

Table of Contents

1. Introduction	1
2. Quantal Phase Factors for Adiabatic Changes	5
2.1 Introduction	5
2.2 Adiabatic Approximation	10
2.3 Berry's Adiabatic Phase	14
2.4 Topological Phases and the Aharonov–Bohm Effect	22
Problems	29
3. Spinning Quantum System in an External Magnetic Field	31
3.1 Introduction	31
3.2 The Parameterization of the Basis Vectors	31
3.3 Mead–Berry Connection and Berry Phase for Adiabatic Evolutions – Magnetic Monopole Potentials....	36
3.4 The Exact Solution of the Schrödinger Equation.....	42
3.5 Dynamical and Geometrical Phase Factors for Non-Adiabatic Evolution	48
Problems	52
4. Quantal Phases for General Cyclic Evolution	53
4.1 Introduction	53
4.2 Aharonov–Anandan Phase	53
4.3 Exact Cyclic Evolution for Periodic Hamiltonians.....	60
Problems	64
5. Fiber Bundles and Gauge Theories	65
5.1 Introduction	65
5.2 From Quantal Phases to Fiber Bundles.....	65
5.3 An Elementary Introduction to Fiber Bundles.....	67
5.4 Geometry of Principal Bundles and the Concept of Holonomy	76
5.5 Gauge Theories	87
5.6 Mathematical Foundations of Gauge Theories and Geometry of Vector Bundles	95
Problems	102

6. Mathematical Structure of the Geometric Phase I:	
The Abelian Phase	107
6.1 Introduction	107
6.2 Holonomy Interpretations of the Geometric Phase	107
6.3 Classification of $U(1)$ Principal Bundles and the Relation Between the Berry–Simon and Aharonov–Anandan Interpretations of the Adiabatic Phase	113
6.4 Holonomy Interpretation of the Non-Adiabatic Phase Using a Bundle over the Parameter Space	118
6.5 Spinning Quantum System and Topological Aspects of the Geometric Phase	123
Problems	126
7. Mathematical Structure of the Geometric Phase II:	
The Non-Abelian Phase	129
7.1 Introduction	129
7.2 The Non-Abelian Adiabatic Phase	129
7.3 The Non-Abelian Geometric Phase	136
7.4 Holonomy Interpretations of the Non-Abelian Phase	139
7.5 Classification of $U(\mathcal{N})$ Principal Bundles and the Relation Between the Berry–Simon and Aharonov–Anandan Interpretations of Non-Abelian Phase	141
Problems	145
8. A Quantum Physical System in a Quantum Environment – The Gauge Theory of Molecular Physics	147
8.1 Introduction	147
8.2 The Hamiltonian of Molecular Systems	148
8.3 The Born–Oppenheimer Method	157
8.4 The Gauge Theory of Molecular Physics	166
8.5 The Electronic States of Diatomic Molecule	174
8.6 The Monopole of the Diatomic Molecule	176
Problems	191
9. Crossing of Potential Energy Surfaces and the Molecular Aharonov–Bohm Effect	195
9.1 Introduction	195
9.2 Crossing of Potential Energy Surfaces	196
9.3 Conical Intersections and Sign-Change of Wave Functions ...	198
9.4 Conical Intersections in Jahn–Teller Systems	209
9.5 Symmetry of the Ground State in Jahn–Teller Systems	213
9.6 Geometric Phase in Two Kramers Doublet Systems	219
9.7 Adiabatic–Diabatic Transformation	222

