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MULITPLE-PRECISION ARITHMETIC AND THE EXACT CALCULATION OF THE 3-j, 6-j, AND 9-j SYMBOLS

Robert M. Baer and Martin G. Redlich
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Multiple-Precision Arithmetic and the Exact Calculation of the $3-j, 6-j$, and $9-j$ Symbols

Robert M. Baer and Martin G. Redilch

Introduction. In recent years the $3-j, 6-j$, and $9-j$ symbols [1] Sor the three-dimensional rotation group have found increasing application in calculations in many fields of physics, expecially in nuclear and atomic spectroscopy. The 3-5, 6-j, and $9-j$ symbols will be written as follows:

$$
\left(\begin{array}{lll}
f_{1} & j_{2} & j_{3} \\
m_{1} & m_{2} & m_{3}
\end{array}\right),\left\{\begin{array}{lll}
j_{1} & j_{2} & j_{3} \\
l_{1} & \imath_{2} & l_{3}
\end{array}\right\},\left\{\begin{array}{lll}
j_{1} & j_{2} & j_{12} \\
j_{3} & j_{4} & j_{34} \\
j_{13} & j_{24} & j^{\prime}
\end{array}\right\}
$$

The $3-j$ symbol equals $\left(2 j_{3}+1\right)^{-1 / 2}$. (-) $j_{1}-j_{2}-m_{3}$ times the vector addition, Clebsch-Gordan, or Wigner coefficient [1]. The vector-adaition coefficient is defined in the theory of the singie- and double-valued representations of the threecimensional rotation group SO(3). The coefficient is an element of the matrix which brings the Kronecker product of two representations labeled by the integers or half-integers $j_{1}$ and $j_{2}$ 1nto reduced form. The $6-j$ symbol equals $(-)^{j_{1}+j_{2}+l_{1}+l_{2}}$ times the Racah coefficient [2].

Many tables of the $3-j$ and $6-j$ symbols have appeared. One of the most complete is that of Rotenberg, Bivins, Metropolis, and Wooten, Jr. (RBMW) [3], which gives these symbols as square roots of products of powers of prime numbers. However, even for calculations made with a desk
calculator, one sometimes needs symbols which go beyond the $j_{1}$ or $l_{1}=8$ limit of this table. Furthermore, symbols with $j_{1} \sim 50$ will be needed in the interpretation of recent experiments in the field of reactions between heavy ions and nucie1. In the present paper, we describe a system for making multi-word calculations on a digital computer in the Ifxed-point (integer) mode, and the application of this system in subroutines for the calculation of the exact values of the $3-j, 6-j$, and $9-j$ symbols. These subroutines are called THREE $J, S I X J$, and NINE J.

Multiple-orecision fixec-Doint arithmetic. Usually, only I1mited accuracy can be obtained for calculations performed. with floating-point arithmetic. In some instances, floatingpoint arithmetic of single or double precision may be insufficient for the required accuracy indornary in a computation, because of the accumulation of truncation errors due to many 'arithmetical operations. In other cases, there may be great loss of accuracy in subtractions of numbers which are nearly equal. Thus there may be considerable uncertainty as to the actual inaccuracy of the result, especially in extencied computations which are too complicated for accurate error analyses. All of these considerations apply at least to some extent to the calculation of the $3-j, 6-j$, and $9-j$ symbols; they apply to a still larger extent to programs in which these subroutines are used. Such difficulties can be obviated for calculations which can be carried out entirely in fixed-point arithmetic.

Then the only reason acainst relying on fixed-point arithmetic in machines with fixed word size is that numbers may occur which exceed the available word length of the machine. Examples of such large numbers sometimes occur in the square brackets of equation (2) given below.

This difficulty is overcome by new multiple-precision fixed-point routines (which we shall refer to as MPF routines). These routines accept as input quantities, and return as output quantities, number-pairs ( $X, N$ ) where $X$ is a (sometimes large) integer and $N$ is the number of (machine) words occupied by $X$. The basic MPF routines are addition, multiplication and division. Their input and output may become larger or smaller freely, restricted only by space considerations relative to the overall program, (and these are usually immaterial as a real restriction).

Another program of the MPF package supplies combinatorial functions [such as the relatively prime numerator and denominator resulting from the square bracket of equation (2)]. Adaitional subroutines supply prime factorizations of large numbers, square roots of large numbers in irreducible form, , the sum of two fractions, and, finally, conversion from MPF to double-precision floating-point form. All of these
... routines* are FORTRAN II callable on the IBM 7090/94. They should prove of considerable use in other areas of physics and mathematics where a convenient way of dealing with large integers is required or desirable.

