JOURNAL OF COMPUTATIONAL PHYSICS 17, 437–439 (1975)

Note

Rapid Computation of Rotation Functions*

I. Introduction

Although properties of the matrix elements of the three-dimensional rotation group are throughly documented in standard texts on angular momentum, little attention is given to efficient means of computing them. Edmonds [1] offers an algorithm which requires first the generation of the entire matrix of constants $\mathbf{d}^J(\pi/2)$ using a circuitous recursion which involves both integral and half-integral angular momenta; these constants are then used to compute the $d^J_{MK}(\beta)$ in a sum over sines and cosines. Fano and Racah [2] describe recursions which give all the $d^J_{MK}(\beta)$ for a fixed J and ranging M and K. A more direct method is desirable if one wants a sequence of the functions $d^J_{MK}(\beta)$ with M and K fixed and J possibly ranging. Such a case occurs when computing scattering amplitudes for rotational excitation in the helicity representation [3].

II. Obtaining the Recursion

Unfortunately, the notation used for the $d^J_{MK}(\beta)$ is not standardized. We will use the notation of Rose [4], in which Edmonds' [1, pp. 54–55] notation becomes

$$d^J_{MK}(\beta, \text{here}) = d^J_{KM}(\beta, \text{Edmonds}). \tag{1}$$

The functions $d^J_{MK}(\beta)$ are related [1, p. 58, Eq. (4.1.23)] to the Jacobi polynomials $P_n^{(a,b)}(\beta)$ according to

$$P_n^{(a,b)}(\beta) = \left[\frac{(n+a)!\,(n+b)!}{n!\,(n+a+b)!}\right]^{1/2} \left(\cos\frac{\beta}{2}\right)^{-b} \left(\sin\frac{\beta}{2}\right)^{-a} d^{n+\frac{1}{2}(a+b)}_{\frac{1}{2}(b-a),\frac{1}{2}(b+a)}(\beta). \tag{2}$$

Combining this relation with a recursion formula for Jacobi polynomials [5],

$$\begin{aligned} &2(n+1)(n+a+b+1)(2n+a+b)\, P_{n+1}^{(a,b)}(\beta) \\ &\quad = [(2n+a+b+1)(a^2-b^2) + (2n+a+b)(2n+a+b+1) \\ &\qquad \times (2n+a+b+2)\cos\beta]\, P_n^{(a,b)}(\beta) \\ &\qquad - 2(n+a)(n+b)(2n+a+b+2)\, P_{n-1}^{(a,b)}(\beta) \end{aligned} \tag{3}$$

* This work was supported by the National Science Foundation and the Louis Block Fund.

gives, after some algebra, the following recursion in terms of the $d^J_{MK}(\beta)$ functions.

$$J[(P^2 - M^2)(P^2 - K^2)]^{1/2}\, d^{J+1}_{MK}(\beta)$$

$$= (2J + 1)(JP \cos\beta - MK)\, d^J_{MK}(\beta) - P[(J^2 - M^2)(J^2 - K^2)]^{1/2}\, d^{J-1}_{MK}(\beta), \quad (4)$$

where we have set $P = J + 1$ for brevity in (4). It is simple to verify that (4) becomes the usual recursion for Legendre polynomials when $M = K = 0$, and simplifies to the recursion for associated Legendre polynomials $P_J{}^K(\cos\beta)$ when $M = 0$, where

$$P_J{}^K(\cos\beta) = [(J + K)!/(J - K)!]\, d^J_{0K}(\beta). \quad (5)$$

III. Starting the Recursion

The three-term recursion (4) requires two initial values to get it started. Without any loss of generality, we may assume that

$$J \geqslant M \geqslant K \geqslant 0. \quad (6)$$

Values of the d^J_{MK} for which (6) does not hold may be found from the well-known symmetry properties [4, p. 54].

$$d^J_{MK}(\beta) = (-1)^{K-M}\, d^J_{KM}(\beta), \quad (7)$$

$$d^J_{MK}(\beta) = (-1)^{K-M}\, d^J_{-M,-K}(\beta). \quad (8)$$

Using (6), we initiate the recursion by recognizing that the first nonzero term will occur for $J = M$, and then use [1, p. 59, Eq. (4.1.27)]

$$d^M_{MK}(\beta) = (-1)^{M-K} \left[\frac{(2M)!}{(M + K)!\,(M - K)!}\right]^{1/2} \left(\cos\frac{\beta}{2}\right)^{M+K} \left(\sin\frac{\beta}{2}\right)^{M-K}. \quad (9)$$

The second term is then easily obtained from a relation derivable from (4),

$$d^{M+1}_{MK}(\beta) = [(M + 1)\cos\beta - K] \left[\frac{(2M + 1)}{(M + K + 1)(M - K + 1)}\right]^{1/2} d^M_{MK}(\beta). \quad (10)$$

At this point, we may freely use (4) to generate the desired sequence of functions $\{d^R_{MK}(\beta),\ R = M, M + 1, \ldots, J\}$.

IV. Conclusions

We have detailed an algorithm (based upon a recursion for Jacobi polynomials) for computing a sequence of the functions $d^J_{MK}(\beta)$ with M and K fixed and J ranging upward from its minimum value. The algorithm works equally well for integral or half-integral angular momenta, and is readily adaptable to computer evaluation of the $d^J_{MK}(\beta)$.

Computed values of $d^J_{MK}(\beta)$ obtained by recursion are more accurate than values obtained by direct summation formula [4, p. 52, Eq. (4.13); 1, p. 57, Eq. (4.1.15)]; the latter suffer from numerical errors at large J ($J \approx 30$) arising from the subtraction of nearly equal terms in the summation. To evaluate the accuracy of the $d^J_{MK}(\beta)$, we checked the unitarity of the matrix $\mathbf{d}^J(\beta)$ (M, K ranging for fixed β and J) for J up to $J = 30$. The matrix product of $\mathbf{d}^J$ (40°) and its transpose in all cases gave the unit matrix to 12 (and usually more) significant figures (on an IBM 370, where double precision gives approximately 16 significant figures). As might be expected, the accuracy decreases as J increases.

References

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Received: November 5, 1974

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