Fundamentals of Quantum Mechanics

Quantum mechanics has evolved from a subject of study in pure physics to one with a wide range of applications in many diverse fields. The basic concepts of quantum mechanics are explained in this book in a concise and easy-to-read manner, leading toward applications in solid state electronics and modern optics. Following a logical sequence, the book is focused on the key ideas and is conceptually and mathematically self-contained. The fundamental principles of quantum mechanics are illustrated by showing their application to systems such as the hydrogen atom, multi-electron ions and atoms, the formation of simple organic molecules and crystalline solids of practical importance. It leads on from these basic concepts to discuss some of the most important applications in modern semiconductor electronics and optics.

Containing many homework problems, the book is suitable for senior-level undergraduate and graduate level students in electrical engineering, materials science, and applied physics and chemistry.

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For Solid State Electronics and Optics

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Preface

Quantum mechanics has evolved from a subject of study in pure physics to one with a vast range of applications in many diverse fields. Some of its most important applications are in modern solid state electronics and optics. As such, it is now a part of the required undergraduate curriculum of more and more electrical engineering, materials science, and applied physics schools. This book is based on the lecture notes that I have developed over the years teaching introductory quantum mechanics to students at the senior/first year graduate school level whose interest is primarily in applications in solid state electronics and modern optics.

There are many excellent introductory text books on quantum mechanics for students majoring in physics or chemistry that emphasize atomic and nuclear physics for the former and molecular and chemical physics for the latter. Often, the approach is to begin from a historic perspective, recounting some of the experimental observations that could not be explained on the basis of the principles of classical mechanics and electrodynamics, followed by descriptions of various early attempts at developing a set of new principles that could explain these 'anomalies.' It is a good way to show the students the historical thinking that led to the discovery and formulation of the basic principles of quantum mechanics. This might have been a reasonable approach in the first half of the twentieth century when it was an interesting story to be told and people still needed to be convinced of its validity and utility. Most students today know that quantum theory is now well established and important. What they want to know is not how to reinvent quantum mechanics, but what the basic principles are concisely and how they are used in applications in atomic, molecular, and solid state physics. For electronics, materials science, and applied physics students in particular, they need to see, above all, how quantum mechanics forms the foundations of modern semiconductor electronics and optics. To meet this need is then the primary goal of this introductory text/reference book, for such students and for those who did not have any quantum mechanics in their earlier days as an undergraduate student but wish now to learn the subject on their own.

This book is not encyclopedic in nature but is focused on the key concepts and results. Hopefully it makes sense pedagogically. As a textbook, it is conceptually and mathematically self-contained in the sense that all the results are derived, or derivable, from first principles, based on the material presented in the book in a logical order without excessive reliance on reference sources. The emphasis is on concise physical explanations, complemented by rigorous mathematical demonstrations, of how things work and why they work the way they do.

A brief introduction is given in **Chapter** 1 on how one goes about formulating and solving problems on the atomic and subatomic scale. This is followed in **Chapter** 2 by a concise description of the basic postulates of quantum mechanics and the terminology and mathematical tools that one will need for the rest of the book. This part of the book by necessity tends to be on the abstract side and might appear to be a little formal to some of the beginning students. *It is not necessary to master all the mathematical details and complications at this stage*. For organizational reasons, I feel that it is better to collect all this information at one place at the beginning so that the flow of thoughts and the discussions of the main subject matter will not be repeatedly interrupted later on by the need to introduce the language and tools needed.

The basic principles of quantum mechanics are then applied to a number of simple prototype problems in **Chapters** 3–5 that help to clarify the basic concepts and as a preparation for discussing the more realistic physical problems of interest in later chapters. **Section** 5.4 on photons is a discussion of the application of the basic theory of harmonic oscillators to radiation oscillators. It gives the basic rules of quantization of electromagnetic fields and discusses the historically important problem of black-body radiation and the more recently developed quantum theory of coherent optical states. For an introductory course on quantum mechanics, this material can perhaps be skipped.

Chapters 6 and 7 deal with the hydrogenic and multi-electron atoms and ions. Since the emphasis of this book is not on atomic spectroscopy, some of the mathematical details that can be found in many of the excellent books on atomic physics are not repeated in this book, except for the key concepts and results. These chapters form the foundations of the subsequent discussions in **Chapter** 8 on the important topics of time-dependent perturbation theory and the interaction of radiation with matter. It naturally leads to Einstein's theory of resonant absorption and emission of radiation by atoms. One of its most important progeny is the ubiquitous optical marvel known as the LASER (Light Amplification by Stimulated Emission of Radiation).

From the hydrogenic and multi-electron atoms, we move on to the increasingly more complicated world of molecules and solids in **Chapter** 9. The increased complexity of the physical systems requires more sophisticated approximation procedures to deal with the related mathematical problems. The basic concept and methodology of time-independent perturbation theory is introduced and applied to covalent-bonded diatomic and simple organic molecules. Crystalline solids are in some sense giant molecules with periodic lattice structures. Of particular interest are the sp^3-bonded elemental and compound semiconductors of diamond and zincblende structures.

Some of the most important applications of quantum mechanics are in semiconductor physics and technology based on the properties of charge-carriers in periodic lattices of ions. Basic concepts and results on the electronic properties of semiconductors are discussed in **Chapter** 10. The molecular-orbital picture and the nearly-free-electron model of the origin of the conduction and valence bands in semiconductors based on the powerful Bloch theorem are developed. From these follow the commonly used concepts and parameters to describe the dynamics of charge-carriers in semiconductors, culminating finally in one of the most important building blocks of modern electronic and optical devices: the p–n junction.

For applications involving macroscopic samples of many particles, the basic quantum theory for single-particle systems must be generalized to allow for the situation where the quantum states of the particles in the sample are not all known precisely. For a uniform sample of the same kind of particles in a statistical distribution over all possible states, the simplest approach is to use the density-matrix formalism. The basic concept and properties of the density operator or the density matrix and their equations of motion are introduced in **Chapter 11**. This chapter, and the book, conclude with some examples of applications of this basic approach to a number of linear and nonlinear, static and dynamic, optical problems. For an introductory course on quantum mechanics, this chapter could perhaps be omitted also.

While there might have been, and may still be in the minds of some, doubts about the basis of quantum mechanics on philosophical grounds, there is no ambiguity and no doubt on the applications level. The rules are clear, precise, and all-encompassing, and the predictions and quantitative results are always correct and accurate without exception. It is true, however, that at times it is difficult to penetrate through the mathematical underpinnings of quantum mechanics to the physical reality of the subject. I hope that the material presented and the insights offered in this book will help pave the way to overcoming the inherent difficulties of the subject for some. It is hoped, above all, that the students will find quantum mechanics a fascinating subject to study, not a subject to be avoided.

I am grateful for the opportunities that I have had to work with the students and many of my colleagues in the research community over the years to advance my own understanding of the subject. I would like to thank, in particular, Joe Ballantyne, Chris Flytzanis, Clif Pollck, Peter Powers, Hermann Statz, Frank Wise, and Boris Zeldovich for their insightful comments and suggestions on improving the presentation of the material and precision of the wording. Finally, without the numerous questions and puzzling stares from the generations of students who have passed through my classes and research laboratory, I would have been at a loss to know what to write about.

A note on the unit system: to facilitate comparison with classic physics literature on quantum mechanics, the unrationalized cgs Gaussian unit system is used in this book unless otherwise stated explicitly.