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Note

Use of Monte Carlo Techniques for Complex Angular Momentum Algebra Calculations*

Introduction

In the last two decades very sophisticated methods have been proposed [1] for the treatment of "realistic" models in nuclear structure and reaction theory. A vexing difficulty of these calculations can be the ever-increasing complexity of the angular momentum algebra required when, e.g., n particles—n holes ($n \geqslant 2$) matrix elements need to be evaluated. To obviate the analytical complexity of these calculations and, at the same time, to reduce the probability of making errors, several graphical methods have been proposed [2]. The "switchyard" or "switchboard" technique originally proposed by Danos [3], is, in our opinion, particularly convenient, because of its simplicity and straightforwardness. In fact, it reduces a matrix element to a set of lines, which can be interchanged, as necessary for a numerical evaluation, through the use of only one tool: the basic 9-j recoupling box. Complex angular momentum algebra calculations are thus reduced to the simple and even amusing task of finding the "best" graph and reading from it the corresponding analytical formula.

A difficulty, however, persists: a large number of intermediate angular momenta are often generated, upon which summation is implied. Consequently, the required computer time can easily escalate to unmanageable amounts, up to many years of computer time, even with the fastest computers presently available. The purpose of the present paper is to show that complex matrix elements, which would require years of computer time to be computed exactly, can be evaluated in a very reasonable computer time through proper use of the Monte Carlo method, with an expected error of about 1 %, which usually can be considered satisfactory.

Since the switchyard technique is explained in detail elsewhere [3–6], we will simply illustrate it with an example in the next section. In the following section we will describe our Monte Carlo calculation and present our results.

The Switchyard Technique

To illustrate with an example the switchyard technique, we present in Fig. 1 a graph representing an identity, which is one of 9 orthogonality relationships, which

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can be obtained from Fig. 16 of Ref. 3. In Fig. 1 each horizontal line represents an angular momentum (a.m.). The 8 a.m. $a, b, \ldots, h$ are initially coupled to the a.m. p, q, r, s, which in turn are coupled to t, u, and v. The a.m. couplings are represented with curved vertical lines. Therefore in its initial stage (reading from left to right, before the 9-j boxes) the graph represents the following combination of a.m.:

$$[[[a\times b]^{[p]}\times[c\times d]^{[q]}]^{[t]}\times[[e\times f]^{[r]}\times[g\times h]^{[s]}]^{[u]}]^{[v]}. \tag{1}$$

The 8 a.m. are subsequently interchanged through the nine "9-j boxes." Note that every 9-j box interchanges the second with the third a.m., leaving the first and fourth a.m. unaltered. This is the only rule of the game, since any operation consists exclusively of 9-j boxes operating on 4 adjacent a.m., with possibly one mock zero a.m. (6-j symbols) or two mock zero a.m. (3-j symbols). This accounts for the simplicity of the method.

The 9-j boxes represent square 9-j symbols. E.g., the first box at top on the right represents

$$\begin{bmatrix} a & b & p \\ c & d & q \\ A & B & t \end{bmatrix}$$

where the couplings are read horizontally before the box and vertically after the box. Square 9-j symbols are related to ordinary 9-j symbols by

$$\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} = \hat{c}\hat{f}\hat{g}\hat{h}\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix} \tag{2}$$

where $\hat{c}=\sqrt{2c+1}$.

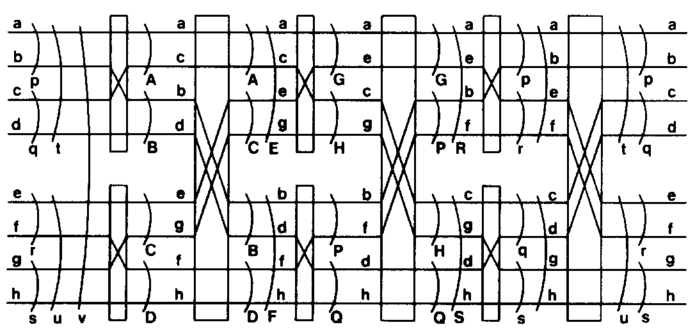

FIG. 1. Graph representing the identity of Eq. 3. Horizontal lines represent angular momenta and the recoupling boxes represent square 9-j symbols.

After all the recouplings by the nine 9-j boxes, we return (right side of Fig. 1) to the original 8 a.m. in the same order and with the same couplings (Eq. 1). Therefore,

$$\sum_{\substack{ABC\\DEF\\GHP\\QRS}} \begin{bmatrix} a & b & p \\ c & d & q \\ A & B & t \end{bmatrix} \begin{bmatrix} e & f & r \\ g & h & s \\ C & D & u \end{bmatrix} \begin{bmatrix} A & B & t \\ C & D & u \\ E & F & v \end{bmatrix} \begin{bmatrix} a & c & A \\ e & g & C \\ G & H & E \end{bmatrix} \begin{bmatrix} b & d & B \\ f & h & D \\ P & Q & F \end{bmatrix}$$
$$\times \begin{bmatrix} G & H & E \\ P & Q & F \\ R & S & v \end{bmatrix} \begin{bmatrix} a & e & G \\ b & f & P \\ p & r & R \end{bmatrix} \begin{bmatrix} c & g & H \\ d & h & Q \\ q & s & S \end{bmatrix} \begin{bmatrix} p & r & R \\ q & s & S \\ t & u & v \end{bmatrix} = 1 \tag{3}$$

where we have summed over all the intermediate a.m., which are generated in the recouplings. If one of the final a.m. had a different value (say $a' \neq a$), the value of the sum of 9-j products would be zero (orthogonality).

