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Automated Angular Momentum Recoupling Algebra

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We describe a code, RACAH, for algebraic solution of angular momentum recoupling problems. The general problem is to find an optimal path from one binary tree (representing the angular momentum coupling scheme for the reduced matrix element) to another (representing the sub-integrals and spin sums to be done). RACAH is implemented on a MS-DOS microcomputer, using the SCHEME dialect of LISP.

Introduction

In this paper we present a code—RACAH—for carrying out quantum angular momentum algebra manipulations. RACAH is effectively an expert system for evaluating reduced matrix elements for transition rates and scattering amplitudes. The code has been developed in PC-SCHEME,¹⁾ a compact dialect of LISP, and it runs on MS-DOS microcomputers.

Angular momentum recoupling computations, while straightforward, are often tedious. Such work can easily lead to errors, with miscalculated phases being the *bête noire* of the industry. This provided a partial motivation for the development of graphical techniques to simplify angular momentum recoupling problems.²⁾

The present work is based on one of these graphical techniques. Danos³⁾ worked out a consistent set of definitions of tensors used within Racah algebra which eliminated practically all the phase difficulties typical of recoupling calculations. While phase problems are considerably alleviated by the Danos scheme, this comes at some cost. For example, spherical harmonics must be re-defined with an unfamiliar phase convention. The Danos technique does save considerable time and effort, but it seems to have attracted only a small community of users, perhaps because of the steep learning curve involved in mastering the method.

The work we present here⁴⁾ uses the Danos graphical technique as a beginning point for a computerized attack on the angular momentum recoupling problem. While lacking the generality of the complete Racah algebra (which the Danos scheme possesses), the RACAH code we have developed further reduces the difficulty of the recoupling algebra. The problem we deal with is the calculation of quantum amplitudes re-expressing them in terms of simpler products of two, three, or four angular momenta coupled by themselves to zero.

The user of RACAH in most cases should be able to move from a statement of the problem expressed in the common language of his or her discipline and obtain from RACAH a result, also expressed in common language, with the details of the intermediate calculations invisible. We believe that this feature alone will make RACAH useful, particularly to infrequent users of angular momentum techniques who do not wish to learn a new technology in order to obtain just one or two straightforward results. Also, the existence of this code may well make some very large recoupling problems tractable, thus making it attractive also to more sophisticated users of Racah algebra.

Angular Momentum Algebra—Review and Problem Statement

For the purpose of defining terms and the problem to be solved, we review briefly the fundamentals of angular momentum algebra. The basic operation within the algebra is one in which two states with good angular momentum quantum numbers are combined to produce a complex system with a good total angular momentum and its z -component:

$$|J, M\rangle = \sum_{m_1, m_2} \langle j_1 m_1, j_2 m_2 | JM \rangle |j_1, m_1\rangle |j_2, m_2\rangle. \quad (1)$$

The symbol $\langle j_1 m_1, j_2 m_2 | JM \rangle$ is a Clebsch-Gordan coefficient. We denote this fundamental operation of coupling angular momentum eigenstates j_1 and j_2 to produce a combined eigenstate J by $[j_1 j_2]^J$.

More complicated systems require sequential application of this binary coupling operation. In systems with more than two angular momenta, the *order* in which we couple the individual components to subtotals, and subtotals to final totals, is crucial to the nature of the final state we describe. For three angular momenta there are several possibilities. For each coupling scheme, the set of states with various values of the intermediate angular momenta form a mathematically complete set of states. This means any such state can be expressed as a linear combination of states from another coupling scheme. For example, $[[j_1 j_2]^{j_{12}} j_3]^J$ is equal to

$$\sum_{j_{23}} (-1)^{j_1+j_2+j_3+J} \widehat{j_{12}} \widehat{j_{23}} \left\{ \begin{matrix} j_1 & j_2 & j_{12} \\ j_3 & J & j_{23} \end{matrix} \right\} [j_1 [j_2 j_3]^{j_{23}}]^J, \quad (2)$$

where $\widehat{j}$ represents $(2j+1)^{1/2}$. The symbol in curly brackets is a 6- j symbol and is defined in terms of sums of products of Clebsch-Gordan coefficients.⁴⁾ Note that it is completely independent of projection quantum numbers, as can be shown using the Wigner-Eckart theorem (described below).

