Automated Angular Momentum Recoupling Algebra

H. T. WILLIAMS

Department of Physics, Washington and Lee University, Lexington, Virginia 24450

AND

RICHARD R. SILBAR

Theoretical Division, Los Alamos National Laboratory, University of California, Los Alamos, New Mexico 87545

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We present a set of heuristic rules for algebraic solution of angular momentum recoupling problems. The general problem reduces to that of finding 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). The method lends itself to implementation on a microcomputer, and we have developed such an implementation using a dialect of LISP. We describe both how our code, called RACAH, works and how it appears to the user. We illustrate the use of RACAH for several transition and scattering amplitude matrix elements occurring in atomic, nuclear, and particle physics. © 1992 Academic Press, Inc.

I. INTRODUCTION

The next generation of computational aids for theoretical scientists has already begun to emerge, and it includes computer codes which can perform symbol manipulation as well as ordinary numerical computation. Software like MACSYMA [1] and REDUCE [2] have been capable for some time of carrying out symbolic computations in higher (college level) mathematics.

In addition to merely speeding up work and making it more accurate, symbolic computing, like numerical computing, can have more profound effects. As an example, with its built-in ability to evaluate traces of products of Dirac gamma matrices, REDUCE has had a significant effect on the progress, as well as the accuracy, of relativistic quantum electrodynamic calculations and the experiments to which they relate.

Until recently, the power necessary to handle symbol manipulation codes has not been available on microcomputers. The developments of more efficient meta-languages for writing such codes and of faster and larger "personal" computers, however, have converged to provide this power. Microcomputer versions of codes such as Mathematica [3] and MAPLE [4] are now being put to practical use.

In this paper we present a code—RACAH—for carrying out manipulations within the specialized physics domain of quantum angular momentum algebra. RACAH is effectively an expert system for solving angular momentum recoupling problems. It is naturally applied to the evaluation of reduced matrix elements for the types of operators found in typical quantum mechanical applications. The code has been developed in PC SCHEME [5], a compact dialect of LISP, and it runs on MS-DOS microcomputers [6].

Section II of this paper presents our motivations for developing the RACAH code. This is followed by a brief review of Racah algebra, which also serves to define the conventions we use. Section IV presents the paradigm problem, the evaluation of a quantum amplitude or "matrix element" in terms of simpler "irreducible invariant matrix elements." The representation of this process in terms of manipulations on a binary tree makes it particularly compatible to solution of the problem using the LISP programming language. The logic of the LISP code will be presented in Section V, which also discusses the heuristic rules we have incorporated in the code to attempt to produce a minimal recoupling result. Section VI shows how the code looks to a user and gives examples of non-trivial recoupling problems from atomic, nuclear, and particle physics. Section VII summarizes and indicates potential future extensions and generalizations.

II. MOTIVATION AND SCOPE

Angular momentum is a vector quantity which has both its length and one component quantized. Its conservation necessitates dealing with the algebra of quantized angular momenta whenever one calculates amplitudes for scattering, reactions, and decays in atomic, molecular, nuclear, and particle physics. The theoretical basis of angular momentum theory is presented in great detail by Biedenharn and Louck [7]. It is presently learned as a practical skill from textbooks such as those of Rose [8], Edmonds [9], or Fano and Racah [10]; we follow the notation and conventions of Edmonds in this paper.

The nature of angular momentum recoupling computations is straightforward although often quite tedious and time consuming. Problems in computing accurately the phase resulting from angular momentum recoupling provided a partial motivation for the development of graphical techniques to simplify angular momentum recoupling problems [11].

Our work here is based on one of these graphical techniques. Danos [12] has worked out a consistent set of definitions of tensors used within Racah algebra which greatly reduces the phase difficulties and which allows a graphical representation of the recoupling process leading directly to the final algebraic result. This technique allows a quick representation of one or several possible recoupling paths which produce a desired re-expression of a quantum amplitude but does not intrinsically suggest minimal solutions [13].

We use 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 further reduces the tedium of the recoupling algebra. Our efforts are directed at the problem of calculating quantum amplitudes—products of an initial quantum state, a tensor interaction operator, and a conjugated final quantum state, coupled together to a net angular momentum of zero—expressed in terms of simpler products of two, three, or four angular momenta coupled by themselves to zero.

The restriction here to the evaluation of angular momentum matrix elements means that we ignore certain kinds of activities for which the Racah algebra is often used. For example, we have little to say about identities among sums and products of 3*j*, 6*j*, and 9*j* symbols, often used to simplify intermediate results of recouplings. The computer techniques we discuss here attempt to derive *minimal* solutions to the recoupling calculations, which preclude the need for such Racah identities.

On the positive side, the RACAH code allows use of a standard set of definitions for spherical harmonics and tensor products [14], and the results it derives are, in a great number of cases, expressed in the most concise algebraic form. The user should be able to move from a statement of the problem expressed in the common language of his or her discipline and receive from RACAH a minimal 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 as well to more frequent and sophisticated users of Racah algebra.

III. ANGULAR MOMENTUM ALGEBRA—A BRIEF REVIEW

The basic operation within angular momentum algebra is one in which two states, each of which has a quantized value of its total angular momentum and one component (by convention, the z-component), are combined to produce a system with a total angular momentum and its z-component, also properly quantized.

We adopt the notation of Dirac and refer to quantum state vectors—"kets"—using the symbol $|j, m\rangle$. This represents a normalized state vector, an eigenfunction of the square of the total angular momentum operator, J^2 (with eigenvalue j(j+1)), and an eigenfunction of the z-component, J_z (with eigenvalue m.) Should the state be composite, with the total angular momentum comprised of sums of angular momenta of constituents, this construction shall be indicated within the brackets. A conjugated state appropriate for a final state vector in an amplitude will be denoted using the Dirac "bra," $\langle j', m' |$.