Monte Carlo Calculation

In Eq. 3 all the a.m. represented by small letters ($a, b, \ldots, v$) can be chosen arbitrarily. Of course p, q, r, s, t, u, and v must satisfy the proper triangular conditions, e.g., $|a-b| \leqslant p \leqslant a+b$. Also the 12 intermediate a.m. $A, B, \ldots, S$ must satisfy the corresponding triangular conditions. Since [7]

$$\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix} = \sum_k (2k+1)\, W(aidh; kg)\, W(bfhd; ke)\, W(aibf; kc) \tag{4}$$

in order to verify Eq. 3, one must evaluate a sum over 21 indexes ($A, B, \ldots, S$ plus nine k's) of terms each consisting of 27 Racah coefficients. Even assuming that each Racah coefficient could be calculated in only 10^{-4} s, the total computer time would be of the order of 10^{12} s (i.e., many thousand years), if the choice of the prefixed a.m. $a, b, \ldots, v$ is not trivial.

In order to demonstrate the usefulness of the Monte Carlo method in a.m. algebra calculations, we have evaluated the left side of Eq. 3 for N choices of random values of the intermediate a.m., each time multiplying for the corresponding weight factor and averaging. As an example, since the a.m. a and c are coupled to the intermediate a.m. A, we have each time chosen A at random between $|a-c|$ and $a+c$ with a weight factor $a+c-|a-c|+1$. To ascertain the validity of the method, we have performed our calculations for 10 different choices of the prefixed a.m. $a, b, \ldots, v$.

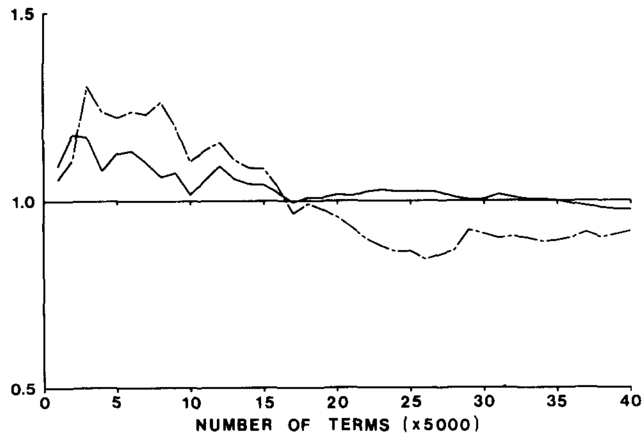

FIG. 2. Results of our Monte Carlo calculations for the best case (solid line) and worst case (dashed line) vs. N (number of terms) in multiples of 5000.

Figure 2 shows the result of our calculations for the best (most "lucky") case (solid line) and for the worst case (dashed line). The exact result (1) is also shown as a straight line. For convenience of representation, we have taken N in multiples of 5000 up to 200,000 (40×5000). It is clear from Fig. 1 that, after some (possibly wild) oscillations above or below the exact value, the averaged result stabilizes itself around 1 with an error that, for $N = 200{,}000$ is of the order of 1%. Better results can be obtained, of course, with more terms. This is not very economical, however, since the accuracy is proportional to $N^{1/2}$, i.e., to obtain an expected accuracy of about 0.1% one would need to include at least 2×10^7 terms. We have also found that, at least in our limited sample, the accuracy does not depend appreciably on the choice of the prefixed a.m. $a, b, \ldots, v$, which are reported for completeness in Table I for the two cases of Fig. 2.

The CPU time required for each complete calculation ($N = 200{,}000$) was about 8 h in our DEC-10 computer. We did not use, however, any of the usual computer tricks (e.g., tabulating the most commonly used Racah coefficients, so that they do not need to be computed each time, etc.). With a faster machine and/or a more efficient code we could have easily gained a factor of 100 or more in the computer

TABLE I

Value of the Prefixed Angular Momenta Chosen for the Best Case and Worst Case (See Fig. 2)

	a	b	c	d	e	f	g	h	p	q	r	s	t	u	v
Best Case	5	1	1	4	1	2	2	1	5	4	1	1	6	2	5
Worst case	1	3	4	1	3	1	1	2	2	3	3	1	3	3	4

time required for each calculation. Proper use of well-known statistical techniques like importance sampling related, for example, to the intermediate angular momenta of the Racah coefficients would further decrease the statistical error.

CONCLUSION

We have demonstrated the usefulness and reliability of the Monte Carlo method in angular momentum algebra calculations, using an identity which can be easily proved with Danos' switchyard technique. We believe that the application of the switchyard technique with a Monte Carlo numerical evaluation of the matrix elements can be very fruitful in future calculations of nuclear structure and reaction theory, in view of the increasing complexity of the nuclear models proposed and of the sophisticated methods which already exist for their treatment.

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P. P. DELSANTO† AND J. D. ALEMAR

Department of Physics,
University of Puerto Rico,
Mayaguez, Puerto Rico 00708

† Present address: Code 5831, Naval Research Lab., Washington, D.C. 20375.