Exact recursive evaluation of 3*j*- and 6*j*-coefficients for quantum-mechanical coupling of angular momenta*

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Algorithms are developed for the exact evaluation of the 3*j*-coefficients of Wigner and the 6*j*-coefficients of Racah. These coefficients arise in the quantum theory of coupling of angular momenta. The method is based on the exact solution of recursion relations in a particular order designed to guarantee numerical stability even for large quantum numbers. The algorithm is more efficient and accurate than those based on explicit summations, particularly in the commonly arising case in which a whole set of related coefficients is needed.

I. INTRODUCTION

Common algorithms for the evaluation of 3*j*- and 6*j*-coefficients are based on the explicit expressions of Wigner[1] and Racah.[2] Calculations involving the quantum mechanical coupling of angular momenta often require the evaluation of whole strings of coupling coefficients of the kind:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \quad \text{for all allowed } j_1, \tag{1}$$

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix} \quad \text{for all allowed } m_2, \tag{2}$$

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} \quad \text{for all allowed } j_1. \tag{3}$$

Numerical examples of these sets of coupling coefficients are given in Figs. 1—3.

The existing algorithms, however, evaluate coupling coefficients separately and do not make use of relationships between the values of neighboring 3*j*- and 6*j*-coefficients. The algorithms, furthermore, are inapplicable for large angular momentum values ($\sim 100\hbar$) which, for example, occur frequently in problems of molecular dynamics.

We have now numerically tested an algorithm for the evaluation of 3*j*- and 6*j*-coefficients based on recursion equations relating the coefficients in the strings (1), (2), or (3). This algorithm simultaneously generates all coupling coefficients within these strings without more numerical effort than is needed to evaluate a single coupling coefficient. Further, this algorithm is numerically applicable for large angular momentum quantum numbers.

In the following, we will present the derivations of the recursion equations which relate the coupling coefficients in (1), (2), or (3). In Sec. II we derive these recursion relations algebraically from certain sum rules satisfied by these coefficients. While this derivation is the shortest available, it is somewhat remote from the definitions of the coefficients. Thus in the Appendix, we supply an alternate derivation starting directly from the basic definitions of angular momentum coupling. In Sec. III we then derive the algorithm for generating the strings of 3*j*- and 6*j*-coefficients (1), (2), and (3). In Sec. IV we demonstrate numerically the accuracy and efficiency of the algorithm. Computer programs for the recursive evaluation of 3*j*- and 6*j*-coefficients will be made available.[3]

Beside being most advantageous for numerical evaluations, the recursion equations serve to make the functional properties of the angular momentum coupling coefficients more transparent. In a second article following this one,[4] it is shown that the recursion equations for 3*j*- and 6*j*-coefficients can be solved using a discrete analog of the uniform WKB approximation to yield simple analytic approximate expressions for individual coupling coefficients, which are quite accurate even for moderate quantum numbers.

II. RECURSION RELATIONSHIPS FOR 3*j*- AND 6*j*-COEFFICIENTS

The recursion relationships which connect the angular momentum coupling coefficients in (1), (2), and (3) had been previously reported. Condon and Shortley[5] derived the recursion relationships for the 3*j*-coefficients in (1), and Rose[6] presented the recursion relationship for the 3*j*-coefficients in (2). In both instances the recursion relationships were obtained from the interpretation of the strings of 3*j*-coefficients in (1) and (2) as the eigenvectors of certain angular momentum operators. Condon and Shortley, and subsequently Rose, suggested that these recursion equations might help evaluate the 3*j*-coefficients. The recursion equation for the 6*j*-coefficients in (3) have been given by Yutsis *et al.*[7] In an appendix following this paper, we show that this recursion equation, too, originates from an eigenvalue problem. Instead of now just quoting the recursion equations of Condon and Shortley, Rose and Yutsis *et al.*, we present a unified derivation for these three recursion equations. This derivation starts off from three basic sum rules which hold for 3*j*- and 6*j*-coefficients.

Let us first consider the 3*j*-coefficients in (1). For the 3*j*-coefficients there is an identity[8]

$$(-1)^{j_2+m_2+j_3-m_3+l_1+m_1'} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & j_3 \\ m_1' & m_2' & -m_3 \end{pmatrix}$$

$$
= \sum_{l_3} (2l_3+1) \begin{pmatrix} j_1 & l_2 & l_3 \\ m_1 & m_2' & m_1'+m_2 \end{pmatrix} \begin{pmatrix} l_1 & j_2 & l_3 \\ -m_1' & -m_2 & m_1'+m_2 \end{pmatrix}
$$

$$
\times \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}. \tag{4}
$$

For $l_1 = \frac{1}{2}$, $l_2 = j_3 + \alpha$, and $m_1' = \beta$ $(\alpha, \beta = \pm\frac{1}{2})$ this identity reduces to the three term recursion relationship

$$
(-1)^{j_2+m_2+j_3-m_3+1/2+\beta} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & j_3+\alpha & j_3 \\ \beta & m_3-\beta & -m_3 \end{pmatrix}
$$

$$
= \sum_{l_3=j_2-1/2}^{j_2+1/2} (2l_3+1) \begin{pmatrix} j_1 & j_3+\alpha & l_3 \\ m_1 & m_3-\beta & m_2+\beta \end{pmatrix}
$$

$$
\times \begin{pmatrix} \frac{1}{2} & j_2 & l_3 \\ -\beta & -m_2 & m_2+\beta \end{pmatrix} \begin{Bmatrix} j_1 & j_2 & j_3 \\ \frac{1}{2} & j_3+\alpha & l_3 \end{Bmatrix} \tag{4'}
$$

which connects the $3j$-coefficients

$$
\begin{pmatrix} j_1 & j_2-\frac{1}{2} & j_3+\alpha \\ m_1 & m_2+\beta & m_3-\beta \end{pmatrix}, \quad \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}
$$

and

$$
\begin{pmatrix} j_1 & j_2+\frac{1}{2} & j_3+\alpha \\ m_1 & m_2+\beta & m_3-\beta \end{pmatrix}.
$$

The factors multiplying these $3j$-coefficients in Eq. (4′) are $3j$- and $6j$-coefficients containing a quantum number $\frac{1}{2}$ for which closed expressions exist. Equation (4′) with $\alpha = -\frac{1}{2}$ and $\beta = -\frac{1}{2}$ is identical with a recursion relationship previously derived by Louck[9] starting from the Clebsch–Gordan series.

