

## CONTENTS

Preface		xi	
The Computer Interface			xiii
1	Sym	nmetry in Physical Systems	1
	1.1	Symmetries and invariances 1	
		1.1.1 Symmetries and conservation laws 2	
		1.1.2 Noether's theorem and Curie's principle 5	
	1.2	Spatial symmetries 7	
		1.2.1 Reflection symmetry in nature 8	
		1.2.2 Translation symmetries; mosaics and crystals 10	
	1.3	Rotational symmetries 12	
		1.3.1 Active and passive rotations; Euler angles 13	
		1.3.2 Coordinate systems for rotations 17	
		1.3.3 Angular momentum and rotations: a cameo portrait 19	
	1.4	Discrete symmetries and quantum systems 21	
		1.4.1 Parity symmetry 22	
		1.4.2 Charge conjugation and time reversal 25	
		1.4.4 <i>BCT</i> and the Bouli principle: Liider's theorem 32	
	15	Ricken symmetries from cosmetology to cosmology 34	
	1.5	Dioken symmetries from cosmology to cosmology 54	
		Problems on symmetry in physical systems 36	

## 2 Mathematical and Quantal Preliminaries

- 2.1 Matrix definitions and manipulations 42
  - 2.1.1 Linear spaces and operator matrix elements 42
  - 2.1.2 Inner and direct products of matrices 45
  - 2.1.3 Operations on matrices, and special properties 50
  - 2.1.4 Phase manipulation rules 52

### 2.2 Transformations and operators 53

- 2.2.1 Similarity and symmetry transformations 53
- 2.2.2 Unitarity: its interpretation in quantum mechanics 57
- 2.2.3 Operator exponentials and commutators 58
- 2.2.4 Raising and lowering operators 59
- 2.3 Eigenvalues and eigenstates 63
  - 2.3.1 Eigenvalues of operators and matrices 63
  - 2.3.2 Diagonalizing matrices 64
  - 2.3.3 Eigenvectors as basis states 66
- 2.4 Spinors and their properties 67
  - 2.4.1 Definitions of spinors 67
  - 2.4.2 Representing spinors; rotations 69
  - 2.4.3 Objects that distinguish turns though  $2\pi$  and  $4\pi$  72
- 2.5 A primer on groups 72
  - 2.5.1 Group examples and definitions 73
  - 2.5.2 Group theory terminology 79
  - 2.5.3 Representations of groups 80
  - 2.5.4 Interesting groups and their uses 84
  - 2.5.5 Irreducibility of a representation 88
- 2.6 Mathematics, groups, and the physical sciences 89 Problems on mathematical and quantal preliminaries 90

#### 3 Rotational Invariance and Angular Momentum

- 3.1 Infinitesimal rotations; the J operators 95
  - 3.1.1 Schemes for describing rotations 96
  - 3.1.2 Commutation relations of J operators 97
  - 3.1.3 The spherical-basis operators  $J_{+1}$ ,  $J_0$ ,  $J_{-1}$  99
- 3.2 Orbital angular momentum operators 100
  - 3.2.1 Infinitesimal rotations applied to spatial functions 100
  - 3.2.2 Components of L in spherical polar coordinates 103
  - 3.2.3 The special role of the operator  $L_z$  105
- 3.3 Other representations of **J** operators 105
  - 3.3.1 The 2 × 2 matrix representation: Pauli matrices 105
  - 3.3.2 Eigenvectors of the Pauli matrices 108
  - 3.3.3 Finite rotations and Pauli matrices 109
  - 3.3.4 Spinor space and its operators 111
- 3.4 Angular momentum eigenvalues and matrix elements 113
  - 3.4.1 Eigenvalues of  $J^2$  and  $J_z$ ; irreducibility 113
  - 3.4.2 Matrix elements in the spherical basis 116
  - 3.4.3 Matrix elements in the Cartesian basis 117
  - 3.4.4 Operator matrices for j = 1/2, 1, and 3/2 119
  - 3.4.5 Angular momentum: geometrical and dynamical 120

