ELEMENTS OF NON-RELATIVISTIC QUANTUM MECHANICS

非相对论量子力学基础

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PREFACE

It is almost a trivial observation that many collective endeavours require the accomplishment of numerous complicated tasks, and that the different individuals that perform them may lose sight of the overall design. Like other creative endeavours, the scientific quest is particularly prone to such a state of affairs, for not only does the difficulty of the tasks absorb the mind but the beauty of what is learnt in performing them engages the soul. Like a diver, who may be so charmed by the nearby coral so as to forget that its beauty is but a minute reflection of the majestic beauty of the ocean, a spectroscopist may be so taken by the beautiful symmetries that the molecules exhibit so as to loose sight of the wonderful structure of quantum mechanics that informs them.

* * *

For many years, I have taught a graduate course on non-relativistic quantum mechanics at the University of British Columbia. As a first graduate course in the subject, it was to provide a good understanding of the principles as well as the necessary basic skills for the application of quantum mechanics to a diversity of fields. The students, coming, as the did, from universities all over the world, had very diverse backgrounds and I could not assume that every one of them had a good grasp of the basic principles of quantum mechanics, all I could assume was that they all had studied the standard elementary applications. Because the course was required of all graduate students in Physics, the prospective fields of its audience ranged widely – from quantum field theory to physical oceanography –, which meant that I could not maintain their interest by centring the lectures on any particular field of application. Faced with these constraints, I felt that the best way of achieving the aims of the course was to present the theory of quantum mechanics taking care to exhibit its coherence and beauty, hoping to maintain the students' interest by appealing to their aesthetic sense. Now that I am nearing the end of my teaching career, I feel that the approach taken was successful, and I have the satisfaction of knowing that this feeling is shared by many of my former students.

The present book was born of the experience gained in teaching the course just described. It is not meant to be a textbook for such a course. It covers less material than the course did, but treated in more depth. As a first approximation, the book might be described as a coherent presentation of the core of the course augmented by the answers to questions that many of my students and some of my colleagues have put to me in the course of the years. Many of these questions I could not answer by reference to the literature, for the available answers were presented at a level not accessible to those that formulated them.

In spite of the suggestions that I received from students and colleagues I would not have undertaken the task of writing this book had it not been for my own desire to have a comprehensive overview of quantum mechanical theory and gain a better appreciation of its beauty. I feel now that the exercise was worth the effort and I hope that the reader would gain as much aesthetic satisfaction from reading this book as the author gained from writing it.

To limit the size of the book, I had to decide what not to include. It was clear to me that those problems which are solved in detail in every textbook (e.g., the hydrogen atom) could be left out, unless they were necessary for the development of the presentation (such as the harmonic oscillator) or particularly useful as illustrations of the theory. More difficult was the decision not to include approximate methods and scattering theory because, although these two subjects have in some sense an ancillary status within the general theory, not only are they of essential importance in the applications but they also have had an enormous influence in the way we think about the physical world. Even more difficult was the decision not to treat the quantization of fields more extensively and just to touch it very briefly in connection with the study of an assembly of particles.

I had no difficulty in deciding not to include a discussion of the interpretations of quantum mechanics nor of the closely related problem of measurement. These extremely interesting questions lie in a "metalevel" above quantum theory and, in my opinion, would require a full volume to be properly discussed.

What is included constitutes the core of non-relativistic quantum-mechanical theory, the *elements* needed to properly understand the developments of the subject and its applications.

As can be gathered from the introductory paragraphs of this preface, these elements are presented with a different emphasis than is common in the standard textbooks, and at a higher level, but without requiring from the reader more than a working knowledge of quantum mechanics on the physical side, and the mathematical background in algebra and analysis normally acquired at the undergraduate level. This book occupies a largely empty niche between the usual textbooks and the more mathematically advanced writings on the subject. I expect it would be of interest both to graduate students and to many practising scientists who would like to delve a little into the structure of quantum mechanics and into the mathematical notions that underlie it.