Recursion relationships (5) properly combined give a recursion relationship which only connects $3j$-coefficients belonging to (1). To be specific, the recursion relationships to be combined are

$$
(-1)^{2m_3} (2j_2+1) [j_3-m_3+1]^{1/2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}
$$

$$
= [(j_1+j_2-j_3)(j_1-j_2+j_3+1)(j_2-m_2)]^{1/2}
$$

$$
\times \begin{pmatrix} j_1 & j_2-\frac{1}{2} & j_3+\frac{1}{2} \\ m_1 & m_2+\frac{1}{2} & m_3-\frac{1}{2} \end{pmatrix}
$$

$$
-[(j_1+j_2+j_3+2)(-j_1+j_2+j_3+1)(j_2+m_2+1)]^{1/2}
$$

$$
\times \begin{pmatrix} j_1 & j_2+\frac{1}{2} & j_3+\frac{1}{2} \\ m_1 & m_2+\frac{1}{2} & m_3-\frac{1}{2} \end{pmatrix}, \tag{5a}
$$

$$
(-1)^{2m_3} 2j_2 [j_3-m_3+1]^{1/2} \begin{pmatrix} j_1 & j_2-\frac{1}{2} & j_3+\frac{1}{2} \\ m_1 & m_2+\frac{1}{2} & m_3-\frac{1}{2} \end{pmatrix}
$$

$$
= -[(j_1+j_2+j_3+1)(-j_1+j_2+j_3)(j_2+m_2)]^{1/2}
$$

$$
\times \begin{pmatrix} j_1 & j_2-1 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}
$$

$$
+[(j_1-j_2+j_3+1)(j_1+j_2-j_3)(j_2-m_2)]^{1/2}
$$

$$
\times \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}, \tag{5b}
$$

and

$$
(-1)^{2m_3} (2j_2+2)[j_3-m_3+1]^{1/2} \begin{pmatrix} j_1 & j_2+\frac{1}{2} & j_3+\frac{1}{2} \\ m_1 & m_2+\frac{1}{2} & m_3-\frac{1}{2} \end{pmatrix}
$$

$$
= -[(j_1+j_2+j_3+2)(-j_1+j_2+j_3+1)(j_2+m_2+1)]^{1/2}
$$

$$
\times \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}
$$

$$
+[(j_1-j_2+j_3)(j_1+j_2-j_3+1)(j_2-m_2+1)]^{1/2}
$$

$$
\times \begin{pmatrix} j_1 & j_2+1 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \tag{5c}
$$

Inserting (5b) and (5c) into (5a) gives a recursion relationship for $3j$-coefficients which may be written

$$
j_1 A(j_1+1) \begin{pmatrix} j_1+1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} + B(j_1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}
$$

$$
+ (j_1+1) A(j_1) \begin{pmatrix} j_1-1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = 0, \tag{6a}
$$

where

$$
A(j_1) = [j_1^2 - (j_2-j_3)^2]^{1/2} [(j_2+j_3+1)^2 - j_1^2]^{1/2} [j_1^2 - m_1^2]^{1/2}, \tag{6b}
$$

$$
B(j_1) = -(2j_1+1)[j_2(j_2+1)m_1 - j_3(j_3+1)m_1 - j_1(j_1+1)(m_3-m_2)]. \tag{6c}
$$

Recursion equation (6), it will be shown below, together with the normalization condition

$$
\sum_{j_1} (2j_1+1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}^2 = 1, \tag{7}
$$

is sufficient to determine except for an overall phase factor the values of the $3j$-coefficients in (1).

There exists yet another recursion equation for $3j$-coefficients, which relates $3j$-coefficients with different magnetic quantum numbers, and which allows the evaluation of the elements in (2). This recursion equation is derived in much the same manner as Eq. (6). Hence, we may only outline this derivation. It had already been pointed out by Edmonds[10] that the identity

$$
\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}
$$

$$
= \sum_m (-1)^{\psi_m} \begin{pmatrix} j_1 & l_2 & l_3 \\ m_1 & m & -m_1-m \end{pmatrix} \begin{pmatrix} l_1 & j_2 & l_3 \\ m_3-m & m_2 & m_1+m \end{pmatrix}
$$

$$
\times \begin{pmatrix} l_1 & l_2 & j_3 \\ m-m_3 & -m & m_3 \end{pmatrix}, \tag{8}
$$

$$
\psi_m = l_1 + l_2 + l_3 + m_1 - m_3 - m,
$$

provides a suitable starting point for the derivation of recursion relationships for $3j$-coefficients. Setting $l_1=\frac{1}{2}$, $l_2=j_3+\beta$, and $l_3=j_2+\alpha$ $(\alpha,\beta=\pm\frac{1}{2})$ gives the three term recursion relationship

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{Bmatrix} j_1 & j_2 & j_3 \\ \frac{1}{2} & j_3+\beta & j_2+\alpha \end{Bmatrix} = \sum_{m=m_3-1/2}^{m_3+1/2} (-1)^{\phi_m} \begin{pmatrix} j_1 & j_3+\beta & j_2+\alpha \\ m_1 & m & -m_1-m \end{pmatrix} \times \begin{pmatrix} \frac{1}{2} & j_2 & j_2+\alpha \\ m_3-m & m_2 & m_1+m \end{pmatrix} \begin{pmatrix} \frac{1}{2} & j_3+\beta & j_3 \\ m-m_3 & -m & m_3 \end{pmatrix} \qquad (8')$$

which connects the $3j$-coefficients

$$\begin{pmatrix} j_1 & j_2+\alpha & j_3+\beta \\ m_1 & m_2+\frac{1}{2} & m_3-\frac{1}{2} \end{pmatrix}, \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \text{ and } \begin{pmatrix} j_1 & j_2+\alpha & j_3+\beta \\ m_1 & m_2-\frac{1}{2} & m_3+\frac{1}{2} \end{pmatrix}.$$

The factors multiplying these $3j$-coefficients are again $3j$- and $6j$-coefficients containing a quantum number $\frac{1}{2}$ for which closed expressions exist. From (8′) can then be obtained by a proper combination of three recursion relationships the following equation which relates the $3j$-coefficients belonging to (2)

$$C(m_2+1)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2+1 & m_3-1 \end{pmatrix} + D(m_2)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} + C(m_2)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2-1 & m_3+1 \end{pmatrix} = 0 \qquad (9a)$$

where

$$C(m_2)=[(j_2-m_2+1)(j_2+m_2)(j_3+m_3+1)(j_3-m_3)]^{1/2}, \qquad (9b)$$

$$D(m_2)=j_2(j_2+1)+j_3(j_3+1)-j_1(j_1+1)+2m_2m_3. \qquad (9c)$$

It will be shown that Eq. (9) together with the normalization condition

$$\sum_{m_2} (2j_1+1)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix}^2 = 1 \qquad (10)$$

is sufficient to determine except for an overall phase factor the values of the $3j$-coefficients in (2).

The recursion equation which selectively connects the $6j$-coefficients belonging to the set (3) is derived in a manner strikingly similar to the recursion equations (6) and (9) above. Now the Biedenharn—Elliot identity[11] serves as the starting point:

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1' & l_2' & l_3' \end{Bmatrix} = \sum_\lambda (-1)^{\phi_\lambda} \begin{Bmatrix} j_1 & l_2' & l_3' \\ \lambda & l_3 & l_2 \end{Bmatrix} \begin{Bmatrix} l_1' & j_2 & l_3' \\ l_3 & \lambda & l_1 \end{Bmatrix} \begin{Bmatrix} l_1' & l_2' & j_3 \\ l_2 & l_1 & \lambda \end{Bmatrix}, \qquad (11)$$

$$\phi_\lambda = j_1+j_2+j_3+l_1+l_2+l_3+l_1'+l_2'+l_3'+\lambda.$$

If one sets $l_1'=\frac{1}{2}$, $l_2'=j_3+\beta$, and $l_3'=j_2+\alpha$ $(\alpha,\beta=\pm\frac{1}{2})$, the sum over λ reduces to two terms with $\lambda=l_1\pm\frac{1}{2}$. One arrives then at the recursion relationship

