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QUANTUM MECHANICS

A Conceptual Approach

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To Charlotte

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PREFACE

The physical laws and mathematical structure that constitute the basis of quantum mechanics were derived by physicists, but subsequent applications became of interest not just to the physicists but also to chemists, biologists, medical scientists, engineers, and philosophers. Quantum mechanical descriptions of atomic and molecular structure are now taught in freshman chemistry and even in some high school chemistry courses. Sophisticated computer programs are routinely used for predicting the structures and geometries of large organic molecules or for the indentification and evaluation of new medicinal drugs. Engineers have incorporated the quantum mechanical tunneling effect into the design of new electronic devices, and philosophers have studied the consequences of some of the novel concepts of quantum mechanics. They have also compared the relative merits of different axiomatic approaches to the subject.

In view of the widespread applications of quantum mechanics to these areas there are now many people who want to learn more about the subject. They may, of course, try to read one of the many quantum textbooks that have been written, but almost all of these textbooks assume that their readers have an extensive background in physics and mathematics; very few of these books make an effort to explain the subject in simple non-mathematical terms.

In this book we try to present the fundamentals and some simple applications of quantum mechanics by emphasizing the basic concepts and by keeping the mathematics as simple as possible. We do assume that the reader is familiar with elementary calculus; it is after all not possible to explain the Schödinger equation to someone who does not know what a derivative or an integral is. Some of the mathematical techniques that are essential for understanding quantum mechanics, such as matrices and determinants, differential equations, Fourier analysis, and so on are

described in a simple manner. We also present some applications to atomic and molecular structure that constitute the basis of the various molecular structure computer programs, but we do not attempt to describe the computation techniques in detail.

Many authors present quantum mechanics by means of the axiomatic approach, which leads to a rigorous mathematical representation of the subject. However, in some instances it is not easy for an average reader to even understand the axioms, let alone the theorems that are derived from them. I have always looked upon quantum mechanics as a conglomerate of revolutionary new concepts rather than as a rigid mathematical discipline. I also feel that the reader might get a better understanding and appreciation of these concepts if the reader is familiar with the background and the personalities of the scientists who conceived them and with the reasoning and arguments that led to their conception. Our approach to the presentation of quantum mechanics may then be called historic or conceptual but is perhaps best described as pragmatic. Also, the inclusion of some historical background makes the book more readable.

I did not give a detailed description of the various sources I used in writing the historical sections of the book because many of the facts that are presented were derived from multiple sources. Some of the material was derived from personal conversations with many scientists and from articles in various journals. The most reliable sources are the original publications where the new quantum mechanical ideas were first proposed. These are readily available in the scientific literature, and I was intrigued in reading some of the original papers. I also read various biographies and autobiographies. I found Moore's biography of Schröedinger, Constance Reid's biographies of Hilbert and Courant, Abraham Pais' reminiscences, and the autobiographies of Elsasser and Casimir particularly interesting. I should mention that Kramers was the professor of theoretical physics when I was a student at Leiden University. He died before I finished my studies and I never worked under his supervision, but I did learn quantum mechanics by reading his book and by attending his lectures.

Finally I wish to express my thanks to Mrs. Alice Chen for her valuable help in typing and preparing the manuscript.

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