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

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Algorithms are developed for the exact evaluation of the 3j-coefficients of Wigner and the 6j-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 3j- and 6j-coefficients are based on the explicit expressions of Wigner and Racah. Calculations involving the quantum mechanical coupling of angular momenta often require the evaluation of whole strings of coupling coefficients of the kind:

\[ \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \quad \text{for all allowed } j_1, \]

\[ \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 - m_1 & m_3 \end{pmatrix} \quad \text{for all allowed } m_2, \]

\[ \begin{pmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{pmatrix} \quad \text{for all allowed } j_1. \]

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 3j- and 6j-coefficients. The algorithms, furthermore, are inapplicable for large angular momentum values (~100\hbar) which, for example, occur frequently in problems of molecular dynamics.

We have now numerically tested an algorithm for the evaluation of 3j- and 6j-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 3j- and 6j-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 3j- and 6j-coefficients will be made available.

Besides 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, it is shown that the recursion equations for 3j- and 6j-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. RECURRENCE RELATIONSHIPS FOR 3J- AND 6J-COEFFICIENTS

The recursion relationships which connect the angular momentum coupling coefficients in (1), (2), and (3) have been previously reported. Condon and Shortley derived the recursion relationships for the 3j-coefficients in (1), and Rose presented the recursion relationship for the 3j-coefficients in (2). In both instances the recursion relationships were obtained from the interpretation of the strings of 3j-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 3j-coefficients. The recursion equation for the 6j-coefficients in (3) have been given by Yutis et al. 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 Yutis et al., we present a unified derivation for these three recursion equations. This derivation starts off from three basic sum rules which hold for 3j- and 6j-coefficients.

Let us first consider the 3j-coefficients in (1). For the 3j-coefficients there is an identity:

\[ (-1)^{l_2 + l_3 + m_1 + m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1' & m_2' & m_3' \end{pmatrix} \]
\[
\begin{aligned}
&= \sum_{l_3} (2l_3 + 1) \left( \frac{j_1 l_2 l_3}{m_1 m_2 m_3} \right) \left( \frac{l_1'}{m_1'} - \frac{l_2'}{m_2'} - \frac{l_3'}{m_3'} \right)
\end{aligned}
\]

\[
\times \left\{ \frac{j_1 j_2 j_3}{l_1 l_2 l_3} \right\}.
\]

(4)

For \( l_1 = \frac{1}{2}, \ l_2 = j_2 + \alpha, \) and \( m_1 = \beta (\alpha, \beta = \pm \frac{1}{2}) \) this identity reduces to the three term recursion relationship

\[
\begin{aligned}
&= \sum_{l_3} (2l_3 + 1) \left( \frac{j_1 j_2 j_3}{m_1 m_2 m_3} \right) \left( \frac{1}{2} j_3 + \alpha \right)
\end{aligned}
\]

\[
\times \left\{ \frac{j_1 j_2 j_3}{l_1 l_2 l_3} \right\}.
\]

which connects the 3j-coefficients

\[
\left( \frac{j_1 j_2 \frac{1}{2} j_3 + \alpha}{m_1 m_2 m_3} \right), \ \left( \frac{j_1 j_2 j_3}{m_1 m_2 m_3} \right)
\]

and

\[
\left( \frac{j_1 j_2 \frac{1}{2} j_3 + \alpha}{m_1 m_2 m_3} \right).
\]

The factors multiplying these 3j-coefficients in Eq. (4) are 3j- and ij-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 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

\[
\begin{aligned}
&= - \left\{ \frac{1}{2} j_2 + \frac{1}{2} j_3 + \frac{1}{2} \right\}, \int \\
&= \left\{ - \frac{1}{2} j_2 + \frac{1}{2} j_3 - \frac{1}{2} \right\}, \int
\end{aligned}
\]

\[
\times \left\{ \frac{j_1 j_2 j_3}{m_1 m_2 m_3} \right\}.
\]

(5a)

\[
\begin{aligned}
&= - \left\{ \frac{1}{2} j_2 - \frac{1}{2} j_3 + \frac{1}{2} \right\}, \int \\
&= \left\{ \frac{1}{2} j_2 + \frac{1}{2} j_3 - \frac{1}{2} \right\}, \int
\end{aligned}
\]

\[
\times \left\{ \frac{j_1 j_2 j_3}{m_1 m_2 m_3} \right\}.
\]

(5b)

\[
\begin{aligned}
&= - \left\{ \frac{1}{2} j_2 + \frac{1}{2} j_3 + \frac{1}{2} \right\}, \int \\
&= - \left\{ \frac{1}{2} j_2 - \frac{1}{2} j_3 - \frac{1}{2} \right\}, \int
\end{aligned}
\]

\[
\times \left\{ \frac{j_1 j_2 j_3}{m_1 m_2 m_3} \right\}.
\]

(5c)