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j_3 \\ \frac{1}{2} & j_3+\beta & j_2+\alpha \end{Bmatrix} = \sum_{\lambda=l_1-1/2}^{l_1+1/2} (-1)^{\phi_\lambda} \begin{Bmatrix} j_1 & j_2+\alpha & j_3+\beta \\ \lambda & l_2 & l_3 \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & j_2 & j_2+\alpha \\ l_3 & \lambda & l_1 \end{Bmatrix} \times \begin{Bmatrix} \frac{1}{2} & j_3+\beta & j_3 \\ l_2 & l_1 & \lambda \end{Bmatrix} \qquad (11')$$

which connects the $6j$-coefficients

$$\begin{Bmatrix} j_1 & j_2+\alpha & j_3+\beta \\ l_1-\frac{1}{2} & l_2 & l_3 \end{Bmatrix}, \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} \text{ and } \begin{Bmatrix} j_1 & j_2+\alpha & j_3+\beta \\ l_1+\frac{1}{2} & l_2 & l_3 \end{Bmatrix}.$$

The factors in this recursion relationship consist of $6j$-coefficients with a quantum number $\frac{1}{2}$ for which closed expressions exist. Proper combination of three recursion relationships (11′) yields

$$j_1E(j_1+1)\begin{Bmatrix} j_1+1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} + F(j_1)\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} + (j_1+1)E(j_1)\begin{Bmatrix} j_1-1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = 0 \qquad (12a)$$

where

$$E(j_1)=\{[j_1^2-(j_2-j_3)^2][(j_2+j_3+1)^2-j_1^2][j_1^2-(l_2-l_3)^2] \times[(l_2+l_3+1)^2-j_1^2]\}^{1/2}, \qquad (12b)$$

$$F(j_1)=(2j_1+1)\{j_1(j_1+1)[-j_1(j_1+1)+j_2(j_2+1)+j_3(j_3+1)] + l_2(l_2+1)[j_1(j_1+1)+j_2(j_2+1)-j_3(j_3+1)] + l_3(l_3+1)[j_1(j_1+1)-j_2(j_2+1)+j_3(j_3+1)] - 2j_1(j_1+1)l_1(l_1+1)\}.$$

Recursion equation (12) together with the normalization condition

$$\sum_{j_1} (2j_1+1)(2l_1+1)\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}^2 = 1 \qquad (13')$$

is sufficient to determine expect for an overall phase factor the $6j$-coefficients in (3).

Racah[11] had pointed out that his explicit formula is not the only pathway for an evaluation of $6j$-coefficients, but that instead the recursion equation (11′) equally well furnishes an approach to the evaluation of $6j$-coefficients. Racah and Fano noted that the coefficients in these recursion equations consisting of $6j$-coefficients with quantum numbers $\frac{1}{2}$ are determined through the unitary property

$$\sum_{j_1} (2j_1+1)(2l_1+1)\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1' & l_2 & l_3 \end{Bmatrix} = \delta_{l_1 l_1'} \qquad (13)$$

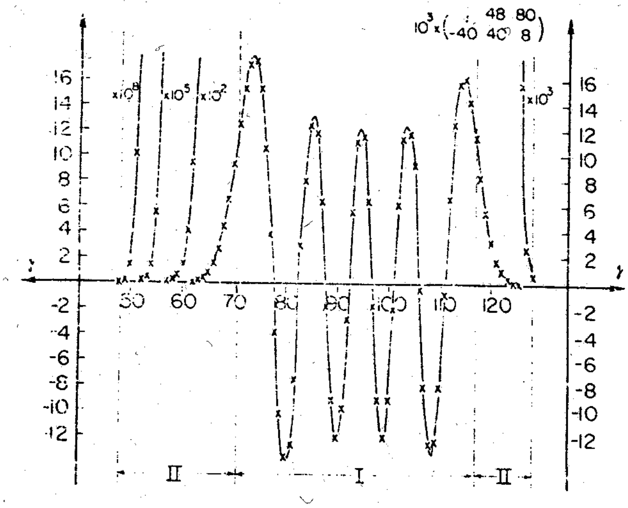

FIG. 1. Functional behavior of 3j-coefficients $f(j_1)=\begin{pmatrix} j_1 & 48 & 80 \\ -40 & 40 & 8 \end{pmatrix}$ $(48 \le j_1 \le 128)$. The evaluation of $f(j_1)$ followed the recursion algorithm described in Sec. 3. The domain of $f(j_1)$ can be divided into a classical and two nonclassical regions (Ref. 4). In the classical region $f(j_1)$ oscillates with slowly varying amplitude; in the nonclassical regions $|f(j_1)|$ monotonically decays to zero.

together with the associative property

$$\sum_{j_1} (-1)^{j_1+l_1+l_1'} (2j_1+1) \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1' & l_3 & l_2 \end{Bmatrix} = \begin{Bmatrix} j_2 & l_3 & l_1 \\ j_3 & l_2 & l_1' \end{Bmatrix}. \tag{14}$$

Hence, the very interesting conclusion can be drawn that the identities (13), (14), and (11) completely determine the 6j-coefficients save an overall phase factor.[11]

The similarity between the recursion equations (6) and (9) for 3j-coefficients and the recursion equation (12) for 6j-coefficients as well as the similarity between the corresponding derivations is explained through the existence of an asymptotic relationship between 3j- and 6j-coefficients[12]:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \lim_{R\to\infty} (-1)^{2l_1-2j_1} \, [2l_1+2R+1]^{1/2} \times \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1+R & l_2+R & l_3+R \end{Bmatrix} \tag{15}$$

where $l_3-l_2=m_1$, $l_1-l_3=m_2$, and $l_2-l_1=m_3$. In fact, Eq. (6) follows from Eq. (12) by taking the asymptotic limit letting l_1, l_2, and l_3 go to infinity, whereas Eq. (9) follows from Eq. (12) by letting j_1, j_2, and l_3 go to infinity. We have chosen the series of 3j- and 6j-coefficients in Figs. 1, 2, and 3 to be related through the asymptotic relationship (15) as may be readily checked. The similarity of these diagrams is therefore an illustration for Eq. (15).

III. ALGORITHM FOR THE RECURSIVE EVALUATION OF 3j- AND 6j-COEFFICIENTS

The three-term recursion equations for 3j- and 6j-coefficients (6), (9), and (12) have been derived and it will now be shown how the Wigner and Racah coefficients can be determined from these recursion equations.

To describe the proposed recursive algorithm, we will first consider the evaluation of the string of 3j-coefficients

$$f(j_1) = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}, \quad j_{1\,\mathrm{min}} \le j_1 \le j_{1\,\mathrm{max}}. \tag{1'}$$

The range of j_1 is finite, the smallest and largest values being

$$j_{1\,\mathrm{min}} = \max\{|j_2-j_3|,\ |m_1|\} \ \text{ and } \ j_{1\,\mathrm{max}} = j_2+j_3.$$

Once proper starting values have been given, the re-

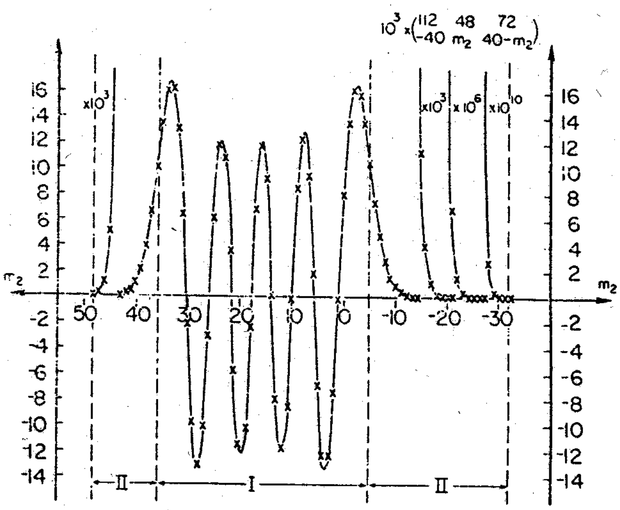

FIG. 2. Functional behavior of the 3j-coefficients $g(m_2) = \begin{pmatrix} 112 & 48 & 72 \\ -40 & m_2 & 40-m_2 \end{pmatrix}$ $(-32 \le m_2 \le 48)$. The evaluation of $g(m_2)$ followed the recursion algorithm described in Sec. 3. The domain of $g(m_2)$ can be divided into a classical region and two nonclassical regions (Ref. 4). In the classical region $g(m_2)$ oscillates with slowly varying amplitude; in the nonclassical regions $|g(m_2)|$ monotonically decays to zero.

