $\Delta E$  of the energy, instead of  $E$  itself.*

To be more precise, here (1) is in analogy with what we know from classical mechanics, where energy  $E$  comes in two flavors too, namely kinetic energy  $T$  and potential energy  $V$ , and with our excuses here for the conflicting  $T, V$  notations, but the alphabet is not long enough for all our physics in this book. As for (2), this is again in analogy with classical mechanics, where the potential energy  $V$  is defined only up to an additive constant, which makes  $E = T + V$  itself be to defined only up to an additive constant too.

In what regards now the physics of  $Q$ , this is heat as we know it, related to the temperature  $T$ . To be more precise here, its main properties are as follows:

**PRINCIPLE 7.20.** *The amount of heat  $Q$  received during a transformation is a thermodynamical quantity, in relation with temperature, and which normally depends on the chosen path in the state space. However, we usually have*

$$Q = C\Delta T$$

*with  $C > 0$  being a constant, called heat capacity of the material, independently on the chosen path in the state space, between the initial and the final point.*

With the above principles in hand, we can now talk about energy, or rather about energy variation, and formulate the first law of thermodynamics, as follows:

**LAW 7.21** (First law of thermodynamics). *During a transformation of a gas, along a path in the state space  $f(P, V, T) = 0$ , we have the formula*

$$\Delta E = Q - W$$

*where  $Q$  is the amount of heat received, and  $W$  is the work performed, with  $\Delta E$  not depending on the precise path chosen between the initial and the final point.*

This first law of thermodynamics, which will replace in what follows Principles 7.19 and Principle 7.20, for most of our practical purposes, might seem a bit head-scratching. You would say that this is just the definition of  $\Delta E$ , or if you want the definition of  $E$  up to a constant. But, more is true. The whole point lies in the last words, stating that  $\Delta E$  is independent of precise path chosen between the initial and the final point.

So, to reformulate. The first law of thermodynamics states two things:

(1) First we have a true law of physics, which is something non-trivial, stating that, while both the quantities  $Q$  and  $W$  generally depend on the chosen path in the state space, between the initial and the final point, their difference  $Q - W$  does not.

(2) And then we have a definition based on this, namely  $\Delta E = Q - W$ , which tells us that the independence of  $Q - W$  on the chosen path comes in fact from the existence of an internal energy function  $E$  of the system, well-defined up to a scalar.

But perhaps most illustrating for all this are some simple examples, as follows:

**PROPOSITION 7.22.** *The following happen:*

- (1) *For a cyclic transformation we have  $Q = W$ , regardless of the chosen path in the state space, between the initial and the final point.*
- (2) *Assuming that the heat received is subject to  $Q = C\Delta T$ , with  $C > 0$ , for a thermally insulated system we have  $\Delta E = -W$ .*

PROOF. Both these assertions are clear from definitions, as follows:

- (1) For a cyclic transformation we have  $\Delta E = 0$ , and so  $Q = W$ , as claimed.
- (2) Our combined assumptions mean  $Q = C\Delta T = 0$ , so  $\Delta E = -W$ , as claimed.  $\square$

Finally, the first law of thermodynamics invites us to introduce, as a complement to the various elementary notions from Definition 7.17:

DEFINITION 7.23. *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 in Proposition 7.22 (2), namely those of the thermally insulated systems obeying to  $Q = C\Delta T$ , with  $C > 0$ . More on adiabatic transformations later, but in any case, not to mess them up with isobaric, isochoric or isothermal transformations.

Let us do now some math, based on all this. We have here the following result:

THEOREM 7.24. *We have the following heat equations,*

$$\begin{aligned} dQ &= \left(\frac{dE}{dP}\right)_V dP + \left[\left(\frac{dE}{dV}\right)_P + P\right] dV \\ dQ &= \left[\left(\frac{dE}{dP}\right)_T + P\left(\frac{dV}{dP}\right)_T\right] dP + \left(\frac{dH}{dT}\right)_P dT \\ dQ &= \left[\left(\frac{dE}{dV}\right)_T + P\right] dV + \left(\frac{dE}{dT}\right)_V dT \end{aligned}$$

where  $H = E + PV$ , called *enthalpy of the system*.

PROOF. This follows indeed by doing some computations, as follows:

- (1) We first have the following formulae, coming from definitions:

$$\begin{aligned} dE(P, V) &= \left(\frac{dE}{dP}\right)_V dP + \left(\frac{dE}{dV}\right)_P dV \\ dE(P, T) &= \left(\frac{dE}{dP}\right)_T dP + \left(\frac{dE}{dT}\right)_P dT \\ dE(V, T) &= \left(\frac{dE}{dV}\right)_T dV + \left(\frac{dE}{dT}\right)_V dT \end{aligned}$$

- (2) In order to advance, we use the work formula in Theorem 7.16, rewritten as:

$$dW = PdV$$

By plugging into formula into the first law, the first law becomes:

$$dQ = dE + dW = dE + PdV$$

(3) Now by using this latter formula, the equations found in (1) become:

$$dQ = \left(\frac{dE}{dP}\right)_V dP + \left[\left(\frac{dE}{dV}\right)_P + P\right] dV$$

$$dQ = \left(\frac{dE}{dP}\right)_T dP + \left(\frac{dE}{dT}\right)_P dT + PdV$$

$$dQ = \left[\left(\frac{dE}{dV}\right)_T + P\right] dV + \left(\frac{dE}{dT}\right)_V dT$$

(4) In what regards the first and third equations, these are those in the statement. In what regards the second equation, we can work a bit more on it, and make it look better. Indeed, we can use here the following formula, coming from definitions:

$$dV = \left(\frac{dV}{dP}\right)_T dP + \left(\frac{dV}{dT}\right)_P dT$$

With this formula in hand, the second equation can be rewritten as:

$$dQ = \left[\left(\frac{dE}{dP}\right)_T + P\left(\frac{dV}{dP}\right)_T\right] dP + \left(\frac{d(E + PV)}{dT}\right)_P dT$$

(5) Still in regards with this second equation, with the aim of making it even better, let us introduce a new state function of the system, called enthalpy, as follows:

$$H = E + PV$$

In terms of this function, the second equation as modified in (4) becomes:

$$dQ = \left[\left(\frac{dE}{dP}\right)_T + P\left(\frac{dV}{dP}\right)_T\right] dP + \left(\frac{dH}{dT}\right)_P dT$$

Thus, we have as well the second equation in the statement, and we are done. □

As an immediate consequence of the above result, we have:

PROPOSITION 7.25. *The heat capacities at constant V and P are*

$$C_V = \left(\frac{dE}{dT}\right)_V$$

$$C_P = \left(\frac{dE}{dT}\right)_P$$

*with the derivatives being taken as usual, as above.*

PROOF. This follows indeed from the formulae in Theorem 7.24. □

Before going ahead, let us comment on the enthalpy function  $H = E + PV$  appearing in Theorem 7.24. We came upon this function via some math, but we have:

COMMENT 7.26. *The enthalpy function of a system, given by*

$$H = E + PV$$

*is what's needed for creating the system out of nothing, and putting it into environment.*

To be more precise, assume that you are a magician, and want to create a rabbit. You first need energy  $E$  for creating the rabbit. But then you also need energy for putting it into environment, with this meaning pushing out the atmosphere, for creating space for the rabbit. And assuming that we are at 1 atm, this extra energy needed is  $PV$ .

Due to this, enthalpy is an important quantity in chemistry computations, and this even for simple reactions like  $2\text{H}_2 + \text{O}_2 = 2\text{H}_2\text{O}$ , because the basic quantum chemistry formulae for them, involving electrons and so on, do not take into account the energy needed for putting the output into environment, and must be therefore fine-tuned.

For more on all this, including a picture of the magician and rabbit, we refer to the lovely book of Schroeder [79]. By the way, speaking books, an excellent reference for thermodynamics is the small red book by Fermi [32], which not only is enjoyable now, 100 years after, but often beats in elegance most of everything else. There are also several good books starting with a bit of thermodynamics and then going ahead with statistical mechanics, such as the classical book of Huang [49]. At the graduate level, well-known books include those by Kadanoff [56] and Pathria and Beale [69]. And of course, you can go as well with your favorite authors, such as Feynman [33], or Shankar [85].

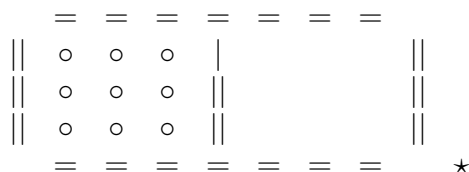
Back to work now, let us try to understand what the theory that we have so far says for the ideal gases. And here, we first have the following important finding:

FACT 7.27 (Joule). *For an ideal gas we have the formula*

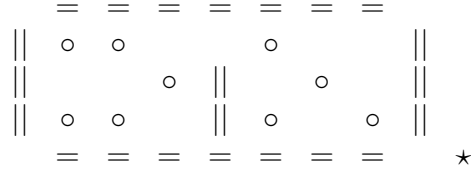
$$E = E(T)$$

*meaning that the total energy depends only on the temperature.*

Joule came upon this via a simple experiment, namely an adiabatic expansion of a gas. His experiment used a double gas chamber with a separation, as follows, with the left side being initially filled with gas, and with the right side being empty:



Everything was taking place inside a calorimeter, which is a device preventing heat from entering or escaping. The calorimeter was containing as well a thermometer  $\star$ . Joule opened the separation, and the gas distended, occupying the whole double chamber:



What Joule noticed is that the thermometer reading did not change much,  $\Delta T \simeq 0$ . And his conclusion came from here, the reasoning being as follows:

- (1) With an ideal gas,  $\Delta T \simeq 0$  could only have meant  $\Delta T = 0$ .
- (2) Due to the calorimeter, the transformation was adiabatic,  $Q = 0$ .
- (3) Equivalently,  $\Delta E = -W$ . But  $W = 0$ , clearly, and so  $\Delta E = 0$ .
- (4) Thus  $\Delta T = 0$  corresponds to  $\Delta E = 0$ , so we must have  $E = E(T)$ .

So, this was the story of the Joule finding. There is actually more to be said here, because Fact 7.27 eventually became a theorem, being possible to be proved by using the second law of thermodynamics, that we have not learned yet. More on this later.

As another comment, our  $E, T$  are defined so far up to a scalar, but this is not an issue for stating  $E = E(T)$ . For a discussion here we refer to our favorite books, Fermi [32] or Schroeder [79]. Now with Fact 7.27 in hand, we can go ahead, as follows:

**THEOREM 7.28.** *For an ideal gas,  $PV = kT$ , we have the equation*

$$C_V dT + PdV = dE$$

*called first law thermodynamics for ideal gases, in Joule formulation.*

**PROOF.** We know from Joule that the following quantity is constant:

$$C_V = \frac{dE}{dT}$$

By integrating, we obtain a formula as follows, with  $\lambda \in \mathbb{R}$  being a constant:

$$E = C_V T + \lambda$$

But with this in hand, the first law becomes the first formula in the statement.  $\square$

Next in line, we have the following key result:

**THEOREM 7.29.** *For an ideal gas,  $PV = kT$ , we have the equation*

$$C_P = C_V + k = \left( \frac{dE}{dT} \right)_P$$

*relating the molecular heats at constant pressure, and constant volume.*

PROOF. By using  $PV = kT$  and Theorem 7.28, we obtain:

$$\begin{aligned} PV = kT &\implies PdV + VdP = kdT \\ &\implies (C_V + k)dT - VdP = dE \end{aligned}$$

With  $dP = 0$ , we are led to the second formula in the statement.  $\square$

As a third important result now, regarding the ideal gases, we have:

THEOREM 7.30. *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. Since for an adiabatic transformation we have  $dE = 0$ , the Joule formula in Theorem 7.28 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 is very interesting, theoretically speaking, and the only thing that is still missing is a discussion about the ideal gases themselves, not necessarily thermodynamic. To be more precisely, given a certain gas  $G$ , that is to say, a chemical substance in gaseous form, we would like to know which number  $k > 0$  makes the ideal gas equation  $PV = kT$  best approximate the equation of state of  $G$  itself, and also to which extent is this approximation reliable, what about correction terms, and so on.

This is obviously more chemistry than physics, and we will talk about such things in the opening part of chapter 8 below, statistical mechanics, which despite what the name might suggest, mathematics or perhaps physics, will be something quite chemical.

In the meantime, just believe us, we are dealing here with usual, real-life gases, up to our silence on  $k > 0$ , and up to some  $\varepsilon \simeq 0$  in the final formulae. More on this later.



### 7c. Carnot, Otto, Diesel

We have seen so far that the first law of thermodynamics, coupled with some theory and findings for the ideal gases, already leads into some interesting math and physics, such as the adiabatics computed in Theorem 7.30. However, the story with theory is not over here. Remember that heat flowing from warm to cold, that we were discussing in the beginning of this chapter? That is something not to be forgotten:

**LAW 7.31** (Second law of thermodynamics). *Heat flows from warm to cold.*

As explained in the beginning of this chapter, this is a quite subtle statement, of statistical nature, which won't work for instance for gases having 2 molecules. As another comment, note that heat flows in Law 7.31 exactly in the opposite direction to that of the wind, which usually blows from cold to warm. But this latter phenomenon is easy to understand, because wind usually blows from higher pressure to lower pressure.

As an important remark now, Law 7.31 is just one of the possible formulations of the second law, and there are many more, with basically all the thermodynamics greats, including Clausius and Lord Kelvin, having made contributions to the matter. Let us just record here a well-known equivalent formulation, very instructive, as follows:

**ADVICE 7.32.** *Don't try to make money by cooling the land, and converting that heat into work, then electricity. This won't work, due to the second law.*

As usual, for more on all this, history, details and everything, we refer to our favorite thermodynamics books, namely Fermi [32], Huang [49] and Schroeder [79].

Getting back now to Law 7.31 as it is, as already said, this is something subtle, of statistical nature. Thus, we can expect some spectacular consequences of it, perhaps even going beyond our imagination. We will see that this is indeed the case.

Our workhorses for exploiting the second law will be the Carnot engines, which are somewhat mathematical objects, constructed as follows:

**DEFINITION 7.33.** *A Carnot engine is a 4-cycle engine, functioning between temperatures  $T_1 < T_2$ , consisting of:*

- (1) *An isothermal expansion at  $T_2$ , absorbing heat.*
- (2) *An adiabatic expansion, down to temperature  $T_1$ .*
- (3) *An isothermal compression at  $T_1$ , expelling heat.*
- (4) *An adiabatic compression, back to temperature  $T_2$ .*

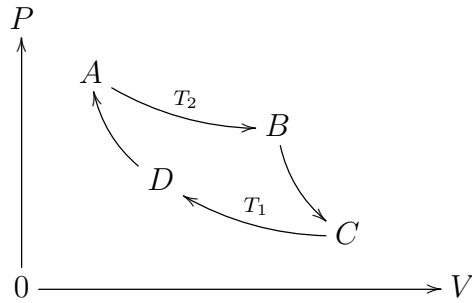
So, what kind of engine is this. In a nutshell, these are the best possible engines, and quite fascinating objects, no one really knowing to which area of science they belong. We will see that, from the perspective of physics, such things rather belong to mathematics.

From the perspective of a mathematician, such things look more as engineering. And from the perspective of an engineer, such things look more like theoretical physics.

In short, and by anticipating a bit, we have:

ADVERTISEMENT 7.34. *Carnot engines are creatures from the outer space, having a deep meaning, and bringing a certain order in the universe.*

In order to get familiar with such engines, let us discuss their functioning. We can represent a Carnot engine on a  $(P, V)$  diagram, as follows, with the horizontals  $AB, CD$  being the isothermals, and the verticals  $BC, DA$  being the adiabatics:



Regarding now the engineering, the Carnot engines can be implemented as 1-cylinder, 4-stroke engines, with the functioning of one full cycle being as follows:

	A	B	C	D	A'
$V_C$			$\perp$		
$V_B$		$\perp$			
$V_D$				$\perp$	
$V_A$	$\perp$				$\perp$
	$T_2$	$T_2$	$\equiv$	$T_1$	$\equiv$

To be more precise, pictured here is the height of the piston  $\perp$  at every step, with the lower data corresponding to the transformations made,  $T_1, T_2$  standing for the temperatures of the isothermals, and  $\equiv$  standing for an insulator, needed for the adiabatics.

Obviously, a Carnot engine is an engine as we know them, converting heat into work. To be more precise, an amount of heat  $Q_2$  is absorbed during the upper isotherm  $AB$ , and is transformed into an amount of work  $W$  during the lower isotherm  $CD$ , with an amount of heat  $Q_1$  expelled as well during this lower isotherm  $CD$ . And with the adiabatics being there for adjusting the machine, as to make it work as a cycle, in the  $[T_1, T_2]$  regime.

To summarize, what is going on here is a conversion of heat into work,  $Q_2 \rightarrow W$ , with a loss  $Q_1$ . Based on this, let us formulate the following definition:

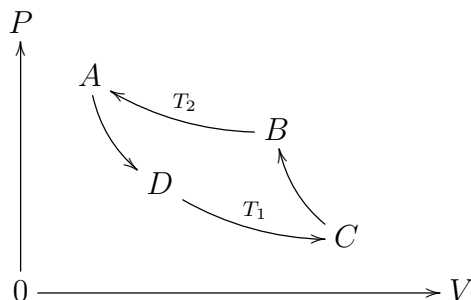
DEFINITION 7.35. *The efficiency of a Carnot engine functioning between temperatures  $T_1 < T_2$  is the quantity  $\eta \in (0, 1)$  given by*

$$\eta = \frac{W}{Q_2} = \frac{Q_2 - Q_1}{Q_2} = 1 - \frac{Q_1}{Q_2}$$

where  $Q_2$  is the heat absorbed at  $T_2$ , from the heat source of the engine,  $W$  is the work done, and  $Q_1$  is the loss in the process  $Q_2 \rightarrow W$ , appearing as heat expelled at  $T_1$ .

We will see in a moment that this Carnot engine efficiency cannot be beaten. But before that, let us make the following remark, of practical use:

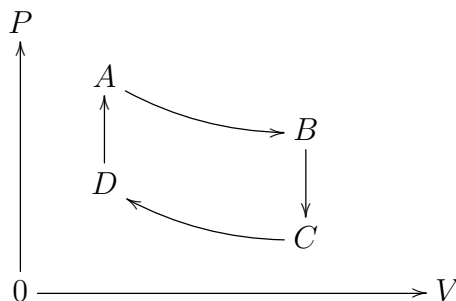
REMARK 7.36. *When running a Carnot engine in the other sense, namely*



what we have is a refrigerator, absorbing heat  $Q_1$  on the isotherm  $DC$ , helped by some input work  $W$ , and expelling it as heat  $Q_2$  during the isotherm  $BA$ .

Observe in passing that due to  $Q_2 > Q_1$ , using a refrigerator for cooling the room during the Summer, with the door wide open, is not a good idea. But are we here for talking about home appliances. Getting back to engines, the Carnot cycle is difficult to implement, due to various reasons, and for powering a car we have much better:

DEFINITION 7.37. *The Otto engine is the 4-stroke engine working as*

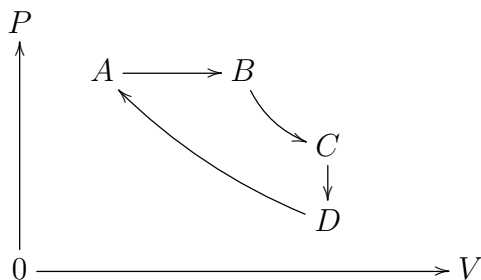


with isochores on the vertical, and adiabats on the horizontal.

To be more precise, during a cycle  $C \rightarrow D \rightarrow A \rightarrow B$  the gas gets compressed on  $CD$ , ignites on  $DA$ , moves the piston on  $AB$ , and gets exhausted on  $BC$ . This cycle was invented by Otto, shortly after Carnot, and is still used nowadays, for powering cars.

Yet another popular engine, invented by Diesel shortly after Otto, is the Diesel one. This makes a bit of a compromise between Carnot and Otto, being certainly less funny to drive than Otto, but a bit more efficient. The functioning is as follows:

DEFINITION 7.38. *The Diesel engine is the 4-stroke engine working as*



*consisting of an isobaric, an isochore, and two adiabatics.*

Here during a cycle  $D \rightarrow A \rightarrow B \rightarrow C$  the gas gets compressed on  $DA$ , heated on  $AB$ , ignites and moves the piston on  $BC$ , and gets cooled on  $CD$ . This cycle is very useful for powering heavy machinery like 20-ton trucks, or big ships of any size.

Getting back now to math, in view of these new engines, and of the many more that can be constructed, let us complement Definition 7.35 above with:

DEFINITION 7.39. *The efficiency of an arbitrary cyclic engine functioning between temperatures  $T_1 < T_2$  is the quantity  $\eta \in (0, 1)$  given by*

$$\eta = \frac{W}{Q_2} = \frac{Q_2 - Q_1}{Q_2} = 1 - \frac{Q_1}{Q_2}$$

*where  $Q_2$  is the heat absorbed at  $T_2$ , from the heat source of the engine,  $W$  is the work done, and  $Q_1$  is the loss in the process  $Q_2 \rightarrow W$ , appearing as heat expelled at  $T_1$ .*

Since we are a bit abstract here, we must comment on the fact that we have indeed  $W > 0$  and  $Q_2 > Q_1 > 0$ . First, we will take  $W > 0$  by definition, with the above word “engine” standing for that, that is, “useful engine”. So we are left with  $W = Q_2 - Q_1 > 0$ , and the problem is whether this really must come from  $Q_2 > Q_1 > 0$ .

This question might seem a bit futile, but it is not. The second law has certainly something to do with this, because that’s the only principle that we have, preventing heat from flowing from cold to warm, and producing weird things like  $Q_1 < 0$ , or  $Q_2 < 0$ . So, let us try now to clarify all this, as our first application of the second law.

In order to discuss this question, let us start with:

LAW 7.40 (Second law, Kelvin’s formulation). *It is impossible to extract heat from a source staying at constant temperature  $T$ , and convert it into work.*

This is something that we have already met, in an informal form, as Advice 7.32. Our claim now is that this Kelvin formulation is equivalent to Law 7.31, due to Clausius:

**PROPOSITION 7.41.** *The second law in Clausius' formulation, Law 7.31 above, is equivalent to the second law in Lord Kelvin's formulation, Law 7.40 above.*

**PROOF.** Following Fermi [32], we'll do this as mathematicians do, via double implication, and cherry on the cake, by reasoning via negation too:

" $\Rightarrow$ " Assume that Kelvin is wrong, so that we can extract heat from a body  $B$  at temperature  $T$ , and convert it into work  $W$ . Consider as well a body  $B'$ , lying nearby, at temperature  $T' < T$ . By friction we can convert  $W$  into heat, and then heat  $B'$  with this heat. Thus heat has flown from  $B$  to  $B'$ , so Clausius was wrong too.

" $\Leftarrow$ " Assume now that Clausius is wrong, so that heat  $Q_2$  can flow from a body  $B_1$  at temperature  $T_1$  to a body  $B_2$  of temperature  $T_2 > T_1$ . With the help of a Carnot engine installed on  $B_2$  and functioning in the  $[T_1, T_2]$  regime we can convert this heat  $Q_2$  into work  $W$ , and with the expelled heat  $Q_1$ , at temperature  $T_1 < T_2$ , not affecting  $B_2$ . Thus  $B_2$  has in fact nothing to do with the whole process, which ultimately consists in extracting heat from  $B_1$  and converting it into work  $W$ . So Kelvin was wrong too.  $\square$

Still following [32], we can now fix the bug in Definition 7.39, as follows:

**PROPOSITION 7.42.** *In the context of Definition 7.39, assuming that the engine there is a true, useful engine,  $W > 0$ , we have indeed  $Q_2 > Q_1 > 0$ .*

**PROOF.** Since  $W = Q_2 - Q_1 > 0$ , we just need to show  $Q_1 > 0$ . So, assume by contradiction  $Q_1 < 0$ , which in the context of Definition 7.39 means that our engine functioning in the  $[T_1, T_2]$  regime manages to absorb heat at the low temperature  $T_1$ . But then we can install an extra device, letting heat flow from status  $T_2$  to status  $T_1$ , during each cycle, exactly as for our machine at status  $T_1$  to absorb  $-Q_1 > 0$  heat. And what we have here, in the end, is a machine leaving things at  $T_1$  status unchanged, and making work  $W > 0$  out of the source at constant temperature  $T_2$ , contradicting Kelvin.  $\square$

Summarizing, everything fine with Definition 7.39, we know now what the efficiency of an engine is. So, let us compare now these engines. We have here:

**THEOREM 7.43.** *Among the engines functioning in a given  $[T_1, T_2]$  regime, the maximum efficiency*

$$\eta = 1 - \frac{Q_1}{Q_2}$$

*is achieved by the reversible engines, including the Carnot ones, and with all these reversible engines having the same efficiency.*

**PROOF.** This is something quite tricky. Following [32], the proof goes as follows:

(1) Our first claim is that is enough to prove the following inequality, for any two engines  $M, M'$ , with the first engine  $M$  being assumed to be reversible:

$$\frac{Q_1}{Q_2} \leq \frac{Q'_1}{Q'_2}$$

Indeed, this certainly proves the first assertion, regarding the maximum efficiency of  $M$ . It also proves the last assertion, because assuming that  $M'$  was reversible too, we can interchange  $M \leftrightarrow M'$ , and by double inequality we obtain equality of the above quotients, and so of efficiencies. Finally, the fact that the Carnot engines are reversible is something that we know well, thier inverses being refrigerators, as explained in Remark 7.36.

(2) Some math first. We want to prove that we have the following inequality:

$$\frac{Q_1}{Q'_1} \leq \frac{Q_2}{Q'_2}$$

So, assume that this is wrong, and pick a rational number in between:

$$\frac{Q_1}{Q'_1} > \frac{N'}{N} > \frac{Q_2}{Q'_2}$$

We must come up with a contradiction, out of these inequalities.

(3) In order to do so, we use a trick. Consider the engine  $\mathcal{M}$  consisting of  $N'$  cycles of  $M'$ , and  $N$  reverse cycles of  $M$ . The data for this new, complex engine  $\mathcal{M}$  is:

$$\mathcal{Q}_1 = N'Q'_1 - NQ_1$$

$$\mathcal{Q}_2 = N'Q'_2 - NQ_2$$

$$\mathcal{W} = N'W' - NW$$

We have then  $\mathcal{W} = \mathcal{Q}_2 - \mathcal{Q}_1$ . On the other hand, the inequalities in (2) read:

$$\mathcal{Q}_1 < 0 \quad , \quad \mathcal{Q}_2 > 0$$

Thus, the total work is positive,  $\mathcal{W} > 0$ , so we have here a true engine, in the sense of Proposition 7.42. But the point now is that, as explained in Proposition 7.42, this should imply  $\mathcal{Q}_2 > \mathcal{Q}_1 > 0$ . Thus, we have our contradiction, and we are done.  $\square$

### 7d. Absolute temperature

We are now ready for one of the most beautiful results in mathematics, physics and engineering combined. You have probably witnessed some episodes of cold, say  $-5^\circ \text{C}$  or  $-10^\circ \text{C}$ , why not  $-20^\circ \text{C}$ , or even  $-30^\circ \text{C}$ , depending on where you live, where you have travelled to, and so on. Things can be sometimes freezing cold, but, in all honesty, in such a situation, have you ever said to yourself “things cannot be colder than that”?

I bet not. I'm sure your thought was something of type "hope tomorrow will be not  $-10^\circ$  colder than today". We are just so used, intuitively, for temperature to be like so many other quantities, like space and time, unbounded from above and from below.

So here comes our point. Not only temperature is bounded from below,  $T > 0$ , after a rescaling, which is something itself quite crazy, as a fact. But you can prove this just armed with your brain, with no need for any weird experiments and scientific machinery. And in addition, the proof is something truly amazing, mixing all the bizarre mathematics, physics and engineering that we have been doing so far, in this chapter.

But perhaps enough advertisement. Here is the result, and its proof:

**THEOREM 7.44.** *The temperature as measured before, with an arbitrarily calibrated thermometer, can be linearly rescaled into an absolute temperature, which is positive,*

$$T > 0$$

*and is given by the following equation, valid for any  $T_1 < T_2$ ,*

$$\frac{T_1}{T_2} = 1 - \eta$$

*where  $\eta$  is the efficiency of a reversible engine operating in the regime  $[T_1, T_2]$ .*

**PROOF.** This follows indeed from the theory developed above, with the idea being as follows, and the whole proof being explained for instance in Fermi's book [32]:

(1) We know from Theorem 7.43 that the efficiency of a reversible engine operating in the regime  $[T_1, T_2]$  is a number  $\eta = \eta(T_1, T_2)$  as follows, depending only  $T_1, T_2$ :

$$\eta(T_1, T_2) = 1 - \frac{Q_1}{Q_2}$$

(2) Consider the following function, defined for any temperatures  $T_1 < T_2$ :

$$f(T_1, T_2) = \frac{1}{1 - \eta(T_1, T_2)} = \frac{Q_2}{Q_1}$$

By combining engines with refrigerators, as in the proof of Theorem 7.43, we conclude that we have the following formula, valid for any temperatures  $T_0 < T_1 < T_2$ :

$$f(T_0, T_2) = f(T_0, T_1)f(T_1, T_2)$$

But this tells us that we can find a certain function  $\theta = \theta(T)$  such that:

$$f(T_1, T_2) = \frac{\theta(T_2)}{\theta(T_1)}$$

Moreover, this function  $\theta = \theta(T)$  must be strictly positive, and increasing.

(3) Getting back now to efficiencies, we have the following formula:

$$\eta(T_1, T_2) = 1 - \frac{1}{f(T_1, T_2)} = 1 - \frac{\theta(T_1)}{\theta(T_2)}$$

The point now is that, for computing  $\theta$ , we can use this formula, and any reversible engine, of our choice. And by choosing here the Carnot engine operating on  $[T_1, T_2]$ , and doing the computation, based on the adiabatics for the ideal gases, we obtain:

$$\eta(T_1, T_2) = 1 - \frac{T_1}{T_2}$$

Thus the absolute temperature  $\theta = \theta(T) \in (0, \infty)$  constructed in (2) is given by  $\theta(T) = \lambda T$ , for some  $\lambda \in \mathbb{R}$ , and we are led to the conclusion in the statement.  $\square$

We can now calibrate our thermometer, as follows:

DEFINITION 7.45. *We can calibrate our thermometer, as follows:*

- (1) *Celsius:  $T = 0$  is where water freezes, and  $T = 100$  is where water boils.*
- (2) *Kelvin:  $T = 0$  is the absolute minimum, and the degrees are as in Celsius.*

In practice, this means  $0^\circ \text{ K} = -273.15^\circ \text{ C}$ . We will use in what follows the Kelvin scale for abstract physics, and Celsius for various engineering matters. We will be also back to all this later on, with various refinements and finer numerics.

So, that was it, and truly amazing, isn't it. Obviously, having  $T > 0$  is something of similar impact to Einstein's  $v < c$ . And, not only this discovery came before Einstein's, but its proof, explained above, was via a sort of enormous Gedankenexperiment, far more technically involved than the trains and clocks needed for special relativity.

Hommage to the thermodynamics greats, Gay-Lussac, Celsius, Joule, Carnot, Otto, Diesel, Clapeyron, Clausius, Lord Kelvin and the others, for this remarkable discovery. More homage to follow in the next chapter, to Maxwell, Boltzmann and others, for further discoveries. And even more homage later, to Max Planck and then Bose, Fermi and others, for even further discoveries, such as the difference between bosons and fermions. And finally, with a special thought for Fermi, and his wonderful book [32], where all the basic thermodynamics, and much more, is explained, much better than here.

## 7e. Exercises

No surprise here, as unique exercise, we have:

EXERCISE 7.46. *Read Fermi's book [32].*

Available from Dover, at 11.95 USD.



## CHAPTER 8

### Statistical mechanics

#### 8a. Molecules and pressure

We have seen in the previous chapter that some basic thermodynamics theory can be developed for the gases, by using the mathematics of their equation of state  $f(P, V, T) = 0$ , regarded as defining a surface in the 3D space of all possible parameters  $P, V, T \in \mathbb{R}$ . As a main finding, we have seen that the obvious conditions  $P > 0$ ,  $V > 0$  can be complemented with  $T > 0$ , and with this finding being something universal, beyond the gas level.

In this chapter we get back to the usual 3D, with the  $x, y, z$  coordinates referring, as before in mechanics, to the usual  $\mathbb{R}^3$  space that we live in. All our substances, be them gases, or liquids or solids, will be bodies  $B \subset \mathbb{R}^3$ . We will be interested in how heat flows between, and inside such bodies  $B \subset \mathbb{R}^3$ , as function of the time  $t \in \mathbb{R}$ .

Obviously, what we want to do here is to unify thermodynamics with mechanics. Or perhaps, more modestly, we want to upgrade our basic knowledge of thermodynamics, dealing so far only with gases, and with such gases being abstract  $(P, V, T)$  creatures, into something more advanced, of mechanical type, and covering liquids and solids too.

The discipline dealing with this is statistical mechanics. Mechanics because what we want to do is some sort of mechanics. And statistical because what we know so far about gases, and thermodynamics in general, suggests that at the level of subtle things, such as the second law of thermodynamics, everything is of deep statistical nature.

As usual, we will be quite brief. Excellent introductions to statistical mechanics are provided by the books of Feynman [33], Schroeder [79], Shankar [85] and Weinberg [92]. There are plenty of advanced books as well, such as Huang [49], Kadanoff [56], Pathria and Beale [69], and many more. We will be back with more references later.

To start with, let us go back to gases, and improve our previous knowledge about them. You surely know that ordinary matter is made of molecules, and that in the case of gases, these molecules are free to move. Let us axiomatize this situation as follows:

**DEFINITION 8.1.** *A gas is made of molecules which are free to move, in a certain volume  $B \subset \mathbb{R}^3$ , with each molecule moving with its own speed. These molecules have perceptible size, and are subject to elastic collisions, when they meet.*

Obviously, this is something quite general. A first simplification is by assuming that the volume  $B \subset \mathbb{R}^3$  is something standard, such as a sphere, or a cube, with this allowing us to forget about  $B$ , and talk instead about the volume of the gas,  $V = \text{vol}(B) > 0$ . With this assumption made, the problem is that of finding the equation of state:

$$f(P, V, T) = 0$$

Another problem appears at the level of speeds. Molecules are of course, by definition, free to move in any direction, but if the speed is assumed to have the same magnitude  $\|v\| > 0$  for all molecules, this will bring of course some simplifications.

Finally, the big problem appears in connection with collisions. We know from chapter 2 above that elastic collisions in 3D, even between bodies of the same mass, and in fact even between bodies of same mass arriving with the same speed, are uniquely determined up to a scattering angle  $\theta$ . Thus, in order to clarify our collision formalism, we need to know more about the chemical structure of the gas, telling us about  $\theta$ .

In order to deal with these latter problems, and with other problems that might appear afterwards, it is convenient to relax a bit our formalism, as follows:

**DEFINITION 8.2.** *We call 1D, 2D or 3D gas a gas as in Definition 8.1, with the molecules allowed to move in 1, 2 or all 3 directions.*

This is of course something purely mathematical, but the 1D and 2D gases will prove to be useful, as toy examples to be worked out before getting into the usual, 3D gas problems. As a first result now, dealing with the non-collision case, we have:

**THEOREM 8.3.** *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 traveling at speed  $v$ . We must compute the pressure  $P$  exerted by this molecule on the right wall:

$$\begin{array}{c} \begin{array}{ccc} = & = & = \\ \parallel & & \parallel \\ \parallel & \nearrow_v & \parallel \\ \parallel & \bullet_m & \parallel \\ = & = & = \end{array} \end{array} \rightarrow P$$

(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,  $V = L_1 L_2 L_3$ . Here the above 1D gas computation carries on, and gives the same result, as follows:

$$P = \frac{F}{L_2 L_3} = \frac{\Delta p}{L_2 L_3 \Delta t} = \frac{2mv}{L_2 L_3 \cdot 2L_1/v} = \frac{mv^2}{L_1 L_2 L_3} = \frac{2K}{V}$$

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:

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

(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.  $\square$

The above result is quite interesting, so let us keep building on it. We will adopt an engineering approach. We would like to know more about the measurement of the pressure, given by the following formula, with  $d = 3$  for the usual, 3D gases:

$$P = \frac{2K}{dV}$$

To be more precise, we would like to better understand the physics of the measuring piston, and we have plenty of interesting questions here, as follows:

**QUESTIONS 8.4.** *In a context of a gas enclosed in a cylinder with a piston, assumed to be formed of point molecules, with no collisions between them:*

- (1) *What is the correct modeling of the elastic collisions between the molecules and the piston, instantaneous,  $\Delta t = 0$ , or in nonzero time,  $\Delta t > 0$ ?*
- (2) *How will the piston exactly move, depending on the chosen model? Will equilibrium lead to some special distribution of the molecular speeds?*
- (3) *How does measured pressure  $P_t$  evolve with time  $t > 0$ ? What is the correct time  $t_f > 0$  for reading the correct, final pressure,  $P_f = 2K/dV$ ?*

These are certainly all good questions, in view of the fact that our only way of knowing more about the gas is via its interaction with the piston. In practice now, obviously (1) is a quite complicated question, and contemplating a good soup cooking, in a pot with a cover, with the cover jiggling under the effect of the steam, will give you a taste of the complexity involved. Question (2) looks more mathematical, and of prime theoretical importance, but in order to have some fun with it, and do some computations, we will need a model for it, to start with, as in (1). As for (3), again this looks like math, but again we need a model for it, in order to get started, in our computations.

So, these are our problems, and this even before getting to the real-life gases, made of molecules having perceptible size, with collisions between them. We will attempt now to solve these questions, with our main focus being on (2), try to have something done there, that can afterwards evolve into the Maxwell-Boltzmann distribution, which is the correct distribution of the molecular speeds for a real-life gas, with collisions.

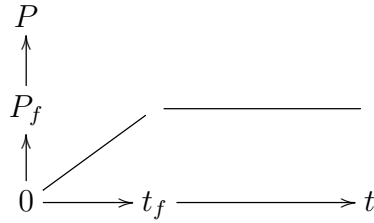
Let us start with discussing (3). Obviously this question is in need of a model, say with a spring for the piston, exactly as in the case of the usual manometers, functioning with

a spring. However, we can actually say something, to start with, purely mathematical, even without a spring or other model for the piston involved, as follows:

**THEOREM 8.5.** *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 8.3 above:

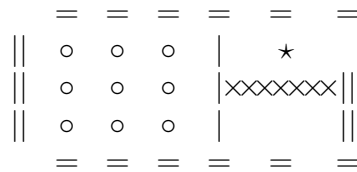
$$v_{i1}^2 = ||v_i||^2/d$$

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 8.3. 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.  $\square$

Going ahead now with the real problem, namely finding models for the piston, and then doing some math afterwards, we have several choices here. First we have:

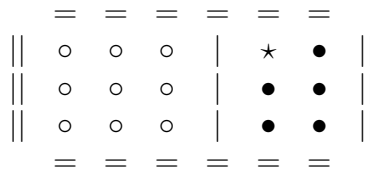
MODEL 8.6 (Spring model). *The piston has a spring on its back, with the energy  $E = mv^2/2$  of each incoming molecule being converted, over a certain period of time  $\Delta t > 0$ , into internal energy  $E_s$  of the spring, until the molecule comes to a stop, and then released back as identical kinetic energy  $E = mv^2/2$ , over the same period of time  $\Delta t > 0$ , of that molecule bouncing back, with speed of same magnitude  $||v||$ .*

In other words, we are proposing here a model for the piston which is similar to the one which can be found inside the usual, real-life manometers. The functioning is as follows, with  $\star$  standing for our displacement measuring devices:



This model surely stands, and certainly brings some fresh air into our physics. Indeed, what we have been doing so far assumes that the collisions with the piston are elastic and instantaneous,  $\Delta t = 0$ , and the problem now is about fine-tuning our theory using collision times  $\Delta t > 0$ , as above. In addition, the model can be further complicated afterwards, say allowing for some friction on the vertical, which amounts in allowing heat diffusion at the piston, having something to do with the temperature  $T$  of the gas.

As a variation of this model, again inspired by usual manometers, the spring used above is just a flexible solid, so why not using instead a liquid, or even a gas. We are led in this way to the following scheme, with  $\bullet$  standing our favorite lab fluid, and with  $\star$  standing as usual for our measurement devices, now floating inside this fluid:



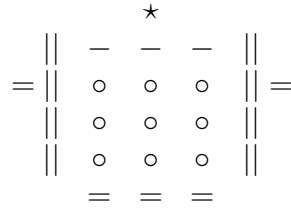
To be more precise, assuming for instance that  $\bullet$  is another gas, initially at lower pressure than the gas to be studied  $\circ$ , the piston will certainly start moving to the right, and then after some time, start to stabilize, with an interesting jiggling to be studied.

But do we really have some lab gas  $\bullet$ , that we know well. Not really, at this point of our story. So we are led into liquids, which are a bit more similar to the solid springs in Model 8.6, but do we really know about compression of liquids, and the answer here is not either. So, we will not use such fluid models, and keep them in mind for later.

As a third model now, which is intuitive and viable as well, we have:

MODEL 8.7 (Cooking pot model). *The cylinder and piston, functioning now vertically, work as a cooking pot with cover. That is, the gas is cooking inside the pot, the cover has a certain weight  $M \gg m$  and is subject to an acceleration  $g > 0$ , not affecting the gas itself, and the molecules  $m$  collide elastically with the cover  $M$ , assumed to travel frictionless on the vertical only, making it jiggle, around an average height  $L$ .*

This model looks quite interesting, and here is the picture, with handles attached, for easy transportation inside the lab, and with  $\star$  standing for our measuring devices:



The same general comments as for the spring model apply, with this model being something preliminary, which can be subject to further improvements. However, there are two notable differences with the spring model. First, in this cooking model the collisions are still assumed to be instantaneous,  $\Delta t = 0$ , and so we have less physics to care about. And also, speaking simplicity, our cooking pot model is purely gravitational, and so no need to go into springs and their functioning, we're just ready to go.

As another comment, if the fact that  $g > 0$  acts by definition on the cover  $M$ , but not on the gas molecules  $m$ , bothers you, you can assume for instance that the cover  $M$  and the acceleration  $g > 0$  are something more modern, say of magnetic nature. But, in what follows, we will refer to what happens as being gravitational, nothing being better in life than a good soup or stew, cooking in an old pot, with old-style gravitational cover.

Here is now our result, regarding the cooking pot model:

THEOREM 8.8. *The following happen, in the context of a gas having  $N$  point molecules, with no collisions between them, cooking in a pot with cover, as in Model 8.7:*

- (1) *In the usual regime,  $N \gg 0$ , the cover mass  $M$  and the acceleration  $g$  must be subject to the formula  $dLMg = 2K$ , with  $d, L, K$  being as before.*
- (2) *At  $N = 1$ , that is to say, when cooking a single molecule, the cover will bounce up and fall, perfectly in tune with the molecule, which keeps its speed  $\|v\|$ .*
- (3) *At  $N = 2$  however, when cooking two molecules, the initial speeds  $v_1, v_2$  of these molecules, even when taken equal, will change over time, due to the cover.*
- (4) *Even worse, at  $N = 2$  the system will exhibit chaotic behavior, and this for all choices of the initial data. And the same will happen at any  $N \geq 2$ .*

PROOF. There are many things to be done here, the idea being as follows:

(1) Let us first assume that we have a 1D gas. The molecular force acting on the cover, upwards, is given by the following formula,  $A$  being the area of the cover:

$$F = PA = \frac{2KA}{V} = \frac{2K}{L}$$

But this force must cancel  $F' = Mg$ , pointing downwards, so we have:

$$\frac{2K}{L} = Mg \implies LMg = 2K$$

In general, the computation is identical, with the parameter  $d = 1, 2, 3$  appearing attached to the volume  $V$ , and so to the length  $L$ , leading to  $dLMg = 2K$ , as stated.

(2) Let us cook now a single molecule,  $N = 1$ . Again, by assuming first that we deal with a 1D gas, the process here will take place in 4 steps, as follows:

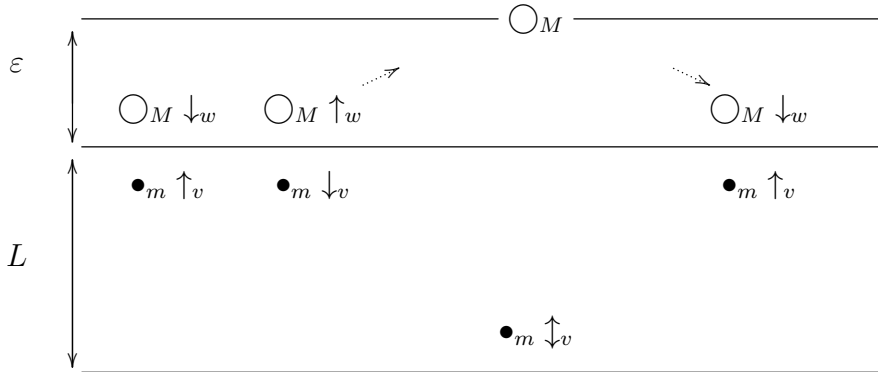
- The molecule, with mass  $m$  and upwards speed  $v$ , meets the cover, with mass  $M$  and downwards speed  $w$ , and has an elastic collision with it. Since we want our molecule to simply switch its speed after the collision,  $v \rightarrow -v$ , we must assume  $Mw = mv$ .

- In the second step, which is also infinitesimal, our molecule is now traveling downwards with speed  $v$ , and the cover is now travelling upwards with speed  $w$ .

- In the third step, the cover travels upwards during some time  $t_c$ , until getting to a halt, under the influence of  $g$ . As for the molecule, this travels downwards, during some time  $t_m$ , until reaching the bottom of the pot, for an elastic collision there.

- Finally, in the fourth step, the cover falls during time  $t_c$ , under the influence of  $g$ , until reaching its initial height  $L$ , with its initial downwards speed  $w$ . As for the molecule, this reaches to the initial height  $L$ , with its upwards speed  $v$ , in time  $t_m$ .

(3) In order now to have a cycle, we must have  $t_c = t_m$ , as for the whole picture of our cycle to look as follows, over this common travelling time  $t_c = t_m$ :





(4) But travelling times are easy to compute. In what regards the molecule, its travelling time during half of the full cycle is given by:

$$t_m = \frac{L}{v}$$

As for the cover, its equation of movement, with respect to the origin taken at height  $L$ , is  $x = wt - gt^2/2$ . We have  $x = 0$  at  $t = 0$ , of course, and then again at  $t = 2w/g$ , and so the travelling time of the cover during half of the full cycle is given by:

$$t_c = \frac{w}{g}$$

Thus, our cycle condition  $t_c = t_m$  amounts in saying that we must have  $gL = vw$ , and so to conclude, our machinery works well when the following conditions are satisfied:

$$Mw = mv \quad , \quad Lg = vw$$

Observe that when multiplying these two equations, as to get rid of the initial cover speed  $w$ , we obtain the following equation, which is the one found in (1) above:

$$LMg = mv^2 = 2K$$

(5) In the general case now, that of a  $d$ -dimensional gas, formed as before by 1 molecule, the analysis is similar. To be more precise, let us get back to Model 8.7, and to the exact prescriptions there, namely that the collisions between the molecule and the cover should be elastic, but with the cover travelling on the vertical only, in a frictionless manner, and managing somehow to absorb the lost horizontal momentum of the molecule, at each collision. Under these assumptions, the above computations carry over, with the only thing that changes being that the molecule speed  $v$  must be replaced by its vertical component  $v_1$ . Thus, the equations found in (4) become:

$$Mw = mv_1 \quad , \quad Lg = v_1 w$$

Also as before, when multiplying these two equations, as to get rid of the initial cover speed  $w$ , we obtain the following equation, which is the one found in (1) above:

$$LMg = mv_1^2 = \frac{m||v||^2}{d} = \frac{2K}{d}$$

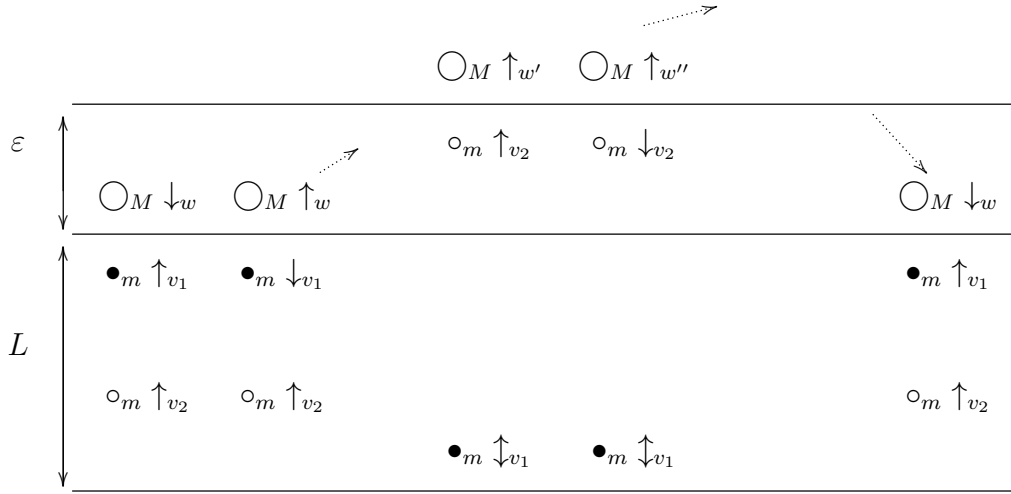
Here, as in the proof of Theorem 8.3 above, we have used the formula  $||v||^2 = dv_1^2$ , which is something of statistical nature, coming from the fact that our molecule is assumed to move in a random direction, inside its allowed  $d$ -dimensional space.

(6) At  $N = 2$  now, when cooking two molecules, some interesting things happen. To be more precise, our claim is that the initial speeds  $v_1, v_2$  of these two molecules, even when taken equal in magnitude initially, will change over time, due to the cover.

Indeed, in the context of the analysis done in (2-4), a second molecule, hitting the cover after the first one, will hit this cover travelling either upwards or downwards, and in

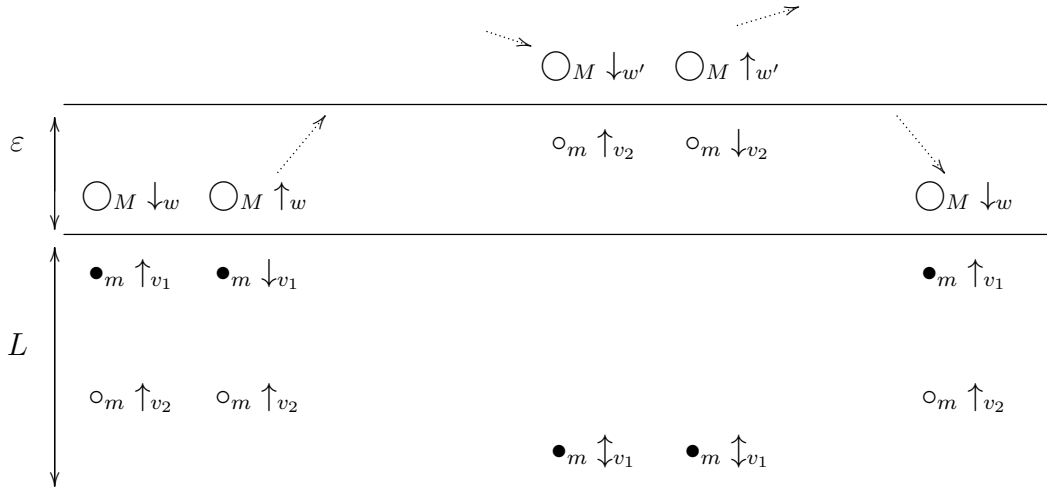
both cases at a speed of different magnitude,  $w' \neq w$ . Thus, when assuming for instance  $v_1 = v_2$  initially, this second collision will be no longer between objects having equal, opposite momenta, and so the speed  $v_2$ , instead of simply getting reversed,  $v_2 \rightarrow -v_2$ , will get modified, into something of type  $v_2 \rightarrow -v'_2$  with  $v'_2 < v_2$ . And so on.

(7) To be more precise, let us show now that there is no possible configuration of the initial parameters as to have a perfect cycle. There are two possible cases. The first case is where the second coming molecule hits the cover during its upwards travel:



But this certainly won't work, because the collision between the cover and the second molecule cannot happen as indicated, on top, due to obvious momentum reasons.

(8) The other case, which is perhaps more realistic, is that when the second coming molecule hits the cover during its downwards travel, as follows:



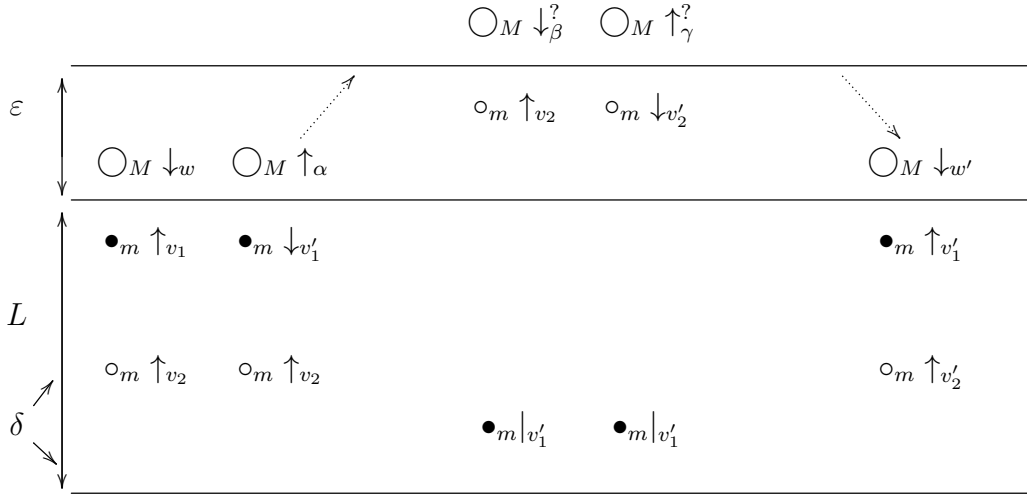
Here both the collisions will perform fine, as indicated, provided that the equal and opposite momenta conditions for them are satisfied, namely:

$$Mw = mv_1 \quad , \quad Mw' = mv_2$$

However, there is a bug at the level of time. On one hand we must have  $v_2 > v_1$ , since the second molecule has to travel  $2\varepsilon$  more than the first one, during the whole cycle. And on the other hand we must have  $v_2 < v_1$  due to the above collision equations, since  $w' < w$ . Thus, contradiction, and this second configuration is ruled out too.

(9) In short, complicated, but as a comment however, frankly, who would have guessed that we can get into such interesting math, just by cooking 2 molecules in a pot.

(10) Moving ahead now, the next problem is that of understanding how the speeds  $w, v_1, v_2$  will modify over the time. Assuming, to start with, that we still want to have some sort of cycle, with the positions of the two molecules and of the cover being unchanged after the cycle, but with the speeds modified, the picture of the problem as follows:



To be more precise, things evolve as indicated, with the upper question marks standing for the fact that we want to deal with all possible orientations there, but we have chosen some orientations, as indicated, for doing our computations, with the convention  $\beta, \gamma \in \mathbb{R}$ . As for the  $|$  signs on the bottom, near the speeds  $v'_1$ , these stand for the orientations of these speeds  $v'_1 > 0$ , which are irrelevant at that exact moment. And finally, as new parameter we have the distance  $\delta > 0$  between the second molecule and the bottom.

(11) Getting now to equations, there are many of them. First we have the two collision equations, momentum and energy, which after simplification for energy are:

$$\begin{aligned} M(w - \alpha) &= m(v'_1 - v_1) \quad , \quad M(\beta - \gamma) = m(v'_2 - v_2) \\ w + \alpha &= v_1 + v'_1 \quad , \quad \beta + \gamma = v_2 + v'_2 \end{aligned}$$

We have then two equations relating the speeds of  $M$ , left to middle, and middle to right, which can be obtained by conservation of energy, and are as follows:

$$\alpha^2 - \beta^2 = w'^2 - \gamma^2 = 2g\varepsilon$$

We have then equations regarding the partial times  $t_1, t_2$  of our two-step cycle, viewed from the perspective of the second molecule, and of the first molecule, as follows:

$$t_1 = \frac{L - \delta + \varepsilon}{v_2} \quad , \quad t_2 = \frac{L + \delta + \varepsilon}{v'_2} \quad , \quad t_1 + t_2 = \frac{2L}{v'_1}$$

And finally we have degree 2 equations for  $t_1, t_2$  from the perspective of the cover, which are as follows, with the  $\pm$  sign standing for upwards vs downwards collision:

$$t_1 = \frac{\alpha \pm \sqrt{\alpha^2 - 2\varepsilon g}}{g} \quad , \quad t_2 = \frac{\gamma + \sqrt{\gamma^2 + 2\varepsilon g}}{g}$$

(12) Looking at these equations, they don't look that bad. The first 6 equations, all regarding speeds, can be used in order to compute  $\alpha, \beta, \gamma$  and  $w', v'_1, v'_2$  in terms of  $w, v_1, v_2$ . And then we have 5 equations for  $t_1, t_2$ , which can be used for computing  $t_1, t_2$ , and then for finding what exact conditions must the initial data  $m, M, g, L, \delta, w, v_1, v_2$  satisfy, as for the positions of our 3 objects to be the same in the end as in the beginning.

(13) Summarizing, the math for some sort of cycle seems to be here, but this must be taken with care. First, because we have seen in (8) above that things can fail due to positivity reasons, which are invisible from the linear algebra viewpoint. And second, importantly, because nothing guarantees that the final data of a first cycle can run well as initial data for a second cycle, and such kind of thing must be checked too.

(14) We can only conclude from all this that things are quite chaotic at  $N = 2$ , and consequently, at  $N \geq 3$  too. With the comment however that with  $N \gg 0$  something interesting must certainly happen, because after all at  $N = \infty$  we have equilibrium, as explained in (1). But we are here with our math on the thin edge between equilibrium and chaos, and such things are reputed to be difficult, so we will just stop here.  $\square$

Summarizing, many interesting things going on here, but at the end of the day, as always in such difficult situations, we are left with asking the cat. And cat says:

*CAT 8.9. Mathematical gases don't work, better learn some physics from Maxwell and Boltzmann. And for dinner, grill a steak.*

This sounds reasonable, as always, especially in regards with the last part. Not only my 2 molecules do not finally smell that tasty, despite my cooking efforts, but I will certainly not touch anymore that crazy pot cover, now that I know how it works. Unless maybe with my welding gloves, but I cannot find them in that mess at my shop.

Regarding the first part, however, I still have some doubts. Sure yes, we got into some complicated equations, and chaos, after some encouraging  $N = 1, \infty$  results, but maybe

our mathematical model was not the best one. And there are so many other models, that can be tried. And, believe me, mathematics has always shown that problems from physics can always be modeled, with patience, from simple to complicated, from 1D to 3D, and so on. And wasn't that the case with everything classical mechanics, and then with relativity too, and then also with electromagnetism, in a certain sense.

So, time perhaps to ask again the cat, although I perfectly know that he doesn't quite appreciate to be bothered too often with physics questions. And cat answers:

CAT 8.10. *Thermodynamics comes after chemistry, which comes after quantum mechanics. By the way, relativity comes after electromagnetism too.*

My goodness. Looks like the spirit of Lev Landau has revived, and talked to me. So yes, what can I say. Sure I know, but what can we do. After all, Feynman and Reagan have won the Cold War, so their civilization is probably not that bad.

In any case, good pieces of advice, and we'll go with Maxwell and Boltzmann.

