

Evaluation of Matrix Elements from a Graphical Representation of the Angular Integral*

JOHN S. BRIGGS†

*Department of Physics, University of Chicago, Chicago, Illinois 60637
Argonne National Laboratory, Argonne, Illinois 60439*

The graphical representation of angular momentum is used as the basis of a procedure for the complete evaluation of the matrix element of a Coulomb or multipole interaction operator between atomic states having any number of open shells. The method is presented in the form of a step-by-step procedure and is designed to permit straightforward extension to the evaluation of the matrix elements of other types of tensor operators and of sums of products of Coulomb matrix elements, such as occur in the perturbation theory of configuration interaction.

CONTENTS

1. Introduction	189
2. Graphical Representation	191
2.1 The Interaction Operators	191
2.2 Many-Electron Wave Functions	193
2.3 Fractional Parentage Expansion	194
3. The Coulomb Matrix Element	195
3.1 Integration over Electron Variables	195
3.2 Phase Factor and Weight Factor	196
4. Evaluation of the Angular Factor	199
4.1 The Coupling Schemes	199
4.2 The j -Coefficient Diagrams	201
4.3 Reduction of Diagrams	202
4.4 Examples	205
5. Multipole Operators	209
5.1 Integration over Electron Variables	209
5.2 The Angular Factor	210
6. Summarized Prescription	212
6.1 Step-by-Step Procedure	212
6.2 Example	214
7. Sums of Products of Matrix Elements	219
7.1 Effective Operators	219
7.2 Example	224
8. General Form of the Matrix Element	228
8.1 Graphical Representation	228
8.2 Evaluation of the Matrix Element	229

1. INTRODUCTION

In atomic and nuclear physics, many-particle wave functions are usually constructed as Slater determinants, i.e., as sums of products of one-particle wave functions. In a central-field approximation the one-particle functions are themselves products of radial, angular, and spin functions. The angular functions describe the symmetry of the wave functions under rotation and a many-particle wave function of a certain symmetry is obtained by coupling the one-particle angular wave functions in a specified way. In a sequence of papers, Racah (R42a, R42b, R43) developed calculational techniques for the evaluation of matrix elements of tensor operators between such many-particle wave functions. The original development concerned matrix elements which occur in theoretical atomic spectroscopy, but since then the methods have been used extensively in nuclear shell theory (deSF63). In this

paper the discussion will be from the standpoint of atomic calculations.

Racah's guiding thought regarding spectroscopic calculations was that multiple integrations over angular coordinates reduce to standard, highly symmetric numerical functions of angular momentum quantum numbers, known today as $3n-j$ coefficients. This reduction has been performed over the years by a variety of techniques, utilizing points of view developed to unravel specific aspects of problems with increasing complication.

Today, sums of products of interaction matrix elements are carried out, or contemplated (RW63); these too can be reduced to a single operation (RS67, W68). The diagrammatic methods of Yutsis, Levinson, and Vanagas (YLV62), which can be combined with Feynman diagram techniques (J67), have been particularly effective in extending the range of application of Racah's concept. Several other points of view, mentioned below, have contributed to recent progress. It seems possible now to attempt a unified formulation which contains features from various sources and can be presented in a fairly self-contained manner.

A general approach of theoretical spectroscopy has been to utilize the analytical results of angular integrations without any attempt to evaluate radial integrals. Coefficients representing these integrals were determined by fitting large numbers of experimental energy levels. Thus the theory was used for the limited purpose of determining relationships among levels which are implied by angular momentum properties, i.e., by symmetries under rotation. Lately, interest has returned to radial integrations. This trend implies a shift in emphasis from a concentration on the effects of rotational symmetries to a more complete formulation which includes all relevant factors. It has been realized, of course, from the beginning that the effects of interaction of an atom with external, static or radiative, multipole fields could be treated on an equal footing with particle interactions within an atom (FR59, Chaps. 17-19). Nowadays, the methods of theoretical spectroscopy are normally applied to the collision phenomena; indeed, the relationship of the two fields is increasingly emphasized (FP63, S466, SM68).

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† Present address: Theoretical Physics Division, A.E.R.E., Harwell, Didcot, Berkshire, England.

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Table of Contents Zica Pilot Papers

1. Understanding the eBook Zica Pilot Papers
 - The Rise of Digital Reading Zica Pilot Papers
 - Advantages of eBooks Over Traditional Books
2. Identifying Zica Pilot Papers
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Zica Pilot Papers
 - User-Friendly Interface
4. Exploring eBook Recommendations from Zica Pilot Papers
 - Personalized Recommendations
 - Zica Pilot Papers User Reviews and Ratings
 - Zica Pilot Papers and Bestseller Lists
5. Accessing Zica Pilot Papers Free and Paid eBooks

- Zica Pilot Papers Public Domain eBooks
- Zica Pilot Papers eBook Subscription Services
- Zica Pilot Papers Budget-Friendly Options
- 6. Navigating Zica Pilot Papers eBook Formats
 - ePub, PDF, MOBI, and More
 - Zica Pilot Papers Compatibility with Devices
 - Zica Pilot Papers Enhanced eBook Features
- 7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Zica Pilot Papers
 - Highlighting and Note-Taking Zica Pilot Papers
 - Interactive Elements Zica Pilot Papers
- 8. Staying Engaged with Zica Pilot Papers
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Zica Pilot Papers
- 9. Balancing eBooks and Physical Books Zica Pilot Papers
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Zica Pilot Papers
- 10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
- 11. Cultivating a Reading Routine Zica Pilot Papers
 - Setting Reading Goals Zica Pilot Papers
 - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Zica Pilot Papers
 - Fact-Checking eBook Content of Zica Pilot Papers
 - Distinguishing Credible Sources
- 13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development

- Exploring Educational eBooks

14. Embracing eBook Trends

- Integration of Multimedia Elements
- Interactive and Gamified eBooks

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