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THE REDUCED ROTATION MATRIX *

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PROGRAM SUMMARY

Title of program: DS

Catalogue number: ABOR

Program obtainable from: CPC Program Library, Queen's University of Belfast, N.Ireland (see application form in this issue)

Computer: IBM 360/91. *Installation*: Princeton University

Operating system: OS360

Programming languages used: FORTRAN IV

High speed store required: 947 words. *No of bits in a word:* 64

Is the program overlaid? No

No. of magnetic tapes required: None

What other peripherals are used? Card Reader; Line Printer

No. of cards in combined program and test deck: 112

Card punching code: EBCDIC

Keywords: Atomic, Molecular, Nuclear, Rotation Matrix, Rotation Group, Representation, Euler Angle, Symmetry, Helicity, Correlation.

Nature of the physical problem

Subprogram DS is a FORTRAN IV DOUBLE PRECISION FUNCTION which calculates the reduced matrix elements of finite rotations [1] in the angular momentum representation, using a standard phase convention [2]. The four arguments of the FUNCTION are: J2, twice the total angular momentum; MI2 and MF2, twice the z-projection of the total angular momentum in the initial and final coordinate systems, respectively and BETA, the Euler angle-of-rotation around y' [2].

Method of solution

A Wigner-closed-sum expression for $d^j_{mm'}(\beta)$ is evaluated. Each term contains products of factorials. Using a method similar to that of Wills [3], a common coefficient (containing factorials) is evaluated by combining the logarithms of the factorials, followed by one exponentiation. The remaining expression is written, without factorials, as a nested product. This method contrasts well, in speed and accuracy, with methods that evaluate factorial products in the closed-sum coefficients term-by-term, before adding.

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References

[1] E.P. Wigner, Gruppentheorie (vieweg, Braunschweig, 1931); A.R. Edmonds, Angular momentum in quantum mechanics (Princeton Univ. Press, Princeton, 1960).
[2] D.M. Brink and G.R. Satchler, Angular momentum (Oxford Univ. Press, London, 1962).
[3] J.G. Wills, Oak Ridge National Laboratory Report ORNL-TM-1949 (1967), unpublished; Computer Phys. Commun. 2 (1971) 381.

LONG WRITE-UP

1. Introduction

The elements of the matrix associated with the rotation operator $R(\alpha,\beta,\gamma) = \exp(-i\alpha Jz)\exp(-i\beta Jy)\exp(-i\gamma Jz)$ are evaluated in the angular momentum representation where they are $\exp(-im\alpha)\, d^j_{mm'}(\beta)\exp(-im'\gamma)$. These matrix elements are complex, with the *real* matrix $d^j_{mm'}(\beta)$ being the only difficult part to evaluate.

The rotation matrix has enjoyed wide use for many problems of interest in quantum mechanics. Although it has been widely used in a formal way, its numerical evaluation is needed if it is to be applied to experimental problems in atomic and nuclear physics. Examples of this application occur in the use of direct reaction scattering theory to predict the angular correlations between two or more radiations [1], and in the expansion of nuclear reaction cross sections in helicity amplitudes [2].

2. Code description

The code being reported is a FORTRAN IV FUNCTION SUBPROGRAM called DS. This subprogram calculates values for the reduced rotation matrix [3] corresponding to an Euler angle-of-rotation of β around the y'axis [4] for both integer and half-integer spins. The method of calculation is to *modify* and evaluate the following Wigner closed-form expression [3].

$$d^j_{mm'}(\beta) = \left[\frac{(j+m')!(j-m')!}{(j-m)!(j+m)!}\right]^{1/2} \sum_\sigma \binom{j+m}{j-m'-\sigma}\binom{j-m}{\sigma}(-1)^{j-m'-\sigma}(\cos\tfrac{1}{2}\beta)^{2\sigma+m'+m}(\sin\tfrac{1}{2}\beta)^{2j-2\sigma-m'-m},$$

where $\binom{N}{K} = N!/(N-K)!K!$ is the binomial coefficient.