95

3.5 Reference frames: spin and orbital angular momenta 122 Problems on rotational invariance and angular momentum 124

## 4 Angular Momentum Eigenstates

- 4.1 Orbital eigenstates and spherical harmonics 127
  - 4.1.1 Legendre functions and their properties 129
  - 4.1.2 Displaying Legendre functions; polar diagrams 131
  - 4.1.3 Calculating and visualizing spherical harmonics 135
  - 4.1.4 Solid harmonics and other variants 143
- 4.2 Spherical-basis vectors and angular momentum in a field 149
  - 4.2.1 Vectors in the spherical basis 150
  - 4.2.2 Infinitesimal rotations of vectors 152
  - 4.2.3 The electromagnetic field and photons 155
- 4.3 Spin eigenstates and their representations 156
  - 4.3.1 What is spin? 156
  - 4.3.2 Intrinsic spin eigenstates 160
  - 4.3.3 Spinor-space representations 162
  - 4.3.4 Time reversal and spin 163

Problems on angular momentum eigenstates 165

#### 5 Angular Momentum in Quantum Systems

5.1 Rotational symmetry and dynamical angular momentum 170

- 5.1.1 Angular momentum and the role of Planck's constant 170
  - 5.1.2 Classical angular momentum: Ehrenfest theorems 172
  - 5.1.3 Larmor precession in magnetic fields 175
- 5.2 Uncertainty relations for angular momentum 179
  - 5.2.1 Heisenberg uncertainty relations for quantum systems 180
  - 5.2.2 Angular momentum uncertainties 183
  - 5.2.3 Uncertainties between angular momentum and angles 186
- 5.3 The semiclassical vector model 189
  - 5.3.1 Constructing the vector model of angular momentum 190
  - 5.3.2 Uses and limitations of the vector model 192

5.4 Angular momentum and wave mechanics 193
5.4.1 Plane waves and centripetal barriers; Bessel functions 193

- 5.4.2 Displaying partial-wave expansions 199
- 5.5 The conceptual development of angular momentum 203 Problems on angular momentum in quantum systems 206

#### 6 Finite Rotations of Angular Momentum Eigenstates

- 6.1 Introduction to rotation matrices 211
  - 6.1.1 Review of rotations and angle schemes 212
  - 6.1.2 Group and factorization properties of rotations 213

## 127

169

211

- 6.2 Determining rotation matrices 213
  - 6.2.1 Rotation of eigenstates about z axes 214
  - 6.2.2 Rotations about the y axis for j = 1 216
  - 6.2.3 Constructing d/ from spinor representations 218
  - 6.2.4 Relation of d' elements to other functions 220
  - 6.2.5 Computing reduced rotation matrix elements 222
- 6.3 Interpreting rotated states 224
  - 6.3.1 Orbital angular momentum states 225
  - 6.3.2 Transformation amplitudes for arbitrary j 227
  - 6.3.3 Visualizing rotation matrix elements 230
- 6.4 Properties of rotation matrices 232
  - 6.4.1 Symmetry properties of  $d^{i}$  and  $D^{i}$  232
  - 6.4.2 Unitarity and orthogonality properties 234
  - 6.4.3 Classical limits of rotation matrices 236
  - 6.4.4 Spherical harmonics as rotation matrix elements 239
- 6.5 Rigid-body rotations in quantum mechanics 240
  - 6.5.1 The  $D^{j}$  as angular momentum eigenfunctions 241
  - 6.5.2 The Hamiltonian of a rigid rotator 242
  - 6.5.3 Rotational states of molecules and nuclei 245

