

APPLICATIONS OF GROUP THEORY TO ATOMS, MOLECULES, AND SOLIDS

The majority of all knowledge concerning atoms, molecules, and solids has been derived from applications of group theory. Taking a unique, applications-oriented approach, this book gives readers the tools needed to analyze any atomic, molecular, or crystalline solid system.

Using a clearly defined, eight-step program, this book helps readers to understand the power of group theory, what information can be obtained from it, and how to obtain it. The book takes in modern topics, such as graphene, carbon nanotubes, and isotopic frequencies of molecules, as well as more traditional subjects: the vibrational and electronic states of molecules and solids, crystal-field and ligand-field theory, transition-metal complexes, space groups, time-reversal symmetry, and magnetic groups.

With over a hundred end-of-chapter exercises, this book is invaluable for graduate students and researchers in physics, chemistry, electrical engineering, and materials science.

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Contents

<i>Preface</i>	<i>page xi</i>
1 Introductory example: Squarene	1
1.1 In-plane molecular vibrations of squarene	1
1.2 Reducible and irreducible representations of a group	12
1.3 Eigenvalues and eigenvectors	27
1.4 Construction of the force-constant matrix from the eigenvalues	30
1.5 Optical properties	31
References	34
Exercises	35
2 Molecular vibrations of isotopically substituted AB_2 molecules	39
2.1 Step 1: Identify the point group and its symmetry operations	39
2.2 Step 2: Specify the coordinate system and the basis functions	39
2.3 Step 3: Determine the effects of the symmetry operations on the basis functions	41
2.4 Step 4: Construct the matrix representations for each element of the group using the basis functions	41
2.5 Step 5: Determine the number and types of irreducible representations	42
2.6 Step 6: Analyze the information contained in the decompositions	42
2.7 Step 7: Generate the symmetry functions	43
2.8 Step 8: Diagonalize the matrix eigenvalue equation	50
2.9 Constructing the force-constant matrix	50
2.10 Green's function theory of isotopic molecular vibrations	52
2.11 Results for isotopically substituted forms of H_2O	60

References	62
Exercises	62
3 Spherical symmetry and the full rotation group	66
3.1 Hydrogen-like orbitals	66
3.2 Representations of the full rotation group	68
3.3 The character of a rotation	72
3.4 Decomposition of $D^{(l)}$ in a non-spherical environment	75
3.5 Direct-product groups and representations	76
3.6 General properties of direct-product groups and representations	79
3.7 Selection rules for matrix elements	83
3.8 General representations of the full rotation group	85
References	88
Exercises	88
4 Crystal-field theory	90
4.1 Splitting of d -orbital degeneracy by a crystal field	90
4.2 Multi-electron systems	95
4.3 Jahn–Teller effects	116
References	119
Exercises	119
5 Electron spin and angular momentum	123
5.1 Pauli spin matrices	123
5.2 Measurement of spin	126
5.3 Irreducible representations of half-integer angular momentum	127
5.4 Multi-electron spin–orbital states	129
5.5 The L – S -coupling scheme	130
5.6 Generating angular-momentum eigenstates	132
5.7 Spin–orbit interaction	138
5.8 Crystal double groups	150
5.9 The Zeeman effect (weak-magnetic-field case)	153
References	155
Exercises	156
6 Molecular electronic structure: The LCAO model	158
6.1 N -electron systems	158
6.2 Empirical LCAO models	162
6.3 Parameterized LCAO models	163
6.4 An example: The electronic structure of squareene	168
6.5 The electronic structure of H_2O	182

<i>Contents</i>		vii
References		188
Exercises		189
7	Electronic states of diatomic molecules	193
7.1	Bonding and antibonding states: Symmetry functions	193
7.2	The “building-up” of molecular orbitals for diatomic molecules	198
7.3	Heteronuclear diatomic molecules	206
	Exercises	209
8	Transition-metal complexes	211
8.1	An octahedral complex	211
8.2	A tetrahedral complex	227
	References	237
	Exercises	237
9	Space groups and crystalline solids	239
9.1	Definitions	239
9.2	Space groups	244
9.3	The reciprocal lattice	246
9.4	Brillouin zones	247
9.5	Bloch waves and symmorphic groups	249
9.6	Point-group symmetry of Bloch waves	252
9.7	The space group of the \mathbf{k} -vector, $g_{\mathbf{k}}^s$	258
9.8	Irreducible representations of $g_{\mathbf{k}}^s$	259
9.9	Compatibility of the irreducible representations of $g_{\mathbf{k}}$	260
9.10	Energy bands in the plane-wave approximation	265
	References	276
	Exercises	276
10	Application of space-group theory: Energy bands for the perovskite structure	280
10.1	The structure of the ABO_3 perovskites	280
10.2	Tight-binding wavefunctions	282
10.3	The group of the wavevector, $g_{\mathbf{k}}$	283
10.4	Irreducible representations for the perovskite energy bands	284
10.5	LCAO energies for arbitrary \mathbf{k}	298
10.6	Characteristics of the perovskite bands	300
	References	301
	Exercises	302

