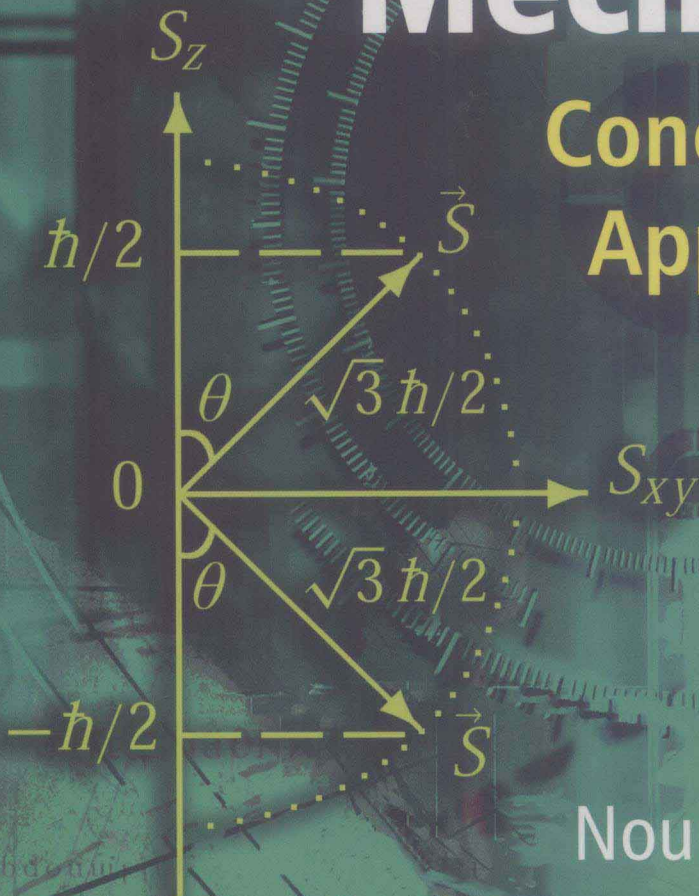


SECOND EDITION

Quantum Mechanics

Concepts and
Applications



Nouredine Zettili

 WILEY

Quantum Mechanics Concepts and Applications

Second Edition

Nouredine Zettili

Jacksonville State University, Jacksonville, USA



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Quantum Mechanics

Second Edition

Preface

Preface to the Second Edition

It has been eight years now since the appearance of the first edition of this book in 2001. During this time, many courteous users—professors who have been adopting the book, researchers, and students—have taken the time and care to provide me with valuable feedback about the book. In preparing the second edition, I have taken into consideration the generous feedback I have received from these users. To them, and from the very outset, I want to express my deep sense of gratitude and appreciation.

The underlying focus of the book has remained the same: to provide a well-structured and self-contained, yet concise, text that is backed by a rich collection of fully solved examples and problems illustrating various aspects of nonrelativistic quantum mechanics. The book is intended to achieve a double aim: on the one hand, to provide instructors with a pedagogically suitable teaching tool and, on the other, to help students not only master the underpinnings of the theory but also become effective practitioners of quantum mechanics.

Although the overall structure and contents of the book have remained the same upon the insistence of numerous users, I have carried out a number of streamlining, surgical type changes in the second edition. These changes were aimed at fixing the weaknesses (such as typos) detected in the first edition while reinforcing and improving on its strengths. I have introduced a number of sections, new examples and problems, and new material; these are spread throughout the text. Additionally, I have operated substantive revisions of the exercises at the end of the chapters; I have added a number of new exercises, jettisoned some, and streamlined the rest. I may underscore the fact that the collection of end-of-chapter exercises has been thoroughly classroom tested for a number of years now.

The book has now a collection of almost six hundred examples, problems, and exercises. Every chapter contains: (a) a number of solved examples each of which is designed to illustrate a specific concept pertaining to a particular section within the chapter, (b) plenty of fully solved problems (which come at the end of every chapter) that are generally comprehensive and, hence, cover several concepts at once, and (c) an abundance of unsolved exercises intended for homework assignments. Through this rich collection of examples, problems, and exercises, I want to empower the student to become an independent learner and an adept practitioner of quantum mechanics. Being able to solve problems is an unailing evidence of a real understanding of the subject.

The second edition is backed by useful resources designed for instructors adopting the book (please contact the author or Wiley to receive these free resources).