10. Experimental Detection of Geometric Phases I:	
Quantum Systems in Classical Environments	225
10.1 Introduction	225
10.2 The Spin Berry Phase Controlled by Magnetic Fields	225
10.2.1 Spins in Magnetic Fields: The Laboratory Frame	225
10.2.2 Spins in Magnetic Fields: The Rotating Frame	231
10.2.3 Adiabatic Reorientation in Zero Field	237
10.3 Observation of the Aharonov–Anandan Phase Through the Cyclic Evolution of Quantum States.....	248
Problems	252
11. Experimental Detection of Geometric Phases II:	
Quantum Systems in Quantum Environments	255
11.1 Introduction	255
11.2 Internal Rotors Coupled to External Rotors.....	256
11.3 Electronic–Rotational Coupling	259
11.4 Vibronic Problems in Jahn–Teller Systems.....	260
11.4.1 Transition Metal Ions in Crystals.....	261
11.4.2 Hydrocarbon Radicals	264
11.4.3 Alkali Metal Trimers.....	265
11.5 The Geometric Phase in Chemical Reactions	270
12. Geometric Phase in Condensed Matter I: Bloch Bands ...	277
12.1 Introduction	277
12.2 Bloch Theory	278
12.2.1 One-Dimensional Case	278
12.2.2 Three-Dimensional Case.....	280
12.2.3 Band Structure Calculation.....	281
12.3 Semiclassical Dynamics	283
12.3.1 Equations of Motion	283
12.3.2 Symmetry Analysis	285
12.3.3 Derivation of the Semiclassical Formulas	286
12.3.4 Time-Dependent Bands	287
12.4 Applications of Semiclassical Dynamics.....	288
12.4.1 Uniform DC Electric Field.....	288
12.4.2 Uniform and Constant Magnetic Field	289
12.4.3 Perpendicular Electric and Magnetic Fields	290
12.4.4 Transport	290
12.5 Wannier Functions.....	292
12.5.1 General Properties	292
12.5.2 Localization Properties.....	293
12.6 Some Issues on Band Insulators	295
12.6.1 Quantized Adiabatic Particle Transport	295
12.6.2 Polarization	297
Problems	299

13. Geometric Phase in Condensed Matter II:	
The Quantum Hall Effect	301
13.1 Introduction	301
13.2 Basics of the Quantum Hall Effect	302
13.2.1 The Hall Effect	302
13.2.2 The Quantum Hall Effect	302
13.2.3 The Ideal Model	304
13.2.4 Corrections to Quantization	305
13.3 Magnetic Bands in Periodic Potentials	307
13.3.1 Single-Band Approximation in a Weak Magnetic Field	307
13.3.2 Harper's Equation and Hofstadter's Butterfly	309
13.3.3 Magnetic Translations	311
13.3.4 Quantized Hall Conductivity	314
13.3.5 Evaluation of the Chern Number	316
13.3.6 Semiclassical Dynamics and Quantization	318
13.3.7 Structure of Magnetic Bands and Hyperorbit Levels ..	321
13.3.8 Hierarchical Structure of the Butterfly	325
13.3.9 Quantization of Hyperorbits and Rule of Band Splitting	327
13.4 Quantization of Hall Conductance in Disordered Systems ...	329
13.4.1 Spectrum and Wave Functions	329
13.4.2 Perturbation and Scattering Theory	331
13.4.3 Laughlin's Gauge Argument	332
13.4.4 Hall Conductance as a Topological Invariant	333
14. Geometric Phase in Condensed Matter III:	
Many-Body Systems	337
14.1 Introduction	337
14.2 Fractional Quantum Hall Systems	337
14.2.1 Laughlin Wave Function	337
14.2.2 Fractional Charged Excitations	340
14.2.3 Fractional Statistics	341
14.2.4 Degeneracy and Fractional Quantization	344
14.3 Spin-Wave Dynamics in Itinerant Magnets	346
14.3.1 General Formulation	346
14.3.2 Tight-Binding Limit and Beyond	348
14.3.3 Spin Wave Spectrum	350
14.4 Geometric Phase in Doubly-Degenerate Electronic Bands ...	353
Problem	359
A. An Elementary Introduction to Manifolds and Lie Groups	361
A.1 Introduction	361
A.2 Differentiable Manifolds	371
A.3 Lie Groups	388

B. A Brief Review of Point Groups of Molecules with Application to Jahn–Teller Systems	407
References	429
Index	437