Problems on finite rotations of angular momentum eigenstates 247

## 7 Combining Two Angular Momentum Eigenstates 251

- 7.1 The semiclassical vector model for addition 252
  - 7.1.1 Vector-addition construction 252
  - 7.1.2 Triangle and projection selection rules 253
  - 7.1.3 Interpreting coupling: spin-orbit interaction 255
  - 7.1.4 Degeneracy of energy states in the Coulomb potential 258
- 7.2 Coupling coefficients: definitions and general properties 263
  - 7.2.1 Combining two angular momenta: Clebsch-Gordan coefficients 264
  - 7.2.2 Unitarity of Clebsch-Gordan coefficients 264
  - 7.2.3 Determining coefficients from spinor representations 266
- 7.3 The 3-j coefficients and their properties 269
  - 7.3.1 Three angular momenta coupled to zero; 3-j coefficients 269
  - 7.3.2 Visualizing symmetry properties 276
  - 7.3.3 Classical limits of 3-j coefficients 278
  - 7.3.4 Expressions for one angular momentum small 280
- 7.4 Computing coupling coefficients 280
  - 7.4.1 Tabulations of coupling coefficients 281
  - 7.4.2 Computing 3-j coefficients efficiently 282
- 7.5 Rotation matrices and coupling coefficients 286
  - 7.5.1 Clebsch-Gordan series for combining  $D^{j}$  elements 286
  - 7.5.2 Special cases of Clebsch-Gordan series 288
  - 7.5.3 Integrals of rotation functions 292
  - 7.5.4 Examples: Celestial bodies and rotator matrix elements 295

Problems on combining two angular momentum eigenstates 300

CONTENTS i x

# 8 Irreducible Spherical Tensors and Spin 305

8.1 Definition of irreducible tensor operators 308
8.1.1 Defining irreducible spherical tensors 308
8.1.2 Racah's definition and its applications 309

#### 8.2 Combining irreducible tensors 312 8.2.1 Building up irreducible spherical tensors 312

8.2.2 Contraction of irreducible tensors to scalars 315

#### 8.3 Wigner-Eckart theorem; reduced matrix elements 316

- 8.3,1 Geometry and dynamics: The Wigner-Eckart theorem 317
- 8.3.2 Conventions for reduced matrix elements 320
- 8.3.3 Determining and using reduced matrix elements 320

#### 8.4 Density matrices and polarization tensors 325

- 8.4.1 Spin density matrices and spin tensors 325
  - 8.4.2 Spin precession in magnetic fields: rotating frames 330
  - 8.4.3 Spin transport through magnetic field gradients 335

Problems on irreducible spherical tensors and spin 341

## 9 Recombining Several Angular Momentum Eigenstates 345

- 9.1 Recoupling three angular momenta 345
  - 9.1.1 Racah and 6-j coefficients for three angular momenta 345
  - 9.1.2 Recoupling tetrahedra, quadrilaterals, and trees 348

#### 9.2 Formulas for 6-j coefficients 350

- 9.2.1 Expansion in terms of 3-j coefficients 350
- 9.2.2 Algebraic expressions for 6-j coefficients 352
- 9.2.3 Tabulations of 6-j coefficients 354

#### 9.3 Properties of recoupling coefficients 354

- 9.3.1 Orthogonality relations of 6-j coefficients 355
- 9.3.2 Symmetries and special values of 6-j coefficients 355
- 9.3.3 Computing 6-j coefficients efficiently 359

#### 9.4 Scalar products of irreducible tensors 361

- 9.4.1 Factorization and projection theorems for tensors 361
- 9.4.2 Matrix elements of multipole expansions 365
- 9.4.3 Tensors in L-S and j-j coupling schemes 367

#### 9.5 Recoupling four angular momenta 370

- 9.5.1 Definition and computation of 9-j coefficients 370
- 9.5.2 Symmetries, special values, and sum rules of 9-j coefficients 374
- 9.5.3 Tensor matrix elements in coupled schemes 376
- 9.5.4 Transformations between L S and j j coupling 377
- 9.5.5 Graphical and automated methods 380

Problems on recombining several angular momentum eigenstates 381

## EPILOGUE

385

## APPENDIX I NOTEBOOKS FOR MATHEMATICA 387

#### x CONTENTS

#### APPENDIX II NUMERICAL COMPUTER PROGRAMS IN C 407 Cl Program for reduced rotation matrix elements 410 C2 Program for 3-j coefficients 412 C3 Program for 6-j coefficients 415 C4 Program for 9-*j* coefficients 417 APPENDIX III **TABLES OF FORMULAS** 421 Legendre functions and spherical harmonics 421 **T**1 Rotation matrix elements 423 T2 The 3-*j* coefficients 425 T3 Irreducible spherical tensor operators 429 T4 The 6-*j* coefficients 431 T5 The 9-j coefficients 433 T6 REFERENCES 437 INDEX 449