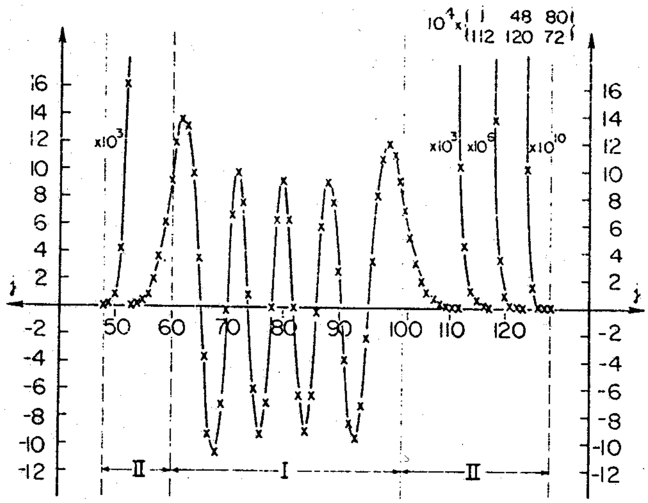

FIG. 3. Functional behavior of the 6j-coefficients $h(j_1) = \begin{Bmatrix} j_1 & 48 & 80 \\ 112 & 120 & 72 \end{Bmatrix}$ $(48 \le j_1 \le 128)$. The evaluation of $h(j_1)$ followed the recursion algorithm described in Sec. 3. The domain of $h(j_1)$ can be divided into a classical and two nonclassical regions (Ref. 4). In the classical region $h(j_1)$ oscillates with slowly varying amplitude; in the nonclassical regions $|h(j_1)|$ monotonically decays to zero.

cursive evaluation of all $f(j_1)$ according to

$$j_1 A(j_1+1) f(j_1+1) + B(j_1) f(j_1) + (j_1+1) A(j_1) f(j_1-1) = 0 \tag{6'}$$

can be performed. But, one should note that such a recursion procedure to generate the quantities $f(j_1)$, $f(j_1+1)$, $f(j_1+2)$, $\cdots$ can be numerically stable only in the direction of *increasing* $f(j_1)$. The semiclassical expressions for $3j$-coefficients,[4] reveal that $f(j_1)$ decreases rapidly to zero at the boundaries of the j_1-domain $j_{1\,\min}$ and $j_{1\,\max}$. This can also be seen from Fig. 1 which illustrates the typical j_1-dependence of $3j$-coefficients. In order to assure numerical stability, the recursive evaluation should therefore proceed from the boundaries $j_{1\,\min}$(left recursion) and $j_{1\,\max}$ (right recursion) of the j_1-domain towards the middle (classical[4,13]) region. The classical region is defined here as the set of j_1-values for which there exists a classical angular momentum vector diagram corresponding to the $3j$-coefficient $f(j_1)$. It is within this region that the typical magnitudes of the $3j$-coefficients $f(j_1)$ are largest.

For the start of the recursion (6′) one observes that $A(j_{1\,\min})=0$ and $A(j_{1\,\max}+1)=0$. The recursion relation at the boundaries $j_{1\,\min}$ and $j_{1\,\max}$ thus becomes

$$B(j_{1\,\min}) f(j_{1\,\min}) + j_{1\,\min} A(j_{1\,\min}+1) f(j_{1\,\min}+1) = 0 \tag{16}$$

and

$$B(j_{1\,\max}) f(j_{1\,\max}) + (j_{1\,\max}+1) A(j_{1\,\max}) f(j_{1\,\max}-1) = 0, \tag{17}$$

i.e., the three term recursion (6′) reduces to two terms. Thus, *one* starting value at each boundary, namely $f(j_{1\,\min})$ and $f(j_{1\,\max})$, is sufficient to start the recursion (6′) in each direction.

Let us now assume that the terminal $6j$-coefficient $f(j_{1\,\min})$ and $f(j_{1\,\max})$ have been given arbitrary values and used to start the recursion (6′). Thus, they are in error by factors c_1 and c_2, respectively. Applications of Eqs. (16) and (17) then yield the quantities $c_1 f(j_{1\,\min})$ and $c_2 f(j_{1\,\max})$. Carrying the recursion further towards the classical regions by means of the linear recursion (6′), the quantities

$c_1 f(j_{1\,\min});\ c_1 f(j_{1\,\min}+1);\ \ldots;\ c_1 f(j_{1\,\mathrm{mid}})$ (left recursion),

$c_2 f(j_{1\,\max});\ c_2 f(j_{1\,\max}-1);\ \ldots;\ c_2 f(j_{1\,\mathrm{mid}})$ (right recursion)

will be generated. The common final j_1-value $j_{1\,\mathrm{mid}}$ for the recursions from left and right should lie within the classical j_1-domain. The recursions from the left and from the right must, however, match at $j_1 = j_{1\,\mathrm{mid}}$, so that we have the condition $c_1 f(j_{1\,\mathrm{mid}}) = c_2 f(j_{1\,\mathrm{mid}})$. We may therefore rescale the left recursion by the factor $c_2 f(j_{1\,\mathrm{mid}})/c_1 f(j_{1\,\mathrm{mid}}) = c_2/c_1$ to get

$$c_2 f(j_{1\,\min});\ c_2 f(j_{1\,\min}+1);\ \ldots;\ c_2 f(j_{1\,\max}-1);\ c_2 f(j_{1\,\max}), \tag{18}$$

i.e., the series of $3j$-coefficients in (1) off by a common factor c_2. To obtain the unknown c_2, we employ the normalization condition (7) which yields the absolute magnitude of c_2. The phase convention

$$\operatorname{sgn}\left\{\begin{pmatrix} j_{1\,\max} & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}\right\} = (-1)^{j_2-j_3-m_1} \tag{19}$$

determines the sign of c_2. Rescaling the series (18) by $1/c_2$ then gives the $6j$-coefficients in (1). It has, hence, been shown that the recursion (6′) can be started with arbitrarily chosen values $c_1 f(j_{1\,\min})$ and $c_2 f(j_{1\,\max})$ to obtain simultaneously all $3j$-coefficients in (1).

