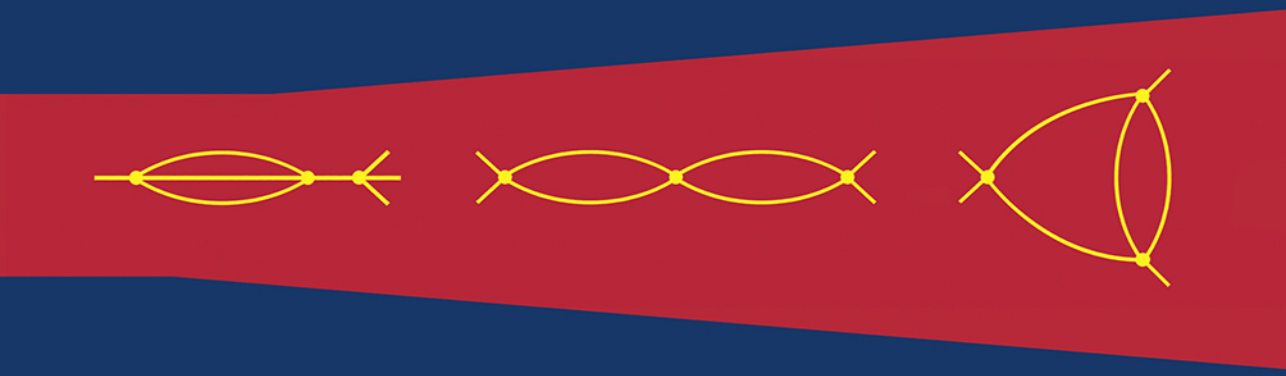
What Is a QUANTUM FIELD THEORY?



A FIRST INTRODUCTION *for* MATHEMATICIANS

Michel **TALAGRAND**

WHAT IS A QUANTUM FIELD THEORY?

Quantum field theory (QFT) is one of the great achievements of physics, of profound interest to mathematicians. Most pedagogical texts on QFT are geared toward budding professional physicists, however, whereas mathematical accounts are abstract and difficult to relate to the physics. This book bridges the gap. While the treatment is rigorous whenever possible, the accent is not on formality but on explaining what the physicists do and why, using precise mathematical language. In particular, it covers in detail the mysterious procedure of renormalization. Written for readers with a mathematical background but no previous knowledge of physics and largely self-contained, it presents both basic physical ideas from special relativity and quantum mechanics and advanced mathematical concepts in complete detail. It will be of interest to mathematicians wanting to learn about QFT and, with nearly 300 exercises, also to physics students seeking greater rigor than they typically find in their courses.

MICHEL TALAGRAND is the recipient of the Loève Prize (1995), the Fermat Prize (1997), and the Shaw Prize (2019). He was a plenary speaker at the International Congress of Mathematicians and is currently a member of the *Académie des sciences* (Paris). He has written several books in probability theory and well over 200 research papers.

"This book accomplishes the impossible task: It explains to a mathematician, in a language that a mathematician can understand, what is meant by a quantum field theory from a physicist's point of view. The author is completely and brutally honest in his goal to truly explain the physics rather than filtering out only the mathematics, but is at the same time as mathematically lucid as one can be with this topic. It is a great book by a great mathematician."

- Sourav Chatterjee, *Stanford University*

"Talagrand has done an admirable job of making the difficult subject of quantum field theory as concrete and understandable as possible. The book progresses slowly and carefully but still covers an enormous amount of material, culminating in a detailed treatment of renormalization. Although no one can make the subject truly easy, Talagrand has made every effort to assist the reader on a rewarding journey though the world of quantum fields."

- Brian Hall, *University of Notre Dame*

"A presentation of the fundamental ideas of quantum field theory in a manner that is both accessible and mathematically accurate seems like an impossible dream. Well, not anymore! This book goes from basic notions to advanced topics with patience and care. It is an absolute delight to anyone looking for a friendly introduction to the beauty of QFT and its mysteries."

- Shahar Mendelson, *Australian National University*

"I have been motivated to try and learn about quantum field theories for some time but struggled to find a presentation in a language that I as a mathematician could understand. This book was perfect for me: I was able to make progress without any initial preparation and felt very comfortable and reassured by the style of exposition."

- Ellen Powell, *Durham University*

"In addition to its success as a physical theory, quantum field theory has been a continuous source of inspiration for mathematics. However, mathematicians trying to understand quantum field theory must contend with the fact that some of the most important computations in the theory have no rigorous justification. This has been a considerable obstacle to communication between mathematicians and physicists. It is why, despite many fruitful interactions, only very few people would claim to be well versed in both disciplines at the highest level.

There have been many attempts to bridge this gap, each emphasizing different aspects of quantum field theory. Treatments aimed at a mathematical audience often deploy sophisticated mathematics. Michel Talagrand takes a decidedly elementary approach to answering the question in the title of his book, assuming little more than basic analysis. In addition to learning what quantum field theory is, the reader will encounter in this book beautiful mathematics that is hard to find anywhere else in such clear pedagogical form, notably the discussion of representations of the Poincaré group and the BPHZ Theorem. The book is especially timely given the recent resurgence of ideas from quantum field theory in probability and partial differential equations. It is sure to remain a reference for many decades."

- Philippe Sosoe, *Cornell University*

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If all mathematics were to disappear, physics would be set back exactly one week.

Richard Feynman

Physics should be made as simple as possible, but not simpler.

Albert Einstein

The career of a young theoretical physicist consists of treating the harmonic oscillator in ever-increasing levels of abstraction.

Sydney Coleman

Contents

Introduction

As a teenager in the sixties reading scientific magazines, countless articles alerted me to "the infinities plaguing the theory of Quantum Mechanics". Reaching 60 after a busy mathematician's life, I decided that it was now or never for me to really understand the subject.[1] The project started for my own enjoyment, before turning into the hardest of my scientific life. I faced many difficulties, the most important being the lack of a suitable introductory text. These notes try to mend that issue.

I knew no physics to speak of, but it was not particularly difficult to get a basic grasp of topics such as Classical Mechanics, Electromagnetism, Special and even General Relativity. They are friendly for mathematicians as they can be made rigorous to our liking.

Quantum Mechanics was a different challenge. Quite naturally, I looked first for books written by mathematicians for mathematicians. By a stroke of bad luck, the first book I tried was to me a shining example of everything one should *not* do when writing a book. Being a mathematician does not mean that I absolutely need to hear about "a one-dimensional central extension of V by a Lie algebra 2-cocycle" just to learn the Heisenberg commutation relations. Moreover, while there is no question that mastery of some high level form of Classical Mechanics will help reaching a deeper understanding of Quantum Mechanics, Poisson Manifolds and Symplectic Geometry are not absolute prerequisites to get started. Other books written by mathematicians are less misguided, but seem to cover mostly topics which barely overlap those in physicists' textbooks with similar titles. To top it all, I was buried by the worst advice I ever received, to learn the topic from Dirac's book itself! The well-known obstacle of the difference of language and culture between mathematics and physics is all too real. To a mathematician's eye, some physics textbooks are chock-full of somewhat imprecise statements made about rather ill-defined quantities. It is not rare that these statements are simply untrue if taken at face value. Moreover arguments full of implicit assumptions are presented in the most authoritative manner. Looking at elementary textbooks can be an even harder challenge. These often use simple-minded approaches

[1] Of course, the realization that I could no longer do research at the level that I wanted to played a major part in this decision.

which need not be fully correct, or try to help the reader with analogies which might be superficial and misleading.[2]

Luckily, in 2012 I ran into the preliminary version of Brian Hall's *Quantum Theory for Mathematicians* [40], which made me feel proud again for mathematicians. I learnt from this book many times faster than from any other place. The "magic recipe" for this was so obvious that it sounds trivial when you spell it out: *explain the theory in complete detail, starting from the very basics, and in a language the reader can understand*. Simple enough, but very difficult to put into practice, as it requires a lot of *humility* from the author, and humility is not the most common quality among mathematicians. I don't pretend to be able to emulate Brian's style, but I really tried and his book has had a considerable influence on mine.

After getting some (still very limited) understanding of Quantum Mechanics came the real challenge: Quantum Field Theory. I first looked at books written by mathematicians for mathematicians. These were obviously not designed as first texts or for ease of reading. Moreover, they focus on building rigorous theories. As of today these attempts seem to be of modest interest for most physicists.[3] More promising seemed studying Gerald Folland's heroic attempt [31] to make Quantum Field Theory accessible. His invaluable contribution is to explain what the physicists do rather than limiting the topic to the (rather small) mathematically sound part of the theory. His book is packed with an unbelievable amount of information, and, if you are stuck with minimum luggage on a desert island, this is a fantastic value. Unfortunately, as a consequence of its neutron-star density, I found it also much harder to read than I would have liked, even in sections dealing with well-established or, worse, elementary mathematics. Sadly, this book has no real competitors and cannot be dispensed with, except by readers able to understand physics textbooks.[4] No doubt my difficulties are due to my own shortcomings, but still, it was while reading Weinberg's treatise [87] that I finally understood what induced representations are, and this is not the way it should have been. So, as the days laboring through Folland's book turned into weeks, into many months, I felt the need to explain his material to myself, and to write the text from which I would have liked to learn the first steps in this area.

In the rest of the introduction I describe what I attempt to do and why. I try to provide an easily accessible introduction to some ideas of Quantum Field Theory for a reader well versed in undergraduate mathematics, but not necessarily knowing any physics beyond the high-school level or any graduate mathematics.

I must be clear about a fundamental point. A striking feature of Quantum Field theory is that it is not mathematically complete. This is what makes it so challenging for mathematicians. Numerous bright people have tried for a long time to make this topic rigorous and have yet to fully succeed. I have nothing new to offer in this direction. This book contains

[2] I am certainly not the first mathematician to be appalled by the way physics students get treated, but it seems futile to discuss this matter further.

[3] This being said, the multiple author treatise [9] is a magnificent piece of work. It is overwhelming at first, but most rewarding once you get into it.

[4] See our Reading Suggestions for physics textbooks on page 732.

statements that nobody knows how to mathematically prove. Still, I try to explain some basic facts *using mathematical language*. I acknowledge right away that familiarity with this language and the suffering I underwent to understand the present material are my only credentials for this task.

My main concern has been to spare the reader some of the difficulties from which I have very much suffered reading others' books (while of course I fear introducing new ones), and I will comment on some of these.

First, there is no doubt that the search for generality and for the "proper setting" of a theory is a source of immense progress in mathematics, but it may become a kind of disease among professional mathematicians.[5] They delight in the "second cohomology group of the Lie algebra" but do not explain why the important theorem holds when the Lie group is $\mathbb{R}$. I feel that in an introductory work generality should be indulged in only when it is useful beyond doubt. As a specific example, I see no need to mention cotangent bundles to explain basic mechanics in Euclidean space, but the use of tensor products *does* clarify Fock spaces. Rather than pursuing generality, I find more instructive to explain in complete detail simple facts and situations, especially when they are not immediately found in the literature.[6] I strive not to refer the reader to extensive specialized works, which may have different notation, and may not have been written to be easily accessible. Of course, other very different approaches are also possible [62].

Second, as an extremely ignorant person, I have suffered from the fact that many textbooks assume much known by the reader, such as "standard graduate courses in mathematics". For mathematics (except on very few occasions), I have assumed nothing that I did not learn in my first three years of university in Lyon, 1969–1972: almost all the more advanced mathematics I need are built from the ground up. For physics, I have tried to assume basically nothing known beyond high-school level.

Third, it was hard at first to recognize that different authors are treating in fact the same material, but each in his own way. I have tried different ways to explain the material which confused me the most.

Fourth, when doing physics, and taking steps of dubious mathematical value (which is often required to proceed) I have tried to be very candid about it and to explain clearly what the problems are.[7]

Fifth, and most importantly, I believe that brevity is not such a desirable goal that it should be reached at the reader's expense. The goal of a textbook is to communicate ideas, not to encrypt them in the shortest possible way (however beautifully this is done). Reading an introductory textbook such as this one *should simply not be a research project*. This book is long because:

[5] I personally found that the only rather accessible article of the volume [18] is due to Edward Witten! But of course this volume is not designed as an introductory course.

[6] This attitude is motivated by the fact that whatever small successes I had in my own mathematical research were always based on a thorough understanding of very simple structures.

[7] I do not believe that authoritative statements, use of implicit assumptions, or contrived arguments as to which obvious problems are not real help the readers.

- *It starts with basic material.*
- *The proofs are very detailed.*[8]

As G. Folland appropriately points out [31], readers of notes such as these are likely to be "tourists": they do not look to acquire professional expertise in the topic. He and I disagree in that I don't think most tourists enjoy extreme sports. My overwhelming concern has been to make the book easy to read, by providing everywhere as high a level of detail as I could manage, and by avoiding anything really complicated until the last chapters. Tourists may not enjoy extreme sports, but they might enjoy leisurely sight-seeing. A number of appendices strive to provide an accessible introduction to a number of rewarding topics which complement the main story.[9]

It seemed most useful not to duplicate what is done everywhere else. First, I acknowledge the fundamental importance of historical perspective in understanding a topic, but I make no attempt whatsoever in this direction: there is no point repeating in a clumsy way what is said excellently elsewhere. Besides, one might gain by presenting early certain central and simple ideas even if they came later in the development of the theory.[10] I am in good company here, see Weinberg's treatise [87]. Second, I concentrate on the points I had the most difficulty understanding, and I treat these in considerable detail, trying also to explain how these points are presented in physics textbooks. The subtitle of this book, a first introduction for mathematicians, *does not mean* that it intends to be the fastest possible introduction to the topic, but rather that the reader is not assumed to know anything whatsoever about it. A bare-bones treatment (covering far more material than I do) has already been written [23], and I am aiming here at a more fulfilling level of understanding.[11] I felt it useful to cover some of the fundamental structures in sufficient detail to provide a solid understanding. One of my most glaring shortcomings is the inability to make sense of a mathematical statement unless I have taken it apart to the very last bolt and reconstructed it entirely. I have tried to do just that for these fundamental structures. This often takes several times longer than in standard textbooks. Obviously in these the reader is expected to produce whatever efforts are required to become a professional and master the field, while I try to be much less demanding. On the other hand, some fundamentally important topics, which I found easier to learn, get only succinct coverage here when detailed understanding is not indispensable.

[8] Yes, for *every* topic, I do *whatever it takes* to complete all details.

[9] The choice of these topics is highly personal and reflects both my interests and the history of my learning of this topic. There are points which I felt I just *had to* understand, but which I am certain many readers will feel comfortable to accept without proof.

[10] Furthermore, it *does help* to entirely forget about some early missteps of the theories.

[11] In practice, I have pursued every thread of thought until I felt I reached some real understanding of it, or until I was forced to accept that some kind of miracle is taking place.

Quantum Field Theory is difficult and voluminous. It involves a great many deep ideas. Not all of them are extremely difficult, but the overall quantity is staggering. Being simultaneously detailed and thorough limits the number of topics I might cover, and difficult choices had to be made. Roger Penrose [63, page 657], characterizes Quantum Field Theory as "this magnificent, profound, difficult, sometimes phenomenonally accurate, and yet often tantalizingly inconsistent scheme of things". As the contribution of the present work is only to describe in a self-contained manner some simple facts in mathematical language, it seemed appropriate that it covers mostly topics where mathematical language brings benefits well beyond a simple matter of notation. This is no longer the case when one ventures in the "inconsistent scheme of things" part of the theory. Still, I briefly enter this territory, in order to provide at least some form of answer to the question which serves as title, and some glimpse at physics methods. I deliberately choose to explain these as clearly as possible on the simplest possible "toy models" without any attempt to study realistic models (where the principles are similar but obscured by many accessory complications). I do not attempt what is already done in so many places, such as describing the tremendous successes of Quantum Electrodynamics. You will not learn here any real physics or what is the Standard Model.[12] Rather, I try to prepare the reader to study books which cover these topics, among which I first recommend Folland's book [31].[13] I have also decided to stay entirely away from path integrals (also known as Feynman's integrals). There is no doubt that from the point of view of physics, path integrals are the correct approach, but they are not well defined mathematically, and I do not see what yet another heuristic discussion of them would bring.

On the other hand, the study of renormalization, the method to circumvent the dreadful infinities, receives far more attention than it does in standard textbooks. The procedure itself is rigorous. It involves only rather elementary (but magnificently clever) mathematics. There seems to exist no other detailed source than the original papers or specialized monographs such as [52] or [70].[14] I prove in full detail the possibility of renormalization at all orders of the so-called ϕ_4^4 and ϕ_6^3 theories, cases of somewhat generic difficulty.

No magic wand will make Quantum Field Theory really easy and some effort will be required from the reader. My goal has been to make this effort easier for the reader than it was for me without sacrificing the potential for enjoyment and enrichment this fascinating topic offers.

A number of people helped me while I wrote this book. Shahar Mendelson had a transformative impact, and there are simply no words by which I can express my gratitude for the time and energy he invested in what was for him a pure labor of love. He and Roy Wilsker rescued me many times from the brink of disaster. Gerald Folland spent considerable time and displayed infinite patience in trying to explain some of the most delicate points of his book [31]. Ellen Powell relentlessly asked for clarification of many imprecise statements.

[12] Nor will you meet any idea that was not well formed fifty years ago.

[13] However demanding, this book is simply brilliant at a number of places, and I see no purpose in repeating the parts which I cannot improve in my own eyes.

[14] The major textbooks do not enter into details on this topic, but only illustrate some ideas on examples, "referring the serious reader to the study of the original papers" see e.g. [58, page 157]. This is even the case of books which primarily deal with renormalization, such as [1, 15].

Guilherme Henrique de Paula Reis and Shuta Nakajima read in detail every single proof, however technical, and contributed in a major way to removing numerous obscurities and outright mistakes.[15] Comments of Sourav Chatterjee, Carlos Guesdes, Brian Hall, Amey Joshi, Bernard Lirola, Patrick Lopatto, Hengrui Luo, David Saunders, Krzysztof Smuteck, Phil Sosoe, Zenyuang Zhang and others on the successive versions had a major impact. It was a pure delight to work with my editor Diana Gillooly.[16] I express my gratitude to them all.

Part of the work involved in this project was performed while the author was employed by C.N.R.S and the author is grateful for this support.

[15] I am solely responsible for the remaining ones.
[16] Unless of course the matter at hand was the length of the book.

Part I

Basics

Our broad goal is to construct models explaining the interactions of elementary particles. The multiple ingredients and fundamental ideas are introduced in succession in the main chapters. We will then discover the bad news: even in simple models, the predictions are non-sensical, being expressed by diverging integrals. Still, a process called renormalization allows finite physical predictions from these infinities. Such is the program of the main chapters. Along the way, a wealth of interesting questions of mathematics will be encountered. Many of these are explored in the appendices, which also contain more advanced material on certain matters of physics.* A minimum reading program does not require you to ever look at an appendix. The goal of such a program would be the central Chapter 13, which explains how the infinities occur and hints at how to remove them. The chapter deals only with spinless particles, so it can be reached without learning any of the material related to spin (which is nonetheless of great mathematical interest), and entirely ignoring Part II of the book. This minimum program can then be extended according to the reader's main interests.

The reader is assumed to be a mathematician. As far as knowledge is concerned, this means little more than the expectation that she will not faint at reading the words "group" and "Hilbert space". As far as attitude is concerned this means that she is expected to be more interested in trying to understand what is going on and why certain assumptions and methods are reasonable rather than in the details of specific computations that can be measured against experiments.

Here seems to be a good place to comment on the level of mathematical rigor of the book. A very significant part (particularly in the appendices) is just standard, fully rigorous mathematics, since after all this is what this author is best qualified to write. Another significant part is "basically rigorous" in the sense that it could (probably) be made rigorous but the complication of doing so would obscure the main purpose, and whenever the choice arises, we choose clarity over formality. The rest of the book takes place outside mathematics, in the physicist's fairyland where one manipulates objects whose very existence is rather

* Even though we have aimed at high standards of detail and clarity throughout, some of the appendices might be a bit more demanding mathematically than the main text.

dubious.[†] Roughly speaking this is the case of Part III, whereas most of Parts I, II and IV are either fully rigorous or basically rigorous. We have tried to help the reader figure out the level of rigor of various sections, but of course the boundaries of "basically rigorous" are somewhat fuzzy. Let us stress, however, that Part IV, treating renormalization (the art to make sense of certain diverging integrals) is fully rigorous.

There are many possible plans one could make to treat the present subject. One could choose to follow the historical development. One could choose the "logical order": explain the basics of Classical Mechanics, Quantum Mechanics and Special Relativity before attacking Quantum Field Theory. We have chosen a less-traveled route, which might be more appealing to mathematicians.

