

Quantum Mechanics: Concepts and Applications

Nouredine Zettili
Jacksonville State University

April 2002

Contents

Preface	xiii
1 Origins of Quantum Physics	1
1.1 Historical Note	1
1.2 Particle Aspect of Radiation	4
1.2.1 Blackbody Radiation	4
1.2.2 Photoelectric Effect	10
1.2.3 Compton Effect	13
1.2.4 Pair Production	15
1.3 Wave Aspect of Particles	17
1.3.1 de Broglie's Hypothesis: Matter Waves	17
1.3.2 Experimental Confirmation of de Broglie's Hypothesis	18
1.3.3 Matter Waves for Macroscopic Objects	20
1.4 Particles versus Waves	21
1.4.1 Classical View of Particles and Waves	21
1.4.2 Quantum View of Particles and Waves	23
1.4.3 Wave-Particle Duality: Complementarity	25
1.4.4 Principle of Linear Superposition	26
1.5 Indeterministic Nature of the Microphysical World	27
1.5.1 Heisenberg Uncertainty Principle	27
1.5.2 Probabilistic Interpretation	29
1.6 Atomic Transitions and Spectroscopy	30
1.6.1 Rutherford Planetary Model of the Atom	30
1.6.2 Bohr Model of the Hydrogen Atom	30
1.7 Quantization Rules	36
1.8 Wave Packets	38
1.8.1 Localized Wave Packets	38
1.8.2 Wave Packets and the Uncertainty Relations	41
1.8.3 Motion of Wave Packets	42
1.9 Concluding Remarks	53
1.10 Solved Problems	54
Exercises	71

2	Mathematical Tools of Quantum Mechanics	79
2.1	Introduction	79
2.2	The Hilbert Space and Wave Functions	79
2.2.1	The Linear Vector Space	79
2.2.2	The Hilbert Space	80
2.2.3	Dimension and Basis of a Vector Space	81
2.2.4	Square-Integrable Functions: Wave Functions	83
2.3	Dirac Notation	84
2.4	Operators	88
2.4.1	General Definitions	88
2.4.2	Hermitian Adjoint	89
2.4.3	Projection Operators	91
2.4.4	Commutator Algebra	92
2.4.5	Uncertainty Relation between Two Operators	94
2.4.6	Functions of Operators	95
2.4.7	Inverse and Unitary Operators	96
2.4.8	Eigenvalues and Eigenvectors of an Operator	97
2.4.9	Infinitesimal and Finite Unitary Transformations	100
2.5	Representation in Discrete Bases	102
2.5.1	Matrix Representation of Kets, Bras and Operators	103
2.5.2	Change of Bases and Unitary Transformations	111
2.5.3	Matrix Representation of the Eigenvalue Problem	114
2.6	Representation in Continuous Bases	117
2.6.1	General Treatment	117
2.6.2	Position Representation	119
2.6.3	Momentum Representation	120
2.6.4	Connecting the Position and Momentum Representations	120
2.6.5	Parity Operator	124
2.7	Matrix and Wave Mechanics	126
2.7.1	Matrix Mechanics	126
2.7.2	Wave Mechanics	127
2.8	Concluding Remarks	128
2.9	Solved Problems	129
	Exercises	148
3	Postulates of Quantum Mechanics	157
3.1	Introduction	157
3.2	The Basic Postulates of Quantum Mechanics	157
3.3	The State of a System	159
3.3.1	Probability Density	159
3.3.2	The Superposition Principle	160
3.4	Observables and Operators	162
3.5	Measurement in Quantum Mechanics	164
3.5.1	How Measurements Disturb Systems	164
3.5.2	Expectation Values	165
3.5.3	Complete Sets of Commuting Operators	167
3.5.4	Measurement and the Uncertainty Relations	169