Let us consider now the evaluation of the $3j$-coefficients in (2),

$$g(m_2) = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix}, \quad m_{2\,\min} \le m_2 \le m_{2\,\max}, \tag{2'}$$

by means of the recursion equation

$$C(m_2+1) g(m_2+1) + D(m_2) g(m_2) + C(m_2) g(m_2-1) = 0. \tag{9'}$$

The range of allowed m_2-values in (2) is finite, the smallest m_2-value is $m_{2\,\min} = \max\{-j_2, -j_3-m_1\}$ and the largest m_2-value is $m_{2\,\max} = \min\{j_2, j_3-m_1\}$. The functional behavior of $g(m_2)$ resembles that of $f(j_1)$ in that $g(m_2)$ in general falls off to zero at the boundaries $m_{2\,\min}$ and $m_{2\,\max}$ of the m_2-domain (see also Fig. 2). To assure numerical stability, it is necessary to perform the recursion (9′) from both ends of the m_2-domain (left and right recursion). As was the case for (6′) the terminal recursions contain only the two terms

$$D(m_{2\,\min}) g(m_{2\,\min}) + C(m_{2\,\min}+1) g(m_{2\,\min}+1) = 0, \tag{20}$$

$$D(m_{2\,\max}) g(m_{2\,\max}) + C(m_{2\,\max}) g(m_{2\,\max}-1) = 0, \tag{21}$$

since $C(m_{2\,\min}) = 0$ and $C(m_{2\,\max}+1) = 0$. Assuming arbitrary starting values $c_1 g(m_{2\,\min})$ and $c_2 g(m_{2\,\max})$, the recursion by means of (20), (9′), and (21), (9′) yields the two series

$c_1 g(m_{2\,\min});\ c_1 g(m_{2\,\min}+1);\ \ldots;$

$c_1 (m_{2\,\mathrm{mid}})$ (left recursion)

and

$c_2 g(m_{2\,\max});\ c_2 g(m_{2\,\max}-1);\ \ldots;$

$c_2 g(m_{2\,\mathrm{mid}})$ (right recursion)

for some $m_{2\,\mathrm{mid}}$ in the classical m_2-domain of the $3j$-coefficients. To assure that the matching condition $c_1 g(m_{2\,\mathrm{mid}}) = c_2 g(m_{2\,\mathrm{mid}})$ hold, the left recursion may be rescaled by the factor $c_2 g(m_{2\,\mathrm{mid}})/c_1 g(m_{2\,\mathrm{mid}})$. One then gets

$$c_2 g(m_{2\,\min});\ c_2 g(m_{2\,\min}+1);\ \ldots;$$

$$c_2 g(m_{2\,\max}-1);\ c_2 g(m_{2\,\max}) \tag{22}$$

which represents the $3j$-coefficients in (2), scaled by the unknown factor c_2. c_2 is readily determined from the normalization condition (10) together with the phase convention

$$\operatorname{sgn}\left\{\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_{2\,\max} & -m_1-m_{2\,\max}\end{pmatrix}\right\} = (-1)^{j_2-j_3-m_1}. \tag{23}$$

The desired $3j$-coefficients are then obtained after multiplying (22) by $1/c_2$.

Finally, we turn to the recursive evaluation of the series of the $6j$-coefficients in (3)

$$h(j_1) = \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}, \quad j_{1\,\min} \leq j_1 \leq j_{1\,\max}. \tag{3'}$$

The smallest and largest j_1-values are $j_{1\,\min} = \max\{|j_2 - j_3|, |l_2 - l_3|\}$, and $j_{1\,\max} = \min\{j_2+j_3, l_2+l_3\}$. The $6j$-coefficients $h(j_1)$ fall off to zero at the boundaries $j_{1\,\min}$ and $j_{1\,\max}$ as can be seen from the example given in Fig. 3 and is revealed for the general case by the semiclassical expression for $6j$-coefficients.[4,11] Hence, the recursion

$$j_1 E(j_1+1)\,h(j_1+1) + F(j_1)\,h(j_1) + (j_1+1)\,E(j_1)\,h(j_1-1) = 0 \tag{12'}$$

which connects all possible $h(j_1)$ should again proceed simultaneously from the boundaries $j_{1\,\min}$ (left recursion) and $j_{1\,\max}$ (right recursion) towards the middle j_1-domain. For the recursions at the boundaries we have $E(j_{1\,\min}) = 0$ and $E(j_{1\,\max}+1) = 0$. Hence

$$F(j_{1\,\min})\,h(j_{1\,\min}) + j_{1\,\min} E(j_{1\,\min}+1)\,h(j_{1\,\min}+1) = 0 \tag{24}$$

and

$$F(j_{1\,\max})\,h(j_{1\,\max}) + (j_{1\,\max}+1)\,E(j_{1\,\max})\,h(j_{1\,\max}-1) = 0 \tag{25}$$

can be generated recursively for $j_{1\,\mathrm{mid}}$ being chosen to lie within the classical[4,13] j_1-domain. The classical domain of $6j$-coefficients is the domain of all quantum numbers for which there exists a classical angular momentum vector tetrahedron corresponding to the $6j$-coefficient. Within this domain, typical magnitudes of the $6j$-coefficients are largest. The matching condition $c_1 h(j_{1\,\mathrm{mid}}) = c_2 h(j_{1\,\mathrm{mid}})$ is satisfied if the left recursion is rescaled by the factor $c_2 h(j_{1\,\mathrm{mid}})/c_1 h(j_{1\,\mathrm{mid}})$ which gives

$$c_2 h(j_{1\,\min});\ c_2 h(j_{1\,\min}+1);\ \ldots;\ c_2 h(j_{1\,\max}-1);\ c_2 h(j_{1\,\max}).$$

c_2 is determined from the normalization condition (13′) together with the phase convention

$$\operatorname{sgn}\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = (-1)^{j_2+j_3+l_2+l_3}, \tag{27}$$

so that finally all $6j$-coefficients in (3) are evaluated.

IV. ACCURACY AND EFFICIENCY OF RECURSIVE ALGORITHM

We would like to demonstrate now our claim that the recursive algorithm for the evaluation of $3j$- and $6j$-coefficients is numerically accurate for small and large quantum numbers and, in general, more efficient than existing algorithms based on the explicit expressions for these coefficients given by Wigner and Racah. As far as numerical effort is concerned, the advantageous character of a recursive evaluation is quite obvious. To obtain the coupling coefficients in (1), (2), and (3), essentially only the series $A(n)$, $B(n)$ or $C(n)$, $D(n)$ or $E(n)$, $F(n)$, respectively, which enter as coefficients the recursion equations (6), (9), and (12), need to be calculated.

The fact that the recursive algorithm evaluates a whole set of coupling coefficients is often an advantage, for in many problems of angular momentum coupling whole sets of coupling coefficients like (1), (2), or (3) enter. To give an example we may turn to the evaluation of $9j$-coefficients, which are given through the expansion

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \\ j_7 & j_8 & j_9 \end{Bmatrix} = \sum_H (-1)^{2H} H \begin{Bmatrix} H & j_1 & j_9 \\ j_3 & j_6 & j_2 \end{Bmatrix} \begin{Bmatrix} H & j_2 & j_6 \\ j_5 & j_4 & j_3 \end{Bmatrix} \begin{Bmatrix} H & j_9 & j_1 \\ j_7 & j_4 & j_8 \end{Bmatrix}. \tag{28}$$

Evidently three strings of $6j$-coefficients are needed in the course of evaluating this expansion, namely

$$\begin{Bmatrix} H & j_1 & j_9 \\ j_3 & j_6 & j_2 \end{Bmatrix}, \tag{3a}$$

$$\begin{Bmatrix} H & j_2 & j_6 \\ j_5 & j_4 & j_3 \end{Bmatrix}, \tag{3b}$$

$$\begin{Bmatrix} H & j_9 & j_1 \\ j_7 & j_4 & j_8 \end{Bmatrix}. \tag{3c}$$

Furthermore, to obtain the N $9j$-coefficients for all allowed j_3-quantum numbers, it is sufficient to evaluate (3b) and (3c) once and (3a) for all N allowed j_3 values. Hence, to determine the values of $9j$-coefficients for all j_3, only $N+2$ $6j$-recursions have to be performed. These considerations exemplify how strings of coupling coefficients like (1), (2), and (3) naturally enter into the problems of angular momentum coupling.