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

\[
\begin{aligned}
&= \left\{ \frac{1}{2} j_2 - \frac{1}{2} j_3 - \frac{1}{2} \right\}, \int \\
&= \left\{ \frac{1}{2} j_2 + \frac{1}{2} j_3 - \frac{1}{2} \right\}, \int
\end{aligned}
\]

\[
\times \left\{ \frac{j_1 j_2 j_3}{m_1 m_2 m_3} \right\}.
\]

(6a)

where

\[
\begin{aligned}
&= \left\{ \frac{1}{2} j_2 - \frac{1}{2} j_3 - \frac{1}{2} \right\}, \int \\
&= \left\{ \frac{1}{2} j_2 + \frac{1}{2} j_3 - \frac{1}{2} \right\}, \int
\end{aligned}
\]

\[
\times \left\{ \frac{j_1 j_2 j_3}{m_1 m_2 m_3} \right\}.
\]

(6b)

\[
\begin{aligned}
&= \left\{ \frac{1}{2} j_2 - \frac{1}{2} j_3 - \frac{1}{2} \right\}, \int \\
&= \left\{ \frac{1}{2} j_2 + \frac{1}{2} j_3 - \frac{1}{2} \right\}, \int
\end{aligned}
\]

\[
\times \left\{ \frac{j_1 j_2 j_3}{m_1 m_2 m_3} \right\}.
\]

(6c)

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

\[
\sum_{l_1} (2l_1 + 1) \left( \frac{j_1 j_2 j_3}{m_1 m_2 m_3} \right)^2 = 1,
\]

(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 that the identity

\[
\begin{aligned}
&= \sum_{m} (-1)^{m+1} \left( \frac{j_1 l_2 l_3}{m_1 m_2 m_3} \right) \left( \frac{l_1 l_2 l_3}{m_2 m_3} \right)
\end{aligned}
\]

\[
\times \left\{ \frac{j_1 j_2 j_3}{m_1 m_2 m_3} \right\}.
\]

(8)

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 \( l_2 = j_2 + \alpha (\alpha, \beta = \pm \frac{1}{2}) \) gives the three term recursion relationship

\[
\begin{align*}
\left( j_1 \ j_2 \ j_3 \right)_{m_1 \ m_2 \ m_3} &= \sum_{m = m_3 - 1/2}^{m_3 + 1/2} (-1)^{m} \left( j_1 \ j_3 + \beta \ j_2 + \alpha \right) \\
&\times \left( \frac{1}{2} \ j_2 \ j_3 + \alpha \right) \left( \frac{1}{2} \ j_3 + \beta \ j_2 + \alpha \right) \\
\end{align*}
\]

(8')

which connects the 3j-coefficients

\[
\left( j_1 \ j_2 + \alpha \ j_3 + \beta \right)_{\left( m_1 \ m_2 + \frac{1}{2} \ m_3 - \frac{1}{2} \right)}, \left( j_1 \ j_3 \ j_2 \right)_{\left( m_1 \ m_2 \ m_3 \right)}
\]

and

\[
\left( j_1 \ j_2 + \alpha \ j_3 + \beta \right)_{\left( m_1 \ m_2 - \frac{1}{2} \ m_3 + \frac{1}{2} \right)}.
\]

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)

\[
\begin{align*}
C(m_2 + 1)
\left( j_1 \ j_2 \ j_3 \right)_{\left( m_1 \ m_2 + 1 \ m_3 - 1 \right)} + D(m_2)
\left( j_1 \ j_2 \ j_3 \right)_{\left( m_1 \ m_2 \ m_3 \right)} \\
+ C(m_2)
\left( j_1 \ j_2 \ j_3 \right)_{\left( m_1 \ m_2 - 1 \ m_3 + 1 \right)} &= 0
\end{align*}
\]

(9a)

where

\[
\begin{align*}
C(m_2) &= \left[ (j_2 - m_2 + 1)(j_2 + m_2)(j_2 + m_3 + 1)(j_3 - m_3) \right]^{1/2}, \\
D(m_2) &= j_2(j_2 + 1) + j_3(j_3 + 1) - j_1(j_1 + 1) + 2m_2m_3.
\end{align*}
\]

(9b)

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

\[
\sum_{m_2} (2j_1 + 1) \left( j_1 \ j_2 \ j_3 \right)_{\left( m_1 \ m_2 \ m_3 \right)} = 1
\]

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 Diederich—Elliot identity \(^{11}\) serves as the starting point:

\[
\begin{align*}
\left( j_1 \ j_2 \ j_3 \right)_{\left( l_1 \ l_2 \ l_3 \right)} &= \sum_{\lambda} (-1)^{\lambda} \left( j_1 \ j_2 \ j_3 \right)_{\left( l_1 \ l_2 \ l_3 \right)} \left( j_1 \ j_2 \ j_3 \right)_{\left( l_1 \ l_2 \ l_3 \right)} \\
&= \sum_{\lambda} (-1)^{\lambda} \left( j_1 \ j_2 \ j_3 \right)_{\left( l_1 \ l_2 \ l_3 \right)} \left( j_1 \ j_2 \ j_3 \right)_{\left( l_1 \ l_2 \ l_3 \right)} \\
\end{align*}
\]