Quantum systems cannot be described in terms of our sensory experience, to understand them it is necessary to use the abstract language provided by the algebra of linear operators on a Hilbert space. For this reason, three mathematical appendices have been included. For ease of reference, their paragraphs are numbered and are often referred to in the main text. Appendix A reviews finite-dimensional vector spaces; the necessary results in the theory of Hilbert spaces are summarized in Appendix B, while Appendix C presents some elements of the theory of distributions leading to an explanation of the mathematical basis of Dirac's formalism. The first four chapters of the book make use of the material in sections 1 to 3 of Appendix A which are mostly intended to serve as a reminder. Before embarking in a thorough reading of the rest of the book, the reader is invited to peruse the final sections of Appendix A as well as appendices B and C. A fourth appendix, D, includes some pertinent results in classical mechanics.

Group theoretical considerations pertaining mostly to the Galilei and to the symmetric groups play an important part in the exposition. It has been possible to develop them without assuming on the part of the reader much more than a knowledge of the definition of group. They are not included in the appendices but in appropriate places in the main body of the text.

A remark on the mathematical aspects of the presentation is in order here. Our experimental instruments are finite, in size, in energy, and in the number of configurations that they can exhibit. This implies that, in principle, only the language of finite-dimensional vector spaces is needed to explain experimental results and to understand the structure of quantum mechanics. However, it is extremely fruitful – and necessary if we want to embed the theory in a space and time continuum – to consider idealized instruments capable of an infinite number of configurations, which require a description cast in the language of infinite-dimensional spaces. Because these infinite instruments are approximations of the actual finite ones, physicists have all reason to ignore those properties of the infinite-dimensional Hilbert space that cannot be obtained from the properties of finite-dimensional ones by some, not necessarily unique, *physically based* limiting procedure. A working knowledge of the mathematical description that results from the adopted limiting procedure is necessary to understand many of the developments of quantum mechanics. The mathematical presentation reflects these considerations: the results pertaining to finite-dimensional spaces, necessary for the understanding of the structure of quantum mechanics, are presented with thoroughness; their generalizations to infinite-dimensional spaces are discussed in less detail, although references to the mathematical literature are given for the benefit of the interested reader.

After an introductory chapter that sets the point of view adopted in the exposition, the main body of the book can be thought of as being divided into two parts. In the first one, Chapters II to IV, are presented and elaborated the basic rules (I prefer this word to "postulates" or "axioms" because it does not imply a mathematical rigour that the exposition does not have) as they apply to model systems describable in the language of finite-dimensional spaces. In this way one can exhibit the basic structure of the theory unencumbered by the mathematical complications that arise in infinite-dimensional spaces.

The second part deals with the generalization of the theory and its applications to different types of systems. The general theory is presented in Chapter V, in which the concept of kinematical symmetries is also introduced and applied to those symmetries that arise from galilean invariance. Chapters VI and VII which discuss the particle without internal degrees of freedom are followed by the study in Chapter VIII of the dynamical symmetries of quantum mechanics; at this point the reader may find it helpful to review the classical results of Appendix D. The particle with spin is discussed in Chapter IX, and composite systems in the remaining two chapters. The connection between galilean invariance and the fundamental observables of a system constitutes the unifying thread that runs through this part of the book.

Notes, mainly but not exclusively bibliographical, to most sections can be found after the appendices, followed by a selected bibliography.

A standard nomenclature has been adopted; minor exceptions are the use of "density operator" in preference to the more generally used "density matrix", of "commensurable observables" that seems more appropriate than "compatible" or "simultaneously measurable observables" and of "maximal observable" instead of the lengthier "complete set of commuting observables".

Dirac's formalism and notation is used throughout the main body of the book. From the mathematical point of view, however, this notation has some disadvantages; for this reason and because the use of Dirac's notation is not universal, the main results of the mathematical appendices are given in ordinary notation. Each section of these appendices ends with an explanation of the connection between the two notations.

For reference, mathematical expressions within a chapter are numbered in the common decimal system. Within each chapter, they are referred to by their number [e.g., (3.5)]. In the references across chapters the expression number is preceded by the chapter number [e.g, (II.3.5)]. Paragraphs in the appendices are also numbered in the decimal system (but not enclosed in parentheses) and referred to in a similar manner (e.g., paragraph 3.2.2 of Appendix B will be referred to as 3.2.2 from within the appendix and as B.3.2.2 from without). Mathematical expressions in the appendices are not numbered.