The material in this book is suitable for three semesters—a two-semester undergraduate course and a one-semester graduate course. A pertinent question arises: How to actually use

the book in an undergraduate or graduate course(s)? There is no simple answer to this question as this depends on the background of the students and on the nature of the course(s) at hand. First, I want to underscore this important observation: As the book offers an abundance of information, every instructor should certainly select the topics that will be most relevant to her/his students; going systematically over all the sections of a particular chapter (notably Chapter 2), one might run the risk of getting bogged down and, hence, ending up spending too much time on technical topics. Instead, one should be highly selective. For instance, for a one-semester course where the students have not taken modern physics before, I would recommend to cover these topics: Sections 1.1–1.6; 2.2.2, 2.2.4, 2.3, 2.4.1–2.4.8, 2.5.1, 2.5.3, 2.6.1–2.6.2, 2.7; 3.2–3.6; 4.3–4.8; 5.2–5.4, 5.6–5.7; and 6.2–6.4. However, if the students have taken modern physics before, I would skip Chapter 1 altogether and would deal with these sections: 2.2.2, 2.2.4, 2.3, 2.4.1–2.4.8, 2.5.1, 2.5.3, 2.6.1–2.6.2, 2.7; 3.2–3.6; 4.3–4.8; 5.2–5.4, 5.6–5.7; 6.2–6.4; 9.2.1–9.2.2, 9.3, and 9.4. For a two-semester course, I think the instructor has plenty of time and flexibility to maneuver and select the topics that would be most suitable for her/his students; in this case, I would certainly include some topics from Chapters 7–11 as well (but not all sections of these chapters as this would be unrealistically time demanding). On the other hand, for a one-semester graduate course, I would cover topics such as Sections 1.7–1.8; 2.4.9, 2.6.3–2.6.5; 3.7–3.8; 4.9; and most topics of Chapters 7–11.

Acknowledgments

I have received very useful feedback from many users of the first edition; I am deeply grateful and thankful to everyone of them. I would like to thank in particular Richard Lebed (Arizona State University) who has worked selflessly and tirelessly to provide me with valuable comments, corrections, and suggestions. I want also to thank Jearl Walker (Cleveland State University)—the author of *The Flying Circus of Physics* and of the Halliday–Resnick–Walker classics, *Fundamentals of Physics*—for having read the manuscript and for his wise suggestions; Milton Cha (University of Hawaii System) for having proofread the entire book; Felix Chen (Powerwave Technologies, Santa Ana) for his reading of the first 6 chapters. My special thanks are also due to the following courteous users/readers who have provided me with lists of typos/errors they have detected in the first edition: Thomas Sayetta (East Carolina University), Moritz Braun (University of South Africa, Pretoria), David Berkowitz (California State University at Northridge), John Douglas Hey (University of KwaZulu-Natal, Durban, South Africa), Richard Arthur Dudley (University of Calgary, Canada), Andrea Durlò (founder of the A.I.F. (Italian Association for Physics Teaching), Ferrara, Italy), and Rick Miranda (Netherlands). My deep sense of gratitude goes to M. Bulut (University of Alabama at Birmingham) and to Heiner Mueller-Krumbhaar (Forschungszentrum Juelich, Germany) and his Ph.D. student C. Gugenberger for having written and tested the C++ code listed in Appendix C, which is designed to solve the Schrödinger equation tested for a one-dimensional harmonic oscillator and for an infinite square-well potential.

Finally, I want to thank my editors, Dr. Andy Slade, Celia Carden, and Alexandra Carrick, for their consistent hard work and friendly support throughout the course of this project.

N. Zettili
Jacksonville State University, USA
January 2009

Preface to the First Edition

Books on quantum mechanics can be grouped into two main categories: textbooks, where the focus is on the formalism, and purely problem-solving books, where the emphasis is on applications. While many fine textbooks on quantum mechanics exist, problem-solving books are far fewer. It is not my intention to merely add a text to either of these two lists. My intention is to combine the two formats into a single text which includes the ingredients of both a textbook and a problem-solving book. Books in this format are practically nonexistent. I have found this idea particularly useful, for it gives the student easy and quick access not only to the essential elements of the theory but also to its practical aspects in a unified setting.

During many years of teaching quantum mechanics, I have noticed that students generally find it easier to learn its underlying ideas than to handle the practical aspects of the formalism. Not knowing how to calculate and extract numbers out of the formalism, one misses the full power and utility of the theory. Mastering the techniques of problem-solving is an essential part of learning physics. To address this issue, the problems solved in this text are designed to teach the student how to calculate. No real mastery of quantum mechanics can be achieved without learning how to derive and calculate quantities.