To answer the important question about the numerical accuracy of the proposed algorithm, a comparison between recursively evaluated coupling coefficients and tabulated values of these coefficients suggests itself. The exact representation of $3j$- and $6j$-coefficients in terms of prime number factors, as given in the table of Rotenberg *et al.*[14] provides the accurate values for these coefficients. In Tables I, II, and III we present a comparison between $3j$- and $6j$-coefficients generated by recursion and those obtained from the tabulation of Rotenberg *et al.* As can be seen, agreement is found for essentially all significant figures provided by the computer representation of numerical constants (i.e., 16 significant digits in the double precision mode on a IBM 360/91).

Perhaps more important is the fact that the recursive algorithm allows the evaluation of coupling coefficients with very large quantum numbers, thus enlarging the realm of coupling coefficients accessible to numerical methods. Since no tabulated values of large quantum number coupling coefficients exist, the accuracy of the recursive algorithm must be demonstrated through a test of its numerical stability. This has been done by carrying out two simultaneous evaluations of $6j$-coefficients for large quantum numbers, the results of which

TABLE I. Accuracy of recursively evaluated 3j-coefficients $\begin{pmatrix} L1 & 9/2 & 7/2 \\ 1 & -7/2 & 5/2 \end{pmatrix}$.

$L1$	Values of 3j-coefficients[a]
1	0.278 886 675 511 3585 (0) I
	0.278 886 675 511 3586 (0) II
2	−0.953 462 589 245 5920 (−1) I
	−9.953 462 589 245 5920 (−1) II
3	−0.674 199 862 463 2420 (−1) I
	−0.674 199 862 463 2420 (−1) II
4	0.153 311 035 167 9666 (0) I
	0.153 311 035 167 9666 (0) II
5	−0.156 446 554 693 6860 (0) I
	−0.156 446 554 693 6859 (0) II
6	0.109 945 041 215 6550 (0) I
	0.109 945 041 215 6550 (0) II
7	−0.553 623 569 313 1718 (−1) I
	−0.553 623 569 313 1718 (−1) II
8	0.179 983 545 113 7785 (−1) I
	0.179 983 545 113 7785 (−1) II

[a] I: Rotenberg *et al.*; II: This paper.

are presented in Table IV. One of the calculations was done in single precision mode (IBM 360/91) which provides 6 significant digits for numerical constants, and the other calculations used double precision with 16 significant digits. Numerical stability is demonstrated since the single precision calculation agrees with the double precision calculation within its full range of significant figures, as is shown for one example in Table IV. It is remarkable that even the small coefficients near the ends of the range are found with the maximum possible relative accuracy.

TABLE II. Accuracy of recursively evaluated 3j-coefficients $\begin{pmatrix} 8 & 15/2 & 13/2 \\ 1 & M & -M-1 \end{pmatrix}$.

M	Values of 3j-coefficients[a]
−15/2	0.209 158 973 288 6152 (−1) I
	0.209 158 973 288 6155 (−1) II
−13/2	0.853 756 555 321 5250 (−1) I
	0.853 756 555 321 5260 (−1) II
−11/2	0.908 295 370 868 6920 (−1) I
	0.908 295 370 868 6930 (−1) II
−9/2	−0.389 054 377 846 4993 (−1) I
	−0.389 054 377 846 4995 (−1) II
−7/2	−0.663 734 970 165 6800 (−1) I
	−0.663 734 970 165 6810 (−1) II
−5/2	−0.649 524 040 528 3890 (−1) I
	−0.649 524 040 528 3900 (−1) II
−3/2	−0.215 894 310 595 4037 (−1) I
	−0.215 894 310 595 4036 (−1) II
−1/2	−0.778 912 711 785 2390 (−1) I
	−0.778 912 711 785 2390 (−1) II
1/2	0.359 764 371 059 5433 (−1) I
	0.359 764 371 059 5431 (−1) II
3/2	0.547 301 500 021 2632 (−1) I
	0.547 301 500 021 2631 (−1) II
5/2	−0.759 678 665 956 7610 (−1) I
	−0.759 678 665 956 7610 (−1) II
7/2	−0.219 224 445 539 8920 (−1) I
	−0.219 224 445 539 8921 (−1) II
9/2	0.101 167 744 280 7722 (0) I
	0.101 167 744 280 7721 (0) II
11/2	0.734 825 726 244 7190 (−1) I
	0.734 825 726 244 7190 (−1) II

[a] Rotenberg *et al.*; II: This work.

TABLE III. Accuracy of recursively evaluated 6j-coefficients $\begin{Bmatrix} L1 & 8 & 7 \\ 13/2 & 15/2 & 15/2 \end{Bmatrix}$.

$L1$	Values of 6j-coefficients[a]
1	0.349 090 513 837 3299 (−1) I
	0.349 090 513 837 3284 (−1) II
2	−0.374 302 503 965 9791 (−1) I
	−0.374 302 503 965 9775 (−1) II
3	0.189 086 639 095 9559 (−1) I
	0.189 086 639 095 9551 (−1) II
4	0.734 244 825 492 8642 (−2) I
	0.734 244 825 492 8610 (−2) II
5	−0.235 893 518 508 1794 (−1) I
	−0.235 893 518 508 1783 (−1) II
6	0.191 347 695 521 5436 (−1) I
	0.191 347 695 521 5427 (−1) II
7	0.128 801 739 772 4172 (−2) I
	0.128 801 739 772 4175 (−2) II
8	−0.193 001 836 629 0526 (−1) I
	−0.193 001 836 629 0531 (−1) II

[a] I: Rotenberg *et al.*; II. This paper.

APPENDIX: DERIVATION OF RECURSION EQUATION FOR 6j-COEFFICIENTS AS SOLUTIONS TO AN EIGENVALUE PROBLEM

The remarkable resemblance between the series of

TABLE IV. Accuracy of recursively evaluated 6j-coefficients $\begin{Bmatrix} L1 & 120 & 120 \\ 112 & 48 & 80 \end{Bmatrix}$.

$L1$	Values of 6j-coefficients[a]
48	0.161 1825 (−8) I
	0.161 1825 (−8) II
56	0.949 0981 (−4) I
	0.949 0977 (−4) II
64	0.964 1119 (−3) I
	0.964 1123 (−3) II
72	0.988 0543 (−3) I
	0.988 0543 (−3) II
80	0.919 9395 (−3) I
	0.919 9396 (−3) II
88	0.918 3130 (−3) I
	0.918 3132 (−3) II
96	0.332 5452 (−3) I
	0.332 5446 (−3) II
104	0.322 0624 (−3) I
	0.322 0624 (−3) II
112	0.115 3951 (−5) I
	0.115 3951 (−5) II
120	0.835 0757 (−10) I
	0.835 0761 (−10) II
128	0.119 3770 (−16) I
	0.119 3771 (−16) II

[a] I: double precision; II: single precision.