First, let us ask why one might be interested in this topic. There are obvious reasons, of course. Any learned person should want to know something about a theory, which is certainly one of the greatest intellectual achievements of all times, and which has been so well confirmed by experiment with the discovery of the Higgs boson.[‡] But more specifically, why might mathematicians be interested in Quantum Field Theory? For the *very* ambitious, there is the fact that putting the theory on a firm mathematical footing remains a formidable challenge. More modestly, an aesthetically appealing aspect of the theory is that so much of it is determined just by the requirement that it should be consistent with Special Relativity, i.e. invariant under Lorentz transformations. Our presentation emphasizes this aspect, culminating in Chapter 10 with simple arguments (using no more than elementary linear algebra) that allow the discovery of the basic free fields. Prior to this chapter, only the minimum is said about Quantum Mechanics, delaying the description of fundamental practical matters such as perturbation theory until they are actually needed, and until motivation has been gained.

Probably the reader would like to have a more precise road map of what lies ahead, but whatever precise information we might try to give at this stage would only make little sense to a reader not knowing the basic concepts of Quantum Mechanics. Consequently, a technical overview of the first few chapters is delayed until the beginning of Chapter 3.

[†] And one even "proves theorems" about them!
[‡] Or, maybe more accurately, of a boson that looked like a Higgs boson at the time of this writing.

1

Preliminaries

As the present project started as an attempt at rewriting Folland's textbook [31], we begin in the same direction, attempting though to give more details.

1.1 Dimension

The numerical value of many physical quantities depends on the unit one chooses to measure them. My height is 1.8 m, or 180 cm, or 1.90×10^{-16} light-years. The use of light-years here as a unit is weird, but not so much more than the use of centimeters to measure distances at the scale of a nucleon as many textbooks do. (A nucleon has a size of about 10^{-15} m $= 10^{-13}$ cm.) Tradition unfortunately has more weight than rationality in these matters.

The concept of "physical dimension" (which definitely differs from dimension in the mathematical sense) expresses how the numerical value of a physical quantity depends on the units you choose to measure it. A distance has dimension $[l]$ where l stands of course for length. If you increase the unit of length by a factor 100, the corresponding measure *decreases* by a factor 100: 100 cm = 1 m. Then a surface has dimension $[l^2]$: $(100)^2\,\text{cm}^2 = 1\,\text{m}^2$. A volume has dimension $[l^3]$: $1\,\text{km}^3 = (10^3)^3\,\text{m}^3 = 10^9\,\text{m}^3$. The unit of time can be chosen independently from the unit of length. Time has dimension $[t]$, so speed, which is a distance divided by a time, has dimension $[lt^{-1}]$. Thus 1 m/s = 3,600 m/h = 3.6 km/h. Acceleration, which is a change of speed divided by a time, has dimension $[lt^{-2}]$. It is of course a convention to choose time and length as fundamental quantities. One could make other choices, such as choosing time and speed as fundamental quantities. This is indeed basically what is actually done. Since 1983, in the international system the speed of light is *defined* to be *exactly*

$$c = 299{,}792{,}458\ \text{m/s} \tag{1.1}$$

and this serves as a definition of the meter given the unit of time.[1]

A formula in physics *must give a correct result independently of the system of units used.* This is a strong constraint. This is why it often makes sense to multiply or divide quantities of different dimensions, but it *never* makes sense to add them. As we learn in kindergarten,

[1] The reason for this definition is that the speed of light is a fundamental constant of Nature, and that it makes little sense to have its value change as the accuracy of measurements improves.

you do not add pears with bananas. Furthermore, when a quantity occurs in a formula as the argument of, say, an exponential, it must be *dimensionless,* i.e. its value must be independent of the unit system. To understand a formula in physics it always helps to check that it makes sense with respect to dimension, a task we will perform many times.

The unit of mass can be chosen independently of the units of length and time. Momentum,[2] the product of a mass and a speed, then has dimension $[lt^{-1}m]$, and angular momentum, the product of a momentum and a distance, has dimension $[l^2t^{-1}m]$. Energy has the dimension of a mass times the square of a speed, that is $[l^2t^{-2}m]$. Less known is the *action* which occurs in Lagrangian Mechanics as the integral over a time interval of a quantity with the dimension of energy, and thus has the same dimension $[l^2t^{-1}m]$ as the angular momentum.

A fundamental constant of Nature is Planck's constant h, which represents the basic quantum of action (and in particular has the dimension of an action). In physical equations it often occurs in combinations with a factor of $1/2\pi$, so one defines the reduced Planck constant

$$\hbar = \frac{h}{2\pi}, \tag{1.2}$$

whose value is about[3]

$$\hbar = 1.0546 \times 10^{-34}\ \mathrm{J}\cdot\mathrm{s}. \tag{1.3}$$

This is small, as becomes more apparent if this value is expressed in units more related to the microscopic world[4] $\hbar \simeq 6.6\times 10^{-16}\ \mathrm{eV}\cdot\mathrm{s}$. It is important to note that energy times time, momentum times length and angular momentum all have the same dimension as $\hbar$ so that their quotients by $\hbar$ are dimensionless. These quotients will occur in countless formulas.

Exercise 1.1.1 The Planck-Einstein relation gives the energy E of a photon of frequency ν as $E = h\nu$. Check that this formula makes sense with respect to dimension.

Exercise 1.1.2 The de Broglie momentum–wavelength relation states that to a particle of momentum p is associated a wavelength $\lambda = h/p$. Check that this formula makes sense with respect to dimension.

1.2 Notation

Since to enjoy this topic one has to read the work of physicists, it is best to adopt their notation from the beginning. Complex numbers play a central role, and the conjugate of a complex number a is denoted by a^*. Even some of the best authors let the reader decide

[2] Please do not worry if you do not have a real feeling for the concepts of momentum, energy, etc. (despite the fact that you should experience them every day). This is not going to be an obstacle.

[3] An action has the dimension of an energy times a time. In the International System of Units, the unit of energy is the joule J and the unit of time is the second s, so action is measured in $\mathrm{J}\cdot\mathrm{s}$. From May 2019, the value of h is *defined* to be exactly $6.62607015 \times 10^{-34}\mathrm{J}\cdot\mathrm{s}$.

[4] A joule is a huge energy at the microscopic scale. A more appropriate unit of energy at this scale is the electron-volt eV, the energy acquired by an electron going through a difference of potential of one volt.

whether i denotes a complex number with $i^2 = -1$ or an integer index. Since this requires no extra work, the complex number will be denoted by i, so that $\mathrm{i}^* = -\mathrm{i}$.

When working with complex Hilbert spaces we adopt the convention that the inner product $(\cdot,\cdot)$ is anti-linear in the *first* variable (while often mathematicians use the convention that it is anti-linear in the second variable). One says that the inner product is *sesqui-linear*. That is, as another example of our notation for complex conjugation, we write

$$(ax, y) = a^*(x, y)$$

for any vectors x, y and any complex number a. Moreover

$$(y, x) = (x, y)^*. \tag{1.4}$$

The norm $\|x\|$ of a vector x is given by $\|x\|^2 = (x, x)$, and we recall the Cauchy-Schwarz inequality

$$|(x, y)|^2 \leq \|x\|^2 \|y\|^2,$$

where $|a|$ denotes the modulus of the complex number a. A basic example of a complex Hilbert space[5] is the space $\mathbb{C}^n$, where the inner product is defined by $(x, y) = \sum_{i \leq n} x_i^* y_i$, with the obvious notation $x = (x_i)_{i \leq n}$. Another very important example is the space $L^2(\mathbb{R})$ of complex-valued functions f on the real line for which $\int_{\mathbb{R}} |f|^2 \mathrm{d}x = \int_{\mathbb{R}} |f(x)|^2 \mathrm{d}x < \infty$, where $|f(x)|$ denotes the modulus of $f(x)$. The inner product is then given by $(f, g) = \int_{\mathbb{R}} f^* g \mathrm{d}x$. A physicist would actually write

$$(f, g) = \int_{-\infty}^{\infty} \mathrm{d}^1 x f(x)^* g(x), \tag{1.5}$$

where the superscript 1 refers to the fact that one integrates for a one-dimensional measure. The reason for which the $\mathrm{d}^1 x$ is put before the function to integrate is that this makes the formula easier to parse when there are multiple integrals. We will use this convention systematically. We will not however mention the dimension in which we integrate when this dimension is equal to one.

An *operator* A on a finite-dimensional Hilbert space $\mathcal{H}$ is simply a linear map $\mathcal{H} \to \mathcal{H}$. Its *adjoint* $A^\dagger$ is defined by

$$(A^\dagger(x), y) = (x, A(y)), \tag{1.6}$$

for all vectors x, y. (Mathematicians would use the notation A^* rather than $A^\dagger$.)

Exercise 1.2.1 (a) If A is an operator and α a number, prove the formula

$$(\alpha A)^\dagger = \alpha^* A^\dagger.$$

(b) If A and B are operators, prove that $(AB)^\dagger = B^\dagger A^\dagger$.

An operator (still on a finite-dimensional space) is called *Hermitian* if $A = A^\dagger$. A Hermitian operator A has the crucial property that if a subspace F is such that $A(F) \subset F$ then the orthogonal complement $F^\perp$ of F is also such that $A(F^\perp) \subset F^\perp$.

[5] In this work we consider only finite-dimensional or, more generally, *separable* Hilbert spaces.

Exercise 1.2.2 Deduce this from the fact that $(A(x), y) = (x, A(y))$ for all x, y.

As a consequence, a Hermitian operator has a simple structure: there exists an orthonormal basis of eigenvectors.[6]

Exercise 1.2.3 Give a complete proof of this fact by induction over the dimension of the space.

Moreover the eigenvalues are real since $(x, A(x))$ is real for all x. Indeed,

$$(x, A(x)) = (A(x), x)^* = (x, A(x))^*,$$

where the second equality uses that A is Hermitian. If $A(x) = \lambda x$ then $(x, A(x)) = \lambda(x, x)$, so that $\lambda(x, x) = \lambda^*(x, x)$ and $\lambda = \lambda^*$. It is this property of having a basis of eigenvectors, with real eigenvalues, which makes the class of Hermitian operators so important.

A few times we will need the notion of *anti-linear* operator. Such a map T does satisfy $T(x + y) = T(x) + T(y)$ but for a scalar a we have $T(ax) = a^* T(x)$.

We should also mention that in physics, vectors and inner products are denoted differently, using Dirac's ubiquitous notation, which we will explain later. In most situations however we prefer to use standard mathematical notation, and it is unlikely that anybody reading this will mind.

1.3 Distributions

Laurent Schwartz invented the theory of distributions to give a rigorous meaning to many formal calculations of physicists. The theory of distributions is a fully rigorous part of mathematical analysis. In the main text however we will use only the very basics of this theory at a purely informal level. In Appendix L the reader may find an introduction to rigorous methods.

We will consider distributions on $\mathbb{R}^n$ but here we assume $n = 1$. The central object is the space $\mathcal{S} = \mathcal{S}(\mathbb{R})$ of *rapidly decreasing functions*, called also *test functions* or *Schwartz functions*. A complex-valued[7] function ζ on $\mathbb{R}$ is a test function if it has derivatives of all orders and if for any integers $k, n \geq 0$ one has[8]

$$\sup_x |x^n \zeta^{(k)}(x)| < \infty. \tag{1.7}$$

A distribution is simply a linear functional (which also satisfies certain regularity conditions which will not concern us before we reach Appendix L, as they will be satisfied in all the examples we will consider). That is, a distribution Φ is a complex linear map from $\mathcal{S}$ to $\mathbb{C}$, and for each test function ζ the number $\Phi(\zeta)$ makes sense. Such a distribution should actually be called a *tempered* distribution, but we will simply say "distribution" since we will

[6] Later we will meet a far-reaching extension of this fact, the spectral theorem for self-adjoint operators.

[7] A test function is typically complex-valued. At times, to avoid complications created by anti-linear operators, we also consider real-valued test functions. The space of such functions is denoted by $\mathcal{S}_{\mathbb{R}}$. Please try to remember that the subscript $\mathbb{R}$ on a space of test functions means that we consider only real-valued functions.

[8] The property is often described in words as follows: As $|x| \to \infty$, the function and each of its derivatives decrease faster than $|x|^{-n}$ for each n. This is what motivates the name "rapidly decreasing function".

hardly consider any other type of distribution. Tempered distributions are also known under the name of *generalized functions.* This name has the advantage of explaining the point of the theory of distributions: it generalizes the theory of functions. Indeed, a sufficiently well-behaved function[9] f defines a distribution (= generalized function) Φ_f by the formula

$$\Phi_f(\zeta) = \int \mathrm{d}x\, \zeta(x) f(x). \tag{1.8}$$

Throughout the book *we maintain the convention that when the domain of integration is not mentioned, this domain is the whole space*. Thus (1.8) means $\Phi_f(\zeta) = \int_{\mathbb{R}} \mathrm{d}x f(x)\zeta(x) = \int_{-\infty}^{\infty} \mathrm{d}x f(x)\zeta(x)$.

As we are going to see, distributions can be strange animals. On the other hand, distributions given by a formula such as (1.8) are much better behaved. The short way to describe the situation where the distribution Φ is of the type Φ_f as in (1.8) is to simply say that Φ *is a function*.

In general a distribution is certainly not given by a formula of the type (1.8). However, when dealing with distributions we will maintain the *notational fiction* that they are functions, i.e. for a test function ζ we will write

$$\int \mathrm{d}x\, \zeta(x)\Phi(x) := \Phi(\zeta). \tag{1.9}$$

The use of the symbol := here is to stress that the right-hand side is a definition of the left-hand side, so that you may be reassured that your memory did not fail and that there is no point in looking back for the definition of the left-hand side. Equation (1.9) indeed defines the left-hand side, since the symbol $\Phi(x)$ is a *notation*, and a priori really *makes no sense whatsoever by itself*. It is only the integral $\int \mathrm{d}x\, \zeta(x)\Phi(x)$ which makes sense for any test function, and the value of this integral is (by definition) the quantity $\Phi(\zeta)$, as expressed in (1.9).[10] The central objects of this work, quantum fields, have precisely the previous property. The value of a quantum field cannot be specified at any given point. This value makes sense only "when it is integrated against a test function", or *smeared* in physics-type language.

Even for distributions, it is however sometimes possible to give a meaning to the quantity $\Phi(x)$ for certain values of x. Given an open interval I of the real line, we say that a distribution *is a function on* I if there exists a well-behaved function f on I such that $\Phi(\zeta) = \int \mathrm{d}x\, \zeta(x) f(x)$ whenever the test function ζ has compact support contained in I.[11] It is then reasonable to define $\Phi(x) = f(x)$ for $x \in I$. However, unless Φ is a function, it is not possible to assign a meaning to the symbol $\Phi(x)$ for each value of x.

[9] The meaning of the expression "well-behaved" varies depending on the context. In the present case, f needs to be locally integrable and "not grow too fast at infinity".

[10] The notational fiction (1.9) is however quite useful when one likes to be informal, as we simply do not distinguish distributions from functions until this leads us into trouble.

[11] When $I = \mathbb{R}$ this looks different from the definition (1.8) because then it is not required that ζ has compact support. However, using the regularity properties that are part of the definition of a distribution, and on which we do not dwell here one may show that these definitions coincide, see Appendix L.

Distributions can be added, or multiplied by a scalar, but in general *cannot be multiplied*.[12] The great appeal of distributions is that they can always be differentiated. The derivative of a distribution Φ is the distribution *defined* by the formula

$$\Phi'(\zeta) := -\Phi(\zeta') \tag{1.10}$$

for every test function ζ. The reason behind this definition is best understood by integrating by parts when Φ is given by the formula (1.8) for a well-behaved function f. Then $\Phi'(\zeta) = \int \mathrm{d}x f'(x)\zeta(x)$.

Exercise 1.3.1 Convince yourself from the preceding definition that "if a distribution is actually a nice function, its derivatives as a function and as a distribution coincide". Hint: Recalling (1.8), prove that $(\Phi_f)' = \Phi_{f'}$.

Pretending that Φ' is also a function, we write $\Phi'(\zeta)$ as $\int \mathrm{d}x\zeta(x)\Phi'(x)$, and equally shamelessly we write (1.10) as

$$\int \mathrm{d}x\, \zeta(x)\Phi'(x) := -\int \mathrm{d}x\, \zeta'(x)\Phi(x). \tag{1.11}$$

In several dimensions, the class of test functions is defined as the class of infinitely differentiable functions such that the product of any partial derivative (of any order) and any polynomial in the variables is bounded. The reader may refer to Section L.1 for more about test functions.

1.4 The Delta Function

Besides reviewing the delta function, this section introduces the idea of a smooth cutoff, how to get rid of the troublesome part of an integral.

Mathematically, the delta "function" δ is simply the distribution given by

$$\delta(\zeta) = \zeta(0) \tag{1.12}$$

for any test function $\zeta \in \mathcal{S}$. Pretending that the delta "function" is actually a true function we will shamelessly write (1.12) as

$$\zeta(0) = \int \mathrm{d}x\zeta(x)\delta(x). \tag{1.13}$$

The name "delta function" is historical. Physicists have been using this object long before distributions were invented.

Exercise 1.4.1 (a) Convince yourself that it makes perfect sense to say that $\delta(x) = 0$ if $x \neq 0$.
(b) Make sure that you understand that despite the terminology, the delta function δ is not a function in the mathematical sense and that the quantity $\delta(0)$ *makes no sense*.

[12] One of the reasons for the dreaded infinities which will occur later is that we will have no other choice to proceed than pretending we can multiply certain distributions.

(c) Convince yourself from (1.13) that, in the words of physicists, "the delta function δ is the function of x which is equal to zero for $x \neq 0$ and to infinity for $x = 0$, but in such a way that its integral is 1".
(d) Convince yourself that the *derivative* of the delta function δ, i.e. the distribution δ' given by $\delta'(\zeta) = -\zeta'(0)$ "does not look at all like a function".

For $a \neq 0$ let us *define* $\delta(ax)$ by

$$\int \mathrm{d}x\zeta(x)\delta(ax) := \frac{1}{|a|}\int \mathrm{d}x\zeta(x/a)\delta(x) = \frac{1}{|a|}\zeta(0), \tag{1.14}$$

so that

$$\delta(ax) = \frac{1}{|a|}\delta(x), \tag{1.15}$$

and in particular $\delta(-x) = \delta(x)$.[13]

Proper mathematical terminology requires one to say "the function f" but sooner or later one always says "the function $f(x)$" to carry at the same time the information that the variable is called x. In the same manner we will use expressions such as "the distribution $\Phi(x)$" which *should not* be interpreted as meaning that the quantity $\Phi(x)$ makes sense for a given x.

We will often write the quantity $\delta(x - y)$. It can be seen as a "function" of x depending on the parameter y. This "function" makes sense only when integrated in x against a test function ζ, and one has

$$\zeta(y) = \int \mathrm{d}x\zeta(x)\delta(x - y). \tag{1.16}$$

It can also be seen as a "function" of y depending on the parameter x, and one has

$$\zeta(x) = \int \mathrm{d}y\zeta(y)\delta(x - y). \tag{1.17}$$

Exercise 1.4.2 The quantity $\delta(x - y)$ can also be seen as a distribution Φ in the variables x, y. For a test function $\xi(x, y)$ one has

$$\iint \mathrm{d}x\mathrm{d}y\xi(x, y)\delta(x - y) := \Phi(\xi) := \int \mathrm{d}x\xi(x, x).$$

Convince yourself that this is consistent with (1.16) and (1.17).

Note also that $\delta(x - y) = \delta(y - x)$. We will shift freely between the previous meanings of the quantity $\delta(x - y)$. More generally we will stay very informal. Everything we say at this stage could be made rigorous, but this is not our objective.[14]

[13] Please be prepared: soon we will start manipulating delta functions as if they were functions, for example taking for granted the first equality in (1.14).
[14] It makes no sense to carefully climb molehills when the Himalayas are waiting for us.

