Computer Physics Communications 11 (1976) 269–278

RECURSIVE EVALUATION OF 3j AND 6j COEFFICIENTS *

K. SCHULTEN
Max-Planck-Institut für biophysikalische Chemie, Göttingen, Fed. Rep. Germany

and

R.G. GORDON
Harvard University, Department of Chemistry,
Cambridge, Massachusetts 02138, USA

Received 23 February 1976

PROGRAM SUMMARY

Title of program: J1-RECURSION OF 3J-COEFFICIENTS

Catalogue number: ACWQ

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

Computer: UNIVAC 1108; *Installation*: Gesellschaft für wissenschaftliche Datenverarbeitung, Göttingen, Fed. Rep. Germany.

Operating system: EXEC 8

Program language used: FORTRAN 4

High speed storage required: 8958 words

No. of bits in a word: 36

Overlay structure: None

No. of magnetic tapes required: None

Other peripherals used: Card reader, lineprinter (for test)

No. of cards in combined program and test deck: 405

Card punching code: BCD

Keywords: General purpose, molecular, rotation group, recoupling coefficient, 3j, Clebsch–Gordan, Wigner, angular momentum, recursion.

Nature of physical problem
Subroutine REC3JJ generates 3j coefficients

$$f(j_1) = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

for all allowed j_1 (j_2, j_3, m_1, m_2, m_3 held fixed) from the exact solution of a recursion equation. The algorithm is more efficient and accurate than those based on explicit expressions, particularly in the commonly arising case in which a complete set of 3j coefficients is needed. The algorithm is numerically stable for large quantum numbers which occur in problems of molecular dynamics.

Methods of solution
To guarantee numerical stability the recursion equation which relates 3j coefficients $f(j_1)$ with contiguous j_1 values j_1-1, j_1, j_1+1 is solved in the direction of increasing $f(j_1)$ from both ends of the allowed j_1 domain, $j_{1\,\min}$ and $j_{1\,\max}$. The linear recursion equation reduces to two terms at $j_{1\,\min}$ and $j_{1\,\max}$ and thus can be started at both ends with arbitrary initial values $f(j_{1\,\min})$ and $f(j_{1\,\max})$, respectively. At an intermediate j_1 forward and backward recursions are matched which leaves all $f(j_1)$ off by a constant factor. This factor is determined from the unitary property of 3j coefficients and Wigner's phase convention.

Typical running time
0.4 msec per 3j coefficient for $j_{1\,\max}-j_{1\,\min} > 20$, somewhat longer for smaller j_1 domains.

Unusual features of the program
Large quantum number 3j coefficients $f(j_1)$ may vary over many orders of magnitude over their j_1 domain. The program prevents underflow and overflow for which purpose the smallest and largest number representable on the computer, TINY and HUGE, respectively, have to be defined. In the recursion process the relative magnitudes of contiguous 3j coefficients $f(j_1)$ are being evaluated exactly, however. The program sets later on all 3j coefficients which are smaller than TINY to zero.

* Supported by the National Science Foundation.

PROGRAM SUMMARY

Title of program: M2-RECURSION OF 3J-COEFFICIENTS

Catalogue number: ACWR

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

Computer: UNIVAC 1108; *Installation*: Gesellschaft für wissenschaftliche Datenverarbeitung, Göttingen, Fed. Rep. Germany.

Operating system: EXEC 8

Program language used: FORTRAN 4

High speed storage required: 8879 words

No. of bits in a word: 36

Overlay structure: None

No. of magnetic tapes required: None

Other peripherals used: Card reader, lineprinter (for test)

No. of cards in combined program and test deck: 392

Card punching code: BCD

Keywords: General purpose, molecular, rotation group, recoupling coefficient, 3*j*, Clebsch–Gordan, Wigner, angular momentum, recursion.

Nature of physical problem
Subroutine REC3JM generates 3*j* coefficients

$$g(m_2) = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix}$$

for all allowed m_2 (j_1, j_2, j_3, m_1 held fixed) from the exact solution of an recursion equation. The algorithm is more efficient and accurate than those based an explicit expressions, particularly, in the commonly arising case in which a complete set of 3*j* coefficients is needed. The algorithm is numerically stable for large quantum numbers which occur in problems of molecular dynamics.

Methods of solution
To guarantee numerical stability the recursion equation which relates 3*j* coefficients $g(m_2)$ with contiguous m_2 values m_2-1, m_2, m_2+1 is solved in the direction of increasing $g(m_2)$ from both ends of the allowed m_2 domain, $m_{2\,\mathrm{min}}$ and $m_{2\,\mathrm{max}}$. The linear recursion equation reduces to two terms at $m_{2\,\mathrm{min}}$ and $m_{2\,\mathrm{max}}$ and thus can be started at both ends with arbitrary initial values $g(m_{2\,\mathrm{min}})$ and $g(m_{2\,\mathrm{max}})$, respectively. At an intermediate m_2 forward and backward recursion are matched which leaves all $g(m_2)$ off by a constant factor. This factor is determined from the unitary property of 3*j* coefficients and Wigner's phase convention.