viii	<i>Contents</i>	
11	Applications of space-group theory: Lattice vibrations	304
11.1	Eigenvalue equations for lattice vibrations	305
11.2	Acoustic-phonon branches	309
11.3	Optical branches: Two atoms per unit cell	314
11.4	Lattice vibrations for the perovskite structure	320
11.5	Localized vibrations	327
	References	334
	Exercises	334
12	Time reversal and magnetic groups	337
12.1	Time reversal in quantum mechanics	337
12.2	The effect of \mathbb{T} on an electron wavefunction	340
12.3	Time reversal with an external field	341
12.4	Time-reversal degeneracy and energy bands	342
12.5	Magnetic crystal groups	346
12.6	Co-representations for groups with time-reversal operators	350
12.7	Degeneracies due to time-reversal symmetry	357
	References	361
	Exercises	361
13	Graphene	363
13.1	Graphene structure and energy bands	363
13.2	The analogy with the Dirac relativistic theory for massless particles	368
13.3	Graphene lattice vibrations	369
	References	381
	Exercises	381
14	Carbon nanotubes	383
14.1	A description of carbon nanotubes	384
14.2	Group theory of nanotubes	386
14.3	One-dimensional nanotube energy bands	393
14.4	Metallic and semiconducting nanotubes	401
14.5	The nanotube density of states	403
14.6	Curvature and energy gaps	406
	References	407
	Exercises	407
<i>Appendix A</i>	Vectors and matrices	410
<i>Appendix B</i>	Basics of point-group theory	415

	<i>Contents</i>	ix
<i>Appendix C</i>	Character tables for point groups	430
<i>Appendix D</i>	Tensors, vectors, and equivalent electrons	442
<i>Appendix E</i>	The octahedral group, O and O_h	449
<i>Appendix F</i>	The tetrahedral group, T_d	455
<i>Appendix G</i>	Identifying point groups	462
	<i>Index</i>	465

Preface

The majority of all knowledge accumulated in physics and chemistry concerning atoms, molecules, and solids has been derived from applications of group theory to quantum systems.

My (T.W.) first encounter with group theory was as an undergraduate in physics, struggling to understand Wigner's *Group Theory and Its Application to the Quantum Mechanics of Atomic Spectra* (1959). I felt there was something magical about the subject. It was amazing to me that it was possible to analyze a physical system knowing only the symmetry and obtain results that were absolute, independent of any particular model. To me it was a miracle that it was possible to find some exact eigenvectors of a Hamiltonian by simply knowing the geometry of the system or the symmetry of the potential.

Many books devote the initial chapters to deriving abstract theorems before discussing any of the applications of group theory. We have taken a different approach. The first chapter of this book is devoted to finding the molecular vibration eigenvalues, eigenvectors, and force constants of a molecule. The theorems required to accomplish this task are introduced as needed and discussed, but the proofs of the theorems are given in the appendices. (In later chapters the theorems needed for the analysis are derived within the discussions.) By means of this applications-oriented approach we are able to immediately give a general picture of how group theory is applied to physical systems. The emphasis is on the process of applying group theory. The various steps needed to analyze a physical system are clearly delineated. By the end of the first chapter the reader should have an appreciation for the power of group theory, what information can be obtained, and how to obtain it. That is, the “magic” of group theory should already be apparent.

In addition to the essential, traditional topics, there are new topics, including the electronic and vibrational properties of graphene and nanotubes, the vibrations of isotopically substituted molecules, localized vibrations, and discussions of the axially symmetric lattice dynamics model. The energy bands and vibrational

normal modes of crystals with the perovskite structure are also discussed in detail.

The material in this book was developed in part from group-theory courses and from a series of lectures presented in courses on special topics at the University of Missouri-Columbia. It is appropriate for science and engineering graduate students and advanced undergraduate seniors. The ideal reader will have had a course in quantum mechanics and be familiar with eigenvalue problems and matrix algebra. However, no prerequisite knowledge of group theory is necessary.

This book may be employed as a primary text for a first course in group theory or as an auxiliary book for courses in quantum mechanics, solid-state physics, physical chemistry, materials science, or electrical engineering. It is intended as a self-teaching tool and therefore the analyses in the early chapters are given in some detail. Each chapter includes a set of exercises designed to reinforce and extend the material discussed in the chapter.

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and
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