Introduction

Why yet another book on quantum mechanics? Quantum mechanics was born in the first quarter of the twentieth century and has received an enormous number of theoretical and experimental confirmations over the years. It is considered to be the fundamental physical paradigm, and has a wide range of applications, from cosmology to chemistry, and from biology to information sciences. It is one of the greatest intellectual achievements of the past century. As an effect of its invention, the very concept of physical reality was changed, and "observation," "measurement," "prediction," and "state of the system" acquired a new and deeper meaning.

Probability was not unknown in physics: it was introduced by Boltzmann in order to control the behavior of a system with a very large number of particles. It was the missing concept in order to understand the thermodynamics of macroscopic bodies, but the structure of the physical laws remained still deterministic. The introduction of probability was needed as a consequence of our lack of knowledge of the initial conditions of the system and of our inability to solve an enormous number of coupled non-linear differential equations.

In quantum mechanics, the tune is different: if we have 10^6 radioactive atoms *no* intrinsic unknown variables decide which of them will decay first. What we observe experimentally seems to be an irreducible random process. The original explanation of this phenomenon in quantum mechanics was rather unexpected. All atoms have the same probability of having decayed: only when we observe the system do we select which atoms have decayed in the past. In spite of the fact that this solution seems to be in contrast with common sense, it is the only possible one in the framework of the conventional interpretation of quantum mechanics. Heisenberg, de Broglie, Pauli, Dirac, and many others invented a formalism that was able to explain and predict the experimental data and this formalism led, beyond the very intention of the men who constructed it, to this conceptual revolution. Then, the old problem of the relations among the observer and the observed object, discussed for centuries by philosophers, had a unexpected evolution and now it must be seen from a new, completely different perspective.

Once established, quantum mechanics became a wonderful and extremely powerful tool. The properties of the different materials, the whole chemistry, became for the first time objects that could be predicted from the theory and not only phenomenological rules deduced from experiments. The technological discovery that shaped the second half of last century, the transistor (i.e. the basis of all the modern electronics and computers) could not have been invented without a deep command of quantum mechanics.

The advances of recent years have not only concentrated on the problems of interpretation that could be (wrongly) dismissed as metaphysical by some people, considering them

to be beyond experimental tests. In the last 30 years, the whole complex of problems connected to quantum mechanics and the meaning of measurements started to be studied from a new perspective. Real, not only *Gedanken* experiments began to be done on some of the most elusive properties of quantum mechanics, i.e. the existence of correlations among spatially separated systems that could not be explained using the traditional concept of probability. The precise quantum mechanical meaning of measurements started to be analyzed in a more refined way (e.g. quantum non-demolition measurements were introduced) and various concepts from statistical mechanics and other fields of physics began to be used.

This is not only an academic or philosophical problem. The possibility of constructing a quantum computer, which would improve the speed of present day computers by an incredible factor, is deeply rooted in these achievements. It is now clear that a quantum computer can solve problems, which on conventional computers take a time exploding as exponent of some parameter (e.g. the factorization into primes of a number of length N), in a time which is only a polynomial in N. The technical problems to be overcome in constructing a quantum computer are not easy to solve, but this result has a high conceptual status, telling us how deeply quantum mechanics differs from classical mechanics. Another quantum-information puzzling phenomenon, i.e. teleportation, has been recently proved experimentally to exist and it is a very active area of experimental research.

The arguments above explain why this new situation imposes the necessity to treat this field in a new way. The idea of writing this book came to one of us in 2000; it has taken more than eight years to accomplish this challenge.

Outline

The book is divided into four parts:

I *Basic features of quantum mechanics*
Part I deals with the basic framework of the theory and the reasons for its birth. Furthermore, starting from the fundamental principles, it explains the nature of quantum observables and states, and presents the dynamics of quantum systems and its main examples.

II *More advanced topics*
In Part II we introduce angular momentum, spin, identical particles, and symmetries. Moreover, we give a special emphasis to the quantum theory of measurement.

III *Matter and light*
We devote Part III to some of the most important applications of quantum theory: approximation methods and perturbation theory, the hydrogen atom, simple molecules, and quantum optics.

IV *Quantum information: state and correlations*
Finally, we deal with the most recent topics: the quantum theory of open systems, state

measurement, quantum correlations and non-locality, and quantum information and computation.

In this book there is material for four one-semester courses. It may also serve as a guide for short courses or tutorials on specific and more advanced topics.

