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Publication Date

1969-08-20

Submitted to Computer Physics
Communications

UCRL-19310
Preprint

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August 20, 1969

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ARBITRARY $3n-j$ SYMBOLS FOR $SU(2)$

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August 20, 1969

ABSTRACT

We present a computer program to write a Fortran
function routine which calculates a given (arbitrary)
 $3n-j$ coefficient given its diagram.

THEORY AND PROCEDURE

In problems involving the coupling of several spins and orbital angular momenta, or of combining several isospins, one often needs recoupling, or $3n-j$ coefficients. While there are essentially only one $6-j$ and one $9-j$ symbol, for higher n the number of different $3n-j$ symbols becomes very large. The symbols are best described by a diagram.¹ Each vertex of the diagram corresponds to a $3j$ Wigner coefficient, with each line emerging from the vertex corresponding to a given angular momentum j and z component m . If the j 's appear in counterclockwise order in the Wigner coefficient, the vertex is labelled (+), otherwise (-). A line entering a vertex just has its m reversed. Thus Fig. 1a corresponds to

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & -m_2 & -m_3 \end{pmatrix}. \quad (1)$$

A line connecting two vertices is to be treated as a sum over m of the vertices with free lines, but with a phase $(-1)^{j-m}$. This is represented by Fig. 1b. With this representation of the Wigner coefficients and z component sums, an arbitrary $3n-j$ symbol is represented by a diagram with $2n$ vertices interconnected with $3n$ directed line segments, with three lines connected to each vertex.

One can then use certain easily proved lemmas to reduce any diagram to a sum of products of $6-j$ symbols. The necessary lemmas are shown in Fig. 2. Figure 2a permits any $3n-j$ symbol with an

internal triangle to be reduced to a $3(n-1)-j$ symbol times a $6j$ symbol. If there are no triangles, a given polygon in the original diagram can be reduced, one side at a time, using Fig. 2b, until one is left with a triangle. Each reduction requires multiplying by a $6-j$ symbol and summing over one angular momentum. Thus for an efficient formula it is important to start with the polygon with the fewest number of sides. In order to use Fig. 2a and 2b, it may be necessary to change the sign at the vertex or the direction of a line. Fig. 2c-2d permit this. One will finally wind up with a $6-j$ symbol (Fig. 2e).

It is possible in the course of reducing a diagram to have a part connected to the rest of the diagram by only one or two lines. These are called degenerate parts and may be reduced until they are of the form of Fig. 2f or 2g. If such diagrams arise in the reduction of a diagram which cannot be divided into two parts by cutting two lines, the particular reduction used was inefficient, introducing an extra sum and Kronecker δ .

STRUCTURE OF THE PROGRAM

The program writes a Fortran function to evaluate a given diagram. The arguments are the $3n$ angular momenta. At the time of asking the program to write the function routine, it must be decided what order the $3n$ angular momenta, j , are to appear, and whether the arguments will be floating, integer = j , or integer = $2j$ (called DOUBLE mode).

In order to tell the subroutine what diagram to evaluate, one labels the vertices in any order, and the lines in the order they are to appear as arguments. Vectors containing the numbers of the vertices at the heads and tails of the lines are then used to describe the diagram. For further details, see comments in the listing.

After writing the header card and converting any mode to DOUBLE, the program rearranges the description of the symbol, adjusting the directions of lines and orders at the vertices into a standard form. At each step in the reduction this form is maintained, and the phase adjusted correspondingly. The subsequent behavior of the program is best understood with the flow chart. The parts are described below. Each step writes some of the function at the end and possibly at the beginning of the function, working towards the middle. This is stored in core and organized and outputted at the end.

DESCRIPTION OF THE PARTS OF THE FLOW DIAGRAM

POLYFIND (800). Finds the polygon with the smallest number of sides. Among those, the polygon first in alphabetical order (in the vertex numbers) is placed in IVP.

POLYREDUCE (300). Uses Fig. 2b to reduce the number of sides one at a time. The side which is "dualized" is the one connecting the second and third highest numbered vertices.

TYPE (500). Puts triangle in standard form and determines how many distinct vertices it is connected to. If three, we have normal triangle (NORM). If one, we are down to the final 6-j symbol (FINAL). Otherwise we have a degenerate graph.