Exercise 1.4.3 For a test function ξ convince yourself of the formula (various versions of which we will use many times)

$$\int \mathrm{d}z\delta(x-z)\delta(z-y)\xi(z) = \delta(x-y)\xi(x). \tag{1.18}$$

We will make massive use of the formula[15]

$$\delta(x) = \frac{1}{2\pi}\int \mathrm{d}y\,\exp(\mathrm{i}xy), \tag{1.19}$$

and we first need to make sense of it. In studying physics, one must keep in mind at all times that the goal is to make predictions about the behavior of the physical world. This is difficult enough. To study the physical world, one makes models of it. One should as far as possible concentrate on problems that arise from the physical world, and stay away from the problems that arise not from the physical world, but from the models we made of it. We may never know for sure whether the physical world is finite or not, but certainly events located very far from our experiments are unlikely to affect very much their outcome, so their inclusion in our model is an idealization, and in (1.19) points very far from the origin should be discounted, for example by a factor $\exp(-ay^2)$ for a very small $a > 0$. This is an example of what is called a "smooth cutoff". Thus, rather than (1.19) we mean

$$\delta(x) = \lim_{a\to 0}\frac{1}{2\pi}\int \mathrm{d}y\,\exp(\mathrm{i}xy - ay^2). \tag{1.20}$$

Here the limit is "in the sense of distributions". *By definition of convergence in the sense of distributions*, this means that for every test function ζ,

$$\zeta(0) = \int \mathrm{d}x\zeta(x)\delta(x) = \lim_{a\to 0}\int \mathrm{d}x\zeta(x)\psi_a(x), \tag{1.21}$$

where

$$\psi_a(x) := \frac{1}{2\pi}\int \mathrm{d}y\,\exp(\mathrm{i}xy - ay^2) = \frac{1}{2\sqrt{a\pi}}\exp(-x^2/4a),$$

the second equality resulting from the computation of the Gaussian integral, see Lemma C.3.3. Making the change of variables $x = \sqrt{a}y$, (1.21) becomes

$$\zeta(0) = \lim_{a\to 0}\int \mathrm{d}y\zeta(y\sqrt{a})\psi_1(y),$$

which holds by dominated convergence since ψ_1 has integral 1 and ζ is uniformly bounded.[16]

A regularization procedure as in (1.20) can make sense only if it is robust enough. You might have chosen an origin different from mine, but this does not matter since for all b it follows from (1.20) that we actually have

$$\delta(x) = \lim_{a\to 0}\frac{1}{2\pi}\int \mathrm{d}y\,\exp(\mathrm{i}xy - a(y-b)^2).$$

[15] $\exp(x)$ is just another notation for e^x.

[16] Certainly the reader has observed the fundamental idea there: a family of functions of integral 1, which peaks more and more narrowly around zero converges to the delta function in the sense of distributions, consistently with Exercise 1.4.1 (a).

Exercise 1.4.4 It would seem at first that the substitution $z = y - b$ in the right-hand side brings a factor $\exp(-\mathrm{i}xb)$. Why is there no such factor? Hint: Where is the delta function different from zero?

We will also need the obvious three-dimensional generalization of (1.19). In this case, not only might you and I have chosen different origins, we might also move at relativistic speed with respect to each other (and consequently we may not agree on the way we measure distances). There is however little point in investigating which specific regularization schemes would take care of this: as we will see later in this section, far more general regularization schemes work.

1.5 The Fourier Transform

Besides reviewing some basic facts about Fourier transforms, this section provides the first example of certain calculations common in physics.

The Fourier transform will play a fundamental role.[17] Let us temporarily denote by $\mathcal{F}_m$ the Fourier transform, that is

$$\mathcal{F}_m(f)(x) = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}y \exp(-\mathrm{i}xy) f(y), \tag{1.22}$$

where the subscript m reminds you that this is the way mathematicians like to define it (whereas our choice of normalization will be different). The right-hand side is defined for f integrable, and in particular for a Schwartz function $f \in \mathcal{S}$. Using integration by parts in the first equality, and differentiation under the integral sign in the second one, we obtain the fundamental facts that for any test function f,

$$\mathcal{F}_m(f')(x) = \mathrm{i}x\mathcal{F}_m(f)(x)\ ;\ \mathcal{F}_m(xf) = \mathrm{i}\mathcal{F}_m(f)', \tag{1.23}$$

where we abuse notation by denoting by xf the function $x \mapsto xf(x)$. An essential fact is that the Fourier transform of a test function is a test function. The details of the proof are a bit tedious, and are given in Section L.1.[18]

The Plancherel formula is the equality

$$(\mathcal{F}_m(f), \mathcal{F}_m(g)) = (f, g), \tag{1.24}$$

for $f, g \in \mathcal{S}$, where $(f, g) = \int \mathrm{d}x f(x)^* g(x)$. It is very instructive to "prove" this formula the way a physicist would, since this is a very simplified occurrence of the type of computations that are ubiquitous in Quantum Field Theory:

$$\begin{aligned}(\mathcal{F}_m(f), \mathcal{F}_m(g)) &= \frac{1}{2\pi} \int \mathrm{d}x \Big(\int \mathrm{d}y_1 \exp(-\mathrm{i}xy_1) f(y_1) \Big)^* \int \mathrm{d}y_2 \exp(-\mathrm{i}xy_2) g(y_2) \\ &= \frac{1}{2\pi} \iint \mathrm{d}y_1 \mathrm{d}y_2 f(y_1)^* g(y_2) \int \mathrm{d}x \exp(\mathrm{i}x(y_1 - y_2))\end{aligned}$$

[17] As will be explained later, it provides a natural correspondence between the "position representation" and the "momentum representation".

[18] The essential point is that iteration of the previous relations and Plancherel's formula show that if f is a test function then for each $n, k \in \mathbb{N}$ the function $x^n \mathcal{F}_m(f)^{(k)}(x)$ belongs to L^2.

$$
\begin{aligned}
&= \iint \mathrm{d}y_1 \mathrm{d}y_2 f(y_1)^* g(y_2) \delta(y_1 - y_2) \\
&= \int \mathrm{d}y_2 f(y_2)^* g(y_2) \\
&= (f, g),
\end{aligned} \tag{1.25}
$$

where we have used (1.19) in the third line and have integrated first in y_1 in the fourth line. Although this type of manipulation might look scary at first to a mathematician, it suffices in fact to insert a factor $\exp(-ax^2)$ in the first line and let $a \to 0$ to make the argument rigorous using (1.20).

As a consequence of Plancherel's formula, for $f \in \mathcal{S}$, the Fourier transform of f has the same L^2 norm as f, i.e. $\mathcal{F}_m$ is an isometry when $\mathcal{S}$ is provided with the L^2 norm. Since $\mathcal{S}$ is dense in L^2 for this norm, an elementary result asserts that we may extend by continuity the Fourier transform as a linear map from L^2 to itself and this extension still satisfies (1.24). Please observe that it is by no means obvious that the right-hand side of the formula (1.22) is well-defined when $f \in L^2$.

One of the miracles of the Fourier transform is that it can be inverted by a formula very similar to (1.22):

$$
\mathcal{F}_m^{-1}(g)(y) = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}x \exp(\mathrm{i}xy) g(x). \tag{1.26}
$$

To justify the notation $\mathcal{F}_m^{-1}$ we observe that, using (1.26) for $g = \mathcal{F}_m(f)$, and using again (1.19),

$$
\begin{aligned}
\mathcal{F}_m^{-1}\left(\mathcal{F}_m(f)\right)(y) &= \frac{1}{2\pi} \int \mathrm{d}x \exp(\mathrm{i}xy) \int \mathrm{d}z \exp(-\mathrm{i}xz) f(z) \\
&= \frac{1}{2\pi} \int \mathrm{d}z f(z) \int \mathrm{d}x \exp(\mathrm{i}x(y - z)) \\
&= \int \mathrm{d}z f(z) \delta(y - z) \\
&= f(y).
\end{aligned} \tag{1.27}
$$

This again can be made rigorous just as (1.25). Let us now look back at (1.21), which we write, using Fubini's theorem,

$$
\zeta(0) = \lim_{a \to 0} \frac{1}{2\pi} \int \mathrm{d}y \exp(-ay^2) \left(\int \mathrm{d}x \exp(\mathrm{i}xy) \zeta(x) \right),
$$

and by dominated convergence we obtain

$$
\zeta(0) = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}y \, \mathcal{F}_m^{-1}(\zeta)(y). \tag{1.28}
$$

Incidentally, it is now quite obvious that the regularization scheme in (1.20) is very robust. To see this, let us investigate for which regularizing families of functions ψ_a, we have in the sense of distributions

$$
\delta(x) = \lim_{a \to 0} \frac{1}{2\pi} \int \mathrm{d}y \exp(\mathrm{i}xy) \psi_a(y).
$$

This means that for any test function $\zeta \in \mathcal{S}$ it holds that

$$\zeta(0) = \lim_{a\to 0} \frac{1}{2\pi} \iint \mathrm{d}x\mathrm{d}y\, \zeta(x) \exp(\mathrm{i}xy)\psi_a(y). \tag{1.29}$$

The right-hand side is

$$\lim_{a\to 0} \frac{1}{\sqrt{2\pi}} \int \mathrm{d}y\, \mathcal{F}_m^{-1}(\zeta)(y)\, \psi_a(y) = \lim_{a\to 0} \int \mathrm{d}y\, \theta(y)\psi_a(y),$$

where $\theta := (2\pi)^{-1/2}\mathcal{F}_m^{-1}(\zeta)$. Since θ is a test function, and since its integral is $\zeta(0)$ by (1.28), (1.29) holds true whenever ψ_a converges to the constant function 1 in the sense of distributions, that is

$$\lim_{a\to 0} \int \mathrm{d}y\, \eta(y)\psi_a(y) = \int \mathrm{d}y\, \eta(y)$$

for each test function η. This is the case for example (using dominated convergence) when $\psi_a(y) = \psi(ay)$ where $\psi \in \mathcal{S}$ satisfies $\psi(0) = 1$, and in particular when $\psi(x) = \exp(-x^2)$ as in (1.20).

Let us also mention that it is possible to define a notion of "Fourier transform of a distribution", and once this is done (1.28) is equivalent to the statement "the delta function is the Fourier transform of the constant function $1/\sqrt{2\pi}$", which is a more elaborate way to describe the way we made sense of (1.19).

Mathematicians love the symmetry between (1.22) and (1.26), but in physics it is better, thinking that x has the dimension of a length and p of a momentum to define the Fourier transform of a function f as

$$\hat{f}(p) = \int \mathrm{d}x \exp(-\mathrm{i}xp/\hbar) f(x) = \sqrt{2\pi}\mathcal{F}_m(f)(p/\hbar) \tag{1.30}$$

and the inverse Fourier transform as

$$\check{\xi}(x) = \int \frac{\mathrm{d}p}{2\pi\hbar} \exp(\mathrm{i}xp/\hbar)\xi(p). \tag{1.31}$$

This makes sense because the quantity $xp/\hbar$ is dimensionless. The Plancherel formula then becomes

$$\int \mathrm{d}x\, |f(x)|^2 = \int \frac{\mathrm{d}p}{2\pi\hbar} |\hat{f}(p)|^2. \tag{1.32}$$

Exercise 1.5.1 Make sure you understand (1.31) by writing out all details. The factor $2\pi\hbar$ will occur constantly.[19]

There are obvious multidimensional versions of these formulas. There is one factor $2\pi\hbar$ per dimension in the analog of (1.31). When integrating in p we will always include these factors.

Exercise 1.5.2 Write the multidimensional versions of these formulas.

[19] According to (1.2), we have $2\pi\hbar = h$ but we write all formulas in term of $\hbar$.

The formula (1.23) now becomes

$$\widehat{-\mathrm{i}\hbar\frac{\mathrm{d}f}{\mathrm{d}x}}(p) = -\mathrm{i}\hbar\widehat{\frac{\mathrm{d}f}{\mathrm{d}x}}(p) = p\,\hat{f}(p). \tag{1.33}$$

The operator $-\mathrm{i}\hbar\mathrm{d}/\mathrm{d}x$ is fundamental in Quantum Mechanics, and (1.33) means that it is much simpler to express on $\hat{f}$ than on f: applying this operator to the function f simply amounts to multiplying the Fourier transform of f by p.

Key facts to remember:

- One should always check that an equation in physics makes sense from the point of view of physical dimension.
- The complex conjugate of a complex number a is denoted by a^* and the adjoint of an operator A by $A^\dagger$.
- Distributions generalize functions but their value is not defined at every point and they make sense only when integrated against a test function. The "delta function" is not a function!
- The ubiquitous Fourier transform is not exactly defined as it would be in mathematics.

2

Basics of Non-relativistic Quantum Mechanics

Quantum Field Theory may be described as an attempt to bring together non-relativistic Quantum Mechanics and Special Relativity. As a first task one has to understand some basics of Quantum Mechanics. In this chapter we review the absolute minimum required. We make no attempt to state axioms in a formal and complete way, since the goal, as so often in this book,[1] is to explain things clearly rather than formally. If you have never heard of Quantum Mechanics, it is unlikely that these basic elements will suffice. Despite the fact that if you pick a textbook at random from your library shelf, it is likely to vampirize your time, there *do exist* good, well-written textbooks, and there is no point in duplicating too much of them here. On the mathematical side, the reader-friendly book by Hall [40] provides a good introduction. On the physics side, Cohen-Tannoudji, Diu, and Laloë's treatise [11] is a masterpiece of pedagogy. These textbooks contain far more material than will actually be needed, but they are excellent pieces to read more if you need to do so.

Different approaches may be tried to provide a sketch of Quantum Mechanics. One could cover right away all the needed topics systematically. The reader may then face neural overload (as I experience myself when being confronted with such texts). Another approach, which we try here, is to introduce every element only when and as needed, and to develop even simple and basic ideas only when required. That may ease the mental overload, but it may then take longer for the reader to form a global mental picture of what is going on. If this is your experience, try Hall's textbook [40] for help.

Another point must be stressed. We do our best to present the basics of Quantum Mechanics in a non-pedantic manner, but still in mathematical language (at the expense, of course, of not always giving complete arguments). It is far from obvious that the principles we will explain have any relevance to the physical world. Yet it is their real justification, and one can only marvel at the depth of insight of the great minds who discovered them. To explain this relevance, one must lay out examples of concrete situations, where the predictions of the model can be compared with lab experiments. Needless to say, this author is not the best qualified to do this, but many such examples are covered in a very progressive manner in Cohen-Tannoudji, Diu, and Laloë's book [11].

More basic facts about Quantum Mechanics are covered at the beginning of Chapter 11 and require only the material of the present chapter as a prerequisite.

[1] The appendices are more often fully mathematical.

2.1 Basic Setting

We must first stress that one does not "prove" the basic concepts of Quantum Mechanics, or of any physical theory. One builds models, and *the ultimate test of the validity of such models is whether they predict correctly the results of experiments.* Still, one strives for mathematical consistency and elegance.[2]

The purpose of Mechanics is to describe the state of mechanical systems and to determine their time-evolution. Consider, for example, one of the simplest mechanical systems: a massive dimensionless point. Its state at a given time is described by its position and velocity. That this, indeed, is the correct way to specify even such a simple system is by itself a deep fact: it is the position and the velocity (and not, say, the acceleration) at a given time that determine the future motion of the point. This fact is delicate enough that apparently it is not understood by the general public, which seems to still believe that an astronaut stepping out of the International Space Station (ISS) will start falling toward Earth.[3]

As we pointed out, it is not easy to relate the principles of Quantum Mechanics to actual physical experiments. On the positive side, this means that there is no real loss in starting to learn them even with little knowledge of Classical Mechanics. A very brief introduction to Classical Mechanics will be given in Sections 6.4 and 6.5.

> **Principle 1** [4] *The state of a physical system is described by a unit vector in a complex*[5] *Hilbert space* $\mathcal{H}$.

This Hilbert space is called the *state space*, and the unit vector is called the *state vector*. The state space will always be either finite-dimensional or separable (i.e. admitting a countable orthonormal basis). As in the case of the lowly classical massive point, the correct description of the state of a system encompasses a huge amount of wisdom. The fact that it is done by a vector in Hilbert space allows some of the most surprising features of Quantum Mechanics. *It makes physical sense to consider linear combinations of different states.*[6] The principles of Quantum Mechanics, and this one in particular, really do not appeal to our everyday intuition. There seems to be no remedy to this situation.

This is a good place to start explaining Dirac's notation, which is nearly ubiquitous in physics textbooks. Dirac's notation (also called bra–ket notation) is not really appropriate for writing mathematical arguments, so our use of it will be somewhat limited. Nonetheless, it must be learned in order to read physics literature. In this notation, vectors (i.e. elements of $\mathcal{H}$) are denoted by $|\alpha\rangle, |\beta\rangle$, and so on. These are called "ket vectors". Let us stress that

[2] This is a critical philosophical difference between mathematicians and physicists: mathematicians have logical systems that they can use to have confidence in systems, and, conversely, experience has made them cautious about vagueness and lack of logical rigor. Physicists, who can never "prove" that something is physically true, look to experimental results (and, occasionally, beauty) to provide confidence in their assumptions or to tell them to go back to the drawing board.

[3] Of course, the ISS too is falling toward Earth, since otherwise, its motion would be in a straight line. What is meant here is that the astronaut falls at a *faster rate*.

[4] Particularly important principles are outlined for the reader's convenience but there is no claim that these form a complete or independent set of axioms. I may use at times the word "axiom" rather than principle.

[5] All Hilbert spaces considered in this work are complex Hilbert spaces. According to the quote of Richard Feynman that opens this book, he apparently considered complex numbers as a part of physics rather than a part of mathematics. That complex numbers play such a major part in our models of the world is a rather awesome fact.

[6] This allows, in particular, for interferences.

in this notation, α is *not* an element of $\mathcal{H}$; it is a *label*. It is the whole symbol $|\alpha\rangle$ that is an element of $\mathcal{H}$. For example, we may very well denote by $\{|i\rangle; 1 \leq i \leq n\}$ a basis of $\mathcal{H}$, where n is the dimension of $\mathcal{H}$. The notation $|i\rangle$ for what a mathematician would write, say, e_i, looks strange at first until one realizes that the real information is carried by the index i, and that the letter e is just a support for this index and is no longer needed in the Dirac notation, where the support for the index is now the symbol $|\cdot\rangle$.

On the other hand, any element x of $\mathcal{H}$ induces a linear functional $y \mapsto (x, y)$ on $\mathcal{H}$. When $x = |\alpha\rangle$, this linear functional is denoted by $\langle\alpha|$ and is called a "bra vector". So $|\alpha\rangle$ is an element of $\mathcal{H}$, while $\langle\alpha|$ is a linear functional on $\mathcal{H}$. The value of the functional $\langle\alpha|$ on the vector $|\beta\rangle$ is denoted by $\langle\alpha|\beta\rangle$ (rather than $\langle\alpha||\beta\rangle$). This is simply the inner product of the vector $|\alpha\rangle$ and the vector $|\beta\rangle$. Thus, corresponding to (1.4) we have

$$\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*. \tag{2.1}$$

Let us observe in particular that $\langle\alpha|\alpha\rangle$ is the square of the norm of $|\alpha\rangle$.

An essential ingredient of any physical theory is the concept of an *observable*, that is, a quantity that can, at least in principle, be measured by an apparatus in an experiment, and the goal of the theory is to predict this measured value. The concept of observable is particularly important in Quantum Mechanics. In this theory, many quantities are *not* observable, and this leads to all kinds of nonsense if forgotten. In the basic example, the position of the point should be such an observable.

To explain more about the principles of Quantum Mechanics, in the first stage, we assume that the state space is *finite-dimensional*.[7]

> **Principle 2** *To each observable $\mathcal{O}$, there corresponds a Hermitian operator A on the state space $\mathcal{H}$.*

The statement is not very precise yet, as it does not say how we use the operator A to measure the observable, but we will come to that soon.

A fundamental fact about operators is that they may not commute. In general, $AB \neq BA$, and this lack of commutativity has immeasurable consequences. As a measure of the "lack of commutativity," we define the *commutator*

$$[A, B] := AB - BA, \tag{2.2}$$

of two operators, which will be of constant use. It should be stressed that operators are a complicated business. To a large extent, this explains the intricacies of Quantum Mechanics.

In the case of $\mathcal{H} = \mathbb{C}^2$, the simplest situation of interest,[8] the space of Hermitian operators is a four-dimensional real vector space. A natural basis consists of the following four matrices:

$$\sigma_0 = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \; ; \; \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \; ; \; \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \; ; \; \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.3}$$

[7] When that is not the case, we have to find the proper generalization of the notion of Hermitian operator, which we will explain later.

[8] Nature has made considerable use of this case, although this cannot be explained yet. In words you might have heard, $\mathbb{C}^2$ is the appropriate state space to describe the spin of particles of spin 1/2.

The matrices σ_1, σ_2 and σ_3 are called the *Pauli matrices* and are of fundamental importance. The reader may try to compute the commutators of these matrices to become convinced that lack of commutativity is already in full force. One should also observe that σ_3 is diagonal, so it is a bit simpler than σ_1 and σ_2. As will become gradually clear, the reason for this choice is that in our laboratories, the vertical direction is privileged.

In Dirac's notation the action of the operator A on the vector $|\alpha\rangle$ is denoted by $A|\alpha\rangle$. In mathematical notation the action of the operator A on the vector $x \in \mathcal{H}$ is denoted by $A(x)$ or sometimes Ax. Physicists like to write Ax, and my own training is to write $A(x)$. This schizophrenic pressure prevents me from being consistent.

