

Contents

1 Basic Concepts	1
1.1 Spin States and Density Matrix of Spin-1/2 Particles	1
1.1.1 Pure Spin States.....	1
1.1.2 The Polarization Vector	4
1.1.3 Mixed Spin States	7
1.1.4 Pure Versus Mixed States	9
1.1.5 The Spin-Density Matrix and Its Basic Properties	11
1.1.6 The Algebra of the Pauli Matrices	17
1.1.7 Summary	20
1.2 Polarization States and Density Matrix of Photons	21
1.2.1 The Classical Concept of Wave Polarization	21
1.2.2 Pure and Mixed Polarization States of Photons	24
1.2.3 The Quantum Mechanical Concept of Photon Spin.....	25
1.2.4 The Polarization Density Matrix	27
1.2.5 Stokes Parameter Description	29
2 General Density Matrix Theory	35
2.1 Pure and Mixed Quantum Mechanical States	35
2.2 The Density Matrix and Its Basic Properties	38
2.3 Coherence Versus Incoherence	43
2.3.1 Elementary Theory of Quantum Beats	43
2.3.2 The Concept of Coherent Superposition.....	45
2.4 Time Evolution of Statistical Mixtures	47
2.4.1 The Time Evolution Operator	47
2.4.2 The Liouville Equation	50
2.4.3 The Interaction Picture	52
2.5 Spin Precession in a Magnetic Field.....	57
2.6 Systems in Thermal Equilibrium	58

3 Coupled Systems	61
3.1 The Nonseparability of Quantum Systems after an Interaction	61
3.2 Interaction with an Unobserved System. The Reduced Density Matrix	63
3.3 Analysis of Light Emitted by Atoms (Nuclei)	67
3.3.1 The Coherence Properties of the Polarization States.....	67
3.3.2 Description of the Emitted Photon	69
3.4 Some Further Consequences of the Principle of Nonseparability....	71
3.4.1 Collisional Spin Depolarization.....	71
3.4.2 “Complete Coherence” in Atomic Excitation	72
3.5 Excitation of Atoms by Electron Impact I.....	74
3.5.1 The Reduced Density Matrix of the Atomic System.....	74
3.5.2 Restrictions due to Symmetry Requirements	78
3.6 Nonseparability, Entanglement, and Correlations in Two-Particle Spin-1/2 Systems	82
3.6.1 Introduction and Basic Definitions.....	82
3.6.2 Two-Particle Density Matrices and Reduced Density Matrices. Criterion for Entanglement	84
3.6.3 Correlation Parameters and Their Interpretation. Joint Probabilities.....	87
3.6.4 Entanglement Versus Classical Correlations. LOCC-Procedures. Entanglement in Mixtures	92
3.6.5 States with Maximal Entanglement. Entropy of Entanglement. Bell States	97
3.6.6 Correlations in the Singlet States. Conditional Probabilities	104
3.6.7 Entanglement and Non-Locality. Bell Inequalities.....	109
3.6.8 Experimental Tests. Conclusions	112
4 Irreducible Components of the Density Matrix	115
4.1 Introduction	115
4.2 The Definition of Tensor Operators	116
4.2.1 The General Construction Rule	116
4.2.2 Transformation Properties Under Rotations. The Rotation Matrix	118
4.2.3 Examples	121
4.2.4 Some Important Properties of the Tensor Operators	122
4.3 State Multipoles (Statistical Tensors).....	124
4.3.1 Definition of State Multipoles.....	124
4.3.2 Basic Properties of State Multipoles	126
4.3.3 Physical Interpretation of State Multipoles. The Orientation Vector and Alignment Tensor	127
4.4 Examples: Spin Tensors	129
4.4.1 Spin Tensors for Spin-1/2 Particles	129
4.4.2 Description of Spin-1 Particles.....	130

4.5 Symmetry Properties. Relation Between Symmetry and Coherence	134
4.5.1 Axially Symmetric Systems.....	134
4.5.2 Classification of Axially Symmetric Systems	135
4.5.3 Examples: Photoabsorption by Atoms (Nuclei).....	139
4.6 Excitation of Atoms by Electron Impact II: State Multipoles	140
4.6.1 Collisional Production of Atomic Orientation	140
4.6.2 General Consequences of Reflection Invariance	142
4.6.3 Axially Symmetric Atomic Systems.....	144
4.6.4 Symmetry Relations in the “Natural System”	145
4.6.5 Coordinate Representation of the Density Matrix. Shape and Spatial Orientation of Atomic Charge Clouds ...	147
4.7 Time Evolution of State Multipoles in the Presence of an External Perturbation	153
4.7.1 The Perturbation Coefficients	153
4.7.2 Perturbation Coefficients for the Fine and Hyperfine Interactions	155
4.7.3 An Explicit Example	160
4.7.4 Influence of an External Magnetic Field.....	161
4.8 Notations Used by Other Authors	162
5 Radiation from Polarized Atoms. Quantum Beats	165
5.1 General Theory I: Density Matrix Description of Radiative Decay Processes	165
5.2 General Theory II: Separation of Dynamical and Geometrical Factors	169
5.3 Discussion of the General Formulas	171
5.3.1 General Structure of the Equations	171
5.3.2 Manifestations of Coherence. Quantum Beats	173
5.4 Perturbed Angular Distribution and Polarization	175
5.4.1 General Theory	175
5.4.2 Quantum Beats Produced by “Symmetry Breaking”	176
5.5 Time Integration Over Quantum Beats	178
5.5.1 Steady-State Excitation.....	178
5.5.2 Depolarization Effects Caused by Fine and Hyperfine Interactions	179
6 Some Applications	183
6.1 Theory of Electron–Photon Angular Correlations in Atomic Physics	183
6.1.1 Singlet–Singlet Transitions.....	183
6.1.2 Influence of Fine and Hyperfine Interactions on the Emitted Radiation	188
6.2 Steady-State Excitation	189
6.2.1 Polarization of Impact Radiation.....	189
6.2.2 Threshold and Pseudothreshold Excitations.....	191