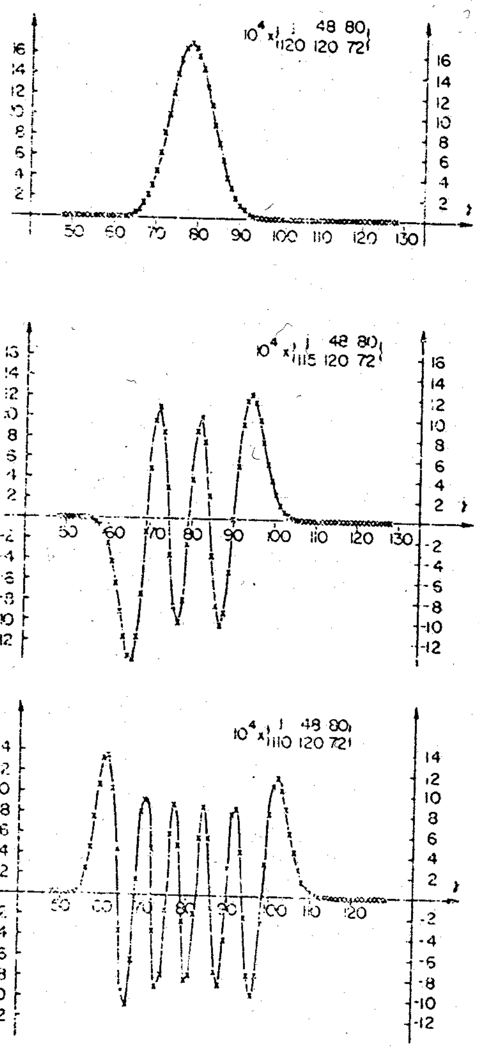

FIG. 4. Comparison of the functional behavior of the $6j$-coefficients $h(j_1)=\begin{Bmatrix} j_1 & 48 & 80 \\ l_1 & 120 & 72 \end{Bmatrix}$ $(48 \le j_1 \le 128)$ evaluated through the recursion algorithm described in Sec. 3. The largest allowed l_1-quantum number is $l_{1\max}=120$. The diagram shows that $l_{1\max}-l_1$ counts the nodes of $h(j_1)$: (a) $l_{1\max}-l_1=0$ (b) $l_{1\max}-l_1=5$; (c) $l_{1\max}-l_1=10$.

$3j$- and $6j$-coefficients in Figs. 1, 2, 3, and bound state eigenfunctions may not have escaped the readers' attention. To carry further a comparison between angular momentum coupling coefficients and eigensolutions of bound state problems we present in Fig. 4 the series of $6j$-coefficients

$$[(2j_1+1)(2l_1+1)]^{1/2} \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}, \quad j_{1\min} \le j_1 \le j_{1\max},$$

for different l_1-values. $j_{1\min}=\max\{|j_2-j_3|, \; |l_2-l_3|\}$ and $j_{1\max}=\min\{j_2+j_3, l_2+l_3\}$ are the smallest and largest values j_1 can assume in order for the $6j$-coefficients not to vanish. It can be seen from Fig. 4 that l_1 takes on the character of a quantum number which counts the nodes $l_{1\max}-l_1$ of the series $(l_{1\max}=\min\{j_2+l_3, \; j_3+l_3\})$. What is the origin of this particular behavior of the coupling coefficients? The answer to this question is that $3j$- and $6j$-coefficients are by definition components of eigenvectors to certain eigenvalue problems. The coupling coefficients in Figs. 1–4 just represent those eigenvectors.

That $3j$-coefficients can be obtained through the diagonalization of certain angular momentum operators has been known since the early days of quantum mechanics. Hence, this will not be demonstrated here, but we may refer the reader to Refs. 5 and 6. However, we will show in the following which eigenvalue problem defines $6j$-coefficients, and will prove that the recursion equations for $6j$-coefficients are a consequence of this eigenvalue problem. The main reason for this algebraic detour is to convince the reader that the recursion equations derived above do indeed follow directly from the definition of the 6-j coefficients.

Let us consider a system composed of four angular momenta $\mathbf{J}_2$, $\mathbf{J}_3$, $\mathbf{L}_2$, and $\mathbf{L}_3$ such that $\mathbf{J}_2+\mathbf{J}_3+\mathbf{L}_2+\mathbf{L}_3=0$. This system may be described by two different *zero* total angular momentum states:

$$|(j_2,j_3)(l_2,l_3)j_1\rangle = \sum_m (-1)^{j_1-m}\,[2j_1+1]^{-1/2} \, |(j_2,j_3)j_1\,m\rangle\,|(l_2,l_3)j_1-m\rangle \tag{A1}$$

and

$$|(j_2,l_3)(l_2,j_3)l_1\rangle = \sum_m (-1)^{l_1-m}[2l_1+1]^{-1/2} \times |(j_2,l_3)l_1 m\rangle\,|(l_2,j_3)l_1-m\rangle. \tag{A2}$$

The transformation matrix element $\langle (j_2,j_3)(l_2,l_3)j_1 | \times (j_2,l_3)(l_2,j_3)l_1\rangle$ defines then the $6j$-coefficient

$$\langle (j_2,j_3)(l_2,l_3)j_1 | (j_2,l_3)(l_2,j_3)l_1\rangle = [(2j_1+1)(2l_1+1)]^{1/2} \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}. \tag{A3}$$

It is a simple exercise in angular momentum algebra to show that this definition is in agreement with the more conventional definition of $6j$-coefficients in terms of $3j$-coefficients.[10] $|(j_2,j_3)(l_2,l_3)j_1\rangle$ and $|(j_2,l_3)(l_2,j_3)l_1\rangle$ are both eigenstates of the angular momentum operators J_2^2, J_3^2, L_2^2, L_3^2, but only the first state is also an eigenfunction of $J_1^2=(\mathbf{J}_2+\mathbf{J}_3)^2$, whereas only the latter is an eigenstate of $L_1^2=(\mathbf{J}_2+\mathbf{L}_3)^2$. From elementary principles of linear algebra it then follows that the columns of $\langle (j_2,j_3)(l_2,l_3)j_1 | (j_2,l_3)(l_2,j_3)l_1\rangle$ are the eigenvectors of the operator L_1^2 in the $|(j_2,j_3)(l_2,l_3)j_1\rangle$-basis.

Let us evaluate L_1^2 in this basis. We first notice that $[\mathbf{J}_2+\mathbf{J}_3+\mathbf{L}_2+\mathbf{L}_3, \; L_1^2]=0$, hence, the application of L_1^2 does not affect the total angular momentum state. We may then express L_1^2 through operators whose action on the intermediate states $|(j_2,j_3)j_1 m\rangle$ and $|(l_2,l_3)j_1-m\rangle$ in (1) are known:

$$L_1^2 = J_2^2 + L_3^2 + J_{2-}L_{3+} + J_{2+}L_{3-} + 2J_{2z}L_{3z}. \tag{A4}$$

We have obviously

$$(J_2^2+L_3^2)\,|(j_2,j_3)(l_2,l_3)j_1\rangle = [j_2(j_2+1)+l_3(l_3+1)]\,|(j_2,j_3)(l_2,l_3)j_1\rangle.$$

The remaining operators in (4) applied to $|(j_2,j_3)(l_2,l_3)j_1\rangle$ give

$$\sum_m \frac{(-1)^{j_1-m}}{[2j_1+1]^{1/2}} \quad \Big\{ \langle (j_2,j_3)j_1 m\,|J_{2-}\; \langle (l_2,l_3)j_1-m\,|L_{3+}$$

$$+\langle (j_2,j_3)j_1 m\,|J_{2+}\langle (l_2,l_3)j_1 - m\,|L_{3-}$$

$$+2\langle (j_2,j_3)j_1 m\,|J_{2z}\langle (l_2,l_3)j_1 - m\,|L_{3z}\Big\}. \quad \text{(A5)}$$