Since A is Hermitian, it has an orthonormal basis of eigenvectors, which we denote by $|i\rangle$, so that $A|i\rangle = \lambda_i|i\rangle$ for some real numbers λ_i (which may or may not be different as i varies). Here i ranges from 1 to the dimension n of $\mathcal{H}$. Since $\{|i\rangle; i \leq n\}$ is an orthonormal basis, we have

$$|\alpha\rangle = \sum_{i \leq n} \langle i|\alpha\rangle |i\rangle, \tag{2.4}$$

because $\langle i|\alpha\rangle$ equals the inner product of the vectors $|i\rangle$ and $|\alpha\rangle$. In mathematical notation one would write $x = \sum_{i \leq n} (e_i, x) e_i$. It is pleasant to rewrite (2.4) as

$$|\alpha\rangle = \sum_{i \leq n} |i\rangle\langle i|\alpha\rangle,$$

or even

$$\mathsf{1} = \sum_{i \leq n} |i\rangle\langle i|, \tag{2.5}$$

where $\mathsf{1}$ is the identity operator.[9] Physicists call such a relation a *resolution of the identity* or a *completeness relation*, because the system of vectors $\{|i\rangle; i \leq n\}$ is complete enough to reconstitute the whole space.

Exercise 2.1.1 If $|\alpha\rangle$ is a unit vector, describe the operator $|\alpha\rangle\langle\alpha|$.

The next two principles relate the operator associated to an observable with the actual measurements of this observable.

> **Principle 3** *When measuring (by an experiment) the value of the observable $\mathcal{O}$ for a system in state $|\alpha\rangle$, the value obtained is always one of the eigenvalues λ_i of the Hermitian operator A associated to $\mathcal{O}$.*

At this stage we can only give trivial examples of physical systems, but let us try to consider a system consisting of one single point, which can be at any of n different locations $(\lambda_i)_{i \leq n}$ on the real line. (In the next few pages, this example will be referred to as the *basic example.*) In this basic example, the position of the point should be such an observable. According to Principle 3, it seems sensible that the state space is just $\mathbb{C}^n$, and that the

[9] This relation holds because by (2.4) it holds whenever applied to a vector $|a\rangle$.

operator corresponding to the position of the point on the real line is such that for $x = (x_i)_{i\leq n} \in \mathbb{C}^n$, one has $A(x) = (\lambda_i x_i)_{i\leq n}$ (where $(\lambda_i)_{i\leq n}$ are the n possible positions of the point on the real line).[10] Equivalently, each vector $e_i = |i\rangle$ of the canonical basis is an eigenvector of eigenvalue λ_i, $A(e_i) = \lambda_i e_i$ or, in Dirac's notation, $A|i\rangle = \lambda_i |i\rangle$.

The amazing thing (amazing at least compared to our macroscopic experience) is that repeating the experiment on identically prepared systems usually gives *different values*, however carefully these systems have been prepared.

Principle 4 *If the system is in state* $|\alpha\rangle$ *(so that* $\langle\alpha|\alpha\rangle = 1$*), then the* probability *of measuring the value* λ_i *for the observable* $\mathcal{O}$ *is*

$$\sum_{j;\lambda_j=\lambda_i} |\langle\alpha|j\rangle|^2. \tag{2.6}$$

Here, *probability* means that if you repeat the experiment many times on identically prepared systems, the frequency of measuring the value λ_i is about the value of the right-hand side (with an accuracy that increases with the number of experiments).

Let us examine Principle 4 in the case of the basic example. If the system is in state $|\alpha\rangle = x = (x_i)_{i\leq n} \in \mathbb{C}^n$ (with $\sum_{j\leq n} |x_j|^2 = 1$), then $x_i = (e_i, x) = \langle i|\alpha\rangle$, so that $|x_i|^2$ is the probability of measuring the system at position λ_i.

As explained, the state of a physical system is described by a unit vector of $\mathcal{H}$, and conversely, every unit vector of $\mathcal{H}$ describes a state of the system.[11] Very often we will consider non-zero vectors that need not be unit vectors. It is very convenient, as we will do without further warning, *to consider that such a vector* x *describes the same state of the system as the unit vector* $x/\|x\|$. With this convention, when the state $|\alpha\rangle$ is not normalized, the expression (2.6) has to be divided by $\langle\alpha|\alpha\rangle$. Please note at this stage that even when we use this convention, the state $|\alpha\rangle$ of a system is a *non-zero vector*.

The statement "the state of a system is described by a unit vector in a complex Hilbert space $\mathcal{H}$" has to be qualified in a precise way. In Classical Mechanics, if you know the state of the system, you can, in principle, know its exact state at any future time and predict the outcome of any future measurement. Quantum Mechanics allows no such prediction. It does not predict with certainty the outcome of a given experiment. What it does is to make *statistical predictions* about the results of many identical experiments. The technically correct way to express this is to say that "an ensemble of identical systems is described by a unit vector in a Hilbert space".[12] For simplicity we will keep saying that "a system is described by a given state vector", but this *does not* mean, even for simple systems consisting of one single particle, that from this state vector one could (even in principle) determine quantities such as the position or the momentum of the particle. What Quantum Mechanics does is to predict (statistically) the results you will get when you *measure* this position or this momentum. In fact in Quantum Mechanics it *does not make sense* to talk about the position of the particle or its momentum except at a time when you measure it. It is a misconception

[10] For what else could A depend on?

[11] The correspondence is not one-to-one, however. If a is a complex number of modulus 1, x and ax describe the same state.

[12] One may try to think of a state as specifying a preparation process. Repeating the same experiment on similarly prepared systems yields results that are only statistically predictable.

to think that in Quantum Mechanics, systems are in a kind of "undetermined state". The state vector should be thought of (at least according to the standard interpretation) as a *complete description of everything that can possibly be known* about the system. (It of course touches philosophical issues to decide whether this state vector is "a complete description of reality".) It is *the result of measurements on the system* that are not determined, not the state of the system itself.

Going back to Principle 4, we are guaranteed to get the value λ_i out of our measurement only in the very special case where $|\langle\alpha|j\rangle| = 0$ for $\lambda_j \neq \lambda_i$, that is, when $|\alpha\rangle$ is an eigenvector of eigenvalue λ_i. In the case of the basic example this means that only one of the components x_i of x is not zero.

Let us examine what happens if we proceed twice in succession to the measurement of $\mathcal{O}$ on the same system. We consider here the idealized situation where the second measurement takes place "immediately after" the first measurement. (What this means at the experimental level will be discussed a few pages later.) Then both measurements must yield the same result.[13] Thus, at the time of the second measurement, the system must be such that any measurement of $\mathcal{O}$ yields a given value (the value obtained in the first measurement) so that the state of the system must be an eigenvector of A. Consequently, if before the first measurement the state of the system was not an eigenvector of A, this first measurement has *changed* the state of the system. In the case of the basic example, this means that measuring position changes the state x of the system as soon as at least two components of x are not zero. *Measurements typically cannot be performed without changing the state of the system.*

In order to form a clearer picture of the situation, let us anticipate Section 2.15. In the absence of measurements, the time-evolution of the state of a system is *entirely deterministic*. The measurement is not producing a temporary disturbance of the system. Rather, the measurement sends the system on a new course for ever after. Which new course exactly depends on the result of the measurement, a result that can be predicted only statistically.

Much ink (and ingenuity) has been expended debating the fact that randomness appears to be intrinsic to Nature at the most fundamental level. As a probabilist, living a full century after this discovery, I must confess that I do not find it more startling than the older discovery that Earth is orbiting the Sun and not the other way around, so I will say no more about this. Far more annoying is the fact that the change of state occurring in a measurement process (which is often called "the collapse of the wave function") is hard to describe within the setting of Quantum Mechanics. In the preceding formulation of the basic principles, we implicitly assumed that Quantum Mechanics applies only to the microscopic world, while the experimental apparatus, as well as the physicist performing the experiment are *outside* its domain of validity. But where, then, is the boundary of the domain of validity? It would be more satisfactory that Quantum Mechanics should itself be able to describe the measuring apparatus as well as the observer performing the experiment. This raises issues that are not fully resolved to this day. For a simple discussion of these issues, we refer to Isham's book [43], and for a more detailed (yet accessible) account to Weinberg's book [88]. In fact there remain a number of other conceptual difficulties within Quantum Mechanics

[13] At least that is the way things behave. Physics would be harder otherwise.

(see e.g. [20]). The legendary question by A. Einstein to N. Bohr offers a glimpse of this: Do you really believe that the moon is not there when nobody looks at it? (According to the standard interpretation of Quantum Mechanics, it makes no sense to assert that the moon is there when nobody looks at it.[14])

In Dirac's notation, $\langle\beta|A|\alpha\rangle$ denotes the inner product of the vectors $|\beta\rangle$ and $A|\alpha\rangle$. To compute this quantity one may use (2.4), but this computation gives us an opportunity to illustrate one of the strengths of Dirac's notation, the use of (2.5) to obtain the following:

$$\langle\beta|A|\alpha\rangle = \sum_{i,j\leq n} \langle\beta|i\rangle\langle i|A|j\rangle\langle j|\alpha\rangle = \sum_{i,j\leq n} \langle\beta|i\rangle\langle\alpha|j\rangle^*\langle i|A|j\rangle. \tag{2.7}$$

This type of manipulation using completeness relations is of constant use in physics.[15]

A consequence of Principle 4 and (2.6) is that for a system in state $|\alpha\rangle$, the expected value,[16] or average value, of the measurement of the observable $\mathcal{O}$ is

$$\sum_{i\leq n} |\langle\alpha|i\rangle|^2\lambda_i = \langle\alpha|A|\alpha\rangle, \tag{2.8}$$

where the equality is obtained using (2.7) together with the fact that $\langle i|A|j\rangle = \langle i|j\rangle\lambda_j = \lambda_i$ if $i = j$ and zero otherwise. To lighten our terminology, we will use expressions such as "average value of the observable" or even "average of the observable" as shorthand for "average value of the measurement of the observable". Similarly we will say "expected value of the observable" for "expected value of the measurement of the observable". Let us note that the expected value $\langle\alpha|A|\alpha\rangle$ of the observable $\mathcal{O}$ does not determine the probability law of Principle 4.

We obviously get the same result in (2.8) if we replace $|\alpha\rangle$ by $a|\alpha\rangle$ where the complex number a is of modulus 1, $|a| = 1$. Thus as far as predicting the result of the measurement of $\mathcal{O}$ (which is the purpose of the model) is concerned, all these vectors represent the same state, and one should say that the state of the system is actually represented by a *unitary ray*, the set of vectors $a|\alpha\rangle$ for $|a| = 1$ and a certain unit vector $|\alpha\rangle$. (The name *unitary ray* is traditional, even though this set is a circle!)

2.2 Measuring Two Different Observables on the Same System

Suppose now that we consider a second observable $\mathcal{O}'$ with a corresponding Hermitian operator B. Then if a system in state $|\alpha\rangle$ is such that it will always yield the same value

[14] One should say that the problem here is formulated in a rather outrageous way to make the point clear. The universe seems to have done fine prior to our existing! The problem is nonetheless real. On the one hand, one may argue that Quantum Mechanics applies only to the microscopic world. Then a measurement process will be anything that interacts with a macroscopic object such as a photosensitive chemical in a photographic emulsion and has nothing to do with a conscious observer. On the other hand, if one refuses this arbitrary and ill-defined boundary between macroscopic and microscopic worlds, the quantum realm extends all the way to the consciousness of the observer. It is then very difficult to escape the conclusion that this consciousness plays a role, and matters become very murky. The theory of *decoherence* tries to address these issues.

[15] Including cases where the mathematical justification is not ironclad.

[16] The measured value of the observable O in state $|\alpha\rangle$ is a random variable, and as such has an expected value. When we repeat the experiment many times and average the corresponding measurements, the quantity we obtain is near this expected value. This is why both names are used.

when $\mathcal{O}$ is measured, and also when $\mathcal{O}'$ is measured, then $|\alpha\rangle$ must be an eigenvector of both A and B. Then $[A, B]|\alpha\rangle = 0$. When no such $|\alpha\rangle$ exists,[17] there does not exist a state for which both $\mathcal{O}$ and $\mathcal{O}'$ can be measured with certainty. It is simply *impossible* to ever know at the same time the values of both $\mathcal{O}$ and $\mathcal{O}'$ for any state of the system. It is fallacious to think that to know them both one just has to measure $\mathcal{O}$ and then $\mathcal{O}'$. After the measurement of $\mathcal{O}'$ has taken place you no longer know the value of $\mathcal{O}$. If you measure $\mathcal{O}$, then measure $\mathcal{O}'$, and "immediately after" measure $\mathcal{O}$ again, the result of this second measurement of $\mathcal{O}$ *will* sometimes be different from the result of the first measurement. This is because, as we explained earlier, the measurement of $\mathcal{O}'$ *has changed* the state of the system. Right after the measurement of $\mathcal{O}'$, the state of the system is an eigenvector of B, and by hypothesis, this eigenvector of B is *not* an eigenvector of A, so that in this state of the system, the result of the measurement of A cannot be predicted with certainty.

To prove at the experimental level that the difference between the first and the second measurements of $\mathcal{O}$ is really due to the measurement of $\mathcal{O}'$, but not to the evolution of the system, one cannot of course perform the measurements of $\mathcal{O}$, $\mathcal{O}'$, and then $\mathcal{O}$ again "immediately after each other". One simply arranges that the time between the measurements is very short compared with the timescale at which the system evolves. This is most easily done when the spontaneous evolution of the system is very slow, as in the case of the spin of an electron in Earth's very weak magnetic field. The actual spectacular physical experiment, where $\mathcal{O}$ and $\mathcal{O}'$ are, for example, the x and y components of the spin of an electron, is described in many introductory textbooks. (Generally speaking, the predictions of Quantum Mechanics are extremely well confirmed by experiments.)

> **Exercise 2.2.1** Consider two observables $\mathcal{O}$ and $\mathcal{O}'$ and the corresponding Hermitian operators A and A'. Assume for simplicity that all the eigenvalues of A are distinct, and all the eigenvalues of A' are distinct. Prove that if A and A' commute, the probability to measure a certain value λ of $\mathcal{O}$ for a system in a given state $|\alpha\rangle$ remains the same if we measure $\mathcal{O}'$ before we measure $\mathcal{O}$. Prove that if A and A' do not commute, there are certain states $|\alpha\rangle$ for which this is not true. Hint: A and A' commute if and only if they have a common basis of eigenvectors.

2.3 Uncertainty

Heisenberg's uncertainty principle, which we will study in the present section, is related to but different from the phenomenon of the previous section. If the system is in state x with $(x, [A, B]x) \neq 0$, one cannot measure both observables $\mathcal{O}$ and $\mathcal{O}'$ with arbitrary accuracy. We are not talking here of successive measurements on the same experiment, where the first measurement changes the state of the system. We are talking of measurements on different experiments. One repeats the experiment many times, each time measuring *either* $\mathcal{O}$ *or* $\mathcal{O}'$. If the results of measuring $\mathcal{O}$ are concentrated in a small interval, then the results of measuring $\mathcal{O}'$ must spread out. In the important special case where $[A, B]$ is a multiple of the

[17] Recall here that since $|a\rangle$ is the state of the system, it must be non-zero. An important particular case is when $[A, B]$ is a multiple of the identity.

identity, whatever the state of the system, you can *never* measure both $\mathcal{O}$ and $\mathcal{O}'$ with arbitrary accuracy. A quantitative version of this statement is given in Proposition 2.3.2.

Definition 2.3.1 Consider an observable $\mathcal{O}$ with associated Hermitian operator A. The *uncertainty* $\Delta_x A \geq 0$ of $\mathcal{O}$ in the state $x \in \mathcal{H}$ is given by

$$(\Delta_x A)^2 := (x, A^2 x) - (x, Ax)^2. \tag{2.9}$$

For instance, in the case of the basic example, the uncertainty of the position in state x is $\sqrt{\sum_{i\leq n} \lambda_i^2 |x_i|^2 - (\sum_{i\leq n} \lambda_i |x_i|^2)^2}$. To make sense of (2.9), one may observe that $(\Delta_x A)^2$ is just the variance of the probability distribution of Principle 4, or in other words, $\Delta_x A$ is the standard deviation of this probability distribution. The physical content of this definition should be stressed. When you make a measurement of the observable $\mathcal{O}$ for a system in state x, you get a *random* result, and $\Delta_x A$ is the standard deviation of this random result.[18]

To explain (2.9) in more mathematical terms, this quantity measures "the square-deviation of $\mathcal{O}$ from its average in state x". Indeed, denoting by $\mathsf{1}$ the identity operator of $\mathcal{H}$ (and since x is of norm 1),

$$(\Delta_x A)^2 = (x, A'^2 x), \tag{2.10}$$

where the Hermitian operator $A' := A - (x, Ax)\mathsf{1}$ is "the deviation of $\mathcal{O}$ from its average in state x". When x is an eigenvector of A, obviously $(\Delta_x A)^2 = 0$. Conversely, when $(\Delta_x A)^2 = 0$, since

$$(x, A'^2 x) = (A'x, A'x) = \|A'x\|^2,$$

then $A'x = 0$ so that x is an eigenvector of A. Therefore, $(\Delta_x A)^2 = 0$ if and only if x is an eigenvector of A, i.e. if and only if the measurement of $\mathcal{O}$ in state x offers no uncertainty, in accord with our calling $\Delta_x A$ the "uncertainty of $\mathcal{O}$ in state x".

Observe finally that $(x, A'x) = 0$, so that (2.10) means

$$(\Delta_x A)^2 = (\Delta_x A')^2. \tag{2.11}$$

Proposition 2.3.2 ([71]) *For two Hermitian operators A and B,*

$$\Delta_x A \Delta_x B \geq \frac{1}{2} |(x, [A, B]x)|. \tag{2.12}$$

When the right-hand side is not zero, this gives a quantitative lower bound on the product of the uncertainty of measuring $\mathcal{O}$ and $\mathcal{O}'$ in state x, a quantitative version of Heisenberg's uncertainty principle. We will soon meet fundamental operators for which $[A, B]$ is a non-zero multiple of the identity and the right-hand side is never zero.

Proof Defining B' in the obvious manner, using (2.11), and observing that $[A, B] = [A', B']$ because $\mathsf{1}$ commutes with everything, we see that it suffices to prove (2.12) for A' and B' or, equivalently, in the case where $(x, Ax) = (x, Bx) = 0$. In that case,

[18] Standard deviation is a statistical measure of how "spread out" a random variable is. Intuitively this means here that the outcomes of different experiments are likely to differ by values of order $\Delta_x A$.

$(\Delta_x A)^2 = (x, A^2 x)$, and similarly for B. The key fact is that, using symmetry (and denoting by $\mathrm{Im}\, z$ the imaginary part of the complex number z),

$$\begin{aligned}(x, [A, B]x) &= (x, ABx) - (x, BAx) = (Ax, Bx) - (Bx, Ax) \\ &= (Ax, Bx) - (Ax, Bx)^* = 2\mathrm{i}\mathrm{Im}\,(Ax, Bx). \end{aligned} \tag{2.13}$$

Therefore, using the Cauchy-Schwarz inequality,

$$|(x, [A, B]x)| \leq 2|(Ax, Bx)| \leq 2\|Ax\|\|Bx\|. \tag{2.14}$$

Now, since $\|Ax\|^2 = (Ax, Ax) = (x, A^2 x) = (\Delta_x A)^2$ and similarly for B, (2.14) proves (2.12). □

2.4 Finite versus Continuous Models

Mathematicians are trained to think of physical space as $\mathbb{R}^3$. But our continuous model of physical space as $\mathbb{R}^3$ is of course an idealization, both at the scale of the very large and at the scale of the very small. This idealization has proved to be very powerful, but in the case of Quantum Field Theory, it creates multiple problems, and in particular the infamous infinities (in the form of diverging integrals).

Can we dispense with continuous models and their analytical problems? A physical measurement is made through a device with finite accuracy, and this measurement is no different from the same measurement rounded to the last significant digit. The result of the measurement is also bounded,[19] so it may yield only finitely many possible values, and we might be able to study physics using only finite-dimensional Hilbert spaces (of huge dimension).

There is a fundamental reason why we stubbornly keep infinite models. Probably the most important guiding principle in finding good models is that a proper theory should be Lorentz invariant,[20] reflecting the fact that physics should be the same for all inertial observers[21] (who undergo no acceleration). There is no way this can be implemented in a finite model, say one which replaces the continuous model of physical space by a finite grid. Lorentz invariance can be recovered from a finite model only "in the infinite limit". Further, there is no canonical choice for such a finite model, so that one has to show that the results obtained by a finite approximation are indeed essentially independent of how this approximation is performed. Heuristically, this is plausible but it is quite another matter to really prove independence. In fact, it can be argued that settling this question is of the same order of difficulty as constructing a continuous model which in some sense would be the limit of the finite model as the grid becomes finer. In the case of Quantum Field Theory, this is a highly non-trivial task. Most importantly, considering finite models does not really solve anything. The infinities reappear in the guise of quantities that blow up as the grid becomes finer, and it is very hard to make sense of this behavior.

[19] For example, as of today, no object at distance from us greater than a few billion light-years has been observed. If you feel like arguing that this bound is not large enough, then try to argue that the bound of 10^{10000} light-years is not large enough.

[20] See Chapter 4.