3.6	Time Evolution of the System's State	170
3.6.1	Time Evolution Operator	170
3.6.2	Stationary States: Time-Independent Potentials	171
3.6.3	Schrödinger Equation and Wave Packets	172
3.6.4	The Conservation of Probability	173
3.6.5	Time Evolution of Expectation Values	174
3.7	Symmetries and Conservation Laws	175
3.7.1	Infinitesimal Unitary Transformations	175
3.7.2	Finite Unitary Transformations	176
3.7.3	Symmetries and Conservation Laws	177
3.8	Connecting Quantum to Classical Mechanics	179
3.8.1	Poisson Brackets and Commutators	179
3.8.2	The Ehrenfest Theorem	181
3.8.3	Quantum Mechanics and Classical Mechanics	182
3.9	Solved Problems	183
	Exercises	199
4	One-Dimensional Problems	205
4.1	Introduction	205
4.2	Properties of One-Dimensional Motion	206
4.2.1	Discrete Spectrum (Bound States)	206
4.2.2	Continuous Spectrum (Unbound States)	207
4.2.3	Mixed Spectrum	207
4.2.4	Symmetric Potentials and Parity	207
4.3	The Free Particle: Continuous States	208
4.4	The Potential Step	210
4.5	The Potential Barrier and Well	213
4.5.1	The Case $E > V_0$	214
4.5.2	The Case $E < V_0$: Tunneling	216
4.5.3	The Tunneling Effect	219
4.6	The Infinite Square Well Potential	220
4.6.1	The Unsymmetric Square Well	220
4.6.2	The Symmetric Potential Well	223
4.7	The Finite Square Well Potential	224
4.7.1	The Scattering Solutions ($E > V_0$)	224
4.7.2	The Bound State Solutions ($0 < E < V_0$)	224
4.8	The Harmonic Oscillator	227
4.8.1	Energy Eigenvalues	229
4.8.2	Energy Eigenstates	231
4.8.3	Energy Eigenstates in Position Space	231
4.8.4	The Matrix Representation of Various Operators	234
4.8.5	Expectation Values of Various Operators	235
4.9	Numerical Solution of the Schrödinger Equation	236
4.9.1	Numerical Procedure	236
4.9.2	Algorithm	237
4.10	Solved Problems	239
	Exercises	263

5	Angular Momentum	269
5.1	Introduction	269
5.2	Orbital Angular Momentum	269
5.3	General Formalism of Angular Momentum	271
5.4	Matrix Representation of Angular Momentum	276
5.5	Geometrical Representation of Angular Momentum	279
5.6	Spin Angular Momentum	280
5.6.1	Experimental Evidence of the Spin	280
5.6.2	General Theory of Spin	283
5.6.3	Spin 1/2 and the Pauli Matrices	284
5.7	Eigenfunctions of Orbital Angular Momentum	287
5.7.1	Eigenfunctions and Eigenvalues of \hat{L}_z	288
5.7.2	Eigenfunctions of \hat{L}^2	289
5.7.3	Properties of the Spherical Harmonics	292
5.8	Solved Problems	295
	Exercises	311
6	Three-Dimensional Problems	317
6.1	Introduction	317
6.2	3D Problems in Cartesian Coordinates	317
6.2.1	General Treatment: Separation of Variables	317
6.2.2	The Free Particle	319
6.2.3	The Box Potential	320
6.2.4	The Harmonic Oscillator	322
6.3	3D Problems in Spherical Coordinates	324
6.3.1	Central Potential: General Treatment	324
6.3.2	The Free Particle in Spherical Coordinates	327
6.3.3	The Spherical Square Well Potential	329
6.3.4	The Isotropic Harmonic Oscillator	330
6.3.5	The Hydrogen Atom	334
6.3.6	Effect of Magnetic Fields on Central Potentials	348
6.4	Concluding Remarks	351
6.5	Solved Problems	351
	Exercises	368
7	Rotations and Addition of Angular Momenta	373
7.1	Rotations in Classical Physics	373
7.2	Rotations in Quantum Mechanics	375
7.2.1	Infinitesimal Rotations	375
7.2.2	Finite Rotations	377
7.2.3	Properties of the Rotation Operator	378
7.2.4	Euler Rotations	379
7.2.5	Representation of the Rotation Operator	380
7.2.6	Rotation Matrices and the Spherical Harmonics	382
7.3	Addition of Angular Momenta	385
7.3.1	Addition of Two Angular Momenta: General Formalism	385
7.3.2	Calculation of the Clebsch–Gordan Coefficients	391