NORM (520). Reduces the triangle to a vertex using Fig. 2a.

FINAL (580). Finishes off final 6-j symbol. The instructions written during the previous execution are edited. If necessary, a statement 1 is added if it has been referred to previously. Control returns to drive program.

TWOLEG (557). We have a degenerate graph connected by two legs. It is reduced to a single line but is not yet in standard form.

STANDARD (561). Checks that we no longer have a degenerate part, and puts diagram into standard form.

INNER (564). If after the reduction of TWOLEG we still have a degenerate part, we reduce that.

ONELEG (570). Reduces part hanging by one leg. The connecting line is now not in standard form.

LIMITATIONS AND TESTS

The dimension statements limit the program to $n \leq 20$. To increase the allowable n 's, change the dimension of JPH, IT, IEND, and ITIP to $3n$, J to $6n$, M and L to $(2n, 3)$, and NJI and IVP to $2n$. There is not enough room in the header and conversion statements for J100, so if $n > 33$ these must be changed. The POLYFIND routine works only if the smallest polygon has fewer than nine sides. This suffices for $n < 23$, but for $n = 23, 31, 47, 63, 95 \dots$ we need 1, 2, 3, \dots extra loops exactly analogous to 846-827.

The program itself has no restrictions on the values of the angular momentum calculated, but the present 6-j function, which is

used together with the output functions, is limited to the sum of the angular momenta < 50 .

The time required on a CDC 6600 to write the functions is under one second for the programs tested. The time these functions require depends very strongly on the values of the angular momenta and erratically on the symbol. For angular momenta ≈ 3 with 15-j symbols, the time was $\sim 6-40$ ms.

Because POLYFIND selects the first smallest polygon, and POLYREDUCE dualizes the next to last leg, it is possible to get several functions for the same diagram by renumbering the vertices (adjusting IVP accordingly). These may differ in their efficiency.

The test run calculates five 9-j symbols which agree with tables. It also uses two different functions for a single 24-j symbol, which agree in a nontrivial calculation.

ACKNOWLEDGMENT

The author wishes to thank his wife, who was of great help in debugging this program.

REFERENCE

1. This graphical representation is developed by A. P. Yutsis, I. B. Levinson, and V. V. Vanagas, The Theory of Angular Momentum (Oldbourne Press, London, 1962). Other authors have developed slightly different notations.

FIGURE CAPTIONS

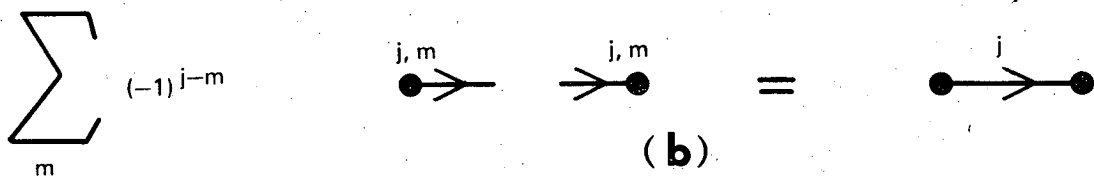
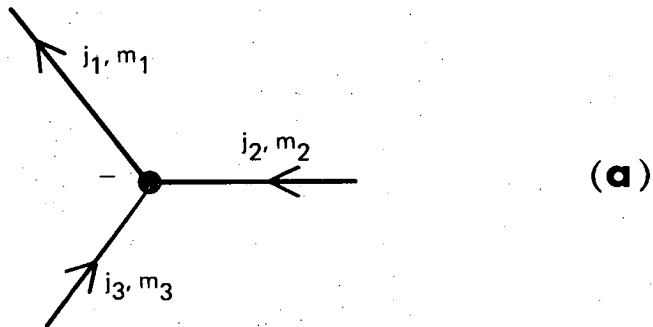
Fig. 1. The graphical representations for

- (a) the Wigner coefficient;
- (b) the z-component sums.

Fig. 2. Basic lemmas for reducing the diagrams.