[21] This fact is extremely well-established experimentally.

For these reasons we uncomfortably but realistically consider continuous models, even though they are not really well defined. Since nobody really knows how to solve the analytical difficulties related to these models, there is little point in working toward a partial solution to these difficulties, and our efforts in this direction will be minimal. It is embarrassing (in particular for this author) to write quantities that do not really make sense, but they would make sense if we replaced the continuous model by a suitable finite approximation.[22] The simple device of "putting the universe in a box" which we study later in Section 3.9 goes a long way in this direction.

2.5 Position State Space for a Particle

In this section we analyze how the previous machinery works to describe a very simple system, a massive point that can be located anywhere on the real line. This provides a first concrete example, and at the same time allows us to discuss the intricacies of considering infinite-dimensional state spaces. Almost nothing of what we explained in the finite-dimensional case will carry on exactly the same, but a suitable infinite-dimensional reinterpretation of the concepts will basically suffice.

The state space $\mathcal{H}$ is the space $L^2 = L^2(\mathbb{R}, \mathrm{d}x)$ of complex-valued square-integrable functions[23] on the real line.[24] An element of $\mathcal{H}$ is thus a complex-valued function[25] f on $\mathbb{R}$. The traditional terminology is to call this function the *wave function*. A wave function of norm 1 therefore describes the possible state of a massive point, which for simplicity we will call a *particle*.

The basic idea is that the position of a particle in state f is not really determined, but that the function $|f|^2$ represents the probability density to find this particle at a given location. This statement will eventually appear as the proper interpretation of (2.6) in the present "continuous case". To develop this idea, consider an interval I of $\mathbb{R}$, and the operator $\mathsf{1}_I$ defined by $\mathsf{1}_I(f)(x) = f(x)$ if $x \in I$ and $\mathsf{1}_I(f)(x) = 0$ if $x \notin I$. This operator is bounded since $\|\mathsf{1}_I(f)\| \leq \|f\|$. After we develop the right generalization of Hermitian operators in infinite dimensions, it will become apparent that this operator corresponds to an observable, and the average value of this observable on the state f is

$$(f, \mathsf{1}_I(f)) = \int_I \mathrm{d}x |f(x)|^2,$$

which is the probability to find the particle in the set I. It is worth repeating the fundamental fact: When you actually measure whether the particle is in I or not, you get a yes/no answer. But you are certain to find the particle in I only if its state vector f is an eigenvector of $\mathsf{1}_I$

[22] As far as we know, there is no other way to give a precise meaning to these quantities. Physicists seriously trying to explain why what they do makes sense use exactly this procedure, see e.g. Duncan's book [24].

[23] In L^2, functions which differ on a set of measure zero are identified, but this is never an issue here.

[24] You may also wonder why we choose such a state space. It is quite natural in view of our "basic example" of a point taking n possible positions on the real line. The true answer that this is the fruitful model which will become only gradually apparent.

[25] For clarity we often denote functions in position state space by Latin letters and functions on momentum state space by Greek letters.

of eigenvalue 1, i.e. $f(x) = 0$ for $x \notin I$, and you are certain not to find it in I only when f is an eigenvector of 1_I of eigenvalue 0, i.e. $f(x) = 0$ for $x \in I$.[26]

In the present setting, the position of the particle is an observable so that it corresponds to a "Hermitian operator" X, which will be called the *position operator*. It is not difficult to guess what the operator X should be. If indeed $|f|^2$ represents the probability density that the particle is at a given location, its average position is given by

$$\int \mathrm{d}x\, x|f(x)|^2 = \int \mathrm{d}x f(x)^*(xf(x)). \tag{2.15}$$

This quantity should be $(f, X(f))$, so that X should be the operator which sends f to the function xf (where of course xf is the function $x \mapsto xf(x)$).

This operator X is not defined everywhere, because the function xf may not be square-integrable. It is defined only for the functions f such that $xf \in L^2$. Accordingly we need to introduce the concept of *unbounded operators*.

Definition 2.5.1 An unbounded operator A on a Hilbert space $\mathcal{H}$ is a linear map from a dense linear subspace $\mathcal{D}(A)$ into $\mathcal{H}$. The space $\mathcal{D}(A)$ on which A is defined is called the *domain* of A.

We will say "operator" rather than "unbounded operator", and when the operator is bounded, i.e. $\|A(y)\| \leq C\|y\|$ for some constant C and all $y \in \mathcal{H}$ we will say "bounded operator".[27] The reason for this terminology is that most of the operators we shall use are unbounded. Not all unbounded operators are of interest. The important class, the so-called "self-adjoint operators", is the proper generalization of the Hermitian operators, and we start to introduce the necessary concepts to define it. These concepts are important in the rigorous study of Quantum Mechanics, but they will be rather marginal for us. If you find their study too demanding, you should jump right after Exercise 2.5.20.

Let us recall from Section 1.2 that in finite dimension the adjoint $A^\dagger$ of an operator A is given by (1.6), i.e. $(A^\dagger(y), x) = (y, A(x))$ for all $x, y \in \mathcal{H}$. We would like to use the same definition (1.6) in infinite dimensions. Certainly this formula can make sense only for $x \in \mathcal{D}(A)$. Looking at the left-hand side, we see that when this formula holds, we have

$$|(y, A(x))| = |(A^\dagger(y), x)| \leq \|A^\dagger(y)\|\|x\|,$$

so that $A^\dagger(y)$ may exist only when $y \in \mathcal{H}$ such that the linear map $x \mapsto (y, A(x))$, which is defined on $\mathcal{D}(A)$, is also bounded; $|(y, A(x))| \leq C\|x\|$ for a constant C independent of x.

These observations point the way to the proper definition of the adjoint of an unbounded operator. We define the subspace $\mathcal{D}(A^\dagger)$ as the set of $y \in \mathcal{H}$ for which there exists a constant C independent of x such that $|(y, A(x))| \leq C\|x\|$ for all $x \in \mathcal{D}(A)$. For such a y, by

[26] Generally speaking, it is not always obvious to understand the meaning of the observable corresponding to a given operator.

[27] The reader may of course wonder why an operator which is not defined everywhere is called an "unbounded operator". The reason is that it can be shown that an operator which is defined everywhere and is not extremely pathological is automatically bounded. It is obvious that the position operator cannot be bounded, because if $\|X(f)\| \leq C\|f\|$, then $(f, X(f)) \leq C$ for $\|f\| = 1$. This is absurd because $(f, X(f))$ is the average of the measured position of the particle, and there exist of course particles that are arbitrarily far away.

continuity, the map $x \mapsto (y, A(x))$ from $\mathcal{D}(A)$ to $\mathbb{C}$ extends to the whole of $\mathcal{H}$. Therefore, by the Riesz representation theorem,[28] there exists an element $A^\dagger(y)$ of $\mathcal{H}$ such that

$$\forall x \in \mathcal{D}(A)\ ,\ (A^\dagger(y), x) = (y, A(x)), \tag{2.16}$$

and $A^\dagger(y)$ is uniquely determined by this condition since $\mathcal{D}(A)$ is dense.

Definition 2.5.2 When $\mathcal{D}(A^\dagger)$ is dense, the operator $A^\dagger$ with domain $\mathcal{D}(A^\dagger)$ defined by (2.16) is called the *adjoint* of A.

Observe that when A is a bounded operator we have $\mathcal{D}(A^\dagger) = \mathcal{H}$.

Definition 2.5.3 An operator A is called *symmetric* if

$$\forall x, y \in \mathcal{D}(A)\ ,\ (A(y), x) = (y, A(x)). \tag{2.17}$$

Exercise 2.5.4 Consider the space $\mathcal{D}$ of continuously differentiable functions f on $[0, 1]$. Consider the operator A on $L^2([0, 1])$ with domain $\mathcal{D}$ defined by $A(f) = \mathrm{i} f'$. Is A symmetric? What happens if one considers instead the domain $\mathcal{D}_\alpha = \{f \in \mathcal{D};\ f(1) = \alpha f(0)\}$, where α is a complex number of modulus 1?

The following should be obvious.

Lemma 2.5.5 *If A is symmetric, then $\mathcal{D}(A) \subset \mathcal{D}(A^\dagger)$*[29] *and $A^\dagger(y) = A(y)$ for $y \in \mathcal{D}(A)$.*

Definition 2.5.6 An operator is called *self-adjoint* if it is symmetric and if $\mathcal{D}(A^\dagger) = \mathcal{D}(A)$.

If we remember that in finite dimensions an operator A is Hermitian if and only if $A = A^\dagger$, we see that the previous definition exactly generalizes this definition to the infinite-dimensional case: A is self-adjoint if it is equal to its adjoint, i.e. $A^\dagger$ has the same domain as A and coincides with A on this domain. The fundamental importance of self-adjoint operators in Quantum Mechanics is that they correspond to observables. In infinite dimensions physicists often call an operator Hermitian when in fact they mean self-adjoint (so, you will hardly ever see the word "self-adjoint" in physics textbooks).

One may stress the point of Definition 2.5.6 as follows. If we *decrease* $\mathcal{D}(A)$ we *increase* $\mathcal{D}(A^\dagger)$. That is if $\mathcal{D}' \subset \mathcal{D}(A)$ and we denote by B the operator with domain $\mathcal{D}'$, given by $B(x) = A(x)$ for $x \in \mathcal{D}'$, then the domain of $B^\dagger$ contains the domain of $A^\dagger$. This should be obvious from the definitions. Thus in a sense a self-adjoint operator is a symmetric operator such that its domain *is as large as possible*.

Exercise 2.5.7 Prove that if the operator A is symmetric and if $A^\dagger$ is symmetric, then $A^\dagger$ is self-adjoint.

[28] The Riesz representation theorem states that given a bounded linear functional φ on $\mathcal{H}$, that is $|\varphi(x)| \leq C\|x\|$ for all x, there exists $y \in \mathcal{H}$ such that $\varphi(x) = (y, x)$.

[29] In particular, $\mathcal{D}(A^\dagger)$ is dense and the adjoint is well defined.

The following exercise is of fundamental importance to get a feeling for self-adjoint operators.

Exercise 2.5.8 Consider the Hilbert space $\mathcal{H}$ of sequences $x = (x_n)_{n\geq 0}$ with norm $\|x\|^2 = \sum_{n\geq 0} |x_n|^2$. Consider a sequence $(\lambda_n)_{n\geq 0}$ of complex numbers.
(a) Prove that the formula

$$A((x_n)_{n\geq 0}) = (\lambda_n x_n)_{n\geq 0}$$

defines an operator on the domain

$$\mathcal{D}(A) = \Big\{ x = (x_n)_{n\geq 0} \in \mathcal{H} \; ; \; \sum_{n\geq 0} |\lambda_n x_n|^2 < \infty \Big\}.$$

(b) Prove that A is symmetric if and only if $\lambda_n \in \mathbb{R}$ for each $n \geq 0$.
(c) Prove that the adjoint of $A^\dagger$ of A has the domain $\mathcal{D}(A^\dagger) = \mathcal{D}(A)$ and is given by the formula

$$A^\dagger((x_n)_{n\geq 0}) = (\lambda_n^* x_n)_{n\geq 0}.$$

(d) Prove that A is self-adjoint when $\lambda_n \in \mathbb{R}$ for each n.

Exercise 2.5.9 Consider a sequence $(\mathcal{H}_n)_{n\geq 0}$ of Hilbert spaces and their direct sum $\bigoplus_{n\geq 0} \mathcal{H}_n$. Thus an element $x \in \bigoplus_{n\geq 0} \mathcal{H}_n$ is a sequence $(x_n)_{n\geq 0}$ where $x_n \in \mathcal{H}_n$, with norm $\|x\|^2 := \sum_{n\geq 0} \|x_n\|^2$. Consider for each $n \geq 0$ a bounded operator A_n from $\mathcal{H}_n$ to $\mathcal{H}_{n+1}$ and the adjoint operator B_n from $\mathcal{H}_{n+1}$ to $\mathcal{H}_n$, that is the operator such that $(x, A_n(y)) = (B_n(x), y)$ for $x \in \mathcal{H}_{n+1}$ and $y \in \mathcal{H}_n$. Consider the following domain:

$$\mathcal{D}(A) = \Big\{ x = (x_n)_{n\geq 0} \; ; \; \sum_{n\geq 0} \|x_n\|^2 < \infty \; , \; \sum_{n\geq 0} \|A_n(x_n)\|^2 < \infty \Big\},$$

and define $\mathcal{D}(B)$ similarly. Then the operator A: $(x_n)_{n\geq 0} \mapsto (0, A_0(x_0), A_1(x_1), \ldots)$ is defined on the domain $\mathcal{D}(A)$. Define the operator B similarly and prove that A and B are adjoint of each other.

Exercise 2.5.10 Recall that $\mathsf{1}$ denotes the identity operator. Prove that a symmetric operator A is self-adjoint if $A + \mathrm{i}\mathsf{1}$ and $A - \mathrm{i}\mathsf{1}$ are onto.[30] Caution: This takes only four lines but is very tricky.

Exercise 2.5.11 If A is as in Exercise 2.5.8 and symmetric, prove that $A + \mathrm{i}\mathsf{1}$ and $A - \mathrm{i}\mathsf{1}$ are onto.

Exercise 2.5.12 Consider the space $\mathcal{D}$ of continuously differentiable functions on the unit circle and the operator on L^2 (of the unit circle) with domain $\mathcal{D}$ given for $f \in \mathcal{D}$ by $A(f) = \mathrm{i}f'$. Prove that A is symmetric. Prove that if f is in the domain of $A^\dagger$ one may find a continuous function g such that $f = g$ a.e. Hint: This is difficult if you do not use Fourier series.

[30] The converse is proved in Theorem J.1.

When we define an operator A by a concrete formula, in typical cases this formula shows that the operator is defined on a dense subspace $\mathcal{D}(A)$, but this subspace is often too small for A to be self-adjoint. When A is the restriction to $\mathcal{D}(A)$ of a self-adjoint operator defined on the larger domain, there is a simple "automatic procedure" to construct this larger domain, based on the following elementary fact.

Definition 2.5.13 The *graph* of the operator A is the set of pairs $(u, v) \in \mathcal{H} \times \mathcal{H}$ with $u \in \mathcal{D}(A)$ and $v = A(u)$.

Lemma 2.5.14 *If A is an unbounded operator on a Hilbert space $\mathcal{H}$, the graph of $A^\dagger$ is a closed subset of $\mathcal{H} \times \mathcal{H}$.*

Proof By definition of the adjoint we have $z \in \mathcal{D}(A^\dagger)$ and $y = A^\dagger(z)$ if and only if for each $x \in \mathcal{D}(A)$ it holds that $(y, x) = (z, A(x))$. Given x, the set of pairs $(z, y) \subset \mathcal{H} \times \mathcal{H}$ which satisfy this condition defines a closed subset of $\mathcal{H} \times \mathcal{H}$. Thus the graph of $A^\dagger$ is the intersection of a family of closed sets and therefore is closed. □

Thus, if A is self-adjoint, its graph is a closed subset of $\mathcal{H} \times \mathcal{H}$. This leads to the following definition:

Definition 2.5.15 An operator A is *essentially self-adjoint* if the closure in $\mathcal{H} \times \mathcal{H}$ of the graph of A is the graph of a self-adjoint operator.

Thus the "automatic procedure" to check if an operator A can be "made self-adjoint" by properly extending its domain of definition is to compute the closure of the graph of A and see if it is the graph of a self-adjoint operator. This method is much used in serious rigorous texts, but we choose here not to concentrate on "technicalities".

Exercise 2.5.16 Consider the subspace $\mathcal{L}_0$ of $L^2 = L^2([0, 1])$ consisting of functions of integral zero. Consider the map $T\colon L^2 \to L^2$ given by $T(f)(x) = \int_0^x \mathrm{d}t f(t)$. Prove that it is one-to-one. Let $\mathcal{D}_0 = T(\mathcal{L}_0)$. Prove that the operator $A = \mathrm{i}T^{-1}$ with domain $\mathcal{D}_0$ is symmetric, that its graph is closed but that it is not self-adjoint.

One rarely uses the actual details of the domain of a self-adjoint operator, and it usually suffices to know that a given operator is essentially self-adjoint. In some sense, self-adjoint operators have a simple structure (while operators which are simply symmetric may have all kinds of pathologies). The most spectacular way to reveal this structure is called the "spectral theory for self-adjoint operators". It is a generalization of the fact that in finite dimensions a Hermitian operator has an orthogonal basis of eigenvectors. This theory is of fundamental importance in Quantum Mechanics. As it is a favorite topic for authors attempting a rigorous presentation of the subject, many proofs are available, and those presented in the textbook of Brian Hall [40] are particularly detailed. The spectral theorem is arguably of less fundamental importance in Quantum Field Theory, for the simple reason that the central parts of Quantum Field Theory are too far from mathematical rigor to really take advantage of this result. While the spectral theory solves some of the difficulties in constructing a suitable continuous model, this is of limited help as other difficulties remain unsolved to this day.

For this reason, and in order to keep the present volume to a reasonable size, we will not enter spectral theory here, which is extensively covered in the treatise by Reed and Simon [68]. We limit ourselves to an intuitive understanding of some of the main conclusions of this theory. For this we return to the "multiplication by x" operator of (2.15), which is obviously self-adjoint since it is symmetric and both its domain and the domain of its adjoint consist of the functions f such that $xf \in L^2$.

Exercise 2.5.17 Prove this last statement concerning the domain of the adjoint. Hint: A function f belongs to this domain if the integral $\int \mathrm{d}x f(x)xg(x)$ exists whenever $g \in L^2$.

It is important to observe that this operator *does not* have any eigenvector (although a function with support near a given point x should be thought of as an approximate eigenvector with eigenvalue x).[31] A more general example of a self-adjoint operator is obtained by considering the "same" "multiplication by x" operator on the space $L^2 = L^2(\mathbb{R}, \mathrm{d}\mu, \mathbb{C})$ of functions which are square-integrable for a more general measure $\mathrm{d}\mu$ than Lebesgue's measure.[32] The measure $\mathrm{d}\mu$ is always assumed to give finite mass to bounded sets.

Exercise 2.5.18 Prove that the "multiplication by x" operator has an eigenvector with eigenvalue a if and only if the measure $\mathrm{d}\mu$ gives positive mass to the point a.

In the previous example the eigenvalues have "multiplicity 1". A more general example consists of the "multiplication by x" operator on the space $L^2(\mathbb{R}^2, \mathrm{d}\mu, \mathbb{C})$, where the coordinates of a point in $\mathbb{R}^2$ are denoted by (x, y). The good news is that the most general self-adjoint operator is just a tad more complicated than this operator.

Exercise 2.5.19 Prove that this operator has an eigenvector with eigenvalue a if and only if the measure $\mathrm{d}\mu$ gives positive mass to the set $\{a\} \times \mathbb{R}$. Prove that this eigenvalue has finite multiplicity n if and only if the restriction of μ to this set is supported by a set of cardinality n but not by a set of cardinality $n - 1$.

Thus in this example, the multiplicity of an eigenvalue can be finite or infinite. Spectral theory then asserts that a "generic" self-adjoint A operator is not more complicated than this, in a sense that we will develop in Section 2.6. When facing a statement on unbounded operators, one should first try to understand what it means for the "multiplication by x" operator.

It is very easy to write all kinds of nonsense if one ignores the fact that unbounded operators are *not* defined everywhere (but only on their domain $\mathcal{D}$). Many such examples are given in this book by Hall [40]. Interestingly enough, in a random sample of physics textbooks on the shelves of my university's library, it turned out that only a very small fraction even mentions potential problems on this matter. Rather, one pretends that every self-adjoint operator[33] is defined everywhere and diagonalizable. Of course, it is more

[31] Thus in general a self-adjoint operator does not have eigenvectors.
[32] Mathematicians love to call Lebesgue's measure the standard volume measure on $\mathbb{R}^n$.
[33] Words like "self-adjoint" themselves are rarely to be found in these books.

admissible in physics than in mathematics to forge ahead and ignore all kinds of potential problems until a looming disaster imposes more caution.

Exercise 2.5.20 Convince yourself that if $|\gamma\rangle = A|\beta\rangle$ then $\langle\gamma| = \langle\beta|A^\dagger$, where $\langle\beta|A^\dagger$ denotes the composition of the operator $A^\dagger$ from $\mathcal{H}$ to itself and the operator $\langle\beta|$ from $\mathcal{H}$ to $\mathbb{R}$.

It would have been an embarrassment not to state Definitions 2.5.1–2.5.6 in this book, but as we manage to mostly skirt spectral theory they will play a rather small part in the sequel.

Going back to our model for a particle on the line, the state space L^2 on which the position operator is represented by the "multiplication by x" operator X will be used many times. We will call it the "position state space" since "the position of the particle" is simply related to the element of L^2 (the wave function) which represents the state of the particle.