## 8b. Basic principles

Back now to true physics, that of the gases made of molecules which are free to move, in a certain volume of  $\mathbb{R}^3$ , with each molecule moving with its own speed, and with these molecules having perceptible size, and elastically colliding, when they meet.

Generally speaking, the idea will be that of incorporating the new physics, coming from collisions, into what we have, namely the pressure equation in Theorem 8.3:

$$PV = \frac{2K}{3}$$

Before anything, we should mention that the internal collisions are a phenomenon of considerable magnitude, which can only substantially modify our physics, due to:

FACT 8.11. *At standard temperature and pressure (STP), meaning freezing water temperature, and pressure a tad lower than the average pressure at sea level,*

$$T = 0^\circ \text{ C} = 273.15$$

$$P = 1 \text{ bar} = 10^5$$

*a gas molecule undergoes about  $10^{10}$  collisions per second, on average.*

Here we refer as usual to standard units, namely meters, kilograms, seconds, coulombs not needed here, and kelvins. Let us also mention that the average pressure at sea level is  $1 \text{ atm} = 1.013 \times 10^5$ , with the previous STP standard, until the 80s, being  $0^\circ \text{ C}$  and  $1 \text{ atm}$ . Not to be confused with normal temperature and pressure (NTP), which means  $20^\circ \text{ C}$  and  $1 \text{ atm}$ . Or with many other standards, the situation here being a bit similar to that of the boxing world, with WBA, WBC, IBF, WBO all involved.

Speaking numbers and STP, let us record as well some data for gases, in order to have a clue on what we are talking about. Here it is, for 1 m<sup>3</sup> of hydrogen H<sub>2</sub>, at STP:

Quantity	Data	Comments
	—	
pressure $P$	1 bar = 10 <sup>5</sup>	STP
volume $V$	1	by assumption
temperature $T$	0° C = 273.15	STP
	—	
number of molecules $N$	$2.689 \times 10^{25}$	idealized
molecular density $\rho$	$2.689 \times 10^{25}$	cf. $V = 1$
molecule mass $m$	$3.347 \times 10^{-27}$	2.016 amu
	—	
total mass $M$	$9 \times 10^{-2}$	$M = Nm$
total energy $K$	$1.5 \times 10^5$	$K = 3PV/2$
	—	
molecular energy $K_0$	$5.578 \times 10^{-21}$	$K_0 = K/N$
molecular speed $v$	$1.825 \times 10^3$	cf. $K_0 = mv^2/2$
molecular momentum $p$	$6.108 \times 10^{-24}$	$p = mv$
	—	
pressure reading $t_f$	$1.896 \times 10^{-3}$	$t_f = 2\sqrt{3}V^{1/3}/v$

Observe, as simple conclusions, to be kept in mind, that 1 m<sup>3</sup> of hydrogen H<sub>2</sub> at STP weights 90 grams, that the molecular speed is about 1-2 km/s, and with this being also the speed of expansion of STP hydrogen in vacuum, and finally that the time needed for measuring pressure of hydrogen H<sub>2</sub> at STP is about 2 milliseconds.

Getting started now, as mentioned before, we must incorporate the about 10<sup>10</sup> collisions per second from Fact 8.11 into our physics. We have promised not long ago to never ever talk about math gases again, but hey, cat is not here, and we can formulate:

THEOREM 8.12. *For a general 1D gas the previous formula, namely*

$$PV = 2K$$

*still holds in the collision setting, and the physics of the 1D gases stops here.*

PROOF. This is something a bit philosophical, as follows:

(1) We know from Theorem 8.3 that at  $d = 1$  we have  $PV = 2K$ , under the assumptions there, and the problem now is to understand what happens when the molecules are assumed to have perceptible size, with elastic collisions between them.

(2) But, for an elastic 1D collision between particles having the same mass  $m$ , we know from chapter 2, as a consequence of the conservation of energy and momentum, that the

only thing that happens is that the speeds of our particles gets switched:

$$v'_1 = v_2 \quad , \quad v'_2 = v_1$$

(3) Thus, during such a 1D collision, formally the particles get switched, and so to say, nothing happens. Thus, we can simply ignore these collisions, and so we are back to the formalism in Theorem 8.3, namely point masses, and we are done.

(4) Finally, in what regards the last assertion, it is pretty much clear, in view of the above, that we cannot speak of the temperature of a 1D gas, or of other more complicated such things, and so the physics of such gases stops here, as claimed.  $\square$

Moving ahead with 2D, 3D, let us first review the collision formulae from chapter 2, in the case where the colliding masses are equal. We have here the following result:

**PROPOSITION 8.13.** *In the context of an elastic 2D collision between particles having the same mass  $m$ , the output speeds are given by the fomulae*

$$v'_1 = v_1 + u \quad , \quad v'_2 = v_2 - u$$

*or alternatively, by the following equivalent formulae*

$$v'_1 = v_2 - w \quad , \quad v'_2 = v_1 + w$$

*where  $u, w$  with  $u + w = v_2 - v_1$  form with  $v_2 - v_1$  a right triangle,  $u \perp w$ .*

**PROOF.** This follows from the collision formulae in chapter 2, as follows:

(1) We recall from there that the general output speeds are  $v'_1 = v_1 + q/m_1$  and  $v'_2 = v_2 - q/m_2$ , with the parameter  $q \in \mathbb{R}^2$  being subject to the following equation:

$$2 < v_2 - v_1, q > = \left( \frac{1}{m_1} + \frac{1}{m_2} \right) \|q\|^2$$

(2) In the case of equal masses,  $m_1 = m_2 = m$ , if we set  $u = q/m$  then we have the first formulae in the statement,  $v'_1 = v_1 + u$  and  $v'_2 = v_2 - u$ , with  $u \in \mathbb{R}^2$  satisfying:

$$< v_2 - v_1, u > = \|u\|^2$$

(3) Now by setting  $w = v_2 - v_1 - u$ , the first formulae in the statement transform into the second ones, namely  $v'_1 = v_2 - w$  and  $v'_2 = v_1 + w$ , and we have:

$$< u, w > = < u, v_2 - v_1 - u > = 0$$

(4) Thus, we are led to the conclusion in the statement, and with the remark that everything depends, equivalently, on the angle  $\theta \in \mathbb{R}$  between  $(u, v_2 - v_1)$ , which fully determines the right triangle  $(u, w, v_2 - v_1)$  in the statement.

(5) To be more precise, when this angle is  $\theta = 0$  we have  $w = 0$  and so, as in the 1D case, the collision simply amounts in an exchange of particles. However, for  $\theta \neq 0$  this exchange is perturbed, by the vector  $w$ , having magnitude  $\|w\| = \|v_2 - v_1\| \sin \theta$ .  $\square$

In the general 3D case, the situation becomes even more complicated, because the output speeds  $v'_1, v'_2$  consist of  $3 + 3 = 6$  unknowns, and conservation of energy and momentum give us only  $1 + 3 = 4$  equations. Thus, we have here 2 free parameters, unless of course we want to declare that the collision stays in the 2D plane  $(v_1, v_2)$ , in which case the problem is fully solved by Proposition 8.13, with just 1 parameter.

However, in practice, this latter assumption is not very realistic, due to the usually complex 3D shape of the gas molecules. As an example here, you can go to your chemistry lab, pick two big plastic  $\text{H}_2\text{O}$  molecules, and make them collide on a table. And, even if you always throw them with the same speeds  $v_1, v_2$ , what happens at the moment of the impact can vary, depending on which side of the first  $\text{H}_2\text{O}$  will hit which side of the second  $\text{H}_2\text{O}$ . To be more precise, you can observe in this way the above-mentioned angle  $\theta$ , and if you throw hard enough, one of the two  $\text{H}_2\text{O}$  might even take off upon impact, making it clear that there is as well a 2nd parameter involved there.

Getting now back to gases, we would like to find their equation of state, relating the pressure  $P$ , volume  $V$  and temperature  $T$  into a single formula, as follows:

$$f(P, V, T) = 0$$

Normally we have a bit of math and physics already, for dealing with such questions. The starting point would be the pressure formula that we already have, namely:

$$PV = \frac{2K}{3}$$

Now imagining that we have a good model for the piston, along the lines of the previous section, and with that model being smart enough as to read the temperature too, via heat diffusion at the piston, and perhaps some friction too, and imagining too that we are good enough at math for incorporating into the physics the  $10^{10}$  collisions per second from Fact 8.11, via the math in Proposition 8.13, and finally imagining that chemists can help us a bit in understanding the basic differences between various gases, in relation with their internal collision mechanisms, well, good news, we can compute the equation of state.

In practice, however, this looks more like insanity. And so modesty, and instead of formulating a theorem, with proof and everything, we'll have to begin with a fact:

FACT 8.14. *The ideal gas is subject to the equation of state*

$$PV = kT \quad : \quad k = Nb$$

*where  $N$  is the number of molecules present, and where*

$$b = 1.380\,649 \times 10^{-23}$$

*is an exact constant, called Boltzmann constant.*



As a first comment, this fact is something old as ever, going back to the 18th century greats, such as Boyle and Charles, and then with further important contributions in the 19th century, by Gay-Lussac and Clausius, and then Maxwell and Boltzmann.

As a second comment, from a modern perspective, this fact lies somewhere between fact and theorem. We know that we have  $PV = 2K/3$ , and somehow the argument would be that the total kinetic energy  $K$  of the gas corresponds to temperature  $T$ , via:

$$\frac{2K}{3} = kT$$

Equivalently, by dividing everything by the number of molecules  $N$ , the individual molecular kinetic energy  $K_0$  should correspond to temperature  $T$ , via:

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

But is this obvious? We know from thermodynamics that temperature  $T$  measures heat  $Q$ , which is a form of energy, and with this in mind, having  $K_0 \sim T$  perfectly makes sense. But finding the precise proportionality factor amounts in doing the math for that  $10^{10}$  collisions per second added to the theory, and with this leading us into countless challenges, as explained before Fact 8.14. And in addition to this, above everything, even if you manage to do the math, you still need afterwards experimental physicists to confirm the fact that your model is indeed the correct one, physically speaking. But such a confirmation can only come via a statement similar to Fact 8.14, so here we are, back to the starting point, after an interesting theoretical physics loop.

But perhaps enough talking for now, let us do a verification. We have here:

VERIFICATION 8.15. *For hydrogen  $H_2$  at STP we have*

$$PV = 0.986 \times kT$$

*based on the  $1 \text{ m}^3$  data from the beginning of this section.*

PROOF. We have indeed the following computation, based on that data:

$$\frac{PV}{NbT} = \frac{10^5 \times 1}{2.689 \times 10^{25} \times 1.381 \times 10^{-23} \times 273.15} = 0.986$$

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

Going ahead now with more talking, as already mentioned, the formula in Fact 8.14 is old as ever, and there are many possible formulations of it, involving mysterious notions like moles, molar mass, molar volume, molar everything, the Avogadro number, the gas constant, and many more. The problem comes, besides from history, from modern chemistry, which uses different units, mole-centered. Or as Feynman was putting it, the problem comes perhaps from the fact that “we physicists use 1 as unit”. We refer to

Feynman's book [33] for a full-scale trashing of chemists, and their units, written some time ago, and with the comment that things have not changed much, since then.

By the way, speaking now books, it is always a big issue on where to put  $PV = kT$ , and with which type of explanations. Shall that be at the beginning, as an honest, simple fact, as history of physics went by? Or in the middle, with some sort of explanations, as we are doing it here? Or, by going fully modern, at the end, with full explanations?

These are all good questions, and good books exist for all tastes. Let us particularly recommend here, for this and for what follows next, Weinberg's book [92]. That is a wonderful, concise book dealing with physics at large, assuming basic math known, and which starts precisely with thermodynamics and statistical mechanics. By the way, the other books of Weinberg, [93], [94], [95] and more, are worth a look too.

Still commenting on Fact 8.14, a common misconception states that the formula there comes from the physics of the internal collisions, needed to keep the gas in place "at perfect equilibrium", with this meaning without container. But this does not make much sense, because, while collisions are certainly responsible for turning back certain molecules willing to escape, they can do nothing against half of the molecules at the boundary, those with speeds oriented towards freedom. And once these molecules are gone, you will never see them again, and then also the boundary will shrink, and more molecules will escape, and so on. In fact, it is always good to remember here that we have:

FACT 8.16. *The average density of the intergalactic space is 1 particle / m<sup>3</sup>.*

Here by particle we mean atom or molecule, depending on the precise story of that particle. Observe that we are here in the region where the Maxwell demon can strike, and also that there might be some gravitation involved too. So we will leave now this trip to the outer space, with as usual, as conclusion, a bit more wisdom and modesty.

Back now to work, as a complement to Fact 8.14, but at a more advanced level, dealing now with the internal mechanism of the  $PV = kT$  formula, we have:

FACT 8.17 (Maxwell). *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 Fact 8.14, 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 discuss the original argument of Maxwell, then go towards 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 the discussion after Fact 8.14 that one of the many equivalent formulations of  $PV = kT$ , using  $PV = 2K/3$ , was as follows:

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

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

Observe that the above proof has little physical content, with the whole thing being obtained by using  $PV = 2K/3$ , a theorem, then  $PV = kT$ , a crucial physics fact, and finally by invoking several times symmetry arguments, and doing some calculus.

However, and here comes our point, the result itself, Fact 8.17 as stated, is something quite deep, having to do with the collisions, and the intimate physics of gases. Which should be in fact not surprising, because after all, modulo some math, Fact 8.17 is a reformulation of Fact 8.14, which itself is surely a deep physics fact.

In short, we are here getting to the essence of things. Fact 8.17 is something very interesting, and the one who manages to find a proof for that, via mechanics and collisions, not only can claim to have proved Fact 8.17, but also to have proved Fact 8.14.

### 8c. Collisions, Boltzmann

In order to discuss this, following Boltzmann, let us go first back to basic thermodynamics, as in chapter 7. As a continuation of the material there, we have:

**THEOREM 8.18.** *Given a gas, with states denoted  $S = (P, V, T) \in \mathbb{R}^3$ , subject to the equation of state  $f(S) = 0$ , define the entropy of a state by the formula*

$$\mathfrak{E}(S) = \int_{S_0}^S \frac{dQ}{T}$$

*where  $S_0$  is a chosen state, and the integral is over a reversible transformation from  $S_0$  to  $S$ . Then  $\mathfrak{E}$  is well-defined up to an additive scalar, and we have the inequality*

$$\mathfrak{E}(S_1) \leq \mathfrak{E}(S_2)$$

*for any transformation  $S_1 \rightarrow S_2$ , with equality when this transformation is reversible. That is, entropy increases, and there is nothing much that you can do about it.*

**PROOF.** This comes as a continuation of the material from chapter 7, and we will use the same methods as there, namely calculus, and Carnot machines:

- (1) Our first claim is that for any cycle  $\circ : S \rightarrow S$  we have:

$$\int_{\circ} \frac{dQ}{T} \leq 0$$

In order to prove this, we approximate the cycle  $\circ$  by a sequence of isothermals  $\gamma_1, \dots, \gamma_k$ , at temperatures  $T_1, \dots, T_k$ . Now let us fix  $T_0 > T_i$ , and for each  $i$  consider a Carnot machine  $C_i$ , refrigerator or engine, which functions in the range  $[T_i, T_0]$ , by absorbing at  $T_i$  the positive or negative heat  $dQ_i$  emitted by our gas during  $\gamma_i$ .

- (2) Let us see how our machinery, consisting of our gas and of the Carnot machines  $C_1, \dots, C_k$ , works, over the full cycle  $\circ$ . At each  $T_i$  nothing happens, because what is

absorbed or expelled by the gas is expelled or absorbed by  $C_i$ , due to our conventions above. So, if there is something that our machinery does, that happens at  $T_0$ .

(3) But at  $T_0$  the gas does nothing, and the system of our Carnot machines  $C_1, \dots, C_k$  extracts or absorbs work, of total quantity, positive or negative, given by:

$$W = T_0 \int_{\circ} \frac{dQ}{T}$$

But we know from the second law of thermodynamics, in Lord Kelvin's formulation, that you cannot extract work from a given temperature  $T_0$ . Thus, our system of Carnot machines  $C_1, \dots, C_k$  works overall as a refrigerator,  $W \leq 0$ , as desired.

(4) Thus our claim in (1) is proved, and all the rest is trivial, just by gluing paths. Indeed, by using (1), we first conclude that  $\mathfrak{E}(S)$  is not dependent on the choice of a reversible path  $S_0 \rightarrow S$ . Moreover, also by using (1), we conclude afterwards that  $\mathfrak{E}(S)$  is well-defined up to an additive scalar, independently of the choice of  $S_0$ . And finally, again by using (1), we conclude that the equality in the statement  $\mathfrak{E}(S_1) \leq \mathfrak{E}(S_2)$  holds indeed, with equality when the transformation  $S_1 \rightarrow S_2$  is reversible.

(5) As for the final conclusion, this is something philosophical, and with that frightening Gothic notation  $\mathfrak{E}$  that we chose for entropy coming from that.  $\square$

So, this was for the basics of entropy, and with the inequality  $\mathfrak{E}(S_1) \leq \mathfrak{E}(S_2)$  being not at all something philosophical, but rather something subtle, true, and of course annoying, regarding our universe. To put it squarely, our universe is slowly dying, over the long long term, basically because the heat flowing from warm to cold never comes back.

Personally, not that I care much about this, busy with science and other, but since cat is passing by, let us ask him too about this, right. Hope he will reply with a gentle piece of advice, instead of one of these raw cat facts. And cat says:

*FACT 8.19. Good scientists will watch the fate of the universe from Heaven. Bad scientists will watch it from Hell.*

Which sounds good to me, for one time we are on the same wavelength. So leaving now cat go for his hunt, let us go back to physics. Following Boltzmann, we have:

*THEOREM 8.20 (Boltzmann). The kinetic theory of gases, taking into account the collisions between molecules, leads to the formula for entropy*

$$\mathfrak{E}(S) = -b \int P(S) \log P(S) dS$$

*with  $P$  being the probability on the state space, around our given state  $S$ .*

PROOF. This is something quite complicated, and for a proof here, we refer to any solid statistical mechanics book. Note in the above the obvious similarity with the Shannon entropy formula from information theory, if you ever came across that. Finally, observe that  $\mathfrak{E}$  as computed above is given by an exact formula, not depending on an additive constant, the point here being that, in the context of Theorem 8.18, we can formally choose the state  $S_0$  there to be the one, which is unique, at temperature  $T = 0$ .  $\square$

Moving ahead now, as a second key result, also due to Boltzmann, we have:

THEOREM 8.21 (Boltzmann). *Given a gas with initial molecular speed distribution  $P$ , the collisions between molecules, leading to equilibrium, will work such as the quantity*

$$H = \int P(v) \log P(v) dv$$

*decreases over time. The final distribution reached, over time, which is the one at equilibrium, is precisely the one which minimizes  $H$ , given by the formula*

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

*which is the Maxwell-Boltzmann distribution, that we knew before from Maxwell.*

PROOF. Again, this is something at the same time a bit complicated, but of utter beauty, and for the proof, we again refer to any solid statistical mechanics book.  $\square$

Observe the obvious similarity between Theorem 8.20 and Theorem 8.21, and also the important theoretical consequences of the above, in view of the comments that we previously made in connection with the Maxwell-Boltzmann distribution.

As a conclusion to all this, Boltzmann's work drags the whole subject into probability theory and computations, which are immensely powerful, as shown by Theorem 8.21. The further developments of the subject, due to Gibbs and others, are along these lines, kinetic theory models, and then lots of probability computations. For more on all this, we refer to any book on physics at large, or statistical mechanics, such as Huang [49], Kadanoff [56], Pathria and Beale [69], Schroeder [79] or Weinberg [92].

#### 8d. States of matter, diffusion

We briefly discuss here all sorts of things, that must be discussed, for the most in relation with matter, subject to heating or cooling. 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  $V = \text{vol}(B) \in \mathbb{R}$ , as it was the case so far.

Let us first record, regarding the gases, at a more advanced level:

THEOREM 8.22. *Beyond the ideal gas setting, stating that we should have*

$$PV = kT$$

*the gases are subject to the Van der Waals equation*

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

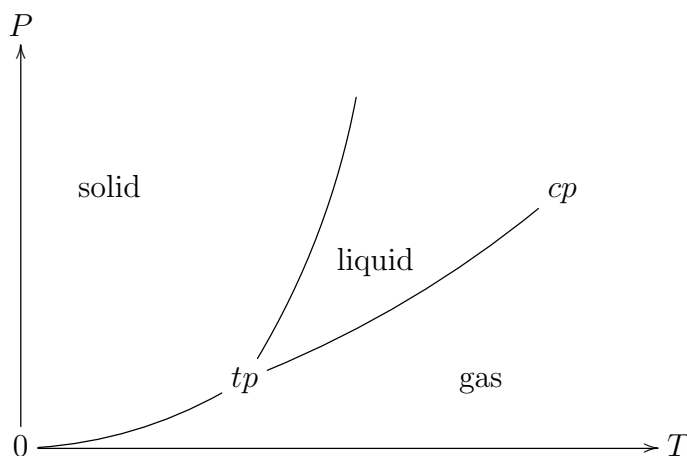
*depending on two parameters  $\alpha, \beta > 0$ .*

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. For an introduction to all this, we refer for instance to Huang [49], or Schroeder [79].  $\square$

The above result is of key importance, and takes us into rethinking everything that what 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, this Van der Waals gas study makes appear some interesting points on the isothermals, called triple and critical points of the gas. Which makes the connection with the general theory of matter, which can be summarized as follows:

FACT 8.23. *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 phenonema like Bose-Einstein condensation, and plasma.*

Needless to say, the quantity of things that can be said about all this is enormous. Passed the gases, that we are starting to be quite familiar with, the problem is with the

liquids and solids, plus of course with all sorts of exotic matter that can appear at the extremes. Good books here include Abrikosov [1], Ashcroft and Mermin [8], Chaikin and Lubensky [17], Goodstein [40], Harrison [47], [48], Kittel [58], Yeomans [98], for what happens here on Earth, including weird things in our labs, and Choudhuri [19], Clayton [20], Ryden [75], [76], [77] and Weinberg [94], [95] for a trip to the outer space.

Finally, let us discuss heat diffusion. Again, there are countless things that can be said here, both at the level of basic thermodynamics, and of the kinetic theory of gases, and as usual we refer to our standard thermodynamics and statistical mechanics books. However, if there is one beautiful thing to be said here, this is as follows:

FACT 8.24. *Heat diffusion is generally described by the heat equation*

$$\dot{\varphi} = \alpha \Delta \varphi$$

where  $\alpha > 0$  is the thermal diffusivity of the medium, and  $\Delta$  is the Laplace operator.

Observe the amazing similarity with the wave equation that we met in chapter 6, when talking electromagnetic waves, namely  $\ddot{\varphi} = v^2 \Delta \varphi$ . More on this later.

So, this was for the basics of statistical mechanics, as a continuation of thermodynamics. Regarding references, as already mentioned, excellent introductions are provided by the books of Feynman [33], Schroeder [79], Shankar [85] and Weinberg [92]. There are plenty of advanced books as well, such as Huang [49], Kadanoff [56], Pathria and Beale [69], which are excellent but not exactly beginner level, with both the math and the physics being a bit opaque to the untrained eye, due to usual issues with statistical mechanics, namely too much new physics, and a new way of doing math too.

Let us also mention that there are many books written by mathematicians too, or perhaps scientists at the interface between applied math and theoretical physics, usually on more advanced topics, such as Anderson, Guionnet and Zeitouni [3], Baxter [14], Di Francesco, Mathieu and Sénéchal [24], or Jones [55]. Although on quite advanced topics, which might seem a bit specialized, these books can be actually a nice intermediate step between the undergraduate physics books [33], [79], [85], [92] and the graduate ones [49], [56], [69] mentioned above, for the simple reason that the math is usually as complicated, but at least you're saved from some of the physics. In any case, this is the situation, and never forget, if you have troubles with learning statistical mechanics, that's normal.

## 8e. Exercises

Things have been difficult in this chapter, and as unique exercise, we have:

EXERCISE 8.25. *Find a nice book on statistical mechanics, and read it.*

Here the first part is the tricky one, due to the bewildering choice, with no clear winner. As for the second part, reading a book that you love, that's certainly easy.



## Part III

# Quantum mechanics

*All aboard, all aboard, ooh  
Come on boy, do you wanna ride?  
All aboard, all aboard, ooh  
Last train to Trancentral*

## CHAPTER 9

### Atomic theory

#### 9a. Quantum mechanics

Welcome to quantum mechanics. This is the main topic of the present book, and good news, we have plenty of time for discussing it. A full 200 pages only for this, as opposed to the previous 200 pages, which were quite condensed, for everything else.

Before anything, in the hope that you have not started this book here, at page 200, unless you know what you're doing. We will be heavily using things that we learned so far, namely classical mechanics, relativity, electromagnetism and thermodynamics. In case you know them, things fine of course. If not, you can either restart at page 1, or read them from somewhere else. Good references here include the books of Feynman [33], [34], Shankar [85], [86] and Weinberg [92]. A pleasant alternative is to start with Griffiths [42], for electromagnetism and love for physics, then complete say with Kibble [57], French [37], Fermi [32], for classical mechanics, relativity and thermodynamics.

So, what is quantum mechanics? The answer is very simple, as follows:

DEFINITION 9.1. *Quantum mechanics is the science of everything, starting from the nanoscale level ( $1 \text{ nm} = 10^{-9} \text{ m}$ ), and all the way below.*

This certainly deserves some explanations. Really everything? Why quantum? Why mechanics? And also, what does  $10^{-9}$  have to do with all this?

In what regards “everything”, yes the claim is that quantum mechanics has answers to everything happening at  $d < 10^{-9}$ , including mathematics, physics, chemistry, biology, engineering, and even things like philosophy, literature and sports. To be more precise, in what regards sports for instance, if one day we'll learn that everything is made of tiny little particles, far smaller than those presently known, who spend their time playing soccer and making fun of us, believe me, it is physicists doing quantum mechanics that will discover them, and not the sports anchors from your local TV station.

In what regards “mechanics”, no surprise here, in view of what we've seen so far in this book. Everything in life is some sort of mechanics, with forces acting, experiments needed for writing equations, and then math needed for solving these equations. So, business as

usual, with mechanics meaning more or less “physics”. In fact, if you hear people talking about “quantum physics”, that is exactly the same thing as quantum mechanics.

In what regards “quantum”, things here are trickier. To start with, we have:

**TERMINOLOGY 9.2.** *Quantum, plural quanta, comes from the Latin quantus, meaning “how much”. In the context of physics, a quantum is the minimum possible amount of any physical quantity. And with quantity coming by the way from quantus, too.*

And isn’t this confusing. Leaving now aside the Latin quantus, and the word quantity naturally derived from it, the key words in the above are “minimum possible amount”. So, that is the precise definition of quantum, in physics parlance.

As an example here, money is quantized, that is, made of quanta, a quantum of money being 1 cent, if you live in the US. Sugar in a sugar box is quantized too, a quantum being here a cube of sugar. And so on. Note in passing that quantum has not necessarily something to do with “small”, in the usual sense. For instance a herd of elephants is quantized too, a quantum here being 1 elephant. But things are relative, and assuming that you are interested in elephants only, 1 elephant is certainly something small.

Getting back now to physics, what is quantized, and what not? Common sense would suggest that all the basic physical quantities, such as distance, mass, energy and so on, vary continuously, and so are not quantized. And here comes the whole point, with quantum mechanics making the following bold statement:

**CLAIM 9.3.** *Quantum mechanics claims that all the basic physical quantities are in fact quantized, and that below the  $10^{-9}$  m range, nothing cannot be really understood, if not taking into account the quantized nature of things.*

Summarizing, in regards with the questions raised after Definition 9.1, we have solved all of them, and by killing two rabbits with one shot, Claim 9.3 explaining both “quantum” and  $10^{-9}$ . So, it simply remains to justify a bit this claim, and then get to work.

So, why should be things quantized in physics, and in life in general. Good question, going back to the cavern men, thinking about it. In the lack of anything spectacular, let us start with some philosophy. Our first piece of support for Claim 9.3 comes from:

**FACT 9.4.** *Life is quantized, the quanta being the cells, and not even need for a microscope for that, the orange cells for instance being big enough. That’s how this world is made, quantized, or at least the fancy, living part of it. So if you look long enough at a rock, as to fall in love with that rock, that rock will become quantized too.*

It is possible to further build along these lines, with this being the occupation of mankind and philosophers for long millennia in a row. In order to reach however to something more precise, as in Claim 9.3, some modern physics is needed.

So, let us review now the physics that we learned so far, and see if we have indication from there that things are quantized. The situation here is as follows:

(1) In what regards classical mechanics, things seem to be going smoothly there. However, as explained afterwards, when doing electromagnetism, the gravitational force is  $10^{42}$  weaker than the electromagnetic one, which is quadratic too, which raises the possibility for gravitation to be the “quantum” of quadratic forces,  $F \sim 1/d^2$ .

(2) Again speaking classical mechanics, we have seen that this naturally evolves into relativity, where  $v < c$  is paramount. So now that speeds are bounded from above, why should they not be bounded from below, either? That is, there might be well an  $\varepsilon > 0$  such that travelling at positive speed  $v < \varepsilon$  is impossible. Who knows.

(3) Still mechanics, Einstein’s energy formula  $\mathcal{E} = mc^2 + mv^2/2 + 3mv^4/8c^2 + \dots$  is something quite perplexing. The rest mass term  $E = mc^2$  suggests that inside any mass  $m$  there is an enormous amount of tiny little forces, which remain to be discovered. And the third term,  $3mv^4/8c^2$ , which is truly tiny, is something quite interesting too.

(4) Less speculatively now, when doing electromagnetism, we inevitably got into electrons, which are the quanta for charge, and these electrons are here to stay. So, that is at least something that we can agree upon, that charge is quantized, and as a consequence, that all the quantities appearing from electromagnetism are quantized too.

(5) In relation now with thermodynamics, things were quite complicated there, suggesting that pressure  $P$  and temperature  $T$  might be quantized. And also, as a rock-solid finding there, we had a theorem stating that  $T > 0$ , which suggests that, even if  $T$  is not quantized, at least it’s not a usual linear quantity, so careful with it.

And that’s pretty much it. Not bad, in any case, we have here some serious evidence for Claim 9.3. Or at least for the quantization claim there, with the precise figure  $10^{-9}$  still needing to be discussed. And so, to end this discussion, Definition 9.1 seems to be justified, we know what quantum mechanics should be, and where its name comes from, and all that is left now is to find this quantum mechanics, its laws and everything.

The first thought goes to experiments, but here we stumble upon:

**FACT 9.5.** *You cannot really measure tiny little things, smaller than the resolution of your machinery. In addition, for the same reasons, measuring might perturb them.*

This is of course something as old as engineering, and the solution is always to wait for long years, for technology to evolve. But in our case, when looking at the above list (1-5), giving some indication about how quantization should appear, and how small the quanta we are looking for should be, this does not look very good. We are really looking

for tiny little things, well beyond the range of usual scientific machinery, so don't really count on that machinery, and better try to develop some theory first.

But what to start with? Looking again at the above list (1-5), nothing very simple going on there. So, we are a bit into an impasse, at this point of things. Fortunately, there is an answer, a very clever answer to all this, as follows:

IDEA 9.6 (Let there be light). *Burning matter, and observing the color of the flame, gives you information about the intimate, infinitesimal structure of that matter.*

And isn't this amazing. This says more or less that when burning some gas, or wood, or salt, or whatever other substance, you're doing first-class quantum mechanics there, observing things so small that you never dreamed of coming upon.

So, this will be our starting point, in order to get into quantum mechanics, burning matter and recording the color of the light. We can in fact do even better, by avoiding the chemical reactions associated with burning, which will affect the matter that we are observing, and proceeding in a perhaps less glamorous way, as follows:

IDEA 9.7 (Let there be heat). *Heating matter, and observing the changing colors, gives you information about the intimate, infinitesimal structure of that matter.*

The above two ideas are of course as old as physics, or perhaps as fire and metallurgy, and the whole human civilization, in what concerns their everyday, macroscopic uses. Try cooking some food, or a blade, and you'll naturally get into them. In what concerns however their microscopic use, as suggested above, things are more recent, and the discipline of modern physics based on them is called spectroscopy. Our plan will be as follows:

(1) We will first need some preliminaries on basic optics, following Newton and others, and machinery like prisms, and also a bit of advanced discussion on light itself, as a continuation of some things started when doing electromagnetism.

(2) Then we will talk spectroscopy, theory and experiments, with all sorts of interesting findings, due to Balmer, Rydberg and others, giving a taste of what quantum mechanics should look like, with some mysterious matrices being involved.

(3) We will make then a connection between light and heat, go back to thermodynamics at the point where we left it, in the previous chapter, and keep building on that, notably with a spectacular result of Max Planck, stating that energy is quantized.

(4) And finally, we will put everything together, with an atomic theory, due to Bohr and others, which is compatible with the findings of Balmer, Rydberg and Planck, and with everything else. And it is all this that will lead us to quantum mechanics.

Before starting with all this, we should mention that there are several possible approaches to quantum mechanics, and good books written on them, for all tastes. As a continuation of our previous discussion about general physics books, from the beginning of this chapter, for quantum mechanics, you have again Feynman [35], Shankar [87] and Weinberg [93]. But that can be also Griffiths [43], Huang [50], Landau-Lifshitz [63], Peres [70], Sakurai [78], Schwinger [83], von Neumann [91] or Weyl [96].

Summarizing, plenty of choices, and in what follows, we will often refer to these books, and with a particular affection for Griffiths [43]. Let us mention too that, historically, all the quantum mechanics greats wrote books, and with the standard reference here, still readable and not obsolete nowadays, being the one by Dirac [25].

Also, an interesting investment and reading is the popular book by Kumar [59], majestically explaining the story of the subject, and with a quite good deal of technical physics and formulae included. Personally I got it in my mailbox long ago on a Friday evening, and it ruined my whole weekend, I just sit and read, all weekend long.

### 9b. Lyman, Balmer, Paschen

Getting started now, we first need to talk about light. This will be our main tool for getting into quantum mechanics, a bit like it was in chapter 4 above, for getting into relativity. And with this being of course a general principle from usual life too. Going down to the cave, or up to the barn? Turn on the light first, to see what's there.

We have met light on two occasions, so far. First in chapter 4, when talking relativity, with the summary of our knowledge from there being as follows:

FACT 9.8 (Einstein principles). *The following happen:*

- (1) *Light travels in vacuum at  $c = 299\,792\,458$  m/s.*
- (2) *This speed  $c$  is the same for all inertial observers.*
- (3) *In non-vacuum, the light speed is lower,  $v < c$ .*
- (4) *Nothing can travel faster than light,  $v \not> c$ .*

To be more precise here, (1) is something known from long ago, with that precise figure being by definition exact, as per latest SI regulations, defining the meter in terms of  $c$ . Regarding (2), this is a tricky thing, due to Einstein, and with the whole theory coming from it, relativity, being verified experimentally. Regarding (3), this is something known for a long time too, and more on it in a moment. As for (4), this is part of Einstein's relativity theory too, and with the whole thing being verified experimentally.

All the above does not tell us what light is, but we reached to a beginning of answer to this question in chapter 6, with our conclusion there being as follows:

FACT 9.9 (Maxwell theory). *In regions of space where there is no charge or current present the Maxwell equations for electrodynamics read*

$$\langle \nabla, E \rangle = \langle \nabla, B \rangle = 0$$

$$\nabla \times E = -\dot{B} \quad , \quad \nabla \times B = \dot{E}/c^2$$

*and both the electric field  $E$  and magnetic field  $B$  are subject to the wave equation*

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

*where  $\Delta = \sum_i d^2/dx_i^2$  is the Laplace operator, and  $c$  is the speed of light.*

To be more precise here, the general Maxwell equations for electrodynamics, which appear as a mixture of math and physics, are globally a physics fact. In the circumstances in the statement these reduce to the equations above, and the verification of the wave equation is a theorem, obtained via some calculus. The speed of light  $c$  has something to do with all this via the key formula  $\varepsilon_0 \mu_0 = 1/c^2$  from the Biot-Savart law, with this numeric observation, namely that we have indeed  $\varepsilon_0 \mu_0 = 1/c^2$ , being due to Maxwell.

So, what is light? Light is the wave predicted by Fact 9.9, with its properties being in tune with what Fact 9.8 says, and with an important extra property being that it depends on a real positive parameter, that can be called, upon taste, frequency, wavelength, or color. And in what regards the creation of light, the mechanism here is as follows:

FACT 9.10. *An accelerating or decelerating charge produces electromagnetic radiation, called light, whose frequency and wavelength can be explicitly computed.*

This phenomenon can be observed in a variety of situations, such as the usual light bulbs, where electrons get decelerated by the filament, acting as a resistor, or in usual fire, which is a chemical reaction, with the electrons moving around, as they do in any chemical reaction, or in more complicated machinery like nuclear plants, particle accelerators, and so on, leading there to all sorts of eerie glows, of various colors.

In view of the above, and especially of the light bulb example, a natural question appears: what about a resistor which is not a light bulb filament, what happens to the light produced there? This is a good question, and we already know a part of answer to it, from the Joule law, saying that the resistor will start heating. The second part of it, that we will discuss in a moment, states that responsible for heat is, guess who, light again, but this time in non-visible wavelengths, typically IR.

Getting back now to Fact 9.10, in its general form, as stated above, this is something which can be deduced via some math, based on the Maxwell equations. However, all this math is not exactly trivial, and we will defer the discussion here for later.

To start with, let us go back to the wave equation  $\ddot{\varphi} = v^2 \Delta \varphi$  from Fact 9.9, and try to understand its simplest solutions. In 1D, the situation is as follows:



THEOREM 9.11. *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 solution of the wave equation appears as a linear combination of such basic solutions.*

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 something standard, coming from Fourier analysis, that we will not really need, in what follows.  $\square$

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:

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

Moving ahead now towards electromagnetism and 3D, let us formulate:

DEFINITION 9.12. *A monochromatic plane wave is a solution of the 3D wave equation which moves in only 1 direction, making it in practice a solution of the 1D wave equation, and which is of the special form found in Theorem 9.11, with no frequencies mixed.*

In other words, we are making here two assumptions on our wave. First is the 1-dimensionality assumption, which gets us into the framework of Theorem 9.11. And second is the assumption, in connection with the Fourier decomposition result from the end of Theorem 9.11, that our solution is of “pure” type, meaning a wave having a well-defined wavelength and frequency, instead of being a “packet” of such pure waves.

All this is still mathematics, and making now the connection with physics and electromagnetism, and more specifically with Fact 9.9 and Fact 9.10, we have:

FACT 9.13. *Physically speaking, a monochromatic plane wave is the electromagnetic radiation appearing as in Fact 9.9 and Fact 9.10, via equations of type*

$$\begin{aligned} E = \operatorname{Re}(\tilde{E}) & : \quad \tilde{E} = \tilde{E}_0 e^{i(\langle k, x \rangle - wt)} \\ B = \operatorname{Re}(\tilde{B}) & : \quad \tilde{B} = \tilde{B}_0 e^{i(\langle k, x \rangle - wt)} \end{aligned}$$

with the wave number being now a vector,  $k \in \mathbb{R}^3$ . Moreover, it is possible to add to this an extra parameter, accounting for the possible polarization of the wave.

To be more precise, what we are doing here is to import the conclusions of our mathematical discussion so far, from Theorem 9.11 and Definition 9.12, into the context of our original physics discussion, from Fact 9.10 and Fact 9.11. And also to add an extra twist coming from physics, and more specifically from the notion of polarization, that we met in chapter 6, without however giving much details. We will be back to this.

In any case, we have now a decent intuition about what light is, and more on this later, and let us discuss now the examples. The idea is that we have various types of light, depending on frequency and wavelength. These are normally referred to as “electromagnetic waves”, but for keeping things simple and luminous, we will keep using the familiar term “light”. The classification, 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 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

Outside visible light we have, as you probably know it, UV on higher frequencies, and IR on lower frequencies. At the high frequency end we have X-rays, that you surely know about too, and  $\gamma$  rays, which are usually associated with various bad things, such as thunderstorms, solar flares, and small bugs with our nuclear energy technology.

As for the lower frequency end of the scale, first we have microwaves, but if you love physics and chemistry you should learn some cooking, that's first-class chemistry, that you can practice every day. And then we have all sorts of radio wavelengths, including FM, followed by AM, and then by several more obscure low-frequency waves.

Importantly, both ends of the table are a bit loose. At the high frequency end there are some restrictions coming from quantum mechanics, and more on them later. As for the low frequency end, what's wave and what's not is a bit of a philosophical question, but which is actually not that philosophical, because waves having huge wavelengths can easily turn around mountains, full countries and so on, and so are of military interest. Secret research here, more of engineering type of course, is still ongoing.

Back now to our business, with all the above in hand, we can do some optics. Light usually comes in “bundles”, with waves of several wavelengths coming at the same time, from the same source, and the first challenge is that of separating these wavelengths.

In order to discuss this, let us start with the following fact:

**FACT 9.14.** *Inside a linear, homogeneous medium, where there is no free charge or current present, the Maxwell equations for electrodynamics read*

$$\langle \nabla, E \rangle = \langle \nabla, B \rangle = 0$$

$$\nabla \times E = -\dot{B} \quad , \quad \nabla \times B = \varepsilon \mu \dot{E}$$

*with  $E, B$  being as before the electric and the magnetic field, and with  $\varepsilon > \varepsilon_0$  and  $\mu > \mu_0$  being the electric permittivity and magnetic permeability of the medium.*

Observe that this is precisely the first part of Fact 9.9, with the vacuum constants  $\varepsilon_0, \mu_0$  being replaced by their versions  $\varepsilon, \mu$ , concerning the medium in question. In what regards now the second part of Fact 9.9, which was a theorem, we have:

**THEOREM 9.15.** *Inside a linear, homogeneous medium, where there is no free charge or free current present, both  $E$  and  $B$  are subject to the wave equation*

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

with  $v$  being the speed of light inside the medium, given by

$$v = \frac{c}{n} \quad : \quad n = \sqrt{\frac{\varepsilon \mu}{\varepsilon_0 \mu_0}}$$

with the quantity on the right  $n > 1$  being called *refraction index* of the medium.

**PROOF.** This is something that we know well in vacuum, from chapter 6, and the proof in general is identical, with the resulting speed being:

$$v = \frac{1}{\sqrt{\varepsilon \mu}}$$

But this formula can be written in a more familiar form, as above. □

As a first observation here, while the above is something quite trivial, mathematically speaking, from the physical viewpoint we are here into complicated things. Materials can be transparent or opaque, with the distinction between them being something very subtle, and advanced, and Theorem 9.15 obviously deals with the transparent case.

In short, we are here inside advanced materials theory, that we cannot really understand, with our knowledge so far. In what follows we will be interested in transparent materials only, such as glass. Regarding the other materials, such as rock, let us just mention that light disappears inside them, converted into heat. Of course glass heats too when light crosses it, with this being related to  $v < c$  inside it. More on this later.

Next in line, and for interest for us, we have:

**FACT 9.16.** *When traveling through a material, and hitting a new material, some of the light gets reflected, at the same angle, and some of it gets refracted, at a different angle, depending both on the old and the new material, and on the wavelength.*

Again, this is something deep, and very old as well, and there are many things that can be said here, ranging from various computations based on the Maxwell equations, to all sorts of considerations belonging to advanced materials theory.

As a basic formula here, we have the famous Snell law, which relates the incidence angle  $\theta_1$  to the refraction angle  $\theta_2$ , via the following simple formula:

$$\frac{\sin \theta_2}{\sin \theta_1} = \frac{n_1(\lambda)}{n_2(\lambda)}$$

Here  $n_i(\lambda)$  are the refraction indices of the two materials, adjusted for the wavelength, and with this adjustment for wavelength being the whole point, which is something quite complicated. For an introduction to all this, we refer for instance to Griffiths [42].

As a simple consequence of the above, we have:

**THEOREM 9.17.** *Light can be decomposed, by using a prism.*

**PROOF.** This follows from Fact 9.16. Indeed, when hitting a piece of glass, provided that the hitting angle is not  $90^\circ$ , the light will decompose over the wavelengths present, with the corresponding refraction angles depending on these wavelengths. And we can capture these split components at the exit from the piece of glass, again deviated a bit, provided that the exit surface is not parallel to the entry surface. And the simplest device doing the job, that is, having two non-parallel faces, is a prism.  $\square$

In the lack of a colored illustration here, in this book, due to various budget reasons, we refer to the cover of the “Dark side of the moon” album, by Pink Floyd.

With this in hand, we can now talk about spectroscopy:

**FACT 9.18.** *We can study events via spectroscopy, by capturing the light the event has produced, decomposing it with a prism, carefully recording its “spectral signature”, consisting of the wavelengths present, and their density, and then doing some reverse engineering, consisting in reconstructing the event out of its spectral signature.*

This is the main principle of spectroscopy, and applications, of all kinds, abound. In practice, the mathematical tool needed for doing the “reverse engineering” mentioned above is the Fourier transform, which allows the decomposition of packets of waves, into monochromatic components. Finally, let us mention too that, needless to say, the event can be reconstructed only partially out of its spectral signature.

As a conclusion to all this, we have learned many things about light, and in particular the method of spectroscopy. And so, we can now go back to atoms, and to the methods mentioned in the beginning of this chapter, and start developing them.

So, getting now back to atoms, there is a long story here, involving many discoveries of many people, around 1890-1900, focusing on hydrogen H. We will present here things a bit retrospectively, as to bet fit with science as we know it now, and with the present book. First on our list is the following discovery, by Lyman in 1906:

FACT 9.19 (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. Due to this fact, namely the invisibility of UV to the human eye, this series, while theoretically being the most important, for certain reasons to be explained later, 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 9.20 (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, and with his original wavelength formula being in fact something equivalent to the above formula, but a bit

more complicated, as follows, with  $B \simeq 3.645 \times 10^{-7}$  being the Balmer constant:

$$\lambda = \frac{Bn^2}{n^2 - 4}$$

As a third main result now, this time in IR, due to Paschen in 1908, we have:

FACT 9.21 (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 9.22 (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
...	...	...	...	...

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.

But from a theoretical physics viewpoint, the main result remains the middle assertion, called Ritz-Rydberg combination principle. This is something at the same time extremely simple, and completely puzzling, the informal conclusion being as follows:

THOUGHT 9.23. *The simplest observables of the hydrogen atom, combining via*

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

*look like quite weird quantities. Why wouldn't they just sum normally.*

Getting now to quantum mechanics, and to our dreams about it, formulated before, well, good news, we have some serious data here. These spectral lines are basic and beautiful, obviously of quantized type, and in order to get started with our theory, we first need to solve the puzzle of the Ritz-Rydberg combination principle.

But, how to do this? Fortunately, matrix theory comes to the rescue, as follows:

THOUGHT 9.24. *The Ritz-Rydberg 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, which are the elementary matrices given by*

$$e_{ij} : e_j \rightarrow e_i$$

*perhaps taken in infinite dimensions, as to allow infinite-ranging indices.*



This looks certainly very interesting, and actually reminds a mathematical speculation that we already did in this book, at a crucial point, namely in chapter 4 when getting into relativity. Remember the Galileo addition formula there for relative speeds, which got converted into the Einstein addition formula for the same relative speeds? Well, the reasoning there was as follows, involving the same sort of weird additions as above:

$$\begin{aligned} v_{AB} +_g v_{BC} &= v_{AC} & : & \quad v_{AC} = v_{AB} + v_{BC} \\ \implies v_{AB} +_e v_{BC} &= v_{AC} & : & \quad v_{AC} = \frac{v_{AB} + v_{BC}}{1 + v_{AB}v_{BC}/c^2} \end{aligned}$$

In short, be that with matrix theory, or with relative speeds in classical mechanics or relativity, we are in familiar territory here, and we can start dreaming of:

**THOUGHT 9.25.** *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.*

And probably enough for now, this is the kind of discovery that should be celebrated with slaughtering 50 sheep and inviting your friends over, for a banquet, as the legend has it that Pythagoras did, after he discovered his  $a^2 + b^2 = c^2$  theorem.

We will be back to all this a bit later, following Bohr, and then Heisenberg, and others, the idea being that Thought 9.25 is the main idea behind Heisenberg's first reasonable formulation of quantum mechanics, as a "matrix mechanics" theory.

For the story here, as a funny fact, Heisenberg did not know in fact about matrices, when starting his work, and rediscovered them by himself. More about this later.

To summarize now, very interesting all this. Lyman, Balmer, Paschen, these will be our new gods, the gods of quantum mechanics. Learn their names, as a prayer, and say this prayer "Lyman, Balmer, Paschen", whenever you'll be lost into the mysteries of quantum mechanics. Or at least that's what I do myself, and it always works.

### 9c. Radiation, Max Planck

We have seen so far that many interesting things can be said about matter, via spectroscopy and light, and with all these experiments and data still in need to be processed, via a clever theory of "quantum mechanics", which remains to be invented.

Our discussion so far implicitly used the fact that heat is light too, and so time now, before getting into quantum mechanics, to get back to the theory of heat, as developed in chapters 7-8, and see what our new viewpoint on it can bring. The main problem here is to compute the radiation of black bodies, and we will discuss this now.

Consider a black body, that is to say, a body at thermal equilibrium, assumed to be at temperature  $T$ . This body radiates heat, and we are interested in computing the energy density of the radiation  $\mathcal{E}(\nu, T)$ , around a given frequency  $\nu$  of this radiation.

Quite surprisingly, the intuitive and honest modeling of the problem, and the subsequent math, done honestly too, lead to a spectacularly wrong result, as follows:

**THEOREM 9.26.** *We have the Rayleigh-Jeans formula for the energy density*

$$\mathcal{E}(\nu, T) = \frac{8\pi bT}{c^3} \nu^2$$

where  $b$  is the Boltzmann constant, leading globally to the divergent integral

$$\mathcal{E} = \frac{8\pi bTV}{c^3} \int_0^\infty \nu^2 d\nu$$

over a volume  $V$ , with this divergence phenomenon being called *UV catastrophe*.

**PROOF.** This is arguably the most famous wrong result in the history of physics, so we will spend some time in trying to understand its proof. And with the comment that this will be no waste of time, because the fix, found later by Max Planck, uses exactly the same ideas and computations, but with an unexpected twist at the end.

(1) Our starting point are the equations for the electromagnetic radiation, that we will now regard as heat, as formulated in Fact 9.13, namely:

$$E = \text{Re}(\tilde{E}) \quad : \quad \tilde{E} = e_n e^{i(\langle k_n, x \rangle - w_n t)}$$

$$B = \text{Re}(\tilde{B}) \quad : \quad \tilde{B} = b_n e^{i(\langle k_n, x \rangle - w_n t)}$$

Here  $n$  is a certain parameter, that will appear later on, and that we can for the moment ignore. Now inserting this data into the Maxwell equations gives the following formulae, connecting the parameters, that we will use several times in what follows:

$$k_n \times b_n + \frac{w_n}{c} e_n = 0$$

$$k_n \times e_n - \frac{w_n}{c} b_n = 0$$

$$\langle k_n, e_n \rangle = \langle k_n, b_n \rangle = 0$$

(2) Let us compute the electromagnetic energy in a finite volume  $V = L^3$ . We will use here the well-known fact, coming from classical electrodynamics, that the energy density in radiation is  $(\|E\|^2 + \|B\|^2)/8\pi$ . Thus, the energy we are looking for is given by:

$$\mathcal{E} = \frac{1}{8\pi} \int_V (\|E\|^2 + \|B\|^2)$$

(3) In order to compute this integral, let us better model our question. Due to obvious periodicity reasons, the wave number  $k$  and the angular frequency  $w$  must be of the following form, with  $n \in \mathbb{Z}^3$  being a vector with integer components:

$$k_n = \frac{2\pi}{L} \cdot n \quad , \quad w_n = c||k_n||$$

Thus, the electric and magnetic fields in our enclosure  $V = L^3$  appear as linear combinations as follows, for certain vectors  $e_n, b_n \perp n$ , related by the formulae in (1):

$$E = Re(\tilde{E}) \quad : \quad \tilde{E} = \sum_n e_n e^{i(<k_n, x> - w_n t)}$$

$$B = Re(\tilde{B}) \quad : \quad \tilde{B} = \sum_n b_n e^{i(<k_n, x> - w_n t)}$$

(4) According to the above formula of  $E$ , we have:

$$\begin{aligned} ||E||^2 &= ||Re(\tilde{E})||^2 \\ &= \frac{1}{4} \left\| \sum_n e_n e^{i(<k_n, x> - w_n t)} + \bar{e}_n e^{-i(<k_n, x> - w_n t)} \right\|^2 \\ &= \frac{1}{4} \sum_{nm} \langle e_n, e_m \rangle e^{i(<k_n - k_m, x> - (w_n - w_m)t)} \\ &\quad + \frac{1}{4} \sum_{nm} \langle e_n, \bar{e}_m \rangle e^{i(<k_n + k_m, x> - (w_n + w_m)t)} \\ &\quad + \frac{1}{4} \sum_{nm} \langle \bar{e}_n, e_m \rangle e^{i(-<k_n + k_m, x> + (w_n + w_m)t)} \\ &\quad + \frac{1}{4} \sum_{nm} \langle \bar{e}_n, \bar{e}_m \rangle e^{i(-<k_n - k_m, x> + (w_n - w_m)t)} \end{aligned}$$

(5) Now by integrating, we obtain the following formula:

$$\begin{aligned} \frac{1}{V} \int_V ||E||^2 &= \frac{1}{4} \sum_n \langle e_n, e_n \rangle + \frac{1}{4} \sum_n \langle e_n, \bar{e}_{-n} \rangle e^{-2iw_n t} \\ &\quad + \frac{1}{4} \sum_n \langle \bar{e}_n, e_{-n} \rangle e^{2iw_n t} + \frac{1}{4} \sum_n \langle \bar{e}_n, \bar{e}_n \rangle \end{aligned}$$

(6) Similarly, according to the above formula of  $B$ , we have:

$$\begin{aligned} \frac{1}{V} \int_V ||B||^2 &= \frac{1}{4} \sum_n \langle b_n, b_n \rangle + \frac{1}{4} \sum_n \langle b_n, \bar{b}_{-n} \rangle e^{-2iw_n t} \\ &\quad + \frac{1}{4} \sum_n \langle \bar{b}_n, b_{-n} \rangle e^{2iw_n t} + \frac{1}{4} \sum_n \langle \bar{b}_n, \bar{b}_n \rangle \end{aligned}$$

(7) Before summing the integrals that we found, let us use the formulae connecting the parameters  $k_n, e_n, b_n$  found in (1) above, namely:

$$k_n \times b_n + \frac{w_n}{c} e_n = 0$$

$$k_n \times e_n - \frac{w_n}{c} b_n = 0$$

$$\langle k_n, e_n \rangle = \langle k_n, b_n \rangle = 0$$

By using these formulae, we obtain the following identities:

$$\langle b_n, b_n \rangle = \frac{c^2}{w_n^2} \langle k_n \times e_n, k_n \times e_n \rangle = \frac{c^2 \|k_n\|^2}{w_n^2} \langle e_n, e_n \rangle = \langle e_n, e_n \rangle$$

$$\langle b_n, \bar{b}_{-n} \rangle = \frac{c^2}{w_n^2} \langle k_n \times e_n, k_{-n} \times \bar{e}_n \rangle = -\frac{c^2 \|k_n\|^2}{w_n^2} \langle e_n, \bar{e}_{-n} \rangle = -\langle e_n, \bar{e}_{-n} \rangle$$

$$\langle \bar{b}_n, b_{-n} \rangle = \frac{c^2}{w_n^2} \langle k_n \times \bar{e}_n, k_{-n} \times e_n \rangle = -\frac{c^2 \|k_n\|^2}{w_n^2} \langle \bar{e}_n, e_{-n} \rangle = -\langle \bar{e}_n, e_{-n} \rangle$$

$$\langle \bar{b}_n, \bar{b}_n \rangle = \frac{c^2}{w_n^2} \langle k_n \times \bar{e}_n, k_n \times \bar{e}_n \rangle = \frac{c^2 \|k_n\|^2}{w_n^2} \langle \bar{e}_n, \bar{e}_n \rangle = \langle \bar{e}_n, \bar{e}_n \rangle$$

(8) We conclude that when summing the integrals computed in (5) and (6), all the terms involving phases will cancel, and we obtain the following formula:

$$\frac{1}{V} \int_V \|E\|^2 + \|B\|^2 = \frac{1}{2} \sum_n \langle e_n, e_n \rangle + \frac{1}{2} \sum_n \langle \bar{e}_n, \bar{e}_n \rangle$$

Now by multiplying everything by  $V/8\pi$ , as explained in (2), we obtain:

$$\mathcal{E} = \frac{V}{16\pi} \sum_n (\langle e_n, e_n \rangle + \langle \bar{e}_n, \bar{e}_n \rangle)$$

(9) The point now is that, by computing this sum, we are led to the Rayleigh-Jeans formula in the statement for the corresponding radiation energy density, namely:

$$\mathcal{E}(\nu, T) = \frac{8\pi b T}{c^3} \nu^2$$

(10) And this is certainly wrong, because the total energy which is radiated by our black body, all over the frequency spectrum, follows to be:

$$\mathcal{E} = \frac{8\pi b T V}{c^3} \int_0^\infty \nu^2 d\nu = \infty$$

More precisely, the Rayleigh-Jeans formula works quite well all across the frequency spectrum, in particular fitting well with the known data, except for the UV range, where things diverge. And with this phenomenon being called “UV catastrophe”.  $\square$

Well well, looks like we are in deep trouble here. Fortunately, the solution to the UV catastrophe, and to the black body problem in general, was found a few years later by Max Plank, his bold new modeling method, and result, being as follows:

**THEOREM 9.27.** *The correct formula for the black body radiation, obtained by assuming that energy is quantized, is the Planck formula*

$$\mathcal{E}(\nu, T) d\nu = \frac{8\pi h_0}{c^3} \cdot \frac{\nu^3 d\nu}{e^{h_0\nu/bT} - 1}$$

with  $h_0$  being a new constant, called Planck constant. This formula fits with all known data, fits as well with Rayleigh-Jeans outside the UV range, and globally leads to

$$\mathcal{E} = \int_0^\infty \mathcal{E}(\nu, T) d\nu = aT^4$$

with the radiation energy constant on the right being given by:

$$a = \frac{16\pi^8 b^4}{15h_0^3 c^3}$$

**PROOF.** This is something quite technical, obtained by further building on the formula found in (8) above, but counting this time in a new way, by assuming that the energy is quantized. For details here, and for more, we refer for instance to Weinberg [93].  $\square$

So, this is the famous Planck formula, whose consequences go far beyond its scope. Indeed, regardless on what the original problem was about, namely black bodies, and who cares after all about them, we have now proof for the fact that the energy is quantized. And this, simply because any attempt of solving the problem without assuming that energy is quantized leads to a catastrophe, as explained before.

Finally, a word about the new constant appearing in the above, namely the Planck constant. Due to some technical reasons, we will use here a non-standard notation for this constant, with the figures and our conventions being as follows:

**FACT 9.28.** *The Planck constant is given by the exact formula*

$$h_0 = 6.626\ 070\ 15 \times 10^{-34}$$

as per latest SI regulations. We will also use the reduced Planck constant, given by

$$h = \frac{h_0}{2\pi}$$

which is numerically given by

$$h \simeq 1.054\ 571\ 817 \times 10^{-34}$$

with everything being as usual in standard units.

To be more precise here, the point is that in quantum mechanics the constant which appears all the time is the reduced Planck constant, usually denoted  $\hbar = h/2\pi$ , with the original Planck constant being denoted  $h$ . However, the point is that, at least in what concerns us, we will heavily use for our quantum mechanics computations both this reduced Planck constant  $\hbar$  and the unnormalized trace of matrices  $tr$ . And the problem is that, in quick handwriting,  $tr$ ,  $\hbar$  often get confused, and when you compute you can't stop cursing, and you end up adopting the convention  $h = h_0/2\pi$ , as above.