(11)

\[
\phi_4 = j_1 + j_2 + j_3 + l_1 + l_2 + l_3 + l_1^2 + l_2^2 + l_3^2 + \lambda.
\]

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

\[
\begin{align*}
\left( j_1 \ j_2 \ j_3 \right)_{\left( l_1 \ l_2 \ l_3 \right)} &= \sum_{\lambda = l_1 - 1/2}^{l_1 + 1/2} (-1)^{\lambda} \left( j_1 \ j_2 \ j_3 \right)_{\left( l_1 \ l_2 \ l_3 \right)} \left( j_1 \ j_2 \ j_3 \right)_{\left( l_1 + \frac{1}{2} \ l_2 \ l_3 \right)} \\
&= \sum_{\lambda = l_1 - 1/2}^{l_1 + 1/2} (-1)^{\lambda} \left( j_1 \ j_2 \ j_3 \right)_{\left( l_1 \ l_2 \ l_3 \right)} \left( j_1 \ j_2 \ j_3 \right)_{\left( l_1 + \frac{1}{2} \ l_2 \ l_3 \right)} \\
&= \sum_{\lambda = l_1 - 1/2}^{l_1 + 1/2} (-1)^{\lambda} \left( j_1 \ j_2 \ j_3 \right)_{\left( l_1 \ l_2 \ l_3 \right)} \left( j_1 \ j_2 \ j_3 \right)_{\left( l_1 + \frac{1}{2} \ l_2 \ l_3 \right)} \\
\end{align*}
\]

(11')

which connects the 6j-coefficients

\[
\left( j_1 \ j_2 + \alpha \ j_3 + \beta \right)_{\left( l_1 - \frac{1}{2} \ l_2 \ l_3 \right)}, \left( j_1 \ j_3 \ j_2 \right)_{\left( l_1 \ l_2 \ l_3 \right)}
\]

and

\[
\left( j_1 \ j_2 + \alpha \ j_3 + \beta \right)_{\left( l_1 + \frac{1}{2} \ l_2 \ l_3 \right)}.
\]

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

\[
\begin{align*}
&j_1E(l_1 + 1) \left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{array} \right\} + F(j_1) \left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{array} \right\} \\
&+ (j_1 + 1)E(l_1) \left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{array} \right\} = 0
\end{align*}
\]

(12a)

where

\[
\begin{align*}
F(j_1) &= \left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{array} \right\} \left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{array} \right\} \\
&= \left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{array} \right\} \left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{array} \right\}
\end{align*}
\]

(12b)

Recursion equation (12) together with the normalization condition

\[
\sum_{l_1} (2j_1 + 1)(2l_1 + 1) \left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{array} \right\}^2 = 1
\]

(13')

is sufficient to determine except 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

\[
\sum_{l_1} (2j_1 + 1)(2l_1 + 1) \left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{array} \right\} \left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{array} \right\} = 5_{11} \frac{1}{2}
\]

(13)
corresponding derivations is explained through the existence of an asymptotic relationship between $3j$- and $6j$-coefficients:

$$\begin{align*}
\frac{f(j_1 \ j_2 \ j_3)}{m_1 \ m_2 \ m_3} &= \lim_{R \to \infty} (-1)^{2j_1 + j_2} \left[ (2I_1 + 2R + 1)^{1/2} \right. \\
&\left. \times \begin{bmatrix} j_1 & j_2 & j_3 \\ I_1 + R & I_2 + R & I_3 + R \end{bmatrix} \right]
\end{align*}$$

(15)

where $I_2 - I_1 = m_1$, $I_3 - I_2 = m_2$, and $I_4 - I_3 = m_3$. In fact, Eq. (6) follows from Eq. (12) by taking the asymptotic limit letting $I_1$, $I_2$, and $I_3$ go to infinity, whereas Eq. (9) follows from Eq. (12) by letting $j_1$, $j_2$, and $I_1$ 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

$$f(j_1) = \frac{(j_1 \ j_2 \ j_3)}{m_1 \ m_2 \ m_3}, \quad j_{1\min} \leq j_1 \leq j_{1\max}$$

(1)