In this book I want to achieve a double aim: to give a self-contained, yet concise, presentation of most issues of nonrelativistic quantum mechanics, and to offer a rich collection of fully solved examples and problems. This unified format is not without cost. Size! Judicious care has been exercised to achieve conciseness without compromising coherence and completeness.

This book is an outgrowth of undergraduate and graduate lecture notes I have been supplying to my students for about one decade; the problems included have been culled from a large collection of homework and exam exercises I have been assigning to the students. It is intended for senior undergraduate and first-year graduate students. The material in this book could be covered in three semesters: Chapters 1 to 5 (excluding Section 3.7) in a one-semester undergraduate course; Chapter 6, Section 7.3, Chapter 8, Section 9.2 (excluding fine structure and the anomalous Zeeman effect), and Sections 11.1 to 11.3 in the second semester; and the rest of the book in a one-semester graduate course.

The book begins with the experimental basis of quantum mechanics, where we look at those atomic and subatomic phenomena which confirm the failure of classical physics at the microscopic scale and establish the need for a new approach. Then come the mathematical tools of quantum mechanics such as linear spaces, operator algebra, matrix mechanics, and eigenvalue problems; all these are treated by means of Dirac's bra-ket notation. After that we discuss the formal foundations of quantum mechanics and then deal with the exact solutions of the Schrödinger equation when applied to one-dimensional and three-dimensional problems. We then look at the stationary and the time-dependent approximation methods and, finally, present the theory of scattering.

I would like to thank Professors Ismail Zahed (University of New York at Stony Brook) and Gerry O. Sullivan (University College Dublin, Ireland) for their meticulous reading and comments on an early draft of the manuscript. I am grateful to the four anonymous reviewers who provided insightful comments and suggestions. Special thanks go to my editor, Dr Andy Slade, for his constant support, encouragement, and efficient supervision of this project.

I want to acknowledge the hospitality of the Center for Theoretical Physics of MIT, Cambridge, for the two years I spent there as a visitor. I would like to thank in particular Professors Alan Guth, Robert Jaffee, and John Negele for their support.

Note to the student

We are what we repeatedly do. Excellence, then, is not an act, but a habit.

Aristotle

No one expects to learn swimming without getting wet. Nor does anyone expect to learn it by merely reading books or by watching others swim. Swimming cannot be learned without practice. There is absolutely no substitute for throwing yourself into water and training for weeks, or even months, till the exercise becomes a smooth reflex.

Similarly, physics *cannot be learned passively*. Without tackling various challenging problems, the student has no other way of testing the quality of his or her understanding of the subject. Here is where the student gains the sense of satisfaction and involvement produced by a genuine understanding of the underlying principles. *The ability to solve problems is the best proof of mastering the subject*. As in swimming, the more you solve problems, the more you sharpen and fine-tune your problem-solving skills.

To derive full benefit from the examples and problems solved in the text, avoid consulting the solution too early. If you cannot solve the problem after your first attempt, try again! If you look up the solution only after several attempts, it will remain etched in your mind for a long time. But if you manage to solve the problem on your own, you should still compare your solution with the book's solution. You might find a shorter or more elegant approach.

One important observation: as the book is laden with a rich collection of fully solved examples and problems, one should absolutely avoid the temptation of memorizing the various techniques and solutions; instead, one should focus on understanding the concepts and the underpinnings of the formalism involved. It is not my intention in this book to teach the student a number of tricks or techniques for acquiring good grades in quantum mechanics classes without genuine understanding or mastery of the subject; that is, I didn't mean to teach the student how to pass quantum mechanics exams without a deep and lasting understanding. However, the student who focuses on understanding the underlying foundations of the subject and on reinforcing that by solving numerous problems and thoroughly understanding them will doubtlessly achieve a double aim: reaping good grades as well as obtaining a sound and long-lasting education.

N. Zettili

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Chapter 1

Origins of Quantum Physics

In this chapter we are going to review the main physical ideas and experimental facts that defied classical physics and led to the birth of quantum mechanics. The introduction of quantum mechanics was prompted by the failure of classical physics in explaining a number of microphysical phenomena that were observed at the end of the nineteenth and early twentieth centuries.

