

GIAN-CARLO ROTA, *Editor*
ENCYCLOPEDIA OF MATHEMATICS AND ITS APPLICATIONS
Volume 9

Section: Mathematics of Physics
Peter A. Carruthers, *Section Editor*

The Racah–Wigner Algebra in Quantum Theory

Lawrence C. Biedenharn

James D. Louck

GIAN-CARLO ROTA, *Editor*
ENCYCLOPEDIA OF MATHEMATICS AND ITS APPLICATIONS
Volume 9

Section: Mathematics of Physics
Peter A. Carruthers, *Section Editor*

The Racah–Wigner Algebra in Quantum Theory

Lawrence C. Biedenharn

Department of Physics
Duke University
Durham, North Carolina

James D. Louck

Theoretical Division
Los Alamos National Laboratory
University of California
Los Alamos, New Mexico

With a Foreword by

Peter A. Carruthers

Los Alamos National Laboratory

Introduction by

George W. Mackey

Harvard University



1981

Addison-Wesley Publishing Company

Advanced Book Program
Reading, Massachusetts

London • Amsterdam • Don Mills, Ontario • Sydney • Tokyo

Library of Congress Cataloging in Publication Data

Biedenharn, L. C.

The Racah-Wigner algebra in quantum theory.

(Encyclopedia of mathematics and its applications ; v. 9. Section, Mathematics of physics)

Includes bibliographies and indexes.

1. Racah algebra. 2. Quantum theory.

I. Louck, James D. II. Title. III. Series: Encyclopedia of mathematics and its applications ; v. 9. IV. Series: Encyclopedia of mathematics and its applications. Section, Mathematics of physics.

QC174.17.R32B53 530.1'2'01512 81-3668

ISBN 0-201-13508-6

AACR2

American Mathematical Society (MOS) Subject Classification Scheme (1980): 05C05, 05C30, 12D10, 12E10, 20C30, 20C35, 22E70, 33A65, 33A75, 46K99, 46L05, 46L10, 47C10, 47D10, 47D15.

Copyright © 1981 by Addison-Wesley Publishing Company, Inc.

Published simultaneously in Canada.

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, recording, or otherwise, without the prior written permission of the publisher, Addison-Wesley Publishing Company, Inc., Advanced Book Program, Reading, Massachusetts 01867, U.S.A.

Manufactured in the United States of America

ABCDEFGHIJ-HA-8987654321

Contents of Volume 8

Contents of companion volume

The Racah-Wigner Algebra in Quantum Theory

by L. C. Biedenharn and J. D. Louck

(ENCYCLOPEDIA OF MATHEMATICS AND ITS
APPLICATIONS, Volume 9)

Editor's Statement

Section Editor's Foreword

Preface

Acknowledgments

PART I

Chapter 1 Introduction

Notes

References

Chapter 2 The Kinematics of Rotations

1. Introduction
2. Properties of Rotations
3. Dirac's Construction
4. Cartan's Definition of a Spinor
5. Relation between $SU(2)$ and $SO(3)$ Rotations
6. Parametrizations of the Group of Rotations
7. Notes
- References

Chapter 3 Standard Treatment of Angular Momentum in Quantum Mechanics

1. Overview
2. Definition of the Angular Momentum Operators
3. The Angular Momentum Multiplets
4. Matrices of the Angular Momentum
5. The Rotation Matrices (General Properties)
6. The Rotation Matrices (Explicit Forms)

7. Wave Functions for Angular Momentum Systems
8. Differential Equations for the Rotation Matrices
9. Orthogonality of the Rotation Matrices
10. Spherical Harmonics
11. The Addition of Angular Momentum
12. The Wigner Coefficients
13. Relations between Rotation Matrices and Wigner Coefficients.
14. Concept of a Tensor Operator
15. The Wigner-Eckart Theorem
16. The Coupling of Tensor Operators
17. Applications of the Wigner-Eckart Theorem
18. Racah Coefficients
19. $9-j$ Coefficients
20. Rotationally Invariant Products
21. Operators Associated with Wigner, Racah, and $9-j$ Coefficients
22. Notes
23. Appendices
- References

Chapter 4 The Theory of Turns Adapted from Hamilton

1. An Alternative Approach to Rotations
2. Properties of Turns (Geometric Viewpoint)
3. Properties of Turns (Algebraic View)
4. The Space of Turns as a Carrier Space
5. Notes
- References