Methodology

(1) In our exposition we have tried to follow a "logical" order, starting from the principles of classical mechanics, the need of quantum mechanics with its fundamental assumptions (superposition, complementarity, and uncertainty principles). Then, we present the main features of observables and states, before going forward to the dynamics and to more sophisticated stuff, applications, and special areas.
(2) We have made an effort to use a pedagogical style. In particular:
   (i) We prove or let the reader prove (through problems that are solved on the book's website) practically all our results: we try to lead the reader to reach them step by step from previous ones.
   (ii) We have made the choice to present Dirac algebra and operatorial formalism from the very beginning, instead of starting with the wave-function formalism. The latter is obtained naturally as a particular representation of the former. This approach has the advantage that we are not obliged to repeat the fundamental mathematical tools of the theory.
   (iii) We present our main principles and results in a pragmatic way, trying to introduce new concepts on the basis of experimental evidence, rather than in an axiomatic way, which may result cumbersome for readers who are learning quantum mechanics.
   (iv) We have made an effort to pay particular attention to cross-references in order to help the (inexpert) reader to quickly find the necessary background and related problems.
(3) We have taken into account some of the most recent developments at theoretical and experimental level, as well as with respect to technological applications: quantum optics, quantum information, quantum non-locality, state measurement, etc.
(4) We believe that measurement theory constitutes a fundamental part of quantum mechanics. As a consequence we have devoted an entire chapter to this issue.
(5) When necessary, we have emphasized interpretational as well as historical issues, such as complementarity, measurement, nature of quantum states, and so on.
(6) We propose to the reader a large number of problems (more than 300), and the less trivial ones (about half of them) are solved in a pedagogical way.
(7) From time to time, we have chosen to treat special topics in "boxes."

Apparatus

Besides a large number of cross-references, we also list the following tools:

(1) The book contains 200 figures among drawings, photographs, and graphs, distributed in all chapters (a sample of color figures can be found on the book's website). We consider this graphic support a very important aspect of our exposition. In this context, figure captions are particularly accurate and often self-contained.
(2) The book contains an extensive bibliography (almost 600 entries, most of which are quoted in the text) and a "Further reading" section at the end of each chapter. Name of authors in italics in citations refer to books, those in roman text refer to journals, papers, and other publications.
(3) The book contains full, accurate, and comprehensive indices (table of contents, subject index, author index, list of figures, list of tables, list of abbreviations, list of symbols, list of boxes, list of theorems, definitions, and so on) together with a summary of the main concepts at the end of each chapter.

Readers

This book is addressed to people who want to learn quantum mechanics or deepen their knowledge of the subject. The requirement for understanding the book is a knowledge of calculus, vectorial analysis, operator algebra, and classical mechanics.

The book is primarily intended for third- and fourth-year undergraduate students in physics. However, it may also be used for other curricula (such as mathematics, engineering, chemistry, computer sciences, etc.). Furthermore, it may well be used as a reference book for graduate students, researchers, and practitioners, who want a rapid access to specific topics. To this purpose the extensive indices and lists are of great help. It may even serve as an introduction to specific areas (quantum optics, entanglement, quantum information, measurement theory) for experienced professionals from different fields of physics. Finally, the book may prove useful for scientists of other disciplines who want to learn something about quantum mechanics.

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Finally, we dedicate this book to our families for their continual support and love, and for tolerating our many absences during the completion of the book.

PART I

BASIC FEATURES OF QUANTUM MECHANICS

1 From classical mechanics to quantum mechanics

In this chapter we shall first summarize some conceptual and formal features of classical mechanics (Sec. 1.1). Modern physics started with the works of Galileo Galilei and Isaac Newton from which classical mechanics, one of the most beautiful and solid intellectual buildings of the human history, came out. The architecture of classical mechanics was developed between the end of the eighteenth century and the second half of the nineteenth century, and its present form is largely due to Lagrange, Jacobi, and Hamilton. As we shall see in this chapter, classical mechanics is built upon the requirement of determinism, a rather complex assumption which is far from being obvious. In Sec. 1.2 we shall present the two main conceptual features of quantum mechanics on the basis of an ideal interferometry experiment: the superposition principle and the principle of complementarity. In Sec. 1.3 a first formal treatment of quantum-mechanical states is developed: quantum states are represented by vectors in a space that turns out to be a Hilbert space. In Sec. 1.4 the significance of probability for quantum mechanics is explained briefly: we will show that probability is not just an ingredient of quantum mechanics, but is rather an intrinsic feature of the theory. Furthermore, we shall see that quantum probability is not ruled by Kolmogorov axioms of classical probability. Finally, we discuss the main evidences which have historically revealed the necessity of a departure from classical mechanics. Our task then is to briefly present the principles upon which quantum mechanics is built (in Secs. 1.2–1.4) and to summarize in Sec. 1.5 the main evidences for this new mechanics.