The $3-1$ Symbol. For programming, we use formula (1.5) of RBMW, but we write it in the following way, which requires only one combinatorial calculation. The definitions of $n_{1}$, $n_{2}, \ldots, n_{12}, x$, and $\lambda$ are given first.

$$
\begin{array}{lll}
n_{1}=j_{2}-m_{2}, & n_{5}=-j_{1}+j_{2}+j_{3}, & n_{9}=j_{2}+m_{2} \\
n_{2}=\jmath_{3}+m_{3}, & n_{6}=j_{1}-j_{2}+j_{3}, & n_{10}=\jmath_{3}-j_{1}-m_{2} \\
n_{3}=\jmath_{3}-m_{3}, & n_{7}=j_{1}+j_{2}-j_{3}, & n_{21}=j_{3}-j_{2}+m_{1} \\
n_{4}=j_{1}+m_{1}, & n_{8}-j_{1}-m_{1}, & n_{12}=j_{1}+j_{2}+j_{3}+1
\end{array}
$$

$$
x=\operatorname{Max}\left(-n_{10},-n_{11}, 0\right), \quad \lambda=\operatorname{M1n}\left(n_{7}, n_{8}, n_{9}\right)
$$

The coefficients $f_{k}$ are defined for $k=k$ by setting $f_{k}=1$, and recursively for $x<k \leq \lambda$ by

$$
\begin{equation*}
f_{k+2}=-f_{k} \frac{(n 7-k)(n 8-k)(n g-k)}{(k+1)\left(n_{10}+k+1\right)\left(n_{12}+k+1\right)} \tag{1}
\end{equation*}
$$

Then the $3-j$ symbol is given by:

$$
\left(\begin{array}{lll}
j_{1} & j_{2} & j_{3}  \tag{2}\\
m_{1} & m_{2} & m_{3}
\end{array}\right)^{\prime}=
$$

$=(-)^{j_{1}-j_{2}-m_{3}+x}$

$$
\left[\frac{n_{1}!n_{2}!n_{3}!n_{4}!n_{5}!n_{6}!n_{7}!n_{8}!n_{9}!}{k!2\left(n_{7}-k\right)!^{2}\left(n_{8}-k\right)!^{2}\left(n_{9}-k\right)!^{2}\left(n_{10}+k\right)!^{2}\left(n_{11}+k\right)!^{2} n_{12}!^{2}}\right]^{1 / 2} \cdot \sum_{k=x}^{\lambda} r_{k}
$$

Examination of the details of the calculations for input $j_{1}, j_{2}$, and $j_{3}$ all $\leqslant 85$ shows that the numbers in intermediate steps and in the result occupy at most six words in computer storage ( 1 word $\approx 3.4 \times 10^{10}$ ). . We have arbitrarily allocated at least eight words for each quantity which becomes large.

The output of the subroutine TriREE $J$ has been checked by comparison with the table of RBMW and by the sum rule for the squares of $3-j$ symbols [RBMW formula (1.14)]. Some examples are given below. Each symbol is given as $\sqrt{S Q} \bar{R} \bar{T} \cdot N U M / D E N$, with obvious abbreviations. (The magnitudes of the symbols in all tables of this paper have been checked by sum rules.)

3-i Symbols

| $2 j_{1}$ | $2 j_{2}$ | $2 j_{3}$ | $2 m_{1}$ | $2 m_{2}$ | $2 \mathrm{~m}_{3}$ |  |  |  | SQRT |  |  | ... NUM |  |  | DEN |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 33 | 35 | 60 | 19 | 35 | -54 |  |  |  |  | 8136 | 72717 | 7 |  |  | 29 | 00794 |
| 50 | 50 | 50 | 10 | 20 | -30 |  | 10477 | 35777 | 10678 | 15050 | 77155 | -2801 | 186 | 61339 | 54893 | 85958 |
| 125 | 105 | 200 | 87 | 103 | -190 | 9655 | 90053 | 31483 | 43182 | 39667 | 40406 | -38 | 746 | 37851 | 43782 | 28977 |

The $6-j$ and $9-j$ Symbols. The expression for the subroutine SIX J is entirely analogous to (2). Formula (2.3) of RBMW is used, again rewritten so that only one combinatorial calculation is needed. Three examples follow:

6-j Symbols


The 9-j symbol is expressed as a sum of products of $6-j$ symbols in RBMW formula (3.1). This formula is used by Subroutine NINE $J$ to calculate the $9-J$ symbol. An alternate subroutine for the calculation of the 9-j symbol has
been programmed; this subroutine uses a modification of RBifiw (3.1) similar to (2) for the $3-j$ symbol, so that only one combinatorial expression appears. Tinis latter subroutine 1s roughly $20 \%$ faster, but requires 2,26410 words storage compared with $426_{10}$ for the former one. The two subroutines have been used to check each other; in addition, their output has been checked by the sum rule of squares of $9-j$ symbols [RBMW (3.6)]. This sum rule also serves as a check on SIX J.