Chapter 5 The Boson Calculus Applied to the Theory of Turns

1. Introduction
2. Excursus on the Boson Calculus
3. The Jordan Mapping
4. An Application of the Jordan Map
5. Generalization of the Jordan Map
6. Application of the Generalized Jordan Map
7. Application of the Generalized Jordan Map to Determine the Wigner Coefficients
8. Wigner Coefficients as "Discretized" Rotation Matrices
9. Appendices
- References

Chapter 6 Orbital Angular Momentum and Angular Functions on the Sphere

1. Rotational Symmetry of a Simple Physical System
 2. Scalar Product of State Vectors
 3. Unitarity of the Orbital Rotation Operator
 4. A (Dense) Subspace of $\mathcal{H}(S)$
 5. Only Integral Values of l can occur in the Quantization of Spatial (Orbital) Angular Momentum
 6. Transformations of the Solid Harmonics under Orbital Rotation
 7. The Elements of the Rotation Matrix $\mathcal{D}^l(R)$ are Homogeneous Polynomials
 8. The Energy Eigenvalue Equation
 9. Tensor Spherical Harmonics
 10. Spinor Spherical Harmonics
 11. Vector Spherical Harmonics
 12. Algebraic Aspects of Vector Spherical Harmonics
 13. Summary of Properties of Vector Solid Harmonics
 14. Decomposition Theorem for Vector Functions Defined on the Sphere
 15. Rotationally Invariant Spherical Functions of Two Vectors
 16. Applications of the Cartan Map to Spherical Functions
 17. Rotationally Invariant Spherical Functions in Several Vectors
 18. Relationship of Solid Harmonics to Potential Theory
 19. The Orbital Rotation Matrices as Forms
 20. The Orbital Rotation Matrices are Equivalent to Real Orthogonal Matrices
 21. The "Double-Valued Representations" of the Proper Orthogonal Group $SO(3)$
 22. Note
- References

PART II

Chapter 7 Some Applications to Physical Problems

1. Introductory Remarks
2. Basic Principles Underlying the Applications
3. The Zeeman Effect

- a. Background
- b. The Normal Zeeman Effect
- c. Quantal Treatment
- d. The Anomalous Zeeman Effect
- e. Relation to the Development of Angular Momentum Theory
- f. Concluding Remarks
- g. Note
- References
- 4. The Nonrelativistic Hydrogen Atom
 - a. Algebraic Aspects
 - b. Properties of the Bound States of the Hydrogen Atom
 - c. Explicit Hydrogen Atom Wave Functions
 - d. Momentum Space Representation
 - e. Relationship between Rotation Matrices and Hyperspherical Harmonics
 - f. Pauli Particle (Hydrogen Atom with Spin)
 - g. Remarks
 - h. Appendix
 - References
- 5. Atomic Spectroscopy
 - a. Introduction
 - b. The Approximate Hamiltonian for Many-Electron Atoms
 - c. The Central-Field Model
 - d. A Short Vocabulary of Spectroscopy Terminology
 - e. Closed Shells
 - f. The One-Electron Problem with Spin-Orbit Coupling
 - g. Two-Electron Configurations
 - h. Equivalent Electron Configurations
 - i. Operator Structures in l^n -Configurations
 - j. Appendix
 - References
- 6. Electromagnetic Processes
 - a. Preliminary Remarks
 - b. Multipole Radiation
 - c. The Hansen Multipole Fields
 - d. Classical Multipole Moments
 - e. Reduction of the Electric Multipole Moments
 - f. The Radiated Multipole Fields
 - g. A Curious Property of the Multipole Expansion (Casimir [9])

- h. The Radiated Power
- i. Angular Momentum Flux
- j. A Vectorial Analog to the Rayleigh Expansion
- k. An Illustrative Example
- l. The Density Matrix for Photon Angular Correlation Measurements
- m. Notes
- References
- 7. Angular Momentum Techniques in the Density Matrix Formulation of Quantum Mechanics
 - a. Preliminaries
 - b. Statistical Tensors
 - c. A Geometric Characterization of the Density Matrices for Pure States of Spin- j
 - d. The Density Matrix for a Relativistic Massive Particle of Spin- j
 - e. The Special Case of Massless Particles
 - f. Coupling of Statistical Tensors
 - g. Some Examples Illustrating the Coupling Formula
 - h. The Majorana Formula
 - References
- 8. Angular Correlations and Angular Distributions of Reactions
 - a. The Nature of the Angular Correlation Process
 - b. Cascades
 - c. Stretched Angular Momenta
 - d. More Involved Correlation Processes
 - e. Relativistic Regime
 - References
- 9. Some Applications to Nuclear Structure
 - a. Qualitative Considerations
 - b. The Nuclear Shell Model of Mayer and Jensen
 - c. The Isospin Quantum Number
 - d. Properties of a Short-Range Interaction
 - e. The Pairing Interaction (Seniority)
 - f. Quasi-Spin
 - g. Quasi-Spin Wave Functions (Seniority Label)
 - h. Application of Quasi-Spin to Tensor Operators
 - i. Seniority in Terms of Casimir Operators
 - j. Concluding Remarks
 - k. Note
 - References
- 10. Body-Fixed Frames: Spectra of Spherical Top Molecules