When two states are combined, each can be thought of as retaining its total angular momentum (j) but losing its particular orientation (m). The combination is itself an eigenstate of J^2 and J_z . The linear combination of product states which comprise the composite system is a function only of this property,

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

The symbol $\langle j_1 m_1, j_2 m_2 | JM \rangle$ represents a Clebsch-Gordan coefficient. In effect, it is an overlap integral between the product states and the combined state of "good" J^2 and J_z . Allowed values of J and M are those for which M is the arithmetic sum of m_1 and m_2 , and J satisfies the triangularity conditions with j_1 and j_2 ,

$$J \leq j_1 + j_2, \qquad J \geq |j_1 - j_2|.$$
 (2)

We will denote this fundamental operation of coupling angular momentum eigenstates j_1 and j_2 to produce a combined eigenstate J by $[j_1 j_2]^J$, and the combined eigenstate will be denoted by $|[j_1 j_2]^J_M \rangle$.

As an example, consider an electron bound to a massive and spinless nucleus. The electron has intrinsic ("spin") angular momentum equal to $\frac{1}{2}$ and an orbital angular momentum of l [15]. These combine to produce the total angular momentum j for the atom:

$$|jm\rangle = \sum_{m_s,m_l} \langle lm_l, \frac{1}{2}m_s | jm \rangle | lm_l \rangle | \frac{1}{2}m_s \rangle$$
$$\equiv |[l\frac{1}{2}]^j_m \rangle. \tag{3}$$

More complicated systems require sequential application of this binary addition operation. In systems of more than two angular momenta to be coupled, 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.

If we are to couple three angular momenta— j_1 , j_2 and j_3 —to a state of good angular momentum J using the previously defined Clebsch–Gordan coupling, there are three possibilities:

$$\begin{bmatrix} [j_1 j_2]^{j_{12}} j_3]^{j_1}; & [[j_1 j_3]^{j_{13}} j_2]^{j_1}; \\ \text{or} & [[j_2 j_3]^{j_{23}} j_1]^{j_2}. \quad (4) \end{bmatrix}$$

Each of these ways of forming the combined state, and in fact each separate allowed value of the intermediate coupling values, leads to states which are physically different. While these states have the same total angular momentum, thy could have quite different masses, decay properties, magnetic dipole moments, etc. For each coupling scheme the set of states with various values of the intermediate angular momenta form a mathematically complete set of states for the description of any state with total angular momentum J made from the original three angular momenta j_1 , j_2 , and j_3 . This means any such state can be expressed as a linear combination of states from one coupling scheme. For example,

$$\begin{bmatrix} [j_1 j_2]^{j_{12}} j_3]^J = \sum_{j_{23}} (-1)^{j_1 + j_2 + j_3 + J} \widehat{j_{12}} \ \widehat{j_{23}} \\ \times \begin{cases} j_1 & j_2 & j_{12} \\ j_3 & J & j_{23} \end{cases} \begin{bmatrix} j_1 [j_2 j_3]^{j_{23}} \end{bmatrix}^J, \quad (5)$$

where \hat{j} represents $(2j+1)^{1/2}$. The symbol in curly brackets is known as a 6-*j* symbol. It is defined in terms of sums of products of Clebsch–Gordon coefficients and can be shown to be completely independent of projection quantum numbers [9].

A similar situation arises in situations where four angular momenta are to be coupled. The simplest scheme for this involves coupling the individual components in pairs, and then joining the coupled pairs. A familar example is the coupling of two particles, with intrinsic angular momenta s_1 and s_2 and orbital angular momenta l_1 and l_2 , respectively. Two possible ways of describing the two-particle system with total angular momentum J are via L-S coupling,

$$[[l_1 l_2]^L [s_1 s_2]^S]^J, (6)$$

and via j-j coupling,

$$[[l_1 s_1]^{j_1} [l_2 s_2]^{j_2}]^J.$$
(7)

As in the case of recoupling of three items, each of these schemes when considered for all the allowed intermediate coupling values is a complete set for the description of any combined state of these four angular momenta summed to J. As a consequence, one can express an L-S coupled state as a linear combination of j-j coupled states as follows:

$$\begin{bmatrix} [l_1 \ l_2]^L \ [s_1 \ s_2]^S \end{bmatrix}^J$$

= $\sum_{j_1, j_2} \hat{S} \hat{L} \hat{j}_1 \ \hat{j}_2 \begin{cases} l_1 \ l_2 \ L \\ s_1 \ s_2 \ S \\ j_1 \ j_2 \ J \end{cases} \begin{bmatrix} [l_1 \ s_1]^{j_1} \ [l_2 \ s_2]^{j_2} \end{bmatrix}^J.$ (8)

The 9-j symbol, i.e., the object delimited by the curly brackets, can be expressed as a sum of products of Clebsch–Gordan coefficients and is also independent of projection quantum numbers [9].

When situations arise involving the coupling and recoupling of more than four angular momenta, the required recoupling coefficients are typically expressed in terms of sums of products of the 6-*j* and 9-*j* symbols. Techniques for deriving these relations using Racah algebra have become a standard part of the arsenal of most atomic, molecular, nuclear, and particle physicists. The present work presents an algorithm which can solve a large class of recoupling problems for an unrestricted number of angular momenta.

IV. AMPLITUDE EVALUATION

The specific problem within Racah algebra to be addressed in this paper is that of evaluation of an amplitude, or a matrix element, of some tensor operator between bra and ket states of a many-body system. The general form of this amplitude is

$$\langle j_f, m_f | \operatorname{Op}(j, m) | j_i, m_i \rangle,$$
 (9)

where

1. The bra and ket represent final and initial states of one or more particles, with orbital (angular) and intrinsic (spin) angular momentum quantities coupled in a specified way to be eigenfunctions of J^2 and J_z with eigenvalues j_f , m_f and j_i , m_i , respectively, 2. The interaction operator, Op(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, and

3. The notation is intended to imply the integration over angular and radial variables and contraction over spin variables of all involved particles, making the amplitude a scalar-valued quantity.

The interaction operator consists of combinations of operators each of which acts on the spatial or spin variables of a single particle [16], coupled together via summations over their tensor component values. These couplings, which often take the form of familiar operations from vector algebra, can be represented as combinations of binary Clebsch-Gordan couplings, e.g.,

$$\mathbf{a} \cdot \mathbf{b} = \sqrt{3} \ [a \ b]^0, \tag{10}$$

$$\boldsymbol{\sigma} \cdot (\mathbf{a} \times \mathbf{b}) = -i\sqrt{6} \left[\sigma [a b]^1 \right]^0. \tag{11}$$

Each of the quantities in the example above—**a**, **b**, and σ —are vectors, that is, tensors of rank one, and thus carry the value of unity into the appropriate Clebsch-Gordan coefficient, with possible projection values of m = +1, 0, and -1.

