

Contents

1. Introduction	1
1.1 Interquanta	1
1.2 The Structure of this Book	2
1.3 The Demonstrations	3
1.4 The Computer Laboratory	3
1.5 Literature	4
2. Free Particle Motion in One Dimension	5
2.1 Physical Concepts	5
2.1.1 Planck's Constant. Schrödinger's Equation for a Free Particle	5
2.1.2 The Wave Packet. Group Velocity. Normalization	6
2.1.3 Analogies in Optics	7
2.2 A First Session with the Computer	9
2.2.1 Starting IQ	9
2.2.2 An Automatic Demonstration	9
2.2.3 A First Dialogue	10
2.2.4 A Little Systematics	12
2.3 The Time Development of a Gaussian Wave Packet	13
2.4 The Spectral Function of a Gaussian Wave Packet	15
2.5 The Wave Packet as a Sum of Harmonic Waves	16
2.6 Exercises	19
3. Bound States in One Dimension	22
3.1 Physical Concepts	22
3.1.1 Schrödinger's Equation with a Potential. Eigenfunctions. Eigenvalues	22
3.1.2 Normalization. Discrete Spectra. Orthonormality	23
3.1.3 The Infinitely Deep Square-Well Potential	23
3.1.4 The Harmonic Oscillator	24
3.1.5 The Step Potential	24
3.1.6 Time-Dependent Solutions	26

3.1.7	Harmonic Particle Motion. Coherent States. Squeezed States	26
3.1.8	Particle Motion in a Deep Square Well	27
3.2	Eigenstates in the Infinitely Deep Square-Well Potential and in the Harmonic-Oscillator Potential	30
3.3	Eigenstates in the Step Potential	32
3.4	Harmonic Particle Motion	36
3.5	Particle Motion in the Infinitely Deep Square-Well Potential	37
3.6	Exercises	39
4.	Scattering in One Dimension	45
4.1	Physical Concepts	45
4.1.1	Stationary Scattering States. Continuum Eigenstates and Eigenvalues. Continuous Spectra	45
4.1.2	Time-Dependent Solutions of the Schrödinger Equation	46
4.1.3	Right-Moving and Left-Moving Stationary Waves of a Free Particle	46
4.1.4	Orthogonality and Continuum Normalization of Stationary Waves of a Free Particle. Completeness	47
4.1.5	Boundary Conditions for Stationary Scattering Solutions in Step Potentials	48
4.1.6	Stationary Scattering Solutions in Step Potentials	49
4.1.7	Constituent Waves	50
4.1.8	Normalization of Continuum Eigenstates	50
4.1.9	Harmonic Waves in a Step Potential	50
4.1.10	Time-Dependent Scattering Solutions in a Step Potential	51
4.1.11	Transmission and Reflection. Unitarity. The Argand Diagram	52
4.1.12	The Tunnel Effect	53
4.1.13	Resonances	54
4.1.14	Phase Shifts upon Reflection at a Steep Rise or Deep Fall of the Potential	54
4.1.15	Transmission Resonances upon Reflection at "More- and Less-Dense Media"	56
4.1.16	The Quantum-Well Device and the Quantum-Effect Device	57
4.2	Stationary Scattering States in the Step Potential	59
4.3	Scattering of a Harmonic Wave by the Step Potential	61
4.4	Scattering of a Wave Packet by the Step Potential	63

