Contents

1	Basi	c Conc	epts	1
	1.1	Spin S	States and Density Matrix of Spin-1/2 Particles	1
		1.1.1	Pure Spin States	1
		1.1.2	The Polarization Vector	7
		1.1.3	Mixed Spin States	
		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	Polari	zation 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	Gen	eral De	nsity Matrix Theory	35
	2.1		nd Mixed Quantum Mechanical States	35
	2.2	The D	ensity Matrix and Its Basic Properties	38
	2.3	Coher	ence Versus Incoherence	43
		2.3.1	Elementary Theory of Quantum Beats	43
		2.3.2	The Concept of Coherent Superposition	45
	2.4	Time l	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 F	Precession in a Magnetic Field	57
	26		ns in Thormal Equilibrium	59

xiv Contents

3	Coup	oled Sys	stems	61
	3.1	The N	onseparability of Quantum Systems after an Interaction	61
	3.2	Interac	ction with an Unobserved System. The Reduced	
		Densit	y Matrix	63
	3.3	Analy	sis 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	Excita	tion 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	Nonse	parability, Entanglement, and Correlations	
		in Two	o-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	Inno	duaibla	Components of the Density Matrix	115
-	4.1		luction	115
	4.1		Definition of Tensor Operators	116
	4.2	4.2.1	The General Construction Rule	116
		4.2.1	Transformation Properties Under Rotations.	110
		4.2.2		118
		4,2,3	The Rotation Matrix	
		4.2.3	Examples	121
	4.3		Some Important Properties of the Tensor Operators	122
	4.3		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.	107
	11	Ever	The Orientation Vector and Alignment Tensor	127
	4.4		ples: Spin Tensors	129
		4.4.1	Spin Tensors for Spin-1/2 Particles	129
		4.4.2	Description of Spin-1 Particles	130

Contents xv

4.5 Symmetry Properties. Relation Between Symmetry				
		and C	oherence	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	Excita	ation of Atoms by Electron Impact II: State Multipoles	140
		4.6.1	Collisonal 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 1	Evolution of State Multipoles in the Presence	
		of an l	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	Notati	ons Used by Other Authors	162
5	Radi	iation f	rom Polarized Atoms. Quantum Beats	165
	5.1	Gener	al Theory I: Density Matrix Description	
			liative Decay Processes	165
	5.2		al Theory II: Separation of Dynamical	
			eometrical Factors	169
	5.3	Discus	ssion 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	Pertur	bed Angular Distribution and Polarization	175
		5.4.1	General Theory	175
		5.4.2	Quantum Beats Produced by "Symmetry Breaking"	176
	5.5	Time l	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	Som		cations	183
	6.1		y of Electron–Photon Angular Correlations	
			mic 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	y-State Excitation	189
		6.2.1	Polarization of Impact Radiation	189
		6.2.2	Threshold and Pseudothreshold Excitations	191

xvi Contents

	6.3		of a Weak Magnetic Field	193
		6.3.1	Perturbation Coefficients for Various Geometries	102
			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	Influen	ce 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	Introdu	action	209
	7.2	Rotatio	onal Polarization. Semiclassical Interpretation	
		of State	e Multipoles: Distribution Functions of Angular	
		Momen	ntum Vectors	210
	7.3		vistributions 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		Parameters: General Description of Axis	
			ation and Alignment	219
		7.4.1	General Theory for Linear Molecules	
			and Examples	219
		7.4.2	Relation Between Angular Momenta and Axis	
		, <u>-</u>	Distributions for Linear Rotors. "Pendulum States"	223
	7.5	Angul	ar Momenta and Axis Distributions	
	,		ors after Photoabsorption. Quantum Mechanical	
			assical Theory	224
		7.5.1	Absorption of Linearly Polarized Light	
		7.5.2	Absorption of Circularly Polarized	227
		7.5.2	and Unpolarized Light	227
	7.6	Distrib	oution Functions for Nonlinear Molecules	221
	7.0	and for Diatomics with Electronic Angular Momentum		
		7.6.1	Molecular Orientation Euler Angles	230 230
		7.6.2	Angular Momentum and Axis Distributions	230
		1.0.2	of Symmetric Tops	231
		7.6.3	Theory of Oriented Symmetric-Top Molecules.	231
		7.0.3		222
		7.6.4	Semiclassical Interpretation	
		7.0.4	Order Parameters for Nonlinear Molecules	235

Contents xvii

	7.7	Electro	onic 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	Dynan	nical 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		ntum T	heory of Relaxation	275
	8.1		ty Matrix Equations for Dissipative	
		Quant	um 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	Kineti	cs of Stimulated Emission and Absorption	288
	8.4	The B	loch 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 Li	iouville Formalism	306
	8.7		Response of a Quantum System to an External	
		Perturl	bation	310
		•		212
Aľ	_		L. A. Till a Diversity Design	313
	A.1		dix A: The Direct Product	313
	B.1		dix B: State Multipoles for Coupled Systems	316
	C .1		dix 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		dix D: The Efficiency of a Measuring Device	
	$\mathbf{E}.1$	Appen	dix E: The Scattering and Transition Operators	323

xviii Contents

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
Referen	ces	337
Index		341