The summation and integration of variables in the definition of the amplitude assure that the overall coupling $(of j_j, j_i)$ and $j_i)$ is to an angular momentum of zero. This particular coupling of three angular momenta to zero, is known as the "invariant triple product" and is independent of the internal coupling scheme. Interchange of the order of the elements can change at most the overall sign.

The dependence of the amplitude of Eq. (9) upon projection operators is rather trivial, and can be separated from the more difficult parts of the calculation by use of the Wigner-Eckart theorem,

$$\langle j_f, m_f | \operatorname{Op}(j, m) | j_i, m_i \rangle$$
$$= \frac{(-1)^{2j}}{\widehat{j_f}} \langle j_i m_i, jm | j_f m_f \rangle [j_f || j || j_i].$$
(12)

The quantity $[j_f || j || j_i]$, known as the "reduced matrix element," is independent of the projection quantum numbers m_f , m, and m_i . 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 sums of products of Clebsch-Gordan coefficients, 6-j and 9-j symbols.

The problem to be addressed is that of symbolically

evaluating the reduced matrix element in terms of *elementary* reduced matrix elements involving the spin or angular variables for a single particle. Each of the elementary reduced matrix elements, since its individual angular variables are integrated or its spin values are contracted appropriately, also represents a set of angular momenta coupled to zero. Examples of the most common of these elementary reduced matrix elements are:

$$[j \| 1 \| j] \equiv [j \| j] = \hat{j}, \tag{13}$$

$$\left[\frac{1}{2} \| \sigma \| \frac{1}{2} \right] = \sqrt{6},$$
 (14)

$$[Y_{l_{f}} || Y_{l} || Y_{l_{i}}] = \frac{\hat{l}_{i} \hat{l}}{\sqrt{4\pi}} \langle l_{i} 0, l0 | l_{f} 0 \rangle, \quad (15)$$

$$\begin{bmatrix} Y_{l_1} \| Y_{l_2} Y_{l_3} \end{bmatrix}^x \| Y_{l_4} \end{bmatrix} \equiv \begin{bmatrix} Y_{l_3} \| [Y_{l_4} Y_{l_1}]^x \| Y_{l_2}]$$
$$= \frac{\widehat{l_2} \, \widehat{l_3} \, \widehat{l_4}}{4\pi} \langle l_4 0, x 0 | l_1 0 \rangle$$
$$\times \langle l_2 0, l_3 0 | x 0 \rangle.$$
(16)

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

The RACAH code calculates the reduced matrix element as defined in Eq. (12). Results are presented in terms of sums of products of phases, algebraic factors (typicaly products of "hat" symbols like \hat{j}), 6- \hat{j} symbols, 9- \hat{j} symbols, and elementary reduced matrix elements. Trivial elementary reduced matrix elements (such as $[j|| 1 || \hat{j}]$) are automatically included in the algebra produced by the code; more complicated elementary reduced matrix elements are presented symbolically, to be specified by the user. 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.

V. LOGIC OF THE CODE RACAH

It is clearly possible to present the fundamental Clebsch–Gordan coupling as a elementary binary tree, e.g.,

$$[a,b]^c \to \swarrow^c \searrow b \tag{17}$$

Based on this identification, any coupling of several angular momenta to a single value can be represented by a corresponding binary tree structure, e.g.,



Properties of the Clebsch–Gordan coefficient assure that the coupling of an angular momentum to a normalized entity of zero angular momentum simply yields the original angular momentum,

$$[a 0]^{a} = [0 a]^{a} = a.$$
(19)

One can, therefore, add to any bottom vertex in the binary tree represention two branches, one of zero and the other of value identical to that of the vertex. This allows any binary tree representation of an angular momentum coupling to be transformed into a "balanced" binary tree—with all roots of equal length—representing a mathematically identical algebraic structure. For example, the coupling of Eq. (19) can be represented as a balanced binary tree as

 $[[a b]^p [q [c d]^e]^r]^s$



As a matter of convention, when zeros are added, they will be added to the right branch.

There are two basic operations upon binary trees in this presentation. First, at any vertex not at the bottom of a tree, one can interchange the two roots. This corresponds to the algebraic identity

$$[a b]^{c} = (-1)^{a+b-c} [b a]^{c}, \qquad (21)$$

and thus when this "switch" operation is done, the appropriate phase must be included in the algebraic result. Second, at any vertex at least two levels up from the bottom of a tree, one can interchange the center two "grandchildren" of the vertex,



This corresponds to

$$\begin{bmatrix} [a b]^{x} [c d]^{y} \end{bmatrix}^{z}$$

$$= \sum_{p,q} \hat{x}\hat{y}\hat{p}\hat{q} \begin{cases} a & b & x \\ c & d & y \\ p & q & z \end{cases} \begin{bmatrix} [a c]^{p} [b d]^{q} \end{bmatrix}^{z} \quad (23)$$

(as in Eq. (8)), and thus when the "9-j" operation is done, the result is altered by the inclusion of two summations, a product of square root factors, and one 9-j symbol.

The 6-*j* transformation is a special case of the 9-*j* transformation,

$$\begin{bmatrix} [a \ b]^{x} \ c \]^{z} = \begin{bmatrix} [a \ b]^{x} \ [c \ 0]^{c} \end{bmatrix}^{z} \\ = \sum_{p} \hat{x} \hat{c} \hat{p} \hat{b} \begin{cases} a \ b \ x \\ c \ 0 \ c \\ p \ b \ z \end{cases} \begin{bmatrix} [a \ c]^{p} \ [b \ 0]^{b} \end{bmatrix}^{z}$$
(24)

with

$$[[a c]^{p} [b 0]^{b}]^{z} = [[a c]^{p} b]^{z}.$$
 (25)

Thus, in discussions of transformations of balanced binary trees it will not be treated as a distinct operation. The disappearance of one of the summation variables is due to the triangularity relation involving a zero. It is clear from comparison of Eqs. (5) and (24) that the 6-*j* symbol is, up to a constant, the same as a 9-*j* symbol with a single zero value.

