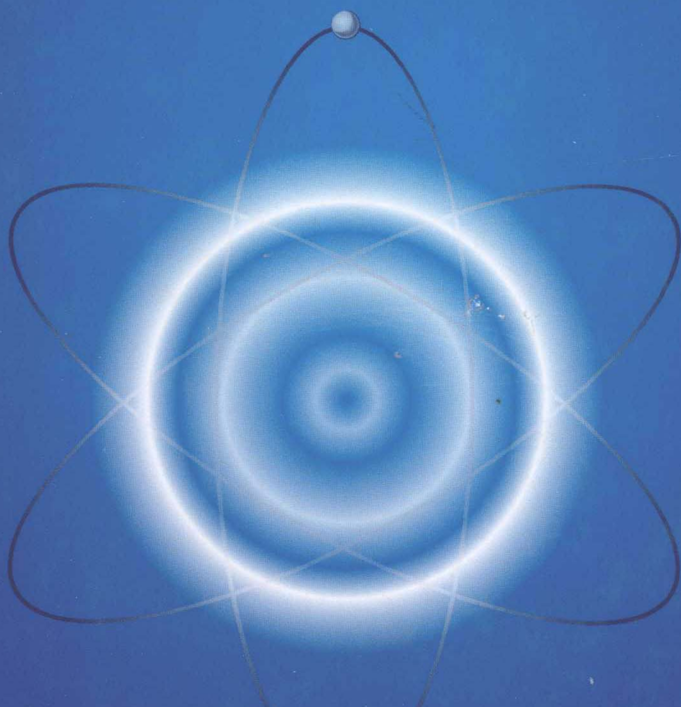
Quantum Mechanics

with Applications to Nanotechnology and Information Science



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QUANTUM MECHANICS

WITH APPLICATIONS TO NANOTECHNOLOGY AND INFORMATION SCIENCE

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PREFACE

Quantum mechanics transcends and supplants classical mechanics at the atomic and subatomic levels. It provides the underlying framework for many subfields of physics, chemistry, and the engineering sciences. It is the only framework for understanding the structure of materials, from the semiconductors in our computers to the metals in our automobiles. It is also the support structure for much of nanotechnology and the promising paradigm of quantum information theory. Moreover, it is the foundation of condensed matter physics, atomic physics, molecular physics, quantum chemistry, materials design, elementary particle, and nuclear physics.

The purpose of this book is to present the fundamentals of quantum theory within a modern perspective, with emphasis on applications to nanoscience and nanotechnology, and information science and information technology. As the frontiers of science have advanced, the sort of curriculum adequate for students in the science and engineering 20 years ago is no longer satisfactory today. Hence, the emphasis is on new topics that are not included in previous books on quantum mechanics [1–11]. These topics include quantum information theory, decoherence and dissipation, quantum measurement theory, disordered systems, and nanotechnology, including spintronics, and reduced dimensional systems such as quantum dots, wires and wells.

The intended readers of this book comprise scientists and engineers, including undergraduate and graduate students in physics, chemistry, materials science, electrical engineering, computer and information science, and nanotechnology. This book can serve as a textbook for a number of courses, including a one-semester undergraduate course in quantum mechanics, a two-semester quantum mechanics undergraduate course, a graduate level quantum mechanics course, an engineering quantum mechanics course, a quantum information and quantum computing course, a nanotechnology course, and a quantum chemistry course. Table 1 specifies the appropriate chapters for each of these courses.

A web page for this book, `https://sites.google.com/site/thequantumbook/`, contains links to interesting web sites related to the subject matter, a link to a list of errors that were found, color versions of the figures of this book, and a means for reporting errors that you find. Please use the e-mail addresses on the web page of the book to contact us with any comments and suggestions regarding this book.

Although we assume the reader is familiar with material ordinarily presented in first-year physics and first-year calculus courses, as well as in linear algebra, Appendices that review the requisite mathematical background material are provided, and a review of classical mechanics is presented in Chapter 16, see `https://sites.google.com/site/thequantumbook/QM_Classical.pdf`.