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

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

Once proper starting values have been given, the re-
cursive evaluation of all $f(j_1)$ according to
\[ j_1 A(j_1 + 1) f(j_1 + 1) + 0 = 0 \]
\[(6') \]
can be performed. But, one should note that such a recursion procedure to generate the quantities $f(j_1)$, $f(j_1 + 1)$, $f(j_1 + 2)$, ... can be numerically stable only in the direction of increasing $f(j_1)$. The semicircular expressions for $3j$-coefficients, reveal that $f(j_1)$ decreases rapidly to zero at the boundaries of the $j_1$-domain $j_1\text{min}$ and $j_1\text{max}$. 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 $j_1\text{min}$ (left recursion) and $j_1\text{max}$ (right recursion) of the $j_1$-domain towards the middle (classical) 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 $A(j_1\text{min}) = 0$ and $A(j_1\text{max} + 1) = 0$. The recursion relation at the boundaries $j_1\text{min}$ and $j_1\text{max}$ thus becomes
\[ B(j_1\text{min}) f(j_1\text{min}) + j_1\text{min} A(j_1\text{min} + 1) f(j_1\text{min} + 1) = 0 \]
\[(16)\]
and
\[ B(j_1\text{max}) f(j_1\text{max}) + j_1\text{max} A(j_1\text{max} + 1) f(j_1\text{max} + 1) = 0, \]
\[(17)\]
i.e., the three term recursion (6') reduces to two terms. Thus, one starting value at each boundary, namely $f(j_1\text{min})$ and $f(j_1\text{max})$, is sufficient to start the recursion (6') in each direction.

Let us now assume that the terminal $6j$-coefficient $f(j_1\text{min})$ and $f(j_1\text{max})$ 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 $c_1 f(j_1\text{min})$ and $c_2 f(j_1\text{max})$. Carrying the recursion further towards the classical regions by means of the linear recursion (6'), the quantities
\[ c_1 f(j_1\text{min}); c_1 f(j_1\text{min} + 1); \ldots; c_1 f(j_1\text{mid}); \]
\[ c_2 f(j_1\text{max}); c_2 f(j_1\text{max} - 1); \ldots; c_2 f(j_1\text{max}) \]
(18)
will be generated. The common final $j_1$-value $j_1\text{mid}$ 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 $j_1 = j_1\text{mid}$, so that we have the condition $c_1 f(j_1\text{mid}) = c_2 f(j_1\text{mid})$. We may therefore rescale the left recursion by the factor $c_2 f(j_1\text{mid})/c_1 f(j_1\text{mid}) = c_2/c_1$ to get
\[ c_2 f(j_1\text{mid}); c_2 f(j_1\text{mid} + 1); \ldots; c_2 f(j_1\text{max}) - 1); c_2 f(j_1\text{max}) \]
(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
\[ \text{sgn} \left( \begin{array}{ccc} j_1\text{max} & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{array} \right) = (-1)^{j_1 - j_2 - m_1} \]
\[(19)\]
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 $c_1 f(j_1\text{mid})$ and $c_2 f(j_1\text{max})$ to obtain simultaneously all $3j$-coefficients in (1).

Let us consider now the evaluation of the $3j$-coefficients in (2),
\[ g(m_2) = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}, \quad m_2\text{min} \leq m_2 \leq m_2\text{max}, \]
\[(2')\]
by means of the recursion equation
\[ C(m_2 + 1) g(m_2 + 1) + D(m_2) g(m_2) + C(m_2) g(m_2 - 1) = 0. \]
\[(9')\]
The range of allowed $m_3$-values in (2) is finite, the smallest $m_3$-value is $m_3\text{min} = \max(-j_1, -j_2 - m_1)$ and the largest $m_3$-value is $m_3\text{max} = \min(j_1, j_2 - m_1)$. 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 $m_2\text{min}$ and $m_2\text{max}$ 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 $m_3$-domain (left and right recursion). As was the case for (6') the terminal recursions contain only the two terms
\[ D(m_2\text{min}) g(m_2\text{min}) + C(m_2\text{min} + 1) g(m_2\text{min} + 1) = 0, \]
\[(20)\]
\[ D(m_2\text{max}) g(m_2\text{max}) + C(m_2\text{max} + 1) g(m_2\text{max} + 1) = 0, \]
\[(21)\]
since $C(m_2\text{min}) = 0$ and $C(m_2\text{max} + 1) = 0$. Assuming arbitrary starting values $c_1 g(m_2\text{min})$ and $c_2 g(m_2\text{max})$, the recursion by means of (20), (9'), and (21), (9') yields the two series
\[ c_1 g(m_2\text{min}) \ldots; \]
\[ c_1 g(m_2\text{min} + 1) \ldots; \]
\[ c_2 g(m_2\text{max}) \ldots; \]
\[ c_2 g(m_2\text{max} - 1) \ldots; \]
\[ c_2 g(m_2\text{max}) \]
\[(22)\]
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
\[
\text{sgn} \left\{ \begin{array}{ccc}
j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \\
- m_1 & - m_2 & m_3
\end{array} \right\} = (-1)^{j_3-j_1-m_1},
\]
(23)
The desired 3j-coefficients are then obtained after multiplying (22) by 1/c_0.