It is also true that the "switch" is another special case of the 9-*j* operation, but involving two zeros:

$$[a b]^{z} = [[0 a]^{a} [b 0]^{b}]^{z}$$
$$= \hat{a}^{2} \hat{b}^{2} \begin{cases} 0 & a & a \\ b & 0 & b \\ b & a & z \end{cases} [[0 b]^{b} [a 0]^{a}]^{z}$$
$$= (-1)^{a+b-c} [b a]^{z}.$$
(26)

Here both summations disappear due to triangularity relations involving zeros, and the 9-*j* symbol with two (or more) zeros is seen to reduce to a simple algebraic product. Despite the redundancy of the "switch" operation with such a 9-*j* symbol, the discussion which follows treats the "switch" as a distinct operation.

In the language of binary trees, the problem of recoupling can be described as 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 fundamental angular momentum labels or zeros. The vertices in between represent intermediate angular momentum couplings and have values consistent with the triangle inequalities.

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 the 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 either have value zero (due to triangularities in the elementary reduced matrix elements), or will acquire values from summations introduced or triangularities enforced during the recoupling process.

The problem addressed by code RACAH is to move from Tree-1 to Tree-2 using the two allowed moves "switch" and "9-*j*" applied at any vertex, as often as necessary. An optimal solution is one in which the resulting algebraic expression is as simple as possible.

The notion of "simplicity" here is not a matter of universal agreement. As an example, consider a recoupling which can be expressed by a single 9-*j* recoupling. This could also be accomplished by a path which reduces to three 6-*j* recouplings and one summation. While many practitioners have a clear preference for the result expressed as a single 9-*j* symbol, the two results are mathematically identical to one another, and a numerical evaluation of the summed 6-*j*'s will be just as quick as an evaluation of the 9-*j* symbol.

In the set of heuristic rules which drives RACAH, the general scoring rules are as follows:

1. The "switch" move, since it contributes at most a sign change to the overall amplitude, is considered free and is done whenever convenient—its cost is zero units.

2. The "9-j" move is carried out at a cost of three units if it has nine non-zero vertices, a cost of one unit if only if one vertex has value zero, and with zero cost if two or more vertices have value zero.

With these rules, a possible solution to the recoupling problem would be to investigate a large class of solutions, score each, and choose the one of lowest cost. For interesting problems involving even a modest number of angular momenta the class of solutions to be investigated becomes so large that such a method would be prohibitively slow. The alternative chosen here, which produces a code which can be used effectively on microcomputers, is to develop a set of heuristic rules based upon solution techniques which produce optimal results in a large number of cases. These cases have been selected from several textbooks and research problems in the fields of atomic, nuclear, and particle physics.

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 builds up the tree for the original amplitude by describing successive couplings, the total eventually coupled to zero. Then the elements in the elementary reduced matrix elements are given—this fully specifies Tree-2 [17]. Given this information, the two binary trees are constructed, and the process of transforming the tree of Tree-1 into Tree-2 is initiated.

As a preconditioning of Tree-1, a 9-*j* may be carried out at the top vertex if this introduces (via triangularity) new zeros at the two vertices immediately below the apex. This check is made in recognition of the fact that often the total interaction operator (e.g., a Hamiltonian) is itself coupled to zero, and in this case, the most efficient recoupling is done if the original coupling is described as

 $[[(initial state)^{J_i} (final state)^{J_j}]^0 (interaction)^0]^0$ (27)

rather than

[(final state)^{J_f} [interaction)⁰ (initial state)^{J_i}]^{J_i}]⁰. (28)

Another preconditioning occurs for Tree-2, representing the elementary reduced matrix elements. These commute with one another, since each separately couples to zero. The code takes advantage of this commutivity by picking an ordering of the subtrees within Tree-2 so that its root (the left-to-right ordered list of elements across the bottom row of the tree) best matches the ordering of the root of Tree-1. This should reduce the amount of recoupling necessary to transform Tree-1 into Tree-2.

After preconditionings, the main part of the algorithm is entered. The procedure loops through the vertices of Tree-1, starting with the apex (vertex 1), moving to the vertex down and to the left (vertex 2), then the one immediately to the right (vertex 3). Things continue this way, left to right, top to bottom until the right-most element, two rows from the bottom (vertex $2^{n-2}-1$ for a tree of *n* horizontal rows) is reached. At each vertex *m*, the code examines the results of three possible actions:

- 1. No change, leave existing tree intact;
- 2. Perform a 9-*j* transformation at vertex *m*;

3. Perform a switch on vertex 2m (immediately down and to the left), followed by a 9-*j* at vertex *m*.

These three options (if followed by appropriate switches at lower vertices) represent all possible reorderings of the four "grandchildren" of the vertex being considered.

As each option is considered, the root of the tree in its present state is compared with the desired final form, i.e., the root of Tree-2. A "goodness of fit" value is assigned to that option. The algorithm giving the goodness-of-fit value is the controlling element of the whole code and encodes the accumulated experience of the "experts" who have contributed to this project. Goodness of fit depends upon how many elements in a particular sub-root of the whole tree match with a similar sub-root of Tree-2. The algorithm also examines the zeros in the root, assigning a fit value sensitive to the eventual goal root and the locations of its zeros. It is this treatment of zeros which causes the code to favor 9-jswitches with zeros to those without. This led to the 3 :1: 0 scoring ratio discussed earlier for the 9-j: 6-j: switch actions.

The action at vertex m which produces the maximum goodness of fit value is then carried out, and consideration moves on to vertex m + 1, where the process is repeated. Once all the appropriate vertices have been so examined, the process returns to vertex 1 and loops through the tree (as reordered) once again. When the root of the altered Tree-1 configuration matches that of Tree-2, the process is complete. It only remains to collect the sums, phases, *j* factors, and 9-*j* symbols resulting from the operations which have brought about this match. This represents the general recoupling coefficient for this process and is the desired result.

The procedure described above represents a heuristic solution to the problem of the minimal recoupling result. When the code produces a result, it is always a *correct* result, although not necessarily a minimal one. In many cases which have been tested, the result is indeed minimal. In cases which produce a *non*-minimal result, a rearrangement of the order of coupling of the initial amplitude usually helps RACAH to find a simpler and often minimal solution. There is also the possibility that a solution might *not* be found. If the code loops through the whole tree without making any transformations, a stalemate is declared and processing halts. In the few such cases examined so far, a rearrangement of the statement of the problem has produced efficient solutions.