The layout of this book is as follows. Chapter 1 contains an introduction to quantum mechanics. It explains what quantum mechanics is and why it is essential to properly describe matter and radiation. It includes a brief introductory of nanotechnology and information science and then provides a first taste of quantum mechanics. [Readers who are not well versed in classical mechanics, may need to read Chp_16_Classical_Mechanics.pdf, which is linked to the web page of the book. It presents classical mechanics, including the Lagrangian and Hamiltonian formulation of mechanics; it provides a contrast with quantum mechanics, yet introduces some concepts that are carried over to quantum mechanics.] Chapter 2 presents the formalism of quantum mechanics, including the mathematical notation required for Hilbert Spaces, Dirac notation, and the various representations of quantum mechanics. Chapter 3 presents angular momentum and spherical symmetry, and Chapter 4 covers spin angular momentum, fine sturcture, hyperfine structure, and magnetic resonance. Chapter 5 considers quantum information, after briefly introducing some concepts from classical information theory. This chapter also introduces the Einstein–Podolsky–Rosen paradox and the Bell's inequalities. The quantum dynamics and quantum correlations of two-level systems (including spin systems), three-level systems, and multi-level systems, as well as wave packet dynamics, and quantum optical control theory are the topics discussed in Chapter 6. The approximation methods described in Chapter 7 include basis-state expansions, semiclassical approximations time-independent and time-dependent perturbation theory, variational methods, sudden and adiabatic approximations, the Berry phase concept, and linear response theory. Chapter 8 on identical particles discusses exchange symmetry of bosons and fermions. Chapter 9 presents the electronic properties of solids, starting from the treatment of the free electron gas and electrons in a periodic potential and then describes metals, semiconductors, and insulators. In Chapter 10, mean-field theories to treat multi-electron systems such as atoms, molecules, and also condensed phase systems are introduced, including Hartree–Fock and configuration interaction, which goes beyond mean field. Some topics for describing molecules are introduced in Chapter 11, including point groups, the Born–Oppenheimer approximation, and the Franck–Condon principle. Scattering theory is presented in Chapter 12, including scattering in one dimension and two dimensions, and scattering in disordered systems. Chapter 13 introduces the quantum mechanics needed to treat low-dimensional systems such as quantum dots, wires, and wells, and other low-dimensional systems. Many-body theory is the topic of Chapter 14, including the basic formulation of second quantization, its application to statistical mechanics, and mean-field theory methods. Finally, density functional theory, the most widely used method for calculating ground-state electronic structure, is the topic of Chapter 15. Appendices on linear algebra and Dirac notation for vectors in Hilbert space (Chapter A), some simple ordinary differential equations required in our treatment of quantum mechanics (B), vector analysis (C), Fourier analysis (D), and group theory (E) are presented at the end of the book.

Because of space limitations, a number of chapters that were originally planned to be part of the book will not appear in the printed version but will be linked to the web page of the book (shortly after printing). Chp_16_Classical_Mechanics.pdf deals with classical mechanics (see above), Chapter_17_Decoherence_Dissipation.pdf considers decoherence and dissipation phenomena and covers the spin-boson model, the Caldeira–Leggett model, master equations, and more generally, the field of *open system dynamics*. Chp_18_Many_Body_Th_Applications.pdf presents field theory methods to treat Landau–Fermi liquid theory, superconductivity, Bose–Einstein condensation, superfluidity, the Hubard model, and the Kondo effect. Finally, Chp_19_Insulators.pdf gives additional detail regarding insulating materials. A list of errors and typos entitled QM_errors_typos.pdf will also be linked to the book web page.

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Table 1 Possible courses based on *Quantum Mechanics with Applications to Nanotechnology and Quantum Information Science* and recommended book chapters.

	Undergrad Quantum Mechanics 1	Undergrad Quantum Mechanics 2	Quantum information and Quantum Computing	Nano-technology	Engineering Quantum Mechanics	Quantum Chemistry (2 Semesters)	Condensed Matter (Solid State)	Graduate Quantum Mechanics
1 Intro. to Quantum Mechanics	x		x		x	x		
2 Formalism of Quantum Mechanics	x		x		x	x		
3 Angular Momentum and Spherical Symmetry	x		Sec. 4.1		x	x		
4 Spin	x		x		x	x		
5 Quantum Information			x					x
6 Quantum Dynamics and Correlations		Optional	x					x
7 Approximation Methods		x			x	x		
8 Identical Particles		x		Optional	x	x		
9 Electronic Properties of Solids		Optional		x	x		x	
10 Electronic Structure of Multi-Electron Systems		x		x	x	x	x	

(Continued)

	Undergrad Quantum Mechanics 1	Undergrad Quantum Mechanics 2	Quantum information and Quantum Computing	Nano-technology	Engineering Quantum Mechanics	Quantum Chemistry (2 Semesters)	Condensed Matter (Solid State)	Graduate Quantum Mechanics
11 Molecules		X				X		
12 Scattering Theory				Optional				X
13 Low-Dimensional Systems			Optional	X			X	Optional
14 Many-Body Theory				Optional		Optional	X	X
15 Density Functional Theory				X		Optional	Optional	Optional
Mathematical Appendices	X					X		
16 Review of Classical Mechanics	X					X		
17 Decoherence and Dissipation			X				X	X
18 Field Theory Applications				Optional		Optional	X	X
19 Insulators				Optional			X	X

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