- a. Introduction
- b. Definition and Kinematics of a Body-Fixed Frame
- c. Form of the State Vectors for Isolated Systems Described in a Body-Fixed Frame
- d. The Instantaneous Principal Axes of Inertia Frame
- e. The Eckart Molecular Frame
- f. Distinguished Particle Frames
- g. Uniform Method of Defining Body-Fixed Frames
- h. Internal Coordinates
 - i. Internal Coordinates for the Eckart Frame
 - j. Internal Coordinates for the Principal Axes Frame
- k. The Linear Momentum Operators
 - l. The Hamiltonian for a Semirigid (Rigid) Polyatomic Molecule
- m. Approximate Form of the Hamiltonian for Spherical Top Molecules
- n. First-Order Energy Spectrum of a Triply Degenerate Vibration in a Spherical Top Molecule
- o. The Point Group of a Rigid Molecule
- p. Higher-Order Corrections: Phenomenological Hamiltonian.
- q. Splitting Patterns
- r. Symmetry Axes and Induced Representations
- s. High Angular Momentum Effects
- t. Selection Rules and Statistical Weights
- u. Spectra of Fundamental Transitions of SF_6
- v. Appendices
- References

Appendix of Tables

Bibliography

List of Symbols

Author Index

Subject Index

Editor's Statement

A large body of mathematics consists of facts that can be presented and described much like any other natural phenomenon. These facts, at times explicitly brought out as theorems, at other times concealed within a proof, make up most of the applications of mathematics, and are the most likely to survive changes of style and of interest.

This **ENCYCLOPEDIA** will attempt to present the factual body of all mathematics. Clarity of exposition, accessibility to the non-specialist, and a thorough bibliography are required of each author. Volumes will appear in no particular order, but will be organized into sections, each one comprising a recognizable branch of present-day mathematics. Numbers of volumes and sections will be reconsidered as times and needs change.

It is hoped that this enterprise will make mathematics more widely used where it is needed, and more accessible in fields in which it can be applied but where it has not yet penetrated because of insufficient information.

GIAN-CARLO ROTA

About the authors:

L. C. Biedenharn earned the Ph.D in Physics at M.I.T. and was research assistant and associate there before going to Oak Ridge National Laboratory. He became Assistant Professor at Yale, and Assistant then Associate Professor, Rice Institute, before becoming Professor of Physics at Duke University.

J. D. Louck, after receiving the Ph.D. in Physics from Ohio State University, became a Staff Member in the Theoretical Division at Los Alamos National Laboratory and then Associate Professor (graduate faculty) at Auburn University, Alabama, from which he had graduated. He returned as a Staff Member to Los Alamos and has been Visiting Professor of Physics at Duke University.

About the book:

The development of the algebraic aspects of angular momentum theory and relationship between angular momentum theory and special topics in physics and mathematics are covered in this volume.

Foreword

The study of the symmetries of physical systems remains one of the principal contemporary theoretical activities. These symmetries, which basically express the geometric structure of the physical system in question, must be clearly analyzed in order to understand the dynamical behavior of the system. The analysis of rotational symmetry, and the behavior of physical quantities under rotations, is the most common of such problems. Accordingly, every professional physicist must achieve a good working knowledge of the "theory of angular momentum."

In addition, the theory of angular momentum is the prototype of continuous symmetry groups of many types now found useful in the classification of the internal symmetries of elementary particle physics. Much of the intuition and mathematical apparatus developed in the theory of angular momentum can be transferred with little change to such research problems of current interest.

If there is a single essential book in the arsenal of the physicist, it is a good book on the theory of angular momentum. I have worn out several earlier texts on this subject and have spent much time checking signs and Clebsch-Gordan coefficients. Such books are the most borrowed and least often returned. I look forward to a long association with the present fine work.

A good book on the theory of angular momentum needs to be thoroughly reliable yet must develop the material with insight and good taste in order to lay bare the elegant texture of the subject. Originality should not be erected in opposition to current practices and conventions if the text is to be truly useful.