When two equivalent statements of a recoupling problem cause RACAH to produce non-identical results, the code has derived a Racah algebra identity. Such identities have been interesting in the past [18], since they allowed reduction of complex recoupling results to more economical representations. Since the intention of RACAH is to produce minimal (or near-minimal) results from the algorithm, the more complex identities are of little interest.

A limitation of the present version of RACAH is that the elementary reduced matrix elements can contain a maximum of four angular momentum entities. For instance, in evaluation of a single-particle amplitude for a spin- $\frac{1}{2}$ particle, the code can easily handle an interaction like $\boldsymbol{\sigma} \cdot \mathbf{X} \boldsymbol{\sigma} \cdot \mathbf{Y}$, which would lead to the elementary reduced matrix element for spin of $[S_f || [\boldsymbol{\sigma} \boldsymbol{\sigma}]^S || S_i]$. However, it cannot presently deal with the interaction $\boldsymbol{\sigma} \cdot \mathbf{A} \boldsymbol{\sigma} \cdot \mathbf{B} \boldsymbol{\sigma} \cdot \mathbf{C}$. This limitation will on occasion require some preliminary recoupling of parts of the original amplitude before use of RACAH. This preliminary recoupling can be done using RACAH as well,

but it is often transparently simple and can be done by hand. For example, in the above case, use of the identity

$$\begin{bmatrix} [\sigma A]^{0} [\sigma B]^{0} \end{bmatrix}^{0} = \sum_{x} \hat{x}^{2} \begin{cases} 1 & 1 & 0 \\ 1 & 1 & 0 \\ x & x & 0 \end{cases} \begin{bmatrix} [\sigma \sigma]^{x} [A B]^{x} \end{bmatrix}^{0}, \quad (29)$$

which is identical to the more familiar

$$\boldsymbol{\sigma} \cdot \mathbf{A}\boldsymbol{\sigma} \cdot \mathbf{B} = \mathbf{A} \cdot \mathbf{B} + i\boldsymbol{\sigma} \cdot \mathbf{A} \times \mathbf{B},\tag{30}$$

will reduce the problem to two separate pieces, each of which can be addressed by RACAH.

VI. EXAMPLES OF THE USE OF RACAH

In order to best demonstrate the power as well as the limitations of the code RACAH, several examples will be given from the fields of atomic, nuclear, and elementary particle physics. The first of these will be given in great detail; those following, more tersely, but each illustrating a further point about how the RACAH code works.

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

$$|J_i, M_i\rangle = \sum_{m_i, \mu_i} \langle l_i m_i, s_i \mu_i | J_i M_i\rangle$$
$$\times f_{l_i}(x) Y_{l_i}^{m_i}(\hat{x}) \chi_{s_i}^{\mu_i}. \tag{31}$$

The final state is of identical construction, and the interaction can be cast in terms of coupled angular momenta as in Eq. (11), $\mathbf{\sigma} \cdot \mathbf{x} = \sqrt{3} [\sigma x]^0$, where the vectors $\mathbf{\sigma}$ and \mathbf{x} are both tensors with angular momentum 1.

The Wigner-Eckart theorem (Eq. (12)) applied to this case gives

$$\langle J_{f}, M_{f} | \mathbf{\sigma} \cdot \mathbf{x} | J_{i}, M_{i} \rangle$$

$$= \sqrt{3} \,\delta_{J_{i}J_{f}} \delta_{M_{i}M_{f}} \frac{1}{\hat{J}_{i}} \langle J_{i}M_{i}, 00 | J_{i}M_{i} \rangle$$

$$\times [[l_{f}s_{f}]^{J_{i}} | [\mathbf{\sigma} x]^{0} | [l_{i}s_{i}]^{J_{i}}], \qquad (32)$$

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. (32) can be evaluated using RACAH. A menu-driven interface guides the user to input the original coupling scheme, which appears as

$$[[l_f s_f]^{J_i} [[\sigma x]^z [l_i s_i]^{J_i}]^{J_j}]^0.$$
(33)

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. The user is then led to describe the sub-integrals and spin-sums (Tree-2, the desired end result), which appears as

$$(l_f x l_i)(s_f \sigma s_i).$$

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 should be identified with the angular momentum value of 1.

With this information, the code will evaluate the reduced matrix element algebraically and display its result:

$$[(s_{f} \sigma s_{i})][(l_{f} x l_{i})](-1)^{J_{i}+l_{i}+s_{f}} \times \left(\frac{2J_{i}+1}{3}\right)^{1/2} \begin{cases} l_{f} & s_{f} & J_{i} \\ s_{i} & l_{i} & 1 \end{cases}.$$
 (34)

The two leading factors in this expression are the elementary reduced matrix elements, referring successively to the spin variables and spatial variables of the involved particle. If the particle has $\text{spin}-\frac{1}{2}$, then

$$\left[\left(s_{f}\,\sigma\,s_{i}\right)\right] = \sqrt{6}.\tag{35}$$

From Eq. (15) (and remembering that x stands for angular momentum 1),

$$[(l_f x l_i)] = \hat{l}_i \sqrt{3/4\pi} \langle l_i 0, 10 | l_f 0 \rangle$$
$$\times \int_0^\infty f_{l_f}(r) f_{l_i}(r) r^3 dr.$$
(36)

3Î.