4.5	Transmission and Reflection. The Argand Diagram	65
4.6	Exercises	68
4.7	Analogies in Optics	78
4.8	Reflection and Refraction of Stationary Electromagnetic Waves	82
4.9	Reflection and Refraction of a Harmonic Light Wave	84
4.10	Scattering of a Wave Packet of Light	86
4.11	Transmission, Reflection and Argand Diagram for a Light Wave	88
4.12	Exercises	91
5.	A Two-Particle System: Coupled Harmonic Oscillators	94
5.1	Physical Concepts	94
5.1.1	The Two-Particle System	94
5.1.2	Initial Condition for Distinguishable Particles	96
5.1.3	Time-Dependent Wave Functions and Probability Distributions for Distinguishable Particles	96
5.1.4	Marginal Distributions for Distinguishable Particles	97
5.1.5	Wave Functions for Indistinguishable Particles. Symmetrization for Bosons. Antisymmetrization for Fermions	97
5.1.6	Marginal Distributions of the Probability Densities of Bosons and Fermions	99
5.1.7	Normal Oscillations	99
5.2	Stationary States	100
5.3	Time Dependence of Global Quantities	101
5.4	Joint Probability Densities	103
5.5	Marginal Distributions	105
5.6	Exercises	106
6.	Free Particle Motion in Three Dimensions	112
6.1	Physical Concepts	112
6.1.1	The Schrödinger Equation of a Free Particle in Three Dimensions. The Momentum Operator	112
6.1.2	The Wave Packet. Group Velocity. Normalization. The Probability Ellipsoid	114
6.1.3	Angular Momentum. Spherical Harmonics	116

6.1.4	The Stationary Schrödinger Equation in Polar Coordinates. Separation of Variables. Spherical Bessel Functions. Continuum Normalization. Completeness	118
6.1.5	Partial-Wave Decomposition of the Plane Wave . . .	119
6.1.6	Partial-Wave Decomposition of the Gaussian Wave Packet	119
6.2	The 3D Harmonic Plane Wave	122
6.2.1	A Cartesian 3D Plot	122
6.2.2	A Polar 3D Plot	123
6.3	The Plane Wave Decomposed into Spherical Waves	124
6.4	The 3D Gaussian Wave Packet	125
6.5	The Probability Ellipsoid	127
6.6	Angular-Momentum Decomposition of a Wave Packet . . .	129
6.7	Exercises	131
7.	Bound States in Three Dimensions	134
7.1	Physical Concepts	134
7.1.1	The Schrödinger Equation for a Particle under the Action of a Force. The Centrifugal Barrier. The Effective Potential	134
7.1.2	Bound States. Scattering States. Discrete and Continuous Spectra	136
7.1.3	The Infinitely Deep Square-Well Potential	137
7.1.4	The Spherical Step Potential	138
7.1.5	The Harmonic Oscillator	141
7.1.6	The Coulomb Potential. The Hydrogen Atom	142
7.1.7	Harmonic Particle Motion	143
7.2	Radial Wave Functions in Simple Potentials	144
7.3	Radial Wave Functions in the Step Potential	149
7.4	Probability Densities	151
7.5	Harmonic Particle Motion	154
7.6	Exercises	156
8.	Scattering in Three Dimensions	160
8.1	Physical Concepts	160
8.1.1	Radial Scattering Wave Functions	160
8.1.2	Boundary and Continuity Conditions. Solution of the System of Inhomogeneous Linear Equations for the Coefficients	162
8.1.3	Scattering of a Plane Harmonic Wave	163

8.1.4	Scattering Amplitude and Phase. Unitarity. The Argand Diagram	167
8.2	Radial Wave Functions	168
8.3	Stationary Wave Functions and Scattered Waves	171
8.4	Differential Cross Sections	173
8.5	Scattering Amplitude. Phase Shift. Partial and Total Cross Sections	175
8.6	Exercises	178
9.	Special Functions of Mathematical Physics	183
9.1	Basic Formulae	183
9.1.1	Hermite Polynomials	183
9.1.2	Harmonic-Oscillator Eigenfunctions	184
9.1.3	Legendre Polynomials and Legendre Functions	184
9.1.4	Spherical Harmonics	185
9.1.5	Bessel Functions	186
9.1.6	Spherical Bessel Functions	187
9.1.7	Laguerre Polynomials	188
9.1.8	Radial Eigenfunctions of the Harmonic Oscillator	189
9.1.9	Radial Eigenfunctions of the Hydrogen Atom	189
9.2	Hermite Polynomials	190
9.3	Eigenfunctions of the One-Dimensional Harmonic Oscillator	191
9.4	Legendre Polynomials and Associated Legendre Functions	192
9.4.1	Type 2 Plots – Functions of x or $\cos \vartheta$	192
9.4.2	Type 2 Plots – Polar Diagrams	193
9.5	Spherical Harmonics	195
9.6	Bessel Functions	196
9.6.1	Type 2 Plots	196
9.6.2	Type 0 Plots	197
9.7	Spherical Bessel Functions	199
9.8	Laguerre Polynomials	200
9.8.1	Type 2 Plots	200
9.8.2	Type 0 Plots	200
9.9	Radial Eigenfunctions of the Harmonic Oscillator	202
9.10	Radial Eigenfunctions of the Hydrogen Atom	203
9.11	Simple Functions of a Complex Variable	204
9.12	Exercises	206
10.	Additional Material and Hints for the Solution of Exercises	208
10.1	Units and Orders of Magnitude	208
10.1.1	Definitions	208