Finally, we turn to the recursive evaluation of the series of the 6j-coefficients in (3)
\[
h(j_1) = \begin{pmatrix} j_1 & j_2 & j_3 \\ i_1 & i_2 & i_3 \end{pmatrix}, \quad j_1 \leq i_1 \leq j_1,
\]
(3')
The smallest and largest j_1-values are \( j_{1,\text{min}} = \max \{ j_2 - i_1, 0 \} \), and \( j_{1,\text{max}} = j_1 + 1 \). The 6j-coefficients \( h(j_1) \) fall off to zero at the boundaries \( j_{1,\text{min}} \) and \( j_{1,\text{max}} \) 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. Hence, the recursion
\[
j_1 E(j_1 + 1) h(j_1 + 1) + F(j_1) h(j_1) + (j_1 + 1) E(j_1) h(j_1 - 1) = 0
\]
(12)
which connects all possible \( h(j_1) \) should again proceed simultaneously from the boundaries \( j_{1,\text{min}} \) (left recursion) and \( j_{1,\text{max}} \) (right recursion) towards the middle \( j_1 \)-domain. For the recursions at the boundaries we have \( E(j_{1,\text{min}}) = 0 \) and \( E(j_{1,\text{max}} + 1) = 0 \). Hence
\[
E(j_{1,\text{min}}) h(j_{1,\text{min}}) + j_{1,\text{min}} E(j_{1,\text{min}} + 1) h(j_{1,\text{min}} + 1) = 0
\]
(24) and
\[
E(j_{1,\text{max}}) h(j_{1,\text{max}}) + (j_{1,\text{max}} + 1) E(j_{1,\text{max}} + 1) h(j_{1,\text{max}} - 1) = 0
\]
(25)
can be generated recursively for \( j_{1,\text{min}} \) 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 \( c_1 h(j_{1,\text{min}}) = c_2 h(j_{1,\text{max}}) \) is satisfied if the left recursion is rescaled by the factor \( c_1 h(j_{1,\text{min}})/c_2 h(j_{1,\text{max}}) \) which gives
\[
c_2 h(j_{1,\text{min}}); c_2 h(j_{1,\text{min}} - 1); \ldots; c_2 h(j_{1,\text{max}} - 1); c_2 h(j_{1,\text{max}}).
\]
(26) is determined from the normalization condition (13') together with the phase convention
\[
\text{sgn} \left\{ \begin{array}{ccc}
j_1 & j_2 & j_3 \\ i_1 & i_2 & i_3 \end{array} \right\} = (-1)^{j_3-j_1-m_1},
\]
(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 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
\[
\begin{pmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \\ j_7 & j_8 & j_9 \end{pmatrix} = \sum_H (-1)^{j_H} \begin{pmatrix} H & j_1 & j_2 \\ j_3 & j_4 & j_5 \\ j_6 & j_7 & j_8 \end{pmatrix} \begin{pmatrix} H & j_1 & j_2 \\ j_3 & j_4 & j_5 \\ j_6 & j_7 & j_8 \end{pmatrix}
\]
(28)
Evidently three strings of 6j-coefficients are needed in the course of evaluating this expansion, namely
\[
\begin{pmatrix} H & j_1 & j_2 \\ j_3 & j_4 & j_5 \end{pmatrix}
\]
(3a)
\[
\begin{pmatrix} H & j_1 & j_2 \\ j_3 & j_4 & j_5 \end{pmatrix}
\]
(3b)
\[
\begin{pmatrix} H & j_1 & j_2 \\ j_3 & j_4 & j_5 \end{pmatrix}
\]
(3c)
Furthermore, to obtain the \( N \) 9j-coefficients for all allowed \( j_1 \)-quantum numbers, it is sufficient to evaluate (3b) and (3c) once and (3a) for all \( N \) allowed \( j_1 \) values. Hence, to determine the values of 9j-coefficients for all \( j_1 \), 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., 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
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