The operators $J_{2-}L_{3+}$, $J_{2+}L_{3-}$ and $J_{2z}L_{3z}$ only couple to states $|(j_2,j_3)j_1'm+1\rangle|(l_2,l_3)j_1''-m-1\rangle\rangle$, $|(j_2,j_3)j_1'm-1\rangle \times|(l_2,l_3)j_1''-m+1\rangle$, and $|(j_2,j_3)j_1'm\rangle|(l_2,l_3)j_1''-m\rangle$ where $j_1'=j_1\pm 1$, 0 and $j_1''=j_1\pm 1$, 0.[15] But, in order that the state (5) carries zero total angular momentum all terms with $j_1'\neq j_1''$ must cancel out, and hence may be disregarded in the following calculation. The matrix elements $\langle (j_2, j_3)j_1 m\,|J_{2-}|(j_2,j_3)j_1'm'\rangle$, $\langle\langle (l_2,l_3)j_1-m\,|L_{3+}|(l_2,l_3)j_1'-m'\rangle$, etc. all split in orientation independent factors $\langle j_1\|J_2\|j_1'\rangle$ and $\langle j_1\|L_3\|j_1'\rangle$ and m-dependent factors (Wigner–Eckart theorem). The m-dependent factors may be obtained from Ref. 15. It should further be noted that the operators $L_{3\pm}$, L_{3z} operate on the second angular momentum l_3 in $|(l_2,l_3)j_1-m\rangle$, whereas the operators $J_{2\pm}$, J_{2z} operate on the first angular momentum j_2 in $|(j_2,j_3)j_1 m\rangle$. This makes it necessary[5] to give negative values to the off-diagonal elements $\langle j_1\|L_3\|j_1\pm 1\rangle$. We obtain then from (5) the expression

$$\sum_m \frac{(-1)^{j_1-m}}{[2j_1+1]^{1/2}}\,\{-\langle j_1-1\|J_2\|j_1\rangle\langle j_1-1\|L_3\|j_1\rangle$$
$$\times[-(j_1-m-1)(j_1-m)\langle (j_2,j_3)j_1-1\;m+1\,|\,\langle (l_2,l_3)j_1-1\;-m-1\,|$$
$$-(j_1+m)(j_1+m-1)\langle (j_2,j_3)j_1-1\;\;m-1\,|\langle (l_2,l_3)j_1-1\;-m+1\,|$$
$$+2(j_1^2-m^2)\langle (j_2,j_3)j_1-1\;\;m\;|\langle (l_2,l_3)j_1-1\;\;-m\,|]$$
$$+\langle j_1\|J_2\|j_1\rangle\langle j_1\|L_3\|j_1\rangle$$
$$\times[(j_1+m+1)(j_1-m)\langle (j_2,j_3)j_1 m+1\,|\,\langle (l_2,l_3)j_1\;\;-m-1\,|$$
$$+(j_1+m)(j_1-m+1)\langle (j_2,j_3)j_1\;m-1\,|\,\langle (l_2,l_3)j_1\;\;-m+1\,|$$
$$-2m^2\,\langle (j_2,j_3)j_1\;\;m\,|\langle (l_2,l_3)j_1\;\;-m\,|]$$
$$-\langle j_1+1\|J_2\|j_1\rangle\langle j_1+1\|L_3\|j_1\rangle$$
$$\times[-(j_1+m+1)(j_1+m+2)\langle (j_2,j_3)j_1+1\;m+1\,|$$
$$\times\langle (l_2,l_3)j_1+1\;\;-m-1\,|$$
$$-(j_1-m+1)(j_1-m+2)\,\langle (j_2,j_3)j_1+1\;m-1\,|$$
$$\times\langle (l_2,l_3)j_1+1\;\;-m+1\,|$$
$$+2[(j_1+1)^2-m^2]\,\langle (j_2,j_3)j_1+1\;m\;\;|\langle (l_2,l_3)j_1+1\;\;-m\,|]\}. \quad \text{(A6)}$$

Collecting terms with equal magnetic quantum numbers leads to the cancellation of all m-dependent prefactors in the sum, except for the phase $(-1)^{-m}$. Carrying out the m-summation gives then

$$2j_1[(2j_1+1)(2j_1-1)]^{1/2}\,\langle j_1-1\|J_2\|j_1\rangle\langle j_1-1\|L_2\|j_1\rangle$$
$$\times\langle (j_2,j_3)(l_2,l_3)j_1-1\,|$$
$$-2j_1(j_1+1)\,\langle j_1\|J_2\|j_1\rangle\langle j_1\|L_3\|j_1\rangle\langle (j_2,j_3)(l_2,l_3)j_1\,|$$
$$+2(j_1+1)[(2j_1+1)(2j_1+3)]^{1/2}$$
$$\times\langle j_1+1\|J_2\|j_1\rangle\langle j_1+1\|L_3\|j_1\rangle\langle (j_2,j_3)\,(l_2,l_3)j_1+1\,| \quad \text{(A7)}$$

and, finally, with the explicit algebraic expression for $\langle j_1\|J_2\|j_1'\rangle$ and $\langle j_1\|L_3\|j_1'\rangle$[5,15]

$$\langle j_1\,|L_1^2|\,j_1-1\rangle=\frac{\{[j_1^2-(j_2-j_3)^2][(j_2+j_3+1)^2-j_1^2][j_1^2-(l_2-l_3)^2][(l_2+l_3+1)-j_1^2]\}^{1/2}}{2j_1[(2j_1-1)(2j_1+1)]^{1/2}}, \quad \text{(A8)}$$

$$\langle j_1\,|L_1^2|\,j_1+1\rangle=\frac{\{[(j_1+1)^2-(j_2-j_3)^2][(j_2+j_3+1)^2-(j_1+1)^2][(j_1+1)^2-(l_2-l_3)^2][(l_2+l_3+1)^2-(j_1+1)^2]\}^{1/2}}{2(j_1+1)[(2j_1+1)(2j_1+3)]^{1/2}}, \quad \text{(A9)}$$

$$\langle j_1\,|L_1^2|\,j_1\rangle=\{j_1(j_1+1)[-j_1(j_1+1)+j_2(j_2+1)+j_3(j_3+1)]+l_2(l_2+1)[j_1(j_1+1)+j_2(j_2+1)-j_3(j_3+1)]+l_3(l_3+1) \quad \text{(A10)}$$
$$\times[j_1(j_1+1)-j_2(j_2+1)+j_3(j_3+1)]\}[2j_1(j_1+1)]^{-1}$$

These matrix elements show that L_1^2 is a symmetric, tridiagonal matrix. L_1^2 is readily diagonalized and must have real, positive eigenvalues. However, such a diagonalization procedure would provide redundant results (eigenvectors and eigenvalues), since the eigenvalues of L_1^2 are known to be $l_1(l_1+1)$ with $l_1=l_{1\,\max}-n$, $n=0,1,2,\ldots$. Hence, it is sufficient to solve the system of homogeneous equations

$$[L_1^2-l_1(l_1+1)]\mathbf{x}=0. \quad \text{(A11)}$$

Because of the tridiagonal form of L_1^2, this leads to three-term recursion equations for the components of **x**. These equations are identical with the recursion equations derived above for 6j-coefficients. The solution of these recursion equations therefore corresponds directly to the solution of the eigenvalue problem (11).

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