* * *

I owe a debt of gratitude to all those that made possible the writing of this book. I am particularly indebted to the many former students whose comments and questions contributed so much to my understanding of quantum mechanics. Among them, I would dare to name Ulrike Närger, Steve Patitsas, Mark Shegelski and Mike Sofer, who collaborated with me in the teaching of the subject. My thanks are also due to all those colleagues with whom I have discussed many of the topics included in this book and, especially, to F.W. Dalby whose provocative questions always demanded an answer. My readings, of course, influenced the shaping of my course and are reflected in my writing. Two books I should mention in this connection: Messiah's *Quantum Mechanics* and Jauch's *Foundations of Quantum Mechanics*. To their authors I express my gratitude.

In the latter stages of the preparation of this book, I received valuable comments from Mark MacLean, who kindly agreed to read the mathematical appendices, and essential technical help from Janet Clark, who typeset the manuscript in TEX. To both of them, my sincere thanks.

In concluding this preface, I must ask the reader to forgive the dryness of my style, for the language in which I am writing is not the language in which I learned to laugh and to cry.

Vancouver, April 1995.

CONTENTS

I INTRODUCTION

The subject matter of this book is Non-relativistic Quantum Mechanics, a theory which, needless to say, explains an enormous wealth of observations. This fact by itself would constitute a sufficient reason to study the theory in some depth. But there are also other reasons. Non-relativistic Quantum Mechanics, which we shall simply call Quantum Mechanics, rests on a sound mathematical basis which means that the basic concepts of the theory can be understood precisely. This precise understanding is essential to understand and to contribute to the development of two broad fields at the limits of our present knowledge. One is the relativistic theory of quantum fields which constitutes today one of the frontiers of theoretical physics. The other, that lies at the boundary between physics and philosophy, is the understanding of the relation between ourselves and the world that we study.

While the physical observations are non-mathematical entities ultimately accessible to our senses, the theory introduces some fundamental concepts that are mathematical and cannot be explained by appealing to our sensory experience. As a consequence it is not possible to understand Quantum Mechanics without understanding the mathematical theory in which those concepts arise.

It is the purpose of this chapter to explain in some detail the brief remarks of the previous paragraph.

1. Description of experiments

There are of course many reasons that may lead physicists to conceive of an experiment. One may want to test a prediction of a more or less well developed theory. Another may be seeking some orientation in the development of a tentative theoretical formulation. Still another may want to determine the properties of some material with an eye to possible applications. Whatever the motivation, in most if not in all cases, the experimenter has in mind some more or less elaborated theoretical framework to guide him in the design of the experiment.

Once the design has been completed the experimenter decides what instruments are needed, proceeds to draft them in detail, and has them built in the technical shop.[1] The important point to be made here is that the detailed plans of the instruments are completely understandable to the shop staff even if they know nothing about the theoretical ideas that guided the design.

After the experimental instruments have been built and assembled, the experiment, which may consist of one or more experimental runs, is performed.

At the start of an experimental run some of the instruments are adjusted by manipulating knobs or other devices until their settings, as verified by the readings of appropriate dials, are the desired ones. Some time later the run is completed by noting another set of dial readings which constitutes the experimental results of the run.

When the predictions of a theory are statistical, as is the case in quantum mechanics, an experiment consists usually of many runs with identical initial settings of the instruments. Although normally these runs are performed in succession, we may think of them as starting simultaneously and using identical copies of the experimental setup.

A proper account of the experiment can be phrased in plain language in the sense that it need not contain any reference to the theoretical ideas that entered in its conception; all that is required is a description of the experimental instruments, the instrumental settings at the start, and the dial readings at the completion of each run. As already remarked, the instruments can be built, and therefore described, without any use of those theoretical ideas, while the readings of the different instruments consist merely of a set of numbers that refer to some variable characteristics incorporated in the construction of those instruments. Of course, in reporting the experiment, the experimenter usually discusses the theoretical ideas that led to its conception and the significance of the results in relation to those ideas but this part of the report constitutes an *interpretation* of the experiment, not an *account* of it.

