

## Contents

### Preface XIII

|          |  |           |
|----------|--|-----------|
| <b>1</b> | <b>Origin of Main Quantum Concepts</b>         | <b>1</b>  |
| 1.1      | Light: Waves or Particles?                     | 1         |
| 1.2      | Planck Constant, Beginning of the Quantum Era  | 2         |
| 1.3      | Photons  | 3         |
| 1.4      | Spectroscopy and Stability of Atoms            | 5         |
| 1.5      | Bohr Postulates                                | 6         |
| 1.6      | Hydrogen Atom                                  | 9         |
| 1.7      | Correspondence Principle                       | 15        |
| 1.8      | Spatial Quantization                           | 18        |
| 1.9      | Spin   | 20        |
| 1.10     | De Broglie Waves                               | 21        |
| <b>2</b> | <b>Wave Function and the Simplest Problems</b> | <b>25</b> |
| 2.1      | Free Motion                                    | 25        |
| 2.2      | Probability Density and Current                | 26        |
| 2.3      | Superposition Principle and Uncertainty        | 29        |
| 2.4      | Potential Wall                                 | 30        |
| 2.5      | Potential Barrier                              | 31        |
| 2.6      | Barrier Penetration                            | 35        |
| 2.7      | Tunneling                                      | 36        |
| <b>3</b> | <b>Bound States</b>                            | <b>43</b> |
| 3.1      | Potential Box                                  | 43        |
| 3.2      | Orthogonality and Completeness                 | 45        |
| 3.3      | Delta-Function*                                | 46        |
| 3.4      | Time Evolution                                 | 49        |
| 3.5      | Shallow Well and Quantum Halo                  | 52        |
| 3.6      | Resonances                                     | 59        |
| 3.7      | Level Density                                  | 60        |
| 3.8      | Periodic Boundary Conditions                   | 62        |
| 3.9      | Counting Levels in a Smooth Potential          | 63        |

|          |  |     |
|----------|--|-----|
| <b>4</b> | <b>Dynamical Variables</b>                 | 67  |
| 4.1      | Momentum Representation                    | 67  |
| 4.2      | Introducing Operators                      | 70  |
| 4.3      | Commutators                                | 72  |
| 4.4      | Eigenfunctions and Eigenvalues             | 74  |
| 4.5      | Momentum as a Translation Generator        | 75  |
| 4.6      | Introduction to Groups*                    | 78  |
| 4.7      | Orbital Momentum as a Rotation Generator   | 79  |
| 4.8      | Transformation of Operators                | 81  |
| <b>5</b> | <b>Uncertainty Relations</b>               | 85  |
| 5.1      | Uncertainty in Wave Mechanics              | 85  |
| 5.2      | Simple Examples                            | 87  |
| 5.3      | Complementarity and Probability            | 91  |
| 5.4      | Wave Packet: Propagation                   | 94  |
| 5.5      | Spreading of a Wave Packet                 | 96  |
| 5.6      | Estimates with Uncertainty Relations       | 100 |
| 5.7      | Classification of Molecular Excitations    | 104 |
| 5.8      | Level Width                                | 107 |
| 5.9      | Line Width and Mössbauer Effect            | 109 |
| 5.10     | Virtual Processes and Relativistic Effects | 112 |
| 5.11     | Spatial Quantization Revisited             | 114 |
| <b>6</b> | <b>Hilbert Space and Operators</b>         | 119 |
| 6.1      | Probability Amplitude                      | 119 |
| 6.2      | Superposition and Interference             | 120 |
| 6.3      | State Vectors                              | 123 |
| 6.4      | Geometry of Hilbert Space*                 | 124 |
| 6.5      | Linear Operators*                          | 128 |
| 6.6      | Hermitian Operators*                       | 130 |
| 6.7      | Properties of Hermitian Operators*         | 132 |
| 6.8      | Diagonalization*                           | 134 |
| 6.9      | Basis Transformations*                     | 136 |
| 6.10     | Continuous Transformations and Generators* | 138 |
| 6.11     | Projection Operators*                      | 140 |
| 6.12     | Operators of Observables                   | 142 |
| 6.13     | Simultaneous Measurability                 | 144 |
| 6.14     | Quantifying Uncertainty Relations          | 146 |
| <b>7</b> | <b>Quantum Dynamics</b>                    | 153 |
| 7.1      | Hamiltonian and Schrödinger Equation       | 153 |
| 7.2      | Single-Particle Hamiltonian                | 155 |
| 7.3      | Continuity Equation                        | 161 |
| 7.4      | Wigner Distribution                        | 165 |
| 7.5      | Heisenberg Picture                         | 167 |
| 7.6      | Operator Dynamics                          | 168 |

