

Contents

Preface — VII

About the author — XIII

Part I: Basic numerical and mathematical tools

- 1 Basic numerical analysis — 3**
 - 1.1 Numerical differentiation — 3
 - 1.2 Numerical quadrature — 4
 - 1.2.1 Elementary quadrature formulas — 4
 - 1.2.2 Gaussian quadrature — 5
 - 1.2.3 The Monte Carlo method — 6
 - 1.3 Ordinary differential equations — 8
 - 1.3.1 Euler method — 8
 - 1.3.2 Adams–Bashforth method — 8
 - 1.3.3 Runge–Kutta method — 9
 - 1.4 Linear second-order differential equations — 10
 - 1.4.1 Numerov algorithm — 10
- 2 Special functions of mathematical physics — 12**
 - 2.1 Legendre polynomials — 12
 - 2.2 Associated Legendre functions — 13
 - 2.3 Bessel functions — 14
 - 2.4 Spherical harmonics — 16
 - 2.5 Confluent hypergeometric functions — 17
 - 2.6 Green function — 18

Part II: Quantum (non-relativistic) theory of elastic scattering and spin

- 3 Partial wave expansion method — 21**
 - 3.1 Wave propagation, plane waves, and spherical waves — 21
 - 3.2 Time-independent Schrödinger equation for the free particle — 23
 - 3.3 Continuity equation — 24
 - 3.4 Differential elastic scattering cross-section — 25
 - 3.5 The radial equation — 28
 - 3.6 Expansion of the plane wave — 31
 - 3.7 Scattering amplitude — 35

- 3.8 Total elastic scattering cross-section and optical theorem — 36
- 3.9 The first Born approximation — 37
- 3.10 Rutherford elastic scattering cross-section — 39

- 4 Spectrum of angular momentum and spin — 41**
 - 4.1 Spectrum of angular momentum — 41
 - 4.2 Spin — 46

- 5 Phase shifts and atomic potential energy — 51**
 - 5.1 An important application of the Numerov algorithm: the eigenvalue problem — 51
 - 5.2 Phase-shift calculation — 51
 - 5.3 Atomic electron density and atomic potential energy — 53
 - 5.3.1 Thomas–Fermi model — 53
 - 5.3.2 Hartree and Hartree–Fock approximations — 59

Part III: Quantum-relativistic equations and scattering

- 6 The Klein–Gordon and the Dirac relativistic equations — 65**
 - 6.1 The natural system of units — 65
 - 6.2 The Lorentz transformation — 66
 - 6.3 Four-vectors and tensors — 67
 - 6.4 The Hamiltonian of a charged particle in an electromagnetic field — 72
 - 6.5 Klein–Gordon equation — 73
 - 6.6 Klein–Gordon particle in an electromagnetic field — 74
 - 6.7 Nonrelativistic limit of the Klein–Gordon equation — 75
 - 6.8 Difficulties of interpretation — 77
 - 6.9 Spin and gyromagnetic ratio of the electron — 80
 - 6.10 Dirac equation — 81

- 7 The Dirac equation and electron spin — 86**
 - 7.1 Manifestly covariant form of the Dirac equation — 86
 - 7.2 The Dirac equation and spin — 88
 - 7.2.1 Properties of commutators and anti-commutators — 88
 - 7.2.2 Spin — 89
 - 7.3 The solution of the Dirac equation for the free particle — 91
 - 7.4 The Pauli equation — 94

- 8 The Dirac theory of atoms — 97**
 - 8.1 Dirac equation in a central field — 97
 - 8.2 Dirac radial equations — 102

8.3	The Dirac theory of one-electron atoms —	104
8.4	The Dirac theory of one-electron atom energy levels —	108
8.5	Many-electron atoms —	109
8.5.1	Screening function —	109
8.5.2	Corrections to the electrostatic potential —	110
9	Relativistic partial wave expansion method —	112
9.1	Scattering amplitudes —	112
9.1.1	The fundamental equation —	112
9.1.2	Effective Dirac potential —	114
9.1.3	Phase shifts —	115
9.1.4	Scattering amplitudes —	115
9.2	Elastic scattering cross-section —	118
9.2.1	Relativistic elastic scattering cross-section —	118
9.2.2	Nonrelativistic limit —	121
9.3	Phase-shift calculation —	122
9.3.1	Lin, Sherman, and Percus transformation —	122
9.3.2	Phase shifts —	123
9.3.3	Numerical approach —	125
9.4	Electron–molecule elastic scattering —	128
10	Density matrix and spin-polarization phenomena —	130
10.1	The density matrix —	130
10.2	The spin-polarization —	132
10.3	Polarization change following a collision —	135
10.4	Polarization of an electron beam initially not polarized —	138
10.5	Double elastic scattering —	140
10.6	Change of the polarization in the general case —	141
10.7	Sherman function for molecules —	142

Part IV: Applications

11	Exercises —	147
11.1	Exercise 1 —	147
11.2	Exercise 2 —	148
11.3	Exercise 3 —	149
11.4	Exercise 4 —	150
11.5	Exercise 5 —	150
11.6	Exercise 6 —	151
11.7	Exercise 7 —	152
11.8	Exercise 8 —	152

XII — Contents

11.9	Exercise 9 —	153
11.10	Exercise 10 —	154
11.11	Exercise 11 —	155
11.12	Exercise 12 —	155
11.13	Exercise 13 —	157
11.14	Exercise 14 —	159
11.15	Exercise 15 —	160
11.16	Exercise 16 —	160
11.17	Exercise 17 —	162
11.18	Exercise 18 —	164
11.19	Exercise 19 —	166
11.20	Exercise 20 —	168
11.21	Exercise 21 —	169
11.22	Exercise 22 —	171
11.23	Exercise 23 —	172
11.24	Exercise 24 —	173
11.25	Exercise 25 —	173
11.26	Exercise 26 —	174
11.27	Exercise 27 —	175

Bibliography — 177

Index — 179