A second fundamental operator is the *momentum operator*[34] P defined by

$$P(f) = -\mathrm{i}\hbar\frac{\mathrm{d}f}{\mathrm{d}x}. \tag{2.18}$$

Its domain consists of the functions f which are differentiable almost everywhere and such that their differential belongs to L^2. It is not at all intuitive that such an operator measures the momentum of a particle, and it is best for us to take this fact for granted as one of those fundamental principles of Quantum Mechanics whose success is every day confirmed by experience.[35] The momentum operator will also appear very naturally when we study Stone's theorem in Section 2.14.

Exercise 2.5.21 Prove that the momentum operator commutes with the translation operators given by $T(f)(x) = f(x+a)$ when $a \in \mathbb{R}$ and explain the physical meaning of this relation.

The momentum operator does not have any eigenvectors. Such an eigenvector would be a function $f(x) = a\exp(\mathrm{i}px/\hbar)$ but such a function is not square-integrable for $a \neq 0$.

A fundamental property is that the position operator and the momentum operator do not commute, but rather satisfy the following so-called *canonical commutation relation*:

$$[X, P] = \mathrm{i}\hbar\mathbf{1}. \tag{2.19}$$

Generally speaking, the domain of the commutator of two unbounded operators might be very small.[36] In the present case, the commutator is defined on well-behaved functions, and in particular on Schwartz functions. Formula (2.19) is a consequence of the formula $(xf)' - xf' = f$.

[34] One may regret that the letter P has not been reserved for the position operator, but in physics it is irrevocably associated to momentum. The letter P comes from the Latin *pulsus*. The occurrence of a "momentum operator", rather than a "velocity operator" is less surprising if one knows that in Classical Mechanics momentum, the product of the mass of the particle and its velocity, is indeed more fundamental than velocity.

[35] At a very intrinsic level, (2.18) has to do with the wave-particle duality. As we shall see soon, particles are also waves. On page 40 we will give arguments making this formula less mysterious.

[36] It might happen that this domain consists only of the 0 vector, even when the domains of the two operators are dense.

It is a good time to mention that $\mathbf{1}$ will always in our notation denote the identity operator of the Hilbert space under study (unless $\mathcal{H} = \mathbb{C}^2$ in which case it will be denoted by I). Many textbooks make the more sweeping convention of simply omitting such an operator and write simply $[X, P] = \mathrm{i}\hbar$. Also, the desire to respect alphabetic order makes us often write (2.19) as $[P, X] = -\mathrm{i}\hbar\mathbf{1}$.

Exercise 2.5.22 Consider two operators A, B which are assumed to be defined everywhere and satisfy $[A, B] = \mathbf{1}$. Prove by induction on n that $[A, B^n] = nB^{n-1}$. Prove that A and B cannot both be bounded.[37] Hint: Arguing by contradiction, prove that $n\|B^{n-1}\| \leq 2\|A\|\|B\|\|B^{n-1}\|$.

The momentum operator looks very different from the position operator, but in some sense it is a very similar operator, but "in a very different position". This will be explained in Section 2.7.

2.6 Unitary Operators

We introduce now unitary operators between Hilbert spaces. It is a fundamental notion in at least two respects:

- Mathematically it provides (as explained in this section) a way to recognize whether two different models "are in fact the same".
- Physically, countless processes are represented by unitary operators. Why this is the case is explained at the beginning of Section 2.10.

Definition 2.6.1 A linear operator U between Hilbert spaces is called *unitary* if it is one-to-one, *onto*, and preserves the norm, $\|U(x)\| = \|x\|$.

Unitary transformations are in a sense the "natural class of isomorphisms between Hilbert spaces". The "polarization identity" $\|x + y\|^2 = \|x\|^2 + \|y\|^2 + 2\mathrm{Re}(x, y)$ shows that a unitary operator preserves the inner product,[38]

$$(U(x), U(y)) = (x, y). \tag{2.20}$$

It is almost obvious that the set $\mathcal{U}(\mathcal{H})$ of unitary operators on a Hilbert space $\mathcal{H}$ forms a group.

Next we reformulate the condition that an operator on a Hilbert space $\mathcal{H}$ is unitary using the notion of adjoint operator. As already noted, for a bounded operator A one has $\mathcal{D}(A) = \mathcal{D}(A^\dagger) = \mathcal{H}$ and

$$\forall x, y \in \mathcal{H}\ ;\ (A^\dagger(x), y) = (x, A(y)). \tag{2.21}$$

A unitary operator on a Hilbert space is bounded, so its adjoint is defined everywhere. Furthermore by (2.21) one has $(U^\dagger U(x), y) = (U(x), U(y))$ and (2.20) is equivalent to

[37] We recall that an operator A is *bounded* if for some constant C and all x we have $\|A(x)\| \leq C\|x\|$. The operator norm $\|A\|$ of A is then the smallest possible value of C.

[38] One has to be careful that an operator preserving the inner product is necessarily one-to-one, but need not be onto.

$U^\dagger U = \mathsf{1}$. Consequently, an operator on a complex Hilbert space is unitary if and only if it is invertible and

$$U^{-1} = U^\dagger. \tag{2.22}$$

Thus a unitary operator also satisfies $UU^\dagger = \mathsf{1}$.

The following trivial fact is stressed because of its considerable importance.

Lemma 2.6.2 *A unitary operator U from a Hilbert space $\mathcal{H}$ to a Hilbert space $\mathcal{H}'$ induces a map*

$$A \mapsto A' = UAU^{-1}$$

from the operators on $\mathcal{H}$ to the operators on $\mathcal{H}'$.

Of course here $\mathcal{D}(A') = U(\mathcal{D}(A))$. The philosophy is that "A' is a copy of A so it has the same properties as A". For example, if A is self-adjoint, so is A'.

If you use the Hilbert space $\mathcal{H}$, the vector x to model a state of a physical system and the operator A to represent an observable, while I use $\mathcal{H}'$, Ux and A' respectively, we will get the same predictions. Such models are called *unitarily equivalent*. This seems to be a trivial observation, but the point is that even if the models are unitarily equivalent, one might be easier to use than the other (because unitary transformations are far from being trivial). Using a basis of eigenvectors of A surely makes computations related to A simpler. Quite accurately, one may think of unitary transformations simply as changes of basis.

2.7 Momentum State Space for a Particle

To put the ideas of the previous section to use we go back to the model of a massive particle on the line which we studied in Section 2.5. Let us consider $\mathcal{H}' = L^2(\mathbb{R}, \mathrm{d}p/(2\pi\hbar))$, where the notation $\mathrm{d}p/(2\pi\hbar)$ means that we include the factor $1/(2\pi\hbar)$ whenever we integrate in p. Consider the Fourier transform $U\colon f \mapsto \hat{f}$ of (1.30) from $\mathcal{H}$ to $\mathcal{H}'$. It is a unitary operator since it preserves the scalar product by (1.32) and since it has an inverse, the inverse Fourier transform $\varphi \mapsto \check{\varphi}$. The state which was represented by $f \in \mathcal{H}$ is now represented by $\varphi = \hat{f} \in \mathcal{H}'$. As in Lemma 2.6.2 the Fourier transform U transports an operator A on $\mathcal{H}$ to the operator $A' = UAU^{-1}$ on $\mathcal{H}'$ given by $A'(\varphi) = \widehat{A(\check{\varphi})}$. Using (1.33) for $f = \check{\varphi}$ yields (provided φ is well behaved)

$$P'(\varphi)(p) = p\varphi(p) \tag{2.23}$$

and, similarly,

$$X'(\varphi) = \mathrm{i}\hbar\frac{\mathrm{d}\varphi}{\mathrm{d}p}. \tag{2.24}$$

(The plus sign here is not surprising since (2.19) implies that $[X', P'] = \mathrm{i}\hbar\mathsf{1}$.) It is now the momentum operator which looks simple and the position operator which looks complicated. Just as in position state space $|f|^2$ represented the probability density of the location of the particle in state f, we can now argue that $|\varphi|^2$ represents the probability density of the

momentum of the particle (when the basic measure is $\mathrm{d}p/2\pi\hbar$). For this reason we will call this space $\mathcal{H}'$ the *momentum state space*. Taking the Fourier transform is the standard way to analyze a wave. Thus it can be said that using momentum state space *amounts to thinking of a particle as wave*. This is the *wave-particle duality*.[39]

So, the probability density of the location of the particle is $|f|^2$, and the probability density of its momentum is $|\varphi|^2$, where φ is the Fourier transform of f. One shows in Fourier analysis that it never happens that both a function and its Fourier transform are sharply concentrated around a single value. This is closely related to Heisenberg's uncertainty principle, which here asserts according to (2.19) that it is impossible that both position and momentum have a sharply defined value. Momentum state space is of fundamental importance (much more so than position state space) because the kinetic energy of a particle depends simply on its momentum (and its mass). The fun however is that particles interact not only according to their momenta, but also according to their respective positions, and this largely contributes to make the universe quite complicated and interesting.

The self-adjoint momentum operator (2.18) on position state space does not look at all like an operator of "multiplication by a function". Yet, after Fourier transform, on momentum state space, this operator is just "multiplication by p". This is a particularly striking instance of the general fact mentioned on page 36: given a self-adjoint operator A on a Hilbert space $\mathcal{H}$ one may find a unitary map U (to a certain L^2 space) such that the operator UAU^{-1} is a "multiplication by a function" operator, refer to Hall's textbook [40, Theorem 10.9].

> **Exercise 2.7.1** Consider a self-adjoint operator which in momentum state space is given by "multiplication by a function $g(p)$". Prove that this operator commutes with the translations of Exercise 2.5.21.

It can be shown that Exercise 2.7.1 has a converse: operators commuting with the translations are of the from "multiplication by a function $g(p)$". Thus the momentum operator must be of this type. The formula (2.23) corresponds to the simplest case of interest of such an operator.

2.8 Dirac's Formalism

It is regrettable that neither the position nor the momentum operator has a basis of eigenvectors, for this would indeed be very convenient. Paul Dirac invented a remarkable formalism to deal with this problem. It is used in almost every physics textbook, where it is typically considered as self-evident. We try to explain some of the basic features and meaning of this formalism here, striving as usual to explain what this means, but with no serious attempt to make matters rigorous.[40]

[39] Not everybody uses the name "momentum state space".

[40] The so-called theory of "rigged Hilbert spaces" can be used to make matters rigorous, but we have chosen to stay on the heuristic level.

Dirac's formalism works beautifully. It allows a great economy of thought and notation. It is however unfriendly to mathematicians, and the mathematically inclined reader must brace for a kind of cold shower, as things are likely to look horrendously confusing at first. Let us stress that it is not necessary to master this formalism to follow most of the rest of this book. Still, we will use it at times, if only to formulate results in the same language as they are found in physics textbooks. The reader who finds the present section overwhelming is encouraged to move on and to come back when the need arises.

As a consequence of the use of Dirac's formalism, if one looks at a physics textbook discussing (say) particles on the real line, one may find it difficult to recognize any of the previous material. First, one is likely to find very early the sentence "let $|x\rangle$ denote the state of a particle located at x…". An element of the position state space $\mathcal{H} = L^2(\mathbb{R}, \mathrm{d}x)$ that could be said to be located at x would have to be an eigenvector of the position operator X with eigenvalue x and these do not exist. The expression $|x\rangle$ can however be given a meaning in a kind of "distributional sense". It makes sense only when integrated against a Schwartz function f, that is for such a function the integral $\int \mathrm{d}x |x\rangle f(x)$ makes sense as an element of $\mathcal{H}$. The value of this integral is simply the function f seen as an element of $\mathcal{H}$. Quite naturally, we denote by

$$|f\rangle \text{ the function } f \in \mathcal{S} \text{ seen as an element of } \mathcal{H}, \tag{2.25}$$

so that

$$|f\rangle = \int \mathrm{d}x \, |x\rangle f(x). \tag{2.26}$$

This should certainly remind us of a basis expansion $f = \sum_i (f, e_i) e_i = \sum_i e_i (f, e_i)$, and physicists think of $|x\rangle$ as a "continuous basis". In this manner we have given a meaning to the quantity $|x\rangle$ as "an element of $\mathcal{H}$ in the distributional sense". The principle at work here is important enough to be stated clearly:[41]

> *To make sense of a formula written in Dirac's formalism, try to integrate it against one or several Schwartz functions.* (2.27)

We will however not stop at considering Dirac formalism as just a way to encode complicated formulas in a simpler manner. Rather, we will try to free our imagination and to give a "mathematical" interpretation of the objects appearing in this formalism, at least at the level of intuition. Matters will get slippery, since to really make mathematical sense[42] of what we shall do would require heavy formalism which we want to avoid. Still, in this way we will develop a way to look at things which *in the long run* helps intuition.[43] Another point which must be stressed is that our manipulations of quantities involving Dirac's formalism, as e.g. in the rest of this section, never pretend to "prove" anything, and simply check on important instances that the formalism is self-consistent.

[41] Thus, you will know what to try first when meeting exercises asking you to make sense of formulas written in this formalism!

[42] However hard this may be for a mathematician, one has to accept that certain things make some kind of sense even if it is not mathematical.

[43] Please trust me on that assertion, even if you suffer now.

Let us then look at $|x\rangle$ again. If we recall (1.16), that is

$$f(y) = \int \mathrm{d}x f(x)\delta(x-y) = \int \mathrm{d}x f(x)\delta_x(y)$$

where $\delta_x(y) = \delta(x-y) = \delta(y-x)$, so that $f = \int \mathrm{d}x f(x)\delta_x$. Comparing with (2.26), we see that in position state space $|x\rangle$ "corresponds to the Dirac function δ_x",[44] even though $\mathcal{H}$ consists of square-integrable functions, which is not the case of "the function δ". This matches very well with the fact that an eigenvector of the position operator of eigenvalue x must take value zero at points different from x.

Let us next try to give a meaning to the quantity $\langle x|$. As a consequence of (2.26), given a test function g we should have

$$\langle g| = \int \mathrm{d}x g(x)^* \langle x|,$$

so that $\langle g|f\rangle = \int \mathrm{d}x g(x)^* \langle x|f\rangle$. Comparing with the formula

$$\langle g|f\rangle = \int \mathrm{d}x g(x)^* f(x) \tag{2.28}$$

we conclude that

$$\langle x|f\rangle = f(x). \tag{2.29}$$

This formula is not really defined for all $f \in L^2 = \mathcal{H}$, but it certainly makes sense for $f \in \mathcal{S}$. This formula also makes $\langle x|$ appear as a linear functional defined on a subspace of $\mathcal{H}$, and in particular on $\mathcal{S}$.[45] The formula (2.29) is also consistent with the interpretation that "$|x\rangle$ corresponds to the function δ_x".

Using (2.29) we reformulate (2.26) as follows: for $f \in \mathcal{S}$,

$$|f\rangle = \int \mathrm{d}x |x\rangle\langle x|f\rangle, \tag{2.30}$$

which looks much better than (2.26) (but means the same). It can be summarized in the formula

$$\int \mathrm{d}x |x\rangle\langle x| = \mathsf{1}, \tag{2.31}$$

which is a kind of continuous version of (2.5). Physicists call (2.31) a "completeness relation", meaning that there are enough elements in the continuous basis $|x\rangle$ to capture the whole space. They are well aware that $|x\rangle \notin \mathcal{H}$, but pretend nonetheless that this is the case and that $|x\rangle$ is an eigenvector of the position operator X with eigenvalue x. They maintain this position until disaster strikes, and then they call the attention of the reader to the fact that "the state $|x\rangle$ is unphysical" or sometimes, that it is "improper".

[44] You might have observed at this stage that one has sometimes to use somewhat ill-defined expressions such as this one. As far as possible they are always between quotes.

[45] Of course the function $f \mapsto f(x)$ is not continuous in the L^2 norm, i.e. there does not exist a number C such that $|f(x)| \leq C\|f\|_2$ for all $f \in \mathcal{S}$. This corresponds to the fact that the functional $\langle x|$ is not defined on all of L^2.

Now, how can we define $\langle y|x\rangle$ for two such "states" x, y? Applying the functional $\langle y|$ to both sides of (2.26), we should get

$$f(y) = \langle y|f\rangle = \int \mathrm{d}x \langle y|x\rangle f(x), \tag{2.32}$$

and since $f(y) = \int \mathrm{d}x f(x)\delta(x-y)$ from (1.16) we can summarize this by the formula

$$\langle y|x\rangle = \delta(x-y)\ (= \delta(y-x)). \tag{2.33}$$

It is important for the sequel that the first part of the next exercise be very clear to you.

Exercise 2.8.1 (a) Convince yourself that (2.33) is *nothing more* than a compact way to write the formula (2.28).

(b) Convince yourself that (2.33) is consistent with the interpretation of $|x\rangle$ as the Dirac function δ_x, that is that the following somehow makes sense:

$$\langle y|x\rangle = \int \mathrm{d}z \delta_y(z)\delta_x(z) = \delta(y-x). \tag{2.34}$$

Given x prove this equality as an equality of distributions in y, that is prove that for any test function f one has

$$\int \mathrm{d}y f(y) \int \mathrm{d}z \delta_y(z)\delta_x(z) = \int \mathrm{d}y \delta(y-x) f(y),$$

by proving that both sides are equal to $f(x)$. (The formula (2.34) can also be seen as a result on convolution of measures.)

Even though (2.33) sounds like a triviality, this is not the case because it defines a kind of normalization of the "states" $|x\rangle$. (Elements of $\mathcal{H}$ can be normalized to norm 1, but $|x\rangle$ is not such an element.) This is obscured here by the simplicity of the situation, but the proper normalization would be less apparent, if, as will occur later, rather than L^2 we would use the Hilbert space with squared norm $\int \mathrm{d}x |f(x)|^2 w(x)$ for a weight function $w(x)$. We will come back to this later in Section 4.10.

Besides the "states" $|x\rangle$, physics textbooks consider for $p \in \mathbb{R}$ the "states $|p\rangle$ of momentum p". Such a state would have to be an eigenvector of the momentum operator P, and the corresponding differential equation yields the solution $a\exp(\mathrm{i}px/\hbar)$, which does not belong to $\mathcal{H}$ for $a \neq 0$. Nonetheless, thinking of $|p\rangle$ as the function $x \mapsto \exp(\mathrm{i}px/\hbar)$ and thus of $\langle p|$ as the function $x \mapsto \exp(-\mathrm{i}px/\hbar)$, at least for $f \in \mathcal{S}$ it makes perfect sense to consider (using again the notation (2.25))

$$\langle p|f\rangle := \int \mathrm{d}x \exp(-\mathrm{i}px/\hbar) f(x) = \hat{f}(p), \tag{2.35}$$

which turns out to be the Fourier transform of f. Also, since $|x\rangle$ corresponds to the case $f = \delta_x$, we get

$$\langle p|x\rangle = \exp(-\mathrm{i}px/\hbar).$$

Moreover, recalling (1.19) and (1.15),

$$\langle p|p'\rangle = \int \mathrm{d}x \exp(\mathrm{i}(p' - p)x/\hbar) = 2\pi\delta((p' - p)/\hbar) = 2\pi\hbar\delta(p' - p).$$

We observe here the factor $2\pi\hbar$ on the right-hand side. Generally speaking delta functions on momentum space go with a factor $2\pi\hbar$ (or more precisely one such factor for each dimension) because we have chosen our normalization in order that the proper measure on this space is $\mathrm{d}p/2\pi\hbar$, and thus the integral of $2\pi\hbar\delta$ is still 1.

We also have the completeness relation

$$\int \frac{\mathrm{d}p}{2\pi\hbar}|p\rangle\langle p| = \mathsf{1}, \tag{2.36}$$

which is a concise way to express that for $f \in \mathcal{S}$ one has

$$|f\rangle = \int \frac{\mathrm{d}p}{2\pi\hbar}|p\rangle\langle p|f\rangle. \tag{2.37}$$

Indeed, $\langle p|f\rangle = \hat{f}(p)$, and recalling that $|p\rangle$ is just the function $x \mapsto \exp(\mathrm{i}px/\hbar)$, so that $\langle x|p\rangle = \exp(\mathrm{i}px/\hbar)$ the required equality

$$\langle x|f\rangle = f(x) = \int \frac{\mathrm{d}p}{2\pi\hbar}\exp(\mathrm{i}px/\hbar)\hat{f}(p)$$

is just the Fourier inversion formula (1.31).

Exercise 2.8.2 Convince yourself that in momentum state space, "$|p\rangle$ corresponds to the function $2\pi\hbar\delta_p$".