### Table I. Accuracy of recursively evaluated 3j-coefficients

| L | Values of 3j-coefficients
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.278 886 675 511 585 (0) I</td>
</tr>
<tr>
<td>1</td>
<td>0.278 886 675 511 586 (0) II</td>
</tr>
<tr>
<td>2</td>
<td>-0.953 462 589 245 5920 (-1) I</td>
</tr>
<tr>
<td>3</td>
<td>-0.953 462 589 245 5920 (-1) II</td>
</tr>
<tr>
<td>4</td>
<td>-0.674 199 862 463 2420 (-1) I</td>
</tr>
<tr>
<td>5</td>
<td>-0.674 199 862 463 2420 (-1) II</td>
</tr>
<tr>
<td>6</td>
<td>0.153 373 316 579 6336 (0) I</td>
</tr>
<tr>
<td>7</td>
<td>0.153 373 316 579 6336 (0) II</td>
</tr>
<tr>
<td>8</td>
<td>-0.156 446 536 693 6860 (0) I</td>
</tr>
<tr>
<td>9</td>
<td>-0.156 446 536 693 6860 (0) II</td>
</tr>
<tr>
<td>10</td>
<td>0.109 315 411 215 5950 (0) I</td>
</tr>
<tr>
<td>11</td>
<td>0.109 315 411 215 5950 (0) II</td>
</tr>
<tr>
<td>12</td>
<td>0.553 263 569 313 7378 (-1) I</td>
</tr>
<tr>
<td>13</td>
<td>0.553 263 569 313 7378 (-1) II</td>
</tr>
<tr>
<td>14</td>
<td>0.179 934 545 113 7785 (-1) I</td>
</tr>
<tr>
<td>15</td>
<td>0.179 934 545 113 7785 (-1) II</td>
</tr>
</tbody>
</table>

*1: Rotenberg et al.; II: This paper.

### Table II. Accuracy of recursively evaluated 3j-coefficients

| M | Values of 3j-coefficients
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.209 587 823 288 6135 (-1) I</td>
</tr>
<tr>
<td>1</td>
<td>0.209 587 823 288 6135 (-1) II</td>
</tr>
<tr>
<td>2</td>
<td>0.653 756 555 321 5250 (-1) I</td>
</tr>
<tr>
<td>3</td>
<td>0.653 756 555 321 5250 (-1) II</td>
</tr>
<tr>
<td>4</td>
<td>0.908 293 370 658 6820 (-1) I</td>
</tr>
<tr>
<td>5</td>
<td>0.908 293 370 658 6820 (-1) II</td>
</tr>
<tr>
<td>6</td>
<td>0.389 654 327 346 4989 (-1) I</td>
</tr>
<tr>
<td>7</td>
<td>0.389 654 327 346 4989 (-1) II</td>
</tr>
<tr>
<td>8</td>
<td>0.663 734 976 165 6396 (-1) I</td>
</tr>
<tr>
<td>9</td>
<td>0.663 734 976 165 6396 (-1) II</td>
</tr>
<tr>
<td>10</td>
<td>0.619 524 916 228 3829 (-1) I</td>
</tr>
<tr>
<td>11</td>
<td>0.619 524 916 228 3829 (-1) II</td>
</tr>
<tr>
<td>12</td>
<td>0.215 894 310 595 4037 (-1) I</td>
</tr>
<tr>
<td>13</td>
<td>0.215 894 310 595 4037 (-1) II</td>
</tr>
<tr>
<td>14</td>
<td>0.778 912 711 785 2390 (-1) I</td>
</tr>
<tr>
<td>15</td>
<td>0.778 912 711 785 2390 (-1) II</td>
</tr>
<tr>
<td>16</td>
<td>0.359 764 371 059 5433 (-1) I</td>
</tr>
<tr>
<td>17</td>
<td>0.359 764 371 059 5433 (-1) II</td>
</tr>
<tr>
<td>18</td>
<td>0.547 301 509 021 2632 (-1) I</td>
</tr>
<tr>
<td>19</td>
<td>0.547 301 509 021 2632 (-1) II</td>
</tr>
<tr>
<td>20</td>
<td>0.755 678 685 956 7610 (-1) I</td>
</tr>
<tr>
<td>21</td>
<td>0.755 678 685 956 7610 (-1) II</td>
</tr>
<tr>
<td>22</td>
<td>0.219 224 445 539 8920 (-1) I</td>
</tr>
<tr>
<td>23</td>
<td>0.219 224 445 539 8920 (-1) II</td>
</tr>
<tr>
<td>24</td>
<td>0.101 167 741 250 7722 (0) I</td>
</tr>
<tr>
<td>25</td>
<td>0.101 167 741 250 7722 (0) II</td>
</tr>
</tbody>
</table>

*1: Rotenberg et al.; II: This work.