Finally, let us mention that a very interesting continuation of Planck's work concerns the black body radiation of the early universe, with the microwave part of it, via a Doppler shift, still permeating the space that we live in. And with this phenomenon, called "cosmic microwave background", being at the origin of all modern cosmology.

This is, and we insist, something amazing. For more on all this, we refer to any book on cosmology, such as Dodelson [28], Ryden [75] or Weinberg [95].

#### 9d. Atoms, Bohr model

Getting back now to quantum mechanics, and to our various hopes about it, expressed before, time to put everything together. 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, to start with, let us agree on:

**CLAIM 9.29.** *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 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 indeed it is so came from several clever experiments. Let us first recall from Fact 9.5 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 9.29.

Of particular importance here was as well the radioactivity theory of Becquerel and Pierre and Marie Curie, involving this time such small beasts, or perhaps some related radiation, peeling off by themselves, in heavy elements such as uranium  ${}_{92}\text{U}$ , polonium  ${}_{84}\text{Po}$  and radium  ${}_{88}\text{Ra}$ . And there was also Einstein's work on the photoelectric effect, light interacting with matter, suggesting that even light itself might have associated to it some kind of particle, called photon. All this goes of course beyond Claim 9.29, with further particles involved, and more on this later, but as a general idea, all this deluge of small particle findings, all coming around 1900-1910, further solidified Claim 9.29.

So, taking now Claim 9.29 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 9.29, but led to an improved version of it, as follows:

CLAIM 9.30. *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. Remember from the beginning of this book the planets orbiting around the Sun, on ellipses, as found by Kepler? Well, the same should happen with electrons orbiting around the core, but this time due to the Coulomb force. And with this in mind, all the pieces of our puzzle start fitting together, and lead to:

CLAIM 9.31 (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, some further claims, also by Bohr and others, are that the theory can be further extended and fine-tuned as to explain many other phenomena, such as the above-mentioned findings of Einstein, and of Becquerel and Pierre and Marie Curie, and generally speaking, all the physics and chemistry known.

And the story is not over here. Following now Heisenberg, the next claim is that the underlying math in all the above can lead to a beautiful axiomatization of quantum mechanics, as a “matrix mechanics”, along the lines of Thought 9.25.

So this was for the main finding about atoms, following Bohr and his disciples, still used nowadays, and all that is left now for us is to explain a bit what that “modified version of electromagnetism” in Claim 9.31 exactly is, and then go get a beer.

Well, that “modified version of electromagnetism” is in fact quantum mechanics, in its full power and mysterious aspects, and it will take us 3 long chapters in order to explain the basics of its functioning. In chapters 10-11 below we will develop the basics, following Heisenberg and Schrödinger, and then in chapter 12 we will prove Claim 9.31.

### 9e. Exercises

Things have been quite experimental in this chapter, and as unique exercise, making you a good quantum mechanic in the becoming, we have:

EXERCISE 9.32. *Get yourself a prism, and start playing with it.*

Personally I used to have one as a kid, and boy did I like it. Although I must admit that my favorite item in my home lab was a small, fuming bottle of  $\text{HNO}_3$ .



## CHAPTER 10

### Schrödinger equation

#### 10a. The hangover

After all the excitement from the previous chapter, and the night after, personally I celebrated with several bottles of champagne, time for the hangover.

Our theory does not work. The Coulomb force is certainly the same thing as the Newton force, up to a rescaling, but electromagnetism itself is not the same thing as gravitation. The equations of movement here are the Maxwell equations, and believe me, I just did the computations, and these damn Maxwell equations, even with all tricks on Earth, prevent any nice, Kepler type elliptical orbit as a solution.

Looks like we're in deep trouble here, and that it will take us a lot of new ideas and skill in order to overcome this problem, and get restarted with our theory. But let us keep being optimistic. There should be a solution to everything, right. Our problem is:

**PUZZLE 10.1.** *We know from experiments that electrons surround the nucleus. These electrons are not fixed, for they would fall into the nucleus, otherwise. But they cannot move either, due to the Maxwell equations, which prevent any clear trajectory for them.*

After some thinking, this does not look, after all, that scary. Why not looking for an approximate trajectory then, perhaps even by allowing some chaos there, if really needed. Remember for instance from thermodynamics that when measuring the pressure  $P$  or the temperature  $T$  of a gas, some complicated things, which can include a bit of chaos, can happen. So why should not such complicated things appear here, too.

The problem, however, is that this does not work either. The math of the Maxwell equations appears to be demonic, and simply makes impossible anything reasonable, inspired from our everyday math and physics. In fact, everything fails for the hydrogen atom already, and as an even more annoying version of Puzzle 10.1, we have:

**PUZZLE 10.2.** *How can the hydrogen atom function, in view of the fact that, with the proton assumed to be fixed, the electron cannot be fixed, but cannot move either.*

Bohr, who was the initiator of the whole program, thought of course about all this, and found nothing. Other people like Sommerfeld thought about this too, and found nothing either. Not to mention Einstein, and many others, all the pioneers of the quantum theory.

This was in fact the puzzle on anyone's mind, at that time. And be said in passing, that must have being enraging, especially for Bohr, being stuck in a puzzle like that.

Relaxing a bit, and taking things easy, it's not exactly a puzzle, what we have here to solve, but rather a precise scientific question, of quite annoying type, as follows:

QUESTION 10.3. *Who's wrong among:*

- (1) *Thomson and Rutherford.*
- (2) *Lyman, Balmer, Paschen.*
- (3) *Bohr and his requirements.*
- (4) *Newton and Maxwell.*

Observe that, with a certain casual lack of modesty, we have ruled ourselves out of this business. So, we are led here into evaluating the findings of some of our illustrious colleagues. And we will do so, what can we do, with this remaining between us:

(1) Regarding the experiments of Thomson and Rutherford, this looks like a very solid discovery. However, since we are now around 1910, trying to figure out what's right and what's wrong, with all this, and their bombarding methods were quite new at that time, there is a bit of uncertainty, and we will grade their discovery with a  $A^-$ .

(2) Regarding Lyman, Balmer, Paschen, all that is rock-solid. By exaggerating a bit, you can rediscover the Balmer  $\alpha, \beta, \gamma, \delta$  lines of hydrogen in your garage, just armed with a prism. And with some IR, UV equipment, say bought from a military surplus store, you can rediscover the Lyman and Paschen lines too. So, grade  $A^+$ .

(3) Regarding Bohr, we're now into theoretical physics, in the  $B, C, D, E, F$  grade range, with  $A$  being of course reserved for convincing experiments only. Since his theory was very new at that time, it is probably wise of thinking of a  $C$  grade. However, in view of the astonishing beauty of his claims, we will grade them with a  $B^-$ .

(4) Finally, regarding Newton and Maxwell, movements of objects under influence of forces, and their precise equations, that is normally confirmed,  $B^+$  grade theory. But since Newton was after all corrected by Einstein, and also since Maxwell seems to cause our main problems with hydrogen, we should probably downgrade them to a  $B^-$ .

So this was the situation around 1910-1920, with everyone hesitating between sinking Bohr and his theory, which would have sunk all the modern physics at that time too, with so many other people involved, or sinking the good old principles of motion and equations of Newton and Maxwell, with no idea at all on what to replace them by.

A solution eventually came from Heisenberg. So Heisenberg was a fresh, young scientist at that time, full of energy and optimism, the kind of young researcher that can

develop you a full theory of “matrix mechanics”, without even knowing what a matrix is. And this is exactly what happened, initially without knowing what a matrix is, Heisenberg developed his “matrix mechanics” theory, along the lines suggested in the previous chapter, with his infinite matrices and their usual multiplication generalizing the spectral lines of Lyman, Balmer, Paschen, and their Ritz-Rydberg combination rule. His findings, to be explained in detail later on, can be informally summarized as follows:

ANSWER 10.4 (Heisenberg). *There is a way of making function the hydrogen atom, with some precise math and equations, which:*

- (1) *Perfectly agrees with Thomson and Rutherford.*
- (2) *Majestically agrees with Lyman, Balmer, Paschen.*
- (3) *Agrees with most of the Bohr requirements.*
- (4) *But does some harm to Newton and Maxwell.*

This was an enormous advance, making the Bohr model function, quite convincingly, for the first time. There were however several technical questions left:

(A) On one hand, a remaining problem was that of extending the theory to heavier atoms, with a puzzling question there being that of accommodating several electrons on the same energy level, but not on the exactly same positions, due to experiments suggesting so. This was solved after by Pauli and others, notably by using a notion of “electron spin”, and a certain “exclusion principle”, and more on this later.

(B) On the other hand, regarding hydrogen itself, the original spectroscopy results of Lyman, Balmer, Paschen became, in the years and decades afterwards, subject to some fine-tunings, due to Lamb and others, and the original theory of Heisenberg had of course to be corrected, on several occasions, as to fit with the new data. But this was, or perhaps still is, since the story continues nowadays, more of a routine thing.

All this was in connection with (3) above, realization of the Bohr model, with here the Heisenberg answer being an enormous success. In connection with (4), however, things were far more complicated. Without getting into details, to be discussed later, and getting back now to Puzzle 10.2, Heisenberg’s solution was something a bit abstract, and obscure, somehow avoiding the problem. To be more precise, the question of the trajectory of the electron around the proton was carefully avoided, via a bizarre mix of opaque mathematics, and head-scratching physical assumptions.

More on this later, when talking about Heisenberg and his precise discoveries, but in order to have a taste of what was going on, please check the following speculation out, which is something purely mathematical, but somehow in the spirit of what Heisenberg was saying, and decide for yourself if you agree or not with such things:

**SPECULATION 10.5.** *Why not regarding the usual matrices  $A \in M_n(\mathbb{C})$  as functions  $A : M_n \rightarrow \mathbb{C}$ , where  $M_n$  is some sort of “quantum space”, in analogy with the fact that the vectors  $v \in \mathbb{C}^N$  correspond to functions  $v : \{1, \dots, N\} \rightarrow \mathbb{C}$ . In addition:*

- (1) *We can do some math for such functions  $A : M_n \rightarrow \mathbb{C}$ , for instance by saying that  $\int A = \text{tr}(A)$ , or that  $A : M_n \rightarrow \mathbb{R}$  when  $A = A^*$ , and so on.*
- (2) *With the warning that our generalized functions  $A : M_n \rightarrow \mathbb{C}$  do not commute in general,  $AB \neq BA$ , and that  $M_n$  is not a space formed of points.*
- (3) *We can do even more math by saying that  $M_n$  formally has  $\dim(M_n(\mathbb{C})) = n^2$  points, and so must appear as a kind of “twist” of  $\{1, \dots, n^2\}$ .*
- (4) *And we can also say that the symmetry group  $S_{n^2}$  of  $\{1, \dots, n^2\}$  gets twisted in this way into the formal symmetry group  $PU_n = U_n/\mathbb{T}$  of  $M_n$ .*

This certainly looks a bit like nonsense, and, somehow, what Heisenberg was saying then, back 100 years ago, on the movement question was a bit of similar nature, involving things like “quantized orbits”, “quantized trajectories” and so on, all sorts of abstractions contradicting Newton and Maxwell, and basic common sense in general.

In short, the Bohr model was certainly proved to be successful by Heisenberg, and on the way for improvements, but in what regards Puzzle 10.2, and the very idea of quantum mechanics in general, things were quite unclear, with many people thinking:

**THOUGHT 10.6.** *Is quantum mechanics wrong, even before starting?*

The true solution to Puzzle 10.2 came a few years later, from Schrödinger. So Schrödinger was a quite different beast, 24 years older than Heisenberg, and than many other young people working with Heisenberg on the subject. And who was also, as an Austrian, having a strong influence from Boltzmann, and his unorthodox methods.

What Schrödinger did, with such a background, including exactly what Heisenberg and others were missing, was to convincingly solve Puzzle 10.2, a bit in the same way as Boltzmann solved before the main problems in thermodynamics. His result being:

**SOLUTION 10.7 (Schrödinger).** *When regarded statistically, the hydrogen atom functions just fine, via some precise math and equations, which:*

- (1) *Perfectly agree with Thomson and Rutherford.*
- (2) *Perfectly agree with Lyman, Balmer, Paschen.*
- (3) *Agree with most of the Bohr requirements.*
- (4) *Agree with Coulomb, with minimal harm to Newton.*

To be more precise, Schrödinger, exactly like Boltzmann before in thermodynamics, noticing that exact mathematics, and so to say geometry, fails for the problem, sent that geometric problem to the trashcan, or rather assigned it to later generations to come, and investigated the problem statistically. And his solution states that, with a certain suitable

probability distribution for the position of the electron inside its orbit, resembling a bit a wave circling inside that orbit, the hydrogen atom functions just fine.

So this was for the story of the Schrödinger discovery. A bit simplified of course, with this involving some other people as well, notably de Broglie, and also, we should insist on this, with Schrödinger's solution being not independent of Heisenberg's, but rather further building on it. And a bit idealized too, because his statistical point of view, why apparently not doing much harm to Newton, reveals at a closer look that the harm is there, and of similar magnitude to Heisenberg's. In fact, Dirac came later with:

VERDICT 10.8 (Dirac). *Modulo a few things that are not in disagreement with the known experiments, and which can be incorporated into a general theory of quantum mechanics, what Heisenberg and Schrödinger say is the same thing.*

We will explain all this in what follows, in the remainder of the present chapter, and in the next one, following Heisenberg, de Broglie, Schrödinger and Dirac. And then, eventually, in chapter 12, we will fully prove the Bohr claim regarding atoms.

Finally, here are some further details on all the above, namely all sorts of problems remaining, and their possible fixes, to be discussed more in depth later on:

(1) In what regards the Maxwell equations, well, time for them, as for any exact law of physics in the long run, to be eventually downgraded to “statistical laws”. They were fixed some time after, by Feynman, with the whole theory of electrodynamics being replaced by a more advanced theory, quantum electrodynamics (QED). Ironically, this new QED theory is of deep statistical nature too. More on this later, in chapters 13-14 below.

(2) Another idea for improving quantum mechanics, this time of radical new nature, developed later by Gell-Mann and others, was that of replacing  $10^{-9}$  by something much smaller, hunting for the particles here, called “quarks”, understanding their physics, called quantum chromodynamics (QCD), and with this done, recovering QED as some kind of thermodynamic limit of QCD. More on this in chapters 15-16 below.

(3) Yet another idea, due to Weyl and von Neumann, was to take things like Speculation 10.5 seriously, and further build on that, by developing some useful pure mathematics, inspired by the matrix mechanics of Heisenberg. Unfortunately things here took some time to get started, with this idea being forgotten, and only reappearing in the 80s, under the influence of Connes and Drinfeld. More on this in chapters 15-16 too.

(4) Another lost and found idea, originally due to Kaluza and Klein, was to fix things by adding more dimensions. In its modern formulation this is “string theory”, the idea being that the various point particles from QED and QCD, and more generally from

quantum field theory, QFT, need a few extra dimensions in order to reveal their true beauty and shape, and basically look like strings. More on this in chapters 15-16 too.

(5) Finally, in what regards the problem sent by Schrödinger to the trashcan, or rather assigned to later generations to come, namely that of finding some reasonable geometry theory describing the exact trajectory of the electron, this is still open, now 100 years after. With many people having thought about it, including Einstein, for a few decades in a row. If you hear about Einstein vs Bohr, it's not about a fight. It's about Einstein trying to solve this remaining problem, and Bohr, like Schrödinger, deciding that the problem is too complicated, to the point that working on it can be a waste of time. But more on this later, once we'll know a bit more about Schrödinger's solution.

Needless to say, (1,2,3,4,5) above are all related, and with scientific research ongoing, on all these topics. And with people, as usual in physics, being extremely split on all this. Personally I would put my money on a combination of (2) and (3), that is, QCD reunderstood via a Weyl-von Neumann idea, and then producing QED as a thermodynamic limit, slightly improving Feynman (1). And with no idea for (4) and (5). But hey, old man speaking here, all this is in need of enthusiastic young people. Like you.

### 10b. Schrödinger equation

Getting started now, following Schrödinger, let us forget about exact things, and try to investigate the hydrogen atom statistically. We have here the following question:

**QUESTION 10.9.** *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 linear motion, with speed  $v$ , we have:

$$\varphi_t(x) = \varphi_0(x) + vt$$

More generally, assuming that we have a particle whose position at time  $t$  is given by  $x_0 + \gamma(t)$ , the evolution of the probability density will be given by:

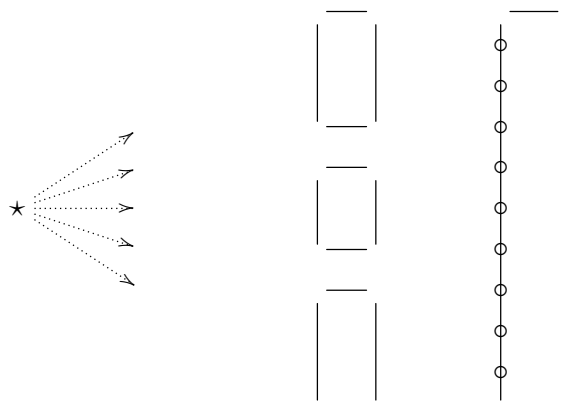
$$\varphi_t(x) = \varphi_0(x) + \gamma(t)$$

These 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 10.10. *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.*

So, here we go again with puzzles. These experiments are nicely described, with extensive comments, in Feynman's book [35]. In what follows, we will present them quickly. We will just need, for our purposes here, the first 4 experiments in the series, which are the most important. These are performed with a machinery as follows:



To be more precise, on the left we have a multi-purpose gun  $\star$ , which can shoot bullets, water waves, or electrons. On the middle we have a wall with two holes in it. On the right we have a solid wall, with sensors  $\circ$ , adapted to the matter that we are shooting.

The first experiment, performed with 22 cal ammo, assumed to be idealized, as to be indestructible, and we refer again to Feynman [35] for full details, goes as follows:

EXPERIMENT 10.11. *When shooting bullets, the density function on the right wall, stopping them, as recorded by our sensors there, is given by*

$$\varphi = \varphi_1 + \varphi_2$$

*where  $\varphi_1$  is the same density, but measured with the lower hole closed, and  $\varphi_2$  is also the same density, but measured with the upper hole closed.*

Nothing surprising so far. Now let us shoot water waves, or rather assume that our gun  $\star$  is a wave source. For this experiment, the sensors at right are set to measure the energy of the incoming wave, which is proportional to the square of the height.

The experiment, best performed with our favorite drinkable, tap water, gives:

EXPERIMENT 10.12. *When shooting waves, the energy density functions at right, measured with one or the other hole open, or both holes open, are related by*

$$\varphi_1 = |\psi_1|^2 \quad , \quad \varphi_2 = |\psi_1|^2 \quad , \quad \varphi = |\psi_1 + \psi_2|^2$$

*where  $\psi_1, \psi_2 \in \mathbb{C}$  are the amplitudes of the waves passing through one hole, with the other hole closed. This phenomenon and formula of  $\varphi$  are due to interference.*

This is again, something not surprising, that we know, coming from the fact that two colliding waves can add up in various ways, depending on their phases.

Now let us shoot electrons. At first sight, these behave like particles, because our sensors beep for them one at the time. However, when examining the results regarding probability distributions, these don't add up as for bullets, the conclusions being:

EXPERIMENT 10.13. *When shooting electrons, these come up one at the time, exactly as bullets. However, in what regards the density functions, these don't add up:*

$$\varphi \neq \varphi_1 + \varphi_2$$

*Thus, we have some interference, and most likely the correct formula is*

$$\varphi_1 = |\psi_1|^2 \quad , \quad \varphi_2 = |\psi_1|^2 \quad , \quad \varphi = |\psi_1 + \psi_2|^2$$

*with  $\psi_1, \psi_2 \in \mathbb{C}$  being certain amplitudes, exactly as for the waves.*

This is a bit surprising, showing that the electrons have a mix of particle and wave behavior, at least with respect to this experiment. Let us also mention too that, contrary to the previous two experiments which are simple and real, this is rather a Gedankenexperiment, and so the wave formulae are to be taken with care. See Feynman [35].

Finally, as a last experiment, again with electrons, we have:

EXPERIMENT 10.14. *When shooting electrons as before, but by putting a light bulb behind one hole, whose light is scattered by electrons passing through that hole:*

$$\varphi = \varphi_1 + \varphi_2$$

*That is, observing the electrons passing through one hole, via them scattering light, has killed the interference process, and we have now usual particles, like bullets.*

And this is probably the most surprising experiment of them all. Indeed, the fact that in Experiment 10.13 we have particles when counting and waves when looking at densities might seem odd, but after all, why not. So these are our beasts, electrons, and this is how their properties are, a bit odd, but at least we know one thing. However, what happens now seems to defy any logic. Observing the electrons has changed their properties, and that's how things are. Welcome to quantum mechanics.



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  $\varphi_t(x) = |\psi_t(x)|^2$ . So, let us reformulate Question 10.9, in the following way:

QUESTION 10.15. *In the context of the hydrogen atom, assuming that the proton is fixed, what is the amplitude function  $\psi_t(x)$  of the position of the electron  $e$ , at time  $t$ ,*

$$P_t(e \in V) = \int_V |\psi_t(x)|^2 dx$$

*as function of an initial amplitude function  $\psi_0(x)$ ? Moreover, can the corresponding equation be solved, and will this prove the Bohr claims for hydrogen, statistically?*

Mathematically, what we did here is to replace the density  $\varphi_t(x) > 0$  by the amplitude function  $\psi_t(x) \in \mathbb{C}$ . 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, experience with math shows that such manipulations can be crucial, raising for instance the possibility that the amplitude function satisfies some simple equation, while the density itself, maybe not. So, let us hope for this to happen.

And this is what happens indeed. Schrödinger was led in this way to:

CLAIM 10.16 (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,  $h$  the modified Planck constant, and  $V$  the Coulomb potential of the proton. The same holds for movements of the electron under an arbitrary 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. There might be of course some speculations to be made here, but passed that, this is certainly not your easy to decipher equation. So, where does this equation come from? Is there a way of deducing it from simpler principles? And so on.

Generally speaking, however, any axiomatic explanation for the Schrödinger equation can only introduce some possible mistakes in our theory. And so we are led by precaution to the following preliminary answer, to such questions, that you might have:

COMMENT 10.17. *The Schrödinger equation comes from Schrödinger.*

And please do not take this as a joke. We are mainly interested in solving the hydrogen atom, and the Schrödinger equation can only solve it, via some calculus. So why not

enjoying this, solving the hydrogen atom by using this equation, and see later what further things, beyond Schrödinger, can be said about quantum mechanics.

This being said, before getting into computations, let us discuss however, a bit in advance, some possible ways of getting into the Schrödinger equation. We first have:

COMMENT 10.18. *The Schrödinger equation appears naturally from an abstract claim of de Broglie, regarding the precise wave properties of the electron.*

To be more precise here, the above-mentioned abstract claim of de Broglie leads to the following equations for the wave function of a free electron:

$$\psi_t = e^{-iEt/\hbar} \psi_0 \quad , \quad E\psi_0 = -\frac{\hbar^2}{2m} \Delta \psi_0$$

Now in the context of movement under a time-independent potential  $V$ , as is the potential coming from the proton, these equations can be naturally modified into:

$$\psi_t = e^{-iEt/\hbar} \psi_0 \quad , \quad E\psi_0 = -\frac{\hbar^2}{2m} \Delta \psi_0 + V\psi_0$$

But this is exactly the simplified form of the general Schrödinger equation from Claim 10.16, in the case of a time-independent potential, as we will soon see.

We have as well a second method for getting into the Schrödinger equation, a bit more powerful, but based on more powerful assumptions too, as follows:

COMMENT 10.19. *The Schrödinger equation appears naturally by invoking a bit of matrix mechanics of Heisenberg type, and the Hamiltonian.*

To be more precise here, according to the viewpoint of Heisenberg, the total energy, or Hamiltonian,  $H = T + V$  is represented by the following “operator”:

$$\hat{H} = -\frac{\hbar^2}{2m} \Delta + V$$

And in terms of this operator, the Schrödinger equation simply appears as:

$$i\hbar \dot{\psi} = \hat{H}\psi$$

This is actually the explanation offered by Schrödinger himself in his paper, and we will comment on this a bit later, when having a better knowledge of the subject. We refer also to Feynman [35], Griffiths [43], Weinberg [93] for more on all this.

Now, let us go back to the Schrödinger equation from Claim 10.16, and try to solve it. Let us start with some computations. As a first question, we would like to see how the probability density  $\varphi = |\psi|^2$  evolves in time, and we have here:

PROPOSITION 10.20. *In the context of the general Schrödinger equation,*

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

*we have the following formula,*

$$\dot{\varphi} = \frac{ih}{2m} (\Delta\psi \cdot \bar{\psi} - \Delta\bar{\psi} \cdot \psi)$$

*for the time derivative of the probability density function  $\varphi = |\psi|^2$ .*

PROOF. According to the Leibnitz product rule, we have the following formula:

$$\dot{\varphi} = \frac{d}{dt}|\psi|^2 = \frac{d}{dt}(\psi\bar{\psi}) = \dot{\psi}\bar{\psi} + \psi\dot{\bar{\psi}}$$

On the other hand, the Schrödinger equation and its conjugate read:

$$\begin{aligned}\dot{\psi} &= \frac{ih}{2m} \left( \Delta\psi - \frac{2m}{h^2}V\psi \right) \\ \dot{\bar{\psi}} &= -\frac{ih}{2m} \left( \Delta\bar{\psi} - \frac{2m}{h^2}V\bar{\psi} \right)\end{aligned}$$

By plugging this data, we obtain the following formula:

$$\dot{\varphi} = \frac{ih}{2m} \left[ \left( \Delta\psi - \frac{2m}{h^2}V\psi \right) \bar{\psi} - \left( \Delta\bar{\psi} - \frac{2m}{h^2}V\bar{\psi} \right) \psi \right]$$

But this gives, after simplifying, the formula in the statement. □

As an important application of Proposition 10.20, we have:

THEOREM 10.21. *The general Schrödinger equation, namely*

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

*conserves probability amplitudes, in the sense that we have*

$$\int_{\mathbb{R}^3} |\psi_0|^2 = 1 \implies \int_{\mathbb{R}^3} |\psi_t|^2 = 1$$

*in agreement with the basic probabilistic requirement,  $P = 1$  overall.*

PROOF. According to the formula in Proposition 10.20, we have:

$$\begin{aligned}\frac{d}{dt} \int_{\mathbb{R}^3} |\psi|^2 dx &= \int_{\mathbb{R}^3} \frac{d}{dt} |\psi|^2 dx \\ &= \int_{\mathbb{R}^3} \dot{\varphi} dx \\ &= \frac{ih}{2m} \int_{\mathbb{R}^3} (\Delta\psi \cdot \bar{\psi} - \Delta\bar{\psi} \cdot \psi) dx\end{aligned}$$

Now by remembering the definition of the Laplace operator, we have:

$$\begin{aligned}
\frac{d}{dt} \int_{\mathbb{R}^3} |\psi|^2 dx &= \frac{ih}{2m} \int_{\mathbb{R}^3} \sum_i \left( \frac{d^2 \psi}{dx_i^2} \cdot \bar{\psi} - \frac{d^2 \bar{\psi}}{dx_i^2} \cdot \psi \right) dx \\
&= \frac{ih}{2m} \sum_i \int_{\mathbb{R}^3} \frac{d}{dx_i} \left( \frac{d\psi}{dx_i} \cdot \bar{\psi} - \frac{d\bar{\psi}}{dx_i} \cdot \psi \right) dx \\
&= \frac{ih}{2m} \sum_i \int_{\mathbb{R}^2} \left[ \frac{d\psi}{dx} \cdot \bar{\psi} - \frac{d\bar{\psi}}{dx} \cdot \psi \right]_{-\infty}^{\infty} \frac{dx}{dx_i} \\
&= \frac{ih}{2m} \sum_i \int_{\mathbb{R}^2} 0 \frac{dx}{dx_i} \\
&= 0
\end{aligned}$$

Here we have used at the end the assumption, which is physically speaking, something reasonable, that the wave function and its derivatives vanish at  $\infty$ . Now with this in hand, since the quantity under consideration is constant, we obtain the result.  $\square$

### 10c. States, observables

Let us do now some computations, in order to get some insight into the quantum mechanics of the particle, as dictated by the Schrödinger equation. We first have:

**THEOREM 10.22.** *The average position and momentum of the particle are*

$$\begin{aligned}
\langle x \rangle &= \int_{\mathbb{R}^3} x |\psi|^2 dx \\
\langle p \rangle &= -ih \int_{\mathbb{R}^3} \nabla \psi \cdot \bar{\psi} dx
\end{aligned}$$

*with the convention that the average speed is the derivative of the average position.*

**PROOF.** This follows again by doing some math, as follows:

(1) The formula for the average position  $\langle x \rangle$  is clear from definitions. Regarding now the average speed  $\langle v \rangle$ , we have here the following computation:

$$\begin{aligned}
\langle v \rangle &= \frac{d \langle x \rangle}{dt} \\
&= \int_{\mathbb{R}^3} x \cdot \frac{d}{dt} |\psi|^2 dx \\
&= \int_{\mathbb{R}^3} x \dot{\varphi} dx \\
&= \frac{ih}{2m} \int_{\mathbb{R}^3} x (\Delta \psi \cdot \bar{\psi} - \Delta \bar{\psi} \cdot \psi) dx
\end{aligned}$$

(2) But each of the components can be computed as follows, by taking into account the vanishing formula found in the proof of Theorem 10.21:

$$\begin{aligned}
 \langle v \rangle_i &= \frac{ih}{2m} \int_{\mathbb{R}^3} x_i (\Delta \psi \cdot \bar{\psi} - \Delta \bar{\psi} \cdot \psi) dx \\
 &= \frac{ih}{2m} \int_{\mathbb{R}^3} x_i \sum_j \left( \frac{d^2 \psi}{dx_j^2} \cdot \bar{\psi} - \frac{d^2 \bar{\psi}}{dx_j^2} \cdot \psi \right) dx \\
 &= \frac{ih}{2m} \sum_j \int_{\mathbb{R}^3} x_i \left( \frac{d^2 \psi}{dx_j^2} \cdot \bar{\psi} - \frac{d^2 \bar{\psi}}{dx_j^2} \cdot \psi \right) dx \\
 &= \frac{ih}{2m} \int_{\mathbb{R}^3} x_i \left( \frac{d^2 \psi}{dx_i^2} \cdot \bar{\psi} - \frac{d^2 \bar{\psi}}{dx_i^2} \cdot \psi \right) dx
 \end{aligned}$$

(3) We can now finish the computation by doing two partial integrations, as follows:

$$\begin{aligned}
 \langle v \rangle_i &= \frac{ih}{2m} \int_{\mathbb{R}^3} x_i \cdot \frac{d}{dx_i} \left( \frac{d\psi}{dx_i} \cdot \bar{\psi} - \frac{d\bar{\psi}}{dx_i} \cdot \psi \right) dx \\
 &= -\frac{ih}{2m} \int_{\mathbb{R}^3} \left( \frac{d\psi}{dx_i} \cdot \bar{\psi} - \frac{d\bar{\psi}}{dx_i} \cdot \psi \right) dx \\
 &= -\frac{ih}{m} \int_{\mathbb{R}^3} \frac{d\psi}{dx_i} \cdot \bar{\psi} dx
 \end{aligned}$$

(4) We conclude that the average speed is given by the following formula:

$$\langle v \rangle = -\frac{ih}{m} \int_{\mathbb{R}^3} \nabla \psi \cdot \bar{\psi} dx$$

By multiplying by the mass, we obtain the formula for  $\langle p \rangle$  in the statement.  $\square$

As an interesting speculation now, based on the above two formulae, and inspired from Heisenberg's idea of matrix mechanics, we have:

**SPECULATION 10.23.** *The average position and momentum formulae, written as*

$$\begin{aligned}
 \langle x \rangle &= \int_{\mathbb{R}^3} \bar{\psi} \cdot x \cdot \psi dx \\
 \langle p \rangle &= \int_{\mathbb{R}^3} \bar{\psi} \cdot (-ih\nabla) \cdot \psi dx
 \end{aligned}$$

*suggest that  $x$  represents position, and  $-ih\nabla$  represents momentum.*

Here we don't quite know what the quantities  $x$  and  $-ih\nabla$  really are, mathematically speaking, so let us call them "operators", and we'll see later for axioms. Now with this convention, the above tells us that for computing the average value of  $x, p$ , we must "sandwich" the corresponding operator between  $\bar{\psi}, \psi$ , and then integrate.

Which is something quite remarkable, and we are now very tempted to formulate something extremely general, and of course still a bit vague, as follows:

SPECULATION 10.24. *The average value of an observable  $O$  should appear as*

$$\langle O \rangle = \int_{\mathbb{R}^3} \bar{\psi} \cdot \hat{O} \cdot \psi \, dx$$

*“sandwich between  $\bar{\psi}, \psi$  and integrate”, where  $\hat{O}$  is the operator associated to  $O$ .*

As an illustration, let us see if this sandwiching method works for the kinetic energy of the particle. The kinetic energy is given by the following formula:

$$T = \frac{m||v||^2}{2} = \frac{\langle p, p \rangle}{2m}$$

Thus, the operator associated to the energy should be given by:

$$\hat{T} = \frac{\langle -ih\nabla, -ih\nabla \rangle}{2m} = -\frac{h^2\Delta}{2m}$$

We obtain in this way something which looks quite reasonable, as follows:

$$\langle T \rangle = -\frac{h^2}{2m} \int_{\mathbb{R}^3} \Delta\psi \cdot \bar{\psi} \, dx$$

More generally now, we can incorporate into this the potential energy too, and we are led in this way to the following interesting, conceptual conclusion:

CONCLUSION 10.25. *According to the above speculations, the operator associated to the total energy, or Hamiltonian,  $H = T + V$  is given by*

$$\hat{H} = -\frac{h^2\Delta}{2m} + V$$

*and so the Schrödinger equation itself appears as*

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

*in terms of this operator, as claimed in Comment 10.19.*

To be more precise, according to the above,  $\hat{H}$  appears indeed via the formula in the statement. But now, let us look back at the Schrödinger equation, namely:

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

We recognize on the right the operator  $\hat{H}$  acting on  $\psi$ , and we are led to the conclusion in the statement. But probably enough for now on this topic, and more later.

Back to computations now, and to the Schrödinger equation as it is, simple and clear equation, let us investigate the case of time-independent potentials, as is the case of the Coulomb potential of the proton, that we are mostly interested in. We have here:

THEOREM 10.26. *In the case of time-independent potentials  $V$ , which include the Coulomb potential of the proton, the solutions of the Schrödinger equation*

$$i\hbar\dot{\psi} = -\frac{\hbar^2}{2m}\Delta\psi + V\psi$$

*which are of the following special form, with the time and space variables separated,*

$$\psi_t(x) = w_t\phi(x)$$

*are given by the following formulae, with  $E$  being a certain constant,*

$$w = e^{-iEt/\hbar}w_0 \quad , \quad E\phi = -\frac{\hbar^2}{2m}\Delta\phi + V\phi$$

*with the equation for  $\phi$  being called time-independent Schrödinger equation.*

PROOF. This follows indeed by doing some math, as follows:

(1) Assuming that we have  $\psi = w\phi$  as in the statement, we obtain:

$$\dot{\psi} = \dot{w}\phi \quad , \quad \Delta\psi = w\Delta\phi$$

Thus, the Schrödinger equation reformulates as follows:

$$i\hbar\dot{w}\phi = -\frac{\hbar^2}{2m}w\Delta\phi + Vw\phi$$

By dividing now everything by  $w\phi$ , our equation becomes:

$$i\hbar \cdot \frac{\dot{w}}{w} = -\frac{\hbar^2}{2m} \cdot \frac{\Delta\phi}{\phi} + V$$

(2) Now observe that the left-hand side depends only on time, and the right-hand side depends only on space. Thus, we must have, for a certain constant  $E$ :

$$i\hbar \cdot \frac{\dot{w}}{w} = -\frac{\hbar^2}{2m} \cdot \frac{\Delta\phi}{\phi} + V = E$$

(3) Let us first examine the first equation, involving time, namely:

$$i\hbar \cdot \frac{\dot{w}}{w} = E$$

This equation can be written more conveniently as follows:

$$\frac{d}{dt} \log w = -\frac{iE}{\hbar}$$

Thus we have  $w = e^{-iEt/\hbar}w_0$ , as claimed in the statement.

(4) Regarding now the second equation, involving space, this is:

$$-\frac{\hbar^2}{2m} \cdot \frac{\Delta\phi}{\phi} + V = E$$

But by multiplying by  $\phi$ , this gives the second equation in the statement. □

As a first remark, the above makes the link with the speculations from Comment 10.18, and we can now formulate, as a complement to Conclusion 10.25:

**CONCLUSION 10.27.** *The Schrödinger equation naturally appears from the de Broglie claim on the wave properties of the electron, as claimed in Comment 10.18.*

This is something very nice, and together with Conclusion 10.25, it brings a more conceptual point of view on the Schrödinger equation. We will be back to all this in a moment, when talking axiomatization, based on these facts.

As a second comment, the above results coupled with some extra computations show that the electron is not a particle in the classical sense, the reason being that a classical particle wave function cannot satisfy the time-independent Schrödinger equation. Thus, to put it squarely, in connection with the considerations from the previous section, the harm to Newton is there, in the Schrödinger approach, but hidden well under the carpet. More on this later, when talking about axiomatization.

#### 10d. Matrix mechanics

We discuss here the axiomatization of quantum mechanics, following Heisenberg and Schrödinger, and de Broglie and Dirac. We will be quite brief, and mostly following in our presentation the books of Feynman [35], Griffiths [43] and Weinberg [93]. These are all well-known books, very nicely explaining the basics, and having a correct attitude towards all sorts of “known cracks” of quantum mechanics, and life in general. We will cite these books quite often, and strongly recommend owing and consulting one of them, from time to time, as a complement to what we will be doing here.

Similar books, with the same cocktail of good physics and modesty, but more advanced, include Huang [50], Sakurai [78], Schwinger [83], Shankar [87]. There are of course many other choices too, for learning quantum mechanics. The unavoidable Landau-Lifshitz [63], [64]. Good old books, like Dirac [25], von Neumann [91], Weyl [96]. Spin-centered books, like Peres [70], Nielsen-Chuang [67], Bengtsson-Życzkowski [15].

In short, plenty of choices, and as long as the book does not claim “I understood quantum mechanics, and I will teach it to you”, which only means that the author has no clue on physics, things fine, and you can probably trust that book.

In order to get started now, we will need some math. Remember that the Heisenberg idea was to use infinite matrices, with some sort of frequencies  $\pm 1/\lambda \in \mathbb{R}$  as entries. However, in view of many other things, including the Schrödinger finding that quantum mechanics naturally lives over  $\mathbb{C}$ , we would like in fact our infinite matrices to be over the complex numbers. So, we are led into the following question:

**QUESTION 10.28.** *How do the matrices  $A \in M_\infty(\mathbb{C})$  act on the vectors  $v \in \mathbb{C}^\infty$ ?*



This is something quite tricky. The problem is that the matrices  $A \in M_\infty(\mathbb{C})$  do not always act on the vectors  $v \in \mathbb{C}^\infty$ . As an example, check this out:

$$\begin{pmatrix} 1 & 2 & 3 & \dots \\ 2 & 3 & 4 & \dots \\ 3 & 4 & 5 & \dots \\ \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \\ \vdots \end{pmatrix} = ?$$

This is actually something doubly wrong, first because the vector  $Av$  is not well-defined, but then also since  $v$  itself is not a good vector, its norm being  $\|v\| = \infty$ .

In order to fix all this, let us start with fixing the vector space  $\mathbb{C}^\infty$ . We would like to replace it with its subspace  $H = l^2(\mathbb{N})$  consisting of vectors having finite norm. But this being said, taking a look at what Schrödinger was saying too, why not including in our theory spaces like  $H = L^2(\mathbb{R}^3)$  too. We are led in this way into:

DEFINITION 10.29. *A Hilbert space is a complex vector space  $H$  with a scalar product  $\langle x, y \rangle$ , which will be linear at left and antilinear at right,*

$$\langle \lambda x, y \rangle = \lambda \langle x, y \rangle \quad , \quad \langle x, \lambda y \rangle = \bar{\lambda} \langle x, y \rangle$$

*and which is complete with respect to corresponding norm*

$$\|x\| = \sqrt{\langle x, x \rangle}$$

*in the sense that any sequence  $\{x_n\}$  which is a Cauchy sequence, having the property  $\|x_n - x_m\| \rightarrow 0$  with  $n, m \rightarrow \infty$ , has a limit,  $x_n \rightarrow x$ .*

Here our convention for scalar products, written  $\langle x, y \rangle$  and being linear at left, is one among others, the rationale behind it being as follows:

(1) Dirac formulated in [25] quantum mechanics in terms of scalar products  $\langle x|y \rangle$  linear at right, the idea being that the components  $\langle x|$  and  $|y \rangle$  can start traveling around, as “bras” and “kets”, and with kets needing more linearity than bras.

(2) But this was some time ago, and things have changed since then. In modern physics bras and kets don’t travel anymore, and passed a few students who still struggle with these bras and kets, for the simple reason that all good old physics books, and by laziness most of the present physics courses too, are written with bras and kets, no one does bras and kets anymore. So, Dirac’s notation becomes  $\langle x, y \rangle$ .

(3) In relation now with linearity, physicists have been generally sticking to Dirac’s convention in [25], linear at right, with no questions asked. Mathematicians however are quite interested in such questions, and for good reason. It’s their job. There are all sorts of choices in math, such as the unit circle being oriented  $\circlearrowright$  instead of  $\circlearrowleft$ , functions acting denoted  $f(x)$  instead of  $x(f)$ , and so on. And mathematicians take such things seriously,

and regularly change their notations, exactly as physicists take the questions regarding units seriously, and regularly update the SI system. And the current trend is towards  $\langle x, y \rangle$  linear at left. So, that's what we will be using,  $\langle x, y \rangle$  linear at left.

(4) Finally, there is a choice between  $\langle x, y \rangle$  and things like  $\langle x, y \rangle$ , which is a matter of taste. Personally I love doing lots of computations, on a daily basis, and with this being actually the job I'm paid for, and since writing acute angles like  $\langle, \rangle$  is 3 times quicker than writing obtuse angles like  $\langle, \rangle$ , I use the former. And not only I use them, but I also find that they are far more beautiful, due to their efficiency. QED.

Getting back now to work, and to Definition 10.29, in its entirety, there is some mathematics encapsulated there, needing some discussion. First, we have:

**THEOREM 10.30.** *Given an index set  $I$ , which can be finite or not, the space of square-summable vectors having indices in  $I$ , namely*

$$l^2(I) = \left\{ (x_i)_{i \in I} \mid \sum_i |x_i|^2 < \infty \right\}$$

*is a Hilbert space, with scalar product as follows:*

$$\langle x, y \rangle = \sum_i x_i \bar{y}_i$$

*When  $I$  is finite,  $I = \{1, \dots, N\}$ , we obtain in this way the usual space  $H = \mathbb{C}^N$ .*

**PROOF.** This can be done in several steps, as follows:

(1) Given a vector  $x \in \mathbb{C}^I$ , let us define its norm by the following formula:

$$\|x\| = \sqrt{\sum_i |x_i|^2}$$

We know that  $l^2(I) \subset \mathbb{C}^I$  is the space of vectors satisfying  $\|x\| < \infty$ . We want to prove that  $l^2(I)$  is a vector space, that  $\langle x, y \rangle$  is a scalar product on it, that  $l^2(I)$  is complete with respect to  $\|\cdot\|$ , and finally that for  $|I| < \infty$  we have  $l^2(I) = \mathbb{C}^{|I|}$ .

(2) The last assertion,  $l^2(I) = \mathbb{C}^{|I|}$  for  $|I| < \infty$ , is clear, because in this case the sums are finite, so the condition  $\|x\| < \infty$  is automatic. So, we know at least one thing.

(3) Regarding the rest, our claim here, which will more or less prove everything, is that for any two vectors  $x, y \in l^2(I)$  we have the Cauchy-Schwarz inequality:

$$|\langle x, y \rangle| \leq \|x\| \cdot \|y\|$$

(4) In order to prove this inequality, consider the following quantity, depending on a real variable  $t \in \mathbb{R}$ , and on a variable on the unit circle,  $w \in \mathbb{T}$ :

$$f(t) = \|twx + y\|^2$$

By developing  $f$ , we see that this is a degree 2 polynomial in  $t$ :

$$\begin{aligned} f(t) &= \langle twx + y, twx + y \rangle \\ &= t^2 \langle x, x \rangle + tw \langle x, y \rangle + t\bar{w} \langle y, x \rangle + \langle y, y \rangle \\ &= t^2 \|x\|^2 + 2t \operatorname{Re}(w \langle x, y \rangle) + \|y\|^2 \end{aligned}$$

Since  $f$  is obviously positive, its discriminant must be negative, and so we have:

$$|\operatorname{Re}(w \langle x, y \rangle)| \leq \|x\| \cdot \|y\|$$

Now the point is that we can arrange for the number  $w \in \mathbb{T}$  to be such that the quantity  $w \langle x, y \rangle$  is real. Thus, we obtain, as desired:

$$|\langle x, y \rangle| \leq \|x\| \cdot \|y\|$$

(5) Now with Cauchy-Schwarz proved, everything is straightforward. We first obtain, by raising to the square and expanding, that for any  $x, y \in l^2(I)$  we have:

$$\|x + y\|^2 \leq (\|x\| + \|y\|)^2$$

Thus  $l^2(I)$  is indeed a vector space, the other vector space conditions being trivial.

(6) Also,  $\langle x, y \rangle$  is surely a scalar product on this vector space, because all the conditions for a scalar product, which are as follows, are satisfied:

- \*  $\langle x, y \rangle$  is linear in  $x$ , and antilinear in  $y$ .
- \*  $\overline{\langle x, y \rangle} = \langle y, x \rangle$ , for any  $x, y$ .
- \*  $\langle x, x \rangle \geq 0$ , for any  $x \neq 0$ .

(7) Finally, the fact that our space  $l^2(I)$  is indeed complete with respect to its norm  $\|\cdot\|$  follows in the obvious way, the limit of a Cauchy sequence  $\{x_n\}$  being the vector  $y = (y_i)$  given by  $y_i = \lim_{n \rightarrow \infty} x_{ni}$ , with all the verifications here being trivial.  $\square$

Going now a bit abstract, we have, more generally, the following result, which shows that our formalism covers as well the Schrödinger spaces of type  $L^2(\mathbb{R}^3)$ :

**THEOREM 10.31.** *Given an arbitrary space  $X$  with a positive measure  $\mu$  on it, the space of square-summable complex functions on it, namely*

$$L^2(X) = \left\{ f : X \rightarrow \mathbb{C} \mid \int_X |f(x)|^2 d\mu(x) < \infty \right\}$$

*is a Hilbert space, with scalar product as follows:*

$$\langle f, g \rangle = \int_X f(x) \overline{g(x)} d\mu(x)$$

When  $X = I$  is discrete, meaning that the measure  $\mu$  on it is the counting measure,  $\mu(\{x\}) = 1$  for any  $x \in X$ , we obtain in this way the previous spaces  $l^2(I)$ .

PROOF. This is something routine, remake of Theorem 10.30, as follows:

(1) The proof of the first, and main assertion is something perfectly similar to the proof of Theorem 10.30, by replacing everywhere the sums by integrals.

(2) With the remark that we forgot to say in the statement that the  $L^2$  functions are by definition taken up to equality almost everywhere,  $f = g$  when  $\|f - g\| = 0$ .

(2) As for the last assertion, when  $\mu$  is the counting measure all our integrals here become usual sums, and so we recover in this way Theorem 10.30.  $\square$

As a third and last theorem about Hilbert spaces, that we will need, we have:

**THEOREM 10.32.** *Any Hilbert space  $H$  has an orthonormal basis  $\{e_i\}_{i \in I}$ , which is by definition a set of vectors whose span is dense in  $H$ , and which satisfy*

$$\langle e_i, e_j \rangle = \delta_{ij}$$

*with  $\delta$  being a Kronecker symbol. The cardinality  $|I|$  of the index set, which can be finite, countable, or worse, depends only on  $H$ , and is called dimension of  $H$ . We have*

$$H \simeq l^2(I)$$

*in the obvious way, mapping  $\sum \lambda_i e_i \rightarrow (\lambda_i)$ . The Hilbert spaces with  $\dim H = |I|$  being countable, including  $l^2(\mathbb{N})$  and  $L^2(\mathbb{R})$ , are all isomorphic, and are called separable.*

PROOF. We have many assertions here, the idea being as follows:

(1) In finite dimensions an orthonormal basis  $\{e_i\}_{i \in I}$  can be constructed by starting with any vector space basis  $\{x_i\}_{i \in I}$ , and using the Gram-Schmidt procedure. As for the other assertions, these are all clear, from basic linear algebra.

(2) In general, the same method works, namely Gram-Schmidt, with one subtlety coming from the fact that the basis  $\{e_i\}_{i \in I}$  will not span in general the whole  $H$ , but just a dense subspace of it, as it is in fact obvious by looking for instance at the standard basis of  $l^2(\mathbb{N})$ . And there is a second subtlety as well, coming from the fact that the recurrence procedure needed for Gram-Schmidt must be replaced by some sort of “transfinite recurrence”, using scary tools from logic, and more specifically the Zorn lemma.

(3) Finally, everything at the end is clear from definitions, except perhaps for the fact that  $L^2(\mathbb{R})$  is separable. But here we can argue that, since functions can be approximated by polynomials, we have a countable algebraic basis, namely  $\{x^n\}_{n \in \mathbb{N}}$ , called the Weierstrass basis, that we can orthogonalize afterwards by using Gram-Schmidt.  $\square$

Observe that, in contrast to Theorem 10.30 and Theorem 10.31, there are several non-trivial things going on with Theorem 10.32. First we have the full proof for the basis, based on the Zorn lemma, which normally takes 1-2 pages, but which can easily take 5-6 pages, if you really want that Zorn lemma proved too, that we have of course avoided. But then, we have also some subtleties at the end, with the space  $L^2(\mathbb{R})$  being in theory

separable, but in practice not really, because the orthogonalization of the Weierstrass basis  $\{x^n\}_{n \in \mathbb{N}}$  is something quite complicated. More on this later.

Moving ahead, now that we know what our vector spaces are, we can talk about infinite matrices with respect to them. And the situation here is as follows:

**THEOREM 10.33.** *Given a Hilbert space  $H$ , consider the linear operators  $T : H \rightarrow H$ , and for each such operator define its norm by the following formula:*

$$\|T\| = \sup_{\|x\|=1} \|Tx\|$$

*The operators which are bounded,  $\|T\| < \infty$ , form then a complex algebra  $B(H)$ , which is complete with respect to  $\|\cdot\|$ . When  $H$  comes with a basis  $\{e_i\}_{i \in I}$ , we have*

$$B(H) \subset \mathcal{L}(H) \subset M_I(\mathbb{C})$$

*where  $\mathcal{L}(H)$  is the algebra of all linear operators  $T : H \rightarrow H$ , and  $\mathcal{L}(H) \subset M_I(\mathbb{C})$  is the correspondence  $T \rightarrow M$  obtained via the usual linear algebra formulae, namely:*

$$T(x) = Mx \quad , \quad M_{ij} = \langle Te_j, e_i \rangle$$

*In infinite dimensions, none of the above two inclusions is an equality.*

**PROOF.** This is something straightforward, well-known by linear algebra in finite dimensions, and the proof in general is similar. As for the last assertion, which is more tricky, in finite dimensions we have of course  $B(H) = \mathcal{L}(H) = M_I(\mathbb{C})$ . However, in infinite dimensions, we have matrices not producing operators, as for instance:

$$M = \begin{pmatrix} 1 & 1 & \dots \\ 1 & 1 & \dots \\ \vdots & \vdots & \end{pmatrix}$$

As for the examples of linear operators which are not bounded, these are more complicated, coming from logic, and we will not need them in what follows.  $\square$

Finally, as a second and last result regarding the operators, we will need:

**THEOREM 10.34.** *Each operator  $T \in B(H)$  has an adjoint  $T^* \in B(H)$ , given by:*

$$\langle Tx, y \rangle = \langle x, T^*y \rangle$$

*The operation  $T \rightarrow T^*$  is antilinear, antimultiplicative, involutive, and satisfies:*

$$\|T\| = \|T^*\| \quad , \quad \|TT^*\| = \|T\|^2$$

*When  $H$  comes with a basis  $\{e_i\}_{i \in I}$ , the operation  $T \rightarrow T^*$  corresponds to*

$$(M^*)_{ij} = \overline{M_{ji}}$$

*at the level of the associated matrices  $M \in M_I(\mathbb{C})$ .*

PROOF. This is standard too, and can be proved in 3 steps, as follows:

(1) The existence of the adjoint operator  $T^*$ , given by the formula in the statement, comes from the fact that the function  $\varphi(x) = \langle Tx, y \rangle$  being a linear map  $H \rightarrow \mathbb{C}$ , we must have a formula as follows, for a certain vector  $T^*y \in H$ :

$$\varphi(x) = \langle x, T^*y \rangle$$

Moreover, since this vector is unique,  $T^*$  is unique too, and we have as well:

$$(S + T)^* = S^* + T^* \quad , \quad (\lambda T)^* = \bar{\lambda} T^* \quad , \quad (ST)^* = T^* S^* \quad , \quad (T^*)^* = T$$

Observe also that we have indeed  $T^* \in B(H)$ , because:

$$\begin{aligned} \|T\| &= \sup_{\|x\|=1} \sup_{\|y\|=1} \langle Tx, y \rangle \\ &= \sup_{\|y\|=1} \sup_{\|x\|=1} \langle x, T^*y \rangle \\ &= \|T^*\| \end{aligned}$$

(2) Regarding now  $\|TT^*\| = \|T\|^2$ , which is a key formula, observe that we have:

$$\|TT^*\| \leq \|T\| \cdot \|T^*\| = \|T\|^2$$

On the other hand, we have as well the following estimate:

$$\begin{aligned} \|T\|^2 &= \sup_{\|x\|=1} |\langle Tx, Tx \rangle| \\ &= \sup_{\|x\|=1} |\langle x, T^*Tx \rangle| \\ &\leq \|T^*T\| \end{aligned}$$

By replacing  $T \rightarrow T^*$  we obtain from this  $\|T\|^2 \leq \|TT^*\|$ , as desired.

(3) Finally, when the Hilbert space  $H$  comes with an orthonormal basis  $\{e_i\}_{i \in I}$ , the formula  $\langle Tx, y \rangle = \langle x, T^*y \rangle$  applied with  $x = e_i$ ,  $y = e_j$  reads:

$$(M^*)_{ij} = \overline{M_{ji}}$$

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

So, this was for the basics of operator theory, extending the basics of linear algebra. For more on all this, including full proofs for certain things in the above, you can check any book labeled functional analysis, or operator theory, or operator algebras, with a good reference here being the functional analysis book by Lax [66].

We are now ready for axiomatizing quantum mechanics. Following Heisenberg and Schrödinger, and then especially Dirac, who did the axiomatization work, we have:

AXIOMS 10.35. *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 our previous “sandwiching” formula, with the operators*

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

*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 our previous “sandwiching” formula holds true, and with this having all sorts of interesting consequences, already discussed before. 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.

All this is of course over-simplified, and as usual, for more on all this, we refer to Feynman [35], Griffiths [43] or Weinberg [93]. And also to Lax [66] for more math, because, as mentioned above, the operators  $T : H \rightarrow H$  can be densely defined, and with this going beyond what we were saying before, in Theorems 10.33 and 10.34. However, as some sort of explanation here, Theorems 10.33 and 10.34 were stated as such for good reason, because we will see later, in chapters 13-16, that more advanced versions of quantum mechanics can be formulated by using bounded operators,  $T \in B(H)$ .

As a first result of our new theory, we have:

THEOREM 10.36 (Heisenberg). *We have the following uncertainty principle,*

$$\sigma_S \cdot \sigma_T \geq \left| \frac{\langle [S, T] \rangle}{2} \right|$$

*regarding the variances of any two observables  $S, T$ . In particular, we have*

$$\sigma_x \cdot \sigma_p \geq \frac{\hbar}{2}$$

*implying that you cannot measure position and momentum at the same time.*

PROOF. This follows indeed by doing some mathematics with operators and their commutators, and for details here, we refer for instance to Griffiths [43].  $\square$

The above uncertainty principle, which is as old as quantum mechanics, is something quite surprising, that you can love or not. There are two schools of thought here:

(1) Bohr school. Adopt the uncertainty principle, and quantum mechanics in general, as axiomatized and developed by Heisenberg, Schrödinger, Dirac, and further build on it as much as you can, with these rules. This Bohr philosophy was widely adopted in the golden years of quantum mechanics, 1920-1940, with spectacular results. In recent times, however, quantum mechanics has enormously evolved, with several successive reformulations, and this philosophy has become more of a mathematician's thing.

(2) Einstein school. Again adopt the uncertainty principle, and the Heisenberg, Schrödinger, Dirac rules for quantum mechanics, and do what's to be done, that is, develop the theory, but this time with the idea in mind of trying to make evolve this theory, towards something deterministic. And this is what physicists have been doing, since 1950-1960, with several improvements of quantum mechanics, namely QED, QCD, QFT, string theory and so on, slowly but surely going towards determinism.

In the remainder of this book we will adopt physicists' philosophy, of course. Einstein all the way. And who cares if we are still so far from the final results. What matters is to fight for the right cause. More on all this in the 150 pages that we still have left.

### 10e. Exercises

Well, young reader, we can only give you here the above-mentioned problem, left by Einstein, Bohr and all the greats, to the generations to come:

EXERCISE 10.37. *Find a reasonable geometry theory describing the exact trajectory of the electron around the proton.*

And don't be afraid. It's just a new idea, that is needed. Exactly like Heisenberg had his new idea. Or like Schrödinger had his new idea. Coming out of nowhere.



## CHAPTER 11

### The hydrogen atom

#### 11a. Laplace operator

Moving ahead towards hydrogen, we are interested in the case where  $V$  is the usual quadratic Coulomb potential of the proton, given by the following formula:

$$V = -\frac{e^2}{4\pi\epsilon_0} \cdot \frac{1}{r}$$

This potential is time-independent, and our main tool here will be the theory of the time-independent Schrödinger equation, as developed in the previous chapter. Let us recall from there that we have the following result:

**THEOREM 11.1.** *In the case of time-independent potentials  $V$ , which include the Coulomb potential of the proton, the solutions of the Schrödinger equation*

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

*which are of the following special form, with the time and space variables separated,*

$$\psi_t(x) = w_t\phi(x)$$

*are given by the following formulae, with  $E$  being a certain constant,*

$$w = e^{-iEt/\hbar}w_0 \quad , \quad E\phi = -\frac{h^2}{2m}\Delta\phi + V\phi$$

*with the equation for  $\phi$  being called time-independent Schrödinger equation.*

**PROOF.** This is something that we know from chapter 10, that we have included here, for convenience. Let us recall too the idea. By dividing by  $\psi$ , the equation becomes:

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

Now since the left-hand side depends only on time, and the right-hand side depends only on space, both quantities must equal a constant  $E$ , and this gives the result.  $\square$

Moving ahead with theory, we can further build on Theorem 11.1, with a number of key observations on the time-independent Schrödinger equation, as follows:

**THEOREM 11.2.** *In the case of time-independent potentials  $V$ , the Schrödinger equation and its time-independent version have the following properties:*

- (1) *For solutions of type  $\psi = w_t \phi(x)$ , the density  $\varphi = |\psi|$  is time-independent, and more generally, all quantities of type  $\langle T \rangle$  are time-independent.*
- (2) *The time-independent Schrödinger equation can be written as  $\hat{H}\phi = E\phi$ , with  $H = T + V$  being the total energy, of Hamiltonian.*
- (3) *For solutions of type  $\psi = w_t \phi(x)$  we have  $\langle H^k \rangle = E^k$  for any  $k$ . In particular we have  $\langle H \rangle = E$ , and the variance is  $\langle H^2 \rangle - \langle H \rangle^2 = 0$ .*

**PROOF.** All the formulae are clear indeed from the fact that, when using the sandwiching formula for computing averages, the phases will cancel:

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

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

All the above is quite interesting, physically speaking, and for a discussion here, we refer to Griffiths [43]. We will be back as well to this, a bit later.