However, this is not the end of the story. Physicists think of the state space as some unspecified abstract Hilbert space, and the state of the system is represented by a vector $|\alpha\rangle$ "independent of any specific representation". Using the "position state space" amounts to describing the state $|\alpha\rangle$ by the function[46] $x \mapsto \langle x|\alpha\rangle$, while using "momentum state space" amounts to describing it by the function $p \mapsto \langle p|\alpha\rangle$. These are related by the completeness relations (2.31) and (2.36)

$$\langle p|\alpha\rangle = \int \mathrm{d}x\langle p|x\rangle\langle x|\alpha\rangle \ = \int \mathrm{d}x \exp(-\mathrm{i}px/\hbar)\langle x|\alpha\rangle \tag{2.38}$$

$$\langle x|\alpha\rangle = \int \frac{\mathrm{d}p}{2\pi\hbar}\langle x|p\rangle\langle p|\alpha\rangle = \int \frac{\mathrm{d}p}{2\pi\hbar}\exp(\mathrm{i}px/\hbar)\langle p|\alpha\rangle \tag{2.39}$$

which simply express that these functions are Fourier and inverse Fourier transforms of each other. We have checked that these claims are indeed correct when one uses the position state space, with the proper interpretation of these formulas. This formalism works beautifully in many more situations. Once it has been developed, it never becomes necessary to use a specific Hilbert space as a state space, which is the way the vast majority of physics

[46] For physicists this function is always well-defined, so please accept their point of view here, as we do not go into technicalities.

textbooks proceed. As we strive to formulate results in a more precise mathematical language we shall mostly not use this point of view.

Let us pursue a bit by a sample computation in the physicist's way [73]. If $\mathcal{O}$ is an observable, why not consider the matrix[47] $\langle x|\mathcal{O}|y\rangle$ for $x, y \in \mathbb{R}$? Let us compute this matrix when $\mathcal{O}$ is the momentum operator (2.18). First, using the completeness relation (2.36),

$$\langle x|P|y\rangle = \int \frac{\mathrm{d}p}{2\pi\hbar} \langle x|P|p\rangle\langle p|y\rangle. \tag{2.40}$$

Now, since we are arguing as physicists, we use that "$|p\rangle$ is an eigenvector for P, of eigenvalue p", so that $P|p\rangle = p|p\rangle$, and thus

$$\langle x|P|p\rangle\langle p|y\rangle = p\langle x|p\rangle\langle p|y\rangle = p\exp(\mathrm{i}p(x-y)/\hbar).$$

Now, recalling (1.19) we have

$$\int \frac{\mathrm{d}p}{2\pi\hbar} \exp(\mathrm{i}p(x-y)/\hbar) = \delta(x-y)$$

and thus (differentiating with respect to x under the integral sign),

$$\int \frac{\mathrm{d}p}{2\pi\hbar} p\exp(\mathrm{i}p(x-y)/\hbar) = -\mathrm{i}\hbar\delta'(x-y),$$

and the above relations yield the formal expression

$$\langle x|P|y\rangle = -\mathrm{i}\hbar\delta'(x-y) = \mathrm{i}\hbar\delta'(y-x). \tag{2.41}$$

In the present case, while the previous computation might seem mysterious to a mathematician, it is easy to understand the result. The quantity $\langle x|P|y\rangle$ can be defined in the distributional sense, requiring that for $f, g \in \mathcal{S}$ one should have

$$\iint \mathrm{d}x\mathrm{d}y g(x)^* f(y)\langle x|P|y\rangle = \langle g|P|f\rangle, \tag{2.42}$$

while, by definition of P, writing f' the derivative of f, $Pf(x) = -\mathrm{i}\hbar f'(x)$, so that

$$\langle g|P|f\rangle = -\mathrm{i}\hbar \int \mathrm{d}x g(x)^* f'(x).$$

Now, using successively (1.16) and (1.11),

$$f'(x) = \int \mathrm{d}y f'(y)\delta(y-x) = -\int \mathrm{d}y f(y)\delta'(y-x),$$

so that one may write

$$-\mathrm{i}\hbar \int \mathrm{d}x g^*(x) f'(x) = \iint \mathrm{d}x\mathrm{d}y\, g(x)^* f(y)(\mathrm{i}\hbar\delta'(y-x)).$$

Thus the right-hand side above equals the left-hand side of (2.42), and this is the meaning of (2.41).

[47] The name "matrix" is Physics terminology.

2.9 Why Are Unitary Transformations Ubiquitous?

Let us go back to the setting of a general Hilbert space, whose elements are denoted $x, y, z, \ldots$. To each observable is associated a self-adjoint operator. Conversely, to each self-adjoint operator is associated an observable (although it is another matter in concrete situations to design an experiment that actually measures it). We now describe a fundamental class of such observables. Given $x \in \mathcal{H}$ of norm 1, $(x,x) = 1$, the projector $P_x(y) := (x,y)x$ is Hermitian since

$$(z, P_x(y)) = (z,x)(x,y) = (x,z)^*(x,y) = ((x,z)x, y) = (P_x(z), y).$$

Exercise 2.9.1 In Dirac's formalism for a norm-1 vector $|\alpha\rangle$ one writes the projector $P_\alpha = |\alpha\rangle\langle\alpha|$. Why does it seem to require no proof that P_α is Hermitian?

Thus the operator P_x corresponds to an observable $\mathcal{O}$. The possible values of $\mathcal{O}$ are the eigenvalues of P, namely 0 and 1. We may describe $\mathcal{O}$ as asking the question: Is the state of the system equal to x?[48] The average value of this operator in state y is given by $(y, P_x(y)) = (y,x)(x,y) = |(x,y)|^2$ and is the probability to obtain the answer "yes" to your question. It is called the *transition probability* between x and y.[49] In physics, the inner product (x,y) is often called an *amplitude*, so that *the transition probability is the square of the modulus of the amplitude*.[50] The transition probability does not change if one multiplies x and y by complex numbers of modulus 1, as expected from the fact that this multiplication does not change the state represented by either x or y.

We should expect that *any transformation*[51] *which preserves the physical properties of a system preserves the transition probabilities*. Transition probabilities are preserved by unitary transformations, since for such a transformation $|(Ux, Uy)|^2 = |(x,y)|^2$. They are also preserved under *anti-unitary* transformations, i.e. anti-linear operators which preserve the inner product. Conversely, which are the transformations of $\mathcal{H}$ which preserve transition probabilities? A deep theorem of Eugene Wigner [92, appendix to Chapter 20] shows that this is the case *only* for unitary and anti-unitary transformations.[52] A fundamental consequence is that any transformation which preserves the physics of the system corresponds to a unitary or anti-unitary transformation. As we explain in the next section, there are many of these, corresponding to the symmetries of Nature. The symmetries of Nature of a certain type naturally form a group, bringing us to group theory. Furthermore time-evolution will also be represented by a unitary transformation.

[48] This *does not* mean that there is any way to "determine" the state y of the system. You may only perform a measurement that will give you a yes/no answer to the question: Is the system in state x? This experiment changes the state of the system.

[49] The reason for this name is that indeed this is the probability that the system exhibits a transition from state y to state x when you measure the observable $\mathcal{O}$.

[50] It would help to remember now the general principle that the square of the modulus of an amplitude represents a probability.

[51] The next section will make clear what is meant exactly by "transformation of the system".

[52] Anti-unitary transformations are much less used than unitary ones. They occur naturally in the study of time-reversal, a topic we do not treat at all.

2.10 Unitary Representations of Groups

Certain types of invariance in Nature are among the most important guiding principles in developing physical theories about the real world. This will be a recurring theme in this book. It forces us to choose models which satisfy certain symmetries and this implies extremely strict restrictions on the possible forms of physical theories.

In this section we start to use this principle in the simplest case, translation invariance. In physics each observer uses a *reference frame* to describe the positions of points in space (or in space-time). These reference frames need not have the same origin, may use different privileged directions and may even move with respect to each other.[53] Here we just consider the situation of different origins. If you study the motion of an object using a different origin for your reference frame than mine, we may disagree on the coordinates of the object, but we should agree that it follows the same laws of physics. Mathematically, the space $\mathbb{R}^3$ acts on itself by translations, and we examine first the effect of these translations at a purely classical level. Suppose that the system you are studying is translated by a vector $\boldsymbol{a}$.[54] The object at position $\boldsymbol{x}$ that you were studying has now been moved to position $\boldsymbol{x}+\boldsymbol{a}$. Say that you use a function f on $\mathbb{R}^3$ to measure e.g. the electrical potential at a point of space. Before you translate the system, the value $f(\boldsymbol{x})$ measures the potential at the point $\boldsymbol{x}$. After the translation this value of the potential occurs at the point $\boldsymbol{x}+\boldsymbol{a}$. Thus the value of the new function $U(\boldsymbol{a})(f)$ you use to measure the potential at this point $\boldsymbol{x}+\boldsymbol{a}$ equals the value of the old function f at the point $\boldsymbol{x}$:

$$U(\boldsymbol{a})(f)(\boldsymbol{x}+\boldsymbol{a}) = f(\boldsymbol{x}),$$

i.e.

$$U(\boldsymbol{a})(f)(\boldsymbol{x}) = f(\boldsymbol{x}-\boldsymbol{a}). \tag{2.43}$$

Observe the all-important minus sign and note the fundamental property $U(\boldsymbol{a}+\boldsymbol{b}) = U(\boldsymbol{a})U(\boldsymbol{b})$.

Suppose now that more generally we study a system whose state is described by a vector x in a Hilbert space $\mathcal{H}$. If the system is translated by a vector $\boldsymbol{a}$ we expect that the system will be described by a new state $U(\boldsymbol{a})(x)$. This new description should not change the physics. The transition probability between x and y should be the same as the transition probability between $U(\boldsymbol{a})(x)$ and $U(\boldsymbol{a})(y)$, i.e. $|(x,y)|^2 = |(U(\boldsymbol{a})(x), U(\boldsymbol{a})(y))|^2$. According to the discussion of the previous section, $U(\boldsymbol{a})$ is either unitary or anti-unitary. Moreover, it is obvious that $U(\boldsymbol{0})$ should be the identity. What becomes very interesting is when we perform two such translations in succession, first by a vector $\boldsymbol{a}$ and then by a vector $\boldsymbol{b}$. The state x is transformed first in $U(\boldsymbol{a})(x)$ and then in $U(\boldsymbol{b})(U(\boldsymbol{a})(x))$. This also amounts to perform the translation by the vector $\boldsymbol{a}+\boldsymbol{b}$, and this transforms the state x into the state $U(\boldsymbol{a}+\boldsymbol{b})(x)$. Therefore $U(\boldsymbol{b})U(\boldsymbol{a})$ and $U(\boldsymbol{a}+\boldsymbol{b})$ should represent the same transformation of the system. We cannot conclude that these transformations are equal, because states are

[53] If you sit in a train, you will typically think of the train as fixed and the landscape as moving.

[54] Equivalently, assume that this system remains fixed, but that you translate your reference frame by a vector $-\boldsymbol{a}$. Translating the system by $\boldsymbol{a}$ is called an *active transformation* whereas translating your reference frame by a vector $-\boldsymbol{a}$ is called a *passive transformation*.

really represented by whole rays rather than points, and operators of the form $c\mathbf{1}$, where c is of modulus 1 and $\mathbf{1}$ is the identity operator, are unitary, but do not change the ray structure. Rather, we expect that

$$U(\boldsymbol{a}+\boldsymbol{b}) = r(\boldsymbol{a},\boldsymbol{b})U(\boldsymbol{a})U(\boldsymbol{b}), \tag{2.44}$$

where $r(\boldsymbol{a},\boldsymbol{b})$ is a complex number of modulus 1. In particular

$$U(\boldsymbol{a}) = r(\boldsymbol{a}/2,\boldsymbol{a}/2)U(\boldsymbol{a}/2)U(\boldsymbol{a}/2).$$

Since the composition of two anti-unitary transformations is unitary, we have shown that $U(\boldsymbol{a})$ is always unitary. This motivates the following definition.

Definition 2.10.1 A map U which associates to each element a in a group G a unitary operator $U(a)$ on $\mathcal{H}$ is called a *projective unitary representation*[55] if for each $a, b \in G$ it satisfies

$$U(ab) = r(a,b)U(a)U(b) \tag{2.45}$$

where the complex number $r(a,b)$ is of modulus 1.

In this definition G denotes a group that is not necessarily commutative, so as customary the group operation is denoted in multiplicative form. In the case $G = \mathbb{R}^3$, (2.45) specializes to (2.44). We may then rephrase the argument which opens this section:

Any quantum system comes equipped with a projective unitary representation of the group of translations. This representation describes how translations affect the state of the system. (2.46)

The word "quantum" in the expression "quantum system" simply stresses the fact that the system is studied through Quantum Mechanics. The same argument shows also that the Euclidean group (generated by translations and rotations) has a projective unitary representation in any quantum system.

Exercise 2.10.2 Using that $(ab)c = a(bc)$ prove that the function r of (2.45) satisfies the identity

$$r(a,bc)r(b,c) = r(ab,c)r(a,b).$$

Our Definition 2.10.1 of projective representations is perfectly adapted to Quantum Mechanics, and follows the way physicists actually think about these objects. Mathematicians however like to look at these somewhat differently. This point of view brings conceptual clarification at the expense of an extra (thin) layer of abstraction, and is explained in Section 2.12. The mathematically inclined reader may like to look at this material now.

[55] These representations are also called *ray representations*.

Definition 2.10.3 A map U which associates to each element a in a group G a unitary operator $U(a)$ on $\mathcal{H}$ is called a *unitary representation* if it satisfies

$$U(ab) = U(a)U(b) \tag{2.47}$$

for $a, b \in G$.

Thus, a unitary representation is simply a projective unitary representation for which $r(a,b) \equiv 1$ for $a, b \in G$.

2.11 Projective versus True Unitary Representations

Let us start the discussion of the concepts involved in Definitions 2.10.1 and 2.10.3. The word "unitary" refers of course to the fact that each of the operators $U(a)$ is unitary. Unless mentioned otherwise, all representations are unitary, so that we shall nearly always omit the word "unitary", and the expressions "representation" and "projective representations" have to be understood by default as "unitary representation" and "projective unitary representations".

To insist that a representation satisfies $r(a,b) = 1$ for all a, b we will sometimes say *true* representation, even though throughout the book, the word "representation" means "true representation". When we consider a representation that is only a projective representation we will always say so explicitly. It is most important to understand the relationship between representations and projective representations.

- The concept of "representation" is *far more restrictive* than the concept of "projective representation".
- From the point of view of mathematics, the nice objects are representations. The study of group representations is a vast subject in mathematics.
- From the point of view of Quantum Mechanics, the natural objects are projective representations.

The following explains an important relationship between representations and projective representations.

Definition 2.11.1 Given a true representation V of G, and for $a \in G$ a number $\lambda(a)$ of modulus 1, the formula

$$U(a) := \lambda(a)V(a) \tag{2.48}$$

defines a projective representation, since (2.45) holds for the function

$$r(a,b) = \lambda(ab)/(\lambda(a)\lambda(b)). \tag{2.49}$$

When this is the case we will say that the projective representation U *arises* from the true representation V.

More generally, there is an important idea behind this definition: two projective representations U, U' such for each $a \in G$ one has $U(a) = \lambda(a)U'(a)$ for some complex number $\lambda(a)$ with $|\lambda(a)| = 1$ are to be thought of as "the same projective representation".

Given a projective representation, the immediate question is whether it arises from a true representation as in Definition 2.11.1. The point here is that even though projective representations are natural for Quantum Mechanics, true representations are much nicer mathematical objects, and it is easier to calculate with them. It would be sad to go through the complications of dealing with a projective representation just because we cannot recognize that this representation is really a true representation in disguise as given by (2.48).

Lemma 2.11.2 *Consider a projective representation U and assume that we can find a function $\lambda(a)$ with $|\lambda(a)| = 1$ such that (2.49) holds. Then U arises from a true representation.*

Proof It is immediate to check that $V(a) = \lambda(a)^{-1}U(a)$ is a true representation, and U arises from V. □

Thus, to prove that a projective representation arises from a true representation, given the function r it "is sufficient" to find a function λ which satisfies (2.49). This might be difficult if r is complicated.

We shall study later a projective representation that does not arise from a true representation, and which will be of constant use. That example motivates the fundamental program of investigating in detail how true and projective representations are related, and what obstacles may prevent a projective representation from arising from a true representation. We shall say a few words about this in Appendix A. We do not pursue this goal in the main text, since our priority is not to understand all possible projective representations, but rather to describe as simply as possible those which are the most important in our topic.

2.12 Mathematicians Look at Projective Representations

This material is not needed to follow the main story. It assumes that you know some very basic group theory. A map U from G to the group $\mathcal{U}(\mathcal{H})$ of unitary transformations of $\mathcal{H}$ is a true representation if and only if it is a group homomorphism. The group $\mathcal{U}(\mathcal{H})$ has a remarkable subgroup, the subgroup consisting of the transformations $\lambda\mathbb{1}$ with $|\lambda| = 1$. Let us denote by $\mathcal{U}_p(\mathcal{H})$ the quotient of $\mathcal{U}(\mathcal{H})$ by this subgroup, and by Φ the quotient map $\mathcal{U}(\mathcal{H}) \to \mathcal{U}_p(\mathcal{H})$. Thus the elements of $\mathcal{U}_p(\mathcal{H})$ are unitary operators "up to a phase", i.e. up to a multiplicative constant of modulus 1. It is immediate to check that a map U from a group G into $\mathcal{U}(\mathcal{H})$ is a projective representation in the sense of Definition 2.10.1 if and only $\Phi \circ U$ is a group homomorphism from G to $\mathcal{U}_p(\mathcal{H})$. The important object is thus the map $\Phi \circ U$. Accordingly, mathematicians *define a projective representation as a group homomorphism from G to $\mathcal{U}_p(\mathcal{H})$*. This formalizes the idea that two projective representations U and U' such that $U(a) = \lambda(a)U'(a)$ "are the same projective representation" (because this is the case if and only if $\Phi \circ U = \Phi \circ U'$). Another benefit of this approach is that it becomes natural to define "continuous projective representations", a topic which is investigated in Section A.2.

In mathematical language, the fundamental question, is, given a projective representation U of G, that is a group homomorphism from G to $\mathcal{U}_p(\mathcal{H})$, whether there exists a true representation V, that is a group homomorphism from G to $\mathcal{U}(\mathcal{H})$, such that $U = \Phi \circ V$.

2.13 Projective Representations of $\mathbb{R}$

We do not investigate in detail how true and projective representations are related in general, but we examine this question in the centrally important case $G = \mathbb{R}$. However, we must first discuss a technical question. In the cases of greatest interest, G is a topological group, and to avoid pathologies, one requires also a mild continuity assumption.

Definition 2.13.1 The map $a \mapsto U(a)$ which associates to each element a of G a unitary operator $U(a)$ is called *strongly continuous* if for each $x \in \mathcal{H}$ the map $a \mapsto U(a)(x)$ from G to $\mathcal{H}$ is continuous.

The topology on $\mathcal{H}$ is the topology induced by its norm, so the condition of strong continuity means that for each $x \in \mathcal{H}$ the norm $\|U(a)(x) - U(a_0)(x)\|$ goes to 0 as $a \to a_0$. Despite the adjective "strong", this condition is much weaker than the continuity of the map $a \mapsto U(a)$ in the operator norm.

A simple but instructive example of a representation is the case where $G = \mathbb{R}$, $\mathcal{H} = L^2(\mathbb{R})$ and $U(a)(f) \in L^2(\mathbb{R})$ is the function $w \mapsto f(w - a)$. The map $a \mapsto U(a)$ is not continuous when the space of unitary operators is provided with the topology induced by the operator norm but it is strongly continuous (as one sees by approximating f with a continuous function of bounded support).

When the map $a \mapsto U(a)$ is strongly continuous, then for $x, y \in \mathcal{H}$ the map $a \mapsto (x, U(a)(y))$ is continuous. This apparently weaker condition is equivalent to strong continuity. To prove this, assume the weaker condition. Then as $a \to a_0$, $(U(a)(x), U(a_0)(x))$ tends to the square of the norm of $U(a_0)(x)$, and since both vectors $U(a)(x)$ and $U(a_0)(x)$ have the same norm they become close to each other (as follows from the relation $\|u - v\|^2 = \|u\|^2 + \|v\|^2 - 2\mathrm{Re}(u, v)$).