- (a) Triangle elimination.
- (b) "Dualizing" to reduce the size of the smallest polygon.
- (c) Reversing directed line segments.
- (d) Reversing the order within a Wigner coefficient.
- (e) The 6-j symbol.
- (f) A two-leg degenerate graph. The term $\{j_1, j_2, j_3\} = 1$ if $|j_1 - j_2| \leq j_3 \leq |j_1 + j_2|$ and $j_1 + j_2 + j_3$ is an integer. Otherwise $\{j_1, j_2, j_3\} = 0$.
- (g) A one leg graph.

Fig. 3. Flow chart for the main (PRG3NJ) subroutine. The numbers are the statement numbers of the beginning of each block.



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Fig. 1

$$\begin{array}{c}
 j_1, m_1 \\
 \swarrow \\
 \bullet \\
 \downarrow \ell_3 \\
 \bullet \\
 \swarrow \ell_2 \quad \searrow \ell_1 \\
 j_2, m_2 \quad j_3, m_3
 \end{array}
 =
 \begin{pmatrix}
 j_1 & j_2 & j_3 \\
 \ell_1 & \ell_2 & \ell_3
 \end{pmatrix}
 \begin{array}{c}
 j_1, m_1 \\
 \swarrow \\
 \bullet \\
 \downarrow \\
 \bullet \\
 \swarrow \quad \searrow \\
 j_2, m_2 \quad j_3, m_3
 \end{array}
 \quad (a)$$

$$\begin{array}{c}
 j_4, m_4 \\
 \swarrow \\
 \bullet \\
 \downarrow \ell \\
 \bullet \\
 \swarrow \quad \searrow \\
 j_2, m_2 \quad j_1, m_1
 \end{array}
 =
 \sum_{\ell'} (2\ell' + 1) (-1)^{2j_3}
 \begin{pmatrix}
 j_4 & \ell & j_3 \\
 j_1 & \ell' & j_2
 \end{pmatrix}
 \begin{array}{c}
 j_4, m_4 \\
 \swarrow \\
 \bullet \\
 \downarrow \ell' \\
 \bullet \\
 \swarrow \quad \searrow \\
 j_2, m_2 \quad j_1, m_1
 \end{array}
 \quad (b)$$

$$\begin{array}{c}
 \ell \\
 \longrightarrow \\
 \bullet \quad \bullet
 \end{array}
 =
 (-1)^{2\ell}
 \begin{array}{c}
 \ell \\
 \longleftarrow \\
 \bullet \quad \bullet
 \end{array}
 \quad (c)$$