We have as well the following result, mathematical this time:

**THEOREM 11.3.** *The solutions of the Schrödinger equation with time-independent potential  $V$  appear as linear combinations of separated solutions*

$$\psi = \sum_n c_n e^{-iE_n t/\hbar} \phi_n$$

*with the absolute values of the coefficients being given by*

$$\langle H \rangle = \sum_n |c_n|^2 E_n$$

$|c_n|$  being the probability for a measurement to return the energy value  $E_n$ .

**PROOF.** This is something standard, which follows from Fourier analysis, which allows the decomposition of  $\psi$  as in the statement, and that we will not really need, in what follows next. As before, for a physical discussion here, we refer to Griffiths [43].  $\square$

Finally, a word about time-dependent potentials too, that we will ignore in this chapter. These are very important, due to the following:

**REMARK 11.4.** *For more complicated situations, like the helium atom, or heavier, the potential  $V$  in the Schrödinger equation is time-dependent, because the electron is subject here to the repulsions from the other electrons, which move in time.*

More on such potentials later, when taking helium and other atoms. In what follows we will be exclusively obsessed by hydrogen, where the math is simpler, and that we want to solve, above everything, anyway. By the way our obsession reminds that of the astrophysicists, who often call anything different from hydrogen “metals”.

Moving ahead towards hydrogen, let us assume that  $V$  is the usual quadratic Coulomb potential of the proton. This potential is rotationally invariant, and it is convenient to use spherical coordinates, which are as follows, with  $s \in [0, \pi]$  and  $t \in [0, 2\pi]$ :

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

We first must reformulate the Schrödinger equation in spherical coordinates. And for this purpose, we will need a well-known, scary computation, as follows:

**THEOREM 11.5.** *The Laplace operator in spherical coordinates is:*

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

**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.  $\square$

We can now reformulate the Schrödinger equation in spherical coordinates, and then separate the variables, which leads to a radial and angular equation, as follows:

**THEOREM 11.6.** *The time-independent Schrödinger equation in spherical coordinates separates, for solutions of type  $\phi = \rho(r)\alpha(s, t)$ , into two equations, as follows,*

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

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

**PROOF.** By using the formula in Theorem 11.5, the time-independent Schrödinger equation reformulates in spherical coordinates as follows:

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

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:

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

In order to solve this equation, we will do two manipulations. First, by multiplying everything by  $2mr^2/(h^2\rho\alpha)$ , this equation takes the following more convenient form:

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

Now observe that by moving the radial terms to the left, and the angular terms to the right, this latter equation can be written as follows:

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

Since this latter equation is now separated between radial and angular variables, both sides must be equal to a certain constant  $-K$ , as follows:

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

But this leads to the conclusion in the statement.  $\square$

### 11b. Spherical harmonics

Let us first study the angular equation, and this for reasons that will become clear later, the idea being that this equation forces the constant  $K$  to be of the form  $K = l(l+1)$  with  $l \in \mathbb{N}$ , which can be used afterwards in the study of the radial equation.

The study will be quite long. We first have the following result:

**PROPOSITION 11.7.** *The angular equation that we found before, namely*

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

*separates, for solutions of type  $\alpha = \sigma(s)\theta(t)$ , into two equations, as follows,*

$$\frac{1}{\theta} \cdot \frac{d^2\theta}{dt^2} = -m^2$$

$$\frac{\sin s}{\sigma} \cdot \frac{d}{ds} \left( \sin s \cdot \frac{d\sigma}{ds} \right) + K \sin^2 s = m^2$$

*with  $m$  being a constant, called azimuthal equation, and polar equation.*

PROOF. This is something elementary, the idea being as follows:

(1) Before anything, for such questions, we need to have a better understanding of the angles  $s, t$ , and the differences between them. So, recall that these angles come from:

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

To be more precise, here  $r \in [0, \infty)$  is the radius,  $s \in [0, \pi]$  is the polar angle, and  $t \in [0, 2\pi]$  is the azimuthal angle. Be said in passing, there are several conventions and notations here, and the above ones, that we use here, come from the general ones in  $N$  dimensions, because further coordinates can be easily added, in the obvious way.

(2) Getting back now to our question, by plugging  $\alpha = \sigma(s)\theta(t)$  into the angular equation, we obtain:

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

By dividing everything by  $\sigma\theta$ , this equation can be written as follows:

$$-\frac{1}{\theta} \cdot \frac{d^2\theta}{dt^2} = \frac{\sin s}{\sigma} \cdot \frac{d}{ds} \left( \sin s \cdot \frac{d\sigma}{ds} \right) + K \sin^2 s$$

Since the variables are separated, we must have, for a certain constant  $m$ :

$$\begin{aligned} \frac{1}{\theta} \cdot \frac{d^2\theta}{dt^2} &= -m^2 \\ \frac{\sin s}{\sigma} \cdot \frac{d}{ds} \left( \sin s \cdot \frac{d\sigma}{ds} \right) + K \sin^2 s &= m^2 \end{aligned}$$

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

Regarding the azimuthal equation, things here are quickly settled, as follows:

PROPOSITION 11.8. *The solutions of the azimuthal equation, namely*

$$\frac{1}{\theta} \cdot \frac{d^2\theta}{dt^2} = -m^2$$

*are the functions as follows, with  $a, b \in \mathbb{C}$  being parameters,*

$$\theta(t) = ae^{imt} + be^{-imt}$$

*and with only the case  $m \in \mathbb{Z}$  being acceptable, on physical grounds.*

PROOF. The first assertion is clear, because we have a second order equation, and two obvious solutions for it,  $e^{\pm imt}$ , and then their linear combinations, and that's all. Regarding the last assertion, the point here is that by using  $\theta(t) = \theta(t + 2\pi)$ , which is a natural physical assumption on the wave function, we are led to  $m \in \mathbb{Z}$ , as stated.  $\square$



We are now about to solve the angular equation, with only the polar equation remaining to be studied. However, in practice, this polar equation is 10 times more difficult than everything what we did so far, and so please be patient. We first have:

PROPOSITION 11.9. *The polar equation that we found before, namely*

$$\frac{\sin s}{\sigma} \cdot \frac{d}{ds} \left( \sin s \cdot \frac{d\sigma}{ds} \right) + K \sin^2 s = m^2$$

with  $m \in \mathbb{Z}$ , translates via  $\sigma(s) = f(\cos s)$  into the following equation,

$$(1 - x^2)f''(x) - 2xf'(x) = \left( \frac{m^2}{1 - x^2} - K \right) f(x)$$

where  $x = \cos s$ , called Legendre equation.

PROOF. Let us first do a number of manipulations on our equation, before making the change of variables. By multiplying by  $\sigma$ , our equation becomes:

$$\sin s \cdot \frac{d}{ds} \left( \sin s \cdot \frac{d\sigma}{ds} \right) = (m^2 - K \sin^2 s) \sigma$$

By differentiating at left, this equation becomes:

$$\sin s (\cos s \cdot \sigma' + \sin s \cdot \sigma'') = (m^2 - K \sin^2 s) \sigma$$

Finally, by dividing everything by  $\sin^2 s$ , our equation becomes:

$$\sigma'' + \frac{\cos s}{\sin s} \cdot \sigma' = \left( \frac{m^2}{\sin^2 s} - K \right) \sigma$$

Now let us set  $\sigma(s) = f(\cos s)$ . With this change of variables, we have:

$$\sigma = f(\cos s)$$

$$\sigma' = -\sin s \cdot f'(\cos s)$$

$$\sigma'' = -\cos s \cdot f'(\cos s) + \sin^2 s \cdot f''(\cos s)$$

By plugging this data, our radial equation becomes:

$$\sin^2 s \cdot f''(\cos s) - 2 \cos s \cdot f'(\cos s) = \left( \frac{m^2}{\sin^2 s} - K \right) f(\cos s)$$

Now with  $x = \cos s$ , which is our new variable, this equation reads:

$$(1 - x^2)f''(x) - 2xf'(x) = \left( \frac{m^2}{1 - x^2} - K \right) f(x)$$

But this is the Legendre equation, as stated. □

Here comes now the difficult point. We have the following non-trivial result:

THEOREM 11.10. *The solutions of the Legendre equation, namely*

$$(1 - x^2)f''(x) - 2xf'(x) = \left(\frac{m^2}{1 - x^2} - K\right)f(x)$$

*can be explicitly computed, via some complicated math, and only the case*

$$K = l(l + 1) \quad : \quad l \in \mathbb{N}$$

*is acceptable, on physical grounds.*

PROOF. The first part is something quite complicated, involving the hypergeometric functions  ${}_2F_1$ , that you don't want to hear about, believe me. As for the second part, analysis and physical speculations, this is something not trivial either.  $\square$

So, what to do? We will not fight with such extreme questions, and instead we will go very slowly, constructing from scratch the solutions which are "acceptable", with full details. And in what regards their uniqueness, well, we will refer here to Theorem 11.10, whose proof can be certainly found somewhere, if you are really interested in that.

In order to construct the solutions, let us start with an extremely basic and fundamental problem. We have seen in chapter 10 that all Hilbert spaces of type  $L^2(X)$  with  $X \subset \mathbb{R}$  are separable, the reason behind this being the fact that we can start with the Weierstrass basis  $\{x^l\}$ , and then orthogonalize by Gram-Schmidt. However, as also mentioned in chapter 10, the Gram-Schmidt orthogonalization, while certainly being something that works in theory, is something quite complicated, if you want to do it explicitly.

Time now to understand this. For the simplest compact space  $X \subset \mathbb{R}$ , or unit ball of  $\mathbb{R}$  if you prefer, which is the interval  $[-1, 1]$ , this problem can be solved as follows:

THEOREM 11.11. *The orthogonal basis of  $L^2[-1, 1]$  obtained by starting with the Weierstrass basis  $\{x^l\}$ , and doing Gram-Schmidt, is the family of polynomials  $\{P_l\}$ , with each  $P_l$  being of degree  $l$ , and with positive leading coefficient, subject to:*

$$\int_{-1}^1 P_k(x)P_l(x) dx = \delta_{kl}$$

*These polynomials, called Legendre polynomials, satisfy the equation*

$$(1 - x^2)P_l''(x) - 2xP_l'(x) + l(l + 1)P_l(x) = 0$$

*which is the Legendre equation at  $m = 0$ , and with  $K = l(l + 1)$ . Moreover,*

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

*which is called the Rodrigues formula for Legendre polynomials.*

PROOF. As a first observation, we are not lost somewhere in abstract math, because of the occurrence of the Legendre equation. As for the proof, this goes as follows:

(1) The first assertion is clear, because the Gram-Schmidt procedure applied to the Weierstrass basis  $\{x^l\}$  can only lead to a certain family of polynomials  $\{P_l\}$ , with each  $P_l$  being of degree  $l$ , and also unique, if we assume that it has positive leading coefficient, with this  $\pm$  choice being needed, as usual, at each step of Gram-Schmidt.

(2) In order to have now an idea about these beasts, here are the first few of them, which can be obtained say via a straightforward application of Gram-Schmidt:

$$\begin{aligned} P_0 &= 1 \\ P_1 &= x \\ P_2 &= (3x^2 - 1)/2 \\ P_3 &= (5x^3 - 3x)/2 \\ P_4 &= (35x^4 - 30x^2 + 3)/8 \\ P_5 &= (63x^5 - 70x^3 + 15x)/8 \end{aligned}$$

(3) Now thinking about what Gram-Schmidt does, this is certainly something by recurrence. And examining the recurrence leads to the Legendre equation, as stated.

(4) As for the Rodrigues formula, by uniqueness no need to try to understand where this formula comes from, and we have two choices here, either by verifying that  $\{P_l\}$  is orthonormal, or by verifying the Legendre equation. And both methods work.  $\square$

Going ahead now, we can solve in fact the Legendre equation at any  $m$ , as follows:

PROPOSITION 11.12. *The general Legendre equation, with parameters  $m \in \mathbb{N}$  and  $K = l(l+1)$  with  $l \in \mathbb{N}$ , namely*

$$(1-x^2)f''(x) - 2xf'(x) = \left( \frac{m^2}{1-x^2} - l(l+1) \right) f(x)$$

*is solved by the following functions, called Legendre functions,*

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

*where  $P_l$  are as before the Legendre polynomials. Also, we have*

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

*called Rodrigues formula for Legendre functions.*

PROOF. The first assertion is something elementary, coming by differentiating  $m$  times the Legendre equation, which leads to the general Legendre equation. As for the second assertion, this follows from the Rodrigues formula for Legendre polynomials.  $\square$

And this is the end of our study. Eventually. By putting together all the above results, the last 6 of them to be more precise, we are led to the following conclusion:

**THEOREM 11.13.** *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.  $\square$

As an inevitable comment here, our study of the angular equation was not complete, with all sorts of easy things missing, but also with something non-trivial not done, namely the uniqueness. This was discussed in Theorem 11.10, redirecting you towards  ${}_2F_1$  and hypergeometric functions. Up to you here, depending on what you want to do in life. The point is that hypergeometric functions can depend on  $N = 1, 2, 3, 4, 5, 6, 7, \dots$  variables, and the bigger your  $N$  that you master, the better your math and physics will be.

As examples here, most scientists get away with  $N = 1, 2$ . A good mathematician must do  $N = 3, 4$ . As for good theoretical physics,  $N = 5, 6, 7$  is usually required. For the story, I once had a difficult problem, and gave it to a  $N = 7$  physicist, who solved it right away. And it took me a few good months to understand his solution.

### 11c. Bohr energy

In order now to finish our study, and eventually get to conclusions about hydrogen, 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 11.14. *The radial equation, written with  $K = l(l + 1)$ ,*

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

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

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

*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:

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

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

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

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.  $\square$

Let us now, eventually, get to hydrogen. Here  $V$  is the usual quadratic Coulomb potential of the proton, given by the following formula, with  $e$  being as usual the charge of the electron, and  $\varepsilon_0$  being the electric permittivity of free space:

$$V = -\frac{e^2}{4\pi\varepsilon_0} \cdot \frac{1}{r}$$

However, before getting into math, we must first discuss units. Remember from chapters 5-6 above the story of the Coulomb constant  $K$ , which was eventually replaced by  $\varepsilon_0 = 1/(4\pi K)$ , due to the Gauss law, and the Maxwell equations? Well, the Maxwell equations being now obsolete, not to say wrong, in quantum mechanics, time to welcome back the Coulomb constant  $K$ . Our new conventions will be as follows:

CONVENTIONS 11.15. *We welcome back the Coulomb constant  $K$ , given by:*

$$K = 8.987\,551\,7923(14) \times 10^9$$

*Also, we welcome as new quantity for energy the electron volt  $eV$ ,*

$$1eV = e = 1.602\,176\,634 \times 10^{-19}$$

*with this being regarded, as per our SI philosophy, as a constant, not a unit.*

As usual, lots of fun here with units. In what regards the Coulomb constant  $K$  and minus the charge of the electron  $e$ , these are given by the formulae in the statement, with the formula of  $e$  being exact, as per latest SI regulations. As for the electron volt eV, this is by definition the amount of kinetic energy gained by an electron accelerating from rest through an electric potential difference of 1 volt in vacuum. Which in practice means that 1 eV is simply the number  $e$ , but regarded as a constant for energy.

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

FACT 11.16. *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.

Getting back now to math, it remains to solve the modified radial equation, for the above potential  $V$ . And we have here the following result, which does not exactly solve this radial equation, but provides us instead with something far better, namely the proof of the original claim by Bohr, which was at the origin of everything:

THEOREM 11.17 (Schrödinger). *In the case of the hydrogen atom, where  $V$  is the Coulomb potential of the proton, the modified radial equation, which reads*

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

leads to the Bohr formula for allowed energies,

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

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, and we will be following Griffiths [43], with some details missing. The idea is as follows:

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

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

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

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

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

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

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

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

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:

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

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

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

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:

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

(8) Thus, we proved the Bohr formula. Regarding now the numerics, the data is as follows, with all formulae being of course approximate:

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



We obtain successively that we have the following formulae:

$$\begin{aligned}\frac{Ke^2}{h} &= \frac{8.988 \times 1.602^2}{1.055} \times \frac{10^9 \times 10^{-38}}{10^{-34}} = 2.186 \times 10^6 \\ \left(\frac{Ke^2}{h}\right)^2 &= 2.186^2 \times 10^{12} = 4.779 \times 10^{12} \\ \frac{m}{2} \left(\frac{Ke^2}{h}\right)^2 &= \frac{9.109 \times 4.779}{2} \times 10^{12-31} = 2.177 \times 10^{-18}\end{aligned}$$

Thus  $E_1$  is as in the statement. In electron volts now, the figure is:

$$\frac{E_1}{e} = \frac{2.177 \times 10^{-18}}{1.602 \times 10^{-19}} = 13.591$$

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

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

THEOREM 11.18. *The Rydberg constant for hydrogen is given by*

$$R = -\frac{E_1}{h_0c}$$

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

$$\frac{1}{\lambda_{n_1n_2}} = R \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

simply reads, via the energy formula in Theorem 11.17,

$$\frac{1}{\lambda_{n_1n_2}} = \frac{E_{n_2} - E_{n_1}}{h_0c}$$

which is in agreement with the Planck formula  $E = h_0c/\lambda$ .

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

$$R = \frac{-E_1}{h_0c} = \frac{2.177 \times 10^{-18}}{6.626 \times 10^{-34} \times 2.998 \times 10^8} = 1.096 \times 10^7$$

As a consequence, and passed now what the experiments exactly say, we can define the Rydberg constant of hydrogen abstractly, by the following formula:

$$R = \frac{m}{2h_0c} \left( \frac{Ke^2}{h} \right)^2$$

Regarding now the second assertion, by dividing  $R = -E_1/(h_0c)$  by any number of type  $n^2$  we obtain, according to the energy convention in Theorem 11.17:

$$\frac{R}{n^2} = -\frac{E_n}{h_0c}$$

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.  $\square$

With these spectacular applications explained, let us go back now to our study of the Schrödinger equation, done throughout this chapter. Our conclusions are:

**THEOREM 11.19.** *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  $p = \gamma r$  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 11.20.** *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  $a = 1/\gamma$  is the inverse of the parameter appearing in our computations above,

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

called Bohr radius of the hydrogen atom. This Bohr radius is the mean distance between the electron and the proton, in the ground state, and is given by the formula

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

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

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

(1) According to the various formulae in the proof of Theorem 11.7, taken at  $n = 1$ , the parameter  $\gamma$  appearing in the computations there is given by:

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

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

(2) Regarding the wave function, according to Theorem 11.19 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.  $\square$

Getting back now to the general setting of Theorem 11.19, the point is that the polynomials  $v(p)$  appearing there are well-known objects in mathematics, as follows:

PROPOSITION 11.21. *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:

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

(1) The orthogonal basis obtained by applying Gram-Schmidt to the Weierstrass basis  $\{x^q\}$  is then the basis formed by the Laguerre polynomials  $\{L_q\}$ .

(2) We have the explicit formula for  $L_q$  in the statement, which is analogous to the Rodrigues formula for the Legendre polynomials.

(3) The first assertion follows from the fact that the coefficients of the associated Laguerre polynomials satisfy the equation for the coefficients of  $v(p)$ .

(4) Alternatively, the first assertion follows as well by using an equation for the Laguerre polynomials, which is very similar to the Legendre equation.  $\square$

With the above result in hand, we can now improve Theorem 11.19, as follows:

THEOREM 11.22. *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, namely Theorem 11.19 and Proposition 11.21, and then doing some remaining work, concerning the normalization of the wave function, which leads to the normalization factor appearing above.  $\square$

And isn't this beautiful. If you want to impress your nerdy friends, or even a random customer in a pub, this is surely the formula that you want to show to them.

### 11d. Fine structure

What is next? All sorts of corrections to the solution that we found, due to various phenomena that we neglected in our computations, or rather in our modelling of the problem, which can be both of electric and relativistic nature. But before getting into that, let us first enjoy what we found, say by taking it as a final, exact result regarding the hydrogen atom. As a first conclusion, of quite philosophical nature, we have:

CONCLUSION 11.23. *The phenomenon of quantization appears, mathematically speaking, from certain equations which generically blow up, and force the various separation constants  $C \in \mathbb{R}$  which appear to be integers,  $C \in \mathbb{N}$ .*

To be more precise, the phenomenon of quantization that we are talking about is of course the Bohr energy one, allowing discrete energies only,  $E_n$  with  $n \in \mathbb{N}$ , which is the mother of everything, in quantum mechanics. Looking back at the proof of this fact, separation constants  $C \in \mathbb{R}$  which mysteriously became integers,  $C \in \mathbb{N}$ , was indeed the mathematical phenomenon behind this. Which appeared no less than 3 times:

(1) First when the azimuthal/polar separation parameter, denoted  $m^2$ , turned to be the square of an integer,  $m \in \mathbb{Z}$ .

(2) Then when the radial/angular separation constant  $K$  turned to be of a similar form,  $K = l(l+1)$  with  $l \in \mathbb{N}$ .

(3) And finally in the context of the radial equation, where the parameter  $S$  there turned to be of the form  $S = 2n$ , with  $n \in \mathbb{N}$ .

This is very nice, we have now a clear mathematical idea about why things are quantized, in quantum mechanics. The 3 space coordinates and the 1 time coordinate, who usually live in peace, get into fights when it comes to differential equations.

As another comment now, in our study we dismissed several times all sorts of solutions, on various physical grounds, usually unacceptable blow up. But, at a more advanced level, some of these solutions make sense of course, due to the following fact:

FACT 11.24. *The hydrogen atom is not the general 2-body problem in quantum mechanics, but rather the case of confined, stable orbits. Some of the solutions which blow up correspond to scattering, in the context of an electron/proton meeting.*

Again, this is something a bit philosophical. In analogy with classical mechanics, what we did is to solve the planetary motion problem. But things like comets and asteroids still need to be investigated, for having a full theory. And which is something quite technical, called “scattering theory”, that we will not get into here, in this book.

Back to work now, let us explain the series of corrections to the Schrödinger solution to the hydrogen atom. We will focus on energy only, so let us start by recalling:

THEOREM 11.25 (Schrödinger). *The energy of the  $\phi_{nlm}$  state of the hydrogen atom is independent on the quantum numbers  $l, m$ , given by the Bohr formula*

$$E_n = -\frac{\alpha^2}{n^2} \cdot \frac{mc^2}{2}$$

where  $\alpha$  is a dimensionless constant, called fine structure constant, given by

$$\alpha = \frac{Ke^2}{hc}$$

which in practice means  $\alpha \simeq 1/137$ .

PROOF. This is the Bohr energy formula that we know, proved by Schrödinger, and reformulated in terms of Sommerfeld’s fine structure constant:

(1) We know from Theorem 11.17 that we have the following formula, which can be written as in the statement, by using the fine structure constant  $\alpha$ :

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

(2) Observe now that our modified Bohr formula can be further reformulated as follows, with  $T_c$  being the kinetic energy of the electron traveling at speed  $c$ :

$$E_n = -\frac{\alpha^2}{n^2} \cdot T_c$$

Thus  $\alpha^2$ , and so  $\alpha$  too, is dimensionless, as being a quotient of energies.

(3) Let us doublecheck however this latter fact, the check being instructive. With respect to the SI system that we use, the units for  $K, e, h, c$  are:

$$U_K = \frac{m^3 \cdot kg}{s^2 \cdot C^2} \quad , \quad U_e = C \quad , \quad U_h = \frac{m^2 \cdot kg}{s} \quad , \quad U_c = \frac{m}{s}$$

Thus the units for the fine structure constant  $\alpha$  are, as claimed:

$$U_\alpha = U_C \cdot U_e^2 \cdot U_h^{-1} \cdot U_c^{-1} = \frac{m^3 \cdot kg}{s^2 \cdot C^2} \cdot C^2 \cdot \frac{s}{m^2 \cdot kg} \cdot \frac{s}{m} = 1$$

(4) In what regards now the numerics, these are as follows:

$$\alpha = \frac{Ke^2/h}{c} \simeq \frac{2.186 \times 10^6}{2.998 \times 10^8} = 7.291 \times 10^{-3} \simeq \frac{1}{137}$$

Here we have used an estimate for  $Ke^2/h$ , from the proof of Theorem 11.17.  $\square$

The fine structure constant  $\alpha$  is a remarkable quantity, as obvious from the above, and more on it in a moment. Among its other magic features, it manages well  $2\pi$  factors. Indeed, by using  $K = 1/(4\pi\epsilon_0)$  and  $h = h_0/2\pi$ , we can write this constant as:

$$\alpha = \frac{e^2}{2\epsilon_0 h_0 c}$$

Finally, let us record the complete official data for  $\alpha$  and its inverse  $\alpha^{-1}$ :

$$\alpha = 0.007\,297\,352\,5693(11)$$

$$\alpha^{-1} = 137.035\,999\,084(21)$$

As a final comment here, all this lengthy discussion about  $\alpha$  might sound a bit like mania, or mysticism. But wait for it. Sometimes soon  $\alpha$  will be part of your life.

Moving ahead now with corrections to Theorem 11.25, we will be very brief, and for further details, we refer as usual to our favorite books, Feynman [35], Griffiths [43] and Weinberg [93]. We first have the following result, which is something non-trivial:

**THEOREM 11.26.** *There is a relativistic correction to be made to the Bohr energy  $E_n$  of the state  $\phi_{nlm}$ , depending on the quantum number  $l$ , given by*

$$\mathcal{E}_{nl} = \frac{\alpha^2 E_n}{n^2} \left( \frac{n}{l + 1/2} - \frac{3}{4} \right)$$

*coming by replacing the kinetic energy by the relativistic kinetic energy.*

**PROOF.** According to Einstein, the relativistic kinetic energy is given by:

$$T = \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \dots$$

The Schrödinger equation, based on  $T = p^2/2m$ , must be therefore corrected with a  $\mathcal{T} = -p^4/(8m^3c^2)$  term, and this leads to the above correction term  $\mathcal{E}_{nl}$ .  $\square$

Equally non-trivial is the following correction, independent from the above one:

**THEOREM 11.27.** *There is a spin-related correction to be made to the Bohr energy  $E_n$  of the state  $\phi_{nlm}$ , depending on the number  $j = l \pm 1/2$ , given by*

$$\mathcal{E}_{nj} = -\frac{\alpha^2 E_n}{n^2} \cdot \frac{n(j - l)}{(l + 1/2)(j + 1/2)}$$

*coming from the torque of the proton on the magnetic moment of the electron.*

PROOF. As we will explain in chapter 12 below, the electron has a spin  $\pm 1/2$ , which is naturally associated to the quantum number  $l$ , leading to the parameter  $j = l \pm 1/2$ . But, knowing now that the electron has a spin, the proton which moves around it certainly acts on its magnetic moment, and this leads to the above correction term  $\mathcal{E}_{nj}$ .  $\square$

So, these are the first two corrections to be made, and again, we refer to Feynman [35], Griffiths [43], Weinberg [93] for details. Obviously we don't quite know what we're doing here, but let us add now the above corrections to  $E_n$ , and see what we get. We obtain in this way one of the most famous formulae in quantum mechanics, namely:

**THEOREM 11.28.** *The energy levels of the hydrogen atom, taking into account the fine structure coming from the relativistic and spin-related correction, are given by*

$$E_{nj} = E_n \left[ 1 + \frac{\alpha^2}{n^2} \left( \frac{n}{j + 1/2} - \frac{3}{4} \right) \right]$$

with  $j = l \pm 1/2$  being as above, and with  $\alpha$  being the fine structure constant.

PROOF. We have the following computation, based on the above formulae:

$$\begin{aligned} \mathcal{E}_{nl} + \mathcal{E}_{nj} &= \frac{\alpha^2 E_n}{n^2} \left( \frac{n}{l + 1/2} - \frac{3}{4} - \frac{n(j - l)}{(l + 1/2)(j + 1/2)} \right) \\ &= \frac{\alpha^2 E_n}{n^2} \left( \frac{n}{l + 1/2} \left( 1 - \frac{j - l}{j + 1/2} \right) - \frac{3}{4} \right) \\ &= \frac{\alpha^2 E_n}{n^2} \left( \frac{n}{j + 1/2} - \frac{3}{4} \right) \end{aligned}$$

Thus the corrected formula of the energy is as follows:

$$\begin{aligned} E_{nj} &= E_n + \mathcal{E}_{nl} + \mathcal{E}_{nj} \\ &= E_n + \frac{\alpha^2 E_n}{n^2} \left( \frac{n}{j + 1/2} - \frac{3}{4} \right) \end{aligned}$$

We are therefore led to the conclusion in the statement.  $\square$

Summarizing, quantum mechanics is more complicated than what originally appears from Schrödinger's solution of the hydrogen atom. Which was something quite complicated too, we must admit that. And the story is not over here, because on top of the above fine structure correction, which is of order  $\alpha^2$ , we have afterwards the Lamb shift, which is an order  $\alpha^3$  correction, then the hyperfine splitting, and more.

As usual, we refer to Feynman [35], Griffiths [43], Weinberg [93] for more on all this. In what concerns us, we will be back to such questions in Part IV below, directly at the advanced level, following Feynman and others, who managed to find a global way of viewing all the phenomena that can appear, corresponding to an infinite series in  $\alpha$ .

To be more precise, the theory here, called quantum electrodynamics (QED), is an advanced version of quantum mechanics, still used nowadays for any delicate computation. Ironically, while providing an exact answer for the hydrogen atom, QED messes up things too, because that exact answer is not exactly computable. More on this later.

As a conclusion now to all this, the battle with the hydrogen atom, and with quantum mechanics in general, seems to be never-ending. And so it is, since all this is still an ongoing story, nowadays. There are in fact several levels of skill here, as follows:

- 1 Dan: Bohr.
- 2 Dan: Heisenberg.
- 3 Dan: Schrödinger.
- 4 Dan: Feynman.
- 5 Dan: Advanced QFT.
- 6 Dan: String theory.
- 7 Dan: Deterministic.

We are now at 3 Dan, but in chapters 13-14 below we will get to 4 Dan, and then in chapters 15-16 we will practice a bit at 5-6 Dan, getting of course a hell of a beating. As for 7 Dan, this means “smarter than Einstein”, that is, solving his problem.

### 11e. Exercises

We have seen in this chapter that the hydrogen atom, which is the 2-body problem in quantum mechanics, can be solved by using the Schrödinger equation, and some basic know-how for such equations, called partial differential equations (PDE).

This was similar to what we did in chapter 1, solving there the planetary motion question, which is the 2-body problem in classical mechanics, by using the Newton equation, and some know-how for such equations, called ordinary differential equations (ODE).

So, time now to seriously get interested in such methods? As exercise, we have:

EXERCISE 11.29. *Learn some basic mathematical analysis, and then some basic theory of the differential equations, say from Rudin, Arnold, Evans.*

To be more precise, for getting started you need to read Rudin’s real and complex analysis book [74], which is a sort of Bible for mathematicians. Especially the chapters there on Fourier analysis, that you will need all the time for ODE, PDE, or for anything else that you might want to do in your life, of mathematical type. And also the chapters there on harmonic functions, that you will need all the time as well.

Then, many choices for equations. You can go here with Arnold [4] for ODE, and check his small PDE book as well, and with Evans [30] for more detailed PDE.



## CHAPTER 12

### Heavier atoms

#### 12a. Angular momentum

We have seen that a theory of quantum mechanics can be developed, as to solve the hydrogen atom, at least approximately, along the lines suggested by Bohr. Our goal here will be to extend these results to the case of heavier atoms, fully realizing Bohr's program. Our grand result will be a new, sharp look at the periodic table of elements.

Which periodic table of elements is the alpha and omega of everything. At least if you live here, on Earth. In short, our results will be impressive, putting quantum mechanics in relation with everything happening at  $10^{-9}$  and below, as claimed in chapter 9.

We will of course need to learn and develop a lot of further quantum mechanics, of quite general type, in order to achieve this goal, following Pauli and Dirac, then Bose and Fermi, and many others. This further quantum mechanics can be of course used for doing all sorts of other things as well, and more on this in chapters 13-16 below.

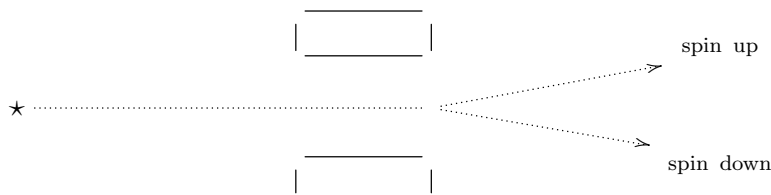
In order to get started, we have seen at the end of the previous chapter that the fine structure correction to the Bohr energy formula involved two things. First we had a relativistic correction, that we have not worked out in detail, but which looks like something within our range, that can only be understood and computed. But then we had as well as spin-related correction, involving the notion of spin, which is totally new to us. So, as a first question that we would like to solve, we have:

**QUESTION 12.1.** *What is the electron spin? That is, what experiments prove that the electron spins? And then, importantly, what is the mathematics of the spin?*

Talking mathematics first, the spin, if that beast exists indeed, is certainly not visible on the wave function  $\psi$ , because this wave function deals with position only. Thus, at least we know one thing, once the spin observed, we will most likely have to incorporate it into our theory by using the matrix mechanics formalism of Heisenberg.

Talking physics now, the main experiment leading to spin is as follows:

FACT 12.2 (Stern-Gerlach experiment). *When passing a beam of electrons through an inhomogeneous magnetic field, these electrons get deflected 50 – 50 up or down,*



*with the only possible explanation being that the electrons have a spin, which is 50 – 50 up or down. The same happens with a beam of neutral atoms, and a magnetic field strong enough, to be put at blame being the statistics of the spins of the constituents.*

So, this was the experiment, and what we call here “up” and “down” is of course the binary choice of the spin orientation, a bit as for usual, round objects in  $\mathbb{R}^3$ . That is, our Earth turns to the right, and in physics we would say that it has “spin up”. Was the Earth turning to the left, we would say in physics that it has “spin down”.

Of course, our presentation above is over-simplified. The original experiment was with neutral particles, namely silver atoms, and this in order to avoid the Lorentz force, which will curve the trajectory of any charged particle, to a much greater extent than the spin up/down deviation to be observed. Later experiments, with charged particles, used some extra apparatus, namely a suitable electric field, positioned after the electromagnet in the above diagram, designed to cancel the effects of the Lorentz force.

As an important observation, the Stern-Gerlach experiment does not observe the absolute, 3D spin up/down feature of the particles, but just a 1D component of it. However, it is possible to cascade experiments, by sending each of the output beams into separate Stern-Gerlach devices, and with these devices having various 3D orientations, and deduce some further conclusions from this. We refer here to Feynman [35].

So long for the Stern-Gerlach experiment. Getting back now to theory and speculations, as a first, innocent observation based on the above, we have:

OBSERVATION 12.3. *A single electron has an interesting life even when fixed, because it spins. Thus, no need for Heisenberg or Schrödinger for getting introduced to quantum mechanics, you can just try to understand the mathematics of a fixed electron.*

Moreover, as a cherry on the cake, as we will soon discover, the above-mentioned mathematics is that of the  $2 \times 2$  complex matrices, which is at the same time something elementary, and fascinating. Which, getting us now into philosophy, leads us into the temptation of burying the physics, and talking right away about  $2 \times 2$  matrices.

And shall we do this or not. Looking at the physics literature, there is a fair mess in the treatment of spin. At one end, you have spin-centered books, taking Observation 12.3 literally, and starting the book with a long, not to say never-ending, discussion about spin. Then you have quantum information related books, such as Bengtsson-Życzkowski [15], Nielsen-Chuang [67], Peres [70], which by a certain desire of brevity and efficiency, rapidly bury the physics of spin, and talk instead about  $2 \times 2$  matrices. And then you have well-known and loved books such as Feynman [35], Griffiths [43], Weinberg [93], presenting all sorts of rather incomprehensible explanations regarding the spin, which vary with authors' taste, for eventually ending, of course, with  $2 \times 2$  matrices.

And so again, what shall we do, talk about  $2 \times 2$  matrices or not. Not clear. But, as usual in such difficult situations, we can always ask the cat. We haven't seen him since chapter 8, when stuck with some difficult questions in thermodynamics, and good news, cat is here, and willing to talk physics. So, what about spin. And cat answers:

CAT 12.4. *Be honest, and say what you have to say. And don't worry about your young readers, they will survive.*

This sounds wise as usual, thanks cat. So, we will follow this advice. But let me get first a huge mug of coffee, or rather huge mug of expresso, because fighting with the physics of the spin with bare hands is something which is reputed impossible.

To start with, and as a matter of reframing our discussion, and having something fresh to rely upon, let us demolish Observation 12.3 above with:

FACT 12.5. *Observation 12.3 is something toxic. You can't really measure spin, and build a serious theory on that alone. What you need to do is to observe spin in context, via its tiny corrections to quantum mechanics. More specifically, spin is an order*

$$\alpha^2 \simeq \frac{1}{10,000}$$

*correction to quantum mechanics, and more precisely to the Bohr energy formula, with the spin correction there appearing as a complement to the relativistic correction. And with this being the correct, healthy and constructive definition of spin.*

In short, we are getting here back to the beginning, general quantum mechanics, with the main conclusion of the Stern-Gerlach experiment, namely “spin exists”, recorded. Of course it is possible to say a bit more from Stern-Gerlach, namely recording the scattering angle, and doing some math there, but this basically does not advance us much. So better forget about Stern-Gerlach, and get back to general quantum mechanics.

The point now is that, with the above fact in hand, not only we are into truth, as we should be, but also we start getting an idea on how to reach to the mathematics of

the spin. To be more precise, we should just think relativity, in the context of quantum mechanics, and with a bit of luck, all this thinking will lead us into spin.

In practice now, all this is doable, but a bit complicated, and was done by Klein, Gordon, Dirac a few years after Uhlenbeck, Goudsmit, Pauli came up with their theory of spin. So, let us briefly explain this idea, which is very beautiful, and we'll come later to Uhlenbeck, Goudsmit, Pauli. Consider the Schrödinger equation for a free electron:

$$i\hbar\dot{\psi} = -\frac{\hbar^2}{2m}\Delta\psi$$

Relativity theory dictates that the 3 space coordinates and the 1 time coordinate should be on the same footing, and so that we should replace  $\dot{\psi}$  by something of type  $\ddot{\psi}$ . But this can be done by replacing the kinetic energy operator  $T = \Delta/2m$  by its relativistic analogue, and also by invoking the invariance under Lorentz transformations, and we are led in this way to the following equation, called Klein-Gordon equation:

$$\left(\Delta - \frac{1}{c^2} \cdot \frac{d^2}{dt^2}\right)\psi = \frac{m^2c^2}{\hbar^2}\psi$$

The point now, which is the key one, discovered by Dirac short after Klein and Gordon, is that it is possible to extract the square root of the Klein-Gordon operator:

$$\Delta - \frac{1}{c^2} \cdot \frac{d^2}{dt^2} = \left(\frac{Pd}{dx} + \frac{Qd}{dy} + \frac{Rd}{dz} + \frac{i}{c} \cdot \frac{Sd}{dt}\right)^2$$

Indeed, we need for this purpose matrices  $P, Q, R, S$  which anticommute,  $AB = -BA$ , and whose squares equal one,  $A^2 = 1$ . But such beasts can be found in  $M_4(\mathbb{C})$ , and then we can take the formal square root of the Klein-Gordon equation:

$$\left(\frac{Pd}{dx} + \frac{Qd}{dy} + \frac{Rd}{dz} + \frac{i}{c} \cdot \frac{Sd}{dt}\right)\psi = \frac{mc}{\hbar}\psi$$

And the thing now, which is truly remarkable, is that this latter equation, called Dirac equation, does work indeed, in the sense that it is a true equation of physics, improving the Schrödinger equation. And a closer look at all this reveals afterwards that the fine structure of hydrogen, comprising the relativistic correction and the spin correction, can be understood in this way, leading to a clear mathematics of the spin.

All this is very beautiful, and leads us into:

THOUGHT 12.6. *Our criticism from Fact 12.5 was probably too harsh, relativity and spin alike being probably more than a mere*

$$\alpha^2 \simeq \frac{1}{10,000}$$

*order correction to quantum mechanics. And this is because the Dirac equation, which is of first order, is something simpler than the Schrödinger equation.*

In fact, we're now again into Observation 12.3, and this time armed with some solid math, and more specifically with a first-grade weapon, the Dirac equation. Which starts to be a bit tiring, yes I know, looks like we're changing our opinion about spin faster than Madonna is changing her shoes. But blame the cat, he came with his advice Cat 12.4.

Moving ahead now, and still following Cat 12.4, after some more thinking, the Dirac equation remains however something a bit speculative, or perhaps something too advanced, and it would be much better, at least to start with, to forget about relativity and abstractions, and have something more solid, regarding the spin.

And fortunately, there is a second way of viewing things, very elementary, inspired from our study of classical mechanics, or even from the movement of our good old Earth, which rotates and spins at the same time, which is as follows:

**PHILOSOPHY 12.7.** *In analogy with classical mechanics, spin should be something of same nature as angular momentum, coming on top of it.*

And good news, this will be our final, stable philosophy. Eventually.

To be more precise, following Uhlenbeck, Goudsmit, Pauli, we will first talk angular momentum, then we will axiomatize spin as being the quantity which naturally “complements” the angular momentum. Then we will talk about  $2 \times 2$  matrices, and review the fine structure corrections to hydrogen as well. And finally, regarding the Klein-Gordon and Dirac equations, we will be back to them in chapter 13 below.

So, let us first talk about angular momentum, and we'll get to spin later. We will need the following basic result, for doing computations:

**PROPOSITION 12.8.** *The components of the position operator  $x = (x_1, x_2, x_3)$  and momentum operator  $p = -ih\nabla$  satisfy the following relations,*

$$[x_i, x_j] = [p_i, p_j] = 0$$

$$[x_i, p_j] = ih\delta_{ij}$$

where  $[a, b] = ab - ba$ , called canonical commutation relations.

**PROOF.** All the above formulae are elementary, as follows:

(1) The components of the position operator  $x = (x_1, x_2, x_3)$  obviously commute with each other,  $x_i x_j = x_j x_i$ , which makes their commutators vanish,  $[x_i, x_j] = 0$ .

(2) Regarding the momentum operator  $p = -ih\nabla$ , its components are as follows:

$$p_1 = -ih \cdot \frac{d}{dx_1} \quad , \quad p_2 = -ih \cdot \frac{d}{dx_2} \quad , \quad p_3 = -ih \cdot \frac{d}{dx_3}$$

Since partial derivatives commute with each other, we obtain  $[p_i, p_j] = 0$ .

(3) It remains to prove the last formula, and we have here:

$$\begin{aligned}
 [x_i, p_j]f &= (x_i p_j - p_j x_i)f \\
 &= -ih \left( x_i \cdot \frac{df}{dx_j} - \frac{d}{dx_j}(x_i f) \right) \\
 &= -ih \left( x_i \cdot \frac{df}{dx_j} - \frac{dx_i}{dx_j} \cdot f - x_i \cdot \frac{df}{dx_j} \right) \\
 &= ih \cdot \frac{dx_i}{dx_j} \cdot f \\
 &= ih \delta_{ij} \cdot f
 \end{aligned}$$

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

The above might look a bit complicated, and the simplest way to remember it is that “everything commutes”, that is,  $ab = ba$ , except for the coordinates and momenta coordinates taken in the same direction, which are subject to the following rule:

$$x_i p_i = p_i x_i + ih$$

Getting now to angular momentum, it is convenient to change notation, with  $(x, y, z)$  instead of  $(x_1, x_2, x_3)$ , due to the vector product involved, which will break the symmetry between coordinates. We have the following result, to start with:

**THEOREM 12.9.** *The components of the angular momentum operator*

$$L = x \times (-ih\nabla)$$

*satisfy the following equations,*

$$[L_x, L_y] = ihL_z$$

$$[L_y, L_z] = ihL_x$$

$$[L_z, L_x] = ihL_y$$

*called commutation relations for the angular momentum.*

**PROOF.** With the more familiar notation  $p = -ih\nabla$  for momentum, or rather for the associated operator, the components of the angular momentum operator are:

$$L_x = yp_z - zp_y$$

$$L_y = zp_x - xp_z$$

$$L_z = xp_y - yp_x$$

Let us prove the first commutation relation. We have:

$$\begin{aligned}
 [L_x, L_y] &= [yp_z - zp_y, zp_x - xp_z] \\
 &= [yp_z, zp_x] - [yp_z, xp_z] - [zp_y, zp_x] + [zp_y, xp_z]
 \end{aligned}$$

By heavily using the commutation relations from Proposition 12.8, we have:

$$[yp_z, zp_x] = yp_z zp_x - zp_x yp_z = y(zp_z - ih)p_x - zyp_x p_z = -ihyp_x$$

$$[yp_z, xp_z] = yp_z xp_z - xp_z yp_z = 0$$

$$[zp_y, zp_x] = zp_y zp_x - zp_x zp_y = 0$$

$$[zp_y, xp_z] = zp_y xp_z - xp_z zp_y = zxp_y p_z - x(zp_z - ih)p_y = ihxp_y$$

We conclude that the commutator that we were computing is given by the following formula, which is precisely the one in the statement:

$$\begin{aligned} [L_x, L_y] &= -ihyp_x + ihxp_y \\ &= ih(xp_y - yp_x) \\ &= ihL_z \end{aligned}$$

The proof of the other two commutation relations is similar, or can be simply obtained by invoking the cyclic invariance  $x \rightarrow y \rightarrow z \rightarrow x$  of our problem, which cyclic invariance is not broken by the vector product  $\times$  used, and so can indeed be invoked.  $\square$

As an interesting consequence of Theorem 12.9, we have:

PROPOSITION 12.10. *The following operator, called square of angular momentum*

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

*commutes with all 3 operators  $L_x, L_y, L_z$ .*

PROOF. We have the following computation, to start with:

$$\begin{aligned} [L^2, L_x] &= (L_x^2 + L_y^2 + L_z^2)L_x - L_x(L_x^2 + L_y^2 + L_z^2) \\ &= L_y^2 L_x + L_z^2 L_x - L_x L_y^2 - L_x L_z^2 \\ &= [L_y^2, L_x] + [L_z^2, L_x] \end{aligned}$$

The first commutator can be computed with a trick, as follows:

$$\begin{aligned} [L_y^2, L_x] &= L_y L_y L_x - L_x L_y L_y \\ &= L_y L_y L_x - L_y L_x L_y + L_y L_x L_y - L_x L_y L_y \\ &= L_y [L_y, L_x] + [L_y, L_x] L_y \\ &= L_y (-ihL_z) + (-ihL_z) L_y \\ &= -ih(L_y L_z + L_z L_y) \end{aligned}$$

The second commutator can be computed with the same trick, as follows:

$$\begin{aligned}
[L_z^2, L_x] &= L_z L_z L_x - L_x L_z L_z \\
&= L_z L_z L_x - L_z L_x L_z + L_z L_x L_z - L_x L_z L_z \\
&= L_z [L_z, L_x] + [L_z, L_x] L_z \\
&= L_z (ihL_y) + (ihL_y) L_z \\
&= ih(L_z L_y + L_y L_z)
\end{aligned}$$

Now by summing we obtain the following commutation relation, as desired:

$$[L^2, L_x] = 0$$

The proof of the other two commutation relations is similar, or we can simply invoke here the cyclic symmetry argument from the end of the proof of Theorem 12.9.  $\square$

Let us discuss now the diagonalization of the momentum operators  $L_x, L_y, L_z$ . Since these operators do not commute, we cannot hope for a joint diagonalization for them. Thus, we must choose one of them, and for reasons that will become clear later, when writing things in spherical coordinates, we will choose  $L_x$ .

In view of Proposition 12.10, this operator  $L_x$  does commute with  $L^2$ , and so we can hope for a joint diagonalization of  $L^2, L_x$ . And, so is what happens:

**THEOREM 12.11.** *The operators  $L^2, L_x$  diagonalize as*

$$L^2 f_l^m = h^2 l(l+1) f_l^m$$

$$L_x f_l^m = hm f_l^m$$

where  $l \in \mathbb{N}/2$  and  $m = -l, -l+1, \dots, l-1, l$ .

**PROOF.** This is something quite long, the idea being as follows:

(1) For reasons that will become clear later on, let us introduce two operators as follows, called raising and lowering operators:

$$L_+ = L_y + iL_z$$

$$L_- = L_y - iL_z$$

We will often deal with these operators at the same time, using the following notation:

$$L_{\pm} = L_y \pm iL_z$$



(2) We have the following computation:

$$\begin{aligned}
 [L_x, L_{\pm}] &= [L_x, L_y] \pm i[L_x, L_z] \\
 &= ihL_z \pm i(-ihL_y) \\
 &= h(iL_z \pm L_y) \\
 &= \pm h(\pm iL_z + L_y) \\
 &= \pm hL_{\pm}
 \end{aligned}$$

(3) Our claim now is that  $L^2 f = \lambda f$ ,  $L_x f = \mu f$  imply:

$$L^2(L_{\pm}f) = \lambda(L_{\pm}f)$$

$$L_x(L_{\pm}f) = (\mu \pm h)(L_{\pm}f)$$

Indeed, the first formula follows from:

$$\begin{aligned}
 L^2(L_{\pm}f) &= L_{\pm}(L^2 f) \\
 &= L_{\pm}(\lambda f) \\
 &= \lambda(L_{\pm}f)
 \end{aligned}$$

As for the second formula, this follows from:

$$\begin{aligned}
 L_x(L_{\pm}f) &= L_x L_{\pm}f \\
 &= (L_x L_{\pm} - L_{\pm} L_x)f + L_{\pm} L_x f \\
 &= \pm h L_{\pm}f + L_{\pm}(\mu f) \\
 &= (\mu \pm h)(L_{\pm}f)
 \end{aligned}$$

(4) Now in view of the formulae found in (3), the raising and lowering operators act on the joint eigenfunctions of  $L^2, L_x$ , by leaving the  $L^2$  eigenvalue unchanged, and by raising and lowering the eigenvalue of  $L_x$ . But both this raising process and lowering process for the eigenvalue of  $L_x$  cannot go on forever, because of the following estimate:

$$\begin{aligned}
 \lambda &= \langle L^2 \rangle \\
 &= \langle L_x^2 \rangle + \langle L_y^2 \rangle + \langle L_z^2 \rangle \\
 &= \mu^2 + \langle L_y^2 \rangle + \langle L_z^2 \rangle \\
 &\geq \mu^2
 \end{aligned}$$

(5) In order to see exactly how the raising and lowering processes terminate, we will need some more computations. We have:

$$\begin{aligned}
 L_{\pm}L_{\mp} &= (L_y \pm iL_z)(L_y \mp iL_z) \\
 &= L_y^2 + L_z^2 \mp i(L_yL_z - L_zL_y) \\
 &= L_y^2 + L_z^2 \mp i(i\hbar L_x) \\
 &= L_y^2 + L_z^2 \pm \hbar L_x \\
 &= L^2 - L_x^2 \pm \hbar L_x
 \end{aligned}$$

Thus, we have the following formula:

$$L^2 = L_{\pm}L_{\mp} + L_x^2 \mp \hbar L_x$$

Now assuming  $L_x f = \hbar l f$ , at termination of the raising process, we have:

$$\begin{aligned}
 L^2(f) &= (L_-L_+ + L_x^2 + \hbar L_x)f \\
 &= (0 + \hbar^2 l^2 + \hbar^2 l)f \\
 &= \hbar^2 l(l+1)f
 \end{aligned}$$

Similarly, assuming  $L_x f = \hbar l' f$ , at termination of the lowering process, we have:

$$\begin{aligned}
 L^2(f) &= (L_+ - L_- + L_x^2 - \hbar L_x)f \\
 &= (0 + \hbar^2 l'^2 - \hbar^2 l')f \\
 &= \hbar^2 l'(l' - 1)f
 \end{aligned}$$

Thus  $l(l+1) = l'(l'-1)$ , and since  $l' = l+1$  is impossible, due to raising vs lowering, we must have  $l' = -l$ , and this leads to the conclusion in the statement.

(6) Finally, for being complete, the full and conceptual understanding of all the above imperatively requires a certain cat climbing a certain ladder, and for full details here, and for other things missing from the above proof, we refer to Griffiths [43].  $\square$

Moving ahead now, let us write everything in spherical coordinates, and find the eigenfunctions. We have here the following remarkable result:

**THEOREM 12.12.** *In spherical coordinates  $r, s, t$  we have*

$$\begin{aligned}
 L_x &= -\frac{i\hbar}{dt} \\
 L_y &= i\hbar \left( \frac{\sin t}{ds} + \frac{\cos s \cos t}{\sin s} \cdot \frac{1}{dt} \right) \\
 L_z &= -i\hbar \left( \frac{\cos t}{ds} - \frac{\cos s \sin t}{\sin s} \cdot \frac{1}{dt} \right)
 \end{aligned}$$

and the spherical harmonics are joint eigenfunctions of  $L^2, L_x$ .

PROOF. We recall that, according to our usual,  $N$ -dimensional looking conventions, the spherical coordinates are as follows, with  $r \in [0, \infty)$  being the radius,  $s \in [0, \pi]$  being the polar angle, and  $t \in [0, 2\pi]$  being the azimuthal angle:

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

(1) We know that we have  $L = -i\hbar x \times \nabla$ , so let us first compute  $\nabla$  in spherical coordinates. We have here, according to the chain rule for derivatives:

$$\begin{aligned} \nabla &= \begin{pmatrix} dr/dx & ds/dx & dt/dx \\ dr/dy & ds/dy & dt/dy \\ dr/dz & ds/dz & dt/dz \end{pmatrix} \begin{pmatrix} d/dr \\ d/ds \\ d/dt \end{pmatrix} \\ &= \begin{pmatrix} dx/dr & dy/dr & dz/dr \\ dx/ds & dy/ds & dz/ds \\ dx/dt & dy/dt & dz/dt \end{pmatrix}^{-1} \begin{pmatrix} d/dr \\ d/ds \\ d/dt \end{pmatrix} \end{aligned}$$

(2) On the other hand, we know from chapter 11 above that we have:

$$\begin{pmatrix} dx/dr & dx/ds & dx/dt \\ dy/dr & dy/ds & dy/dt \\ dz/dr & dz/ds & dz/dt \end{pmatrix} = \begin{pmatrix} \cos s & -r \sin s & 0 \\ \sin s \cos t & r \cos s \cos t & -r \sin s \sin t \\ \sin s \sin t & r \cos s \sin t & r \sin s \cos t \end{pmatrix}$$

We also know from chapter 11 that this latter matrix, say  $A$ , satisfies:

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

Now if we call  $D$  the diagonal matrix on the right, we conclude that the matrix, say  $B$ , appearing in the above formula of  $\nabla$  is given by:

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

(3) Thus, the angular momentum operator that we are looking for,  $L = -i\hbar x \times \nabla$ , written more conveniently as  $L = -i\hbar x/r \times r\nabla$ , is given by:

$$L = -i\hbar \begin{pmatrix} \cos s \\ \sin s \cos t \\ \sin s \sin t \end{pmatrix} \times \begin{pmatrix} r \cos s & -\sin s & 0 \\ r \sin s \cos t & \cos s \cos t & -\sin t/\sin s \\ r \sin s \sin t & \cos s \sin t & \cos t/\sin s \end{pmatrix} \begin{pmatrix} d/dr \\ d/ds \\ d/dt \end{pmatrix}$$

And computing now the vector product gives the formula for  $L$  in the statement.

(4) Now with our explicit formula for  $L$  in hand, we next find that the raising and lowering operators are given by:

$$L_{\pm} = \pm \hbar e^{\pm it} \left( \frac{d}{ds} \pm i \frac{\cos s}{\sin s} \cdot \frac{1}{dt} \right)$$

Next, we find that these two operators satisfy the following formula:

$$L_+ L_- = -\hbar^2 \left( \frac{d^2}{ds^2} + \frac{\cos s}{\sin s} \cdot \frac{d}{ds} + \frac{\cos^2 s}{\sin^2 s} \cdot \frac{d^2}{dt^2} + i \frac{d}{dt} \right)$$

And finally, by using this latter formula, we find that  $L^2$  is given by:

$$L^2 = -\hbar^2 \left( \frac{1}{\sin s} \cdot \frac{d}{ds} \left( \sin s \cdot \frac{d}{ds} \right) + \frac{1}{\sin^2 s} \cdot \frac{d^2}{dt^2} \right)$$

(5) With all these formulae in hand, we can now finish. The eigenfunction equation for the above operator  $L^2$ , with eigenvalue  $\hbar^2 l(l+1)$ , is as follows:

$$-\hbar^2 \left( \frac{1}{\sin s} \cdot \frac{d}{ds} \left( \sin s \cdot \frac{d}{ds} \right) + \frac{1}{\sin^2 s} \cdot \frac{d^2}{dt^2} \right) f = \hbar^2 l(l+1) f$$

But this is precisely the angular equation from chapter 11. As for the eigenfunction equation for the operator  $L_x$ , with eigenvalue  $\hbar m$ , this is as follows:

$$-\frac{i\hbar}{dt} f = \hbar m f$$

But this latter equation is equivalent to the azimuthal equation, also from chapter 11. Thus, we are dealing here with equations that we already know, and the solutions are the spherical harmonics that we found in chapter 11 above, as claimed.  $\square$

So long for angular momentum. And even more magic in a moment, when talking about spin. For more on all the above, we refer to Griffiths [43] or Weinberg [93].

## 12b. Electron spin

In order to talk now about spin, we will regard, a bit as in the classical mechanics case, the spin and the angular momentum as being similar quantities. Thus, in analogy with the basic equations for angular momentum, we should have:

DEFINITION 12.13. *The components of the spin operator are subject to*

$$[S_x, S_y] = i\hbar S_z$$

$$[S_y, S_z] = i\hbar S_x$$

$$[S_z, S_x] = i\hbar S_y$$

*called commutation relations for the spin operator.*

What we did here, with these axioms, is of course a bit heuristic. But this is quite reasonable, and for a more detailed version of the story, invoking rotational invariance as for getting to the above equations, for the angular momentum, spin, or any kind of “generalized angular momentum”, in some reasonable sense, we refer for instance to Weinberg [93]. In what follows we will take Definition 12.13 as it is, and do some rotational invariance work later, in chapter 13 below, directly in the relativistic framework.