|           |  |            |
|-----------|--|------------|
| 7.7       | Virial Theorem                                       | 171        |
| 7.8       | Survival Probability                                 | 173        |
| 7.9       | Sum Rules  | 174        |
| 7.10      | Conservation Laws                                    | 178        |
| 7.11      | Path Integral Formulation                            | 180        |
| 7.12      | Relation to Classical Mechanics                      | 183        |
| 7.13      | Back to the Schrödinger Picture                      | 184        |
| <b>8</b>  | <b>Discrete Symmetries</b>                           | <b>187</b> |
| 8.1       | Time-Reversal Invariance                             | 187        |
| 8.2       | Time-Reversal Transformation of Operators            | 189        |
| 8.3       | Inversion and Parity                                 | 191        |
| 8.4       | Scalars and Pseudoscalars, Vectors and Pseudovectors | 192        |
| 8.5       | Parity Conservation                                  | 193        |
| 8.6       | Symmetry of a Crystal Lattice                        | 197        |
| 8.7       | Quasimomentum and Bloch Functions                    | 198        |
| 8.8       | Energy Bands   | 201        |
| 8.9       | Symmetry of Molecules                                | 203        |
| 8.10      | More Group Theory: Conjugate Classes*                | 206        |
| 8.11      | Group Representations*                               | 207        |
| 8.12      | Orthogonality and Completeness*                      | 209        |
| 8.13      | Characters*  | 212        |
| <b>9</b>  | <b>One-Dimensional Motion: Continuum</b>             | <b>217</b> |
| 9.1       | Eigenvalue Problem                                   | 217        |
| 9.2       | Continuous Spectrum                                  | 218        |
| 9.3       | Degeneracy in the Continuum                          | 221        |
| 9.4       | Transfer Matrix                                      | 224        |
| 9.5       | Delay Time   | 225        |
| 9.6       | Uniform Field  | 228        |
| 9.7       | Airy and Bessel Functions*                           | 229        |
| 9.8       | Asymptotic Behavior*                                 | 232        |
| 9.9       | Asymptotics of the Airy Function*                    | 234        |
| 9.10      | Green Function for One-Dimensional Scattering        | 237        |
| 9.11      | Potential as Perturbation                            | 241        |
| 9.12      | Quasistationary States                               | 244        |
| <b>10</b> | <b>Variational Approach and Diagonalization</b>      | <b>247</b> |
| 10.1      | Variational Principle                                | 247        |
| 10.2      | Direct Variational Method                            | 249        |
| 10.3      | Diagonalization in a Truncated Basis                 | 251        |
| 10.4      | Two-State System                                     | 252        |
| 10.5      | Level Repulsion and Avoided Crossing                 | 254        |
| 10.6      | Time Evolution of a Two-State System                 | 257        |
| 10.7      | Bright State and Fragmentation                       | 259        |
| 10.8      | Collective States                                    | 261        |

