

contents

preface, v

1

introduction

- 1-1. Stationary States, 1
- 1-2. Excitation Potentials, 1
- 1-3. Selection Rules for Transitions, 2
- 1-4. Bohr Theory of Hydrogen Atom, 3
- 1-5. Sommerfeld's Action Integral, 5
- 1-6. Applications of Bohr Theory, 6
- 1-7. Limitations of the Bohr Theory, 7
- 1-8. The Wave Properties of Particles, 7
- 1-9. Wave Mechanics, 9

2

wave theory

- 2-1. Introduction, 11
- 2-2. Harmonic Waves, 11
- 2-3. Superposition of Waves, 13

ix

- 2-4. Real Wave Functions, 15
- 2-5. Standing Waves, 16
- 2-6. The Wave Equation and Its Solutions, 17
- 2-7. The Stationary Wave Equation, 20
- 2-8. Boundary Conditions and Quantization, 22
- 2-9. Interpretation of K_n and Quantization of Frequencies, 26
- 2-10. Harmonic Analysis, 27
- 2-11. Orthogonal Functions, 30
- 2-12. Transforms, 33
- 2-13. General Expansion in Terms of Orthogonal Functions, 35
- 2-14. Orthonormal Sets; Degenerate Eigenfunctions, 38
- 2-15. Summary, 40

wave packets and the uncertainty principle

- 3-1. Introduction, 42
- 3-2. Distribution Functions of Some Wave Packets, 42
- 3-3. The Uncertainty Principle, 47
- 3-4. Dispersion of Wave Packets, 48
- 3-5. Summary, 53

de Broglie's hypotheses applied to electron beams

- 4-1. Introduction, 54
- 4-2. de Broglie's Hypotheses, 54
- 4-3. The Wave Equation for Free-electron Beams, 56
- 4-4. Solutions of the Wave Equation for the Free-particle Beam, 57
- 4-5. Attempted Isolation of an Electron from a Beam, 58
- 4-6. The Effect of Mass on the Dispersion, 59
- 4-7. Summary, 61

the postulates of wave mechanics

- 5-1. Introduction, 62
- 5-2. The First Postulate of Wave Mechanics, 62

- 5-3. The Second Postulate of Wave Mechanics, 63
- 5-4. Schrödinger's Wave Equation, 63
- 5-5. Proper Behavior of Operators in Wave Mechanics, 65
- 5-6. The Third Postulate, 66
- 5-7. Hermitian Conjugation and Hermitian Operators, 67
- 5-8. Applications of the Three Postulates, 68
- 5-9. Fluctuations, 71
- 5-10. Eigenstates, 73
- 5-11. Expansion in Terms of Eigenfunctions, 75
- 5-12. Stationary States, 76
- 5-13. An Example of a Nonstationary State, 77
- 5-14. Summary, 80

the uncertainty principle

- 6-1. Introduction, 81
- 6-2. Derivation of the General Uncertainty Relation, 82
- 6-3. Application of the General Uncertainty Relation, 84
- 6-4. Conjugate Variables and Their Eigenfunctions, 85
- 6-5. Summary, 88

a physical interpretation of the wave and distribution functions

- 7-1. Introduction, 89
- 7-2. The Distribution Coefficients, 89
- 7-3. The Probability Density, 92
- 7-4. The Probability Current, 93
- 7-5. Superposition of Densities and Current, 96
- 7-6. Summary, 98

trapped and travelling electrons

- 8-1. Introduction, 99
- 8-2. Discontinuities in the Potential-energy Function, 100

- 8-3. Splicing Solutions at Finite Discontinuities in the Potential, 102
- 8-4. Classically Accessible and Classically Inaccessible Regions, 103
- 8-5. Reflection and Transmission of Electrons at a Discontinuity in the Potential, 104
- 8-6. Transmission and Reflection at Potential Barriers of Finite Width, 107
- 8-7. Potential Wells, 110
- 8-8. Periodic Potentials, 114
- 8-9. The Bloch Function, 117
- 8-10. Energy Bands, 118
- 8-11. Summary, 119

9

electrons in small fields

- 9-1. Introduction, 122
- 9-2. Relaxation Method for Solving the Wave Equation, 122
- 9-3. Physical Interpretation of the WBK Expression, 127
- 9-4. Electrons in a Uniform Field, 128
- 9-5. Summary, 130

10

**development of operator algebra
for the harmonic oscillator**

- 10-1. Introduction, 131
- 10-2. Rules of Operator Algebra for the Linear Harmonic Oscillator, 131
- 10-3. Solution of the Wave Equation for the Linear Harmonic Oscillator, 132
- 10-4. Normalization in the Linear Harmonic Oscillator, 133
- 10-5. Termination of the Generating Procedures, 134
- 10-6. Uniqueness of the Set of Eigenfunctions, 135
- 10-7. The Ground State of the Linear Harmonic Oscillator, 137
- 10-8. Higher-energy States of the Linear Harmonic Oscillator, 140
- 10-9. Recursion Formula Relating the Eigenfunctions of the Linear Harmonic Oscillator, 143

- 10-10. Selection Rule for the Linear Harmonic Oscillator, 144
- 10-11. The Three-dimensional Harmonic Oscillator, 145
- 10-12. The Isotropic Three-dimensional Harmonic Oscillator, 148
- 10-13. Summary, 149