The point now is that, with the above relations in hand, which are identical to the commutation relations for the angular momentum, all the general results from the previous section, based on that commutation relations, extend to our present setting, simply by changing  $L$  into  $S$  everywhere. And in particular, we are led in this way to:

THEOREM 12.14. *We have the following diagonalization formulae*

$$S^2 f_s^m = \hbar^2 s(s+1) f_s^m$$

$$S_x f_s^m = \hbar m f_s^m$$

$$S_{\pm} f_s^m = \hbar \sqrt{s(s+1) - m(m \pm 1)} f_s^{m \pm 1}$$

*involving the operators  $S^2 = S_x^2 + S_y^2 + S_z^2$ ,  $S_x$  and  $S_{\pm} = S_y \pm iS_z$ .*

PROOF. Here the first two formulae are something that we already know, from the previous section, with  $L, j$  being replaced by  $S, s$ . As for the last formula, this is something that we did not need, in the  $L, j$  context, but that we will need now. We want to compute the constants  $C_{s,\pm}^m$  making work the raising and lowering formula, namely:

$$S_{\pm} f_s^m = C_{s,\pm}^m f_s^{m \pm 1}$$

But this can be done by using  $S^2 = S_{\pm} S_{\mp} + S_x^2 \mp \hbar S_x$  and  $S_{\pm}^* = S_{\mp}$ , and we get:

$$C_{s,+}^m = \hbar \sqrt{s(s+1) - m(m+1)}$$

$$C_{s,-}^m = \hbar \sqrt{s(s+1) - m(m-1)}$$

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

In practice now, let us look for the simplest mathematical realization of spin. We know from the Stern-Gerlach experiment that the spin is something binary, that can be either up, or down. Thus, we are led, for fixed particles, to a quantum mechanics over  $H = \mathbb{C}^2$ , with spin up and down being represented by the following two vectors:

$$e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad e_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

It remains now to see how the equations in Theorem 12.14 reformulate, in this  $H = \mathbb{C}^2$  setting. But here, not many choices, and we are led to:

DEFINITION 12.15. *In the quantum mechanics of the spin, over  $H = \mathbb{C}^2$ , with*

$$e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad e_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

*being spin up and down, the spin is subject to the following equations, for  $f = e_1, e_2$ ,*

$$S^2 f = h^2 s(s+1) f$$

$$S_x f = h m_f f$$

$$S_{\pm} f = h \sqrt{s(s+1) - m_f(m_f \pm 1)} \check{f}$$

*with parameters  $s = 1/2$ ,  $m_{e_1} = 1/2$ ,  $m_{e_2} = -1/2$ , and with  $\{e_1, e_2\} = \{f, \check{f}\}$ .*

Here all the choices, and notably  $s = 1/2$ , are very natural in view of Theorem 12.14, because these are the choices providing a “minimal” realization of the equations in Theorem 12.14, in the smallest possible number of dimensions, namely  $N = 2$ . However, all this comes with a shade of mystery, or at least is not rock-solid enough as to be called theorem, and it is probably safer to use the term “definition”, as we did above.

The point now is that the above questions can be solved, the result being:

THEOREM 12.16. *In the above  $H = \mathbb{C}^2$  context, of the mechanics of a single, fixed electron, the components of the normalized spin  $\sigma = 2S/h$  are as follows,*

$$\sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad \sigma_y = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma_z = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

*called Pauli matrices. In the general, dynamic context, where we already have a Hilbert space  $H$  for the wave function, spin can be introduced by using the space*

$$H' = H \otimes \mathbb{C}^2$$

*and using the above Pauli matrices for it, acting on the  $\mathbb{C}^2$  part.*

PROOF. The equations in Definition 12.15, written in full detail, are as follows:

$$\begin{aligned} S^2 \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= \frac{3h^2}{4} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad S^2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{3h^2}{4} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ S_x \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= \frac{h}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad S_x \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{h}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ S_+ \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad , \quad S_+ \begin{pmatrix} 0 \\ 1 \end{pmatrix} = h \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ S_- \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= h \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad , \quad S_- \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \end{aligned}$$

Thus, we have the following formulae, for the various matrices involved:

$$\begin{aligned} S^2 &= \frac{3h^2}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad , \quad S_x = \frac{h}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ S_+ &= h \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad , \quad S_- = h \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \end{aligned}$$

In relation with what we want to prove, we have obtained the formula of  $S_x$ . Regarding now the formulae of  $S_y, S_z$ , these follow by solving the following system:

$$\begin{aligned} S_+ &= S_y + iS_z \\ S_- &= S_y - iS_z \end{aligned}$$

To be more precise, the computation for  $S_y$  goes as follows:

$$S_y = \frac{S_+ + S_-}{2} = \frac{h}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

As for the computation for  $S_z$ , this goes as follows:

$$S_z = \frac{S_+ - S_-}{2i} = \frac{h}{2i} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \frac{h}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

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

As a first consequence of the above, looking quite good, we have:

**EUREKA 12.17.** *Electrons have spin 1/2.*

This is motivated of course by the formula  $s = 1/2$  in Definition 12.15, but this being said, at least from the perspective of what we know so far about electrons, this does not make much sense, logically speaking. Remember indeed that we are still living under the sword of Heisenberg's uncertainty principle, and so the electrons themselves, and therefore their spin too, remain rather mathematical objects, far away from concrete things like, say planets in the Solar system, turning around the Sun and spinning. And also, there is some unclarity with  $1/2$  vs  $\pm 1/2$ , because the spin can be up or down.

This being said, some speculations are certainly possible. For instance the Pauli matrices all square up to one,  $\sigma_i^2 = 1$ , and a well-known interpretation of this is that “it takes  $720^\circ$  instead of the usual  $360^\circ$  to turn an electron back in place”, leading to the conclusion that the spin of the electron is  $360/720 = 1/2$ .

In any case,  $s = 1/2$  for the electron is good to know, and we will heavily use this formula in what follows, for all sorts of purposes. And we will talk about spin  $\neq 1/2$  too, in chapter 13, with a general particle discussion, involving bosons and fermions.

### 12c. Hydrogen, again

As a first and main application of the above, we can now review the fine structure of the hydrogen atom, with a proof for the following result, announced in chapter 11:

**THEOREM 12.18.** *The energy levels of the hydrogen atom, taking into account the fine structure coming from the relativistic and spin-related correction, are given by*

$$E_{nj} = E_n \left[ 1 + \frac{\alpha^2}{n^2} \left( \frac{n}{j + 1/2} - \frac{3}{4} \right) \right]$$

with  $j = l \pm 1/2$  being as before, and with  $\alpha$  being the fine structure constant.

**PROOF.** We will be doing here something far more precise than what we did in chapter 11, but still with considerable gaps, namely the usage without proof of some methods from perturbation theory, for which we refer to Griffiths [43], and then some silence of a deep topic, namely the formula of the magnetic dipole of the electron, for which we refer to Griffiths [43] and Weinberg [93]. Anyway, here is what we have, for what’s worth:

(1) We will use a general principle from perturbation theory, stating that the perturbed energy appears as expectation of the added Hamiltonian operator:

$$\mathcal{E} = \langle \mathcal{H} \rangle$$

(2) Let us compute first the relativistic correction. According to the general Einstein energy formula, from chapter 4, the relativistic kinetic energy is given by:

$$T = \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \dots$$

The Schrödinger equation, which is based on the non-relativistic formula for kinetic energy  $T = p^2/2m$ , must be therefore corrected with a term as follows:

$$\mathcal{T} = -\frac{p^4}{8m^3c^2}$$



But this leads to the following correction term  $\mathcal{E}_{nl}$ , with the computation using the Schrödinger equation  $p^2\psi = 2m(E - V)\psi$  at the end:

$$\begin{aligned}\mathcal{E}_{nl} &= \langle \mathcal{T} \rangle \\ &= -\frac{1}{8m^3c^2} \langle p^4\psi, \psi \rangle \\ &= -\frac{1}{8m^3c^2} \langle p^2\psi, p^2\psi \rangle \\ &= -\frac{1}{2mc^2} \langle (E_n - V)^2 \rangle\end{aligned}$$

(3) Now by expanding and using some standard expectation computations, for which we refer as before to Griffiths [43], all in terms of the Bohr radius  $a$ , we obtain:

$$\begin{aligned}\mathcal{E}_{nl} &= -\frac{1}{2mc^2} (E_n^2 - 2E_n \langle V \rangle + \langle V^2 \rangle) \\ &= -\frac{1}{2mc^2} \left( E_n^2 + 2E_n K e^2 \left\langle \frac{1}{r} \right\rangle + (K e^2)^2 \left\langle \frac{1}{r^2} \right\rangle \right) \\ &= -\frac{1}{2mc^2} \left( E_n^2 + \frac{2E_n K e^2}{n^2 a} + \frac{(K e^2)^2}{(l + 1/2)n^3 a^2} \right) \\ &= -\frac{E_n}{2mc^2} \left( \frac{4n}{l + 1/2} - 3 \right) \\ &= \frac{\alpha^2 E_n}{n^2} \left( \frac{n}{l + 1/2} - \frac{3}{4} \right)\end{aligned}$$

(4) Regarding now the spin correction, the reasons for it are very intuitive. The electron, as any spinning charge, has a magnetic field, and the proton, which moves around the electron, will exert some torque on this magnetic field, which must be taken into account, and so which will modify the Hamiltonian, and also the energy  $E_n$ .

(5) In practice now, in order to compute the correction we will use the same method as before, namely perturbation theory, but the data will be more delicate to gather.

(6) To start with, when regarding the electron as being fixed, the proton turns around it, and forms an electric loop. The intensity of the corresponding magnetic field can be computed by using the Biot-Savart law, the formula being as follows, with  $I = e/T$  being the intensity of the current, and  $T$  being the loop time:

$$||B|| = \frac{\mu_0 I}{2r} = \frac{\mu_0 e}{2rT} = \frac{2K\pi e}{c^2 r T}$$

On the other hand, recall that the angular momentum of the electron satisfies:

$$||L|| = rm||v|| = \frac{2\pi m r^2}{T}$$

Since both  $B$  and  $L$  point in the same direction, we conclude that we have:

$$B = \frac{Ke}{mc^2 r^3} L$$

(7) The thing now is that  $B$  acts on the magnetic dipole of the electron, which is formally given, for our computation, by the following formula:

$$M = -\frac{e}{2m} \cdot S$$

And there is a long story with this formula, because this is what comes out from a classical electrodynamics computation, so things looking fine. But there is a correction to be made to it, consisting of a rather standard  $1/2$  factor called Thomas precession, and on the other hand there is another correction to it, found by Dirac via a non-trivial relativistic computation, consisting of a  $2$  factor. And these  $1/2$  and  $2$  factors kill each other. For more on the story here, we refer to Griffiths [43] or Weinberg [93].

(8) Moving ahead, based on the formulae of  $B, M$  found above, we can compute the correction to the Hamiltonian operator to be made, which is given by:

$$\mathcal{H} = \langle B, M \rangle = \frac{Ke^2}{2} \cdot \frac{1}{m^2 c^2 r^3} \langle L, S \rangle$$

Thus, we are now in familiar territory, and we can use perturbation theory. By skipping some details here, the correction to the energy formula is as follows, with  $J = L + S$ :

$$\begin{aligned} \mathcal{E}_{nj} &= \langle \mathcal{H} \rangle \\ &= \frac{Ke^2}{4} \cdot \frac{1}{m^2 c^2 r^3} \langle J^2 - L^2 - S^2 \rangle \\ &= \frac{Ke^2}{4} \cdot \frac{1}{m^2 c^2 r^3} \cdot \frac{h^2}{2} (j(j+1) - l(l+1) - s(s+1)) \left\langle \frac{1}{r^3} \right\rangle \\ &= \frac{Ke^2}{4} \cdot \frac{1}{m^2 c^2 r^3} \cdot \frac{h^2}{2} \left( j(j+1) - l(l+1) - \frac{3}{4} \right) \cdot \frac{1}{l(l+1/2)(l+1)n^3 a^3} \\ &= \frac{E_n^2}{mc^2} \cdot \frac{n(j(j+1) - l(l+1) - 3/4)}{l(l+1/2)(l+1)} \\ &= -\frac{\alpha^2 E_n}{n^2} \cdot \frac{n(j-l)}{(l+1/2)(j+1/2)} \end{aligned}$$

(9) Finally, as computed in chapter 11, the revised energy  $E_{nj} = E_n + \mathcal{E}_{nl} + \mathcal{E}_{nj}$ , using the formulae in (3,8), is given by the formula in the statement.  $\square$

As mentioned in chapter 11, the story is not over with the above result, because there are several other corrections, which are smaller, coming of top of the fine structure correction, such as the Lamb shift, the hyperfine splitting, and more. In fact, there is an

infinite series of corrections, with  $\alpha$  as parameter, and the theory designed for solving this problem is quantum electrodynamics, that we will discuss in chapters 13-15 below.

### 12d. The periodic table

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 12.19. *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  $i\hbar\dot{\psi} = \hat{H}\psi$ , with Hamiltonian as follows,*

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

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

As before with the one-particle Schrödinger equation, there is a long story with all this, and for cutting short with the discussion here, this is what experiments lead to.

In general, and in fact at any  $Z > 1$ , and so even at  $Z = 2$ , the Schrödinger equation in Definition 12.19 is pretty much impossible to solve, due to the Coulomb repulsion term, which makes the math 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 are 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 12.20. *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*

$$i\hbar\dot{\psi} = \hat{H}\psi$$

*with Hamiltonian as follows,*

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

*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 12.21. *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  $E_0 = -79 \text{ eV}$ .*

As a partial conclusion to what we have so far, things not going on every well, and in order to advance, we will probably need to invest a lot of time in learning how to solve complicated Schrödinger equations, and why not buying a super-computer too.

Moving ahead, let us focus on a more modest question, that at the end of Problem 12.20, 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 not very far from reality, and is actually quite close to reality, if we add the spin to our discussion. For some explanations here, we refer to Griffiths [43].

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

So, this is the famous Pauli exclusion principle, giving the golden key to the understanding of  $Z \geq 2$  atoms. There are of course many things that can be said about it. A sample quantum mechanics book will probably tell you first something about bosons and fermions, coming with exactly 0 evidence, then some more things about electrons, of type “they are the same, but not really, and everything is entangled, but is it really entangled”, and finally formulate the Pauli exclusion principle, as a theorem.

We will not get into this here, and take the Pauli exclusion principle as it is, a physics fact. However, talking philosophy, personally I always think at it as coming from the “human nature of electrons”. To be more precise, when I’m at my office typing the present book, I feel like occupying some precise quantum numbers, with precise spin. And if 30 colleagues, all typing physics books too, manage to come by surprise to my

office, and squeeze there like sardines, I will surely find a way of getting rid of them, and disposing of their bodies. So now that a poor human like me can do this, why shouldn't a mighty electron be able to do the same. This is the Pauli exclusion principle.

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	$\frac{\text{Cs}}{55}$	$\frac{\text{Ba}}{56}$	$l$	$\frac{\text{Lu}}{71}$	$\frac{\text{Hf}}{72}$	$\frac{\text{Ta}}{73}$	$\frac{\text{W}}{74}$	$\frac{\text{Re}}{75}$	$\frac{\text{Os}}{76}$	$\frac{\text{Ir}}{77}$	$\frac{\text{Pt}}{78}$	$\frac{\text{Au}}{79}$	$\frac{\text{Hg}}{80}$	$\frac{\text{Tl}}{81}$	$\frac{\text{Pb}}{82}$	$\frac{\text{Bi}}{83}$	$\frac{\text{Po}}{84}$	$\frac{\text{At}}{85}$	$\frac{\text{Rn}}{86}$
7	$\frac{\text{Fr}}{87}$	$\frac{\text{Ra}}{88}$	$a$	$\frac{\text{Lr}}{103}$	$\frac{\text{Rf}}{104}$	$\frac{\text{Db}}{105}$	$\frac{\text{Sg}}{106}$	$\frac{\text{Bh}}{107}$	$\frac{\text{Hs}}{108}$	$\frac{\text{Mt}}{109}$	$\frac{\text{Ds}}{110}$	$\frac{\text{Rg}}{111}$	$\frac{\text{Cn}}{112}$	$\frac{\text{Nh}}{113}$	$\frac{\text{Fl}}{114}$	$\frac{\text{Mc}}{115}$	$\frac{\text{Lv}}{116}$	$\frac{\text{Ts}}{117}$	$\frac{\text{Og}}{118}$
			$l:$	$\frac{\text{La}}{57}$	$\frac{\text{Ce}}{58}$	$\frac{\text{Pr}}{59}$	$\frac{\text{Nd}}{60}$	$\frac{\text{Pm}}{61}$	$\frac{\text{Sm}}{62}$	$\frac{\text{Eu}}{63}$	$\frac{\text{Gd}}{64}$	$\frac{\text{Tb}}{65}$	$\frac{\text{Dy}}{66}$	$\frac{\text{Ho}}{67}$	$\frac{\text{Er}}{68}$	$\frac{\text{Tm}}{69}$	$\frac{\text{Yb}}{70}$		
			$a:$	$\frac{\text{Ac}}{89}$	$\frac{\text{Th}}{90}$	$\frac{\text{Pa}}{91}$	$\frac{\text{U}}{92}$	$\frac{\text{Np}}{93}$	$\frac{\text{Pu}}{94}$	$\frac{\text{Am}}{95}$	$\frac{\text{Cm}}{96}$	$\frac{\text{Bk}}{97}$	$\frac{\text{Cf}}{98}$	$\frac{\text{Es}}{99}$	$\frac{\text{Fm}}{100}$	$\frac{\text{Md}}{101}$	$\frac{\text{No}}{102}$		

Here the horizontal parameter  $1, \dots, 18$  is called the group, and the vertical parameter  $1, \dots, 7$  is called the period. The two rows on the bottom consist of lanthanum  $_{57}\text{La}$  and its followers, called lanthanides, and of actinium  $_{89}\text{Ac}$  and its followers, called actinides. These are to be inserted in the main table, where indicated, lanthanides between barium  $_{56}\text{Ba}$  and lutetium  $_{71}\text{Lu}$ , and actinides between radium  $_{88}\text{Ra}$  and lawrencium  $_{103}\text{Lr}$ .

Thus, the periodic table, when correctly drawn, but no one does that because of obvious typographical reasons, is in fact a  $7 \times 32$  table. Note here that, according to our  $7 \times 18$  convention, which is the standard one, lanthanides and actinides don't have a group number  $1, \dots, 18$ . Their group is by definition "lanthanides" and "actinides".

We will comment in a moment on all this, but before anything:

ADVICE 12.23. *Learn their names.*

This is a serious advice, the periodic table being the main theorem of mathematics, physics, chemistry, biology and engineering combined. So if there's one theorem to be learned, full statement, that is the one. In case you're out of memory, just erase from your brain everything that you learned so far from this book of mine, and learn instead that 118 elements. Please do it for me, this being my final wish, from the death bed.

Actually, in order to get started here, here are the names up to krypton  ${}_{36}\text{Kr}$ , which are absolutely needed for everything, and must be all learned, to start with:

NAMES 12.24. *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*  ${}_{36}\text{Kr}$ .

Observe that all names fit with the abbreviations, expect for sodium  ${}_{11}\text{Na}$ , coming from the Latin natrium, potassium  ${}_{19}\text{K}$ , coming from the Latin kalium, iron  ${}_{26}\text{Fe}$  coming from the Latin ferrum, and also copper  ${}_{29}\text{Cu}$ , coming from the Latin cuprum.

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:

NAMES 12.25. *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 abbreviations not fitting with English names come from the Latin or sometimes Greek argentum  ${}_{47}\text{Ag}$ , aurum  ${}_{47}\text{Au}$ , hydrargyrum  ${}_{80}\text{Hg}$ , plumbum  ${}_{82}\text{Pb}$  and stannum  ${}_{50}\text{Sn}$ . 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.

But let us not forget about quantum mechanics, and what we wanted to do, namely discuss electron structure. As a first observation, we have:

**FACT 12.26.** *Any  $Z = 1, \dots, 118$  corresponds to a unique element, having  $Z$  protons in the core, and  $Z$  electrons around it. This element might come with isotopes, depending on the number of neutrons in the core, can be in ground state or excited states, can get ionized, and so on, but all there versions are “family”, and the element is unique.*

This fact is something which might look very natural, with no need for explanation for it, but after some thinking, is this really that natural. And the answer here is that no, if you don't know quantum mechanics, and yes, if you know some, as we do:

(1) For the purposes of our question, we can assume that we are in the context of Problem 12.20, and with the Coulomb repulsions between electrons ignored.

(2) But then, we are a bit in the same situation as in Fact 12.21, and the analysis there, based on hydrogen theory modified via  $e \rightarrow Ze$ , carries over.

(3) And so, the  $Z$  electrons will arrange on various energy levels, subject to Pauli exclusion, as to occupy a state of lowest possible energy, so the solution is unique.

In fact, we can now understand the electron structure of the various elements, and also how the periodic table is exactly made, the conclusions here being as follows:

**FACT 12.27.** *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 [35] or Griffiths [43].

With this in hand, we can now start doing some chemistry. There is an enormous quantity of things that can be said here, the simplest of which being:

**THEOREM 12.28.** *The group 18 elements, helium  ${}_2\text{He}$ , neon  ${}_{10}\text{Ne}$ , argon  ${}_{18}\text{Ar}$ , krypton  ${}_{36}\text{Kr}$ , xenon  ${}_{54}\text{Xe}$  and radon  ${}_{86}\text{Rn}$ , called noble gases, are allergic to chemistry.*

**PROOF.** This follows from the above discussion, because the group 18 elements are precisely those with all possible electron positions fully occupied, up to a certain  $n \in \mathbb{N}$ , which makes them very unfriendly to any chemistry proposition from the outside. By the way, oganesson  ${}_{118}\text{Og}$  is normally part of this group too, but since this element has only been created and observed for a tiny fraction of a second, who really knows, and by the standard scientific etiquette, in the lack of experiments, no comment about it.  $\square$

So long for the chemical elements, and the periodic table. Unfortunately business is business, and we will have to stop here, and in the remainder of this book, we will rather go into the opposite direction, namely towards the very small, sub-atomic.

Observe however that, in relation with what we originally wanted to do, explained in chapter 9 above, job done. We have now proof that quantum mechanics is in relation with everything happening at  $10^{-9}$  and below, as claimed in chapter 9.

Finally, as a last philosophical comment, while quantum mechanics still remains as incomprehensible as usual, and with this being fine with us, our daily life, thinking a bit on what quantum mechanics can finally do in the context of the  $N$ -body problem, compared to what classical mechanics can do in the context of the same  $N$ -body problem, leads to the conclusion that quantum mechanics might be, after all, simpler than classical mechanics. And isn't this amazing. And more on this in chapters 13-16 below, which will be written precisely with this idea in mind, power and optimism all the way.

### 12e. Exercises

Here is an exercise, which is very interesting, and certainly quite time-consuming too, and that I warmly recommend, coming from the bottom of my heart:

EXERCISE 12.29 (The Periodic Table experience). *Find 20 minutes/day, over the next 4 months, say before going to sleep, and at each session:*

- (1) *Go to Wikipedia, or similar website, periodic table, and take a quick look at the elements there, from hydrogen  ${}_1\text{H}$  to oganesson  ${}_{118}\text{Og}$ .*
- (2) *And depending on your mood, and on what you learned the day before too, pick a new element, and spend 20 minutes in reading its page.*

This is surely something that can do with pleasure, and you will learn a lot of interesting things in this way, that any scientist should know. But more is true. During these next 4 months your learning or work on abstract math and physics will drastically improve, because by some magic reason, this math and physics will appear "trivial".

And isn't this magic. Of course, the Periodic Table experience can be repeated afterwards too, anytime when needed, with each time spending your 20 minutes on things that you previously skipped. And for a change, you can try some biology too, classification of species. Or why not history, isn't that complicated too. And so on.

Hope you will find this interesting. That's a good trick, be at any time interested in something else, of really tough type, like chemistry, biology and so on. So that your regular, daily work on theoretical math and physics to appear as something easy.



## Part IV

# Particle physics

*Looking at my watch time 3am  
Got to see that everywhere I turn  
Will point to the fact  
That time is eternal*

## CHAPTER 13

### Dirac equation

#### 13a. Klein-Gordon

We have seen in previous chapters that quantum mechanics provides explanations and equations for all the basic phenomena appearing at the atomic level. Among others, we have reached to a quite decent level of understanding of the hydrogen atom, and we also understood the basic functioning of the heavier atoms.

The natural continuation of all this would consist in picking up the heavier atoms, one by one, from helium  ${}_2\text{He}$  to oganesson  ${}_{118}\text{Og}$ , and working out their properties, by using the Schrödinger equation, and other tools from quantum mechanics. And with here, fun guarantee, because passed a few common things, these 117 heavier atoms all have a different mathematics, leading to a different physics, which is worth investigating, on a case by case basis. And so, with 117 more books in need to be written.

In the remainder of this book we will do instead something more modest. We will be interested in abstract aspects, and more specifically in “fixing quantum mechanics”. And by this we mean not that quantum mechanics is wrong, but that there are certainly a few things that we came upon, which are not very clear, and need to be fixed, as follows:

- (1) We would like our theory to be relativistic. Among others, for getting rid of the “relativistic correction” to the hydrogen atom, a correction never being a good thing.
- (2) In fact, we would like to have a conceptual understanding of the spin correction too, as to get rid of the whole “fine structure correction” to the hydrogen atom.
- (3) We would like our electrons to be joined by more particles, with the minimum here including the protons, the neutrons, and also the photons, representing light.
- (4) And then, why not looking too into phenomena that we have not investigated yet, such as radioactivity. Or splitting protons and neutrons into smaller particles.

We will discuss here all these questions. Quite remarkably, there is a common mathematical framework for investigating all these questions, called quantum field theory (QFT). So, we will develop QFT, and then we will turn to questions (1,2) above, and present an amazing answer to them, involving a QFT called quantum electrodynamics

(QED). Then we will turn to questions (3,4), and discuss a bit the status here, notably with a few words on quantum chromodynamics (QCD), which is the quantum field theory obtained by splitting protons and neutrons into smaller particles.

Before starting, let us mention that things won't be easy. Our present level in quantum mechanics, now at this page 300 of the present book, corresponds more or less to things known since the 1920s. We will of course make big efforts for understanding what happened in the 1930s, then 1940s, then 1950s and so on, but so many things that happened, and the remainder to this book will be just a modest introduction to all this.

At the level of books, standard references are Feynman [36], Griffiths [44], Huang [50], Itzykson-Zuber [53], Landau-Lifshitz [64], Peskin-Schroeder [71], Zinn-Justin [99], as well as a 3-volume monster by Weinberg, coming as a continuation of [93]. Nice popular books include Griffiths [45] and Huang [52]. There are also many books on more advanced aspects of QFT, such as string theory, and more on these later.

Getting started, let us formulate a clear objective:

**OBJECTIVE 13.1.** *We would like to have a relativistic version of quantum mechanics, and with the electron being joined by the photon, representing light. If possible, we would like our theory to cover as well the proton, and the neutron.*

Here the relativistic requirement is very natural in regards with all that has been said above, this being certainly the gate towards a better quantum mechanics.

Regarding the other particles, intuition and common sense would dictate to go first towards the proton and neutron, because aren't these, along with the electron, the constituents of normal matter, that we are normally interested in. However, and here comes our point, mathematically speaking, the electron can certainly live without protons and neutrons, because in order to move, it just needs a positive charge attracting it, and this positive charge can be well something abstract, as per general field theory philosophy.

In contrast, however, the electron cannot live without the photon. The point is that in the context of the basic physics of atoms, electrons can jump between energy levels, emitting or absorbing photons, and with this being known to happen even in the absence of external stimuli. Thus, and for concluding, the true "brother" of the electron is not the proton or the neutron, but rather the photon. And so, the minimal extension of quantum mechanics that we are trying to build should deal with electrons and photons.

Let us first look into the photon, try to understand how to make it fit into our theory, and leave the electron for later. As a starting point, we have:

FACT 13.2. *The master equation for free electromagnetic radiation, that is, for free photons, is the wave equation at speed  $v = c$ , namely:*

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

*This equation can be reformulated in the more symmetric form*

$$\left( \frac{1}{c^2} \cdot \frac{d^2}{dt^2} - \Delta \right) \varphi = 0$$

*with the operator on the left being called the d'Alembertian.*

To be more precise here, these are things that we know well, from chapter 9, or even from chapter 6, when first talking about the wave equation, and radiation. In addition, and importantly, we also know from chapters 6 and 9 that the wave equation, at any speed  $v$ , is relativistic, in the sense that it is invariant under Lorentz transformations, which are as follows, with  $\gamma = 1/\sqrt{1 - v^2/c^2}$  being as usual the Lorentz factor:

$$x' = \gamma(x - vt)$$

$$y' = y$$

$$z' = z$$

$$t' = \gamma(t - vx/c^2)$$

So far, so good. In relation now with the electron, there is an obvious similarity here with the free Schrödinger equation, without potential  $V$ , which reads:

$$\left( i \frac{d}{dt} + \frac{h}{2m} \Delta \right) \psi = 0$$

This similarity suggests looking for a relativistic version of the Schrödinger equation, which is compatible with the wave equation at  $v = c$ . And coming up with such an equation is not very complicated, the straightforward answer being as follows:

DEFINITION 13.3. *The following abstract mathematical equation,*

$$\left( -\frac{1}{c^2} \cdot \frac{d^2}{dt^2} + \Delta \right) \psi = \frac{m^2 c^2}{h^2} \psi$$

*on a function  $\psi = \psi_t(x)$ , is called the Klein-Gordon equation.*

To be more precise, what we have here is some sort of a speculative equation, formally obtained from the Schrödinger equation, via a few simple manipulations, as to make it relativistic. And with the relation with photons being something very simple, the thing being that at zero mass,  $m = 0$ , we obtain precisely the wave equation at  $v = c$ .

All this is very nice, looks like we have a beginning of theory here, both making the electrons relativistic, and unifying them with photons. And isn't this too beautiful to be true. Going ahead now with physics, the following question appears:

QUESTION 13.4. *What does the Klein-Gordon equation really describe?*

And here, unfortunately, bad news all the way. A closer look at the Klein-Gordon equation reveals all sorts of bugs, making it unusable for anything reasonable. And with the main bug, which is enough for disqualifying it, being that, unlike the Schrödinger equation which preserves probability amplitudes  $|\psi|^2$ , the Klein-Gordon equation does not have this property. Thus, even before trying to understand what the Klein-Gordon equation really describes, we are left with the conclusion that this equation cannot really describe anything reasonable, due to the formal nature of the function  $\psi$  involved.

So, this was for the story of the Klein-Gordon equation. Actually this equation was first discovered by Schrödinger himself, in the context of his original work on the Schrödinger equation. But noticing the above bugs with it, Schrödinger dismissed it right way, and then downgraded his objectives, looking for something non-relativistic instead, and then found the Schrödinger equation, leading to the story that we know.

This being said, the Klein-Gordon equation found later a number of interesting applications, the continuation of the story being as follows:

(1) Dirac found a clever way of extracting the “square root” of the Klein-Gordon equation. And this square root equation, called Dirac equation, turned out to be the correct one, making exactly what the Klein-Gordon equation was supposed to do.

(2) Technically speaking, the Klein-Gordon equation is very useful for investigating the Dirac equation, because the components of the solutions of the Dirac equation satisfy the Klein-Gordon equation. More on this later, when discussing the Dirac equation.

(3) Finally, the Klein-Gordon equation was later recognized to describe well the spin 0 particles. But with these particles being something specialized, including the unstable and somewhat fringe “pions”, and the Higgs boson, which is something complicated.

We will discuss all this, in what follows. In any case, we have here a beginning of good discussion, with our cocktail of thoughts and ideas including electrons, photons, relativity and spin, which are exactly the things that we wanted to include in our discussion. So, all that is left is to clarify all this, and we will do so, following Dirac.

### 13b. Dirac equation

The legend has it that Dirac, watching an apple falling, came upon. Sorry, take two. The legend has it that Dirac, watching some logs burning in the fireplace, came upon the idea of extracting the square root of the Klein-Gordon operator, as follows:

PROPOSITION 13.5. *We can extract the square root of the Klein-Gordon operator, via a formula as follows,*

$$-\frac{1}{c^2} \cdot \frac{d^2}{dt^2} + \Delta = \left( \frac{i}{c} \cdot \frac{Pd}{dt} + \frac{Qd}{dx} + \frac{Rd}{dy} + \frac{Sd}{dz} \right)^2$$

by using matrices  $P, Q, R, S$  which anticommute,  $AB = -BA$ , and whose squares equal one,  $A^2 = 1$ .

PROOF. We have the following computation, valid for any matrices  $P, Q, R, S$ , with the notation  $\{A, B\} = AB + BA$ :

$$\begin{aligned} \left( \frac{i}{c} \cdot \frac{Pd}{dt} + \frac{Qd}{dx} + \frac{Rd}{dy} + \frac{Sd}{dz} \right)^2 &= -\frac{1}{c^2} \cdot \frac{P^2 d^2}{dt^2} + \frac{Q^2 d^2}{dx^2} + \frac{R^2 d^2}{dy^2} + \frac{S^2 d^2}{dz^2} \\ &+ \frac{i}{c} \left( \frac{\{P, Q\} d^2}{dt dx} + \frac{\{P, R\} d^2}{dt dy} + \frac{\{P, S\} d^2}{dt dz} \right) \\ &+ \frac{\{Q, R\} d^2}{dx dy} + \frac{\{Q, S\} d^2}{dx dz} + \frac{\{R, S\} d^2}{dy dz} \end{aligned}$$

Thus, in order to obtain in this way the Klein-Gordon operator, the conditions in the statement must be satisfied.  $\square$

As a technical comment here, normally when extracting a square root, we should look for a self-adjoint operator. In view of this, observe that we have:

$$\left( \frac{i}{c} \cdot \frac{Pd}{dt} + \frac{Qd}{dx} + \frac{Rd}{dy} + \frac{Sd}{dz} \right)^* = -\frac{i}{c} \cdot \frac{P^* d}{dt} + \frac{Q^* d}{dx} + \frac{R^* d}{dy} + \frac{S^* d}{dz}$$

Thus, we should normally add the conditions  $P^* = -P$  and  $Q^* = Q, R^* = R, S^* = S$  to those above. But, the thing is that due to some subtle reasons, the natural square root of the Klein-Gordon operator is not self-adjoint. More on this later.

Looking for matrices  $P, Q, R, S$  as above is not exactly trivial, and the simplest solutions appear in  $M_4(\mathbb{C})$ , in connection with the Pauli matrices, as follows:

PROPOSITION 13.6. *The simplest matrices  $P, Q, R, S$  as above appear as*

$$P = \gamma_0 \quad , \quad Q = i\gamma_1 \quad , \quad R = i\gamma_2 \quad , \quad S = i\gamma_3$$

with  $\gamma_0, \gamma_1, \gamma_2, \gamma_3$  being the Dirac matrices, given by

$$\gamma_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad \gamma_i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}$$

where  $\sigma_1, \sigma_2, \sigma_3$  are the Pauli spin matrices, given by:

$$\sigma_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad \sigma_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma_3 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

PROOF. We have  $\gamma_0^2 = 1$ , and by using  $\sigma_i^2 = 1$  for any  $i = 1, 2, 3$ , we have as well the following formula, which shows that we have  $(i\gamma_i)^2 = 1$ , as needed:

$$\gamma_i^2 = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

As in what regards the commutators, we first have, for any  $i = 1, 2, 3$ , the following equalities, which show that  $\gamma_0$  anticommutes indeed with  $\gamma_i$ :

$$\begin{aligned} \gamma_0 \gamma_i &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \\ \gamma_i \gamma_0 &= \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & -\sigma_i \\ -\sigma_i & 0 \end{pmatrix} \end{aligned}$$

Regarding now the remaining commutators, observe here that we have:

$$\gamma_i \gamma_j = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma_j \\ -\sigma_j & 0 \end{pmatrix} = \begin{pmatrix} -\sigma_i \sigma_j & 0 \\ 0 & -\sigma_i \sigma_j \end{pmatrix}$$

Now since the Pauli matrices anticommute, we obtain  $\gamma_i \gamma_j = -\gamma_j \gamma_i$ , as desired.  $\square$

We can now put everything together, and we obtain:

THEOREM 13.7. *The following operator, called Dirac operator,*

$$D = i \left( \frac{\gamma_0 d}{cdt} + \frac{\gamma_1 d}{dx} + \frac{\gamma_2 d}{dy} + \frac{\gamma_3 d}{dz} \right)$$

*has the property that its square is the Klein-Gordon operator.*

PROOF. With notations from Proposition 13.5 and Proposition 13.6, and by making the choices in Proposition 13.6, we have:

$$\begin{aligned} \frac{i}{c} \cdot \frac{Pd}{dt} + \frac{Qd}{dx} + \frac{Rd}{dy} + \frac{Sd}{dz} &= \frac{i}{c} \cdot \frac{\gamma_0 d}{dt} + \frac{i\gamma_1 d}{dx} + \frac{i\gamma_2 d}{dy} + \frac{i\gamma_3 d}{dz} \\ &= i \left( \frac{\gamma_0 d}{cdt} + \frac{\gamma_1 d}{dx} + \frac{\gamma_2 d}{dy} + \frac{\gamma_3 d}{dz} \right) \end{aligned}$$

Thus, we have here a square root of the Klein-Gordon operator, as desired.  $\square$

We can now extract the square root of the Klein-Gordon equation, as follows:

DEFINITION 13.8. *We have the following equation, called Dirac equation,*

$$ih \left( \frac{\gamma_0 d}{cdt} + \frac{\gamma_1 d}{dx} + \frac{\gamma_2 d}{dy} + \frac{\gamma_3 d}{dz} \right) \psi = mc\psi$$

*obtained by extracting the square root of the Klein-Gordon equation.*



As usual with such theoretical physics equations, extreme caution is recommended, at least to start with. We will slowly examine this equation, in what follows, and the good news will be that, passed a few difficulties, this will turn to be a true, magic equation.

As a first observation, all this is very related to spin. In fact, as we will see later, the Dirac equation is the correct relativistic equation describing the spin 1/2 particles.

### 13c. Positrons, Pandora's box

The Dirac equation comes with a price to pay, which is that of opening Pandora's box of particles. To be more precise, once we adopt this equation, we must surely adopt all its free solutions. And bad news here, the solution which is complementary to the electron is not the proton, but rather a weird new particle, called the positron.

In order to explain all this, let us start with the following observation:

PROPOSITION 13.9. *For a particle at rest, meaning under the assumption*

$$\frac{d\psi}{dx} = \frac{d\psi}{dy} = \frac{d\psi}{dz} = 0$$

*the Dirac equation takes the form*

$$\frac{ih}{c} \cdot \gamma_0 \cdot \frac{d\psi}{dt} = mc\psi$$

*with  $\gamma_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$  being as usual the first Dirac matrix.*

PROOF. Consider indeed the Dirac equation, as formulated in Definition 13.8:

$$ih \left( \frac{\gamma_0 d}{cdt} + \frac{\gamma_1 d}{dx} + \frac{\gamma_2 d}{dy} + \frac{\gamma_3 d}{dz} \right) \psi = mc\psi$$

With the above rest assumption, we are led to the equation in the statement. □

The above equation at rest is very easy to solve, the result being as follows:

THEOREM 13.10. *The solutions of the Dirac equation for particles at rest are*

$$\psi = \begin{pmatrix} e^{-imc^2 t/h} \xi \\ e^{imc^2 t/h} \eta \end{pmatrix}$$

*with  $\xi, \eta \in \mathbb{R}^2$  being arbitrary vectors.*

PROOF. In order to solve the Dirac equation in Proposition 13.9, let us write:

$$\psi = \begin{pmatrix} \varphi \\ \phi \end{pmatrix}$$

With this notation, the Dirac equation at rest takes the following form:

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} d\varphi/dt \\ d\phi/dt \end{pmatrix} = -\frac{imc^2}{h} \begin{pmatrix} \varphi \\ \phi \end{pmatrix}$$

Now by looking at the components, the equations are as follows:

$$\frac{d\varphi}{dt} = -\frac{imc^2}{h} \varphi \quad , \quad \frac{d\phi}{dt} = \frac{imc^2}{h} \phi$$

But the solutions of these latter equations are as follows, with  $\xi, \eta \in \mathbb{R}^2$ :

$$\varphi = e^{-imc^2 t/h} \xi \quad , \quad \phi = e^{imc^2 t/h} \eta$$

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

The question is now, is the above result good news or not? Not really, because in view of what we know from quantum mechanics, an  $e^{-iEt/h}$  factor should correspond to the time dependence of a quantum state with energy  $E$ , which at rest is  $E = mc^2$ . And from this perspective, while the above  $\varphi$  functions look very good, the other components, the  $\phi$  functions, look bad, seemingly coming from particles having “negative energy”.

So, what to do? In order to avoid particles with negative energy, which is something that definitely looks very bad, the solution is that of talking about antiparticles with positive energy, and to formulate, as a continuation of Theorem 13.10:

**THEOREM 13.11.** *The basic solutions of the Dirac equation for particles at rest are*

$$\psi^1 = e^{-imc^2 t/h} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad , \quad \psi^2 = e^{-imc^2 t/h} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

*corresponding to the electron with spin up, and spin down, plus*

$$\psi^3 = e^{imc^2 t/h} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad , \quad \psi^4 = e^{imc^2 t/h} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

*corresponding to a new particle, the positron, with spin up, and spin down.*

**PROOF.** Here the mathematics comes from what we found in Theorem 13.10, and the terminology and philosophy comes from the above discussion. With the remark that the newly introduced positron is rather an antiparticle, but more on this later.  $\square$

Not very good, all this. Dirac himself could not believe it, and it took some joint effort of Weyl, Pauli, Oppenheimer and others to convince him that yes, unfortunately the positrons predicted by his equation are not the usual protons. And so that goodbye reasonable physics, goodbye common sense, and welcome positrons.

In what concerns us, we have been extremely reluctant, throughout this book, to talk about new particles, but no choice now, we will have to back up, and adopt the positrons. But, passed this, we will slam down the cover of Pandora's box, right away. We definitely don't want all sorts of fringe, short-lived particles to invade our theory, and multiply like mushrooms, and transform our carefully built theory into something apocalyptic.

Be said in passing, after some thinking, positrons are not that bad, as particles. If there's one sort of bad particles in this life, these are the short-lived ones, which appear as some sort of "mathematical complications", which do not really exist in the real, statistical life, which takes place over substantial time  $t > 0$ . And positrons are not like this, they are nice and stable, exactly as the electrons. Their only fault is that of not being very frequent, a positron's fate being that of being quickly eaten by an electron passing by. But to be blamed for this lack of symmetry is not quantum mechanics, but rather the mechanism of the Big Bang, and once we're fine with this, we're fine with positrons.

More about positrons later, when talking about Feynman diagrams and QED. We will see at that time that positrons are in fact something very natural, and we will get to know and love them on the same level as the usual electrons.

Moving now forward, let us attempt to solve the following question:

QUESTION 13.12. *What are the plane wave solutions*

$$\psi(s) = ae^{-i\langle k, s \rangle} u$$

*of the Dirac equation?*

To be more precise, we are using here, as argument of the function  $\psi$ , the standard relativistic space-time position  $s \in \mathbb{R}^4$  of our particle, namely:

$$s = \begin{pmatrix} ct \\ r \end{pmatrix} \quad , \quad r = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Next, we have in the above a constant  $a \in \mathbb{R}$ , which will be quite irrelevant to our computations, the Dirac equation being linear. Regarding now  $k$ , it is convenient to write this vector split over components, as we did in the above with  $s$ , as follows:

$$k = \begin{pmatrix} f \\ g \end{pmatrix} \quad , \quad g = \begin{pmatrix} g_1 \\ g_2 \\ g_3 \end{pmatrix}$$

With these conventions, along with the standard relativistic convention that the space coordinates contribute with  $-$  signs, the scalar product in Question 13.12 is given by:

$$\langle k, s \rangle = cft - \langle g, r \rangle$$

Now observe that the real part of the exponential in Question 13.12 is given by:

$$\operatorname{Re}(e^{-i\langle k, s \rangle}) = \cos(cft - \langle g, r \rangle)$$

Thus, what we have here, justifying the terminology, is a sinusoidal wave propagating in the direction  $g$ , with angular frequency and wavelength as follows:

$$\omega = cf \quad , \quad \lambda = 2\pi/||g||$$

In order to answer Question 13.12, we must first plug into the Dirac equation our special function  $\psi$ . We are led in this way to a quite simple equation, as follows:

PROPOSITION 13.13. *The Dirac equation for plane wave functions*

$$\psi(s) = ae^{-i\langle k, s \rangle}u$$

*takes the following special form, no longer involving derivatives,*

$$h(\gamma_0 f - \gamma_1 g_1 - \gamma_2 g_2 - \gamma_3 g_3)u = mcu$$

*with the above conventions for indices and vectors.*

PROOF. Consider indeed the Dirac equation, as formulated in Definition 13.8:

$$ih \left( \frac{\gamma_0 d}{cdt} + \frac{\gamma_1 d}{dx} + \frac{\gamma_2 d}{dy} + \frac{\gamma_3 d}{dz} \right) \psi = mc\psi$$

For the function  $\psi$  in the statement, the derivatives are given by:

$$\frac{d\psi}{ds_i} = -ik_i\psi$$

Thus, with our above conventions for indices and vectors, we have:

$$\frac{d\psi}{cdt} = -if\psi \quad , \quad \frac{d\psi}{dr_i} = ig_i\psi$$

By plugging these quantities in the Dirac equation, this equation becomes:

$$h(\gamma_0 f - \gamma_1 g_1 - \gamma_2 g_2 - \gamma_3 g_3)\psi = mc\psi$$

Now by using again  $\psi = ae^{-i\langle k, s \rangle}u$ , this equation takes the following form:

$$h(\gamma_0 f - \gamma_1 g_1 - \gamma_2 g_2 - \gamma_3 g_3)ae^{-i\langle k, s \rangle}u = mcae^{-i\langle k, s \rangle}u$$

Thus, by simplifying, we are led to the equation in the statement.  $\square$

Let us study now the equation that we found. As a first observation, we can further fine-tune the equation in Proposition 13.13, via some simple manipulations, as follows:

PROPOSITION 13.14. *In the context of Proposition 13.13, with the notation*

$$u = \begin{pmatrix} v \\ w \end{pmatrix}$$

*the Dirac equation takes the following form, in terms of the components  $v, w$ ,*

$$v = \frac{\langle g, \sigma \rangle}{f - mc/h} w, \quad w = \frac{\langle g, \sigma \rangle}{f + mc/h} v$$

*where  $\sigma_1, \sigma_2, \sigma_3$  stand as usual for the Pauli spin matrices.*

PROOF. According to the definition of the Dirac matrices, in terms of the Pauli ones, we have the following computation, for the operator appearing in Proposition 13.13:

$$\begin{aligned} \gamma_0 f - \gamma_1 g_1 - \gamma_2 g_2 - \gamma_3 g_3 &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} f - \sum_{i=1}^3 \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix} g_i \\ &= \begin{pmatrix} f & 0 \\ 0 & -f \end{pmatrix} - \begin{pmatrix} 0 & \langle g, \sigma \rangle \\ -\langle g, \sigma \rangle & 0 \end{pmatrix} \\ &= \begin{pmatrix} f & -\langle g, \sigma \rangle \\ \langle g, \sigma \rangle & -f \end{pmatrix} \end{aligned}$$

Thus, the quantity which must vanish in Proposition 13.13 is given by:

$$\begin{aligned} &\left( h(\gamma_0 f - \gamma_1 g_1 - \gamma_2 g_2 - \gamma_3 g_3) - mc \right) u \\ &= \begin{pmatrix} hf - mc & -h\langle g, \sigma \rangle \\ h\langle g, \sigma \rangle & -hf - mc \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix} \\ &= \begin{pmatrix} (hf - mc)v - h\langle g, \sigma \rangle w \\ h\langle g, \sigma \rangle v - (hf + mc)w \end{pmatrix} \end{aligned}$$

We therefore conclude that, in our case, the Dirac equation reads:

$$(hf - mc)v = h\langle g, \sigma \rangle w$$

$$h\langle g, \sigma \rangle v = (hf + mc)w$$

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

In order to solve now our equation, let us make the following observation:

PROPOSITION 13.15. *In the context of Proposition 13.14 we must have*

$$\|g\|^2 = f^2 - \left(\frac{mc}{h}\right)^2$$

*under the assumption that the solution is nonzero,  $u \neq 0$ .*

PROOF. Consider the equations found in Proposition 13.14, namely:

$$v = \frac{\langle g, \sigma \rangle}{f - mc/h} w, \quad w = \frac{\langle g, \sigma \rangle}{f + mc/h} v$$

By substituting, we are led to the following formulae:

$$v = \frac{\langle g, \sigma \rangle^2}{f^2 - (mc/h)^2} v, \quad w = \frac{\langle g, \sigma \rangle^2}{f^2 - (mc/h)^2} w$$

Thus, assuming that the solution is nonzero,  $u \neq 0$ , we must have:

$$\frac{\langle g, \sigma \rangle^2}{f^2 - (mc/h)^2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Now, let us compute the left term. According to our various conventions above, and to the formulae for the Pauli matrices, we have the following formula:

$$\begin{aligned} \langle g, \sigma \rangle &= g_1 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + g_2 \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + g_3 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &= \begin{pmatrix} g_3 & g_1 - ig_2 \\ g_1 + ig_2 & -g_3 \end{pmatrix} \end{aligned}$$

By raising this quantity to the square, we obtain:

$$\begin{aligned} \langle g, \sigma \rangle^2 &= \begin{pmatrix} g_3 & g_1 - ig_2 \\ g_1 + ig_2 & -g_3 \end{pmatrix} \begin{pmatrix} g_3 & g_1 - ig_2 \\ g_1 + ig_2 & -g_3 \end{pmatrix} \\ &= \begin{pmatrix} g_3^2 + (g_1 - ig_2)(g_1 + ig_2) & g_3(g_1 - ig_2) - (g_1 - ig_2)g_3 \\ (g_1 + ig_2)g_3 - g_3(g_1 + ig_2) & (g_1 + ig_2)(g_1 - ig_2) + g_3^2 \end{pmatrix} \\ &= \begin{pmatrix} g_1^2 + g_2^2 + g_3^2 & 0 \\ 0 & g_1^2 + g_2^2 + g_3^2 \end{pmatrix} \\ &= \|g\|^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned}$$

Thus, the condition that we found above, coming from  $u \neq 0$ , reads:

$$\frac{\|g\|^2}{f^2 - (mc/h)^2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

We conclude that we must have the following equality:

$$\|g\|^2 = f^2 - \left(\frac{mc}{h}\right)^2$$

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

The point now is that the above result invites us to use the rescaled energy-momentum four-vector as variable,  $k = \pm p/h$ , and we are led in this way to the following result:

THEOREM 13.16. *The basic plane wave solutions, of type*

$$\psi(s) = ae^{-i\langle k, s \rangle} u$$

*of the Dirac equation, come from the functions*

$$u^1 = \frac{1}{E + mc^2} \begin{pmatrix} E + mc^2 \\ 0 \\ cp_z \\ cp_x + icp_y \end{pmatrix}, \quad u^2 = \frac{1}{E + mc^2} \begin{pmatrix} 0 \\ E + mc^2 \\ cp_x - icp_y \\ -cp_z \end{pmatrix}$$

*corresponding to particle solutions, plus from the functions*

$$u^3 = \frac{1}{E + mc^2} \begin{pmatrix} cp_z \\ cp_x + icp_y \\ E + mc^2 \\ 0 \end{pmatrix}, \quad u^4 = \frac{1}{E + mc^2} \begin{pmatrix} cp_x - icp_y \\ -cp_z \\ 0 \\ E + mc^2 \end{pmatrix}$$

*corresponding to antiparticle solutions.*

PROOF. This comes by putting together all the above. Indeed, with  $k = \pm p/h$ , as suggested above, we have four choices, which are as follows:

$$\begin{aligned} v &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} & , & \quad w = \frac{c}{E + mc^2} \begin{pmatrix} p_z \\ p_x + ip_y \end{pmatrix} \\ v &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} & , & \quad w = \frac{c}{E + mc^2} \begin{pmatrix} p_x - ip_y \\ -p_z \end{pmatrix} \\ w &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} & , & \quad v = \frac{c}{E + mc^2} \begin{pmatrix} p_z \\ p_x + ip_y \end{pmatrix} \\ w &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} & , & \quad v = \frac{c}{E + mc^2} \begin{pmatrix} p_x - ip_y \\ -p_z \end{pmatrix} \end{aligned}$$

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

Regarding the exact physical interpretation of the above plane wave solutions that we found, this is something quite tricky, and we will discuss this later.

In any case, we have now in our theory the electron accompanied by the positron and the photon. There are in fact many other particles which satisfy the Dirac equation, with this equation being in fact the one which describes the spin 1/2 particles. More on this later, when we will know more about the various particles that can appear.

As a last topic, from this preliminary discussion on the Dirac equation, let us discuss now the normalization of the solutions that we found above. We will need:

PROPOSITION 13.17. *For the basic plane wave solutions found above, we have*

$$||u||^2 = \frac{2E}{E + mc^2}$$

*with the norm being computed with respect to the usual complex scalar product.*

PROOF. According to our formulae above, for  $u = u^1, u^2, u^3, u^4$  we have:

$$\begin{aligned} ||u||^2 &= \frac{1}{(E + mc^2)^2} ((E + mc^2)^2 + c^2(p_x^2 + p_y^2 + p_z^2)) \\ &= \frac{1}{(E + mc^2)^2} ((E + mc^2)^2 + c^2||p||^2) \end{aligned}$$

Now recall that for the energy-momentum vector  $\tilde{p} = (E/c, p)$  we have  $||\tilde{p}|| = mc$ . Thus, the norm of the momentum vector component is given by:

$$||p||^2 = \left(\frac{E}{c}\right)^2 - ||\tilde{p}||^2 = \frac{E^2}{c^2} - m^2c^2$$

With this formula in hand, we can finish our computation, as follows:

$$\begin{aligned} ||u||^2 &= \frac{1}{(E + mc^2)^2} \left( (E + mc^2)^2 + c^2 \left( \frac{E^2}{c^2} - m^2c^2 \right) \right) \\ &= \frac{1}{(E + mc^2)^2} (E^2 + m^2c^4 + 2Emc^2 + E^2 - m^2c^4) \\ &= \frac{1}{(E + mc^2)^2} (2E^2 + 2Emc^2) \\ &= \frac{2E}{E + mc^2} \end{aligned}$$

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

In what regards now the normalization of the solutions  $u$  found in Theorem 13.16, there are several possible useful conventions here, as follows:

$$||Nu||^2 = \frac{2E}{c} \quad , \quad ||Nu||^2 = \frac{E}{mc^2} \quad , \quad ||Nu||^2 = 1$$

The corresponding normalizations constants  $N$  can be computed by using Proposition 13.17, and are respectively given by the following formulae:

$$N = \sqrt{\frac{E + mc^2}{c}} \quad , \quad N = \sqrt{\frac{E + mc^2}{2mc^2}} \quad , \quad N = \sqrt{\frac{E + mc^2}{2E}}$$

As before with the exact physical interpretation of the plane wave solutions that we found, their normalization is also something quite tricky, and we will discuss this later.



### 13d. Invariance questions

Let us discuss now invariance questions for the solutions of the Dirac equation. As already mentioned in the above, this equation was meant to be a relativistic version of the Schrödinger equation, but the fact that this equation is indeed relativistic, from the point of view of the invariance of solutions, is still something that we must establish.

We recall from chapter 4 that the frame change, with respect to moving with speed  $v$  along  $Ox$ , is given by the following formulae, where  $\beta = v/c$  and  $\gamma = 1/\sqrt{1 - \beta^2}$ :

$$ct' = \gamma(ct - \beta x)$$

$$x' = \gamma(x - \beta ct)$$

$$y' = y$$

$$z' = z$$

Equivalently, in matrix form, we have the following formula:

$$\begin{pmatrix} ct' \\ x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \gamma & -\gamma\beta & 0 & 0 \\ -\gamma\beta & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix}$$

Regarding the reverse frame change, this is obtained via  $v \rightarrow -v$ , which gives the following formulae, with  $\beta = v/c$  and  $\gamma = 1/\sqrt{1 - \beta^2}$  as before:

$$ct = \gamma(ct' + \beta x')$$

$$x = \gamma(x' + \beta ct')$$

$$y = y'$$

$$z = z'$$

Equivalently, in matrix form, we have the following formula:

$$\begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \gamma & \gamma\beta & 0 & 0 \\ \gamma\beta & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} ct' \\ x' \\ y' \\ z' \end{pmatrix}$$

We refer to chapter 4 for more on these formulae, and to chapter 6 too, for a proof of the fact that the Maxwell equations are invariant under these transformations.

In what regards now the Dirac equation, we have the following result:

THEOREM 13.18. *A solution  $\psi$  of the Dirac equation leads, infinitesimally, to the following solution of the same equation, with respect to a frame change as above,*

$$\psi' = A\psi$$

*with the matrix  $A$  being given by the following formula,*

$$A = \begin{pmatrix} a & 0 & 0 & b \\ 0 & a & b & 0 \\ 0 & b & a & 0 \\ b & 0 & 0 & a \end{pmatrix}$$

*where the parameters are given by the following formulae,*

$$a = \sqrt{\frac{\gamma + 1}{2}} \quad , \quad b = -\sqrt{\frac{\gamma - 1}{2}}$$

*with  $\gamma = 1/\sqrt{1 - v^2/c^2}$  being the Lorentz factor.*

PROOF. This is something quite tricky, the idea being as follows:

(1) Consider indeed the Dirac equation, as formulated in Definition 13.8:

$$ih \left( \frac{\gamma_0 d}{cdt} + \frac{\gamma_1 d}{dx} + \frac{\gamma_2 d}{dy} + \frac{\gamma_3 d}{dz} \right) \psi = mc\psi$$

It is convenient to use the relativistic space-time position vector, given by:

$$s = \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix}$$

With this convention, the Dirac equation, as formulated above, becomes:

$$ih \sum_{i=0}^3 \gamma_i \frac{d\psi}{ds_i} = mc\psi$$

(2) Now let us write as well this equation in the new frame, as follows:

$$ih \sum_{i=0}^3 \gamma_i \frac{d\psi'}{ds'_i} = mc\psi'$$

We can compute the derivation operators  $d/ds'_i$  in terms of the original derivation operators  $d/ds_i$  by using the chain rule, starting from:

$$\begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \gamma & \gamma\beta & 0 & 0 \\ \gamma\beta & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} ct' \\ x' \\ y' \\ z' \end{pmatrix}$$

Indeed, if we denote by  $L^{-1}$  the  $4 \times 4$  matrix appearing above, that of the reverse frame change, then the above formula reads, in terms of space-time position vectors:

$$s = L^{-1}s'$$

Now by using the chain rule, we obtain from this the following formula:

$$\begin{aligned} \frac{d}{ds'_i} &= \sum_j \frac{ds_j}{ds'_i} \cdot \frac{d}{ds_j} \\ &= \sum_j \frac{d(L^{-1}s')_j}{ds'_i} \cdot \frac{d}{ds_j} \\ &= \sum_{jk} \frac{d((L^{-1})_{jk}s'_k)}{ds'_i} \cdot \frac{d}{ds_j} \\ &= \sum_{jk} (L^{-1})_{jk} \frac{ds'_k}{ds'_i} \cdot \frac{d}{ds_j} \\ &= \sum_j (L^{-1})_{ji} \frac{d}{ds_j} \\ &= \sum_j (L^{-1})_{ij} \frac{d}{ds_j} \end{aligned}$$

Here we have used at the end the fact that  $L^{-1}$  is symmetric. In vector notation now, the conclusion is that we have the following formula:

$$\frac{d}{ds'} = L^{-1} \frac{d}{ds}$$

(3) With this formula in hand, let us go back to the Dirac equation in the new frame, and try to find a solution of type  $\psi' = A\psi$  for it. Our equation reads:

$$ih \sum_{i=0}^3 \gamma_i \frac{dA\psi}{ds'_i} = mcA\psi$$

By using the linearity of the derivatives, and then the formula found in (2), the left term of this new Dirac equation is given by the following formula:

$$\begin{aligned} ih \sum_{i=0}^3 \gamma_i \frac{dA\psi}{ds'_i} &= ih \sum_{i=0}^3 \gamma_i A \frac{d\psi}{ds'_i} \\ &= ih \sum_{i=0}^3 \gamma_i A L^{-1} \frac{d\psi}{ds_i} \end{aligned}$$

Summarizing, with  $\psi' = A\psi$ , our equation takes the following form:

$$ih \sum_{i=0}^3 \gamma_i AL^{-1} \frac{d\psi}{ds_i} = mcA\psi$$

Equivalently, by multiplying everything by  $A^{-1}$ , our equation becomes:

$$ih \sum_{i=0}^3 A^{-1} \gamma_i AL^{-1} \frac{d\psi}{ds_i} = mc\psi$$

(4) Now let us compare this new equation that we found with the original Dirac equation, from (1), which was as follows:

$$ih \sum_{i=0}^3 \gamma_i \frac{d\psi}{ds_i} = mc\psi$$

In order to have solutions  $\psi' = A\psi$  as above, in a plain, non-infinitesimal sense, the obvious possibility is that when we have the following formulae, for any  $i$ :

$$A^{-1} \gamma_i AL^{-1} = \gamma_i$$

Thus, as a conclusion to this discussion, in order to prove our theorem, in a plain formulation, it would be enough to establish the following formulae, for any  $i$ :

$$A^{-1} \gamma_i A = \gamma_i L$$

(5) With this done, let us have a look at the matrix  $A$  in the statement. That matrix is constructed by using two numbers  $a, b$ , which are given by:

$$a = \sqrt{\frac{\gamma+1}{2}} \quad , \quad b = -\sqrt{\frac{\gamma-1}{2}}$$

Our first claim is that we have the following useful formulae, relating  $a, b$ :

$$a^2 - b^2 = 1$$

$$a^2 + b^2 = \gamma$$

$$2ab = -\gamma\beta$$

Indeed, the first two formulae are clear, and the third formula comes from:

$$\begin{aligned}
 2ab &= -\sqrt{\gamma^2 - 1} \\
 &= -\sqrt{\frac{1}{1 - \beta^2} - 1} \\
 &= -\sqrt{\frac{\beta^2}{1 - \beta^2}} \\
 &= -\frac{\beta}{\sqrt{1 - \beta^2}} \\
 &= -\gamma\beta
 \end{aligned}$$

Observe also that the above formula  $a^2 - b^2 = 1$  suggests using a notation of type  $a = \cosh p, b = \sinh p$ , but we will not need this here.