### Table III. Accuracy of recursively evaluated 6j-coefficients

| L | Values of 6j-coefficients
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.349 090 513 837 3299 (-1) I</td>
</tr>
<tr>
<td>2</td>
<td>0.349 090 513 837 3284 (-1) II</td>
</tr>
<tr>
<td>3</td>
<td>-0.374 302 503 965 9791 (-1) I</td>
</tr>
<tr>
<td>4</td>
<td>-0.374 302 503 965 9775 (-1) II</td>
</tr>
<tr>
<td>5</td>
<td>0.189 086 639 895 9599 (-1) I</td>
</tr>
<tr>
<td>6</td>
<td>0.189 086 639 895 9581 (-1) II</td>
</tr>
<tr>
<td>7</td>
<td>0.734 244 825 492 8642 (-2) I</td>
</tr>
<tr>
<td>8</td>
<td>0.734 244 825 492 8680 (-2) II</td>
</tr>
<tr>
<td>9</td>
<td>-0.235 939 518 508 1794 (-1) I</td>
</tr>
<tr>
<td>10</td>
<td>-0.235 939 518 508 1733 (-1) II</td>
</tr>
<tr>
<td>11</td>
<td>0.191 347 695 521 5436 (-1) I</td>
</tr>
<tr>
<td>12</td>
<td>0.191 347 695 521 5427 (-1) II</td>
</tr>
<tr>
<td>13</td>
<td>0.128 801 739 772 4172 (-2) I</td>
</tr>
<tr>
<td>14</td>
<td>0.128 801 739 772 4172 (-2) II</td>
</tr>
<tr>
<td>15</td>
<td>-0.193 001 836 629 0235 (-1) I</td>
</tr>
<tr>
<td>16</td>
<td>-0.193 001 836 629 0231 (-1) II</td>
</tr>
</tbody>
</table>

*1: Rotenberg et al.; II: This paper.

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.

### Appendix: Derivation of Recursion Equation for 7j-coefficients as Solutions to an Eigenvalue Problem

The remarkable resemblance between the action of
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 $6j$-coefficients.

Let us consider a system composed of four angular momenta $J_2$, $J_3$, $L_2$, and $L_3$ such that $J_2 + J_3 + L_2 + L_3 = 0$. This system may be described by two different zero total angular momentum states:

$$|J_2(J_3)(L_2)(L_3)| = \sum_m (-1)^{J_3+m} [2J_3 + 1]^{1/2} \langle J_3 | J_3 \rangle_{J_1} m \langle L_2 | L_3 | J_3 - m \rangle$$  \hspace{1cm} (A1)

and

$$|J_2(L_3)(J_3)| = \sum_m (-1)^{J_3-m} [2J_3 + 1]^{1/2} \times |J_2 | L_3 | J_3 \rangle m \langle L_2 | J_3 | J_3 - m \rangle.$$ \hspace{1cm} (A2)

The transformation matrix element $\langle J_2, J_3 | L_2, L_3 | J_3 \rangle$ defines then the $6j$-coefficient

$$\langle J_2, J_3 | L_2, L_3 | J_3 \rangle = \frac{[2J_3 + 1]^{1/2} \langle J_2 | J_3 \rangle L_2 \langle L_2 | J_3 \rangle L_3} {\begin{vmatrix} J_2 & J_3 & \frac{1}{2} \\ L_2 & L_3 & \frac{1}{2} \end{vmatrix}}.$$ \hspace{1cm} (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,$^{10}$ $|J_2(J_3)(L_2)(L_3)|$ and $|J_2(L_3)(J_3)|$ 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 $J_3^2 = (J_2 + J_3)^2$, whereas the latter is only an eigenstate of $L_1^2 = (L_2 + L_3)^2$. From elementary principles of linear algebra it then follows that the columns of $\langle J_2, J_3 | L_2, L_3 | J_3 \rangle$ and $\langle L_2, L_3 | J_3 \rangle$ are the eigenvectors of the operator $L_1^2$ in the $|J_2 | J_3 \rangle$, $|L_2 | L_3 \rangle$-basis.

Let us evaluate $L_1^2$ in this basis. We first notice that $[J_2^2, J_3^2 + L_2^2 + L_3^2] = 0$, 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 $|J_2, J_3 \rangle \langle J_2, J_3 | L_2, L_3 \rangle$ and $|L_2, L_3 \rangle \langle L_2, L_3 | J_3 \rangle$ in (1) are known:

$$L_1^2 = J_2^2 - L_2^2 + J_3^2 - L_3^2 + 2J_2 J_3.$$ \hspace{1cm} (A4)

We have obviously

$$(J_2^2 + L_2^2) |J_2(J_3)(L_2)(L_3)| = \langle J_2(j_2 + 1 + l_2(l_2 + 1)) |J_2, J_3| L_2, L_3 \rangle.$$ \hspace{1cm} (A5)

