Contents

1 Review of Quantum Mechanics 1
1.1 Wave Functions and Equations of Motion 1
1.1.1 States and Wave Functions 1
1.1.2 Linear Operators and Observables 3
1.1.3 The Hamiltonian and Equations of Motion 7
1.2 Symmetries 9
1.2.1 Constants of Motion and Symmetries 9
1.2.2 The Radial Schrödinger Equation 12
1.2.3 Example: The Radially Symmetric Harmonic Oscillator 14
1.3 Bound States and Unbound States 16
1.3.1 Bound States 16
1.3.2 Unbound States 19
1.3.3 Examples 23
1.3.4 Normalization of Unbound States 28
1.4 Processes Involving Unbound States 30
1.4.1 Wave Packets 30
1.4.2 Transmission and Reflection 33
1.4.3 Time Delays and Space Shifts 35
1.5 Resonances and Channels 40
1.5.1 Channels 41
1.5.2 Feshbach Resonances 43
1.5.3 Potential Resonances 48
1.6 Methods of Approximation 50
1.6.1 Time-independent Perturbation Theory 50
1.6.2 Ritz's Variational Method 54
1.6.3 Semiclassical Approximation 57
1.6.4 Inverse Power-Law Potentials 67
1.7 Angular Momentum and Spin 72
1.7.1 Addition of Angular Momenta 74
1.7.2 Spin 75
1.7.3 Spin-Orbit Coupling 77

Problems 79
References 83

2 Atoms and Ions 85
2.1 One-Electron Systems 85
2.1.1 The Hydrogen Atom 85
2.1.2 Hydrogenic Ions 87
2.1.3 The Dirac Equation 88
2.1.4 Relativistic Corrections to the Schrödinger Equation . . . 93
2.2 Many-Electron Systems 95
2.2.1 The Hamiltonian 95
2.2.2 Pauli Principle and Slater Determinants 96
2.2.3 The Shell Structure of Atoms 100
2.2.4 Classification of Atomic Levels 103
2.3 The N-Electron Problem 107
2.3.1 The Hartree-Fock Method 107
2.3.2 Correlations and Configuration Interaction 112
2.3.3 The Thomas−Fermi Model 115
2.3.4 Density Functional Methods 118
2.4 Electromagnetic Transitions 120
2.4.1 Transitions in General, "Golden Rule" 121
2.4.2 The Electromagnetic Field 124
2.4.3 Interaction Between Atom and Field 129
2.4.4 Emission and Absorption of Photons 130
2.4.5 Selection Rules 135
2.4.6 Oscillator Strengths, Sum Rules 138
Problems 140
References 142

3 Atomic Spectra 145
3.1 Long-Ranged and Shorter-Ranged Potentials 146
3.1.1 Very-Long-Ranged Potentials 146
3.1.2 Shorter-Ranged Potentials 147
3.1.3 The Transition From a Finite Number to Infinitely Many Bound States, Inverse-Square Tails 152
3.1.4 Example: Truncated Dipole Series in the H^- Ion 158
3.2 One Electron in a Modified Coulomb Potential 164
3.2.1 Rydberg Series, Quantum Defects 164
3.2.2 Seaton's Theorem, One-Channel Quantum Defect Theory 171
3.2.3 Photoabsorption und Photoionization 172
3.3 Coupled Channels 177
3.3.1 Close-Coupling Equations 177
3.3.2 Autoionizing Resonances 181
3.3.3 Configuration Interaction, Interference of Resonances . . 186

3.3.4 Perturbed Rydberg Series . . . 191
3.4 Multichannel Quantum Defect Theory (MQDT) . . . 193
3.4.1 Two Coupled Coulomb Channels . . . 193
3.4.2 The Lu-Fano Plot . . . 200
3.4.3 More Than Two Channels . . . 203
3.5 Atoms in External Fields . . . 211
3.5.1 Atoms in a Static, Homogeneous Electric Field . . . 212
3.5.2 Atoms in a Static, Homogeneous Magnetic Field . . . 219
3.5.3 Atoms in an Oscillating Electric Field . . . 232
Problems . . . 235
References . . . 239

4 Simple Reactions . . . 243
4.1 Elastic Scattering . . . 243
4.1.1 Elastic Scattering by a Shorter-Ranged Potential . . . 243
4.1.2 Mean Scattering Lengths . . . 254
4.1.3 Near-Threshold Feshbach Resonances . . . 257
4.1.4 Semiclassical Description of Elastic Scattering . . . 259
4.1.5 Elastic Scattering by a Pure Coulomb Potential . . . 265
4.1.6 Elastic Scattering by a Modified Coulomb Potential, DWBA . . . 268
4.1.7 Feshbach Projection. Optical Potential . . . 271
4.2 Spin and Polarization . . . 273
4.2.1 Consequences of Spin-Orbit Coupling . . . 273
4.2.2 Application to General Pure Spin States . . . 276
4.2.3 Application to Mixed Spin States . . . 279
4.3 Inelastic Scattering . . . 281
4.3.1 General Formulation . . . 281
4.3.2 Coupled Radial Equations . . . 287
4.3.3 Threshold Effects . . . 292
4.3.4 An Example . . . 295
4.4 Exit Channels with Two Unbound Electrons . . . 298
4.4.1 General Formulation . . . 298
4.4.2 Application to Electrons . . . 305
4.4.3 Example . . . 309
4.4.4 Threshold Behaviour of Ionization Cross Sections . . . 313
Problems . . . 317
References . . . 321

5 Special Topics . . . 325
5.1 Multiphoton Absorption . . . 326
5.1.1 Experimental Observations on Multiphoton Ionization . 326
5.1.2 Calculating Ionization Probabilities via Volkov States . . 330
5.1.3 Calculating Ionization Probabilities via Floquet States . 333
5.2 Classical Trajectories and Wave Packets . . . 336

5.2.1 Phase Space Densities . . . 337
5.2.2 Coherent States . . . 341
5.2.3 Coherent Wave Packets in Real Systems . . . 347
5.3 Regular and Chaotic Dynamics in Atoms . . . 351
5.3.1 Chaos in Classical Mechanics . . . 351
5.3.2 Traces of Chaos in Quantum Mechanics . . . 356
5.3.3 Semiclassical Periodic Orbit Theory . . . 363
5.3.4 Scaling Properties for Atoms in External Fields . . . 368
5.3.5 Examples . . . 378
5.4 Bose-Einstein Condensation in Atomic Gases . . . 392
5.4.1 Quantum Statistics of Fermions and Bosons . . . 392
5.4.2 The Effect of Interactions in Bose-Einstein Condensates 396
5.4.3 Realization of Bose-Einstein Condensation in Atomic Gases . . . 400
5.5 Some Aspects of Atom Optics . . . 402
5.5.1 Atom-Wall Interactions . . . 404
5.5.2 Evanescent-Wave Mirrors . . . 411
5.5.3 Quantum Reflection . . . 416
Problems . . . 428
References . . . 431

A Special Mathematical Functions . . . 439
A.1 Legendre Polynomials, Spherical Harmonics . . . 439
A.2 Laguerre Polynomials . . . 441
A.3 Gamma Function . . . 442
A.4 Bessel Functions . . . 443
A.5 Whittaker Functions, Coulomb Functions . . . 446
References . . . 447

Solutions to the Problems . . . 449
References . . . 495

Index . . . 497