(6) Before getting to the matrix  $A$  in the statement, let us further study the above numbers  $a, b$ . With the help of the formulae connecting them, from (5), we obtain:

$$\begin{pmatrix} a & b \\ b & a \end{pmatrix} \begin{pmatrix} a & b \\ b & a \end{pmatrix} = \begin{pmatrix} a^2 + b^2 & 2ab \\ 2ab & a^2 + b^2 \end{pmatrix} = \begin{pmatrix} \gamma & -\gamma\beta \\ -\gamma\beta & \gamma \end{pmatrix}$$

We recognize here the upper left block of  $L$ , and so we have:

$$L = \begin{pmatrix} a & b & 0 & 0 \\ b & a & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}^2$$

A similar discussion goes for the inverse Lorentz matrix. Indeed, we have:

$$\begin{pmatrix} a & b \\ b & a \end{pmatrix} \begin{pmatrix} a & -b \\ -b & a \end{pmatrix} = \begin{pmatrix} a^2 - b^2 & 0 \\ 0 & a^2 - b^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Thus, we have the following matrix inversion formula:

$$\begin{pmatrix} a & b \\ b & a \end{pmatrix}^{-1} = \begin{pmatrix} a & -b \\ -b & a \end{pmatrix}$$

We conclude that the inverse of the Lorentz matrix is given by:

$$L^{-1} = \begin{pmatrix} a & -b & 0 & 0 \\ -b & a & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}^2$$

(7) Now let us look at the matrix in the statement, namely:

$$A = \begin{pmatrix} a & 0 & 0 & b \\ 0 & a & b & 0 \\ 0 & b & a & 0 \\ b & 0 & 0 & a \end{pmatrix}$$

This matrix, and its inverse, are then given by the following formulae:

$$A = a + b\gamma_0\gamma_2$$

$$A^{-1} = a - b\gamma_0\gamma_2$$

Indeed, in what regards the formula of  $A$ , this comes from:

$$\begin{aligned} \gamma_0\gamma_2 &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & \sigma_2 \\ -\sigma_2 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

As for the formula of  $A^{-1}$ , this comes from the following computation, with  $J = \gamma_0\gamma_2$ , which satisfies  $J^2 = 1$ , by using the formula  $a^2 - b^2 = 1$  from (5):

$$\begin{aligned} (a + bJ)(a - bJ) &= a^2 + abJ - abJ - b^2J^2 \\ &= a^2 - b^2 \\ &= 1 \end{aligned}$$

(8) In relation now with the formulae needed in (4), our first claim is that:

$$A\gamma_0A = \gamma_0$$

$$A^{-1}\gamma_1A = \gamma_1$$

$$A\gamma_2A = \gamma_2$$

$$A^{-1}\gamma_3A = \gamma_3$$

(9) Indeed, the first formula comes from the following computation:

$$\begin{aligned} A\gamma_0A &= (a + b\gamma_0\gamma_2)\gamma_0(a + b\gamma_0\gamma_2) \\ &= a^2\gamma_0 + ab\gamma_0\gamma_0\gamma_2 + ab\gamma_0\gamma_2\gamma_0 + b^2\gamma_0\gamma_2\gamma_0\gamma_0\gamma_2 \\ &= a^2\gamma_0 - b^2\gamma_0 \\ &= \gamma_0 \end{aligned}$$

The second formula comes from a similar computation, as follows:

$$\begin{aligned}
 A^{-1}\gamma_1 A &= (a + b\gamma_0\gamma_2)\gamma_1(a - b\gamma_0\gamma_2) \\
 &= a^2\gamma_1 - ab\gamma_1\gamma_0\gamma_2 + ab\gamma_0\gamma_2\gamma_1 - b^2\gamma_0\gamma_2\gamma_1\gamma_0\gamma_2 \\
 &= a^2\gamma_1 - b^2\gamma_1 \\
 &= \gamma_1
 \end{aligned}$$

The third formula again comes from a similar computation, as follows:

$$\begin{aligned}
 A\gamma_2 A &= (a + b\gamma_0\gamma_2)\gamma_2(a + b\gamma_0\gamma_2) \\
 &= a^2\gamma_2 + ab\gamma_2\gamma_0\gamma_2 + ab\gamma_0\gamma_2\gamma_2 + b^2\gamma_0\gamma_2\gamma_2\gamma_0\gamma_2 \\
 &= a^2\gamma_2 - b^2\gamma_2 \\
 &= \gamma_2
 \end{aligned}$$

As for the fourth formula, this comes again from a similar computation, namely:

$$\begin{aligned}
 A^{-1}\gamma_3 A &= (a + b\gamma_0\gamma_2)\gamma_3(a - b\gamma_0\gamma_2) \\
 &= a^2\gamma_3 - ab\gamma_3\gamma_0\gamma_2 + ab\gamma_0\gamma_2\gamma_3 - b^2\gamma_0\gamma_2\gamma_3\gamma_0\gamma_2 \\
 &= a^2\gamma_3 - b^2\gamma_3 \\
 &= \gamma_3
 \end{aligned}$$

(10) Now observe that, with respect to the formulae needed in (4), the second and the fourth formulae found in (8) are what we need. As for the first and third formulae, these are not exactly what we need, and we must fine-tune them. We first have:

$$\begin{aligned}
 A^{-1}\gamma_0 A &= (a - b\gamma_0\gamma_2)\gamma_0(a + b\gamma_0\gamma_2) \\
 &= a^2\gamma_0 + ab\gamma_0\gamma_0\gamma_2 - ab\gamma_0\gamma_2\gamma_0 - b^2\gamma_0\gamma_2\gamma_0\gamma_0\gamma_2 \\
 &= (a^2 + b^2)\gamma_0 + 2ab\gamma_2 \\
 &= \gamma \cdot \gamma_0 - \gamma\beta \cdot \gamma_2
 \end{aligned}$$

Similarly, we have the following computation:

$$\begin{aligned}
 A^{-1}\gamma_2 A &= (a - b\gamma_0\gamma_2)\gamma_2(a + b\gamma_0\gamma_2) \\
 &= a^2\gamma_2 + ab\gamma_2\gamma_0\gamma_2 - ab\gamma_0\gamma_2\gamma_2 - b^2\gamma_0\gamma_2\gamma_2\gamma_0\gamma_2 \\
 &= (a^2 + b^2)\gamma_2 - 2ab\gamma_0 \\
 &= \gamma \cdot \gamma_2 + \gamma\beta \cdot \gamma_0
 \end{aligned}$$

(11) Time now to review the conditions found in (4). These conditions, corresponding to the plain Lorentz invariance of the solutions of the Dirac equation, were  $A^{-1}\gamma_i A = \gamma_i L$ . But because of  $\gamma_i^2 = 1$ , we can reformulate them in the following way:

$$L = \gamma_i A^{-1} \gamma_i A$$

Now in view of the above, it makes sense to introduce the following matrices:

$$L_i = \gamma_i A^{-1} \gamma_i A$$

According to the computations in (9), we have the following formulae:

$$L_1 = L_3 = 1$$

On the other hand, according to the computations in (10), we have as well:

$$L_0 = \gamma_0(\gamma \cdot \gamma_0 - \gamma\beta \cdot \gamma_2) = \gamma - \gamma\beta \cdot \gamma_0\gamma_2$$

$$L_2 = \gamma_2(\gamma \cdot \gamma_2 + \gamma\beta \cdot \gamma_0) = \gamma - \gamma\beta \cdot \gamma_0\gamma_2$$

Thus, in usual matrix form, we have the following formulae:

$$L_0 = L_2 = \begin{pmatrix} \gamma & 0 & 0 & -\gamma\beta \\ 0 & \gamma & -\gamma\beta & 0 \\ 0 & -\gamma\beta & \gamma & 0 \\ -\gamma\beta & 0 & 0 & \gamma \end{pmatrix}$$

(12) The point now is that, based on what we found above, we can say that  $\psi' = A\psi$  satisfies the Dirac equation in the new frame, in an infinitesimal sense, as claimed.  $\square$

### 13e. Exercises

This was a quite difficult chapter, going both into difficult mathematics and difficult physics, and as exercises on all this, chosen rather elementary, we have:

EXERCISE 13.19. *Let us set  $\bar{\psi} = \psi^* \gamma_0$ . Prove, by using the equality  $A\gamma_0 A = \gamma_0$  established above, that the quantity*

$$\bar{\psi}\psi = |\psi_1|^2 + |\psi_2|^2 - |\psi_3|^2 - |\psi_4|^2$$

*is invariant under the transformations  $\psi \rightarrow A\psi$ . Show also that this quantity is invariant under the parity operator  $(x, y, z) \rightarrow -(x, y, z)$ .*

EXERCISE 13.20. *Verify that  $\gamma_5 = i\gamma_0\gamma_2\gamma_3\gamma_1$  anticommutes with all the Dirac matrices, and then prove that the following quantity, with  $\bar{\psi} = \psi^* \gamma_0$  as above,*

$$\bar{\psi}\gamma_5\psi$$

*is invariant under the transformations  $\psi \rightarrow A\psi$ . Show also that this quantity changes the sign under the parity operator  $(x, y, z) \rightarrow -(x, y, z)$ .*

As bonus exercise, which is definitely recommended, further clarify the meaning of the infinitesimal Lorentz invariance established above.



## CHAPTER 14

### Particle physics

#### 14a. Decay, scattering

We have seen in the previous chapter that, with Dirac and others helping, it is relatively easy to escape from the electron/photon world we have been living in, so far in this book, with the introduction of other particles, appearing from equations inspired from the Schrödinger equation for the electron, and the wave equation for the photon.

However, I don't know about you, but personally, all this rather leaves me with some bitter taste, instead of the expected enthusiasm. Not only the Dirac equation was something quite difficult, both for me to present, and for you to decipher too, I guess, but in what regards its “new” solutions, the straightforward one was this beast called positron, instead of the good old proton, or good old neutron, that we secretly wished for.

Of course, we made some comments on this, in relation with the Big Bang and other, trying somehow to persuade ourselves that yes, what Dirac says is correct, and the positron is very welcome in our physics, and such good news that we came across it. But all this remains a bit twisted, matter of acknowledging a strange conclusion, imposed to us.

In short, time to ask the cat. And cat answers:

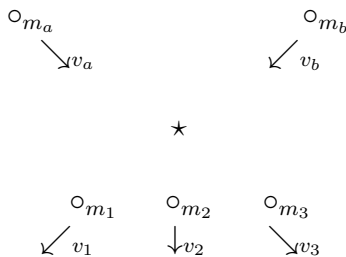
CAT 14.1. *Forget about the proton, not only its mass is different from that of the electron, but its exact charge too. Better stick with the particles that you have, try to understand how these interact. And don't forget, you still have unfinished business with the electron, coming from all that corrections to the hydrogen atom.*

Thanks cat, this sounds wise. So let's leave the proton for later, and the neutron too, these familiar particles might be some sort of cousins of the electron, but as you say, the mechanism behind this is most likely something quite complicated. And instead, let us try to understand how the few particles that we have interact with each other. And with a bit of luck, this might advance us too on that hydrogen business, who knows.

Getting to work now.. but wait, cat still has something to say, let's hear him:

CAT 14.2. *Congratulations boss, from what you say, you're about to develop quantum electrodynamics. And that is good theory, you won't regret it.*

Okay cat, thanks again, and getting to work now, we need to talk about interactions between our particles. But here, we already have some experience from classical mechanics, with the typical picture of what can happen being as follows:



To be more precise, this diagram describes a collision between two particles, but we can of course allow further particles entering the collision, and then the several particles emerging from this collision. The data of each particle, which in classical mechanics means mass  $m$  and speed  $v$ , is carefully recorded, with of course the aim of recovering the output data from the input data. Finally, all this can take place in arbitrary dimensions, and also, importantly, the collision can be elastic, or plastic, or any mixture of these.

This was for basic interactions in classical mechanics. In our present setting, particle physics, things are a bit more complicated than this, due to a variety of reasons, and experimental physics suggests looking at two main types of interactions, as follows:

FACT 14.3. *In particle physics, we have two main types of interactions, namely:*

- (1) *Decay.* This is when a particle decomposes, as a result of whatever internal mechanism, into a sum of other particles,  $*_0 \rightarrow *_1 + \dots + *_n$ .
- (2) *Scattering.* This is when two particles meet, by colliding, or almost, and combine and decompose into a sum of other particles,  $*_a + *_b \rightarrow *_1 + \dots + *_n$ .

Obviously, all this departs a bit from our classical mechanics knowledge, as explained above, and several comments are in order here, as follows:

(1) In what regards decay, something that we talked a lot about, when doing thermodynamics, and then quantum mechanics, is an electron of an atom changing its energy level, and emitting a photon. But this can be regarded as being decay.

(2) As for scattering, the simplest example here appears again from an electron of an atom, changing its energy level, but this time by absorbing a photon. Of course, there are many other possible examples, such as the electron-positron annihilation.

(3) Regarding now the mechanisms at work, for decay we certainly have some intuition from classical mechanics, and we can label that process as being some sort of “explosion”. With of course the comment that usual explosions are rather something chemical.

(4) As for scattering, this normally stands for some sort of “collision”, a bit as in classical mechanics, but with the comment that we are really talking here about general scattering, not only collisions. More on this, which is something quite subtle, later.

Getting to work for good now, let us first gather some knowledge and data about decay. However, this is no easy business, in view of the physics that we know, and it is helpful at this point to take off, and get into our popular physics knowledge, regarding radioactivity. Or at least that is easy for me, during Chernobyl 1986 I used to be a teenager in the nearby Romania, and we all duly learned, in a hurry, all that theory. But you surely know a bit about this too, say from Fukushima 2011, don't you.

So, decay and its mathematics. Ignoring the physics, this is basically a matter of probability and statistics, and the basics here can be summarized as follows:

**THEOREM 14.4.** *In the context of decay, the quantity to look at is the decay rate  $\lambda$ , which is the probability per unit time that the particle will disintegrate. With this:*

- (1) *The number of particles remaining at time  $t > 0$  is  $N_t = e^{-\lambda t} N_0$ .*
- (2) *The mean lifetime of a particle is  $\tau = 1/\lambda$ .*
- (3) *The half-life of the substance is  $t_{1/2} = (\log 2)/\lambda$ .*

**PROOF.** As said above, this is basic probability, as follows:

- (1) In mathematical terms, our definition of the decay rate reads:

$$\frac{dN}{dt} = -\lambda N$$

By integrating, we are led to the formula in the statement, namely:

$$N_t = e^{-\lambda t} N_0$$

- (2) Let us first convert what we have into a probability law. We have:

$$\int_0^\infty N_t dt = \int_0^\infty N_0 e^{-\lambda t} dt = \frac{N_0}{\lambda}$$

Thus, the density of the probability decay function is given by:

$$f(t) = \frac{\lambda}{N_0} \cdot N_0 e^{-\lambda t} = \lambda e^{-\lambda t}$$

We can now compute the mean lifetime, by integrating by parts, as follows:

$$\begin{aligned}
 \tau &= \langle t \rangle \\
 &= \int_0^\infty t f(t) dt \\
 &= \int_0^\infty \lambda t e^{-\lambda t} dt \\
 &= \int_0^\infty t (-e^{-\lambda t})' dt \\
 &= \int_0^\infty e^{-\lambda t} dt \\
 &= \frac{1}{\lambda}
 \end{aligned}$$

(3) Finally, regarding the half-life, this is by definition the time  $t_{1/2}$  required for the decaying quantity to fall to one-half of its initial value. Mathematically, this means:

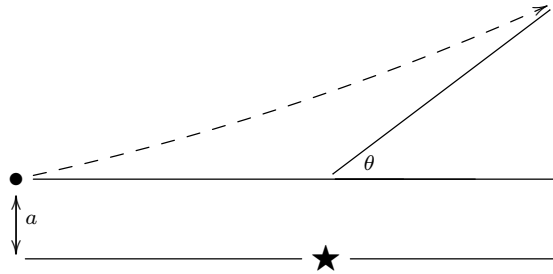
$$N_t = 2^{-\frac{t}{t_{1/2}}} N_0$$

Now by comparing with  $N_t = e^{-\lambda t} N_0$ , this gives  $t_{1/2} = (\log 2)/\lambda$ , as stated.  $\square$

So long for decay, and we will temporarily stop here, with the preliminaries. And no worries, decay will be back very soon, with physics, formulae and everything.

Getting now to scattering, this is something far more familiar, because we can fully use here our experience from classical mechanics. Let us start with:

DEFINITION 14.5. *The generic picture of scattering is as follows,*



with  $a \geq 0$  being the impact parameter, and  $\theta \in [0, \pi]$  being the scattering angle.

In other words, we assume here that the particle misses its target by  $a \geq 0$ , with the limiting case  $a = 0$  corresponding of course to exactly hitting the target, and we are interested in computing the scattering angle  $\theta \in [0, \pi]$  as a function  $\theta = \theta(a)$ .

Many things can be said here, and more on this in a moment, but as an answer to a question that you might certainly have, we are interested in  $a > 0$  because this is what happens in particle physics, there is no need for exactly hitting the target for having a collision-type interaction. By the case, the limiting case  $a = 0$  is rather unwanted in the context of our scattering question, because by symmetry this would normally force the scattering angle to be  $\theta = 0$  or  $\theta = \pi$ , which does not look very interesting.

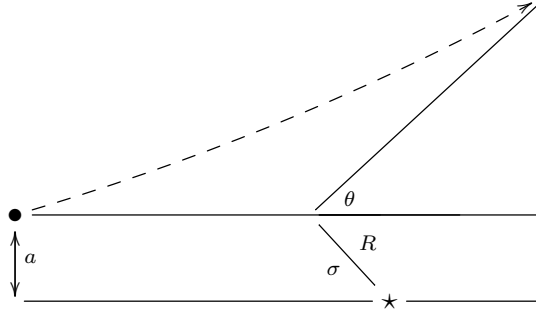
But probably too much talking, let us do a computation. We have here:

**PROPOSITION 14.6.** *In the context of classical particle colliding elastically with a hard sphere of radius  $R > 0$ , we have the formula*

$$a = R \cos \frac{\theta}{2}$$

and so the scattering angle is given by  $\theta = 2 \arccos(a/R)$ .

**PROOF.** In the context from the statement, which is all classical mechanics, and more specifically is a basic elastic collision, between a point particle and a hard sphere, if the impact factor is  $a > R$ , nothing happens. In the case  $a \leq R$  we do have an impact, and a bounce of our particle on the hard sphere, the picture of the event being as follows:



Here the sphere is missing, due to budget cuts, with only its center  $\star$  being pictured, but you get the point. Now with  $\sigma$  being the angle in the statement, we have the following two formulae, with the first one being clear on the above picture, and with the second one coming from the fact that, at the rebound, the various angles must sum up to  $\pi$ :

$$a = R \sin \sigma \quad , \quad 2\sigma + \theta = \pi$$

We deduce that the impact factor is given by the following formula:

$$a = R \sin \left( \frac{\pi}{2} - \frac{\theta}{2} \right) = R \cos \frac{\theta}{2}$$

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

With this understood, let us try to make something more 3D, and statistical, out of this. We can indeed further build on Definition 14.5, as follows:

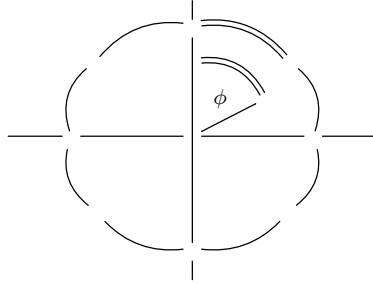
DEFINITION 14.7. *In the general context of scattering, we can:*

- (1) *Extend our length/angle correspondence  $a \rightarrow \theta$  into an infinitesimal area/solid angle correspondence  $d\sigma \rightarrow d\Omega$ .*
- (2) *Talk about the inverse derivative  $D(\theta)$  of this correspondence, called differential cross section, according to the formula  $d\sigma = D(\theta)d\Omega$ .*
- (3) *And finally, define the total cross section of the scattering event as being the quantity  $\sigma = \int d\sigma = \int D(\theta)d\Omega$ .*

And good news, the notion of total cross section  $\sigma$ , as constructed above, is the one that we will need, in what follows, with this being to scattering something a bit similar to what the decay rate  $\lambda$  was to decay, that is, the main quantity to look at.

In order to understand how the cross section works, we have:

PROPOSITION 14.8. *Assuming that the incoming beam comes as follows,*



*subtending a certain angle  $\phi$ , the differential cross section is given by*

$$D(\theta) = \left| \frac{a}{\sin \theta} \cdot \frac{da}{d\theta} \right|$$

*and the total cross section is given by  $\sigma = \int D(\theta)d\Omega$ .*

PROOF. Assume indeed that we have a uniform beam as the one pictured in the statement, enclosed by the double lines appearing there, and with the need for a beam instead of a single particle coming from what we do in Definition 14.7, which is rather of continuous nature. Our claim is that we have the following formulae:

$$d\sigma = |a \cdot da \cdot d\phi| \quad , \quad d\Omega = |\sin \theta \cdot d\theta \cdot d\phi|$$

Indeed, the first formula, at departure, is clear from the picture above, and the second formula is clear from a similar picture at the arrival. Now with these formulae in hand,

by dividing them, we obtain the following formula for the differential cross section:

$$\begin{aligned} D(\theta) &= \frac{d\sigma}{d\Omega} \\ &= \left| \frac{a \cdot da \cdot d\phi}{\sin \theta \cdot d\theta \cdot d\phi} \right| \\ &= \left| \frac{a}{\sin \theta} \cdot \frac{da}{d\theta} \right| \end{aligned}$$

As for the total cross section, this is given as usual by  $\sigma = \int D(\theta) d\Omega$ .  $\square$

As an illustration for this, in the case of a hard sphere scattering, we have:

**THEOREM 14.9.** *In the case of a hard sphere scattering, the cross section is*

$$\sigma = \pi R^2$$

*with  $R > 0$  being the radius of the sphere.*

**PROOF.** We know from Proposition 14.6 that, with the notations there, we have:

$$a = R \cos \frac{\theta}{2}$$

At the level of the corresponding differentials, this gives the following formula:

$$\frac{da}{d\theta} = -\frac{R}{2} \sin \frac{\theta}{2}$$

We can now compute the differential cross section, as above, and we obtain:

$$\begin{aligned} D(\theta) &= \left| \frac{a}{\sin \theta} \cdot \frac{da}{d\theta} \right| \\ &= \frac{R \cos(\theta/2)}{\sin \theta} \cdot \frac{R \sin(\theta/2)}{2} \\ &= \frac{R^2 (\sin \theta)/2}{2 \sin \theta} \\ &= \frac{R^2}{4} \end{aligned}$$

Now by integrating, we obtain from this, via some calculus, the following formula:

$$\sigma = \int \frac{R^2}{4} d\Omega = \pi R^2$$

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

Summarizing, for a hard sphere scattering, the cross section turns to be something very simple, namely the area of the sphere met by the beam. This is of course something quite particular, and when using more complicated targets, the formula of  $\sigma$  gets more complicated too. We will come back to this, with further examples, later on.

### 14b. Golden Rule

Time now to get into the real thing, namely quantum electrodynamics (QED) and Feynman diagrams, which correctly explain the behavior of the electron, and of other particles that we know. And to be followed later by quantum chromodynamics (QCD), which does even better, dealing with smaller beasts, quarks and related gnomes.

We will be following for our presentation the lovely particle physics book of Griffiths [44]. That is a remarkable book, taking the challenge of explaining such things, which are normally quite advanced, to undergraduates. Of course, in case you are not exactly an undergraduate, say you are a professional mathematical physicist, and struggle with what comes next, do not worry. This is normal, can happen to everyone, and I must admit that I struggled too, sometimes quite late in my career, with such things.

Skipping a discussion here with cat, whose sardonic smile, when hearing all this, does not look very inviting, let us get to work. As a main principle regarding particle decay, following Fermi and others, we have the following simple and useful fact:

**PRINCIPLE 14.10** (Fermi Golden Rule). *In the context of a particle physics decay,  $*_0 \rightarrow *_1 + \dots + *_n$ , the decay rate is given by*

$$\lambda = \int |M|^2 dp$$

*with  $M = M(p_0, \dots, p_n)$  being the amplitude of the interaction, and with the integration being restricted to the part of the phase space allowed by basic physics.*

Obviously, several things going on here, that will take us some time, to understand. To start with, the above Golden Rule looks quite reasonable, namely getting  $\lambda$  by integrating something on the phase space. It remains to understand two things, namely what the formula of the amplitude  $M$  is, and where does the integration exactly take place.

Leaving the formula of the amplitude  $M$  for later, let us try to answer the second question, regarding the allowed phase space. According to the Golden Rule, that is simply the phase space allowed by basic physics, and here that basic physics is:

**ADDENDUM 14.11.** *In the above context, the basic physics is as follows:*

- (1) *The total energy and momentum must be conserved.*
- (2) *Each outgoing particle must keep its mass constant.*
- (3) *Each outgoing particle must have positive energy.*

Summarizing, all common sense things that we have here. In mathematical terms now, it is better to add integrands corresponding to the above conditions (1,2,3), instead of exactly specifying the allowed state space. And with both (1) and (2) requiring Dirac masses  $\delta$ , and with (3) requiring a Heaviside function  $H = \chi_{(0,\infty)}$ , we are led to:



PRINCIPLE 14.12 (Golden Rule 2). *In the context of a particle physics decay,  $*_0 \rightarrow *_1 + \dots + *_n$ , the decay rate is given by*

$$\lambda = \int |M|^2 \delta \left( p_0 - \sum_{i=1}^n p_i \right) \prod_{i=1}^n \delta(p_i^2 - m_i^2 c^2) H(p_i^0) dp$$

with  $M = M(p_0, \dots, p_n)$  being the amplitude of the interaction.

Which looks quite neat, but there is actually a subtlety here, in relation with the Dirac masses, which take as arguments squares of variables, instead of the variables themselves. In order to clarify this, let us make the following computation, with  $a > 0$ :

$$\begin{aligned} \int_{\mathbb{R}} f(x) \delta(x^2 - a^2) dx &= \int_{-\infty}^0 f(x) \delta(x^2 - a^2) dx + \int_0^{\infty} f(x) \delta(x^2 - a^2) dx \\ &= \int_{-\infty}^a f(y - a) \delta(y^2 - 2ay) dy + \int_{-a}^{\infty} f(y + a) \delta(y^2 + 2ay) dy \\ &\simeq \int_{-\infty}^a f(y - a) \delta(-2ay) dy + \int_{-a}^{\infty} f(y + a) \delta(2ay) dy \\ &= \int_{-\infty}^{2a^2} f\left(\frac{z}{2a} - a\right) \delta(-z) \frac{dz}{2a} + \int_{-2a^2}^{\infty} f\left(\frac{z}{2a} + a\right) \delta(z) \frac{dz}{2a} \\ &= \frac{f(-a)}{2a} + \frac{f(a)}{2a} \\ &= \int_{\mathbb{R}} f(x) \frac{\delta(x - a) + \delta(x + a)}{2a} dx \end{aligned}$$

Sounds like physics, you would say, and in answer, yes physics that is, but in any case, we have in this way the definition for our quadratic Dirac masses, as follows:

$$\delta(x^2 - a^2) = \frac{\delta(x - a) + \delta(x + a)}{2a}$$

With this understood, and before getting into what the amplitude  $M$  is, let us make some normalizations. Here these normalizations are, and you will have to believe me here, all of them are made for good reasons, as we will discover in a moment:

(1) We have  $\lambda \sim S$ , with  $S = 1/\prod_i (m_i!)$ , where  $m_i \in \mathbb{N}$  with  $\sum m_i = n$  are the multiplicities of the output particles, and it is better to leave  $S$  outside the integral.

(2) Also,  $\lambda \sim 1/(2hm_0)$ , with  $h$  being as usual the reduced Planck constant, and  $m_0$  being the initial mass, and it is better to leave  $1/(2hm_0)$  outside the integral too.

(3) Each Dirac mass  $\delta$  behaves better in computations when multiplied by a  $2\pi$  factor. Also, each individual  $dp_i$  symbol behaves better when divided by a  $2\pi$  factor.

Now by doing all these normalizations, which amounts in correspondingly rescaling the amplitude  $M$ , and with this being certainly not a big deal, because we haven't even talked yet about what this amplitude  $M$  is, so free to do this, we are led to:

PRINCIPLE 14.13 (Golden Rule 3). *In the context of a particle physics decay,  $*_0 \rightarrow *_1 + \dots + *_n$ , the decay rate is given by*

$$\lambda = \frac{S}{2hm_0} \int |\mathcal{M}|^2 (2\pi)^4 \delta \left( p_0 - \sum_{i=1}^n p_i \right) \prod_{i=1}^n 2\pi \delta(p_i^2 - m_i^2 c^2) H(p_i^0) \frac{dp_i}{(2\pi)^4}$$

with  $\mathcal{M} = \mathcal{M}(p_0, \dots, p_n)$  being the normalized amplitude of the interaction, and with  $S = 1/\prod_i(m_i!)$ , where  $m_i \in \mathbb{N}$  with  $\sum m_i = n$  are the multiplicities of the output.

And good news, this will be normally the final form of the Golden Rule for decays, that we will be using, in what follows. In practice, however, we will see in a moment that the integration with respect to time is easy to perform, and this will lead to yet another formulation of the Golden Rule, which is the most useful one, for applications.

Before that, however, some philosophical comments. The Golden Rule has become now something quite complicated, and there is still a discussion about  $\mathcal{M}$ , which will certainly bring its part of complicated mathematics. But remember that, in the end, everything comes from Principle 14.10, which is something quite simple. So, no fear.

This being said, even when looking at Principle 14.10, you might wonder, is that really correct, and where that really comes from. In answer, common sense as explained above, then lots of experiments too, confirming it, or rather confirming the formula of  $\mathcal{M}$ , that we haven't talked about yet, and finally quantum field theory, which is something advanced, that can actually prove this Golden Rule, starting from simple principles.

Back to our business now, we will take Principle 14.13 for granted, and further build on it, with examples, the formula of  $\mathcal{M}$ , and more. Before that, however, let us do what was suggested above, namely integrating with respect to time. This leads to:

THEOREM 14.14 (Golden Rule 4). *In the context of a particle physics decay,  $*_0 \rightarrow *_1 + \dots + *_n$ , the decay rate is given, in standard  $\tilde{p} = (E/c, p)$  notation, by*

$$\lambda = \frac{S}{2hm_0} \int |\mathcal{M}|^2 (2\pi)^4 \delta \left( \tilde{p}_0 - \sum_{i=1}^n \tilde{p}_i \right) \prod_{i=1}^n \frac{1}{2\sqrt{||p_i||^2 + m_i^2 c^2}} \cdot \frac{dp_i}{(2\pi)^3}$$

with  $\mathcal{M} = \mathcal{M}(p_0, \dots, p_n)$  being the normalized amplitude,  $S = 1/\prod_i(m_i!)$  being the statistical factor, and with the convention  $E_i/c = \sqrt{||p_i||^2 + m_i^2 c^2}$ , both in  $\mathcal{M}$  and  $\delta$ .

PROOF. We use the formula from Principle 14.13, written with our standard notation for energy-momentum vectors  $\tilde{p} = (E/c, p)$  from chapter 13, which is as follows:

$$\lambda = \frac{S}{2hm_0} \int |\mathcal{M}|^2 (2\pi)^4 \delta \left( \tilde{p}_0 - \sum_{i=1}^n \tilde{p}_i \right) \prod_{i=1}^n 2\pi \delta(\tilde{p}_i^2 - m_i^2 c^2) H \left( \frac{E_i}{c} \right) \frac{d\tilde{p}_i}{(2\pi)^4}$$

In order to further process this formula, let us look at each of the  $n$  products on the right. According to our conventions for quadratic Dirac masses, explained after Principle 14.12, the Dirac mass appearing there is given by the following formula:

$$\begin{aligned} \delta(\tilde{p}_i^2 - m_i^2 c^2) &= \delta \left( \frac{E_i^2}{c^2} - \|p_i\|^2 - m_i^2 c^2 \right) \\ &= \delta \left( \left( \frac{E_i}{c} \right)^2 - \left( \sqrt{\|p_i\|^2 + m_i^2 c^2} \right)^2 \right) \\ &= \frac{\delta \left( \frac{E_i}{c} - \sqrt{\|p_i\|^2 + m_i^2 c^2} \right) + \delta \left( \frac{E_i}{c} + \sqrt{\|p_i\|^2 + m_i^2 c^2} \right)}{2\sqrt{\|p_i\|^2 + m_i^2 c^2}} \end{aligned}$$

Thus we have two possibilities, and since the Heaviside term  $H(E_i/c)$  equals 1 on the first one, and vanishes on the second one, we are led to the following formula:

$$\delta(\tilde{p}_i^2 - m_i^2 c^2) H \left( \frac{E_i}{c} \right) = \frac{\delta \left( \frac{E_i}{c} - \sqrt{\|p_i\|^2 + m_i^2 c^2} \right)}{2\sqrt{\|p_i\|^2 + m_i^2 c^2}}$$

But this leads to the conclusion in the statement. □

As an illustration, for two-particle decays many things simplify, and we have:

THEOREM 14.15. *For two-particle decays,  $*_0 \rightarrow *_1 + *_2$ , the Golden Rule reads*

$$\lambda = \frac{S \|p\|}{8\pi h m_0^2 c} |\mathcal{M}|^2$$

with  $\mathcal{M}$  being the amplitude,  $\|p\|$  being the magnitude of either outgoing momentum,

$$\|p\| = \frac{c}{2m_0} \sqrt{m_0^4 + m_1^4 + m_2^4 - 2m_0^2 m_1^2 - 2m_0^2 m_2^2 - 2m_1^2 m_2^2}$$

and the statistical factor being  $S = 1$  if  $*_1 \neq *_2$ , and  $S = 1/2$  if  $*_1 = *_2$ .

PROOF. In the case of two-particle decays, the formula in Theorem 14.14 takes the following form, with the statistical factor  $S$  being the one in the statement:

$$\begin{aligned}\lambda &= \frac{S}{2hm_0} \int |\mathcal{M}|^2 (2\pi)^4 \delta(\tilde{p}_0 - \tilde{p}_1 - \tilde{p}_2) \prod_{i=1}^2 \frac{1}{2\sqrt{||p_i||^2 + m_i^2 c^2}} \cdot \frac{dp_i}{(2\pi)^3} \\ &= \frac{S}{32\pi^2 hm_0} \int |\mathcal{M}|^2 \frac{\delta(\tilde{p}_0 - \tilde{p}_1 - \tilde{p}_2)}{\sqrt{||p_1||^2 + m_1^2 c^2} \sqrt{||p_2||^2 + m_2^2 c^2}} dp_1 dp_2\end{aligned}$$

Let us look now at the Dirac function. This decomposes over components, as follows:

$$\delta(\tilde{p}_0 - \tilde{p}_1 - \tilde{p}_2) = \delta\left(\frac{E_0}{c} - \frac{E_1}{c} - \frac{E_2}{c}\right) \delta(p_0 - p_1 - p_2)$$

With the particle  $*_0$  being supposed to be at rest, we have the following formulae:

$$\frac{E_0}{c} = m_0 c \quad , \quad p_0 = 0$$

On the other hand, recall from Theorem 14.14 that the machinery there leads to:

$$\frac{E_1}{c} = \sqrt{||p_1||^2 + m_1^2 c^2} \quad , \quad \frac{E_2}{c} = \sqrt{||p_2||^2 + m_2^2 c^2}$$

Thus, the above Dirac mass is in fact given by the following formula:

$$\delta(\tilde{p}_0 - \tilde{p}_1 - \tilde{p}_2) = \delta\left(m_0 c - \sqrt{||p_1||^2 + m_1^2 c^2} - \sqrt{||p_2||^2 + m_2^2 c^2}\right) \delta(p_1 + p_2)$$

Getting back now to the formula of the decay rate, that becomes:

$$\begin{aligned}\lambda &= \frac{S}{32\pi^2 hm_0} \int |\mathcal{M}|^2 \frac{\delta\left(m_0 c - \sqrt{||p_1||^2 + m_1^2 c^2} - \sqrt{||p_2||^2 + m_2^2 c^2}\right)}{\sqrt{||p_1||^2 + m_1^2 c^2} \sqrt{||p_2||^2 + m_2^2 c^2}} \\ &\quad \times \delta(p_1 + p_2) dp_1 dp_2\end{aligned}$$

Since we must have  $p_2 = -p_1$ , this expression further simplifies to:

$$\lambda = \frac{S}{32\pi^2 hm_0} \int |\mathcal{M}|^2 \frac{\delta\left(m_0 c - \sqrt{||p_1||^2 + m_1^2 c^2} - \sqrt{||p_1||^2 + m_2^2 c^2}\right)}{\sqrt{||p_1||^2 + m_1^2 c^2} \sqrt{||p_1||^2 + m_2^2 c^2}} dp_1$$

In spherical coordinates, this expression takes the following form:

$$\lambda = \frac{S}{32\pi^2 hm_0} \int |\mathcal{M}|^2 \frac{\delta\left(m_0 c - \sqrt{r^2 + m_1^2 c^2} - \sqrt{r^2 + m_2^2 c^2}\right)}{\sqrt{r^2 + m_1^2 c^2} \sqrt{r^2 + m_2^2 c^2}} r^2 \sin s dr ds dt$$

The point now is that by physics, to be explained later, the amplitude must be of the form  $\mathcal{M} = \mathcal{M}(r)$ . Thus the angular integrals contribute with factors as follows:

$$\int_0^\pi \sin s ds = 2 \quad , \quad \int_0^{2\pi} dt = 2\pi$$

We conclude that in the end we are left with a real integral, over  $r$ , as follows:

$$\lambda = \frac{S}{8\pi\hbar m_0} \int_0^\infty |\mathcal{M}|^2 \frac{\delta\left(m_0c - \sqrt{r^2 + m_1^2c^2} - \sqrt{r^2 + m_2^2c^2}\right)}{\sqrt{r^2 + m_1^2c^2}\sqrt{r^2 + m_2^2c^2}} r^2 dr$$

In order to compute this integral, consider the following variable:

$$u = \sqrt{r^2 + m_1^2c^2} + \sqrt{r^2 + m_2^2c^2}$$

Now observe that by differentiating, we obtain the following formula:

$$\begin{aligned} \frac{du}{dr} &= \frac{2r}{2\sqrt{r^2 + m_1^2c^2}} + \frac{2r}{2\sqrt{r^2 + m_2^2c^2}} \\ &= r \left( \frac{1}{\sqrt{r^2 + m_1^2c^2}} + \frac{1}{\sqrt{r^2 + m_2^2c^2}} \right) \\ &= \frac{ur}{\sqrt{r^2 + m_1^2c^2}\sqrt{r^2 + m_2^2c^2}} \end{aligned}$$

Thus, in terms of this new variable  $u$ , we have the following formula:

$$\begin{aligned} \lambda &= \frac{S}{8\pi\hbar m_0} \int_{m_1c+m_2c}^\infty |\mathcal{M}|^2 \delta(m_0c - u) \frac{r}{u} du \\ &= \frac{Sr}{8\pi\hbar m_0^2c} |\mathcal{M}|^2 \end{aligned}$$

Here in the last formula  $r$  stands for the value of the variable  $r$  evaluated at the place where the Dirac mass takes the value 1, that we can compute as follows:

$$\begin{aligned} u = m_0c &\iff \sqrt{r^2 + m_1^2c^2} + \sqrt{r^2 + m_2^2c^2} = m_0c \\ &\iff r^2 + m_1^2c^2 = r^2 + m_2^2c^2 + m_0^2c^2 - 2m_0c\sqrt{r^2 + m_2^2c^2} \\ &\iff 2m_0\sqrt{r^2 + m_2^2c^2} = (m_0^2 - m_1^2 + m_2^2)c \\ &\iff 4m_0^2(r^2 + m_2^2c^2) = (m_0^2 - m_1^2 + m_2^2)^2c^2 \\ &\iff 4m_0^2r^2 = ((m_0^2 - m_1^2 + m_2^2)^2 - 4m_0^2m_2^2)c^2 \\ &\iff r = \frac{c}{2m_0} \sqrt{m_0^4 + m_1^4 + m_2^4 - 2m_0^2m_1^2 - 2m_0^2m_2^2 - 2m_1^2m_2^2} \end{aligned}$$

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

So long for particle decays,  $*_0 \rightarrow *_1 + \dots + *_n$ . We will be back to them later in this chapter, once we will know more about the amplitude  $\mathcal{M}$ .

### 14c. Cross sections

With the particle decays understood, let us turn now to the other phenomenon that can appear, namely collision, or scattering,  $*_a + *_b \rightarrow *_1 + \dots + *_n$ . Here, as you can imagine, the situation is quite similar to that for the decays, as follows:

(1) The Golden Rule in its first formulation, Principle 14.10, holds again, this time with a new amplitude for the interaction, of the form  $N = N(p_a, p_b, p_1, \dots, p_n)$ , which remains, as before in the case of the decays, to be suitably normalized.

(2) The basic physics from Addendum 14.11, which complements Principle 14.10, namely conservation of total energy and total momentum, and constant mass and positive energy requirement for each outgoing particle, holds unchanged.

Thus, we led to the following analogue of Principle 14.12, or Golden Rule 2:

PRINCIPLE 14.16 (Golden Rule 2'). *In the context of a particle physics scattering,  $*_a + *_b \rightarrow *_1 + \dots + *_n$ , the cross section is given by*

$$\sigma = \int |N|^2 \delta \left( p_a + p_b - \sum_{i=1}^n p_i \right) \prod_{i=1}^n \delta(p_i^2 - m_i^2 c^2) H(p_i^0) dp$$

with  $N = N(p_a, p_b, p_1, \dots, p_n)$  being the amplitude of the interaction.

Regarding now the normalization of the amplitude, which is a key point, some things change at the level of physics, the situation being as follows:

(1) We have  $\lambda \sim S$ , with  $S = 1/\prod_i (m_i!)$ , where  $m_i \in \mathbb{N}$  with  $\sum m_i = n$  are the multiplicities of the output particles, exactly as before.

(2) Next, and importantly, at the level of the physics we have the following new formula, that we will discuss more in detail later, instead of the previous  $\lambda \sim 1/(2hm_0)$ , because we are doing now something else, with two particles colliding instead of one decaying, and by computing a cross section  $\sigma$  instead of a decay rate  $\lambda$ :

$$\lambda \sim \frac{h^2}{4\sqrt{\langle p_a, p_b \rangle^2 - (m_a m_b c^2)^2}}$$

(3) Finally, as before, each Dirac mass  $\delta$  behaves better in computations when multiplied by a  $2\pi$  factor, and each  $dp_i$  behaves better when divided by a  $2\pi$  factor.

Now by doing all these normalizations, and with some amplitude magic helping, we are led to the following analogue of Principle 14.13, or Golden Rule 3:

PRINCIPLE 14.17 (Golden Rule 3'). *In the context of a particle physics scattering,  $*_a + *_b \rightarrow *_1 + \dots + *_n$ , the cross section is given by*

$$\sigma = \frac{Sh^2}{4\sqrt{< p_a, p_b >^2 - (m_a m_b c^2)^2}} \int |\mathcal{M}|^2 (2\pi)^4 \delta \left( p_a + p_b - \sum_{i=1}^n p_i \right) \\ \times \prod_{i=1}^n 2\pi \delta(p_i^2 - m_i^2 c^2) H(p_i^0) \frac{dp_i}{(2\pi)^4}$$

with  $\mathcal{M} = \mathcal{M}(p_a, p_b, p_1, \dots, p_n)$  being the normalized amplitude of the interaction, and with  $S = 1/\prod_i (m_i!)$ , where  $m_i \in \mathbb{N}$  with  $\sum m_i = n$  are the multiplicities of the output.

Observe that we have used here the same  $\mathcal{M}$  symbol as in Principle 14.13. Obviously, this is something heavy, and deep, and the whole point with everything lies here. But in the lack of advanced physics tools in order to explain this, which as already mentioned on the occasion of Principle 14.13, come from quantum field theory, we will have to leave it like this, with of course the comment that “all this is verified by experiments”.

Excuse me, but cat is here, meowing something. In English translation, what he says is not very funny, “with your lack of understanding of physics, that you practice every day, and share with your students too, you will end up destroying the whole planet”. Well, dear cat, what can I answer. Physics is not everything in life, let’s not forget about chemistry, and then especially biology, big and slow animals like dinosaurs, or nowadays humans, usually rule, and there is nothing much we can do about this.

Moving ahead now, with Principle 14.17 agreed upon, we can integrate as before over time, and we have the following analogue of Theorem 14.14, or Golden Rule 4:

THEOREM 14.18 (Golden Rule 4'). *In the context of scattering,  $*_a + *_b \rightarrow *_1 + \dots + *_n$ , the cross section is given, in standard  $\tilde{p} = (E/c, p)$  notation, by*

$$\sigma = \frac{Sh^2}{4\sqrt{< \tilde{p}_a, \tilde{p}_b >^2 - (m_a m_b c^2)^2}} \int |\mathcal{M}|^2 (2\pi)^4 \delta \left( \tilde{p}_a + \tilde{p}_b - \sum_{i=1}^n \tilde{p}_i \right) \\ \times \prod_{i=1}^n \frac{1}{2\sqrt{||p_i||^2 + m_i^2 c^2}} \cdot \frac{dp_i}{(2\pi)^3}$$

with  $\mathcal{M} = \mathcal{M}(p_a, p_b, p_1, \dots, p_n)$  being the normalized amplitude,  $S = 1/\prod_i (m_i!)$  being the statistical factor, and with the convention  $E_i/c = \sqrt{||p_i||^2 + m_i^2 c^2}$ , both in  $\mathcal{M}$  and  $\delta$ .

PROOF. This is indeed nearly identical to the proof of Theorem 14.14, with all the manipulations there applying unchanged, to the present situation.  $\square$

Getting now to illustrations, let us work out the analogue of Theorem 14.15, by looking at situations of type  $*_a + *_b \rightarrow *_1 + *_2$ . The result here is as follows:

THEOREM 14.19. *For events of type  $*_a + *_b \rightarrow *_1 + *_2$ , the Golden Rule for scattering, in the center of mass frame, gives the differential cross section formula*

$$\frac{d\sigma}{d\Omega} = \frac{Sh^2c^2|\mathcal{M}|^2}{64\pi^2(E_a + E_b)^2} \cdot \frac{\|p_1\|}{\|p_a\|}$$

with  $\mathcal{M}$  being the amplitude,  $\|p_a\| = \|p_b\|$  and  $\|p_1\| = \|p_2\|$  being the magnitudes of the incoming and outgoing momenta, and  $S = 1$  if  $*_1 \neq *_2$ , and  $S = 1/2$  if  $*_1 = *_2$ .

PROOF. In the case  $n = 2$ , the formula in Theorem 14.18 takes the following form, with the statistical factor  $S$  being the one in the statement:

$$\begin{aligned} \sigma &= \frac{Sh^2}{4\sqrt{\langle \tilde{p}_a, \tilde{p}_b \rangle^2 - (m_a m_b c^2)^2}} \int |\mathcal{M}|^2 \frac{(2\pi)^4 \delta(\tilde{p}_a + \tilde{p}_b - \tilde{p}_1 - \tilde{p}_2)}{4\sqrt{\|p_1\|^2 + m_1^2 c^2} \sqrt{\|p_2\|^2 + m_2^2 c^2}} \cdot \frac{dp_1 dp_2}{(2\pi)^6} \\ &= \frac{Sh^2}{64\pi^2 \sqrt{\langle \tilde{p}_a, \tilde{p}_b \rangle^2 - (m_a m_b c^2)^2}} \int |\mathcal{M}|^2 \frac{\delta(\tilde{p}_a + \tilde{p}_b - \tilde{p}_1 - \tilde{p}_2)}{\sqrt{\|p_1\|^2 + m_1^2 c^2} \sqrt{\|p_2\|^2 + m_2^2 c^2}} \cdot dp_1 dp_2 \end{aligned}$$

Our claim now is that, assuming that we are in the center of mass frame, where  $p_b = -p_a$ , the square root in the normalization factor is given by the following formula:

$$\sqrt{\langle \tilde{p}_a, \tilde{p}_b \rangle^2 - (m_a m_b c^2)^2} \simeq \frac{E_a + E_b}{c} \|p_a\|$$

With the notation  $P = \|p_a\|^2 = \|p_b\|^2$ , coming from our assumption  $p_b = -p_a$ , this is the same as proving that the following quantity is negligible:

$$K = c^2 (\langle \tilde{p}_a, \tilde{p}_b \rangle^2 - (m_a m_b c^2)^2) - (E_a + E_b)^2 P$$

In order to prove our claim, the first observation is that, according to our conventions for four-vectors, and to  $p_b = -p_a$ , we have the following formula:

$$\langle \tilde{p}_a, \tilde{p}_b \rangle = \frac{E_a E_b}{c^2} - \langle p_a, p_b \rangle = \frac{E_a E_b}{c^2} + P$$

We deduce from this that the above quantity  $K$  is given by:

$$\begin{aligned} K &= c^2 \left( \left( \frac{E_a E_b}{c^2} + P \right)^2 - (m_a m_b c^2)^2 \right) - (E_a + E_b)^2 P \\ &= \frac{E_a^2 E_b^2}{c^2} + c^2 P^2 + 2E_a E_b P - m_a^2 m_b^2 c^6 - E_a^2 P - E_b^2 P - 2E_a E_b P \\ &= \frac{E_a^2 E_b^2}{c^2} + c^2 P^2 - m_a^2 m_b^2 c^6 - (E_a^2 + E_b^2) P \end{aligned}$$



In terms of Lorentz factors, we obtain from this the following formula:

$$\begin{aligned}
K &= \frac{(\gamma_a m_a c^2)^2 (\gamma_b m_b c^2)^2}{c^2} + c^2 P^2 - m_a^2 m_b^2 c^6 - ((\gamma_a m_a c^2)^2 + (\gamma_b m_b c^2)^2) P \\
&= \gamma_a^2 \gamma_b^2 m_a^2 m_b^2 c^6 + c^2 P^2 - m_a^2 m_b^2 c^6 - \gamma_a^2 m_a^2 c^4 P - \gamma_b^2 m_b^2 c^4 P \\
&= (\gamma_a^2 \gamma_b^2 - 1) m_a^2 m_b^2 c^6 + c^2 P^2 - (\gamma_a^2 m_a^2 + \gamma_b^2 m_b^2) c^4 P
\end{aligned}$$

Now observe that, for a particle with relativistic momentum  $p = \gamma m v$ , the corresponding Lorentz factor  $\gamma$  can be computed by using the following formula:

$$\begin{aligned}
\sqrt{1 + \left(\frac{\|p\|}{mc}\right)^2} &= \sqrt{1 + \frac{\gamma^2 \|v\|^2}{c^2}} \\
&= \sqrt{1 + \frac{1}{1 - \|v\|^2/c^2} \cdot \frac{\|v\|^2}{c^2}} \\
&= \sqrt{\frac{c^2}{c^2 - \|v\|^2}} \\
&= \frac{1}{\sqrt{1 - \|v\|^2/c^2}} \\
&= \gamma
\end{aligned}$$

By using this formula for both our particles  $*_a$  and  $*_b$ , for which  $\|p_a\|^2 = \|p_b\|^2 = P$ , we can finish our computation of the above quantity  $K$ , and we obtain, as desired:

$$\begin{aligned}
K &= (\gamma_a^2 \gamma_b^2 - 1) m_a^2 m_b^2 c^6 + c^2 P^2 - (\gamma_a^2 m_a^2 + \gamma_b^2 m_b^2) c^4 P \\
&= \left( \left(1 + \frac{P}{m_a^2 c^2}\right) \left(1 + \frac{P}{m_b^2 c^2}\right) - 1 \right) m_a^2 m_b^2 c^6 \\
&\quad - \left( \left(1 + \frac{P}{m_a^2 c^2}\right) m_a^2 + \left(1 + \frac{P}{m_b^2 c^2}\right) m_b^2 \right) c^4 P \\
&= (m_a^2 c^4 P + m_b^2 c^4 P + c^2 P^2) - (m_a^2 c^4 P + m_b^2 c^4 P + 2c^2 P^2) \\
&= -c^2 P^2 \\
&\simeq 0
\end{aligned}$$

Thus, claim proved, and with this in hand, our previous formula of the cross section, from the beginning of the present proof, takes the following form:

$$\sigma = \frac{Sh^2 c}{64\pi^2 (E_a + E_b) \|p_a\|} \int |\mathcal{M}|^2 \frac{\delta(\tilde{p}_a + \tilde{p}_b - \tilde{p}_1 - \tilde{p}_2)}{\sqrt{\|p_1\|^2 + m_1^2 c^2} \sqrt{\|p_2\|^2 + m_2^2 c^2}} \cdot dp_1 dp_2$$

Let us look now at the Dirac function. This decomposes over components, as follows:

$$\delta(\tilde{p}_a + \tilde{p}_b - \tilde{p}_1 - \tilde{p}_2) = \delta\left(\frac{E_a}{c} + \frac{E_b}{c} - \frac{E_1}{c} - \frac{E_2}{c}\right) \delta(p_1 + p_2)$$

Now recall from Theorem 14.18 that the machinery there leads to:

$$\frac{E_1}{c} = \sqrt{||p_1||^2 + m_1^2 c^2} \quad , \quad \frac{E_2}{c} = \sqrt{||p_2||^2 + m_2^2 c^2}$$

Thus, the above Dirac mass is in fact given by the following formula:

$$\delta(\tilde{p}_a + \tilde{p}_b - \tilde{p}_1 - \tilde{p}_2) = \delta\left(\frac{E_a + E_b}{c} - \sqrt{||p_1||^2 + m_1^2 c^2} - \sqrt{||p_2||^2 + m_2^2 c^2}\right) \delta(p_1 + p_2)$$

Getting back now to the formula of the cross section, that becomes:

$$\begin{aligned} \sigma &= \frac{Sh^2 c}{64\pi^2(E_a + E_b)||p_a||} \int |\mathcal{M}|^2 \frac{\delta\left(\frac{E_a + E_b}{c} - \sqrt{||p_1||^2 + m_1^2 c^2} - \sqrt{||p_2||^2 + m_2^2 c^2}\right)}{\sqrt{||p_1||^2 + m_1^2 c^2} \sqrt{||p_2||^2 + m_2^2 c^2}} \\ &\quad \times \delta(p_1 + p_2) dp_1 dp_2 \end{aligned}$$

Since we must have  $p_2 = -p_1$ , this expression further simplifies to:

$$\sigma = \frac{Sh^2 c}{64\pi^2(E_a + E_b)||p_a||} \int |\mathcal{M}|^2 \frac{\delta\left(\frac{E_a + E_b}{c} - \sqrt{||p_1||^2 + m_1^2 c^2} - \sqrt{||p_1||^2 + m_2^2 c^2}\right)}{\sqrt{||p_1||^2 + m_1^2 c^2} \sqrt{||p_1||^2 + m_2^2 c^2}} dp_1$$

In spherical coordinates, this expression takes the following form:

$$\begin{aligned} \sigma &= \frac{Sh^2 c}{64\pi^2(E_a + E_b)||p_a||} \int |\mathcal{M}|^2 \frac{\delta\left(\frac{E_a + E_b}{c} - \sqrt{r^2 + m_1^2 c^2} - \sqrt{r^2 + m_2^2 c^2}\right)}{\sqrt{r^2 + m_1^2 c^2} \sqrt{r^2 + m_2^2 c^2}} \\ &\quad \times r^2 \sin s dr ds dt \end{aligned}$$

The problem now is that, with respect to what we did before for decay, something changes here in the physics, because the quantity  $|\mathcal{M}|^2$  depends this time on the direction of  $p_1$ , and so we cannot do the angular integrations, trivially, as before. More on this later, when talking in detail about the amplitude  $\mathcal{M}$ , and in the meantime, let us finish our computation, by using some other methods and tricks. The idea will be very simple. Consider the solid angle  $\Omega$  on the sphere, whose differential is given by:

$$d\Omega = \sin s ds dt$$

Now observe that we have the following formula, with the quantity on the left being something that we certainly want to compute, namely the differential cross section:

$$\frac{d\sigma}{d\Omega} = \frac{Sh^2 c}{64\pi^2(E_a + E_b)||p_a||} \int_0^\infty |\mathcal{M}|^2 \frac{\delta\left(\frac{E_a + E_b}{c} - \sqrt{r^2 + m_1^2 c^2} - \sqrt{r^2 + m_2^2 c^2}\right)}{\sqrt{r^2 + m_1^2 c^2} \sqrt{r^2 + m_2^2 c^2}} r^2 dr$$

The point now is that the integral on the right is something familiar to us, and can be computed as before, in the decay case, in the proof of Theorem 14.15. To be more precise, following the proof there, consider the following quantity:

$$u = \sqrt{r^2 + m_1^2 c^2} + \sqrt{r^2 + m_2^2 c^2}$$

As before by differentiating, we obtain the following formula:

$$\frac{du}{dr} = \frac{ur}{\sqrt{r^2 + m_1^2 c^2} \sqrt{r^2 + m_2^2 c^2}}$$

Thus, in terms of this new variable  $u$ , we have the following formula:

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \frac{Sh^2 c}{64\pi^2 (E_a + E_b) \|p_a\|} \int_{m_1 c + m_2 c}^{\infty} |\mathcal{M}|^2 \delta\left(\frac{E_a + E_b}{c} - u\right) \frac{r}{u} du \\ &= \frac{Sh^2 c^2 r}{64\pi^2 (E_a + E_b)^2 \|p_a\|} |\mathcal{M}|^2 \end{aligned}$$

Here in the last formula  $r$  stands for the value of the variable  $r$  evaluated at the place where the Dirac mass takes the value 1, that we can compute as follows:

$$\begin{aligned} u &= \frac{E_a + E_b}{c} \\ \Leftrightarrow \sqrt{r^2 + m_1^2 c^2} + \sqrt{r^2 + m_2^2 c^2} &= \frac{E_a + E_b}{c} \\ \Leftrightarrow r^2 + m_1^2 c^2 &= r^2 + m_2^2 c^2 + \left(\frac{E_a + E_b}{c}\right)^2 - \frac{2(E_a + E_b)}{c} \sqrt{r^2 + m_2^2 c^2} \\ \Leftrightarrow \frac{2(E_a + E_b)}{c} \sqrt{r^2 + m_2^2 c^2} &= \left(\frac{E_a + E_b}{c}\right)^2 + (m_2^2 - m_1^2) c^2 \\ \Leftrightarrow 2\sqrt{r^2 + m_2^2 c^2} &= \frac{E_a + E_b}{c} + \frac{m_2^2 - m_1^2}{E_a + E_b} c^3 \\ \Leftrightarrow 4r^2 + 4m_2^2 c^2 &= \left(\frac{E_a + E_b}{c}\right)^2 + \left(\frac{m_2^2 - m_1^2}{E_a + E_b}\right)^2 c^6 + 2(m_2^2 - m_1^2) c^2 \\ \Leftrightarrow 4r^2 &= \left(\frac{E_a + E_b}{c}\right)^2 + \left(\frac{m_2^2 - m_1^2}{E_a + E_b}\right)^2 c^6 - 2(m_1^2 + m_2^2) c^2 \\ \Leftrightarrow r &= \frac{1}{2} \sqrt{\left(\frac{E_a + E_b}{c}\right)^2 + \left(\frac{m_2^2 - m_1^2}{E_a + E_b}\right)^2 c^6 - 2(m_1^2 + m_2^2) c^2} \end{aligned}$$

Equivalently, with  $r = \|p\|_1$ , we are led to the formula in the statement.  $\square$

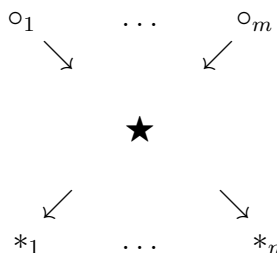
### 14d. Amplitude, diagrams

With the above discussed, generalities of the Golden Rule in particle physics, for both decays and scattering, it remains to say what the amplitude  $\mathcal{M}$  of the interactions is. With this being the missing ingredient, for what we have been doing, so far.