Combining the results of Eqs. (32)-(36), the final result can be obtained:

$$\langle J_f, M_f | \mathbf{\sigma} \cdot \mathbf{x} | J_i, M_i \rangle$$

$$\times \begin{cases} l_{f} & s_{f} & J_{i} \\ s_{i} & l_{i} & 1 \end{cases} \int_{0}^{\infty} f_{l_{f}}(r) f_{l_{i}}(r) r^{3} dr.$$
(37)

EXAMPLE 2. The relationship between states coupled in various ways can be expressed using RACAH to calculate

overlap integrals between the states—matrix elements of the unit operator. A straightforward example of this is given in Eq. (8), which shows the relationship between a two-body state coupled in an *L-S* scheme, and the state coupled in a j-j scheme. The problem is to find an expression for the coefficient α in the equation

$$\begin{bmatrix} [l_1 \ l_2]^L \ [s_1 \ s_2]^S \end{bmatrix}^J{}_M \rangle$$

= $\sum_{j_1, j_2} \alpha \mid [[l_1 \ s_1]^{j_1} \ [l_2 \ s_2]^{j_2}]^J{}_M \rangle.$ (38)

Due to the orthogonality of eigenstates of angular momentum with different eigenvalues, it is easy to solve this for the coefficient α :

$$\alpha = \langle [[l_1 \, s_1]^{j_1} \, [l_2 \, s_2]^{j_2}]^J | 1 | [[l_1 \, l_2]^L \, [s_1 \, s_2]^S]^J \rangle.$$
(39)

The Wigner-Eckart theorem in this case, like the last, has a Clebsch-Gordan coefficient which evaluates to unity, so

$$\alpha = \frac{1}{\hat{j}} \left[\left[\left[l_1 \, s_1 \, \right]^{j_1} \left[l_2 \, s_2 \, \right]^{j_2} \right]^J \| 1 \| \left[\left[l_1 \, l_2 \, \right]^L \left[s_1 \, s_2 \, \right]^S \right]^J \right], \quad (40)$$

and the reduced matrix element on the right can be evaluated by RACAH.

The initial coupling is described to the machine as

$$\left[\left[\left[l_{1}' s_{1}'\right]^{j_{1}} \left[l_{2}' s_{2}'\right]^{j_{2}}\right]^{J'} \left[\left[l_{1} l_{2}\right]^{L} \left[s_{1} s_{2}\right]^{s}\right]^{J}\right]^{0}, \quad (41)$$

similarly, the four elementary reduced matrix elements as

$$(l'_1 l_1) \quad (l'_2 l_2) \quad (s'_1 s_1) \quad (s'_2 s_2).$$
 (42)

The value produced by the code is

$$\hat{j}_{2}\hat{j}_{1}\hat{J}\hat{L}\hat{S}\begin{cases} l_{1} & l_{2} & L\\ s_{1} & s_{2} & S\\ j_{1} & j_{2} & J \end{cases}.$$
(43)

Combining this with the Wigner-Eckart theorem factor produces a result in agreement with Eq. (8).

particular matrix element of the Coulomb interaction of two electrons between three-electron states [19]. Consider three electrons coupled in the following scheme

$$[[[l_1 l_2]^{l_1 2} l_3]^L [[s_1 s_2]^{s_{12}} s_3]^S]^J.$$
(44)

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

$$\frac{1}{|\mathbf{r}_{2} - \mathbf{r}_{3}|} = 4\pi \sum_{k} \frac{(-1)^{k}}{k} \frac{r_{<}^{k}}{r_{>}^{k+1}} \times [Y_{k}(\hat{\mathbf{r}}_{2}) Y_{k}(\hat{\mathbf{r}}_{3})]^{0}$$
(45)

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

$$\langle [[l'_{1} l'_{2}]^{l'_{12}} l'_{3}]^{L'} [[s'_{1} s'_{2}]^{s'_{12}} s'_{3}]^{S'}]^{J}_{M} | \\ \times [Y_{k}(\hat{\mathbf{f}}_{2}) Y_{k}(\hat{\mathbf{f}}_{3})]^{0} \\ \times |[[[l_{1} l_{2}]^{l'_{12}} l_{3}]^{L} [[s_{1} s_{2}]^{s_{12}} s_{3}]^{S}]^{J}_{M} \rangle \\ = \frac{1}{\hat{j}} [[[[l'_{1} l'_{2}]^{l'_{12}} l'_{3}]^{L'} [[s'_{1} s'_{2}]^{s'_{12}} s'_{3}]^{S'}]^{J} | \\ \times [k_{2} k_{3}]^{0} | \\ \times [[[l_{1} l_{2}]^{l'_{12}} l_{3}]^{L} [[s_{1} s_{2}]^{s_{12}} s_{3}]^{S}]^{J}].$$
(46)

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

$$(-1)^{l_{1}'+l_{2}'+l_{3}-l_{12}-l_{12}'-l_{12}'}\frac{\hat{l_{12}}}{\hat{k}}\hat{l}_{12}\hat{l}_{12}\hat{l}_{12}\hat{l}_{12}\|k\| l_{3}][l_{2}'\|k\| l_{2}]$$

$$\times \begin{cases} l_{12} \quad l_{3} \quad L \\ l_{3}' \quad l_{12}' \quad k \end{cases} \begin{cases} l_{2} \quad l_{2}' \quad k \\ l_{12}' \quad l_{12}' \quad l_{12}' \end{cases} .$$
(47)

Evaluating the reduced matrix elements using Eq. (15), and combining Eqs. (45)-(47) leads straightforwardly to the complete result:

$$(-1)^{l_{1}^{\prime}+l_{2}^{\prime}+l_{3}-l_{12}-l_{12}^{\prime}-L^{\prime}} \widehat{l_{12}^{\prime}} \widehat{l_{2}} \widehat{l_{2}} \widehat{l_{3}} \sum_{k} (-)^{k}$$

$$\times \langle l_{3}0, k0 | l_{3}^{\prime}0 \rangle \langle l_{2}0, k0 | l_{2}^{\prime}0 \rangle$$

$$\times \begin{cases} l_{12} \quad l_{3} \quad L \\ l_{3}^{\prime} \quad l_{12}^{\prime} \quad k \end{cases} \begin{cases} l_{2} \quad l_{2}^{\prime} \quad k \\ l_{12}^{\prime} \quad l_{12} \quad l_{1} \end{cases}$$

$$\times \int_{0}^{\infty} dr_{2} r_{2}^{2} \int_{0}^{\infty} dr_{3} r_{3}^{2} f^{\prime}(r_{2}) f^{\prime}(r_{3}) \frac{r^{k}}{r^{k+1}} f(r_{2}) f(r_{3}).$$

$$(48)$$

EXAMPLE 4. Consideration of one of the interactions involved in the calculation of photon absorption on nuclei will demonstrate the evaluation of elementary reduced matrix elements of product operators in a single space. The Hamiltonian representing the interaction between a photon (moving with momentum q in the z direction) and a nucleon current, \mathbf{p}/M , has the form

$$e^{i\mathbf{q}\cdot\mathbf{x}}\frac{p_{\lambda}}{M} = \frac{\sqrt{4\pi}}{M} \sum_{L,\Lambda} i^{L} \hat{L} \langle L0, 1\lambda | \Lambda\lambda \rangle$$
$$\times j_{L}(qr) [Y^{L}p^{1}]_{\lambda}^{\Lambda}. \tag{49}$$