1.1 Review of the foundations of classical mechanics

Classical mechanics is founded upon several principles and postulates, sometimes only implicitly assumed. In the following we summarize and critically review such assumptions.[1]

First of all, in classical mechanics a *principle of perfect determination* is assumed: all properties of a physical system $\mathcal{S}$ are perfectly determined at any time. Here, we define a *physical system* as an object or a collection of objects (somehow interrelated) that can be (directly or indirectly) experienced through human senses, and a *property* as the value that can be assigned to a physical variable or observable describing $\mathcal{S}$. *Perfectly determined* means then that each (observable) variable describing $\mathcal{S}$ has at all times a definite value.

[1] See [Auletta 2004].

Some of these properties will have a value that is a real number, e.g. the position of a particle, others an integer value, e.g. the number of particles that constitute a compound system.

It is also assumed that all properties can be in principle perfectly known, e.g. they can be perfectly measured. In other terms, the measurement errors can be – at least in principle – always reduced below an arbitrarily small quantity. This is not in contrast with the everyday experimental evidence that any measurement is affected by a finite resolution. Hence, this assumption can be called the postulate of *reduction to zero of the measurement error*. We should emphasize that this postulate is not a direct consequence of the principle of perfect determination because we could imagine the case of a system that is objectively determined but cannot be perfectly known.

Moreover, the variables associated with a system $\mathcal{S}$ are in general supposed to be continuous, e.g. given two arbitrary values of a physical variable, all intermediate possible real values are also allowed. This assumption is known as the *principle of continuity*.

At this point we can state the first consequence of the three assumptions above: If the state of a system $\mathcal{S}$ is perfectly determined at a certain time t_0 and its dynamical variables are continuous and known, then, knowing also the conditions (i.e. the forces that act on the system), it should be possible (at least in principle) to predict with certainty (i.e. with probability equal to one) the future evolution of $\mathcal{S}$ for all times $t > t_0$. This in turn means that the future of a classical system is unique. Similarly, since the classical equations of motion (as we shall see below) are invariant under time reversal (the operation which transforms t into $-t$) also the past behavior of the system for all times $t < t_0$ is perfectly determined and knowable once its present state is known. Such a consequence is usually called *determinism*. Determinism is implemented by assuming that the system satisfies a set of first-order differential equations of the form

$$\frac{d}{dt}\mathbf{S} = F[\mathbf{S}(t)], \tag{1.1}$$

where $\mathbf{S}$ is a vector describing the state of the system. It is also assumed that these equations (called equations of motion) have one and only one solution, and this situation is usual if the functional transformation F is not too nasty.

Another very important principle, implicitly assumed since the early days of classical mechanics but brought into the scientific debate only in the 1930s, is the *principle of separability*: given two non-interacting physical systems $\mathcal{S}_1$ and $\mathcal{S}_2$, all their physical properties are separately determined. Stated in other terms, the outcome of a measurement on $\mathcal{S}_1$ cannot depend on a measurement performed on $\mathcal{S}_2$.

We are now in the position to define what a *state* in classical mechanics is. Let us first consider for the sake of simplicity a particle moving in one dimension. Its initial state is well defined by the position x_0 and momentum p_0 of the particle at time t_0. The knowledge of the equations of motion of the particle would then allow us to infer the position $x(t)$ and the momentum $p(t)$ of the particle at all times t.

It is straightforward to generalize this definition to systems with n degrees of freedom. For such a system we distinguish a coordinate configuration space $\{q_1, q_2, \ldots, q_n\} \in \mathbb{R}^n$ and a momentum configuration space $\{p_1, p_2, \ldots, p_n\} \in \mathbb{R}^n$, where the q_j's $(j = 1, \ldots, n)$ are the generalized coordinates and the p_j's $(j = 1, \ldots, n)$ the generalized momenta. On

the other hand, the phase space Γ is the set $\{q_1, q_2, \ldots, q_n; p_1, p_2, \ldots, p_n\} \in \mathbb{R}^{2n}$. The state of a system with n degrees of freedom is then represented by a point in the $2n$-dimensional phase space Γ.

Let us consider what happens by making use of the Lagrangian approach. Here, the equations of motion can be derived from the knowledge of a Lagrangian function. Given a generalized coordinate q_j, we define its *canonically conjugate variable* or *generalized momentum* p_j as the quantity

$$p_j = \frac{\partial}{\partial \dot{q}_j} \mathrm{L}(q_1, \ldots, q_n; \dot{q}_1, \ldots, \dot{q}_n), \tag{1.2}$$

where the $\dot{q}_k$ are the generalized velocities. In the simplest case (position-independent kinetic energy and velocity-independent potential) we have

$$\mathrm{L}(q_1, \ldots, q_n, \dot{q}_1, \ldots : \dot{q}_n) = T(\dot{q}_1, \ldots, \dot{q}_n) - V(q_1, \ldots, q_n), \tag{1.3}$$

where L is the *Lagrangian function* and T and V are the kinetic and potential energy, respectively. The kinetic energy is a function of the generalized velocities $\dot{q}_j$ $(j = 1, \ldots, n)$ and may also be written as

$$T = \sum_j \frac{p_j^2}{2m_j}, \tag{1.4}$$

i.e. as a function of the generalized momenta p_j $(j = 1, \ldots, n)$, where m_j is the mass associated with the j-th degree of freedom.