The present text, written by two well-known contributors to the field, satisfies all these criteria and more. Subtleties and scholarly comments are presented clearly yet unobtrusively. Moreover, the footnotes contain fascinating historical material of which I was previously unaware. The two chapters on the "theory of turns" and "boson calculus" are significant new additions to the pedagogical literature on angular momentum. Much of the theory of turns presented here was developed by the authors. By means of this approach the concept of "double group" is made very clear. The development of the boson calculus employs Gel'fand patterns in an essential way, in addition to the more traditional Young tableaux. This section provides an excellent prototype for the analysis of all compact groups.

The representation theory is developed in the complete detail required for physical applications. This exposition of the lore of rotation matrices is especially thorough, including the Euler angle parametrization as well as others of practical value.

The text ends with a long chapter on applications well chosen to illustrate the power of the general techniques. The book concludes with a masterly development of the group theoretical description of the spectra of spherical top molecules. To my mind the recent experimental confirmation of this theory in high resolution laser spectrometry experiments is one of the most spectacular confirmations of quantum theory.

The present text is really a book for physicists. Nevertheless, the theory generates substantial material of interest for mathematicians. Recent research (for example in non-Abelian gauge field theory) has produced topics of common interest to both mathematicians and physicists. Some of the more interesting mathematical outgrowths of the theory of angular momentum are developed in the companion volume currently in press.

PETER A. CARRUTHERS

General Editor, Section on Mathematics of Physics

Preface

"The art of doing mathematics," Hilbert¹ has said, "consists in finding that *special* case which contains all the germs of *generality*." In our view, angular momentum theory plays the role of that "special case," with symmetry—one of the most fruitful themes of modern mathematics and physics—as the "generality." We would only amend Hilbert's phrase to include physics as well as mathematics. In the Preface to the second edition of his famous book *Group Theory and its Applications to the quantum Mechanics of Atomic Spectra*, Wigner² records von Laue's view of how remarkable it is that "almost all the rules of [atomic] spectroscopy follow from the symmetry of the problem." The symmetry at issue is *rotational symmetry*, and the spectroscopic rules are those implied by *angular momentum conservation*. In this monograph, we have tried to expand on these themes.

The fact that this monograph is part of an encyclopedia imposes a responsibility that we have tried to take seriously. This responsibility is rather like that of a library. It has been said that a library must satisfy two disparate needs: One should find the book one is looking for, but one should also find books that one had no idea existed. We believe that much the same sort of thing is true of an encyclopedia, and we would be disappointed if the reader did not have both needs met in the present work. To accomplish this objective, we have found it necessary to split our monograph into two volumes, one dealing with the "standard" treatment of angular momentum theory and its applications, the other dealing in depth with the fundamental concepts of the subject and the interrelations of angular momentum theory with other areas of mathematics.

Fulfilling this responsibility further, we have made an effort to address readers who seek *very* detailed answers on *specific* points—hence, we have a large index, and many notes and appendices—as well as readers who seek an overview of the subject, especially a description of its unique and appealing aspects. This accounts for the uneven level of treatment which varies from chapter to chapter, or even within a chapter, quite unlike a

¹Quoted in M. Kac, "Wiener and Integration in Function Spaces," *Bull. Amer. Math. Soc.* 72 (1966), p. 65. (The italics are in the original; Kac notes that the statement may be apocryphal.)

²E. P. Wigner, *Group Theory and Its Applications to the Quantum Mechanics of Atomic Spectra*, Academic Press, New York, 1959, p. v. (We have added in brackets the word "atomic," since this was clearly von Laue's intended meaning.)

textbook with its uniformly increasing levels of difficulty. The variation in the treatment applied particularly to the Remarks. Quite often these Remarks contain material that has not been developed or explained earlier. Such material is intended for the advanced reader, and it can be disregarded by others. We urge the reader to browse and skip, rather than trying, at first, any more systematic approach.

These considerations apply also to the applications. Some applications may be almost too elementary, whereas others are at the level of current research. The field of applications is so broad that we have surely failed to do justice in many cases, but we do hope that the treatment of some applications is successful.

In discussing a particular subject, we have given more detail than is usual in mathematical books, where terseness is considered the cardinal virtue. Here we have followed the precepts of Littlewood³ who points out that "two trivialities omitted can add up to an *impasse*."

Let us acknowledge one idiosyncrasy of our treatment: We have not explicitly used the methods of group theory, per se, but have proceeded algebraically so that the group theory, if it appears at all, appears naturally as the treatment develops. No doubt this method of treatment is an overreaction to the censure—(now disappearing?)—with which many physicists greeted the *Gruppenpest*.⁴ In any event, we think that this treatment does make the material more accessible to some readers.