A similar situation arises for the coupling of four angular momenta. The simplest scheme for this involves coupling the individual components in pairs and then joining the coupled pairs to a state of good angular momentum. A familiar example is the expression giving an L - S coupled state as a linear combination of j - j coupled states:

$$[[l_1 l_2]^L [s_1 s_2]^S]^J = \sum_{j_1 j_2} \widehat{S} \widehat{L} \widehat{j_1} \widehat{j_2} \left\{ \begin{matrix} l_1 & l_2 & L \\ s_1 & s_2 & S \\ j_1 & j_2 & J \end{matrix} \right\} [[l_1 s_1]^{j_1} [l_2 s_2]^{j_2}]^J. \quad (3)$$

The 9- j symbol is also independent of projection quantum numbers. It can be expressed as a sum of products of Clebsch-Gordan coefficients or as a sum of products of 6- j symbols.⁴⁾

The specific problem within Racah algebra to be addressed here is that of evaluation of an amplitude, or matrix element, of a tensor operator between states of a many-body system,

$$\langle j_f, m_f | \mathcal{O}(j, m) | j_i, m_i \rangle. \quad (4)$$

Here the interaction operator, $\mathcal{O}(j, m)$, is the m th spherical component of a tensor of rank j operating in the space of the angular and spin variables of the particles in the initial and final state. The notation implies an integration over angular and radial variables and contraction over spin indices of all involved particles, making the amplitude a scalar-valued quantity.

The dependence of the amplitude of Eq. (4) upon projection quantum numbers can be separated from the more difficult parts of the calculation by use of the Wigner-Eckart theorem,

$$\langle j_f, m_f | \mathcal{O}(j, m) | j_i, m_i \rangle = \frac{(-1)^{2j}}{\hat{j}_f} \langle j_i m_i, j m | j_f m_f \rangle [j_f \| j \| j_i]. \quad (5)$$

The reduced matrix element, $[j_f \| j \| j_i]$, is also independent of the projection quantum numbers. This expression, which includes a collection of three or more angular momenta coupled to a net value of zero, is at worst a weighted sum of radial integrals, with weight factors which are products of algebraic factors, 6- j , and 9- j symbols.

RACAH evaluates the reduced matrix element symbolically in terms of *elementary* reduced matrix elements for the spin or angular variables for each particle in the problem. Each of these, since its individual angular variables are integrated over or its spin indices are contracted appropriately, also represents a set of angular momenta coupled to zero. Examples of some common elementary reduced matrix elements are:

$$[j \| 1 \| j] \equiv [j \| j] = \hat{j}, \quad (6)$$

$$[\frac{1}{2} \| \sigma \| \frac{1}{2}] = \sqrt{6}, \quad (7)$$

$$[Y_{l_f} \| Y_l \| Y_{l_i}] = \frac{\hat{l}_i \hat{l}}{\sqrt{4\pi}} \langle l_i 0, l 0 | l_f 0 \rangle, \quad (8)$$

Other such identities can be derived by straightforward evaluation of the indicated matrix element and use of the Wigner-Eckart theorem.

Radial integrals and other factors which, while not explicitly involved in the recoupling process, might carry dependence upon angular momentum values are also to be incorporated into the final result by the user. These factors can be formally considered as part of the elementary reduced matrix elements for angular variables.

Logic of RACAH

The operation of RACAH depends on a representation of successive couplings of angular momenta as a binary tree structure.⁵⁾ In these terms the problem of recoupling is a transformation from one binary tree to another. Let Tree-1 be a balanced binary tree representing the reduced matrix element as originally coupled. Its topmost vertex has value zero and the bottom vertices are denoted by the fundamental (or root) angular momentum labels. The interior vertices of the tree represent intermediate angular momentum couplings.

The target, Tree-2, represents the amplitude recoupled into elementary reduced matrix elements. It is another balanced binary tree of the same size as the first, with topmost vertex also having value zero. The bottom vertices of Tree-2 are exactly the same as those of Tree-1 *but in a different sequence*. Vertices between the top and bottom rows will acquire values from summations introduced, subject to triangularity condition enforced during the recoupling process.

The code RACAH makes a series of step-wise moves from Tree-1 to Tree-2. It turns out that, at any step, there are essentially only two allowed moves which can be applied. These lead to a factor which is either a phase or a 9- j symbol. These steps are performed as often as necessary. An optimal solution is one in which the resulting algebraic expression (summations, phases, square root factors, and 9- j symbols) is as simple as possible. To find an optimal

solution RACAH contains a set of heuristic rules and a scoring scheme to determine what is actually done at any vertex.

