An Introduction to Groups and Their Matrices for Science Students

Group theory, originating from algebraic structures in mathematics, has long been a powerful tool in many areas of physics, chemistry, and other applied sciences, but it has seldom been covered in a manner accessible to undergraduates. This book from renowned educator Robert Kolenkow introduces group theory and its applications starting with simple ideas of symmetry, through quantum numbers, and working up to particle physics. It features clear explanations, accompanying problems and exercises, and numerous worked examples from experimental research in the physical sciences. Beginning with key concepts and necessary theorems, topics are introduced systematically, including molecular vibrations and lattice symmetries; matrix mechanics; wave mechanics; rotation and quantum angular momentum; atomic structure; and finally particle physics. This comprehensive primer on group theory is ideal for advanced undergraduate topics courses, reading groups, or self-study, and it will help prepare graduate students for higher-level courses.

Robert Kolenkow was formerly Associate Professor of Physics at Massachusetts Institute of Technology and was awarded the Everett Moore Baker Award for Outstanding Teaching. He was the lead author of *Physical Geography Today* and coauthor, with Daniel Kleppner, of *An Introduction to Mechanics* (also published by Cambridge University Press).

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To Marcia
my help and support

Contents

PREFACE

This is not a math book, although a quick flip of the pages might give that impression. It is an introduction to group theory and matrix representations, a subject usually treated with mathematical rigor, theorems, and proofs. This book is intended to introduce the subject and to clear a path to more advanced treatments.

INTRODUCTION

Like typical undergraduates in science I took math courses every semester for three years, beginning with the wonders of calculus, differential equations, and advanced calculus. An elective course in linear algebra was my first contact with matrices. In graduate school I heard that group theory is a powerful tool for treating physical problems, so I took a course taught by a renowned theorist, but it was difficult for me. The term "transforms like" puzzled me – what was "transforming" and what was it "like"?

While on the physics faculty of the Massachusetts Institute of Technology I agreed to develop an elective course in group theory for juniors and seniors, having learned by then that a good way to understand a subject is to teach it. The course was popular, with 30–40 majors in physics, chemistry, and math attending.

This is the book I wish I had as a student and the book I would have wanted to teach from. A few proofs are omitted as unsuited to a text at this level, but often made plausible by examples. There are only a few uses of the crutch "it can be shown." Experimental results taken from original research papers are included to show how group theory helps us understand physical phenomena.

After studying this text, the student will be prepared to tackle more advanced texts and to understand, at least in part, research papers that employ group theory.

OVERVIEW

Most chapters end with a "Brief Bios" section to recognize the lives of experimentalists and theorists.

Chapter 1 Fundamental Concepts introduces the idea of symmetry by illustrations and elementary algebra of operations. The **32** group and the isomorphic permutation group illustrate the group axioms, and a matrix representation is derived using algebraic geometry. Matrix types are defined.

Chapter 2 Matrix Representations of Discrete Groups is entirely mathematical by necessity. The major concepts of basis functions, similarity transformations, character, and reducibility are defined and illustrated.

Chapter 3 Molecular Vibrations defines normal modes using Newtonian mechanics and group theory. The water molecule is taken as an example and its vibration modes are calculated and visualized in physical terms. IR active and Raman active modes are predicted from character tables.

Chapter 4 Crystalline Solids deals with ideal crystalline solids and their translation and rotation symmetries. Vibration of a 1-dimensional diatomic chain is calculated from mechanics to show the origin of branches.

Chapter 5 Bohr's Quantum Theory and Matrix Mechanics begins with a summary of Bohr's quantum theory followed by Born's recognition that Heisenberg's difference equations represent matrix algebra. The single quantization condition of matrix mechanics is based on a commutator and is applied to deriving physical principles such as conservation of energy and angular momentum. Heisenberg's uncertainty principle is made plausible by his thought experiments.

Chapter 6 Wave Mechanics, Measurement, and Entanglement Schrödinger's wave equation expresses the dispersion of matter waves. Quantization is illustrated by rotational spectra. A model 2×2 Hermitian matrix is diagonalized. Probability is challenged by the EPR thought experiment that local measurements should not produce distant results. Hidden variable theory and quantum mechanics are compared.

Chapter 7 Rotation uses algebraic geometry to develop matrices for rotation of a vector. Groups U(1) and SU(2) are defined, and SO(3) is derived from SU(2) by a similarity transformation. Euler angles are defined by sketches and matrices.

Chapter 8 Quantum Angular Momentum is a key chapter for applications of group theory. The Stern–Gerlach experiment introduces spatial quantization and angular momentum quantum numbers. Exponential operators are defined and commutators are calculated from matrices. Angular momentum labels for irreducible representations are developed. Spherical harmonics are generated using group theory. Combining quantum mechanical angular momentum is illustrated by positronium and Wigner *3-j* coefficients are generated. Selection rules for electric dipole transitions are derived from spherical harmonics, from the Wigner–Eckart theorem, and from parity.

Chapter 9 The Structure of Atoms summarizes Zeeman's experiments and uses the Zeeman effect to motivate numerous applications including diagonalization with spin-orbit coupling in any field. Group theory applied to He derives the singlet and triplet states. The Pauli principle applied to electron configurations determines allowed states. The building-up principle and Hund's rules give a qualitative account of multi-electron atoms and the periodic table.

Chapter 10 Particle Physics begins by listing the fundamental forces. SU(2) supports isospin of nucleons for strong interactions. Properties of Lagrangians are discussed. U(1) gauge invariance of Schrödinger's equation is demonstrated. The quark model is applied to hadrons. Conservation laws are applied to reactions. SU(3) is introduced and applied to the three-quark model and to color charge.

Appendix A Character Tables from Class Sums
Appendix B Born–Jordan Proof of the Quantization Condition
Appendix C Weyl Derivation of the Heisenberg Uncertainty Principle
Appendix D EPR Thought Experiment
Appendix E Photon Correlation Experiment
Appendix F Tables of Some *3-j* Coefficients
Appendix G Proof of the Wigner–Eckart Theorem

TO THE INSTRUCTOR

There is more than enough material for a one-semester junior-senior course. A solid introduction to group theory and applications would include Chapters 1 Fundamental Concepts, 2 Matrix Representations of Discrete Groups, 3 Molecular Vibrations, 6 Wave Mechanics, Measurement, and Entanglement, 7 Rotation, 8 Quantum Angular Momentum, and 9 The Structure of Atoms. Chapter 10 Particle Physics would be popular with students.

Chapter 5 Bohr's Quantum Theory and Matrix Mechanics and the Sections 6.6 and 6.7 on measurement and entanglement in Chapter 6 deal with topics not commonly treated in texts at this level. The inclusion of these special topics is intended to stimulate student interest, but they could be treated as material for a short course, for a reading course, or for self-study.