10.1.2	SI Units	208
10.1.3	Scaled Units	209
10.1.4	Atomic and Subatomic Units	211
10.1.5	Data-Table Units	212
10.1.6	Special Scales	213
10.2	Argand Diagrams and Unitarity for One-Dimensional Problems	215
10.2.1	Probability Conservation and the Unitarity of the Scattering Matrix	215
10.2.2	Time Reversal and the Scattering Matrix	217
10.2.3	Diagonalization of the Scattering Matrix	218
10.2.4	Argand Diagrams	220
10.2.5	Resonances	221
10.3	Hints and Answers to the Exercises	224
Appendix A. A Systematic Guide to IQ		252
A.1	Dialog Between the User and IQ	252
A.1.1	A Simple Example	252
A.1.2	The General Form of Commands	255
A.1.3	The Descriptor File	256
A.1.4	The Descriptor (Record)	259
A.1.5	The PLOT Command	261
A.1.6	The STOP Command	262
A.1.7	HELP: The Commands HE and PH	262
A.2	Coordinate Systems and Transformations	263
A.2.1	The Different Coordinate Systems	263
A.2.2	Defining the Transformations	265
A.3	The Different Types of Plot	269
A.3.1	Choosing a Plot Type: The Command CH	269
A.3.2	Cartesian 3D Plots (Type 0 Plots)	270
A.3.3	Polar 3D Plots (Type 1 Plots)	270
A.3.4	2D Plots (Type 2 Plots)	272
A.3.5	3D Column Plots (Type 3 Plots)	275
A.3.6	Special 3D Plots (Type 10 Plots)	276
A.4	The Background in the Plots	276
A.4.1	Boxes and Coordinate Axes: The Command BO	277
A.4.2	Scales	277
A.4.3	Arrows	280
A.4.4	Text and Numbers	282
A.4.5	Mathematical Symbols and Formulae	284
A.5	Further Commands	286

- A.5.1 Line Styles 286
- A.5.2 Multiple Plots 288
- A.5.3 Combined Plots 288
- A.5.4 Using Different Plotting Devices 289
- A.5.5 The Different Running Modes 290
- A.5.6 Definition of Physical Variables:
The Commands V0 to V9 293
- A.5.7 Reserved Commands 293
- Appendix B. How to Install IQ 294**
 - B.1 Hardware Requirements 294
 - B.2 Operating-System Requirements 294
 - B.3 Diskette Format 295
 - B.4 Installation 295
 - B.5 Reformatting IQ for Different Types of Diskette 296
- Appendix C. Lists of All Files Provided 298**
 - C.1 Command Files 298
 - C.2 Program Files 298
 - C.3 Descriptor Files for Examples and Exercises 299
 - C.4 Command Input Files and Associated Descriptor Files
for Demonstrations 299
 - C.5 Data Files 299
 - C.6 Help Files 300
- Appendix D. Graphics Devices and Metafiles 301**
- Index of IQ Commands 307**
- Subject Index 309**