When using RACAH, a series of queries leads the user to inform the program of the exact definition of the amplitude (Tree-1) and then the desired recoupled states (Tree-2). The user first builds up the tree for the original amplitude by inputting successive couplings, the total eventually coupled to zero. Then the elements in the elementary reduced matrix elements are given—this fully specifies Tree-2. Given this information, the process of transforming the tree of Tree-1 into Tree-2 is initiated. Soon afterwards, the final algebraic result is displayed.

Examples of the Use of RACAH

In order to demonstrate the power of the code RACAH, we present two example calculations. Both examples are somewhat simpler than the typical problem RACAH can do easily.

EXAMPLE 1: Consider the matrix element of the interaction $\sigma \cdot \mathbf{x}$ between normalized single-particle wave functions in configuration space. The initial wave function, an eigenfunction of the total angular momentum, has the form

$$|J_i, M_i\rangle = \sum_{m_i, \mu_i} \langle l_i m_i, s_i \mu_i | J_i M_i \rangle f_i(x) Y_{l_i}^{m_i}(\hat{x}) \chi_{s_i}^{\mu_i}. \quad (9)$$

The final state is of identical construction, and the interaction can be cast in terms of coupled angular momenta, $\sigma \cdot \mathbf{x} = \sqrt{3} [\sigma \ x]^0$, where the vectors σ and $\mathbf{x}$ are both tensors with angular momentum 1.

The Wigner-Eckart Theorem [Eq. (5)] applied to this case gives

$$\begin{aligned} \langle J_f, M_f | \sigma \cdot \mathbf{x} | J_i, M_i \rangle &= \sqrt{3} \delta_{J_f, J_i} \delta_{M_f, M_i} \frac{1}{J_i} \langle J_i M_i, 00 | J_i M_i \rangle \\ &\times [[l_f \ s_f]^{J_f}] [[\sigma \ x]^0] [[l_i \ s_i]^{J_i}], \end{aligned} \quad (10)$$

where the Kronecker deltas result from triangularity relations applied to the matrix element as a whole. The Clebsch-Gordan coefficient in this example is equal to unity.

The reduced matrix element from Eq. (10) is evaluated, using RACAH, by inputting the original coupling scheme by coupling pairs of angular momenta one at a time. A menu-driven interface guides the user through this input process, which ends when the user denotes the value of the sum of two coupled angular momenta by the symbol 0. For the present example, the input is the initial tree, $[[l_f \ s_f]^{J_f}] [[\sigma \ x]^0] [[l_i \ s_i]^{J_i}]^0$. RACAH also asks the user to indicate which, if any, of the symbols used should have the value zero. In this case z is such a symbol.

Following input of the initial tree, there is a menu-driven interface for inputting the sub-integrals and spin-sums (specifying Tree-2). The input for this problem is $(l_f \ x \ l_i) (s_f \ \sigma \ s_i)$. Finally, the variables defined by the user are displayed, and one can choose to give them particular non-zero numerical values. These values will be displayed in the final result in lieu of the names, but will be treated numerically only in the evaluation of the phase. In the present case, the two vector operators x and σ are identified with the angular momentum value of 1.

With this information, the code will evaluate the reduced matrix element algebraically, and present its result on the computer screen in a two-dimensional display mimicking the usual mathematical form:

$$[(s_f \ \sigma \ s_i)] [(l_f \ x \ l_i)] (-1)^{J_i + l_i + s_f} \left(\frac{2J_i + 1}{3} \right)^{1/2} \left\{ \begin{matrix} l_f & s_f & J_i \\ s_i & l_i & 1 \end{matrix} \right\}. \quad (11)$$

Making use of Eqs. (7) and (8), the matrix element $\langle J_f, M_f | \sigma \cdot \mathbf{x} | J_i, M_i \rangle$ becomes

$$\delta_{J_i J_f} \delta_{M_i M_f} (-1)^{J_i + l_i + s_f} \frac{3 \hat{l}_i}{\sqrt{2\pi}} \langle l_i 0, 10 | l_f 0 \rangle \begin{Bmatrix} l_f & s_f & J_i \\ s_i & l_i & 1 \end{Bmatrix} \times \int_0^\infty f_{l_f}(r) f_{l_i}(r) r^3 dr. \quad (12)$$