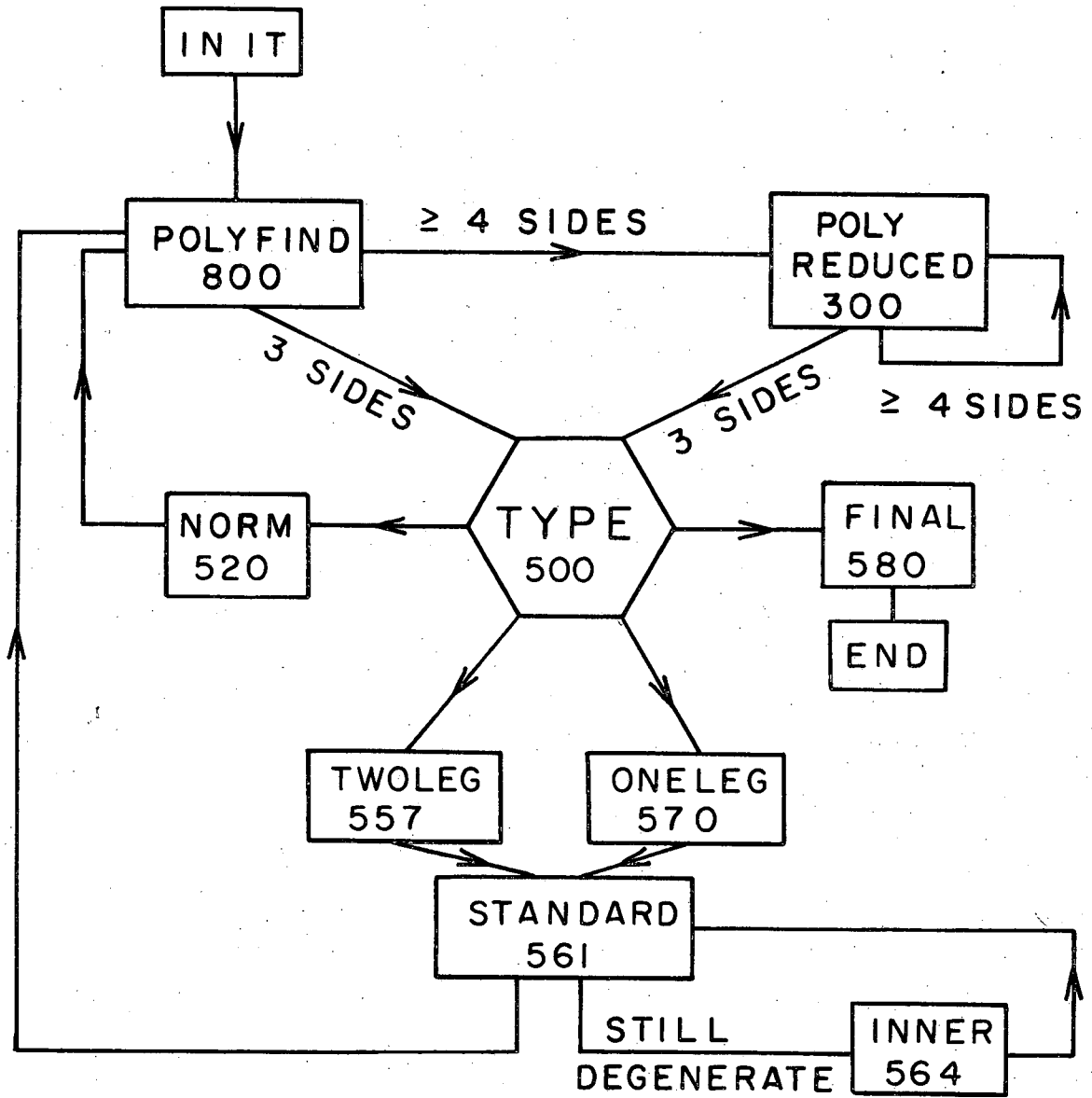
$$\begin{array}{c}
 j_1, m_1 \\
 \swarrow \\
 \bullet \\
 \downarrow \ell \\
 \bullet \\
 \swarrow \quad \searrow \\
 j_2, m_2 \quad j_3, m_3
 \end{array}
 =
 (-1)^{j_1+j_2+j_3}
 \begin{array}{c}
 j_1, m_1 \\
 \swarrow \\
 \bullet \\
 \downarrow \\
 \bullet \\
 \swarrow \quad \searrow \\
 j_2, m_2 \quad j_3, m_3
 \end{array}
 \quad (d)$$

$$\begin{array}{c}
 \bullet \\
 \swarrow \quad \searrow \\
 j_2 \quad j_1 \\
 \downarrow \ell_1 \quad \downarrow \ell_2 \\
 \bullet \\
 \downarrow \ell_3 \\
 \bullet
 \end{array}
 =
 \begin{pmatrix}
 j_1 & j_2 & j_3 \\
 \ell_1 & \ell_2 & \ell_3
 \end{pmatrix}
 \quad (e)$$

$$\begin{array}{c}
 j_2 \\
 \curvearrowright \\
 \bullet \quad \bullet \\
 \downarrow \ell \quad \downarrow \ell \\
 \bullet \quad \bullet \\
 \downarrow \ell \\
 \bullet
 \end{array}
 =
 \frac{\delta_{j_1, j_4} \{j_1, j_2, j_3\}}{2j_1 + 1}
 \begin{array}{c}
 j_1 \\
 \longrightarrow \\
 \bullet \quad \bullet
 \end{array}
 \quad (f)$$

$$\begin{array}{c}
 j_1 \\
 \swarrow \\
 \bullet \\
 \downarrow \ell \\
 \bullet \\
 \swarrow \quad \searrow \\
 j_2 \quad k
 \end{array}
 =
 \delta_{\ell, 0} \delta_{j_1, j_2} \sqrt{\frac{2k+1}{2j_1+1}}
 \begin{array}{c}
 j_1 \\
 \longrightarrow \\
 \bullet \quad \bullet
 \end{array}
 \quad (g)$$

Fig. 2



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Fig. 3

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