However, this is something quite tricky. To start with, we have been talking about decays  $*_0 \rightarrow *_1 + \dots + *_n$  and scattering  $*_a + *_b \rightarrow *_1 + \dots + *_n$ , and the obvious good framework for discussing both situations is that of more complex events, as follows:

$$\circ_1 + \dots + \circ_m \rightarrow *_1 + \dots + *_n$$

Generally speaking, we can think at what happens here as being a quite general type of collision, with several input and output particles. So, let us draw a collision scheme, in the spirit of those what we drew some time ago, when doing classical mechanics:



If you are already a bit familiar with Feynman diagrams, you will recognize here an order 0 such diagram, drawn a bit in an upside-down way. So, thanks for the remark, and in answer, we will be using in the remainder of this book the following convention:

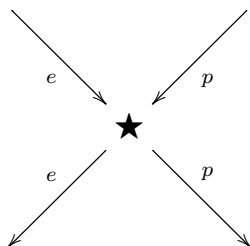
**CONVENTION 14.20.** *For everything diagrams, we use the following conventions, which are commonplace in mathematics, and in modern theoretical physics too:*

- (1) *The vertical direction is for action, going from up to down.*
- (2) *The horizontal direction is for scalars, and other mathematics.*

We will be actually not using in this book scalars and other mathematics as in (2), which are rather advanced things, but it is useful I think to learn the basics in this way, so that you can understand later what modern mathematicians and physicists are doing, without being confused by notations and orientation. And as a joke here, to finish this discussion, all this is quite natural, because if we changed Dirac's notation for the scalar products, we should change Feynman's conventions for diagrams too, right.

Back to work now, we already have some knowledge about decays and scattering, in the particle physics context, but if there is something where we really do have some decent knowledge, that is the movement of the electron  $e$  around the proton  $p$ , in the context of the hydrogen atom, that we spent the whole Part III of the present book in studying.

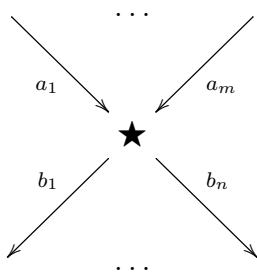
So, this will be our starting point, the mechanics of the hydrogen atom, with the electron  $e$  moving around the proton  $p$ . Obviously, what happens here is some sort of scattering,  $e + p \rightarrow e + p$ , so let us draw right away diagram for this situation:



You might say, end of the story here, this is the relevant diagram, and with that middle  $\star$  symbol being actually a bit inappropriate, because nothing special happens anyway, electron  $e$  spinning smoothly around the proton  $p$ , with no fight or anything.

However, this is wrong. Remember all that corrections to the hydrogen atom, that we had troubles in understanding, and with what we understood being the tip of the iceberg, anyway? The whole point in advanced quantum mechanics lies there, in all that corrections, and quantum electrodynamics comes with the following bright idea:

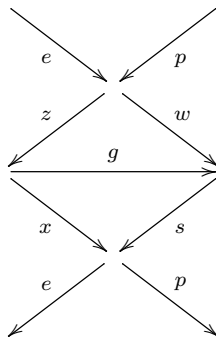
**IDEA 14.21.** *Even for simple situations, like the hydrogen atom  $e + p \rightarrow e + p$ , the interactions should come in a hierarchic way, with the basic order 0 diagram*



*being followed by order 1, order 2 and so on diagrams, and with the corresponding amplitude  $\mathcal{M}$  being computed accordingly, as a power series in a certain variable  $\alpha$ .*

And isn't this bright. Everything illuminates now. So, we should blame all that mysterious corrections to the hydrogen atom on higher order interactions and diagrams, describing our  $e + p \rightarrow e + p$  process, coming in complement to the order 0 diagram

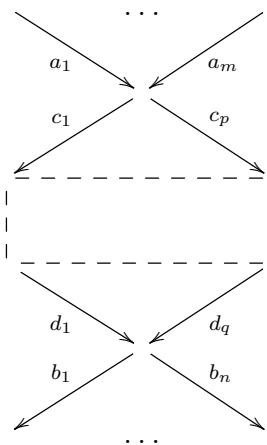
pictured above, with the typical higher order diagram being something as follows:



Here we have used some random letters,  $z, w, g, x, s$ , for the mysterious, very short lived particles that might appear at any time in our process  $e + p \rightarrow e + p$ , that we can hold responsible for the various corrections to the hydrogen atom, that we studied in Part III. Of course, once our theory formally established, we will have to understand, via some further theory, and experiments too, what these beasts  $z, w, g, x, s$  really are.

In short, bright idea that we have, but enormous work still lying ahead, for making all this really work. Getting started now, inspired by the above, let us formulate:

**DEFINITION 14.22.** *A Feynman diagram for a multiple scattering and decay event  $a_1 + \dots + a_m \rightarrow b_1 + \dots + b_n$  is a diagram of type*



*with  $c_i, d_i$  being short-lived particles appearing in the event, and with the middle box being allowed to contain any such configuration of temporary particles too.*

Very nice all this, and getting now to work for good, so many things to be done. Let us start with the general recipe, since I am sure that you are very curious at this point about how all this works, and we will understand later what this really means:

PRINCIPLE 14.23. *The amplitude  $\mathcal{M}$  coming from a given Feynman diagram  $F$  can be computed as follows:*

- (1) *Label each vertex with the corresponding four-momentum vector.*
- (2) *Put factors  $-ig$  at each vertex,  $g$  being the coupling constant.*
- (3) *Install Feynman propagators  $\frac{i}{p_j^2 - m_j^2 c^2}$  on each internal line.*
- (4) *Install rescaled Dirac masses  $(2\pi)^4 \delta(\sum_i p_i)$  at each vertex.*
- (5) *Put integration factors  $\frac{dp_j}{(2\pi)^4}$  on each internal line, and integrate.*
- (6) *Erase the global  $(2\pi)^4 \delta(\sum_i p_i)$  factor appearing after integrating.*
- (7) *Multiply the answer by  $i$ . That is your amplitude  $\mathcal{M}$ .*

Sounds exciting, doesn't it. Obviously, it will take us some time to understand, how all this works. To start with, passed the notations that we used in the above, which are a bit sloppy, but that we chose so in order not to overly complicate things, at least at this preliminary stage of things, what we are doing is quite simple, namely:

(1) The amplitude  $\mathcal{M}$  appears by integrating over the state space, with conservation of energy and momentum being taken into account, at each internal vertex.

(2) What we are integrating are, basically, modulo some rescalings and other mathematical manipulations, the Feynman propagators, on each internal line.

(3) And with these mathematical manipulations including, crucially, the one at the end, namely erasing the final energy and momentum conservation term.

Which looks quite reasonable, physically speaking. However, a more careful look at Principle 14.23 reveals some sort of bug, coming from the coupling constant  $g$  appearing in (2) there. You would probably say, after all, what is this joke, we spent this whole chapter in waiting for the formula of the amplitude  $\mathcal{M}$ , and now here that formula comes, but by relegating everything to yet another beast, this coupling constant  $g$ . Good point, and in answer right away, there is no cheating of any kind here, because we have:

RULE 14.24. *In quantum electrodynamics, the coupling constant is*

$$g = \sqrt{4\pi\alpha}$$

*with  $\alpha \simeq 1/137$  being the fine structure constant.*

In short, with this rule complementing Principle 14.23, that principle is meant to produce something numeric, as amplitude  $\mathcal{M}$ . We will see examples of this in a moment. We have opted for stating Rule 14.24 independently of Principle 14.23, as a complement to it, because Principle 14.23 can work as well beyond quantum electrodynamics, for even finer theories, which require the use of other coupling constants  $g$ . More on this later.

As an example now for the above, chosen as simple as possible, we have:

**THEOREM 14.25.** *For a two-particle decay  $*_0 \rightarrow *_1 + *_2$  the order 0 amplitude is  $\mathcal{M} = g$ , which gives via the Golden Rule an order 0 decay rate of*

$$\lambda = \frac{S||p||\alpha}{2hm_0^2c}$$

with  $||p||$  being the magnitude of either outgoing momentum,

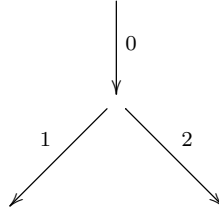
$$||p|| = \frac{c}{2m_0} \sqrt{m_0^4 + m_1^4 + m_2^4 - 2m_0^2m_1^2 - 2m_0^2m_2^2 - 2m_1^2m_2^2}$$

and the statistical factor being  $S = 1$  if  $*_1 \neq *_2$ , and  $S = 1/2$  if  $*_1 = *_2$ .

**PROOF.** We know from Theorem 14.15 that for two-particle decays,  $*_0 \rightarrow *_1 + *_2$ , the Golden Rule takes the following form, with  $S$  and  $||p||$  being as in the statement:

$$\lambda = \frac{S||p||}{8\pi hm_0^2c} |\mathcal{M}|^2$$

In order to compute the amplitude  $\mathcal{M}$ , we use Principle 14.23. At order 0 we only have one Feynman diagram, which is the obvious one, namely:



Now let us apply Principle 14.23. We have a  $-ig$  factor, no propagators, then a  $(2\pi)^4\delta(p_0 - p_1 - p_2)$  factor which appears and disappears, and so we get, right away:

$$\mathcal{M} = i(-ig) = g$$

Thus  $|\mathcal{M}|^2 = g^2 = 4\pi\alpha$ , which gives the formula of  $\lambda$  in the statement.  $\square$

The above example was of course extremely simple, without propagators, or integration work. However, do not worry, for decays at order 1, or for basic scatterings,  $*_a + *_b \rightarrow *_1 + *_2$ , such things will appear. We will discuss them in the next chapter.

### 14e. Exercises

This was a quite tough chapter, and as unique exercise on this, we have:

**EXERCISE 14.26.** *Explore decay at order 1, and scattering at order 0 too.*

And, as said above, do not worry, we will come back to this in the next chapter.



## CHAPTER 15

### Feynman diagrams

#### 15a. Interactions, revised

Welcome to particle physics, take two. Or rather take three, because in chapter 13 we struggled with the Dirac equation, somehow without clear conclusion, and then in chapter 14 we struggled with the Fermi Golden Rule, rather unrelated to chapter 13, without clear conclusion either. Our goal here will be that of putting this material, from chapters 13 and 14, in a together form, and then getting beyond that. Technically, this means to develop quantum electrodynamics (QED), and then getting into quantum chromodynamics (QCD) too, with an introduction to the Standard Model.

This sounds good as a plan, doesn't it, but in practice, I am a bit worried about the exact mathematics and formalism that we will need, for talking about all this. In relation with everything mechanics, including these damn particle things, fellow mathematical and theoretical physicists are usually split between being Lagrangian, and being Hamiltonian. So, shall we upgrade our mathematics and formalism to one of these, and which.

And good question that is, with discussions about it regularly flooding our university coffee rooms, and this for good reason, because the choice of the formalism can dramatically simplify or complicate the math, and you can't really tell in advance. Fortunately cat is here, so let's ask him, are you cats Lagrangian, or Hamiltonian?

CAT 15.1. *Math is trivial anyway, you can safely stay Newtonian.*

Which sounds quite deep, as a piece of advice, and is certainly convenient for us, so we will just follow it, without questions asked, not change anything, and keep going on. Sometimes naivety and ignorance can be the key to good knowledge.

Getting started now, as mentioned above, our main job will be that of merging the material from chapters 13 and 14, by developing quantum electrodynamics.

Before that, however, as a complement to our basic two-particle decay computation, done at the end of the previous chapter, let us do as well some basic computations for scattering, for abstract particles. We first have here the following result:

THEOREM 15.2. *For events of type  $*_a + *_b \rightarrow *_1 + *_2$ , the order 0 amplitude is*

$$\mathcal{M} = \frac{4\pi\alpha}{(p_1 - p_b)^2 - m_e^2 c^2} + \frac{4\pi\alpha}{(p_2 - p_b)^2 - m_e^2 c^2}$$

*which gives via the Golden Rule an order 0 differential cross section of*

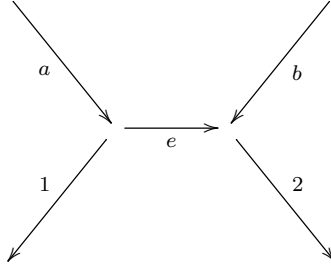
$$\frac{d\sigma}{d\Omega} = \frac{1}{2} \left( \frac{hc\alpha}{4E||p||^2 \sin^2 \theta} \right)^2$$

*in the case  $m_a = m_b = m_1 = m_2$ , with  $||p||$  being the magnitude of outgoing momenta.*

PROOF. We know from chapter 14 that for events of type  $*_a + *_b \rightarrow *_1 + *_2$ , the Golden Rule, in the center of mass frame, gives the following differential cross section formula, with  $\mathcal{M}$  being the amplitude,  $||p_a|| = ||p_b||$  and  $||p_1|| = ||p_2||$  being the magnitudes of the incoming and outgoing momenta, and  $S = 1$  if  $*_1 \neq *_2$ , and  $S = 1/2$  if  $*_1 = *_2$ :

$$\frac{d\sigma}{d\Omega} = \frac{Sh^2 c^2 |\mathcal{M}|^2}{64\pi^2 (E_a + E_b)^2} \cdot \frac{||p_1||}{||p_a||}$$

In order to compute now the amplitude  $\mathcal{M}$ , things are quite simple, because at order 0 we only have two Feynman diagrams. The first one is the obvious one, namely:



Now let us apply the general recipe, explained in the previous chapter:

- We have two vertices, with each being assigned a  $-ig$  factor.
- Then we have an internal line, with propagator as follows:

$$P = \frac{i}{p_e^2 - m_e^2 c^2}$$

- We have then rescaled Dirac masses at the vertices, as follows:

$$(2\pi)^4 \delta(p_a - p_1 - p_e) \quad , \quad (2\pi)^4 \delta(p_b + p_e - p_2)$$

- And finally, we have an integration factor as follows, on the internal line:

$$I = \frac{dp_e}{(2\pi)^4}$$

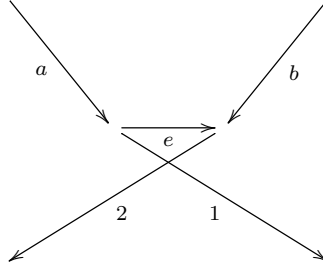
Now by integrating, we obtain the following formula, for the first pre-amplitude:

$$\begin{aligned}
 \mathcal{M}'_1 &= \int (-ig)^2 \frac{i}{p_e^2 - m_e^2 c^2} (2\pi)^4 \delta(p_a - p_1 - p_e) (2\pi)^4 \delta(p_b + p_e - p_2) \frac{dp_e}{(2\pi)^4} \\
 &= -(2\pi)^4 i g^2 \int \frac{1}{p_e^2 - m_e^2 c^2} \delta(p_a - p_1 - p_e) \delta(p_b + p_e - p_2) dp_e \\
 &= -\frac{(2\pi)^4 i g^2}{(p_2 - p_b)^2 - m_e^2 c^2} \delta(p_a + p_b - p_1 - p_2)
 \end{aligned}$$

In order to obtain the first amplitude itself, we must erase the global  $(2\pi)^4 \delta(\sum_i p_i)$  factor appearing after integrating, and multiply the answer by  $i$ . We obtain:

$$\mathcal{M}_1 = \frac{g^2}{(p_2 - p_b)^2 - m_e^2 c^2}$$

Next, the point is that we have as well a second Feynman diagram, obtained by twisting the outgoing lines of the previous diagram, which looks as follows:



But here, no need to do the computation all over again, because we can simply argue that the computation is exactly as the one before, with the change  $p_1 \leftrightarrow p_2$ . Thus, the second amplitude, coming from the above twisted diagram, is given by:

$$\mathcal{M}_2 = \frac{g^2}{(p_1 - p_b)^2 - m_e^2 c^2}$$

As a conclusion to this, the amplitude at order 0, coming from the two possible Feynman diagrams at order 0, pictured above, is given by the following formula:

$$\mathcal{M} = \frac{g^2}{(p_1 - p_b)^2 - m_e^2 c^2} + \frac{g^2}{(p_2 - p_b)^2 - m_e^2 c^2}$$

Moreover, in the context of quantum electrodynamics, where the coupling constant is  $g = \sqrt{4\pi\alpha}$ , with  $\alpha \simeq 1/137$  being the fine structure constant, we obtain:

$$\mathcal{M} = \frac{4\pi\alpha}{(p_1 - p_b)^2 - m_e^2 c^2} + \frac{4\pi\alpha}{(p_2 - p_b)^2 - m_e^2 c^2}$$

Let us compute now the differential cross section, in the center of mass frame. For simplicity, we assume that all the incoming and outgoing masses are equal:

$$m_a = m_b = m_1 = m_2$$

Also, we will make the assumption  $m_e = 0$ , which is something quite natural. Now if we denote by  $\theta$  the scattering angle, we have the following formula:

$$\begin{aligned} (p_1 - p_b)^2 - m_e^2 c^2 &= (p_1 - p_b)^2 \\ &= \langle p_1, p_1 \rangle + \langle p_b, p_b \rangle - 2 \langle p_1, p_b \rangle \\ &= -2||p||^2(1 + \cos \theta) \end{aligned}$$

Similarly, we have the following formula, for the other denominator:

$$\begin{aligned} (p_2 - p_b)^2 - m_e^2 c^2 &= (p_2 - p_b)^2 \\ &= \langle p_2, p_2 \rangle + \langle p_b, p_b \rangle - 2 \langle p_2, p_b \rangle \\ &= -2||p||^2(1 - \cos \theta) \end{aligned}$$

Thus, in this situation, the amplitude for our interaction is given by:

$$\begin{aligned} \mathcal{M} &= \frac{4\pi\alpha}{(p_1 - p_b)^2 - m_e^2 c^2} + \frac{4\pi\alpha}{(p_2 - p_b)^2 - m_e^2 c^2} \\ &= -\frac{2\pi\alpha}{||p||^2(1 + \cos \theta)} - \frac{2\pi\alpha}{||p||^2(1 - \cos \theta)} \\ &= -\frac{2\pi\alpha}{||p||^2} \left( \frac{1}{1 + \cos \theta} + \frac{1}{1 - \cos \theta} \right) \\ &= -\frac{2\pi\alpha}{||p||^2} \cdot \frac{2}{1 - \cos^2 \theta} \\ &= -\frac{4\pi\alpha}{||p||^2 \sin^2 \theta} \end{aligned}$$

On the other hand, the general Golden Rule formula, in the center of mass frame, gives in our situation the following differential cross section formula:

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \frac{Sh^2 c^2 |\mathcal{M}|^2}{64\pi^2 (E_a + E_b)^2} \cdot \frac{||p_1||}{||p_a||} \\ &= \frac{(1/2)h^2 c^2 |\mathcal{M}|^2}{64\pi^2 (2E)^2} \\ &= \frac{h^2 c^2 |\mathcal{M}|^2}{512\pi^2 E^2} \end{aligned}$$

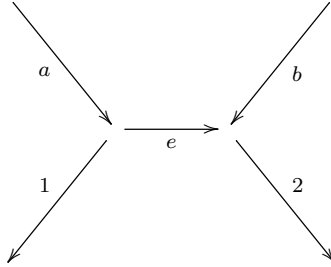
Now by plugging in the above value for  $\mathcal{M}$ , we obtain the following formula:

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= \frac{h^2 c^2}{512\pi^2 E^2} \cdot \frac{16\pi^2 \alpha^2}{||p||^4 \sin^4 \theta} \\ &= \frac{h^2 c^2 \alpha^2}{32E^2 ||p||^4 \sin^4 \theta} \\ &= \frac{1}{2} \left( \frac{hc\alpha}{4E ||p||^2 \sin^2 \theta} \right)^2\end{aligned}$$

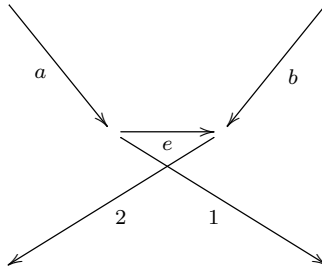
Thus, we are led to the differential cross section formula in the statement.  $\square$

At higher order now, things get considerably more complicated, and we will briefly explore this now. To start with, we have many diagrams at order 1, as follows:

**FACT 15.3.** *For events of type  $*_a + *_b \rightarrow *_1 + *_2$  we have 8 order 1 diagrams, appearing by suitably modifying the basic order 0 diagram, namely*

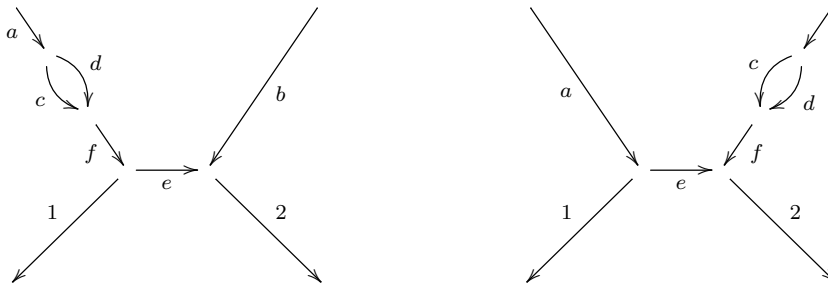


along with 8 more diagrams, appearing by modifying the second order 0 diagram,

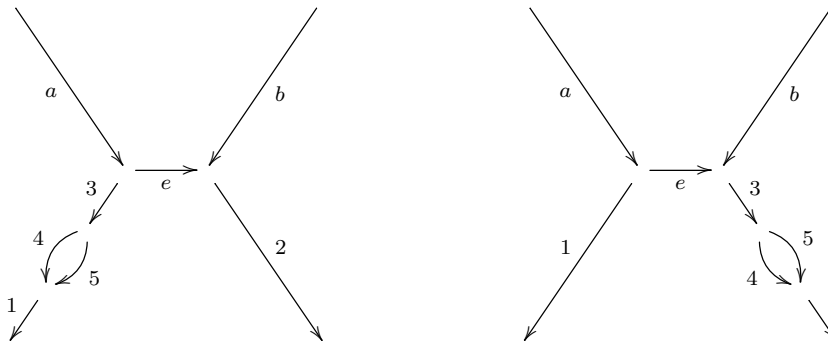


with the modifications appearing by allowing loops, producing 2 more vertices.

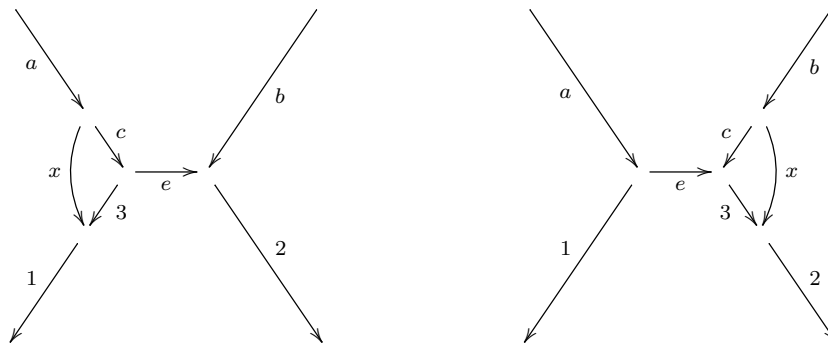
To be more precise here, we first have the following two diagrams, obtained by allowing loops on the incoming lines of the first basic order 0 diagram:



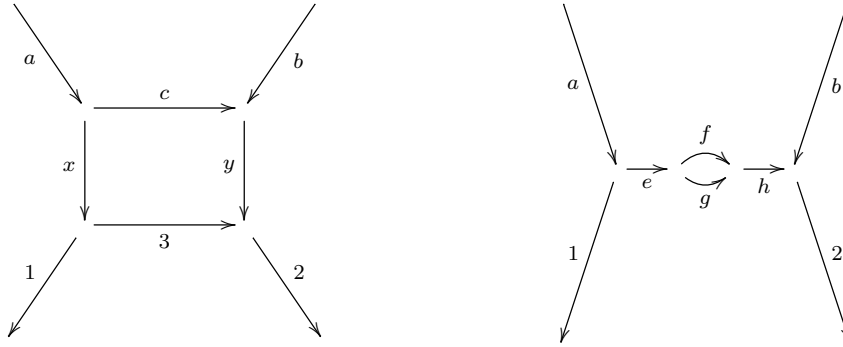
Next, and similarly, we have the following two diagrams, obtained by allowing loops on the outgoing lines of the first basic order 0 diagram:



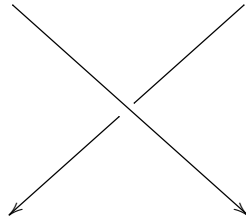
But then, we have as well the following two diagrams, again obtained from the basic order 0 diagram, this time with the left and right vertices becoming triangles:



And finally, again obtained from the basic 0 diagram, we have the following two diagrams, with a square, and then a loop, appearing in the middle:

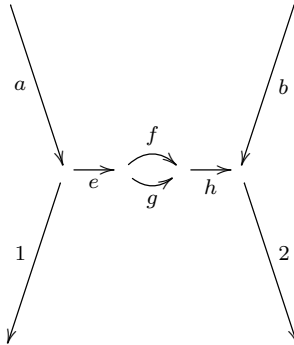


So, these are the 8 order 1 diagrams obtained by modifying the basic order 0 diagram, and then we have 8 more diagrams, obtained by similarly modifying the second order 0 diagram, which amounts in adding the following crossing to the above 8 diagrams:



Obviously, many computations are waiting to be done here. However, as a bad surprise, here is a particular one, where we run into some trouble:

**THEOREM 15.4.** *For the order 1 diagram with a loop in the middle,*



*the amplitude computation diverges. But, there is a fix to this.*

PROOF. This follows from some computations which are quite similar to those in the proof of Theorem 15.2. Let us apply indeed the general Feynman diagram recipe:

- We have four vertices, with each being assigned a  $-ig$  factor.
- Then we have four internal lines, with propagators as follows:

$$P_e = \frac{i}{p_e^2 - m_e^2 c^2} \quad , \quad P_f = \frac{i}{p_f^2 - m_f^2 c^2}$$

$$P_g = \frac{i}{p_g^2 - m_g^2 c^2} \quad , \quad P_h = \frac{i}{p_h^2 - m_h^2 c^2}$$

- We have then rescaled Dirac masses at the vertices, as follows:

$$(2\pi)^4 \delta(p_a - p_1 - p_e) \quad , \quad (2\pi)^4 \delta(p_e + p_f - p_g)$$

$$(2\pi)^4 \delta(p_f - p_g - p_h) \quad , \quad (2\pi)^4 \delta(p_b + p_h - p_2)$$

- And finally, we have integration factors as follows, on the internal lines:

$$I_e = \frac{dp_e}{(2\pi)^4} \quad , \quad I_f = \frac{dp_f}{(2\pi)^4} \quad , \quad I_g = \frac{dp_g}{(2\pi)^4} \quad , \quad I_h = \frac{dp_h}{(2\pi)^4}$$

Now by integrating, we obtain the following formula, for the pre-amplitude:

$$\begin{aligned} \mathcal{M}' &= \int (-ig)^4 \frac{i}{p_e^2 - m_e^2 c^2} \cdot \frac{i}{p_f^2 - m_f^2 c^2} \cdot \frac{i}{p_g^2 - m_g^2 c^2} \cdot \frac{i}{p_h^2 - m_h^2 c^2} \\ &\quad (2\pi)^{16} \delta(p_a - p_1 - p_e) \delta(p_e + p_f - p_g) \delta(p_f - p_g - p_h) \delta(p_b + p_h - p_2) \\ &\quad \frac{dp_e}{(2\pi)^4} \cdot \frac{dp_f}{(2\pi)^4} \cdot \frac{dp_g}{(2\pi)^4} \cdot \frac{dp_h}{(2\pi)^4} \end{aligned}$$

Thus, we have the following formula, for the pre-amplitude:

$$\mathcal{M}' = g^4 \int \frac{\delta(p_a - p_1 - p_e) \delta(p_e + p_f - p_g) \delta(p_f - p_g - p_h) \delta(p_b + p_h - p_2)}{(p_e^2 - m_e^2 c^2)(p_f^2 - m_f^2 c^2)(p_g^2 - m_g^2 c^2)(p_h^2 - m_h^2 c^2)} dp_e dp_f dp_g dp_h$$

Now let us do the integration. To start with, when integrating over  $p_e$ , the first Dirac mass replaces  $p_e \rightarrow p_a - p_1$ , so we are led to a integral as follows:

$$\mathcal{M}' = g^4 \int \frac{\delta(p_a - p_1 + p_f - p_g) \delta(p_f - p_g - p_h) \delta(p_b + p_h - p_2)}{((p_a - p_1)^2 - m_e^2 c^2)(p_f^2 - m_f^2 c^2)(p_g^2 - m_g^2 c^2)(p_h^2 - m_h^2 c^2)} dp_f dp_g dp_h$$



Next, and similarly, when integrating over the last variable  $p_h$ , the last Dirac mass replaces  $p_h \rightarrow p_2 - p_b$ , so we are led to a integral as follows:

$$\mathcal{M}' = g^4 \int \frac{\delta(p_a - p_1 + p_f - p_g) \delta(p_f - p_g - p_2 + p_b)}{((p_a - p_1)^2 - m_e^2 c^2)(p_f^2 - m_f^2 c^2)(p_g^2 - m_g^2 c^2)((p_2 - p_b)^2 - m_h^2 c^2)} dp_f dp_g$$

Summarizing, the pre-amplitude is given by the following formula:

$$\mathcal{M}' = \frac{g^4}{((p_a - p_1)^2 - m_e^2 c^2)((p_2 - p_b)^2 - m_h^2 c^2)} \int \frac{\delta(p_a - p_1 + p_f - p_g) \delta(p_f - p_g - p_2 + p_b)}{(p_f^2 - m_f^2 c^2)(p_g^2 - m_g^2 c^2)} dp_f dp_g$$

Now by integrating over  $p_f$ , the first Dirac mass replaces  $p_f \rightarrow p_1 + p_g - p_a$ , so we are left in the end with the following formula, for the pre-amplitude:

$$\mathcal{M}' = \frac{g^4}{((p_a - p_1)^2 - m_e^2 c^2)((p_2 - p_b)^2 - m_h^2 c^2)} \int \frac{\delta(p_1 - p_a - p_2 + p_b)}{((p_1 + p_g - p_a)^2 - m_f^2 c^2)(p_g^2 - m_g^2 c^2)} dp_g$$

In order to obtain the first amplitude itself, we must erase the global  $(2\pi)^4 \delta(\sum_i p_i)$  factor appearing after integrating, and multiply the answer by  $i$ . We obtain:

$$\mathcal{M} = \left(\frac{g}{2\pi}\right)^4 \frac{i}{((p_a - p_1)^2 - m_e^2 c^2)((p_2 - p_b)^2 - m_h^2 c^2)} \int \frac{1}{((p_1 + p_g - p_a)^2 - m_f^2 c^2)(p_g^2 - m_g^2 c^2)} dp_g$$

Now let us look at the integral which is to be computed. With simplified notations, which are self-explanatory, this integral is something of the following type:

$$I = \int \frac{1}{((p+x)^2 - y)(p^2 - z)} dp$$

And the point is that this integral diverges with  $p \rightarrow \infty$ . Indeed, in spherical coordinates we have  $dp = r^3 dr d\Omega$ , with  $d\Omega$  being the angular part, and with  $p \rightarrow \infty$  the function to be integrated is approximately  $1/r^4$ . Thus, ignoring the angular part, we have:

$$I \approx \int \frac{r^3 dr}{r^4} = \int \frac{dr}{r} = \infty$$

As a conclusion to this, when applying the Feynman rules as stated, to the particular diagram in the statement, we are led to a catastrophe, namely:

$$\mathcal{M} = \infty$$

But hey, there is a fix to this, which was found by physicists after nearly two decades of work. The idea is that of introducing an extra factor in the integral, as follows:

$$F = -\frac{M^2 c^2}{p_g^2 - M^2 c^2}$$

Here  $M$  is an abstract cutoff mass, assumed to be big,  $M \gg 0$ . And the point is that, with this done, the integral can be computed, and separated into two parts, one which converges, and the other one which blows up with  $M \rightarrow \infty$ . And then, a suitable interpretation of the components, known as renormalization, allows us to eventually get rid of the cutoff mass  $M$ , and have a finite figure for the amplitude  $\mathcal{M}$  to be computed. Which is the correct one, in agreement with the results from experimental physics.  $\square$

So long for the brief story of scattering at order 1, and related renormalization issues. We will be back to this later, with more details, directly in the QED context.

### 15b. Quantum electrodynamics

The theory developed above was quite abstract, involving generic particles, without further properties. At a more concrete level now, our main task will be that of merging the material from chapter 13, dealing with explicit particles, with everything that we have been doing since 14, by developing quantum electrodynamics (QED), following Dirac, Pauli, Kramers, Weisskopf, Bethe, Tomonaga, Schwinger, Feynman and others.

Let us first recall that the theory developed in chapter 13 was dealing with the three main particles, or at least with the three main particles from the perspective of very general theoretical physics, which are the electrons, photons and positrons. So, we first need to fine-tune the general rules for the Feynman diagrams, explained at the end of the previous chapter, and heavily used since, in the case of these three types of particles.

In what regards electrons and positrons, we know from chapter 13 that these are related by some sort of time reversal procedure, so we will draw the incoming electrons as usual arrows, and the incoming positrons as reversed arrows:

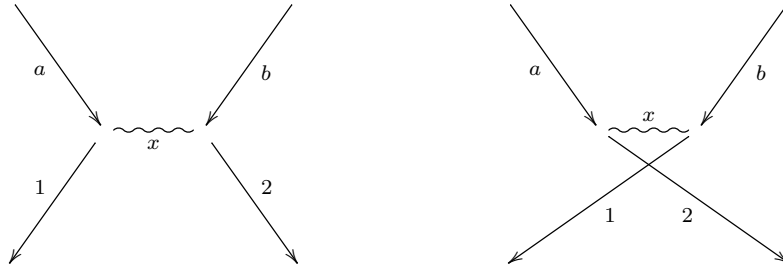
$$\begin{array}{ccc} \longrightarrow & & \longleftarrow \\ \textit{electron} & & \textit{positron} \end{array}$$

As for our third type of particles in our theory, the photons, it is traditional to use for the incoming photons the following special type of arrows:

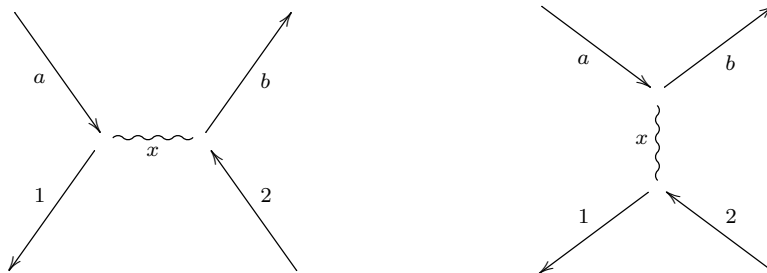
$$\begin{array}{c} \text{~~~~~} \longrightarrow \\ \textit{photon} \end{array}$$

Before getting to the Feynman rules, let us specify as well the main interactions, that we will be interested in. First we have the basic elastic interactions, as follows:

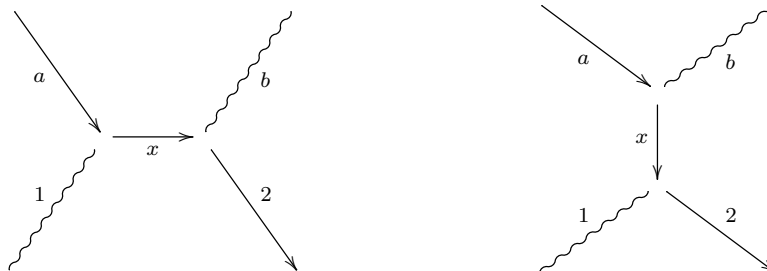
FACT 15.5. *The basic elastic interactions in QED are*



*corresponding to electron-electron, or Møller scattering, then*



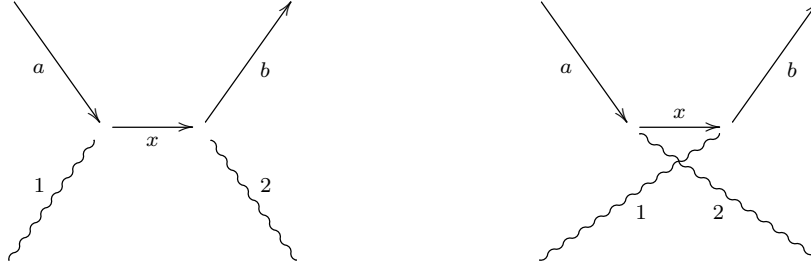
*corresponding to electron-positron, or Bhabha scattering, and then*



*corresponding to electron-photon, or Compton scattering.*

We have as well the basic inelastic interactions, as follows:

FACT 15.6. *The basic inelastic interactions in QED are*



*called electron-positron annihilation, and*



*called electron-positron creation.*

This was for the diagrams of the basic interactions. At higher order there are many interesting diagrams too, with some of these being responsible for the higher order corrections to the hydrogen atom, that we did in chapter 11. But more on these later.

Getting now to the Feynman rules, as formulated in general in chapter 14, these must be updated in the QED context, according to our findings from chapter 13. So, let us begin with a brief reminder of the mathematics of the free electrons, positrons and photons, that we found in chapter 13. In what regards the electrons, we have:

FACT 15.7 (Electrons). *The wave functions for free electrons are as follows,*

$$\psi(x) = ae^{-i\langle k, x \rangle} u^s(p)$$

*with  $k = p/\hbar$ , and  $s = 1, 2$  standing for the two spin states. The functions  $u^s$  satisfy*

$$\sum_i (\gamma_i p_i - mc) u = 0$$

*and their adjoints  $\bar{u}^s = (u^s)^* \gamma_0$  satisfy  $\sum_i \bar{u}(\gamma_i p_i - mc) = 0$ .*

We refer to the material in chapter 13 for more on all this, as well as for the explicit formulae of the functions  $u^s$ , which for our purposes here, can be taken as follows:

$$u^1 = \frac{1}{\sqrt{(E + mc^2)c}} \begin{pmatrix} E + mc^2 \\ 0 \\ cp_z \\ cp_x + icp_y \end{pmatrix}, \quad u^2 = \frac{1}{\sqrt{(E + mc^2)c}} \begin{pmatrix} 0 \\ E + mc^2 \\ cp_x - icp_y \\ -cp_z \end{pmatrix}$$

Regarding now the positrons, the situation for them is quite similar, modulo changing some signs, with the main finding here, also from chapter 13, being as follows:

FACT 15.8 (Positrons). *The wave functions for free positrons are as follows,*

$$\psi(x) = ae^{i\langle k, x \rangle} v^s(p)$$

with  $k = p/h$ , and  $s = 1, 2$  standing for the two spin states. The functions  $v^s$  satisfy

$$\sum_i (\gamma_i p_i + mc) v = 0$$

and their adjoints  $\bar{v}^s = (v^s)^* \gamma_0$  satisfy  $\sum_i \bar{v} (\gamma_i p_i + mc) = 0$ .

As before with electrons, we refer to chapter 13 for more on this, including for the explicit formulae of the functions  $v^s$ , which can be taken as follows:

$$v^1 = \frac{1}{\sqrt{(E + mc^2)c}} \begin{pmatrix} cp_x - icp_y \\ -cp_z \\ 0 \\ E + mc^2 \end{pmatrix}, \quad v^2 = -\frac{1}{\sqrt{(E + mc^2)c}} \begin{pmatrix} cp_z \\ cp_x + icp_y \\ E + mc^2 \\ 0 \end{pmatrix}$$

Finally, in what regards our third type of basic particles in our theory, which are the photons, again following chapter 13, we have here a similar result, as follows:

FACT 15.9 (Photons). *The wave functions for free photons are as follows,*

$$\psi(x) = ae^{-i\langle k, x \rangle} e_i^s$$

with  $k = p/h$ , and  $s = 1, 2$  standing for the two spin states. The functions  $e^s$  satisfy

$$\sum_i p_i e_i = 0$$

for any choice of the spin state, or polarization.

To be more precise, all this follows from the discussion from the beginning of chapter 13, with the photons satisfying the Klein-Gordon equation for a massless particle, namely  $\square\psi = 0$ , and with this equation leading to the above plane wave solutions.

As before with the electrons and positrons, we can be more explicit here, with the following concrete, straightforward formulae for the functions  $e^s$  appearing above:

$$e^1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad e^2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

Good news, with these preliminaries discussed, we can now get back to the Feynman diagrams, and formulate some precise rules for them in QED, as follows:

**PRINCIPLE 15.10.** *The amplitude  $\mathcal{M}$  coming from a given Feynman diagram  $F$  can be computed as follows:*

- (1) *Label each vertex with the corresponding four-momentum vector.*
- (2) *Put factors  $ig\gamma_j$  at each vertex,  $g = \sqrt{4\pi\alpha}$  being the coupling constant.*
- (3) *Install Feynman propagators  $\frac{i(\gamma_j p_j + mc)}{p^2 - m^2 c^2}$  on each charged internal line.*
- (4) *Install Feynman propagators  $-\frac{ig_{ij}}{p^2}$  on each photon internal line.*
- (5) *Install rescaled Dirac masses  $(2\pi)^4 \delta(\sum_i p_i)$  at each vertex.*
- (6) *Put integration factors  $\frac{dp_j}{(2\pi)^4}$  on each internal line, and integrate.*
- (7) *Erase the global  $(2\pi)^4 \delta(\sum_i p_i)$  factor appearing after integrating.*
- (8) *Multiply the answer by  $i$ . That is your amplitude  $\mathcal{M}$ .*

In addition to this, we have an antisymmetrization rule, consisting in including in the final amplitude sum, over the various Feynman diagrams of the same order, a  $-$  sign between diagrams that differ only in the interchange of two incoming electrons, of outgoing electrons, or incoming positrons, or outgoing positrons, or of an incoming electron with an outgoing positron, or of an incoming positron with an outgoing electron.

### 15c. Basic amplitudes

With the above general theory discussed, and getting now to explicit amplitude computations, there are many of them to be done, at the very basic level, according to the lists in Fact 15.5 and Fact 15.6. We will discuss this slowly, with all the details.

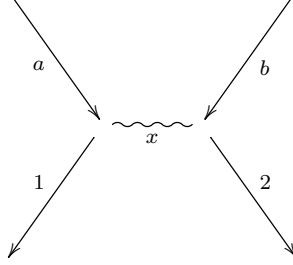
Let us first study the electron-electron scattering. We have here the following result:

**THEOREM 15.11.** *The amplitude for electron-electron scattering is*

$$\begin{aligned} \mathcal{M} = & -\frac{g^2}{(p_a - p_1)^2} \sum_j [\bar{u}(1)\gamma_j u(a)][\bar{u}(2)\gamma_j u(b)] \\ & + \frac{g^2}{(p_a - p_2)^2} \sum_j [\bar{u}(2)\gamma_j u(a)][\bar{u}(1)\gamma_j u(b)] \end{aligned}$$

*with  $a, b$  being the incoming electrons, and  $1, 2$  being the outgoing electrons.*

PROOF. Consider indeed the first diagram for electron-electron scattering:



Let us apply now the Feynman rules for QED, as formulated in Principle 15.10:

– We have two vertices, with the factors assigned to them being as follows:

$$ig\gamma_i \quad , \quad ig\gamma_j$$

– Then we have an internal line, with propagator as follows:

$$P_x = -\frac{ig_{ij}}{p_x^2}$$

– We have then rescaled Dirac masses at the vertices, as follows:

$$(2\pi)^4\delta(p_a - p_1 - p_x) \quad , \quad (2\pi)^4\delta(p_b + p_x - p_2)$$

– And finally, we have an integration factor as follows, on the internal line:

$$I_x = \frac{dp_x}{(2\pi)^4}$$

By integrating, we obtain the following formula, for the first pre-amplitude:

$$\begin{aligned} \mathcal{M}'_1 &= (2\pi)^4 \int \sum_{ij} [\bar{u}(1)(ig\gamma_i)u(a)] \left( -\frac{ig_{ij}}{p_x^2} \right) [\bar{u}(2)(ig\gamma_j)u(b)] \\ &\quad \delta(p_a - p_1 - p_x) \delta(p_b + p_x - p_2) dp_x \end{aligned}$$

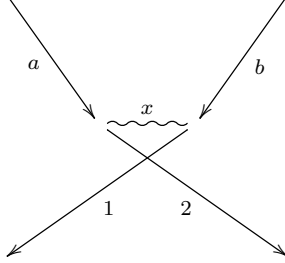
Now by integrating over  $p_x$ , the first Dirac mass makes the following replacement:

$$p_x \rightarrow p_a - p_1$$

Thus, we are left in the end with the following formula, for the first amplitude itself:

$$\mathcal{M}_1 = -\frac{g^2}{(p_a - p_1)^2} \sum_j [\bar{u}(1)\gamma_j u(a)] [\bar{u}(2)\gamma_j u(b)]$$

Regarding now the second possible diagram for the electron-electron scattering, that we must study too, for our computation to be complete, this is as follows:



Let us apply now the Feynman rules for QED, as formulated in Principle 15.10:

– We have two vertices, with the factors assigned to them being as follows:

$$ig\gamma_i \quad , \quad ig\gamma_j$$

– Then we have an internal line, with propagator as follows:

$$P_x = -\frac{ig_{ij}}{p_x^2}$$

– We have then rescaled Dirac masses at the vertices, as follows:

$$(2\pi)^4\delta(p_a - p_2 - p_x) \quad , \quad (2\pi)^4\delta(p_b + p_x - p_1)$$

– And finally, we have an integration factor as follows, on the internal line:

$$I_x = \frac{dp_x}{(2\pi)^4}$$

Now by integrating, we obtain the following formula, for the second pre-amplitude:

$$\begin{aligned} \mathcal{M}'_2 = & (2\pi)^4 \int \sum_{ij} [\bar{u}(1)(ig\gamma_i)u(a)] \left(-\frac{ig_{ij}}{p_x^2}\right) [\bar{u}(2)(ig\gamma_j)u(b)] \\ & \delta(p_a - p_2 - p_x)\delta(p_b + p_x - p_1)dp_x \end{aligned}$$

Now by integrating over  $p_x$ , the first Dirac mass replaces:

$$p_x \rightarrow p_a - p_2$$

Thus, we are left with the following formula, for the second amplitude itself:

$$\mathcal{M}_2 = -\frac{g^2}{(p_a - p_2)^2} \sum_j [\bar{u}(2)\gamma_j u(a)][\bar{u}(1)\gamma_j u(b)]$$



In order to finish now, we must add, or rather subtract, according to the rule discussed after Principle 15.10, the amplitudes that we found. We obtain:

$$\begin{aligned}\mathcal{M} = & -\frac{g^2}{(p_a - p_1)^2} \sum_j [\bar{u}(1)\gamma_j u(a)][\bar{u}(2)\gamma_j u(b)] \\ & + \frac{g^2}{(p_a - p_2)^2} \sum_j [\bar{u}(2)\gamma_j u(a)][\bar{u}(1)\gamma_j u(b)]\end{aligned}$$

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

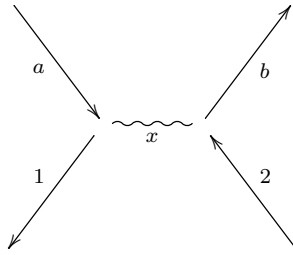
Next, we have the following result, which is quite similar:

**THEOREM 15.12.** *The amplitude for the electron-positron scattering is*

$$\begin{aligned}\mathcal{M} = & -\frac{g^2}{(p_a - p_1)^2} \sum_j [\bar{u}(1)\gamma_j u(a)][\bar{v}(b)\gamma_j v(2)] \\ & + \frac{g^2}{(p_a + p_b)^2} \sum_j [\bar{u}(1)\gamma_j v(2)][\bar{v}(b)\gamma_j u(a)]\end{aligned}$$

with  $a, b$  being the incoming particles, and  $1, 2$  being the outgoing particles.

**PROOF.** The computation here is very similar to the one that we just did. Consider indeed the first diagram for electron-positron scattering:



Let us apply now the Feynman rules for QED, as formulated in Principle 15.10:

– We have two vertices, with the factors assigned to them being as follows:

$$ig\gamma_i \quad , \quad ig\gamma_j$$

– Then we have an internal line, with propagator as follows:

$$P_x = -\frac{ig_{ij}}{p_x^2}$$

– We have then rescaled Dirac masses at the vertices, as follows:

$$(2\pi)^4 \delta(p_a - p_1 - p_x) \quad , \quad (2\pi)^4 \delta(p_x + p_2 - p_b)$$

– And finally, we have an integration factor as follows, on the internal line:

$$I_x = \frac{dp_x}{(2\pi)^4}$$

By integrating, we obtain the following formula, for the first pre-amplitude:

$$\begin{aligned} \mathcal{M}'_1 = (2\pi)^4 \int \sum_{ij} [\bar{u}(1)(ig\gamma_i)u(a)] \left( -\frac{ig_{ij}}{p_x^2} \right) [\bar{v}(b)(ig\gamma_j)v(2)] \\ \delta(p_a - p_1 - p_x) \delta(p_x + p_2 - p_b) dp_x \end{aligned}$$

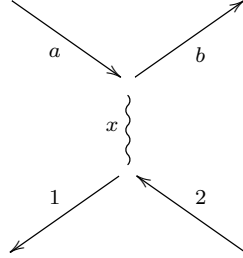
Now by integrating over  $p_x$ , the first Dirac mass makes the following replacement:

$$p_x \rightarrow p_a - p_1$$

Thus, we are left in the end with the following formula, for the first amplitude:

$$\mathcal{M}_1 = -\frac{g^2}{(p_a - p_1)^2} \sum_j [\bar{u}(1)\gamma_j u(a)] [\bar{v}(b)\gamma_j v(2)]$$

Regarding now the second possible diagram for the electron-positron scattering, that we must study too, for our computation to be complete, this is as follows:



Let us apply now the Feynman rules for QED, as formulated in Principle 15.10:

– We have two vertices, with the factors assigned to them being as follows:

$$ig\gamma_i \quad , \quad ig\gamma_j$$

– Then we have an internal line, with propagator as follows:

$$P_x = -\frac{ig_{ij}}{p_x^2}$$

– We have then rescaled Dirac masses at the vertices, as follows:

$$(2\pi)^4 \delta(p_a - p_b - p_x) \quad , \quad (2\pi)^4 \delta(p_x + p_2 - p_1)$$

– And finally, we have an integration factor as follows, on the internal line:

$$I_x = \frac{dp_x}{(2\pi)^4}$$

By integrating, we obtain the following formula, for the second pre-amplitude:

$$\mathcal{M}'_2 = (2\pi)^4 \int \sum_{ij} [\bar{u}(1)(ig\gamma_i)v(2)] \left( -\frac{ig_{ij}}{p_x^2} \right) [\bar{v}(b)(ig\gamma_j)u(a)] \\ \delta(p_a - p_b - p_x) \delta(p_x + p_2 - p_1) dp_x$$

Now by integrating over  $p_x$ , the first Dirac mass makes the following replacement:

$$p_x \rightarrow p_a - p_b$$

Thus, we are left in the end with the following formula, for the second amplitude:

$$\mathcal{M}_2 = -\frac{g^2}{(p_a + p_b)^2} [\bar{u}(1)\gamma_j v(2)] [\bar{v}(b)\gamma_j u(a)]$$

Now by summing, we obtain the following formula:

$$\mathcal{M} = -\frac{g^2}{(p_a - p_1)^2} \sum_j [\bar{u}(1)\gamma_j u(a)] [\bar{v}(b)\gamma_j v(2)] \\ + \frac{g^2}{(p_a + p_b)^2} \sum_j [\bar{u}(1)\gamma_j v(2)] [\bar{v}(b)\gamma_j u(a)]$$

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

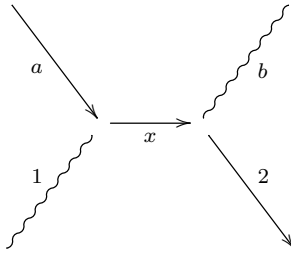
Along the same lines, we have as well the following result:

**THEOREM 15.13.** *The amplitude for the Compton scattering is*

$$\mathcal{M} = \frac{g^2}{(p_a - p_1)^2 - m^2 c^2} [\bar{u}(2)e'(b)(p'_a - p'_1 + mc)e'(1)^* u(a)] \\ + \frac{g^2}{(p_a + p_b)^2 - m^2 c^2} [\bar{u}(2)e'(1)(p'_a + p'_b + mc)e'(b)^* u(a)]$$

with  $r' = \sum_j r_j \gamma_j$ , with  $a, b$  and  $1, 2$  being the incoming and outgoing particles.

**PROOF.** Consider indeed the first diagram for the Compton scattering:



Let us apply now the Feynman rules for QED, as formulated in Principle 15.10:

- We have two vertices, with the factors assigned to them being as follows:

$$ig\gamma_i \quad , \quad ig\gamma_j$$

- Then we have an internal line, with propagator as follows:

$$P_x = \frac{i(p'_x + mc)}{p_x^2 - m^2c^2}$$

- We have then rescaled Dirac masses at the vertices, as follows:

$$(2\pi)^4\delta(p_a - p_1 - p_x) \quad , \quad (2\pi)^4\delta(p_x - p_2 - p_b)$$

- And finally, we have an integration factor as follows, on the internal line:

$$I_x = \frac{dp_x}{(2\pi)^4}$$

By integrating, we obtain the following formula, for the first pre-amplitude:

$$\begin{aligned} \mathcal{M}'_1 = & (2\pi)^4 \int \sum_{ij} e_i(b) [\bar{u}(2)(ig\gamma_i) \frac{i(p'_x + mc)}{p_x^2 - m^2c^2} (ig\gamma_j) u(a)] e_j(1) \\ & \delta(p_a - p_1 - p_x) \delta(p_x - p_2 - p_b) dp_x \end{aligned}$$

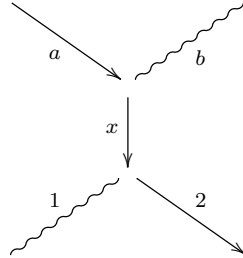
Now by integrating over  $p_x$ , the first Dirac mass makes the following replacement:

$$p_x \rightarrow p_a - p_1$$

Thus, we are left in the end with the following formula, for the first amplitude:

$$\mathcal{M}_1 = \frac{g^2}{(p_a - p_1)^2 - m^2c^2} [\bar{u}(2)e'(b)(p'_a - p'_1 + mc)e'(1)^*u(a)]$$

Regarding now the second possible diagram for the Compton scattering, that we must study too, for our computation to be complete, this is as follows:



Let us apply now the Feynman rules for QED, as formulated in Principle 15.10:

- We have two vertices, with the factors assigned to them being as follows:

$$ig\gamma_i \quad , \quad ig\gamma_j$$

– Then we have an internal line, with propagator as follows:

$$P_x = \frac{i(p'_x + mc)}{p_x^2 - m^2c^2}$$

– We have then rescaled Dirac masses at the vertices, as follows:

$$(2\pi)^4\delta(p_a - p_x - p_b) \quad , \quad (2\pi)^4\delta(p_x - p_1 - p_2)$$

– And finally, we have an integration factor as follows, on the internal line:

$$I_x = \frac{dp_x}{(2\pi)^4}$$

By integrating, we obtain the following formula, for the second pre-amplitude:

$$\begin{aligned} \mathcal{M}'_2 &= (2\pi)^4 \int \sum_{ij} e_i(1) [\bar{u}(2)(ig\gamma_i) \frac{i(p'_x + mc)}{p_x^2 - m^2c^2} (ig\gamma_j) u(a)] e_j(b) \\ &\quad \delta(p_a - p_x - p_b) \delta(p_x - p_1 - p_2) dp_x \end{aligned}$$

Now by integrating over  $p_x$ , the first Dirac mass makes the following replacement:

$$p_x \rightarrow p_a - p_b$$

Thus, we are left in the end with the following formula, for the second amplitude:

$$\mathcal{M}_2 = \frac{g^2}{(p_a + p_b)^2 - m^2c^2} [\bar{u}(2)e'(1)(p'_a + p'_b + mc)e'(b)^*u(a)]$$

Now by summing, we obtain the following formula:

$$\begin{aligned} \mathcal{M} &= \frac{g^2}{(p_a - p_1)^2 - m^2c^2} [\bar{u}(2)e'(b)(p'_a - p'_1 + mc)e'(1)^*u(a)] \\ &\quad + \frac{g^2}{(p_a + p_b)^2 - m^2c^2} [\bar{u}(2)e'(1)(p'_a + p'_b + mc)e'(b)^*u(a)] \end{aligned}$$

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

The remaining basic amplitudes in QED, for electron-positron creation and annihilation from Fact 15.6, can be computed too, by using similar methods. For more on this, and for the story of the higher order diagrams too, including renormalization, and applications to hydrogen, we refer to any quantum field theory book, such as [71].

Importantly, in relation with general QED, the following question is still open:

QUESTION 15.14. *What is the formula of the fine structure constant  $\alpha$ ?*

To be more precise, QED is certainly a very complete, accurate and successful theory, solving all the problems within its range. However, at the theoretical level, QED still involves the fine structure constant  $\alpha$ , which remains something quite mysterious.