7.3.3	Coupling of Orbital and Spin Angular Momenta	397
7.3.4	Addition of More Than Two Angular Momenta	401
7.3.5	Rotation Matrices for Coupling Two Angular Momenta	402
7.3.6	Isospin	404
7.4	Scalar, Vector and Tensor Operators	407
7.4.1	Scalar Operators	408
7.4.2	Vector Operators	408
7.4.3	Tensor Operators: Reducible and Irreducible Tensors	410
7.4.4	Wigner-Eckart Theorem for Spherical Tensor Operators	412
7.5	Solved Problems	415
	Exercises	431
8	Identical Particles	437
8.1	Many-Particle Systems	437
8.1.1	Schrödinger Equation	437
8.1.2	Interchange Symmetry	439
8.1.3	Systems of Distinguishable Noninteracting Particles	440
8.2	Systems of Identical Particles	442
8.2.1	Identical Particles in Classical and Quantum Mechanics	442
8.2.2	Exchange Degeneracy	444
8.2.3	Symmetrization Postulate	445
8.2.4	Constructing Symmetric and Antisymmetric Functions	446
8.2.5	Systems of Identical Noninteracting Particles	446
8.3	The Pauli Exclusion Principle	449
8.4	The Exclusion Principle and the Periodic Table	451
8.5	Solved Problems	457
	Exercises	466
9	Approximation Methods for Stationary States	469
9.1	Introduction	469
9.2	Time-Independent Perturbation Theory	470
9.2.1	Nondegenerate Perturbation Theory	470
9.2.2	Degenerate Perturbation Theory	476
9.2.3	Fine Structure and the Anomalous Zeeman Effect	479
9.3	The Variational Method	488
9.4	The Wentzel–Kramers–Brillouin Method	495
9.4.1	General Formalism	495
9.4.2	Bound States for Potential Wells with No Rigid Walls	498
9.4.3	Bound States for Potential Wells with One Rigid Wall	504
9.4.4	Bound States for Potential Wells with Two Rigid Walls	505
9.4.5	Tunneling through a Potential Barrier	507
9.5	Concluding Remarks	510
9.6	Solved Problems	510
	Exercises	542

10 Time-Dependent Perturbation Theory	549
10.1 Introduction	549
10.2 The Pictures of Quantum Mechanics	549
10.2.1 The Schrödinger Picture	550
10.2.2 The Heisenberg Picture	550
10.2.3 The Interaction Picture	551
10.3 Time-Dependent Perturbation Theory	552
10.3.1 Transition Probability	554
10.3.2 Transition Probability for a Constant Perturbation	555
10.3.3 Transition Probability for a Harmonic Perturbation	557
10.4 Adiabatic and Sudden Approximations	560
10.4.1 Adiabatic Approximation	560
10.4.2 Sudden Approximation	561
10.5 Interaction of Atoms with Radiation	564
10.5.1 Classical Treatment of the Incident Radiation	565
10.5.2 Quantization of the Electromagnetic Field	566
10.5.3 Transition Rates for Absorption and Emission of Radiation	569
10.5.4 Transition Rates within the Dipole Approximation	570
10.5.5 The Electric Dipole Selection Rules	571
10.5.6 Spontaneous Emission	572
10.6 Solved Problems	575
Exercises	591
11 Scattering Theory	595
11.1 Scattering and Cross Section	595
11.1.1 Connecting the Angles in the Lab and CM frames	596
11.1.2 Connecting the Lab and CM Cross Sections	598
11.2 Scattering Amplitude of Spinless Particles	599
11.2.1 Scattering Amplitude and Differential Cross Section	601
11.2.2 Scattering Amplitude	602
11.3 The Born Approximation	606
11.3.1 The First Born Approximation	606
11.3.2 Validity of the First Born Approximation	607
11.4 Partial Wave Analysis	609
11.4.1 Partial Wave Analysis for Elastic Scattering	609
11.4.2 Partial Wave Analysis for Inelastic Scattering	613
11.5 Scattering of Identical Particles	614
11.6 Solved Problems	617
Exercises	627
A The Delta Function	629
A.1 One-Dimensional Delta Function	629
A.1.1 Various Definitions of the Delta Function	629
A.1.2 Properties of the Delta Function	630
A.1.3 Derivative of the Delta Function	631
A.2 Three-Dimensional Delta Function	631

B Angular Momentum in Spherical Coordinates	633
B.1 Derivation of Some General Relations	633
B.2 Gradient and Laplacian in Spherical Coordinates	634
B.3 Angular Momentum in Spherical Coordinates	635
C Computer Code for Solving the Schrödinger Equation	637
References	641
Index	643

Preface

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 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

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 too early the solution. If you cannot solve the problem after your first attempt, try again! If you look up the solution 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.

Nouredine Zettili