Let us make some brief suggestions as to how to use the first volume, *Angular Momentum in Quantum Physics* (AMQP). Part I: (i) Chapters 2 and 3 and parts of Chapter 6 constitute the standard treatment of angular momentum theory and will suffice for many readers who wish to learn the mechanics of the subject. The methods used are elementary (but by no means imprecise), and the whole treatment flows from the fundamental commutation relations of angular momentum. (ii) Chapters 4 and 5 are recommended to the reader who wishes a general overview of the subject with methods capable of great generalization. Paradoxically, although these two chapters contain much new material, this material also belongs to the very beginnings of the subject—in the multiplication of forms of Clebsch and Gordan, and in the ξ - η calculus of Weyl—all of which are now incorporated under the rubric of the "boson calculus." Part II: The applications given in Chapter 7 are totally independent of one another, and can be understood from the results given in Chapter 3.

The second volume, *Racah-Wigner Algebra in Quantum Theory* (RWA), is also presented in two parts. (The Contents for RWA appears also at the

³J. E. Littlewood, *A Mathematician's Miscellany*, Methuen and Co., London, 1953, p. 30. (The italics are in the original.)

⁴B. G. Wybourne, "The Gruppenpest yesterday, today, and tomorrow," *International Journal of Quantum Chemistry*, Symposium No. 7 (1973), pp. 35-43.

beginning of AMQP.) Part I: In Chapters 2, 3, and 4 the algebra of the operators associated with the two basic quantities in angular momentum theory—the Wigner and Racah coefficients—is developed within the framework of the algebra of bounded operators acting in Hilbert space. These chapters are intended to rephrase the concept of a “Wigner operator” (tensor operator) in algebraic terms, using methods from Gel’fand’s development of Banach algebras. This approach to angular momentum theory is rather new, and is intended for the reader who wishes to pursue the subject from the viewpoint of mathematics. Part II: The twelve topics developed in Chapter 5 establish diverse interrelations between concepts in angular momentum theory and other areas of mathematics. These topics are independent of one another, but do draw for their development on the material of Chapter 3 of AMQP, and to a lesser extent on Chapters 1–3 of RWA. This material should be of interest to both mathematicians and physicists.

Acknowledgments

This monograph could not have been completed without the extensive help of friends and colleagues. Professor L. P. Horwitz performed the vital chore of a thorough reading and criticism of the entire two volumes; his help is gratefully acknowledged.

Other colleagues who have helped us by reading and criticizing particular chapters, the applications, or topics in *Angular Momentum in Quantum Physics* and in *Racah-Wigner Algebra in Quantum Theory* are: (i) AMQP. D. Giebink, Chapters 2-4; Professors H. Bacry and B. Wolf, Chapter 4; Professor R. Rodenberg and Dr. M. Danos, Chapters 2-6; Professor B. R. Judd, Chapter 7, Section 5; Drs. H. W. Galbraith, C. W. Patterson, and B. J. Krohn, Chapter 7, Section 10; (ii) RWA. Professor L. Michel, Chapters 2-4; Drs. H. Ruch and R. Petry, Topic 2; Dr. M. M. Nieto, Professors M. Reed, N. Mukunda, and H. Bacry, Topic 7; Professor T. Regge, Topic 9; Dr. B. J. Krohn, Topic 10; Dr. C. W. Patterson and Professor J. Paldus, Topic 12. Dr. W. Holman read both volumes to assist us with the indexing and suggested many improvements. Further acknowledgment of help from those not mentioned here is indicated in the relevant chapters.

In a more general way, we are indebted also to Professors H. van Dam, E. Merzbacher, A. Bohm, and Dr. N. Metropolis for discussions and help extending over several years.

This monograph is dedicated to Professor Eugene P. Wigner, whose picture (courtesy of the Niels Bohr Library of the American Institute of Physics) appears as the frontispiece. We not only acknowledge the inspiration of Wigner's research, but also record his personal encouragement and help, and we are honored that he has accepted this dedication. We wish also to acknowledge our great indebtedness to the late Professor Giulio Racah, who encouraged our work at its most critical time, the very beginning. Professor Ugo Fano also helped us greatly in this same period.

Special thanks are due to Professor Gian-Carlo Rota, editor of this Encyclopedia, for encouraging us to write at length on the subject of this monograph.

Most monographs begin as course notes and lectures series. The present monograph is no exception and evolves from such notes and lectures given over the years. We are particularly indebted to Dr. H. William Koch for urging us to write up the lectures on angular momentum theory (based on