- 10.9 Lanczos Algorithm 265
- 11 Discrete Spectrum and Harmonic Oscillator 267**
  - 11.1 One-Dimensional Bound States 267
  - 11.2 Linear Harmonic Oscillator 269
  - 11.3 Hermite Polynomials\* 275
  - 11.4 Harmonic Oscillator in Plane: Separation of Variables 278
  - 11.5 Isotropic Oscillator 280
  - 11.6 Solving the Problem in Polar Coordinates 282
  - 11.7 Ladder Construction 285
  - 11.8 Creation and Annihilation Operators 286
  - 11.9 Operator Solution for the Harmonic Oscillator 288
- 12 Coherent and Squeezed States 293**
  - 12.1 Introducing Coherent States 293
  - 12.2 Displacements in the Phase Plane 294
  - 12.3 Properties of Coherent States 296
  - 12.4 Coherent States of the Harmonic Oscillator 298
  - 12.5 Linear Source 299
  - 12.6 Semiclassical Limit, Number of Quanta and the Phase 302
  - 12.7 Pairwise Source 304
  - 12.8 Squeezed States 307
  - 12.9 More about Squeezed States 310
- 13 Introducing Magnetic Field 315**
  - 13.1 Magnetic Field in Classical Mechanics 315
  - 13.2 Quantum Formulation and Gauge Invariance 317
  - 13.3 Are Electromagnetic Potentials Observable? 320
  - 13.4 Landau Levels: Energy Spectrum 321
  - 13.5 Landau Levels: Degeneracy and Wave Functions 323
  - 13.6 Quantum Hall Effect 327
  - 13.7 Arbitrary Dispersion Law 331
  - 13.8 Symmetric Gauge 335
  - 13.9 Coherent States in the Magnetic Field 336
- 14 Macroscopic Quantum Coherence 339**
  - 14.1 Ideas of Macroscopic Coherence 339
  - 14.2 Macroscopic Wave Function 340
  - 14.3 Hydrodynamic Description 341
  - 14.4 Dynamics of the Macroscopic Coherent State 344
  - 14.5 Josephson Effects 346
  - 14.6 Quantization of Circulation and Quantum Vortices 349
  - 14.7 Magnetic Fluxoid Quantization and London Electrodynamics 353
- 15 Semiclassical (WKB) Approximation 357**
  - 15.1 Heuristic Introduction 357
  - 15.2 Semiclassical Approximation 360

- 15.3 Asymptotic Expansion 363
- 15.4 Stationary Phase 364
- 15.5 Matching Conditions 365
- 15.6 Bohr–Sommerfeld Quantization 369
- 15.7 Semiclassical Matrix Elements 371
- 15.8 Solutions in the Complex Plane\* 373
- 15.9 Going Around the Complex Plane\* 376
- 15.10 Connection Formulae Revisited\* 378
- 15.11 Close Turning Points\* 379
- 15.12 Path Integral Approach 383
  
- 16 Angular Momentum and Spherical Functions 387**
- 16.1 Angular Momentum as a Generator of Rotations 387
- 16.2 Spin 389
- 16.3 Angular Momentum Multiplets 390
- 16.4 Matrix Elements of Angular Momentum 396
- 16.5 Realization of the Algebra for Orbital Momentum 399
- 16.6 Constructing a Set of Spherical Functions\* 401
- 16.7 Simplest Properties of Spherical Functions\* 403
- 16.8 Scalars and Vectors\* 404
- 16.9 Second Rank Tensors\* 408
- 16.10 Spherical Functions and Legendre Polynomials\* 410
- 16.11 Angular Momentum in an External Field 414
  
- 17 Motion in a Central Field 417**
- 17.1 Reduction to the One-Body Problem 417
- 17.2 Separation of Angular Variables 420
- 17.3 Radial Part of the Schrödinger Equation 422
- 17.4 Free Motion 426
- 17.5 Plane and Spherical Waves 430
- 17.6 Spherical Well 432
- 17.7 Short-Range Potential 435
- 17.8 Adding the Second Center 436
- 17.9 Three-Dimensional Harmonic Oscillator 439
  
- 18 Hydrogen Atom 445**
- 18.1 Bound States 445
- 18.2 Ground State 447
- 18.3 Discrete Spectrum 450
- 18.4 Operator Solution 458
- 18.5 On the Way to Precision Spectroscopy 460
- 18.6 Solution in Parabolic Coordinates\* 462
- 18.7 Continuum States 463
  
