

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

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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.

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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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