Quantum Physics

Arno Bohm • Piotr Kielanowski •
G. Bruce Mainland

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States, Observables and Their Time Evolution

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Arno Bohm
Department of Physics
University of Texas
Austin
TX, USA

Piotr Kielanowski
Department of Physics
CINVESTAV
Mexico City
Mexico

G. Bruce Mainland
Department of Physics
Ohio State University
Columbus
OH, USA

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Preface

> "Quantum Mechanics" is the description of the behavior of matter and light in all its details and, in particular, of the happenings on an atomic scale. Things on a very small scale behave like nothing you have any direct experience about. They do not behave like waves, they do not behave like particles, they do not behave like clouds, or billiard balls, or weights on springs, or like anything you have ever seen.—*Richard Feynman*

This book has been written to serve as a text for an introductory graduate course; much of the material can also be used for an advanced, undergraduate course. Its precursor[1] has been used many times in a 1-year, introductory, graduate course.

Throughout the text either theoretical developments have been motivated by experimental observations or theory has been used to explain experimental data. The authors have made a significant effort to make the material more easily accessible by (a) providing systematic explanations, (b) presenting logical step-by-step derivations, (c) imbedding solved examples in the text at appropriate places to clarify the ongoing discussion, (d) summarizing key ideas at the end of each chapter, and (e) providing an extensive set of problems at the end of each chapter.

Some chapters may be appropriate for courses in quantum chemistry since many physical applications in this book have been chosen from molecular spectra and molecular structure,[2] which serves as a fertile ground for examples of non-relativistic quantum physics.

The sections "Precession of a Spinning Particle in a Magnetic Field: The Interpretation of the Schrödinger and Heisenberg Pictures" and "Magnetic Resonance" can be used in a special topics course as an introduction to nuclear magnetic resonance.

Complicated quantum systems can often be more profitably analyzed, not in terms of their constituents, but instead in terms of more general substructures: specifically, molecules can be analyzed in terms of rotations, oscillations, and

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[1] A. Bohm, *Quantum Mechanics: Foundations and Applications*, Springer-Verlag, New York, 2nd Edition (1986), 3rd Edition (1993), soft-cover printing (2001).

[2] G. Herzberg, *Molecular Spectra and Molecular Structure*, Van Nostrand, New York, 1939–1966.

single-electron excitations,[3] and nuclei can be described in terms of their collective motions.[4] It is remarkable that this way of understanding can also be extended to relativistic systems where the hadron spectra can be analyzed in terms of relativistic rotators and oscillators.[5] This analysis of quantum physical systems in terms of collective motions rather than constituents is also used here to analyze molecular spectra and molecular structure in terms of rotational and vibrational motions.

The objective of this book is to present quantum mechanics in its general form by stressing the operator approach. A major new development in physics usually necessitates a corresponding development in mathematics. For example, differential and integral calculus were developed for classical mechanics, and no one today would teach an advanced course without using this mathematical language. Although the mathematics of linear, scalar-product spaces and linear operators were created and developed to fulfill the needs of quantum physics, quantum mechanics is still often taught without using its mathematical language. By restricting much of a course on quantum mechanics to differential equations and a discussion of their solutions, students may initially find the material easier to grasp because the mathematics is familiar. However, many quantum concepts are difficult to present in this narrow mathematical language that emphasizes only one of the many complementary aspects of quantum physics. There is much more to quantum mechanics than the overemphasized, wave-particle dualism presented in terms of differential equations, and there is no principle that a priori places position and momentum at the forefront. Every observable needs to receive the emphasis that is appropriate for the particular situation being considered.

The mathematics of quantum mechanics, which involves linear, scalar-product spaces and algebras of linear operators, is discussed in Appendix. Rather than treating the mathematics abstractly, each operation in a general, linear space is motivated by first examining the corresponding operation in the familiar three-dimensional vector space. Also, when the properties of scalar-product spaces are discussed, each property is first shown to exist both for the scalar product in three-dimensional vector space and for the scalar product expressed as an integral. The emphasis is on providing an introduction to the mathematics required to perform quantum calculations, not on providing mathematical justification (proofs). This elementary mathematical tutorial has been written for the reader who has no prior knowledge of the general mathematical structure of quantum mechanics. Thus the reader who has some familiarity with the mathematics of linear operators in linear, scalar-product spaces can skip the Appendix. If the reader then finds some aspect of the mathematics in Chap. 1 or in later chapters unfamiliar, the Appendix can be used as a reference.

The discussion of quantum mechanics begins with some basic postulates of quantum mechanics that are formulated and made plausible by using the example of

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[3] Ibid.

[4] A. Bohr, B. R. Mottelson, and J. Rainwater, 1975 Nobel Prize in Physics.

[5] A. Bohm, Y. Neeman, A. O. Barut et al. *Dynamical Groups and Spectrum Generating Algebras*, World Scientific Publishing Co., 1988.

the harmonic oscillator realized by the diatomic molecule. Further basic postulates are introduced in later chapters when the scope of the theory is extended. These basic postulates are not mathematical axioms from which all predictions of the theory can be derived. Such an axiomatic approach does not appear to be possible in physics. Instead, the basic postulates are a concise way of expressing the essence of many experimental results and the successes of various theoretical ideas. In Chap. 1 representations of the algebra of the harmonic oscillator are first determined. The interpretation of experimental data from an energy loss experiment is used to motivate the introduction of the statistical operator—with matrix elements that form the "density matrix"—and to formulate the relationship between average values measured in an experiment and expectation values calculated theoretically. Radiative transitions between harmonic oscillator energy levels and the Einstein coefficients are discussed.

Representations of the algebra of angular momentum are calculated in Chap. 2. The algebra of angular momentum is enlarged by adding the position operator so that the algebra can be used to describe rigid and non-rigid rotating molecules. Theoretical predictions are compared with the experimental spectra of rotating diatomic molecules.

The combination of quantum physical systems using direct-product spaces is discussed in Chap. 3. The theory is used to describe a vibrating rotator, and the theoretical predictions are then compared with data for a vibrating, rotating diatomic molecule. The addition of angular momentum (Clebsch-Gordan coefficients) is discussed. Tensor operators are introduced so that the Wigner-Eckart theorem can be used to relate various experimental data.

The formalism of first- and second-order, non-degenerate perturbation theory and first-order, degenerate perturbation theory is derived in Chap. 4. The basic ideas associated with stationary perturbation are motivated by examining a rotator in a uniform magnetic field. Perturbation theory is used to explain the Stark effect.

Time development is described in Chap. 5 using either the time-dependent Schrödinger equation or Heisenberg's equation of motion. The Schrödinger picture, Heisenberg picture, and interaction picture are discussed. The precession of a spinning particle in a magnetic field is described in both the Schrödinger and Heisenberg pictures to help clarify the relationship between the two pictures. Magnetic resonance is discussed in the Schrödinger picture. The Gibb's distribution and a magnetic resonance experiment are discussed.

Since a discussion of the experimental and theoretical developments that presaged quantum mechanics is necessarily brief, in this book prior knowledge of classical mechanics, some electromagnetic theory, and some atomic physics is required. A basic knowledge of differential and integral calculus is assumed. Some familiarity with matrices, vector algebra, and linear spaces would be helpful.

Austin, TX, USA — Arno Bohm
Mexico City, Mexico — Piotr Kielanowski
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