Theorem 2.13.2 *A strongly continuous projective unitary representation of $\mathbb{R}$ arises from a true representation. That is, for such a projective representation $U(u)$ we have $U(u) = \lambda(u)V(u)$ where $V(u)$ is a true representation.*

Physicist's proof of Theorem 2.13.2 Since $U(u)$ is unitary, it is invertible. Since $U(0) = r(0,0)U(0)^2$, it holds that $r(0,0)U(0) = 1$. Since U is unitary, we have $|r(0,0)| = 1$, and $U'(u) := r(0,0)U(u)$ is a strongly continuous projective representation with $U'(0) = 1$. To prove that U arises from a true representation, it is sufficient to prove that U' arises from a true representation. Thus we may assume that $U(0) = 1$. A physicist will by default assume that for u small,[56] one has

$$U(u) = 1 + u\mathrm{i}H + O(u^2), \tag{2.50}$$

for a certain operator H. Since $U(u)$ is unitary,

$$1 = U(u)U(u)^\dagger = 1 + u\mathrm{i}(H - H^\dagger) + O(u^2),$$

[56] We will comment a bit later on this.

so that $H - H^\dagger = 0$, i.e. H is Hermitian. Let us then set $V(u) = \exp(\mathrm{i}uH)$. This operator is unitary since

$$V(u)^\dagger = \exp(-\mathrm{i}uH^\dagger) = \exp(-\mathrm{i}uH) = V(u)^{-1},$$

and we thus define a true unitary representation. (If you find the first equality mysterious, please think of the finite-dimensional case, where the exponential is given by the usual power series.) Next, we prove that $U(u) = \lambda(u)V(u)$ where $\lambda(u)$ is of modulus 1. For this we fix u and we observe that for an integer n (and because u/n is small for n large),

$$U(u/n) = \mathsf{1} + \mathrm{i}\frac{u}{n}H + O(n^{-2}) = V(u/n) + O(n^{-2}),$$

so that one should have

$$U(u/n)^n = V(u) + O(n^{-1}).$$

Since U is a projective representation, $U(u/n)^n = \lambda(n)U(u)$ where $|\lambda(n)| = 1$, and thus $U(u) = \lambda(n)^{-1}V(u) + O(n^{-1})$. Considering a subsequence (n_k) such that $\lambda(n_k)$ converges as $k \to \infty$ and letting $k \to \infty$ we conclude that $U(u) = \lambda V(u)$ where $|\lambda| = 1$.[57] □

Even in finite dimension the previous proof assumes more about U than what the theorem states. The relation (2.50) holds if and only if the map $u \mapsto U(u)$ is differentiable at $u = 0$ and this is not one of the hypotheses of the theorem. There is *no reason whatsoever* why a continuous projective representation should be differentiable since we may obtain a projective representation from a true representation using (2.48) for a nasty function λ. Furthermore, the previous argument fails in infinite dimension, because (2.50) cannot possibly be true. Even for a true representation there exist in general many vectors x for which the map $u \mapsto U(u)(x)$ is not differentiable at 0. A mathematician's proof of Theorem 2.13.2 may be found in Section A.1.

We may also define the concept of (not necessarily unitary) projective representation by keeping the relation (2.45) but dropping the requirement that the operators are unitary. Similarly we may define the concept of (not necessarily unitary) representation. When we consider representations that are not unitary we will say so explicitly.

2.14 One-parameter Unitary Groups and Stone's Theorem

A (strongly continuous) one-parameter unitary group is simply a (strongly continuous) unitary representation of $\mathbb{R}$, that is a map which associates to $t \in \mathbb{R}$ a unitary operator $U(t)$ on Hilbert space $\mathcal{H}$ in such a manner that

$$U(s)U(t) = U(s+t), \tag{2.51}$$

and (the continuity condition)

$$\forall x, y \in \mathcal{H}\ ,\ \lim_{t\to 0}(x, U(t)(y)) = (x, y). \tag{2.52}$$

[57] In Quantum Mechanics a *phase* is a complex number of modulus 1. To lighten terminology we will say that "$U(u) = V(u)$ up to a phase".

The archetypical example is the operator $U(t)$ on $L^2(\mathbb{R})$ given for $f \in L^2$ and $w \in \mathbb{R}$ by

$$U(t)(f)(w) = \exp(\mathrm{i}tw/\hbar)f(w). \tag{2.53}$$

This is simply the operator "multiplication by the function $\exp(\mathrm{i}t \cdot /\hbar)$." Another example is the operator $V(t)$ on $L^2(\mathbb{R})$ given for $f \in L^2$ and $w \in \mathbb{R}$ by

$$V(t)(f)(w) = f(w + t). \tag{2.54}$$

In both cases it is a nice exercise of elementary analysis to prove that these operators are strongly continuous. These one-parameter groups are closely related by the Fourier transform. Indeed,

$$\widehat{V(t)(f)} = U(t)\hat{f}. \tag{2.55}$$

Exercise 2.14.1 Make sure you understand every detail of the proof of the important formula (2.55).

Theorem 2.14.2 (Stone's theorem) *There is a one-to-one correspondence between the strongly continuous one-parameter unitary groups on a Hilbert space $\mathcal{H}$ and the self-adjoint operators on $\mathcal{H}$. Given the unitary group U, the corresponding self-adjoint operator A is called the* infinitesimal generator *of U. It is defined by the formula*[58]

$$A(x) = \lim_{t \to 0} \frac{\hbar}{\mathrm{i}t}(U(t)(x) - x). \tag{2.56}$$

and its domain $\mathcal{D} = \mathcal{D}(A)$ is the set of x for which the previous limit exists.

The most important part of Stone's theorem is the statement that the formula (2.56) defines a self-adjoint operator. Recalling that the domain of a self-adjoint operator "is large", the mathematical content of this part of Stone's theorem can be understood as a differentiability statement: there are many points x for which the map $t \mapsto U(t)(x)$ is differentiable at $t = 0$.

The impact on Quantum Mechanics of this part of Stone's theorem is simply staggering. Each time we are given a one-parameter unitary group, we can construct a self-adjoint operator, which means that there is a new fundamental quantity with physical meaning which we can measure. One-parameter unitary groups occur e.g. as follows:

- From the operation of space translation in a given direction (to be detailed later in the present section). The corresponding operator is called the *momentum operator in that direction.*
- From the operation of rotation around a given axis. The corresponding operator is called *angular momentum about this axis*.[59]
- From time-evolution, with the construction of the fundamental Hamiltonian operator, as studied in the next section.

[58] The use of the factor i in the denominator of (2.56) is precisely to ensure that A is self-adjoint (as opposed to skew-adjoint i.e. $A^\dagger = -A$) since self-adjoint operators are the class of interest in physics. Conventions such as this one often differ between mathematicians and physicists.

[59] The theory of angular momentum occupies a large part in Quantum Mechanics textbooks. We say a few words about it in Section 8.7.

Given the self-adjoint operator A, the converse part of Stone's theorem constructs a corresponding one-parameter group denoted by

$$U(t) = \exp(\mathrm{i}tA/\hbar). \tag{2.57}$$

It is easy to understand what this means when $\mathcal{H}$ is finite-dimensional (so that A is then simply a Hermitian operator). Then the exponential of an operator is simply given by the usual power series, and it should then be obvious that $\exp(B)^\dagger = \exp(B^\dagger)$. Since A is Hermitian ($A = A^\dagger$), it holds that $U(t)^\dagger = \exp(-\mathrm{i}tA/\hbar) = U(-t) = U(t)^{-1}$ so that $U(t)$ is indeed unitary. It should also be obvious that when A and B *commute* one has $\exp(A+B) = \exp(A)\exp(B)$ and this implies the formula $U(s+t) = U(s)U(t)$. If one has developed spectral theory, it is easy to understand (2.57). A self-adjoint operator A is essentially a "multiplication by x operator" and $\exp(\mathrm{i}tA/\hbar)$ is simply "multiplication by $\exp(\mathrm{i}tx/\hbar)$", see Exercise 2.14.3. In Appendix B we provide a self-contained construction of the operator $\exp(\mathrm{i}tA/\hbar)$ which does not use spectral theory.

The following exercise should not be missed, as it provides some intuition for Stone's theorem. It requires some fluency with integration theory.

> **Exercise 2.14.3** (a) Consider a real-valued measurable function h on $\mathbb{R}$. Prove that the operators $U(t)$ defined by $U(t)(f) = \exp(\mathrm{i}th/\hbar)f$ form a strongly continuous one-parameter group of unitary operators of $L^2 = L^2(\mathbb{R}, \mathrm{d}x, \mathbb{C})$.
> (b) Prove that the operator A of (2.56) has domain $\mathcal{D} = \{f \in L^2; hf \in L^2\}$ and that for $f \in \mathcal{D}$ one has $A(f) = hf$.
> (c) Consider the self-adjoint operator A "multiplication by the function h" given by $A(f) = hf$ for $f \in \mathcal{D} = \{f \in L^2; hf \in L^2\}$. Prove that the corresponding one-parameter group is the group $U(t)$ considered in (a).

Let us now suppose that we are given a one-parameter unitary group $U(t)$. We no longer assume that $\mathcal{H}$ is finite-dimensional, and we proceed to prove the truly remarkable fact that the formula (2.56) defines a self-adjoint operator. The proof takes about three pages, and is rather rewarding. The underlying ideas however are not needed for the sequel, so this material may be skipped without harm.

> **Lemma 2.14.4** *The operator A is symmetric, that is $(A(y), x) = (y, A(x))$ for $x, y \in \mathcal{D}$.*

Proof We observe the obvious but important fact that

$$(U(t)(y) - y, x) = (y, U(-t)(x) - x) \tag{2.58}$$

so that

$$\left(\frac{\hbar}{\mathrm{i}t}(U(t)(y) - y), x\right) = \left(y, \frac{\hbar}{-\mathrm{i}t}(U(-t)(x) - x)\right), \tag{2.59}$$

and letting $t \to 0$ gives the result. □

> **Lemma 2.14.5** *The domain $\mathcal{D}$ where the limit (2.56) exists is a dense subspace of $\mathcal{H}$.*

Assuming this lemma for a moment, to help the reader form an understanding of the situation, we complete the proof of Theorem 2.14.2 when $\mathcal{H}$ is finite-dimensional (the general case requires extra work). Then a dense subspace of $\mathcal{H}$ can be only $\mathcal{H}$ itself, and since A is symmetric it is Hermitian. Moreover, taking the derivative of $t \mapsto U(t+s) = U(t)U(s)$ at $t = 0$ yields $U'(s) = (\mathrm{i}/\hbar)AU(s)$ hence the formula $U(t) = \exp(\mathrm{i}tA/\hbar)$. In the finite-dimensional case this formula makes it obvious that there is a one-to-one correspondence between A and U.

Our proof of Stone's theorem is rather elementary, but it requires the concept of integration of a continuous Hilbert-space-valued function $h(s)$ with compact support. This integral is defined in a quite straightforward manner by approximation by step functions. We shall use that[60]

$$\Big\| \int \mathrm{d}s h(s) \Big\| \leq \int \mathrm{d}s \|h(s)\|, \tag{2.60}$$

and that for a bounded linear operator B (possibly valued in another Hilbert space) one has

$$B\Big(\int \mathrm{d}s h(s) \Big) = \int \mathrm{d}s B(h(s)). \tag{2.61}$$

Proof of Lemma 2.14.5 Consider an infinitely differentiable function f with compact support, an element $x \in \mathcal{H}$ and define

$$y := \int \mathrm{d}s U(s)(x) f(s), \tag{2.62}$$

the integral of the Hilbert-space-valued function $h(s) = U(s)(x)f(s)$. We prove first that $y \in \mathcal{D}$. First we note the formula

$$\begin{aligned} U(t)(y) &= \int \mathrm{d}s U(t)U(s)(x) f(s) = \int \mathrm{d}s U(t+s)(x) f(s) \\ &= \int \mathrm{d}s U(s)(x) f(s-t), \end{aligned} \tag{2.63}$$

using (2.61) in the first equality and change of variables in the last one. The dependence on t in the right-hand side is then through the differentiable function $f(s-t)$, and we are in a situation where we may differentiate under the integral sign. It is then straightforward to see that $y \in \mathcal{D}(A)$ and $A(y) = \mathrm{i}\hbar \int \mathrm{d}s U(s)(x) f'(s)$.

Next, we prove that the elements of the type (2.62) are dense in $\mathcal{H}$. Given $x \in \mathcal{H}$ we construct f such that the element (2.62) of $\mathcal{D}$ is arbitrarily close to x. Since U is strongly continuous, for each $\varepsilon > 0$ there exists $\alpha > 0$ such that $\|U(t)(x) - x\| \leq \varepsilon$ for $|t| < \alpha$. Choosing $f \geq 0$ supported in $[-\alpha, \alpha]$ and of integral 1 we obtain, using (2.60),

$$\|y - x\| = \Big\| \int \mathrm{d}s U(s)(x) f(s) - \int \mathrm{d}s x f(s) \Big\| \leq \int \mathrm{d}s f(s) \|U(s)(x) - x\| \leq \varepsilon.$$

□

Our next observation is that $\mathcal{D}$ is stable under the action of the operators $U(s)$.

[60] As usual when the domain of integration is not specified, the integration is over the whole space, here $\mathbb{R}$.

Lemma 2.14.6 *For each $s \in \mathbb{R}$ and each $x \in \mathcal{D}$ we have $U(s)(x) \in \mathcal{D}$ and $AU(s)(x) = U(s)A(x)$. Furthermore for $x \in \mathcal{D}$ the function $\varphi(s) = U(s)(x)$ is differentiable and*

$$\varphi'(s) = \frac{\mathrm{i}}{\hbar} U(s)A(x) = \frac{\mathrm{i}}{\hbar} AU(s)(x). \tag{2.64}$$

Proof Let s and x be as above and $y = \varphi(s) = U(s)(x)$. We first note the formula

$$\varphi(t+s) - \varphi(s) = U(t)(y) - y = U(s)(U(t)(x) - x).$$

Taking the derivative in t at $t = 0$ in the equality $\varphi(t+s) - \varphi(s) = U(s)(U(t)(x) - x)$ implies that φ is differentiable and $\varphi'(s) = (\mathrm{i}/\hbar)U(s)A(x)$, whereas taking the same derivative in the equality $\varphi(t+s) - \varphi(s) = U(t)(y) - y$ implies that $y \in \mathcal{D}(A)$ and $\varphi'(s) = (\mathrm{i}/\hbar)A(y)$. □

Now comes the key idea of the proof. For $x \in \mathcal{D}$ there is an explicit formula for $U(s)(x) - x$, and moreover this formula demonstrates that $x \in \mathcal{D}$. This allows a complete understanding of $\mathcal{D}$.

Lemma 2.14.7 *If $x \in \mathcal{D}$ then for all s we have*

$$U(s)(x) - x = \frac{\mathrm{i}}{\hbar} \int_0^s \mathrm{d}v U(v)A(x) = \frac{\mathrm{i}}{\hbar} \int_0^s \mathrm{d}v A(U(v)(x)). \tag{2.65}$$

Conversely, if

$$U(s)(x) - x = \frac{\mathrm{i}}{\hbar} \int_0^s \mathrm{d}v U(v)(z) \tag{2.66}$$

for all $s \in \mathbb{R}$ and some $z \in \mathcal{H}$ then $x \in \mathcal{D}$ and $A(x) = z$.

Proof First, (2.64) implies (2.65). Conversely, if (2.66) holds then

$$\frac{U(t)(x) - x}{t} - \frac{\mathrm{i}}{\hbar} z = \frac{\mathrm{i}}{\hbar t} \int_0^t \mathrm{d}v (U(v)(z) - z)$$

and the right-hand side goes to 0 as $t \to 0$ because $v \mapsto U(v)$ is strongly continuous, so that $v \mapsto U(v)(z)$ is continuous. □

Here starts the tricky part: we have to prove that A is self-adjoint, that is (since we know that A is symmetric) that every element of the domain of $A^\dagger$ is an element of $\mathcal{D}$. So, let us consider an element y in the domain of $A^\dagger$, with the goal of proving that $y \in \mathcal{D}$. By definition of the domain of $A^\dagger$, there exists $z \in \mathcal{H}$ for which

$$\forall x \in \mathcal{D}\ ,\ (y, A(x)) = (z, x). \tag{2.67}$$

We will prove that

$$U(s)(y) - y = \frac{\mathrm{i}}{\hbar} \int_0^s \mathrm{d}v U(v)(z), \tag{2.68}$$

which implies that $y \in \mathcal{D}$ according to the second part of Lemma 2.14.7. To prove (2.68) the idea is to prove that both sides have the same inner product with every element x in the dense space $\mathcal{D}$. Considering such x, let us recall that by (2.58) we have

$$(U(s)(y) - y, x) = (y, U(t)(x) - x), \tag{2.69}$$

for $t = -s$. Now, (2.65) implies

$$U(t)(x) - x = \frac{\mathrm{i}}{\hbar} \int_0^t \mathrm{d}v A(U(v)(x)),$$

so that, using (2.61) for the operator $B\colon x \mapsto (y, x)$ in the first line, and (2.67) in the second line,

$$\begin{aligned}(y, U(t)(x) - x) &= \frac{\mathrm{i}}{\hbar} \int_0^t \mathrm{d}v (y, A(U(v)(x))) \\ &= \frac{\mathrm{i}}{\hbar} \int_0^t \mathrm{d}v (z, U(v)(x)) \\ &= \frac{\mathrm{i}}{\hbar} \int_0^t \mathrm{d}v (U(-v)(z), x) \\ &= \Big(-\frac{\mathrm{i}}{\hbar} \int_0^t \mathrm{d}v U(-v)(z), x \Big).\end{aligned}$$

Using (2.69), and since $\mathcal{D}$ is dense, we obtain

$$U(s)(y) - y = -\frac{\mathrm{i}}{\hbar} \int_0^{-s} \mathrm{d}v U(-v)(z).$$

Changing v into $-v$ in the integral implies (2.68) and we have proved one direction in Stone's theorem. We recall that a self-contained proof of the converse can be found in Appendix B.

Let us note the following easy but important fact.

Proposition 2.14.8 *We have $x \in \mathcal{D}(A)$ and $Ax = \lambda x$ if and only if $U(t)(x) = \exp(\mathrm{i}t\lambda/\hbar)x$.*

Proof It is obvious from (2.56) that if $U(t)(x) = \exp(\mathrm{i}t\lambda/\hbar)x$ then $x \in \mathcal{D}(A)$ and $Ax = \lambda x$. To prove the converse we observe that the first equality in (2.65) implies $\mathrm{d}U(s)(x)/\mathrm{d}s = \mathrm{i}\lambda U(s)(x)/\hbar$ and $U(0)(x) = x$. □

Let us investigate the contents of Stone's theorem in the case of the one-parameter groups (2.53) and (2.54) given by

$$U(t)(f)(w) = \exp(\mathrm{i}tw/\hbar) f(w)\ ;\ V(t)(f)(w) = f(w + t).$$

As the state space is now $L^2(\mathbb{R})$ its generic element is denoted f, while x and y now denote elements of $\mathbb{R}$. It should be obvious that the infinitesimal generator of the group (2.53) is

the "multiplication by x" operator X. The infinitesimal generator P of the group (2.54) is given by

$$P(f)(x) = \lim_{t\to 0} \frac{\hbar}{\mathrm{i}t}(f(x+t) - f(x)) = -\mathrm{i}\hbar \frac{\partial}{\partial x} f(x),$$

and this is the momentum operator $P = -\mathrm{i}\hbar\partial/\partial x$. As the group is really natural, it is less surprising that its infinitesimal generator should be fundamental. It is quite instructive in this case to look at the relation (2.57) which here becomes

$$V(t) = \exp(\mathrm{i}tP/\hbar) = \exp(t\partial/\partial x). \tag{2.70}$$

Applied on a well-behaved function this is Taylor's formula:

$$f(x+t) = \sum_{n\geq 0} \frac{t^n}{n!}\Big(\frac{\partial}{\partial x}\Big)^n (f)(x) = \exp(\mathrm{i}tP/\hbar)(f)(x). \tag{2.71}$$

It bears repeating the considerable importance of Stone's theorem as a means of *constructing* self-adjoint operators: each time we construct a one-parameter unitary group we construct such an operator. Here is a fundamental example.

Definition 2.14.9 Assume that the one-parameter group $U_i(s)$ describes the action of translation of physical space by s in the ith direction. Then the momentum operator P_i in the same direction is *defined* by

$$U_i(s) = \exp(-\mathrm{i}sP_i/\hbar). \tag{2.72}$$

At first it sounds strange to define the momentum operator in this way because we might feel that we know it from the physics of the model, but at a deeper level the important relation is (2.72). We will soon meet situations where it is the unitary group $U_i(t)$ rather than P_i which is naturally constructed.[61]

To understand the reason behind the definition (2.72), and in particular the reason behind the minus sign in the exponent, let us look at a special case. We go back to the relation (2.43) (in one dimension), where f is not a potential, but a wave function in position state space, measuring the probability density of the presence of a particle. Then the action $U(s)$ of translation of physical space by s on the wave function f is given by

$$U(s)(f)(x) = f(x-s) = \exp(-\mathrm{i}sP/\hbar)(f)(x),$$

where we use (2.71) in the second equality. This is indeed a special case of (2.72).

Let us recall that the operators P and X satisfy the canonical commutation relation (2.19):

$$[X, P] = \mathrm{i}\hbar\mathbf{1}. \tag{2.73}$$

It is absolutely fundamental that in a precise sense there is a *unique* pair of "nice" operators which satisfy it. "Nice" operators satisfy a slightly stronger form of the relation (2.73) which we explain now. First, recalling the operators U, V of (2.53) and (2.54), we observe that

[61] This is also related to a fundamental principle of Classical Mechanics: Noether's theorem relating symmetries of Lagrangians with invariants of the corresponding theory.