A common factor is extracted from the above form and the phase is modified by $(-1)^{m-m'}$ to follow the Brink and Satchler convention [4]. This results in the following numerically-convenient expression for the reduced rotation matrix:

$$d^j_{mm'}(\beta) = (-1)^{K_3-K_L} C^{K_8} S^{K_9} \frac{(K_1!K_2!K_3!K_4!)^{1/2}}{K_5!K_6!K_7!K_L!}\left\{1 - \frac{C^2}{S^2}\frac{(1+K_6-K_U)(1+K_7-K_U)}{(K_5+K_U)(K_L+K_U)}\right.$$

$$\times\left[1 - \frac{C^2}{S^2}\frac{(2+K_6-K_U)(2+K_7-K_U)}{(K_5+K_U-1)(K_L+K_U-1)}\left[1 - \frac{C^2}{S^2}\frac{(3+K_6-K_U)(3+K_7-K_U)}{(K_5+K_U-2)(K_L+K_U-2)}\left[1 - \ldots\right.\right.\right\},$$

where $K_1 = j-m'$, $K_3 = j-m$, K_L = maximum of $(0, m-m')$, $K_5 = m'+m+K_L$, $K_7 = K_3-K_L$, $K_2 = j+m'$, $K_4 = j+m$, K_U = minimum of (K_1, K_3), $K_6 = K_1-K_L$, $K_8 = K_5+K_L$, $K_9 = K_1+K_2-K_8$, $C = \cos\frac{1}{2}\beta$ and $S = \sin\frac{1}{2}\beta$.

The factorial terms in the coefficient of the nested product above are evaluated by combining the logarithms of the factorials and exponentiating [5]. This expression is:

$$\exp\left\{\tfrac{1}{2}\left[\ln(K_1!) + \ln(K_2!) + \ln(K_3!) + \ln(K_4!)\right] - \left[\ln(K_5!) + \ln(K_6!) + \ln(K_7!) + \ln(K_L!)\right]\right\},$$

where the logarithms of the factorials are provided in a lookup table for arguments from 0 to 150 and approximated by a 5-term Stirling's formula [6] for arguments exceeding 150.

For the special case of rotations through $n\pi$ (where $n = 0, \pm 1, \pm 2, \pm 3, \ldots$) the reduced rotation matrix is either zero or equal to the coefficient of the nested product provided that the term is included where the *power* of $\sin\frac{1}{2}\beta$ or ($\cos\frac{1}{2}\beta$) is zero when $\sin\frac{1}{2}\beta$ or ($\cos\frac{1}{2}\beta$) is zero. These rotations are given special attention in the program, thus ensuring that all the end point roots of $d^j_{mm'}(\beta)$ are properly accounted for [7, 8].

3. Test deck and test run

The test program evaluates the reduced rotation matrix for several argument values where it is approximately zero [7, 8].

References

[1] J.G. Cramer and W.W. Eidson, Nucl. Phys. *55* (1964) 593.
[2] M. Jacob and G.C. Wick, Ann. Phys. N.Y. *7* (1959) 404.
[3] A.R. Edmonds, Angular momentum in quantum mechanics (Princeton Univ. Press, Princeton, 1960).
[4] D.M. Brink and G.R. Satchler, Angular momentum (Oxford Univ. Press, London, 1962).
[5] J.G. Wills, Oak Ridge National Laboratory Report ORNL-TM-1949 (1967), unpublished; Computer Phys. Commun. 2 (1971) 381.
[6] M. Abramowitz and I.A. Stegun, eds., in: Handbook of mathematical functions(U.S. Govt. Printing Office, Washington, 1964) p. 257.
[7] W.J. Braithwaite and J.G. Cramer, Nuclear Physics Laboratory Annual Report, University of Washington (1970) p. 50, unpublished.
[8] J.G. Cramer and W.J. Braithwaite, Nuclear Data Tables A, to be published.

TEST RUN OUTPUT

```
DS(2*J,2*MI,2*MF,BETA)
NEAR ROOT VALUES OF BETA

DS (3,1,1,  70.529) =-0.000004
DS (4,0,0,  54.736) =-0.000009
DS (4,0,0, 125.264) =-0.000010
DS (4,2,2,  60.000) = 0.000000
DS (5,1,1,  46.378) =-0.000001
DS (5,0,0, 106.852) = 0.0
DS (5,3,1,  78.463) =-0.000001
DS (5,3,3,  53.130) = 0.000003
DS (6,0,0,  39.231) = 0.000017
DS (6,0,0, 140.768) = 0.000016
DS (6,2,0,  63.435) = 0.000001
DS (6,2,0, 116.565) = 0.000002
DS (6,2,2,  40.977) = 0.000007
DS (6,2,2,  95.066) =-0.000001
DS (6,4,2,  70.529) = 0.000005
DS (6,4,4,  48.190) =-0.000008
```