Calculating the matrix element of this operator, whether between multi-nucleon states or single particle states will eventually involve the reduced matrix element of $[Y^L p^1]^A$ between single particle states of good orbital angular momentum

$$[L_f \| [Y^L p^1]^A \| L_i].$$
 (50)

To evaluate this we introduce the completeness relation for spherical harmonics,

$$\sum_{l} \hat{l} [Y^{l}(\hat{\mathbf{r}}) \ Y^{l}(\hat{\mathbf{r}}')]^{0} = \delta^{(2)}(\hat{\mathbf{r}} - \hat{\mathbf{r}}'), \tag{51}$$

to separate the matrix element of a product into the product of two matrix elements of single operators. The evaluation proceeds as

$$\begin{bmatrix} L_{f} \| [Y^{L}p]^{A} \| L_{i}] \\ = \sum_{l} \hat{l} [L_{f} \| [Y^{l}Y^{l}]^{0} [Y^{L}p]^{A} \| L_{i}] \\ = \sum_{l} \hat{l} \beta [L_{f} \| Y^{L} \| Y^{l}] [Y^{l} \| p \| L_{i}], \qquad (52)$$

with β being the coefficient provided by the code RACAH. Providing as code input the initial coupling in the form

$$[L_{f}[[[ll]^{0} [Lp]^{A}]^{A} L_{i}]^{L_{f}}]^{0}$$
(53)

and the desired recouplings as

$$(L_f L l)(l p L_i), (54)$$

RACAH returns

$$\beta = (-1)^{L_i + l} \frac{\hat{A}}{\hat{l}} \begin{cases} L_i & l & 1 \\ L & A & L_f \end{cases}$$
$$\times [(L_f L l)] [(l p L_i)]. \tag{55}$$

The first of the two elementary reduced matrix elements on

the right side of Eq. (55) is evaluated in accordance with coordinates of the relative motion. Similarly, the final state Eq. (15), and the second according to the rules $\lceil 12 \rceil$

$$[L ||p|| L] = 0 \tag{56}$$

$$[L ||p|| L-1] = i\sqrt{L} \int_0^\infty r^2 f_L(r) \left(\frac{L-1}{r} - \frac{d}{dr}\right) f_{L-1}(r) dr,$$
(57)

$$[L \| p \| L+1] = i\sqrt{L+1} \int_0^\infty r^2 f_L(r) \left(\frac{L+2}{r} + \frac{d}{dr}\right) f_{L+1}(r) dr.$$
(58)

Since the complete set which was introduced was only in the angular variables, the remaining radial integral is only in one variable, and the derivative operator p in Eq. (55) operates only upon the initial state radial wave function. Which of the forms this operator takes depends, however, on the relationship between L_i and l, not on that between L_i and L_{f} . Combining results from Eqs. (52) and (55) and using Eqs. (15), (57), and (58) to evaluate the elementary reduced matrix elements leads to

$$\left\langle L_{f} \left| e^{i\mathbf{q} \cdot \mathbf{x}} \frac{p_{\lambda}}{M} \right| L_{i} \right\rangle$$

$$= -\frac{1}{M} \sum_{l,L,A} (i)^{L+1} \frac{\hat{L}^{2} \hat{A} \hat{l}}{\hat{L}_{f}} \left\langle L0, 1\lambda \right| A\lambda \right\rangle$$

$$\times \left\langle L_{i}0, A\lambda \right| L_{f}\lambda \right\rangle \left\langle l0, L0 \right| L_{f}0 \right\rangle \left\{ \begin{matrix} L_{i} & l & 1 \\ L & A & L_{f} \end{matrix} \right\}$$

$$\times \int_{0}^{\infty} r^{2} f_{L_{f}}(r) j_{L}(qr) \left[\delta_{lL_{i}+1} \sqrt{L_{i+1}} \left(\frac{L_{i}}{r} - \frac{d}{dr} \right) \right]$$

$$+ \delta_{lL_{i}-1} \sqrt{L_{i}} \left(\frac{L_{i}+1}{r} + \frac{d}{dr} \right) \right] f_{L_{i}}(r) dr.$$

$$(59)$$

EXAMPLE 5. An amplitude of interest in the low-energy quark model is the electric quadrupole transition amplitude from the three-quark state of a nucleon, to that of a Δ (spin $\frac{3}{2}$, isospin $\frac{3}{2}$) resonance. The interaction operator is the L=2term from the expansion of the charge operator

$$Q_i e^{i\mathbf{q}\cdot\mathbf{r}} = Q_i \sqrt{4\pi} \sum_L i^L \hat{L} j_L(qr) Y_L^0(\hat{\mathbf{r}}), \qquad (60)$$

where **q** has been taken as the z-axis.

The nucleon is assumed to be constructed of three quarks, each of isospin $\frac{1}{2}$, spin $\frac{1}{2}$,

$$|J_{i}, M_{i}; T_{i}, t_{i}\rangle = |[[[\frac{1}{2}\frac{1}{2}]^{s}\frac{1}{2}]^{s} [\rho^{l_{1}}\lambda^{l_{2}}]^{L}]^{J_{i}}_{M_{i}}: [[\frac{1}{2}\frac{1}{2}]^{t}\frac{1}{2}]^{T_{i}}_{t_{i}}\rangle, \quad (61)$$

where $T_i = \frac{1}{2}$ is the total isospin of the nucleon state, $J_i = \frac{1}{2}$ is the total nucleon spin, and ρ and λ are Jacobi (vector) of the \varDelta -resonance is

$$\langle \frac{3}{2} M_f; \frac{3}{2} t_i | = \langle [[[\frac{1}{2} \frac{1}{2}]^{s'} \frac{1}{2}]^{s'} \\ \times [\rho^{I_1} \lambda^{I_2}]^{L'}]^{3/2} _{M_f}; [[\frac{1}{2} \frac{1}{2}]^{1/2} \frac{1}{2}]^{3/2} _{I_i} |.$$
(62)