In practice it is generally true that the instructions for the construction of the experimental instruments are phrased in plain language. On the other hand, in an article intended to describe an experiment to other workers in the field one often finds sentences such as "the proton beam was focused on the target" which

[1] Some instruments may, of course, have been designed by somebody else and be available from the shelf but this and other such details are clearly irrelevant for our purposes.

is certainly not expressed in plain language, for it contains an obvious reference to the theoretical ideas used in designing the experiment. That sentence, however, could have been replaced by something like "the current in the coils labelled A in the diagram was adjusted until a maximum signal was obtained in the detector". Another experimenter will know that that was precisely what was done and what he would have to do if he wanted to repeat the experiment. The original sentence is expressed in a sort of shorthand which is based on shared theoretical ideas. Such a shorthand is extremely useful and even essential, for without it communication among physicists would be unbearably slow, but it should be used with care if one wants to avoid ambiguities. Indeed the history of the development of Quantum Mechanics shows that its uncritical use can lead to apparent paradoxes and conceptual errors.

2. The concept of physical system

In analyzing an experiment which can be satisfactorily explained by classical physics, it is not the experimental instruments which are stressed in the analysis but rather the *system* on which the experiment is done. This is so because the concept of system as some physical object separate from the other instruments used in the experimental setup is easy to define precisely.

To illustrate the last remark let us look at a simple example from classical mechanics. Imagine an experiment designed to determine the range of an artillery piece. In each run one measures the velocity of the shell when it leaves the nozzle as well as the horizontal distance that it travels. To analyze the experiment one may choose the shell as "the system". The *state of the system* at any time is given by the values at that time of an appropriate set of coordinates and velocities of the shell. We say that the theory of classical mechanics (including in this case aerodynamics) explains the experiment because it permits us to write a closed system of equations that describes the time evolution of the state of the shell in accordance with the experimental results.

There are three important properties of a classical mechanical system that need to be stressed here.

(i) The system (in our example, the shell) is a part of the experimental setup, constructed as a piece separate from the other experimental instruments, and can therefore be described precisely in plain language.

(ii) The state of the system can be determined, at least in principle, at any time (for example by stroboscopic photography) without altering the predicted states at future times.

(iii) The state uniquely determines the value of every mechanical property (that is, every dynamical variable) of the system.

The precise definition of a classical mechanical system requires, first of all, that a complete set of coordinates be specified, in the sense that prescriptions must be given on how to measure them. It is, of course, possible to define the complete set of coordinates in different ways but the sets so defined are all equivalent because their coordinates are functions of the coordinates of any particular set. The characterization of the system is completed by giving certain intrinsic (that is, pertaining to the system, not to the rest of the experimental setup) parameters, such as masses or moments of inertia.

Systems that share the same complete set of coordinates will be said to belong to the same *type*. Thus the shell of the above example belongs to the type of rigid bodies. But for two shells to constitute identical systems they must have the same moment of inertia and geometrical shape (because the aerodynamic forces depend on the latter). In general we call two systems identical if they belong to the same type and have the same intrinsic parameters.

A parenthetical remark about nomenclature is in order here. In the above description we have implicitly assumed that one characteristic of a system is that its state at any given time uniquely determines, through a *closed* system of equations of motion, the state at any future time. A part of a classical mechanical system can also be assigned a state which is a subset of the set of coordinates and velocities that constitute the state of the system. Although such a part should properly be called a *subsystem*, the prefix is often omitted and the word "system" is loosely applied to it. As we know, the state of a subsystem at a given time does not, in general, determine the state at future times, for the motion may depend on the values of the remaining coordinates and velocities.

There are theories in classical physics in which a system can be defined which does not have property (i) above. An example is classical electromagnetism. In many cases it is convenient in this theory to regard the electromagnetic field as being "the system", although it is obviously not a piece of equipment that can be constructed in the shop separately from the rest of the experimental instruments. The field can be thought of as a physical agent which is produced by some of the experimental instruments and causes the observed correlations between measurements. However, within the domain of applicability of classical physics, it is possible, even in this case, to regard the state of the system, i.e., the field, as given by a set, albeit infinite, of generalized coordinates and velocities such that properties (ii) and (iii) still hold.[2] Thus, the field can be treated as a kind of mechanical

[2] Admittedly property (ii) requires the introduction of idealized test bodies with vanishingly small charges.