In an alternative approach, a classical system is defined by the function

$$H = T(p_1, p_2, \ldots, p_n) + V(q_1, q_2, \ldots, q_n), \tag{1.5}$$

which is known as the Hamiltonian or the energy function, simply given by the sum of kinetic and potential energy. Differently from the Lagrangian function, H is directly observable because it represents the energy of the system. The relationship between Lagrangian and Hamiltonian functions is given by

$$H = \sum_j \dot{q}_j p_j - \mathrm{L}(q_1, \ldots, q_n, \dot{q}_1, \ldots : \dot{q}_n) \tag{1.6}$$

in conjunction with (1.2).

For the sake of simplicity we have assumed that the Lagrangian and the Hamiltonian functions are not explicitly time-dependent. The coordinate q_k and momentum p_k, together with their time derivatives $\dot{q}_k$, $\dot{p}_k$, are linked – through the Hamiltonian – by the Hamilton canonical equations of motion

$$\dot{q}_k = \frac{\partial H}{\partial p_k}, \quad \dot{p}_k = -\frac{\partial H}{\partial q_k}, \tag{1.7}$$

which can also be written in terms of the Poisson brackets as

$$\dot{q}_k = \{q_k, H\}, \quad \dot{p}_k = \{p_k, H\}. \tag{1.8}$$

The Poisson brackets for two arbitrary functions f and g are defined as

$$\{f,g\}=\sum_j\left(\frac{\partial f}{\partial q_j}\frac{\partial g}{\partial p_j}-\frac{\partial f}{\partial p_j}\frac{\partial g}{\partial q_j}\right), \tag{1.9}$$

and have the following properties:

$$\{f,g\}=-\{g,f\}, \tag{1.10a}$$
$$\{f,C\}=0, \tag{1.10b}$$
$$\{Cf+C'g,h\}=C\{f,h\}+C'\{g,h\}, \tag{1.10c}$$
$$0=\{f,\{g,h\}\}+\{g,\{h,f\}\}+\{h,\{f,g\}\}, \tag{1.10d}$$
$$\frac{\partial}{\partial t}\{f,g\}=\left\{\frac{\partial f}{\partial t},g\right\}+\left\{f,\frac{\partial g}{\partial t}\right\}, \tag{1.10e}$$

where C, C' are constants and h is a third function. Equation (1.10d) is known as the Jacobi identity. The advantage of this notation is that, for any function f of q and p, we can write

$$\frac{d}{dt}f=\{f,H\}. \tag{1.11}$$

It is easy to see that Newton's second law can be derived from Hamilton's equations. In fact, from Eq. (1.8) we have

$$\dot{q}_k=\{q_k,H\}=\frac{p_k}{m_k}, \tag{1.12a}$$
$$\dot{p}_k=\{p_k,H\}=-\frac{\partial V}{\partial q_k}. \tag{1.12b}$$

From Eq. (1.12a) one obtains $p_k=m_k\dot{q}_k$ (the definition of generalized momentum), which, substituted into Eq. (1.12b), gives

$$m_k\ddot{q}_k=-\frac{\partial V}{\partial q_k}. \tag{1.13}$$

Since $F_k=-\partial V/\partial q_k$ is the generalized force relative to the k-th degree of freedom, Eq. (1.13) can be regarded as Newton's second law. As a consequence, Newton's second law can be written in terms of a first-order differential equation (as anticipated above). However, in this case we need both the knowledge of position and of momentum for describing a system.

In classical mechanics the equations of motion may also be determined by imposing that the action

$$\mathrm{S}=\int_{t_1}^{t_2}dt\mathrm{L}(q_1,\ldots,q_n,\dot{q}_1,\ldots,\dot{q}_n) \tag{1.14}$$

has an extreme value. This is known as the *Principle of least action* or Maupertuis–Hamilton principle.

The application of this principle yields the *Lagrange equations*

$$\frac{d}{dt}\left(\frac{\partial \mathrm{L}}{\partial \dot{q}_k}\right)-\frac{\partial \mathrm{L}}{\partial q_k}=0, \tag{1.15}$$