6.3	Effect of a Weak Magnetic Field	193
6.3.1	Perturbation Coefficients for Various Geometries Coherence Phenomena	193
6.3.2	Magnetic Depolarization. Theory of the Hanle Effect	197
6.3.3	Physical Interpretation of Zeeman Quantum Beats. Rotation of the Atomic Charge Cloud	200
6.4	Influence of Electric Fields. Orientation – Alignment Conversion...	203
6.4.1	Time Evolution of State Multipoles	203
6.4.2	Variation of Shape and Spatial Direction of Atomic Charge Clouds	205
6.4.3	Creation of Orientation Out of Alignment.....	208
6.4.4	Comparison Between Electric and Magnetic Field Influences	208
7	The Role of Orientation and Alignment in Molecular Processes	209
7.1	Introduction	209
7.2	Rotational Polarization. Semiclassical Interpretation of State Multipoles: Distribution Functions of Angular Momentum Vectors.....	210
7.3	Axis Distributions of Linear Rotors	214
7.3.1	Basic Relations. States with Sharp J and M	214
7.3.2	General Equations. Examples and Experimental Studies	216
7.4	Order Parameters: General Description of Axis Orientation and Alignment.....	219
7.4.1	General Theory for Linear Molecules and Examples	219
7.4.2	Relation Between Angular Momenta and Axis Distributions for Linear Rotors. “Pendulum States”	223
7.5	Angular Momenta and Axis Distributions of Rotors after Photoabsorption. Quantum Mechanical and Classical Theory	224
7.5.1	Absorption of Linearly Polarized Light	224
7.5.2	Absorption of Circularly Polarized and Unpolarized Light.....	227
7.6	Distribution Functions for Nonlinear Molecules and for Diatomics with Electronic Angular Momentum	230
7.6.1	Molecular Orientation Euler Angles	230
7.6.2	Angular Momentum and Axis Distributions of Symmetric Tops.....	231
7.6.3	Theory of Oriented Symmetric-Top Molecules. Semiclassical Interpretation	233
7.6.4	Order Parameters for Nonlinear Molecules	235

7.7	Electronic Orbital Orientation and Alignment	237
7.7.1	Basic Concepts. Space-Fixed Molecules: Excited State Coherence	237
7.7.2	Rotating Molecules. States with Definite Parity: Spatial Orientation and Selective Population.....	241
7.7.3	Combined Description of Rotational Polarization and Orbital Anisotropies	245
7.7.4	Vector Correlations. Analysis of Emitted Light	249
7.7.5	Photoabsorption and Photofragmentation	253
7.8	Dynamical Stereochemistry	256
7.8.1	General Expressions and Definition of Steric Factors	256
7.8.2	Discussion and Examples	263
7.8.3	Product Rotational Polarization. Quantum Mechanical Theory and Semiclassical Approximation	267
7.8.4	Alignment-Induced Chemical Reactions	271
8	Quantum Theory of Relaxation	275
8.1	Density Matrix Equations for Dissipative Quantum Systems	275
8.1.1	Conditions of Irreversibility. Markoff Processes	275
8.1.2	Time Correlation Functions. Discussion of the Markoff Approximation	278
8.1.3	The Relaxation Equation. The Secular Approximation	280
8.2	Rate (Master) Equations	284
8.3	Kinetics of Stimulated Emission and Absorption	288
8.4	The Bloch Equations	294
8.4.1	Magnetic Resonance.....	294
8.4.2	Longitudinal and Transverse Relaxation. Spin Echoes	298
8.4.3	The “Optical” Bloch Equations	301
8.5	Some Properties of the Relaxation Matrix	302
8.5.1	General Constraints.....	302
8.5.2	Relaxation of State Multipoles	304
8.6	The Liouville Formalism	306
8.7	Linear Response of a Quantum System to an External Perturbation	310
Appendices	313
A.1	Appendix A: The Direct Product	313
B.1	Appendix B: State Multipoles for Coupled Systems	316
C.1	Appendix C: Formulas from Angular Momentum Theory	318
C.1.1	Rotation Matrix Elements	320
C.1.2	Matrix Elements of Irreducible Tensor Operators.....	321
C.1.3	Spherical Harmonics	321
D.1	Appendix D: The Efficiency of a Measuring Device	321
E.1	Appendix E: The Scattering and Transition Operators	323

F.1	Appendix F: Some Consequences of Density Matrix Theory for Polarization Vectors and Tensors.....	324
G.1	Appendix G: Derivation of Equation (3.66b)	328
H.1	Appendix H: Conditions for Maximal Entanglement.....	329
I.1	Appendix I: Properties of Maximally Entangled States	330
J.1	Appendix J: Eigenvalues of Density Matrices Condition for Separability Schmidt–Decomposition	333
References.....		337
Index.....		341