### 15d. Further particles

All the above was something very nice, explaining the basic mechanisms of QED, which itself clarifies many things about the hydrogen atom, which were left open after our discussion from Part III. However, QED is not everything, and we have:

QUESTION 15.15. *What about protons, and neutrons?*

Indeed, remember that life as we know it is basically made of atoms, which means protons, electrons and neutrons, and light, which means photons. So, with electrons and photons relatively well understood, in the QED framework, the question is now, how to further improve what we have, as to include the protons and neutrons.

And good question this is. The point indeed is that, despite this being something very simple and natural, and we can even say, by ignoring the neutrons, dealing again with our old friend the hydrogen atom, there is no simple answer to it. That is, there is no simple minimal theory comprising both the electrons and the protons, and with all this being related to the various considerations for chapter 13, and the “catastrophe” explained there, coming from the fact that the positrons are not the same thing as protons.

In short, in order to answer our question, here we are back to the basics, trying to add new particles to what know, by whatever means. And with a bit of luck, we will need less than a few dozen of them, in order to properly talk about protons and neutrons.

Getting started now, in order to have more particles, the traditional way is by looking at radioactivity. The story here is long, twisted, and particularly fascinating:

(1) The fact that uranium  ${}_{92}\text{U}$ , which is not that uncommon in the earth, at certain places, is naturally radioactive has been known since ages, with various items such as pottery being decorated with uranium based paint, as to glow in the dark.

(2) Official science started to investigate this phenomenon quite late, at the end of the 19th century, with the work of Henri Becquerel and Marie Curie on uranium salts. A bit later, many others joined, and there was particular excitement in regards with polonium  ${}_{84}\text{Po}$  and radium  ${}_{88}\text{Ra}$ . In fact, looking a bit retrospectively, there are 8 culprits of this type, relatively light chemical elements having no stable isotopes, namely technetium, promethium, bismuth, polonium, astatine, radon, francium and radium:



(3) As for uranium itself, this is part of a series of 15 heavy elements, called actinides, coming right after radium in the periodic table, which are actinium, thorium, protactinium, uranium, neptunium, plutonium, americium, curium, berkelium, californium,

einsteinium, fermium, mendelevium, nobelium and lawrencium:

$_{89}\text{Ac}$	$_{90}\text{Th}$	$_{91}\text{Pa}$	$_{92}\text{U}$	$_{93}\text{Np}$	$_{94}\text{Pu}$	$_{95}\text{Am}$	$_{96}\text{Cm}$
	$_{97}\text{Bk}$	$_{98}\text{Cf}$	$_{99}\text{Es}$	$_{100}\text{Fm}$	$_{101}\text{Md}$	$_{102}\text{No}$	$_{103}\text{Lr}$

(4) All this, notably with polonium, radium and uranium, was happening at the beginning of the 20th century, roughly at the same time when Rydberg, Planck, Einstein, later joined by Bohr, Thomson, Rutherford and many others were trying to make some sense of quantum mechanics, and develop a reasonable atomic theory. And this soon became job done, with Heisenberg and then Schrödinger, later joined by De Broglie, Pauli, Dirac and others, developing a mathematical theory of quantum mechanics, and proving the Bohr model for the hydrogen atom, and in fact for all the other atoms too, true.

(5) However, the mechanism of radioactivity proved to be much harder to understand than the basic atomic functioning itself, with the reason for this coming from the fact that, in contrast to the latter which deals with a modified version of electromagnetism, negative electrons spinning around a positive nucleus, the former involves the nucleus only, and some subtle forces keeping it together, namely the weak and strong force. Understanding these two new forces, and putting them in the context of quantum mechanics, required a lot of new physics, coming from numerous civilian and military experiments, around WW2 and afterwards, and a lot of theoretical efforts too, with the whole story being over, if ever, in the 1970s, with the Standard Model for particle physics.

In short, quite complicated all this, and getting back now to Question 15.15, here is how the answer to it can be found, starting from what we know, and radioactivity:

RECIPE 15.16. *In order to properly talk about protons, electrons and neutrons:*

- (1) *Start with QED, and include some other spin 1/2 particles.*
- (2) *Include weak interactions, which are responsible for radioactivity.*
- (3) *Include as well the strong force, which is responsible for nuclear fusion.*
- (4) *And with this, your theory will be complete, including protons and neutrons.*

So, this is how advanced particle physics works, and with the complete theory at the end being called the Standard Model of particle physics. In practice, explaining all this is the business of graduate school, and we will not get into this, in the present book.

Let us record, however, as a main finding here, the list of the main particles in the Standard Model. Here they are, with their names, accompanied by their spin and charges,

indicated on top, and masses indicated on the bottom, expressed in  $\text{eV}/c^2$ :

$1/2, 2/3$ up quark $\approx 2.16\text{M}$	$1/2, 2/3$ charm quark $\approx 1.27\text{G}$	$1/2, 2/3$ top quark $\approx 172.57\text{G}$	$1, 0$ gluon 0	$0, 0$ Higgs boson $\approx 125.2\text{G}$
$1/2, -1/3$ down quark $\approx 4.7\text{M}$	$1/2, -1/3$ strange quark $\approx 93.5\text{M}$	$1/2, -1/3$ bottom quark $\approx 4.18\text{G}$	$1, 0$ photon 0	
$1/2, -1$ electron $\approx 0.51\text{M}$	$1/2, -1$ muon $\approx 105.66\text{M}$	$1/2, -1$ tau $\approx 1.78\text{G}$	$1, 0$ Z boson $\approx 91.19\text{G}$	
$1/2, 0$ electron neutrino $< 0.8$	$1/2, 0$ muon neutrino $< 0.17\text{M}$	$1/2, 0$ tau neutrino $< 18.2\text{M}$	$1, \pm 1$ W boson $\approx 80.37\text{G}$	

And please don't ask me what all this stands for. As already mentioned, there is a lot of further physics to be learned, in order to understand what all this is about, and in the hope of course that, with what that you learned from here, you are ready for that.

And we will stop here, with our particle physics discussion. But we will be somehow back to it, in the next chapter, with some cosmology considerations.

### 15e. Exercises

This was a particularly tough chapter, that no one in this world properly understands, with this being something notorious, and as unique exercise on this, we have:

**EXERCISE 15.17.** *Read more particle physics, and preferably from the experimental physicists, that is what you mostly need to know, for a better understanding.*

As bonus exercise, have a look as well at what various mathematicians and theoretical physicists have said, about all this. The truth is, probably, somewhere over there.



## CHAPTER 16

### Beyond physics

#### 16a. Into chemistry

Time to end this book. But how, we have learned so many interesting things, and there are so many possible continuations, and choices for a final chapter. For instance, as mentioned at the end of the previous chapter, it is certainly possible to go ahead with a lot of further basic learning on that Standard Model topics, and with all this being both very modern, and very interesting. But, can we really substantially advance on that in a further 20 pages, probably not. So nice try, and we will have to find something else.

Getting back to the basics, what we learned so far in this book, basic physics accompanied by basic mathematics, is certainly meant to be used, in the real life. That is, basic physics and mathematics are, after all, just a prelude to engineering, so it should be about engineering that we should talk about now, with an introduction to the subject.

This being said, I don't know about you, but personally I'm more of a philosopher, with my engineering needs in life basically reducing to a knife, that I use for cooking and other things, and that I would certainly have troubles in reproducing, starting from iron ore and coal. So, shall we talk about metallurgy, which is certainly a fascinating topic, and an excellent introduction to engineering, as a crowning of what we learned?

Not quite sure about this, but since our engineering expert is here, he's often in the local creek, which passes through my garden, let's ask him about engineering:

BEAVER 16.1. *To be honest, there is little to no mathematics and theoretical physics in what I do. Engineering is a matter of having things done.*

Thanks beaver, and think you're right, engineering remains indeed a bit away from what we've been doing in this book, which was overly theoretical and philosophical, and better finish with something else, that would be more appropriate, and honest.

Fortunately, our chemistry expert, the crocodile, is present too, doing his usual activities also there in the creek, so let's ask him. And crocodile, with a big smile, answers:

CROCODILE 16.2. *You should go with chemistry, then biology, these are quite philosophical as sciences, as you like them. And not far from engineering, either.*

Thanks crocodile, this sounds like a good idea indeed. So leaving you to your daily activities, and by the way please stay as usual at safe distance from both me and cat, theoretical math and physics deserve a minimum of friendship and respect, right, let us make a plan for the present final chapter, with chemistry ideas in mind:

(1) We will first talk about, you guess it right, basic chemistry, as a continuation of the basic quantum mechanics that we learned in Part III. We already know what the atoms are, and passing to some basic molecules will be certainly a pleasure.

(2) Then we will briefly get into organic chemistry, biology and life. This will be quite away from what we know, but eventually there will be some math to be done here, for populations regarded statistically, in relation with the thermodynamics from Part II.

(3) With some biology learned, we will turn to brain, and other types of computers. And here, good news, there are many possible types of computers, with some, called quantum, potentially using the quantum mechanics material from Part III.

(4) Finally, how far the human or computer brain can go, and so on, these are all beautiful questions. You would probably say here “the Standard Model”, and we will comment precisely on this, Standard Model bugs coming from stars and cosmology.

Getting started now, chemistry, many things to be learned. We only have a few pages for this, so don’t expect more than a quick introduction to the subject. But before anything, we should reset our brains, and methods of learning and work, due to:

**WARNING 16.3.** *Chemistry is not the same type of science as math and physics. The methods used are quite different, the situation being as follows:*

- (1) *Math is rigorous, unless of course you do mistakes in your computations, and don’t doublecheck 10 times your final theorem, before publishing.*
- (2) *Physics is less rigorous, but unless doing some weird stuff, say of advanced quantum type, you will always have experiments to confirm your findings.*
- (3) *Chemistry is mostly based on experiments and common sense. Which in practice makes it, contrary to math and physics, 100% correct, or almost.*

Which sounds quite fun, even a bit psychedelic, but please believe me, this is how things are. Also, I certify that the present chapter was written using tap water only.

Getting to work now, the key in understanding chemistry, and the alpha of omega of everything, is the periodic table that we learned at the end of Part III. So that periodic

table will be our starting point, and here that magnificent table is, again:

	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	$\frac{\text{Cs}}{55}$	$\frac{\text{Ba}}{56}$	$l$	$\frac{\text{Lu}}{71}$	$\frac{\text{Hf}}{72}$	$\frac{\text{Ta}}{73}$	$\frac{\text{W}}{74}$	$\frac{\text{Re}}{75}$	$\frac{\text{Os}}{76}$	$\frac{\text{Ir}}{77}$	$\frac{\text{Pt}}{78}$	$\frac{\text{Au}}{79}$	$\frac{\text{Hg}}{80}$	$\frac{\text{Tl}}{81}$	$\frac{\text{Pb}}{82}$	$\frac{\text{Bi}}{83}$	$\frac{\text{Po}}{84}$	$\frac{\text{At}}{85}$	$\frac{\text{Rn}}{86}$
7	$\frac{\text{Fr}}{87}$	$\frac{\text{Ra}}{88}$	$a$	$\frac{\text{Lr}}{103}$	$\frac{\text{Rf}}{104}$	$\frac{\text{Db}}{105}$	$\frac{\text{Sg}}{106}$	$\frac{\text{Bh}}{107}$	$\frac{\text{Hs}}{108}$	$\frac{\text{Mt}}{109}$	$\frac{\text{Ds}}{110}$	$\frac{\text{Rg}}{111}$	$\frac{\text{Cn}}{112}$	$\frac{\text{Nh}}{113}$	$\frac{\text{Fl}}{114}$	$\frac{\text{Mc}}{115}$	$\frac{\text{Lv}}{116}$	$\frac{\text{Ts}}{117}$	$\frac{\text{Og}}{118}$
			$l$ :	$\frac{\text{La}}{57}$	$\frac{\text{Ce}}{58}$	$\frac{\text{Pr}}{59}$	$\frac{\text{Nd}}{60}$	$\frac{\text{Pm}}{61}$	$\frac{\text{Sm}}{62}$	$\frac{\text{Eu}}{63}$	$\frac{\text{Gd}}{64}$	$\frac{\text{Tb}}{65}$	$\frac{\text{Dy}}{66}$	$\frac{\text{Ho}}{67}$	$\frac{\text{Er}}{68}$	$\frac{\text{Tm}}{69}$	$\frac{\text{Yb}}{70}$		
			$a$ :	$\frac{\text{Ac}}{89}$	$\frac{\text{Th}}{90}$	$\frac{\text{Pa}}{91}$	$\frac{\text{U}}{92}$	$\frac{\text{Np}}{93}$	$\frac{\text{Pu}}{94}$	$\frac{\text{Am}}{95}$	$\frac{\text{Cm}}{96}$	$\frac{\text{Bk}}{97}$	$\frac{\text{Cf}}{98}$	$\frac{\text{Es}}{99}$	$\frac{\text{Fm}}{100}$	$\frac{\text{Md}}{101}$	$\frac{\text{No}}{102}$		

Here the horizontal parameter  $1, \dots, 18$  is called the group, and the vertical parameter  $1, \dots, 7$  is called the period. The two rows on the bottom consist of lanthanum  $_{57}\text{La}$  and its followers, called lanthanides, and of actinium  $_{89}\text{Ac}$  and its followers, called actinides. These are to be inserted in the main table, where indicated, lanthanides between barium  $_{56}\text{Ba}$  and lutetium  $_{71}\text{Lu}$ , and actinides between radium  $_{88}\text{Ra}$  and lawrencium  $_{103}\text{Lr}$ .

We already talked a bit about this table in chapter 12, notably with the suggestion of learning the names of all the above elements, and some of their properties too. Now that we are chemists, this is no longer a suggestion, but rather something mandatory:

ADVICE 16.4. *Learn their names.*

Getting now to properties and discussion, from a basic chemistry perspective, the first 8 elements in the periodic table are those which matter the most.

Here is a table with that first 8 elements, containing some basic data about each, whose knowledge is mandatory too:

Element	H	He	Li	Be	B	C	N	O
Atomic number	1	2	3	4	5	6	7	8
Electrons	$1s^1$	$1s^2$	$2s^1$	$2s^2$	$2s^2 2p^1$	$2s^2 2p^2$	$2s^2 2p^3$	$2s^2 2p^4$
Name	Hydrogen	Helium	Lithium	Beryllium	Boron	Carbon	Nitrogen	Oxygen

As a first objective, let us first try to better understand these atoms. In addition, in view of our chemistry objectives, we should learn about ions and isotopes too.

So, getting started for real now, we will need some general theory for the many-particle systems in quantum mechanics. Let us start with a basic fact, as follows:

DEFINITION 16.5. *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  $i\hbar\dot{\psi} = \hat{H}\psi$ , with Hamiltonian as follows,*

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

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

As before with the one-particle Schrödinger equation, there is a long story with all this, and for cutting short with the discussion here, this is what experiments lead to.

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 16.6. *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*

$$i\hbar\dot{\psi} = \hat{H}\psi$$

*with Hamiltonian as follows,*

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

*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 16.7. *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 16.6, 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:

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

In general now, we will be interested in what happens to a system of  $Z$  electrons  $e_1, \dots, e_Z$ , surrounding a central positive charge  $Z'e$ . For a usual atom, which is globally electrically neutral, we have  $Z = Z'$ , but for isotopes and ions we can have  $Z < Z'$  or  $Z > Z'$ . Thus, we will assume that the numbers  $Z, Z'$  are unrelated.

In practice, this corresponds to the following version of Problem 16.6:

PROBLEM 16.8. *Consider a system of atomic number  $Z'$ , meaning a fixed  $Z'e$  charge, surrounded by electrons  $e_1, \dots, e_Z$ . The problem is to solve the Schrödinger equation*

$$i\hbar\dot{\psi} = \hat{H}\psi$$

*with Hamiltonian as follows,*

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

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

As explained in the discussion following Problem 16.6, a first idea is to simply ignore the Coulomb repulsion term on the right. Indeed, this simplifies a lot the mathematics, and by separation of variables we are led to a product of wave functions, with the numerics being worked out, in the simplest case of the helium atom, in Fact 16.7.

So, let us see how this works in general, in the framework of Problem 16.8. As before with helium, in view of the fact that the interactions between the electrons are ignored, this amounts in decomposing the Hamiltonian into  $Z$  components, as follows:

$$\hat{H} = \hat{H}_1 + \dots + \hat{H}_Z$$

By separation of variables, we are led to products of wave functions as follows, called Hartree products, with the prime signs standing for the modification of the central charge,  $e \rightarrow Z'e$ , from the case of hydrogen, to the case of the system under investigation:

$$\phi(x_1, \dots, x_Z) = \phi'(x_1) \dots \phi'(x_Z)$$

Here we have opted, for simplifying notations, to not include the quantum numbers, as in Fact 16.7, at least in the present, preliminary stage of our study.

With this done, we are quite far from something reliable, because as explained in Fact 16.7, such an approximation gives quite average results, with respect to the observed values, even in the simplest case of helium. So, the following question appears:

**QUESTION 16.9.** *How to further improve the Hartree products, without however getting into Problem 16.8 as stated, which is something of extreme difficulty?*

In order to solve this question, let us get back to helium,  $Z = Z' = 2$ . If we denote for simplifying by 1, 2 the first two lowest energy orbits, we have two possible Hartree functions for the simplest excited state of our helium atom, namely:

$$\phi_{12}(x_1, x_2) = \phi'_1(x_1)\phi'_2(x_2) \quad , \quad \phi_{21}(x_1, x_2) = \phi'_2(x_1)\phi'_1(x_2)$$

A natural idea, in order to have some symmetry going on, for our solution, is that of considering a suitable linear combination of these solutions. But since the overall electron density function  $|\phi|^2$  must be invariant under electron exchange, we are led, up to a normalization of the wave function, to linear combinations as follows:

$$\phi = \pm\phi_{12} \pm \phi_{21}$$

Moreover, by taking now into account spin, the Pauli exclusion principle tells us that the correct symmetry property of  $\phi$  is actually antisymmetry. Thus, up to a global  $\pm$  sign, and again up to a normalization of the wave function, the solution must be:

$$\begin{aligned} \phi &= \phi_{12} - \phi_{21} \\ &= \phi'_1(x_1)\phi'_2(x_2) - \phi'_2(x_1)\phi'_1(x_2) \\ &= \begin{vmatrix} \phi'_1(x_1) & \phi'_2(x_1) \\ \phi'_1(x_2) & \phi'_2(x_2) \end{vmatrix} \end{aligned}$$

Getting now to the normalization factor, a simple computation shows that this factor is  $1/\sqrt{2}$ . Thus, as a conclusion, our symmetrization method leads to:

$$\phi = \frac{1}{\sqrt{2}} \begin{vmatrix} \phi'_1(x_1) & \phi'_2(x_1) \\ \phi'_1(x_2) & \phi'_2(x_2) \end{vmatrix}$$

More generally now, the above method applies in the same way to a system of  $Z$  electrons, and we are led to the following preliminary answer to Question 16.9:

ANSWER 16.10. *The correct linear combinations of Hartree products, having the correct antisymmetrization property for the electrons, are the quantities*

$$\phi = \frac{1}{\sqrt{Z!}} \begin{vmatrix} \phi'_1(x_1) & \dots & \phi'_Z(x_1) \\ \vdots & & \vdots \\ \phi'_1(x_Z) & \dots & \phi'_Z(x_Z) \end{vmatrix}$$

*with the subscripts standing for the hydrogen-like energy levels, and the primes standing for the central charge modification  $e \rightarrow Z'e$ , called Slater determinants.*

To be more precise here, the fact that we must indeed consider a determinant is standard, by reasoning as above, and with this actually corresponding to a well-known theorem in mathematics, stating that the determinant is the unique antisymmetric multilinear form  $\det : \mathbb{R}^N \rightarrow \mathbb{R}$ , normalized as to produce 1 for the standard basis of  $\mathbb{R}^N$ . As for the computation of the normalization factor, this is again standard, as above.

Moving ahead now, the electron spin was certainly taken into account when formulating the above answer, due to the Pauli exclusion principle which was used. However, when fully taking spin into account, we are led to the following refinement of the above formula, valid this time for a system of  $Z = 2N$  electrons, with the subscripts ignoring spin, and with the bars, and lack of bars, standing for spin up and down:

$$\phi = \frac{1}{\sqrt{Z!}} \begin{vmatrix} \phi'_1(x_1) & \bar{\phi}'_1(x_1) & \dots & \dots & \phi'_N(x_1) & \bar{\phi}'_N(x_1) \\ \phi'_1(x_2) & \bar{\phi}'_1(x_2) & \dots & \dots & \phi'_N(x_2) & \bar{\phi}'_N(x_2) \\ \vdots & \vdots & & & \vdots & \vdots \\ \vdots & \vdots & & & \vdots & \vdots \\ \phi'_1(x_{Z-1}) & \bar{\phi}'_1(x_{Z-1}) & \dots & \dots & \phi'_N(x_{Z-1}) & \bar{\phi}'_N(x_{Z-1}) \\ \phi'_1(x_Z) & \bar{\phi}'_1(x_Z) & \dots & \dots & \phi'_N(x_Z) & \bar{\phi}'_N(x_Z) \end{vmatrix}$$

However, we will not get into full details here, because an even better approximation method, called Hartree-Fock approximation, beating the above, is still to come.

As an example, however, for all this, let us discuss the case of the beryllium atom  ${}_4\text{Be}$ . Here the Slater determinant, taking into account spin, as above, is as follows:

$$\phi = \frac{1}{\sqrt{24}} \begin{vmatrix} \phi'_1(x_1) & \bar{\phi}'_1(x_1) & \phi'_2(x_1) & \bar{\phi}'_2(x_1) \\ \phi'_1(x_2) & \bar{\phi}'_1(x_2) & \phi'_2(x_2) & \bar{\phi}'_2(x_2) \\ \phi'_1(x_3) & \bar{\phi}'_1(x_3) & \phi'_2(x_3) & \bar{\phi}'_2(x_3) \\ \phi'_1(x_4) & \bar{\phi}'_1(x_4) & \phi'_2(x_4) & \bar{\phi}'_2(x_4) \end{vmatrix}$$

Getting now to the excited states of the same beryllium  ${}_4\text{Be}$ , we need to add here a third orbital, that we will label 3. And then, following a discussion about spin, which

must be subject to certain rules, we are led to the conclusion that the correct linear combination of Hartree products is a difference of two Slater determinants, as follows:

$$\begin{aligned} \phi &= \frac{1}{\sqrt{24}} \begin{vmatrix} \phi'_1(x_1) & \bar{\phi}'_1(x_1) & \phi'_2(x_1) & \bar{\phi}'_3(x_1) \\ \phi'_1(x_2) & \bar{\phi}'_1(x_2) & \phi'_2(x_2) & \bar{\phi}'_3(x_2) \\ \phi'_1(x_3) & \bar{\phi}'_1(x_3) & \phi'_2(x_3) & \bar{\phi}'_3(x_3) \\ \phi'_1(x_4) & \bar{\phi}'_1(x_4) & \phi'_2(x_4) & \bar{\phi}'_3(x_4) \end{vmatrix} \\ &- \frac{1}{\sqrt{24}} \begin{vmatrix} \phi'_1(x_1) & \bar{\phi}'_1(x_1) & \bar{\phi}'_2(x_1) & \phi'_3(x_1) \\ \phi'_1(x_2) & \bar{\phi}'_1(x_2) & \bar{\phi}'_2(x_2) & \phi'_3(x_2) \\ \phi'_1(x_3) & \bar{\phi}'_1(x_3) & \bar{\phi}'_2(x_3) & \phi'_3(x_3) \\ \phi'_1(x_4) & \bar{\phi}'_1(x_4) & \bar{\phi}'_2(x_4) & \phi'_3(x_4) \end{vmatrix} \end{aligned}$$

Along the same lines, but at a more advanced level, an even better approximation method, called Hartree-Fock approximation, is available. And good news, once this Hartree-Fock method is learned and mastered, you can talk about molecules.

Indeed, the idea here is that a molecule can be investigated a bit like a multi-electron atom, by replacing the central charge with a system of positive charges.

Many things can be said here, notably with a number of more advanced models for the simplest molecule of them all, which is the hydrogen molecule. Also, of particular interest is the water molecule  $\text{H}_2\text{O}$ , and its various remarkable properties.

So long for molecules, or rather for the basic story of the molecules, from the perspective of quantum physics. As for the continuation of the story, this is basic chemistry as you learned it from school, involving acids, bases, salts, and various chemical reactions, and with the remark that quantum physics provides explanations for all this.

At an even more advanced level, as a continuation of basic chemistry, we have organic molecules, and ultimately cells and life. This is something considerably more complicated to understand, than mathematics and physics, but as a somewhat nice surprise, for us mathematicians and physicists, the various living beings, be them something very complicated, tend to organize into groups, and compete for food and other, and with everything here reminding a bit thermodynamics, as we previously learned it in this book.

And so, all in all, by a strange twist of fate, all these complications coming from biology and life ultimately lead to some simple mathematics, which is similar to that of thermodynamics. For more on all this, we refer to any basic social science book.



### 16b. Some engineering

Now that we know about biology and living beings, an interesting question that we would like to discuss is computing and brain. Many things can be said here, and with a fundamental question, of engineering and computer science flavor, being as follows:

QUESTION 16.11. *How to compute time?*

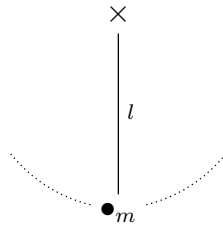
Easy question, you would say, and no need here to be an advanced living being, as us humans, in order to figure out the answer, just look at the Sun, and its position on the sky will give you the time. Which sounds very good, so let us record:

ANSWER 16.12. *The simplest computer is the Sun.*

This being said, and aiming now higher, for times when it rains, or at night, and so on, can we humans invent some sort of portable Sun, giving right away the time?

And good question this is. In order to answer it, the idea will still be to use gravity, as our main computing power, but implemented differently. Let us start our discussion with something basic, coming as a complement to the mechanics from Part I, namely:

DEFINITION 16.13. *A simple pendulum is a device of type*



*consisting of a bob of mass  $m$ , attached to a rigid rod of length  $l$ .*

In order to study the physics of the pendulum, which can easily lead to a lot of complicated computations, when approached with bare hands, the most convenient is to use the notion of energy. For a particle moving under the influence of a force  $F$ , the position  $x$ , speed  $v$  and acceleration  $a$  are related by the following formulae:

$$v = \dot{x} \quad , \quad a = \dot{v} = \ddot{x} \quad , \quad F = ma$$

The kinetic energy of our particle is then given by the following formula:

$$T = \frac{mv^2}{2}$$

By differentiating with respect to time  $t$ , we obtain the following formula:

$$\dot{T} = mv\dot{v} = mva = Fv$$

Now by integrating, also with respect to  $t$ , this gives the following formula:

$$T = \int F v dt = \int F \dot{x} dt = \int F dx$$

But this suggests to define the potential energy  $V$  by the following formula, up to a constant, with the derivative being with respect to the space variable  $x$ :

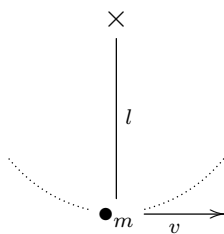
$$V' = -F$$

Indeed, we know from the above that we have  $T' = F$ , so if we define the total energy to be  $E = T + V$ , then this total energy is constant, as shown by:

$$E' = T' + V' = 0$$

Very nice all this, and by getting back now to the pendulum from Definition 16.13, we can have this understood with not many computations involved, as follows:

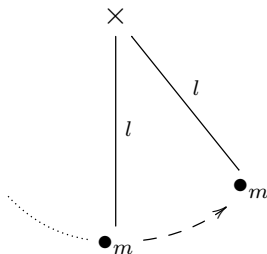
**THEOREM 16.14.** *For a pendulum starting with speed  $v$  from the equilibrium position,*



*the motion will be confined if  $v^2 < 4gl$ , and circular if  $v^2 > 4gl$ .*

**PROOF.** There are many ways of proving this result, along with working out several other useful related formulae, for which we will refer to the proof below, and with a quite elegant approach to this, using no computations or almost, being as follows:

(1) Let us first examine what happens when the bob has traveled an angular distance  $\theta > 0$ , with respect to the vertical. The picture here is as follows:



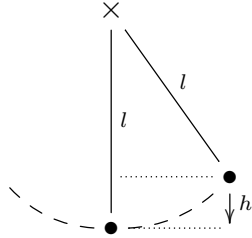
The distance traveled is then  $x = l\theta$ . As for the force acting, this is  $F_{total} = mg$  oriented downwards, with the component alongside  $x$  being given by:

$$\begin{aligned} F &= -||F_{total}|| \sin \theta \\ &= -mg \sin \theta \\ &= -mg \sin \left( \frac{x}{l} \right) \end{aligned}$$

(2) But with this, we can compute the potential energy. With the convention that this vanishes at the equilibrium position,  $V(0) = 0$ , we obtain the following formula:

$$\begin{aligned} V' = -F &\implies V' = mg \sin \left( \frac{x}{l} \right) \\ &\implies V = mgl \left( 1 - \cos \left( \frac{x}{l} \right) \right) \\ &\implies V = mgl(1 - \cos \theta) \end{aligned}$$

(3) Alternatively, in case this sounds too wizarding, we can compute the potential energy in the old fashion, by letting the bob fall, the picture being as follows:



The height of the fall is then  $h = l - l \cos \theta$ , and since for this fall the force is constant,  $\mathcal{F} = -mg$ , we obtain the following formula for the potential energy:

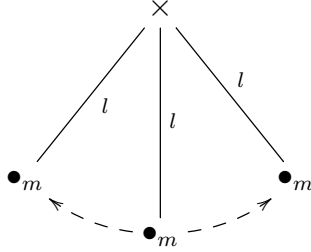
$$\begin{aligned} V' = -\mathcal{F} &\implies V' = mg \\ &\implies V = mgh \\ &\implies V = mgl(1 - \cos \theta) \end{aligned}$$

Summarizing, one way or another we have our formula for the potential energy  $V$ .

(4) Now comes the discussion. The motion will be confined when the initial kinetic energy, namely  $E = mv^2/2$ , satisfies the following condition:

$$\begin{aligned} E < \sup_{\theta} V = 2mgl &\iff \frac{mv^2}{2} < 2mgl \\ &\iff v^2 < 4gl \end{aligned}$$

In this case, the motion will be confined between two angles  $-\theta, \theta$ , as follows:



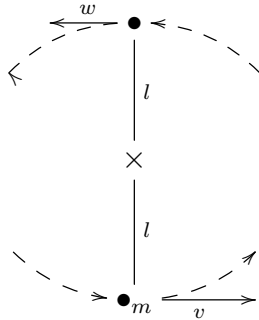
To be more precise here, the two extreme angles  $-\theta, \theta \in (-\pi, \pi)$  can be explicitly computed, as being solutions of the following equation:

$$\begin{aligned} V = E &\iff mgl(1 - \cos \theta) = \frac{mv^2}{2} \\ &\iff 1 - \cos \theta = \frac{v^2}{2gl} \end{aligned}$$

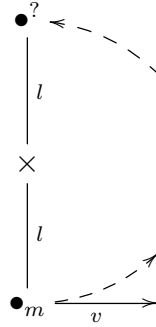
(5) Regarding now the case  $v^2 > 4gl$ , here the bob will certainly reach the upwards position, with the speed  $w > 0$  there being given by the following formula:

$$\begin{aligned} \frac{mw^2}{2} = E - 2mgl &\implies \frac{mw^2}{2} = \frac{mv^2}{2} - 2mgl \\ &\implies w^2 = v^2 - 4gl \\ &\implies w = \sqrt{v^2 - 4gl} \end{aligned}$$

Thus, with the convention in the statement for  $v$ , that is, going to the right, the motion of the pendulum will be counterclockwise circular, and perpetual:



(6) Finally, in the case  $v^2 = 4gl$ , the bob will also reach the upwards position, but with speed  $w = 0$  there, and then, at least theoretically, will remain there:



(7) Actually, it is quite interesting in this latter situation,  $v^2 = 4gl$ , to further speculate on what can happen, when making our problem more realistic. Exercise for you.  $\square$

In practice, in order to talk about clocks, we have to take into account friction. As a first observation, our generalities about motion and energy provide us with:

**THEOREM 16.15.** *For a particle moving near an equilibrium point  $x = 0$ , the following equivalent conditions must be satisfied, infinitesimally:*

- (1) *The potential energy is  $V = kx^2/2$ , when assuming  $V(0) = 0$ .*
- (2) *The force acting on our particle is  $F = -kx$ .*
- (3) *The equation of motion is  $m\ddot{x} + kx = 0$ , with  $m$  being the mass.*

**PROOF.** This is something very standard, the idea being as follows:

(1) Let us start with some generalities regarding the potential energy  $V$ . Around any given point, that we can choose by translation to be  $x = 0$ , we can write:

$$V(x) = V(0) + V'(0)x + \frac{V''(0)x^2}{2} + \frac{V'''(0)x^3}{6} + \dots$$

By definition of  $V$ , we can assume  $V(0) = 0$ . Regarding now the second term, this vanishes too, because our condition of equilibrium reads:

$$V'(0) = -F(0) = 0$$

Thus, with the above normalizations  $x = 0$  and  $V(0) = 0$  made, our general formula above for  $V$  takes at equilibrium the following form, with  $k = V''(0)$ :

$$V(x) = \frac{kx^2}{2} + \dots$$

Thus, we are led to the conclusion in the statement, provided that we are indeed in the non-degenerate case, where  $k \neq 0$ , which amounts in saying that  $F'(0) \neq 0$ .

(2) This follows indeed from (1), and from  $V' = -F$ .

(3) This follows indeed from (2), and from  $F = ma = m\ddot{x}$ .  $\square$

The above result suggests formulating the following definition:

DEFINITION 16.16. *A harmonic oscillator is a particle moving as above, following*

$$m\ddot{x} + kx = 0$$

*with  $k \neq 0$ . In the case  $k > 0$ , we say that we have a simple harmonic oscillator.*

There the last convention comes from the fact that our oscillator is unstable when  $k < 0$ , and stable  $k > 0$ , and it is in this latter case that we are mostly interested in. And with this, stability depending on the sign of  $k$ , coming either from some abstract reasoning along the lines of Theorem 16.15, or from the explicit formulae below.

Very nice, so let us solve now the equation of motion. We have here:

THEOREM 16.17. *The solutions of the equation of motion  $m\ddot{x} + kx = 0$  for the harmonic oscillators are as follows:*

- (1)  $x = ae^{pt} + be^{-pt}$  with  $p = \sqrt{-k/m}$ , when  $k < 0$ .
- (2)  $x = c \cos wt + d \sin wt$  with  $w = \sqrt{k/m}$ , when  $k > 0$ .

PROOF. This is standard mathematics, as follows:

(1) Assume first that we are in the case  $k < 0$ . Here, with  $p = \sqrt{-k/m}$  as in the statement, the equation of motion takes the following form:

$$\ddot{x} = p^2 x$$

But the functions  $e^{pt}$ ,  $e^{-pt}$  being solutions of this equation, by linearity we obtain that the solutions are exactly the linear combinations of these two functions, as claimed.

(2) Assume now that we are in the case  $k > 0$ . Here, with  $w = \sqrt{k/m}$  as in the statement, the equation of motion takes the following form:

$$\ddot{x} = -w^2 x$$

But the functions  $\cos wt$ ,  $\sin wt$  being solutions, by linearity we obtain that the solutions are exactly the linear combinations of these two functions, as claimed.  $\square$

Observe that, as already mentioned above, the formulae that we obtained make it clear that our oscillator is unstable when  $k < 0$ , and stable when  $k > 0$ . In fact, we have the following simple consequences of the general formulae obtained above:

PROPOSITION 16.18. *The short and long time behavior of a harmonic oscillator, moving according to  $m\ddot{x} + kx = 0$ , are as follows:*

- (1) *In the case  $k < 0$ , with  $x = ae^{pt} + be^{-pt}$  as above, we have  $x \simeq (a + b) + p(a - b)t$  for  $t > 0$  small, and  $x \simeq ae^{pt}$  for  $t \gg 0$ .*
- (2) *In the case  $k > 0$ , with  $x = c \cos wt + d \sin wt$  as above, we have  $x \simeq c + dwt$  for  $t > 0$  small, and there is no asymptotics for  $t \gg 0$ .*

PROOF. This is indeed standard mathematics based on Theorem 16.17, as follows:

(1) In the case  $k < 0$ , with  $x = ae^{pt} + be^{-pt}$  as in Theorem 16.17, in the  $t > 0$  small regime we have indeed the following estimate, coming from  $e^z \simeq 1 + z$ :

$$\begin{aligned} x &= ae^{pt} + be^{-pt} \\ &\simeq a(1 + pt) + b(1 - pt) \\ &= (a + b) + p(a - b)t \end{aligned}$$

As for the other estimate, namely  $x \simeq ae^{pt}$  for  $t \gg 0$ , this is clear.

(2) In the case  $k > 0$ , with  $x = c \cos wt + d \sin wt$  as in Theorem 16.17, in the  $t > 0$  small regime we have indeed the following estimate, coming from standard calculus:

$$\begin{aligned} x &= c \cos wt + d \sin wt \\ &\simeq c(1 + o(t)) + dwt \\ &\simeq c + dwt \end{aligned}$$

As for the last assertion, regarding the lack of asymptotics at  $k > 0$  in the  $t \gg 0$  regime, this is clear, because neither  $\cos$ , nor  $\sin$  have such asymptotics, and the same happens for any linear combination of them, with non-trivial coefficients. Of course, interesting exercise for you to figure out all this, abstractly, this being not hard.  $\square$

As a last piece of mathematics, using this time complex numbers, we have:

**THEOREM 16.19.** *The solutions of the equation  $m\ddot{x} + kx = 0$  are as follows, regardless of the sign of  $k$ , and with  $a, b, c, d \in \mathbb{C}$  chosen as to have  $x \in \mathbb{R}$ :*

- (1)  $x = ae^{pt} + be^{-pt}$ , with  $p = \sqrt{-k/m}$ .
- (2)  $x = c \cos wt + d \sin wt$ , with  $w = \sqrt{k/m}$ .

PROOF. This is standard complex number business, the idea being as follows:

(1) As before in the proof of Theorem 16.17 (1), but by using this time complex numbers, we are led to the conclusion in the statement. With two remarks, namely:

– In the case  $k < 0$  we have  $p \in \mathbb{R}$ , and so  $a, b \in \mathbb{R}$ , and we recover in this way Theorem 16.17 (1) itself.

– As for the case  $k > 0$ , here we can write  $p = iw$  with  $w = \sqrt{k/m} \in \mathbb{R}$ , and the formula that we get, according to the above, is as follows:

$$x = ae^{iwt} + be^{-iwt}$$

Now in order to have  $x \in \mathbb{R}$ , which is the same as saying that  $x = \bar{x}$ , we need:

$$a = \bar{b}$$

Thus we can write  $a = c - id$ ,  $b = c + id$  with  $c, d \in \mathbb{R}$ , and with these substitutions made, the solution found above takes the following form:

$$\begin{aligned} x &= ae^{iwt} + be^{-iwt} \\ &= (c - id)(\cos wt + i \sin wt) + (c + id)(\cos wt - i \sin wt) \\ &= 2(c \cos wt + d \sin wt) \end{aligned}$$

Thus at  $k > 0$ , up to a 2 factor, we obtain the formula from Theorem 16.17 (2).

(2) Things are similar here. Indeed, as before in the proof of Theorem 16.17 (2), we are led to the conclusion in the statement, and with two remarks to be made, namely:

– In the case  $k > 0$  we have  $w \in \mathbb{R}$ , and so  $c, d \in \mathbb{R}$ , and we recover in this way Theorem 16.17 (2) itself.

– As for the case  $k < 0$ , here we can write  $w = -ip$  with  $p = \sqrt{-k/m} \in \mathbb{R}$ , and the formula that we get, according to the above, is as follows:

$$\begin{aligned} x &= c \cos wt + d \sin wt \\ &= c \cos(-ipt) + d \sin(-ipt) \\ &= c \cos(ipt) - d \sin(ipt) \\ &= c \cdot \frac{e^{i(ipt)} + e^{-i(ipt)}}{2} - d \cdot \frac{e^{i(ipt)} - e^{-i(ipt)}}{2i} \\ &= c \cdot \frac{e^{-pt} + e^{pt}}{2} - d \cdot \frac{e^{-pt} - e^{pt}}{2i} \\ &= \frac{1}{2} \left( \left( c + \frac{d}{i} \right) e^{pt} + \left( c - \frac{d}{i} \right) e^{-pt} \right) \end{aligned}$$

Now observe that in order to have  $x \in \mathbb{R}$ , we must have  $c \pm d/i \in \mathbb{R}$ . Thus  $c \in \mathbb{R}$ , and  $d = if$  with  $f \in \mathbb{R}$ , and with this latter substitution made, and then afterwards with the notations  $a = (c + f)/2$  and  $b = (c - f)/2$ , we obtain:

$$\begin{aligned} x &= \frac{1}{2} ((c + f)e^{pt} + (c - f)e^{-pt}) \\ &= ae^{pt} + be^{-pt} \end{aligned}$$

Thus at  $k < 0$ , we obtain the formula from Theorem 16.17 (1). □

Let us study now the damped oscillators, obtained by adding to the picture friction, of some other extra force, which will bring us closer to clocks. We have here:

**THEOREM 16.20.** *For a damped oscillator, which is subject by definition to a force of type  $F = -kx - \lambda\dot{x}$ , the equation of motion is*

$$m\ddot{x} + \lambda\dot{x} + kx = 0$$

*with  $m$  being as before the mass.*



PROOF. This is clear indeed from  $F = ma = m\ddot{x}$ , which gives:

$$\begin{aligned} F = -kx - \lambda\dot{x} &\iff m\ddot{x} = -kx - \lambda\dot{x} \\ &\iff m\ddot{x} + \lambda\dot{x} + kx = 0 \end{aligned}$$

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

Now let us try to solve the equation of motion. When looking for solutions of type  $x = e^{pt}$ , with  $p \in \mathbb{C}$  constant, the equation of motion takes the following form:

$$mp^2 + \lambda p + k = 0$$

But this is a degree 2 equation, that we can solve right away, and we get:

$$p = \frac{-\lambda \pm \sqrt{\lambda^2 - 4mk}}{2m}$$

It is convenient to write these solutions that we found, and the overall final result about damping, in the following more convenient way:

**THEOREM 16.21.** *The generic solutions of  $m\ddot{x} + \lambda\dot{x} + kx = 0$  are the real linear combinations of the functions  $e^{pt}$ , with the parameter  $p \in \mathbb{C}$  being given by*

$$p = -\gamma \pm \sqrt{\gamma^2 - w^2} \quad , \quad \gamma = \frac{\lambda}{2m} \quad , \quad w = \sqrt{\frac{k}{m}}$$

with on the right  $w$  being the frequency of the usual, undamped oscillator.

PROOF. This follows indeed from the formula of  $p$  found above, by dividing everything by  $2m$ . Observe that  $w$  is indeed the frequency of the usual, undamped oscillator.  $\square$

Now assume that we are in the case  $\lambda > 0$ , which is the most usual one, in practice, meaning that our oscillator loses energy. We have then three cases, as follows:

**PROPOSITION 16.22.** *The oscillator damping with  $\lambda > 0$ , with this assumption meaning that our oscillator loses energy over the time, can be of three types:*

- (1) *Large damping, with  $\lambda > 0$  being such that  $\gamma > w$ . Here the roots found above  $p = -\gamma \pm \sqrt{\gamma^2 - w^2}$  are both real, negative, and distinct.*
- (2) *Small damping, with  $\lambda > 0$  being such that  $\gamma < w$ . In this case the roots that we found  $p = -\gamma \pm \sqrt{\gamma^2 - w^2}$  are complex and conjugate.*
- (3) *Critical damping, with  $\lambda > 0$  being such that  $\gamma = w$ . Here we have a double root, which is real and negative, namely  $p = -\gamma$ .*

PROOF. All this is clear indeed from the formula found in Theorem 16.21.  $\square$

Now let us study more in detail the above three types of damping. In what regards the large damping, things here are very simple and intuitive, as follows:

PROPOSITION 16.23. *For large oscillator damping, the trajectory is given by*

$$x = ae^{-\gamma_+ t} + be^{-\gamma_- t}$$

*with the parameters  $\gamma_+ > \gamma_- > 0$  being given by the formulae*

$$\gamma_{\pm} = \gamma \pm \sqrt{\gamma^2 - w^2}$$

*and with  $a, b \in \mathbb{R}$ . With  $t \gg 0$  we have  $x \simeq be^{-\gamma_- t} \rightarrow 0$ .*

PROOF. All this is indeed self-explanatory, and clear from the formula that we found in Theorem 16.21, under the large damping assumption from Proposition 16.22 (1).  $\square$

In what regards the small damping, things here are again simple and intuitive, involving this time complex numbers and trigonometric functions, as follows:

PROPOSITION 16.24. *For small oscillator damping, the trajectory is given by*

$$x = 2re^{-\gamma t} \cos(\rho t - \theta)$$

*with  $\gamma = \lambda/2m$  as before, with the parameter  $\rho > 0$  being given by the formula*

$$\rho = \sqrt{w^2 - \gamma^2}$$

*and with  $r > 0$  and  $\theta \in \mathbb{R}$ . With  $t \gg 0$  we have  $x \rightarrow 0$ , exponentially.*

PROOF. Assume indeed that we are in the small damping regime, where  $\lambda > 0$  is such that  $\gamma < w$ . The roots that we found are then complex conjugate, as follows:

$$p = -\gamma \pm i\rho \quad , \quad \rho = \sqrt{w^2 - \gamma^2}$$

As for the solution itself, this is given by the following formula, with  $c, d \in \mathbb{C}$ :

$$\begin{aligned} x &= ce^{p_+ t} + de^{p_- t} \\ &= ce^{-\gamma t + i\rho t} + de^{-\gamma t - i\rho t} \\ &= e^{-\gamma t} (ce^{i\rho t} + de^{-i\rho t}) \end{aligned}$$

Now in order to have  $x \in \mathbb{R}$ , which is the same as saying  $x = \bar{x}$ , we must have  $c = \bar{d}$ . Thus we can write  $c = re^{-i\theta}$  and  $d = re^{i\theta}$  with  $r > 0$  and  $\theta \in \mathbb{R}$ , and we obtain:

$$\begin{aligned} x &= e^{-\gamma t} (ce^{i\rho t} + \bar{c}e^{-i\rho t}) \\ &= 2e^{-\gamma t} \operatorname{Re}(ce^{i\rho t}) \\ &= 2re^{-\gamma t} \operatorname{Re}(e^{i(\rho t - \theta)}) \\ &= 2re^{-\gamma t} \cos(\rho t - \theta) \end{aligned}$$

Finally, the fact that we have indeed  $x \rightarrow 0$ , exponentially, is clear.  $\square$

As for the critical damping case, the result here is as follows:

THEOREM 16.25. *For critical oscillator damping, the trajectory is given by*

$$x = (a + bt)e^{-\gamma t}$$

*with the parameter  $\gamma > 0$  being given as usual by the formula*

$$\gamma = \frac{\lambda}{2m}$$

*and with  $a, b \in \mathbb{R}$ . With  $t \gg 0$  we have  $x \simeq bte^{-\gamma t} \rightarrow 0$ .*

PROOF. Assume indeed that we are in the critical damping regime, where  $\lambda > 0$  is such that  $\gamma = w$ . In this case the roots that we found in Theorem 16.21 are both given by  $p = -\gamma$ , and so that result provides us with solutions as follows, with  $a \in \mathbb{R}$ :

$$x = ae^{-\gamma t}$$

Thus, we must find in this case some further solutions of the equation  $m\ddot{x} + \lambda\dot{x} + kx = 0$ , and our claim is that the following functions are solutions too:

$$x = bte^{-\gamma t}$$

Indeed, let us verify this, under the above critical damping assumption. By linearity it is enough to do this for  $b = 1$ , and here the derivatives are computed as follows:

$$\begin{aligned} x &= te^{-\gamma t} \\ \Rightarrow \dot{x} &= e^{-\gamma t} - \gamma te^{-\gamma t} = (1 - \gamma t)e^{-\gamma t} \\ \Rightarrow \ddot{x} &= -\gamma e^{-\gamma t} - \gamma(1 - \gamma t)e^{-\gamma t} = -\gamma(2 - \gamma t)e^{-\gamma t} \end{aligned}$$

We can verify now that the equation is indeed satisfied, as follows:

$$\begin{aligned} m\ddot{x} + \lambda\dot{x} + kx &= -m\gamma(2 - \gamma t)e^{-\gamma t} + \lambda(1 - \gamma t)e^{-\gamma t} + kte^{-\gamma t} \\ &= (-2m\gamma + m\gamma^2 t + \lambda - \lambda\gamma t + kt)e^{-\gamma t} \\ &= (m\gamma^2 t - \lambda\gamma t + kt)e^{-\gamma t} \\ &= (m\gamma^2 - \lambda\gamma + k)te^{-\gamma t} \\ &= 0 \end{aligned}$$

Here we have used at the end the fact, that we know from Theorem 16.21 and its proof, that the solutions of the equation  $mp^2 + \lambda p + k = 0$  are given by  $p = -\gamma \pm \sqrt{\gamma^2 - w^2}$ . Indeed, in the present critical damping regime these solutions are both given by  $p = -\gamma$ , and so substituting this particular value in the equation gives zero, as needed:

$$m\gamma^2 - \lambda\gamma + k = 0$$

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

And with this, good news, we have all the needed math for starting building clocks, and other fancy pieces of machinery. Which is a question that I will leave to you:

EXERCISE 16.26. *Build a clock, then other machinery, and computers.*

At a more advanced level, appearing as a ramification of this, we can talk about abstract computer science. Again, many things that can be said here, but with the situation being a bit similar to that with life and biology, with computers basically competing with each other, and with the mathematics being similar to that of thermodynamics.

As an interesting open question here, we have the question of creating a monster “quantum computer”, based on our knowledge of particle spin from Part III. For more on all this, many quantum computing books, including [15], [67], are available.

### 16c. Further relativity

I don’t know about you, but personally I find what we have been talking about recently, namely chemistry, life and biology, and various engineering and computing matters, while certainly very interesting, a bit too terrestrial. So, let us go back to physics, and ask:

QUESTION 16.27. *What forms of smartness can we find in the outer space, or at really tiny scales, or back in the distant past, or forward in the distant future?*

And good question this is. In order to have some discussion started, the best is to go back to the beginning of the present book, and start browsing slowly, looking for scary things. And, in what regards such scary things, the answer is pretty much clear, these quite often come from Einstein’s theory of relativity, speeds of type  $v \simeq c$  are certainly no joke, and it is by further learning about this, that we should reach to scary things.

So, let us start our discussion with a continuation of what we learned in chapter 4, about special relativity. We first have the following result:

THEOREM 16.28. *In the relativistic case, the general frame change formula is*

$$x' = x + (\gamma - 1) \frac{\langle v, x \rangle v}{\|v\|^2} - \gamma tv$$

$$t' = \gamma \left( t - \frac{\langle v, x \rangle}{c^2} \right)$$

where  $\gamma = 1/\sqrt{1 - \|v\|^2/c^2}$ , and the reverse frame change is obtained via  $v \rightarrow -v$ .

PROOF. This is something quite tricky, with some vector calculus involved, and we will take our time, and try to understand how this works:

(1) As a first illustration, let us first see what happens at  $N = 1$ . Here both the position variable  $x$  and the speed  $v$  are usual real numbers, and our first formula becomes:

$$\begin{aligned} x' &= x + (\gamma - 1) \frac{vx \cdot v}{v^2} - \gamma tv \\ &= x + (\gamma - 1)x - \gamma tv \\ &= \gamma x - \gamma tv \\ &= \gamma(x - tv) \end{aligned}$$

Thus, our first formula is correct. As for the second formula, this is correct too:

$$t = \gamma \left( t - \frac{vx}{c^2} \right)$$

(2) As a second illustration, let us move to arbitrary  $N \in \mathbb{N}$  dimensions, including the case  $N = 3$  that we are mostly interested in, and test our formula in the case where the configuration is standard, that is, where the speed vector is of the following form:

$$v = \begin{pmatrix} \nu \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

In this case, we obtain the correct formula for the position vector, as follows:

$$\begin{aligned} x' &= x + (\gamma - 1) \frac{\nu x_1 \cdot v}{\nu^2} - \gamma tv \\ &= x + (\gamma - 1)x_1 \cdot \frac{v}{\nu} - \gamma tv \\ &= \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix} + (\gamma - 1)x_1 \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} - \gamma t \begin{pmatrix} \nu \\ 0 \\ \vdots \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} \gamma x_1 - \gamma t \nu \\ x_2 \\ \vdots \\ x_N \end{pmatrix} \end{aligned}$$

As for the resulting time, this is the correct one too, as follows:

$$t' = \gamma \left( t - \frac{\nu x_1}{c^2} \right)$$

(3) Summarizing, the formula in the statement generalizes well everything that we know. In order to prove now this formula, the general idea is that of decomposing the

position vectors  $x, x'$  as follows, with respect to  $v$  and its complement:

$$\begin{aligned} x &= \lambda v + y \quad , \quad y \perp v \\ x' &= \lambda' v + y' \quad , \quad y' \perp v \end{aligned}$$

Indeed, this can only give the result, by using the standard configuration formulae from chapter 4, and various abstract or concrete rotation arguments.

(4) In practice now, there are several ways of doing this. As a first observation, the above decomposition argument shows that our time formula is indeed the correct one:

$$t' = \gamma \left( t - \frac{\langle v, x \rangle}{c^2} \right)$$

But with this in hand, it is possible to trick with an abstract argument, saying on one hand that  $x'$  must be linear in  $x, t$ , and on the other hand that we must have:

$$\|x'\|^2 - ct'^2 = \|x\|^2 - ct^2$$

(5) Going instead on a more pedestrian way, we certainly know that the formula of  $t'$  is correct, and it remains to justify the formula of  $x'$ . But here, the best is to do first the computation in  $N = 2$  dimensions, along the lines suggested in (3). This gives:

$$x' = x + (\gamma - 1) \frac{\langle v, x \rangle v}{\|v\|^2} - \gamma tv$$

Thus, we have the formula  $x'$  at  $N = 2$ , and the extension to  $N = 3$  and higher is straightforward, either by using a similar computation, or a rotation argument.  $\square$

As a second task now, let us recover the speed addition formula, first established in 1D in chapter 4, from the Lorentz transform. We can do this in general, as follows:

**THEOREM 16.29.** *The speed addition formula in  $N$ -dimensional relativity is*

$$u +_e v = \frac{1}{1 + \langle u, v \rangle} \left( u + v + \frac{\langle u, v \rangle u - \langle u, u \rangle v}{1 + \sqrt{1 - \|u\|^2}} \right)$$

in  $c = 1$  units.

**PROOF.** This is something very standard, the idea being as follows:

(1) As before, the idea will be that of differentiating  $x_1, \dots, x_N$  and  $t$  in the formulae for the inverse Lorentz transform. With the replacement  $v \rightarrow u$  for the moving speed, this inverse Lorentz transform is, according to Theorem 16.28, given by:

$$\begin{aligned} x_i &= x'_i + (\gamma - 1) \frac{\langle u, x' \rangle u_i}{\|u\|^2} + \gamma t' u_i \\ t &= \gamma \left( t' + \frac{\langle u, x' \rangle}{c^2} \right) \end{aligned}$$

(2) Now by differentiating, we obtain from this the following formulae:

$$dx_i = dx'_i + (\gamma - 1) \frac{\langle u, dx' \rangle u_i}{||u||^2} + \gamma u_i dt'$$

$$dt = \gamma \left( dt' + \frac{\langle u, dx' \rangle}{c^2} \right)$$

(3) By dividing now the first formula by the second one, we obtain:

$$\frac{dx_i}{dt} = \frac{1}{\gamma} \cdot \frac{dx'_i + (\gamma - 1) \langle u, dx' \rangle u_i / ||u||^2 + \gamma u_i dt'}{dt' + \langle u, dx' \rangle / c^2}$$

(4) Next, by dividing everything on the right by  $dt'$ , we get from this:

$$\frac{dx_i}{dt} = \frac{1}{\gamma} \cdot \frac{dx'_i/dt' + (\gamma - 1) \langle u, dx'/dt' \rangle u_i / ||u||^2 + \gamma u_i}{1 + \langle u, dx'/dt' \rangle / c^2}$$

(5) In terms of speeds now, this means that we have, with  $w = u +_e v$ :

$$w_i = \frac{1}{\gamma} \cdot \frac{v_i + (\gamma - 1) \langle u, v \rangle u_i / ||u||^2 + \gamma u_i}{1 + \langle u, v \rangle / c^2}$$

(6) Now in  $c = 1$  units, this formula is as follows, still with  $w = u +_e v$ :

$$w_i = \frac{1}{\gamma} \cdot \frac{v_i + (\gamma - 1) \langle u, v \rangle u_i / ||u||^2 + \gamma u_i}{1 + \langle u, v \rangle}$$

(7) In vector notation now, the above formula shows that we have:

$$\begin{aligned} u +_e v &= \frac{1}{1 + \langle u, v \rangle} \cdot \frac{1}{\gamma} \left( v + (\gamma - 1) \frac{\langle u, v \rangle u}{||u||^2} + \gamma u \right) \\ &= \frac{1}{1 + \langle u, v \rangle} \left( u + \frac{v}{\gamma} + \left( 1 - \frac{1}{\gamma} \right) \frac{\langle u, v \rangle u}{||u||^2} \right) \\ &= \frac{1}{1 + \langle u, v \rangle} \left( u + v + \left( 1 - \frac{1}{\gamma} \right) \left( \frac{\langle u, v \rangle u}{||u||^2} - v \right) \right) \\ &= \frac{1}{1 + \langle u, v \rangle} \left( u + v + \left( 1 - \frac{1}{\gamma} \right) \frac{\langle u, v \rangle u - \langle u, u \rangle v}{||u||^2} \right) \\ &= \frac{1}{1 + \langle u, v \rangle} \left( u + v + \frac{\langle u, v \rangle u - \langle u, u \rangle v}{1 + \sqrt{1 - ||u||^2}} \right) \end{aligned}$$

(8) Here we have used at the end the following formula, for the Lorentz factor:

$$\begin{aligned} 1 - \frac{1}{\gamma} &= 1 - \frac{1}{1/\sqrt{1 - ||u||^2}} \\ &= 1 - \sqrt{1 - ||u||^2} \\ &= \frac{||u||^2}{1 + \sqrt{1 - ||u||^2}} \end{aligned}$$

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

And with this, good news, we have now a correct theoretical understanding of the special relativity basics, going beyond what we previously knew from chapter 4.

### 16d. Stars, cosmology

With relativity theory properly understood, many interesting questions appear about space, time, and our universe itself. It is beyond our goals to get now into this, at the end of the present book, but here are a few questions, which are of particular interest:

(1) How does gravity exactly fit into relativity theory? What about the Standard Model? These are not easy questions, because gravity leads to a lot of beasts, such as black holes, and dark matter and energy, which have troubles in fitting in the Standard Model. In fact, even usual, basic gravity does not fit well into the Standard Model.

(2) What happened in the past, at the beginnings of our universe? Also, what will happen in the future? Again, these are not easy questions, with the best known theory for the past, called Big Bang, allowing for a strange procedure, called “cosmic inflation”, which does not fit very well with relativity. As for the future, no one knows.

And so, plenty of scary things, and open questions, happening at the universal scale, basically defying our human physics, as we know it. At a more modest level, however, somehow midway between our human physics, and the above-mentioned difficult cosmology questions, we have the stars. There are stars indeed everywhere, and their physics comes as a natural continuation of our terrestrial physics. Always aim for them.

### 16e. Exercises

Congratulations for having read this book, and no exercises for this chapter. Instead, you can have a look at the various books referenced below, and just pick one.



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