11

the central field

- 11-1. Introduction, 150
- 11-2. The Angular-momentum Operator, 151
- 11-3. The Total Angular Momentum, 155
- 11-4. Generation of the Eigenfunctions of the \mathfrak{L}_z and \mathfrak{L}^2 , 156
- 11-5. Termination of the Generating Procedure, 157
- 11-6. Eigenvalues of the Total Angular Momentum, 158
- 11-7. The Uncertainty Principle Applied to the Central-field Problem, 162
- 11-8. Uniqueness of the Ladder, 165
- 11-9. Angular Distribution of the Electron Charge in Atoms, 165
- 11-10. Schroedinger's Equation in Polar Coordinates, 168
- 11-11. Orbitals and Hybridization, 169
- 11-12. Spectroscopic Notation, 170
- 11-13. The Rotational Energy of Diatomic Molecules, 171
- 11-14. Summary, 171

12

spherical harmonics and selection rules

- 12-1. Introduction, 173
- 12-2. Normalization, 173
- 12-3. Legendre's Differential Equations, 175
- 12-4. Rodrigues's Formula, 175
- 12-5. Recursion Relations between Spherical Harmonics, 177
- 12-6. Selection Rules for the Central Field, 179
- 12-7. The Rotational Spectra of Diatomic Molecules, 183
- 12-8. Summary, 184

13

**radial dependence of wave functions
in a coulomb field**

- 13-1. Introduction, 185
- 13-2. Solution of Schrödinger's Equation for a Coulomb Field, 186
- 13-3. Generation of the Eigenfunctions of the Hamiltonian Operator, 187
- 13-4. Termination of the Generating Procedure, 191
- 13-5. Uniqueness of the Ladders, 193
- 13-6. Some Low-energy States of the Hydrogen Atom; Comparison with Bohr's Model, 195
- 13-7. Selection Rules, 201
- 13-8. Summary, 201

14

the hydrogen molecule-ion

- 14-1. Introduction, 203
- 14-2. The Hamiltonian for the Hydrogen Molecule-Ion, 203
- 14-3. Solution of Schrödinger's Equation, 205
- 14-4. Energy as a Function of Proton-Proton Distance, 208
- 14-5. The Stationary Wave Functions, 211
- 14-6. Time-dependent Wave Functions of the Hydrogen Molecule-Ion, 213
- 14-7. The Interaction of Electromagnetic Radiation with H_2^+ , 214
- 14-8. The Limiting Case of Very Large Proton-Proton Distance, 216
- 14-9. Resonance Energy: The Double-well Potential, 216
- 14-10. Summary, 217

15

separation of variables

- 15-1. Introduction, 218
- 15-2. Eigenfunctions and Separation of Variables, 218
- 15-3. Separation of Variables in an Operator, 221
- 15-4. Summary, 223

16

electron spin and the exclusion principle

- 16-1. Introduction, 224
- 16-2. The Spin Operators, Their Eigenfunctions and Eigenvalues, 224
- 16-3. The Orthonormality of α and β , 227
- 16-4. Systems of Two Electrons, 229
- 16-5. Vector Representation for the Spin Functions $\alpha(1) \alpha(2)$ and $(\beta(1) \beta(2))$, 232
- 16-6. Vector Representation of the Spin Functions $\alpha(1)\beta(2)$ and $\beta(1)\alpha(2)$, 232
- 16-7. The Four Eigenfunctions of σ^2 , 235
- 16-8. Indistinguishability of Electrons, 238
- 16-9. The Orbital Wave Functions of a Two-electron System, 240
- 16-10. The Fourth Postulate: The Exclusion Principle, 244
- 16-11. The Vector Diagram for Addition of Electron Spins, 245
- 16-12. Summary, 246

17

perturbation theory

- 17-1. Introduction, 247
- 17-2. Perturbations, 247
- 17-3. Approximation to the Energy Levels, 250
- 17-4. First-order Perturbation Theory, 252
- 17-5. Second-order Perturbation Theory, 254
- 17-6. The Perturbed Wave Functions, 255
- 17-7. An Anharmonic Oscillator, 257
- 17-8. Summary, 260

18

the helium atom

- 18-1. Introduction, 261
- 18-2. The Ground State of the Helium Atom, 261

contents

- 18-3. The Sixteen First Excited States, 263
- 18-4. Degenerate Perturbation Theory, 264
- 18-5. Physical Interpretation of J and K , 269
- 18-6. The Term-value Diagram for Helium, 271
- 18-7. Summary, 271

19

electronic configurations of atoms

- 19-1. Introduction, 273
- 19-2. The Exclusion Principle, 273
- 19-3. Resolution of the Orbital Degeneracies, 275
- 19-4. Resolution of Spin Degeneracies, 277
- 19-5. Multiplet Structure; Symmetric Spin Function of Three Electrons, 278
- 19-6. Other Spin Functions of Three-electron Systems, 281
- 19-7. Hund's Rule, 282
- 19-8. Hybridization and Hund's Rule, 283
- 19-9. The Aufbau Principle, 285

appendix 1 Reference Books, 289

index, 291