A comparison was made with a sample consisting of 2155 symbols from a table of $9-j$ symbols calculated in the floatingpoint mode [4]. Eleven of the symbols in the sample differed In the fifth significant figure from the values calculated and checked by the present subroutines. One other 9-j symbol of this sample, the first of those given below, differed in the first significant figure from the value calculated and checked by MPF subroutines. Again, some examples follow:

## 9-1 Symbols

|  | $2 j_{2}$ | ${ }^{2} j_{12}$ | $2 j_{3}$ | $2 j_{4}$ | $2 j_{34}$ | ${ }^{2} j_{13}$ | ${ }^{2} j_{34}$ | $2{ }^{1}$ |  |  | SQRT | NUM |  | DEN |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 5 | . 8 | 5. | 7 | 12 | 10 |  | 14 |  |  | 154 | -1 |  | 8316 |
| 1 | 15 | 28 | -15 | 15 | 26 | 30 | 24 | 40 |  | 129 | 64479 | 719 | 2307087 | 96750 |
| 1 | 16 | 16 | 16 | 16 | 16 | 30 | 26 | 32 | 2 | 09778 | 98214 | -143 | 729644 | 80675 |

Storage Space and Timing: The total space allocation required for THREE $J, S I X J$, and NINE $J$ t is approximately $3000_{10}$ words; the space allocation required for the set of MPF routines is approximately 400010 words.

The execution time of THREE J varies from $\sim 10 \mathrm{milil-}$ sec. to $\sim 26$ milil-sec. for input $\left(j_{1}, j_{2}, j_{3}\right)$ varying from $(1,1,1)$ to $(16,16,16)$. For $S I X J$, the range 1 from $\sim 12$ milli-sec. to $\sim 1$ sec. corresponding to input areument values ranging Erom all j's and l's $\sim 1$ to all g's and l's ~ 26. This execution time increases sharpiy with increasing size of input values; for all argument values $\sim 8$, the time is about 160 milli-sec. For NINE $J$ the execution time ranges from $\backsim 60$ milli-sec. for all j's $\sim 1$ to 6 sec. for all j's $\sim 8:$

It must be emphasized that the iimiting input values to the present subroutines can be made as large as may foreseeably, be desired. This is accomplished by a trivial change in space allocations and in a corresponding input to a combinatorial subroutine.

Check of Calculations. It is difficult to be certain that any computer program is entirely correct, and especially difficult to know exactly what its limitations are. In order to ensure the correctness of any long calculation, it appears most desirable to have two separate, independent programs, and thus to use the computer to check its own work. Fortunately, in anguiar-momentum algebra it is usually possible to develop two independent formulas for the same quantity. Therefore, it is possible to be nearly certain about the correctness of results even of long calculations.

In particular, two long, independent programs for the same matrix elements of nuclear interactions have been

Written here; using MPF arithmetic. These programs both, use the subroutines THREE $J$ and SIX $J$ hundreds of times for each set of input values. The results of the two programs have checked exactly for many such sets, thus giving further indication of the accuracy of these subroutines.

For the construction of some of the MPF routines we are indented to Mr. G. Johnson, and Mrs. E. Krasnow, of the Computer Center, Berkeley, and Mr. J. Brillhart of the University of San Francisco.

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## Footnotes

* These routines are available from SHARE as Al BC MPAS, MPFT, MPRD, MPDV, $G 8$ BC KOMO, and A1 BC MPFA.

Ttrese routines are submitted to SHARE under the desicnation C3 BC JSYM: they require the package of routines mentioned in the preceding footnote. Another package, C3 BC PHYS, contains some simple multiple-precision physical subroutines.A
CThese include Racah's reduced $c(k)$ matrix element [2] and the SL-jJ transformation coefficients for two particles.

Footnote for First Page
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## References

1. E.P. Wigner, "On the matrices which Reduce the Kronecker Products of Representations of Simply Reducible Groups" (c1rca 1939, unpublished).
2. G. Racah, Phys. Rev. 62, 438 (1942).
3. M. Rotenberf, R. Bivins, N. Metropolis, and J.K. Wooten, Jr.; The $3-j$ anc 6-j Symbols (Technology Press, Campridge, Mass., 2959).
4. K. Smith and J.W. Stevenson, Argonne National Laboratory Report 5776 (2957, unpubilshed); K. Smith, Argonne National Laboratory Report 5860 (1958, unpublished).