EXAMPLE 2: A more complex example from the field of atomic physics can be demonstrated via the evaluation of a particular matrix element of the Coulomb interaction of two electrons between three-electron states.⁶⁾ Consider three electrons coupled in the following scheme

$$[[[l_1 l_2]^{l_{12}} l_3]^L [[s_1 s_2]^{s_{12}} s_3]^S]^J. \quad (13)$$

It is desired to find the matrix element of the Coulomb interaction,

$$\frac{1}{|\mathbf{r}_2 - \mathbf{r}_3|} = 4\pi \sum_k \frac{(-1)^k}{\hat{k}} \frac{r_{<}^k}{r_{>}^{k+1}} [Y_k(\hat{\mathbf{r}}_2) Y_k(\hat{\mathbf{r}}_3)]^0 \quad (14)$$

between two such states. The matrix element to be evaluated is thus

$$\begin{aligned} & \langle [[l'_1 l'_2]^{l'_{12}} l'_3]^{L'} [[s'_1 s'_2]^{s'_{12}} s'_3]^{S'}]^J_M | \\ & \quad \times [Y_k(\hat{\mathbf{r}}_2) Y_k(\hat{\mathbf{r}}_3)]^0 | [[l_1 l_2]^{l_{12}} l_3]^L [[s_1 s_2]^{s_{12}} s_3]^S]^J_M \rangle \\ & = \frac{1}{\hat{J}} \langle [[l'_1 l'_2]^{l'_{12}} l'_3]^{L'} [[s'_1 s'_2]^{s'_{12}} s'_3]^{S'}]^J \| \\ & \quad \times \| [k_2 k_3]^0 \| | [[l_1 l_2]^{l_{12}} l_3]^L [[s_1 s_2]^{s_{12}} s_3]^S]^J \rangle. \end{aligned} \quad (15)$$

The reduced matrix element in this relation is evaluated by RACAH as

$$\begin{aligned} & (-1)^{l'_1 + l'_2 + l_3 - l_{12} - l'_{12} - L'} \frac{\widehat{l'_{12}} \widehat{l_{12}} \widehat{J}}{\hat{k}} [l'_3 \| k \| l_3] [l'_2 \| k \| l_2] \\ & \times \begin{Bmatrix} l_{12} & l_3 & L \\ l'_3 & l'_{12} & k \end{Bmatrix} \begin{Bmatrix} l_2 & l'_2 & k \\ l'_{12} & l_{12} & l_1 \end{Bmatrix}. \end{aligned} \quad (16)$$

Evaluating the reduced matrix elements using Eq. (8), and combining Eqs. (14-16) leads straightforwardly to the complete result:

$$\begin{aligned} & (-1)^{l'_1 + l'_2 + l_3 - l_{12} - l'_{12} - L'} \widehat{l'_{12}} \widehat{l_{12}} \widehat{l_2} \widehat{l_3} \sum_k (-1)^k \langle l_3 0, k 0 | l'_3 0 \rangle \\ & \times \langle l_2 0, k 0 | l'_2 0 \rangle \begin{Bmatrix} l_{12} & l_3 & L \\ l'_3 & l'_{12} & k \end{Bmatrix} \begin{Bmatrix} l_2 & l'_2 & k \\ l'_{12} & l_{12} & l_1 \end{Bmatrix} \\ & \times \int_0^\infty dr_2 r_2^2 \int_0^\infty dr_3 r_3^2 f'(r_2) f'(r_3) \frac{r_{<}^k}{r_{>}^{k+1}} f(r_2) f(r_3). \end{aligned} \quad (17)$$

Summary

It is possible to automate the manipulations of angular momentum algebra and achieve useful algebraic results using a computer. RACAH presently runs efficiently ("in real time") on an IBM-XT with 512KB of RAM, and, of course, more powerful MS-DOS compatibles. It is expected that a version will be available early in 1991 which runs on MacIntosh microcomputers as well.

When used properly, RACAH will always produce a correct result, and in many cases, one of minimal algebraic complexity. RACAH's ability to solve quite complex problems should encourage scientists to perform calculations which have not been previously attempted because of the time involved in doing the angular momentum algebra.

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