The isospin amplitude can be completely factored from the spin-space amplitude and computed separately. The charge of the *i*th quark can be expressed in terms of the isospin operator τ ,

$$Q_i = e(\frac{1}{6} + \frac{1}{2}\tau_0^i). \tag{63}$$

The matrix element of the constant term between nucleon (isospin $\frac{1}{2}$) and Δ (isospin $\frac{3}{2}$) vanishes, so we need only treat the second term. For the third quark $(r \rightarrow \lambda)$, for example, the Wigner-Eckhart theorem yields

$$\left\langle \left[\left[\frac{1}{2} \frac{1}{2} \right]^{1} \frac{1}{2} \right]^{3/2} \left| \frac{1}{2} \tau_{0}^{3} \right| \left[\left[\frac{1}{2} \frac{1}{2} \right]^{\prime} \frac{1}{2} \right]^{1/2} \right\rangle$$

$$= \frac{1}{4} \left\langle \frac{1}{2} t_{i}, 10 \right| \frac{3}{2} t_{f} \right\rangle$$

$$\times \left[\left[\left[\frac{1}{2} \frac{1}{2} \right]^{1} \frac{1}{2} \right]^{3/2} \|\tau\| \left[\left[\frac{1}{2} \frac{1}{2} \right]^{\prime} \frac{1}{2} \right]^{1/2} \right].$$

$$(64)$$

Recoupling the reduced matrix element to the form

$$(\frac{1}{2}\frac{1}{2})$$
 $(\frac{1}{2}\frac{1}{2})$ $(\frac{1}{2}\tau\frac{1}{2}),$ (65)

RACAH gives

$$2\sqrt{2} \begin{cases} \frac{1}{2} & \frac{1}{2} & 1\\ \frac{1}{2} & \frac{3}{2} & 1 \end{cases} [(\frac{1}{2}\tau \frac{1}{2})]. \tag{66}$$

The elementary reduced matrix element of τ is $\sqrt{6}$, as for the Pauli spin operator above. Combining results, using the explicit value of the 6-j coefficient, gives for the isospin matrix element

$$\left\langle \left[\left[\frac{1}{2} \frac{1}{2} \right]^{1} \frac{1}{2} \right]^{3/2} | \mathcal{Q}_{3} | \left[\left[\frac{1}{2} \frac{1}{2} \right]^{\ell} \frac{1}{2} \right]^{1/2} \right\rangle = -\frac{\sqrt{2}}{3}.$$
 (67)

The remaining spin-space amplitude,

$$\langle \left[\left[\left[\frac{1}{2} \frac{1}{2} \right]^{s'} \frac{1}{2} \right]^{s'} \left[\hat{\rho}^{I'_1} \hat{\lambda}^{I'_2} \right]^{L'} \right]^{J'_i} | j_2(q\lambda) \\ \times Y_2^0(\hat{\lambda}) | \left[\left[\left[\frac{1}{2} \frac{1}{2} \right]^s \frac{1}{2} \right]^s \left[\hat{\rho}^{I_1} \hat{\lambda}^{I_2} \right]^L \right]^{J_i} \rangle,$$
 (68)

can be similarly computed, producing the overall result

$$e(-1)^{J+S+L+L'+l_1+l_2+1} \frac{5\sqrt{2}}{3} \hat{J}\hat{I}\hat{L}\hat{L'}$$

$$\times \langle JM, 20|J'M' \rangle \langle l_20, 20|l'_20 \rangle$$

$$\times \begin{cases} L & L' & 2 \\ J' & J & S \end{cases} \begin{cases} L' & l'_2 & l_1 \\ l_2 & L & 2 \end{cases}$$

$$\times \int_0^\infty \lambda^2 f'(\lambda) j_L(q\lambda) f(\lambda) d\lambda. \qquad (69)$$

VII. CONCLUSION

When used properly, RACAH will always produce a correct result, and in many cases, one of minimal algebraic complexity. It can certainly be used to check results derived "by hand," and this activity can quickly lead to a confidence in RACAH which will elevate it into the position of replacing one's traditional techniques. RACAH's ability to solve quite complex problems should enable calculations which have not been previously attempted because of the time involved in doing the angular momentum algebra.

The utility of this tool to physicists in the several areas mentioned previously and to chemists working in the area of spectroscopy and atomic and molecular theory will be enhanced by the suggestions of users. Preliminary versions of the code have already been put in the hands of a few physicists whose work frequently involves angular momentum algebra. Our intention in this early distribution was to receive these persons' reactions and to respond by further refining the software. A production version of the RACAH program is now available for serious use. Persons interested in using RACAH should contact one of the authors [20].

There are several extensions of this work which seem useful to pursue in the near future. RACAH presently runs efficiently on an IBM-XT with 512KB of RAM, and, of course, more powerful MS-DOS compatibles. A version under development will run at least as well on MacIntosh microcomputers. Conversion of RACAH to run on other computers, in particular UNIX and NeXT workstations and mainframes, should be straightforward in situations where SCHEME dialects of LISP are available. Another enhancement of RACAH would allow the generation of, for example, Fortran coding for the angular momentum parts of the solution. RACAH could also be embedded into the context of a larger code which addresses a particular subset of physical problems; for example, we have developed a prototype program to compute partial wave amplitudes for baryon-baryon scattering via one meson exchange. The Racah algbra discussed in this paper is based upon the SU(2) symmetry of spin (or isospin) and ordinary space rotations. In principle, recoupling problems in higher symmetries such as SU(3) could be carried out using the same techniques as were exercised in development of RACAH

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- 13. A more precise definition of the term "minimal solution" will be discussed in detail in Section IV.
- 14. Indeed, it can be used with any set of such definitions by an appropriate choice of the irreducible invariant matrix elements. We use definitions here that we believe to be in most common use within the physics community.
- 15. We choose units such that $\hbar = 1$.
- 16. Since isospin operators obey the same SU(2) symmetry of the angular and spin quantities of this discussion, the techniques discussed in this paper are straightforwardly extended to include isospin. A problem involving isospin quantities will be illustrated in Section VI of this paper.
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- Preferably, query RRS (electronic mail, SILBAR@LAMPF.BIT-NET). We will provide our software free of charge, but it requires PC-SCHEME software [5] (available at a cost of less than \$100).