The remaining operators in (4) applied to $|J_2(J_3)(L_2)(L_3)|$ give

$$\sum_{m} (-1)^{J_3-m} [2J_2 + 1]^{1/2} \langle J_2 | J_3 \rangle m | J_2^2, \langle L_2 | L_3 | J_3 - m \rangle | L_3.$$
The operators \( J_{2s}, L_{2s}, J_{2s} L_{2s}, \) and \( J_{2s} L_{2s}^* \) only couple to states \( |(j_s,j_s)j_s(m+1)\rangle, |(j_s,j_s)j_s(m)\rangle, \) \( |(j_s,j_s)j_s(m-1)\rangle, \) and \( |(j_s,j_s)j_s(m)\rangle \) \( |(l_s, l_s)j_s(m)\rangle \) where \( j_s = j_s \pm 1, 0 \) and \( j_s^* = j_s \pm 1, 0. \) In order that the state (5) carries zero total angular momentum all terms with \( j_s^* \neq j_s \) must cancel out, and hence may be disregarded in the following calculation. The matrix elements \( \langle j_s, j_s j_s j_s(m) | J_{2s} L_{2s} | j_s, j_s j_s j_s(m') \rangle, \) \( \langle j_s, j_s j_s j_s(m) | L_{2s} | j_s, j_s j_s j_s(m') \rangle, \) and \( \langle j_s, j_s j_s j_s(m) | j_s L_{2s}^* j_s | j_s, j_s j_s j_s(m') \rangle \) and \( m \)-dependent factors (Wigner–Eckart theorem). The \( m \)-dependent factors may be obtained from Ref. 15. It should be noted that the operators \( L_{2s}, L_{2s}^* \) operate on the second angular momentum \( l_s \) in \( |(l_s, l_s)j_s(m)\rangle, \) whereas the operators \( J_{2s}, J_{2s}^* \) operate on the first angular momentum \( j_s \) in \( |(l_s, l_s)j_s(m)\rangle. \) This makes it necessary\(^5\) to give negative values to the off-diagonal elements \( |j_s, L_{2s} j_s(m)\rangle \). We obtain then from (5) the expression

\[
\sum_{m} \frac{(-1)^{j_s-m}}{(2j_s + 1)^{3/2}} \langle j_s, L_{2s} j_s(m) | j_s, L_{2s} j_s(m) \rangle \langle j_s - 1, L_{2s} j_s(m) \rangle \]

\[
\times \langle j_s, l_s j_s(m) | j_s, l_s j_s(m) \rangle |(l_s, l_s)j_s(m+1)\rangle |(l_s, l_s)j_s(m-1)\rangle \]

\[= \langle j_s, L_{2s}^* j_s | j_s, L_{2s}^* j_s \rangle |(l_s, l_s)j_s(m+1)\rangle |(l_s, l_s)j_s(m-1)\rangle \]

\[= \langle j_s, L_{2s}^* j_s | j_s, L_{2s}^* j_s \rangle |(l_s, l_s)j_s(m)\rangle |(l_s, l_s)j_s(m)\rangle \].

(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

\[2j_s[(2j_s + 1)(2j_s + 1)^{1/2}] \langle j_s + 1, L_{2s} j_s(m) \rangle \langle j_s - 1, L_{2s} j_s(m) \rangle \]

\[= 2j_s[(2j_s + 1)(2j_s + 1)^{1/2}] \langle j_s + 1, L_{2s} j_s(m) \rangle \langle j_s - 1, L_{2s} j_s(m) \rangle \]

\[= 2j_s[(2j_s + 1)(2j_s + 1)^{1/2}] \langle j_s + 1, L_{2s} j_s(m) \rangle \langle j_s - 1, L_{2s} j_s(m) \rangle \]

\[= 2j_s[(2j_s + 1)(2j_s + 1)^{1/2}] \langle j_s + 1, L_{2s} j_s(m) \rangle \langle j_s - 1, L_{2s} j_s(m) \rangle \]

\[= 2j_s[(2j_s + 1)(2j_s + 1)^{1/2}] \langle j_s + 1, L_{2s} j_s(m) \rangle \langle j_s - 1, L_{2s} j_s(m) \rangle \].

(A7)

and, finally, with the explicit algebraic expression for \( \langle j_s, L_{2s}^* j_s \rangle \) and \( \langle j_s, L_{2s} j_s \rangle \),

\[\langle j_s, L_{2s}^* j_s | j_s, L_{2s} j_s \rangle = \frac{\langle j_s, L_{2s}^* j_s | j_s, L_{2s} j_s \rangle}{2j_s[(2j_s + 1)(2j_s + 1)^{1/2}]}, \]

(A8)

\[\langle j_s, L_{2s}^* j_s | j_s, L_{2s} j_s \rangle = \frac{\langle j_s, L_{2s}^* j_s | j_s, L_{2s} j_s \rangle}{2j_s[(2j_s + 1)(2j_s + 1)^{1/2}]}, \]

(A9)

\[\langle j_s, L_{2s}^* j_s | j_s, L_{2s} j_s \rangle = \frac{\langle j_s, L_{2s}^* j_s | j_s, L_{2s} j_s \rangle}{2j_s[(2j_s + 1)(2j_s + 1)^{1/2}]}, \]

(A10)

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

\[L_{2s}^2 - l_s(l_s + 1)x = 0. \]

(A11)

These terms are known as the recursion equations derived above for \( j_s \)-coefficients. The solution

\[x = \frac{1}{l_s(l_s + 1)} \frac{1}{2j_s[(2j_s + 1)(2j_s + 1)^{1/2}]}. \]

(A12)

of these recursion equations therefore corresponds directly to the solution of the eigenvalue problem (11).

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