1.1 Historical Note

At the end of the nineteenth century, physics consisted essentially of classical mechanics, the theory of electromagnetism¹, and thermodynamics. Classical mechanics was used to predict the dynamics of *material bodies*, and Maxwell's electromagnetism provided the proper framework to study *radiation*; *matter* and *radiation* were described in terms of *particles* and *waves*, respectively. As for the interactions between matter and radiation, they were well explained by the Lorentz force or by thermodynamics. The overwhelming success of classical physics—classical mechanics, classical theory of electromagnetism, and thermodynamics—made people believe that the ultimate description of nature had been achieved. It seemed that all known physical phenomena could be explained within the framework of the general theories of matter and radiation.

At the turn of the twentieth century, however, classical physics, which had been quite unsailable, was seriously challenged on two major fronts:

- **Relativistic domain:** Einstein's 1905 theory of relativity showed that the validity of Newtonian mechanics ceases at very high speeds (i.e., at speeds comparable to that of light).
- **Microscopic domain:** As soon as new experimental techniques were developed to the point of probing atomic and subatomic structures, it turned out that classical physics fails miserably in providing the proper explanation for several newly discovered phenomena. It thus became evident that the validity of classical physics ceases at the microscopic level and that *new* concepts had to be invoked to describe, for instance, the structure of atoms and molecules and how light interacts with them.

¹Maxwell's theory of electromagnetism had unified the, then ostensibly different, three branches of physics: electricity, magnetism, and optics.

The failure of classical physics to explain several microscopic phenomena—such as blackbody radiation, the photoelectric effect, atomic stability, and atomic spectroscopy—had cleared the way for seeking new ideas outside its purview.

The first real breakthrough came in 1900 when Max Planck introduced the concept of the *quantum* of energy. In his efforts to explain the phenomenon of blackbody radiation, he succeeded in reproducing the experimental results only after postulating that the energy exchange between *radiation* and its surroundings takes place in *discrete*, or *quantized*, amounts. He argued that the energy exchange between an *electromagnetic wave* of frequency ν and matter occurs *only in integer multiples* of $h\nu$, which he called the energy of a *quantum*, where h is a fundamental constant called *Planck's constant*. The quantization of electromagnetic radiation turned out to be an idea with far-reaching consequences.

Planck's idea, which gave an accurate explanation of blackbody radiation, prompted new thinking and triggered an avalanche of new discoveries that yielded solutions to the most outstanding problems of the time.

In 1905 Einstein provided a powerful consolidation to Planck's quantum concept. In trying to understand the photoelectric effect, Einstein recognized that Planck's idea of the quantization of the *electromagnetic waves* must be valid for *light* as well. So, following Planck's approach, he posited that *light itself is made of discrete bits of energy (or tiny particles)*, called *photons*, each of energy $h\nu$, ν being the frequency of the light. The introduction of the photon concept enabled Einstein to give an elegantly accurate explanation to the photoelectric problem, which had been waiting for a solution ever since its first experimental observation by Hertz in 1887.

Another seminal breakthrough was due to Niels Bohr. Right after Rutherford's experimental discovery of the atomic nucleus in 1911, and combining Rutherford's atomic model, Planck's quantum concept, and Einstein's photons, Bohr introduced in 1913 his model of the hydrogen atom. In this work, he argued that atoms can be found only in *discrete states* of energy and that the interaction of atoms with radiation, i.e., the emission or absorption of radiation by atoms, takes place only in *discrete amounts* of $h\nu$ because it results from transitions of the atom between its various discrete energy states. This work provided a satisfactory explanation to several outstanding problems such as atomic stability and atomic spectroscopy.

Then in 1923 Compton made an important discovery that gave the most conclusive confirmation for the corpuscular aspect of light. By scattering X-rays with electrons, he confirmed that the X-ray photons behave like particles with momenta $h\nu/c$; ν is the frequency of the X-rays.

This series of breakthroughs—due to Planck, Einstein, Bohr, and Compton—gave both the theoretical foundations as well as the conclusive experimental confirmation for the particle aspect of waves; that is, the concept that waves exhibit particle behavior at the microscopic scale. At this scale, classical physics fails not only quantitatively but even qualitatively and conceptually.

As if things were not bad enough for classical physics, de Broglie introduced in 1923 another powerful new concept that classical physics could not reconcile: he postulated that not only does radiation exhibit particle-like behavior but, conversely, *material particles* themselves display *wave-like* behavior. This concept was confirmed experimentally in 1927 by Davisson and Germer; they showed that interference patterns, a property of waves, can be obtained with material particles such as electrons.

Although Bohr's model for the atom produced results that agree well with experimental spectroscopy, it was criticized for lacking the ingredients of a theory. Like the "quantization" scheme introduced by Planck in 1900, the postulates and assumptions adopted by Bohr in 1913