- 19 Stationary Perturbations 469**
- 19.1 Introduction 469
- 19.2 Perturbation Theory With No Degeneracy 470

|           |  |            |
|-----------|--|------------|
| 19.3      | Convergence  | 474        |
| 19.4      | Case of Close Levels                                       | 477        |
| 19.5      | Adiabatic Approximation                                    | 478        |
| 19.6      | Molecular Ion of Hydrogen                                  | 482        |
| 19.7      | Interactions of Atoms at Large Distances                   | 486        |
| <b>20</b> | <b>Spin 1/2</b>  | <b>489</b> |
| 20.1      | $SU(2)$ Group  | 489        |
| 20.2      | Spin 1/2: Algebra  | 490        |
| 20.3      | Spinors  | 494        |
| 20.4      | Magnetic Resonance   | 499        |
| 20.5      | Time-Reversal Transformation and Kramers Theorem           | 501        |
| 20.6      | Time-Conjugate States                                      | 503        |
| 20.7      | Spinors as Qubits  | 504        |
| <b>21</b> | <b>Finite Rotations and Tensor Operators</b>               | <b>509</b> |
| 21.1      | Matrices of Finite Rotations                               | 509        |
| 21.2      | Spherical Functions as Matrix Elements of Finite Rotations | 511        |
| 21.3      | Addition Theorem*  | 514        |
| 21.4      | Transformation of Operators                                | 516        |
| 21.5      | Introduction to Selection Rules                            | 518        |
| 21.6      | Electromagnetic Multipoles                                 | 519        |
| <b>22</b> | <b>Angular Momentum Coupling</b>                           | <b>523</b> |
| 22.1      | Two Subsystems   | 523        |
| 22.2      | Decomposition of Reducible Representations                 | 525        |
| 22.3      | Two Particles of Spin 1/2                                  | 528        |
| 22.4      | Tensor Operators and Selection Rules Revisited             | 532        |
| 22.5      | Applying to Electromagnetic Multipoles                     | 533        |
| 22.6      | Vector Coupling of Angular Momenta                         | 534        |
| 22.7      | Wigner–Eckart Theorem                                      | 538        |
| 22.8      | Vector Model   | 539        |
| 22.9      | Electric Dipole Moment and Anapole Moment                  | 541        |
| 22.10     | Clebsch–Gordan Series*                                     | 543        |
| <b>23</b> | <b>Fine and Hyperfine Structure</b>                        | <b>545</b> |
| 23.1      | Spin–Orbit Coupling  | 545        |
| 23.2      | Spin–Orbit Splitting                                       | 547        |
| 23.3      | Hydrogen Fine Structure                                    | 550        |
| 23.4      | Fine Structure in Complex Atoms                            | 553        |
| 23.5      | Magnetic Moment with Spin–Orbit Coupling                   | 555        |
| 23.6      | Magnetic Hyperfine Structure                               | 558        |
| 23.7      | Example: One Valence Electron                              | 560        |
| 23.8      | Quadrupole Hyperfine Structure                             | 562        |
| <b>24</b> | <b>Atom in a Static Field</b>                              | <b>567</b> |
| 24.1      | Polarizability in a Static Electric Field                  | 567        |

|       |  |     |
|-------|--|-----|
| 24.2  | Stark Effect                                       | 569 |
| 24.3  | Polarizability of the Hydrogen Atom                | 570 |
| 24.4  | Stark Effect in the Hydrogen Atom                  | 572 |
| 24.5  | Non-uniform Electric Field and Additional Comments | 573 |
| 24.6  | Classical Zeeman Effect                            | 574 |
| 24.7  | A Quantum System in a Magnetic Field               | 575 |
| 24.8  | Normal Quantum Zeeman Effect                       | 576 |
| 24.9  | Anomalous Quantum Zeeman Effect                    | 578 |
| 24.10 | Stronger Magnetic Field                            | 579 |
| 24.11 | Diamagnetism                                       | 581 |
| 24.12 | Towards Really Strong Magnetic Fields              | 583 |
|       | <b>References</b>                                  | 587 |
|       | <b>Further Readings</b>                            | 591 |
|       | <b>Index</b>                                       | 597 |