Typical running time
0.3 msec per 3*j* coefficient for $m_{2\,\mathrm{max}}-m_{2\,\mathrm{min}} > 20$, somewhat longer for smaller m_2 domains.

Unusual features of the program
Large quantum number 3*j* coefficients $g(m_2)$ may vary over many orders of magnitude over their m_2 domain. The program prevents underflow and overflow for which purpose the smallest and largest number representable on the computer, TINY and HUGE, respectively, have to be defined. In the recursion process the relative magnitude of contiguous 3*j* coefficients $g(m_2)$ are being evaluated exactly, however. The program sets later on all 3*j* coefficients which are smaller than TINY to zero.

PROGRAM SUMMARY

Title of program: J1-RECURSION OF 6J-COEFFICIENTS

Catalogue number: ACWS

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

Computer: UNIVAC 1108; *Installation*: Gesellschaft für wissenschaftliche Datenverarbeitung, Göttungen, Fed. Rep. Germany.

Operating system: EXEC 8

Programming language used: FORTRAN 4

High speed storage required: 9178 words

No. of bits in a word: 36

Overlay structure: None

No. of magnetic tapes required: None

Other peripherals used: Card reader, lineprinter (for tests)

No. of cards in combined program and test deck: 431

Card punching code: BCD

Keywords: General purpose, molecular, rotation group, recoupling coefficient, 6*j*, Racah, Wigner, angular momentum, recursion.

Nature of physical problem
Subroutine REC6J generates 6*j* coefficients

$$h(j_1) = \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}$$

for all allowed j_1 (j_2, j_3, l_1, l_2, l_3 held fixed) from the exact solution of a recursion equation. The algorithm is more efficient and accurate then those based on explicit expressions, particularly in the commonly arising case in which a complete set of 6j coefficients is needed. The algorithm is numerically stable for large quantum numbers which occur in problems of molecular dynamics.

Methods of solution
To guarantee numerical stability the recursion equation which relates 6j coefficients $h(j_1)$ with contiguous j_1 values $j_1 - 1, j_1, j_1 + 1$ is solved in the direction of increasing $h(j_1)$ from both ends of the allowed j_1 domain, j_1 min and j_1 max. The linear recursion equation reduces to two terms at j_1 min and j_1 max and thus can be started at both ends with arbitrary initial values $h(j_1\,\text{min})$ and $h(j_1\,\text{max})$, respectively. At an intermediate j_1 forward and backward recursions are matched which leaves all $f(j_1)$ off by a constant factor. This factor is determined from the unitary property of 6j coefficients and Wigner's phase convention.

Typical running time
0.5 msec per 6j coefficient for $j_1\,\text{max}-j_1\,\text{min} > 20$, somewhat longer for smaller j_1 domains.

Unusual features of the program
Large quantum number 6j coefficients $h(j_1)$ may vary over many orders of magnitude over their j_1 domain. The program prevents underflow and overflow for which purpose the smallest and largest number representable on the computer, TINY and HUGE, respectively, have to be defined. In the recursion process the relative magnitudes of contiguous 6j coefficients $h(j_1)$ are being evaluated exactly, however. The program sets later on all 6j coefficients which are smaller than TINY to zero.

LONG WRITE-UP

1. Introduction

3j and 6j coefficients occur in the quantum mechanical algebra of angular momentum addition. Calculations involving the coupling of angular momenta commonly require the evaluation of whole strings of coupling coefficients of the kind

$$f(j) = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}, \qquad \text{for all allowed } j_1; \quad j_{1\,\text{min}} \leqslant j_1 \leqslant j_{1\,\text{max}}, \tag{1a}$$

$$g(m_2) = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix}, \quad \text{for all allowed } m_2; \quad m_{2\,\text{min}} \leqslant m_2 \leqslant m_{2\,\text{max}}, \tag{2a}$$

$$h(j_1) = \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}, \qquad \text{for all allowed } j_1; \quad j_{1\,\text{min}} \leqslant j_1 \leqslant j_{1\,\text{max}}. \tag{3a}$$

Existing algorithms evaluate coupling coefficients separately and do not make use of relationships between the values of contiguous 3j and 6j coefficients in eqs. (1a), (2a) and (3a). The algorithms, furthermore, are inapplicable for large angular momentum quantum numbers (~ 100) which, for example, frequently occur in problems of molecular dynamics.

We have pointed out recently that 3j and 6j coefficients can be evaluated most efficiently and accurately from recursion equations [1]. Condon and Shortley [2], and subsequently Rose [3] have called attention to this possibility for the evaluation of 3j coefficients. The recursion equations are particularly suitable for the evaluation of large quantum number coupling coefficients. In fact, they yield in the limit of very large quantum numbers a simple second-order difference equation from which the semiclassical expressions of 3j and 6j coefficients follow by means of the WKB approximation [4]. The semiclassical expressions reveal that the quantum number domain of 3j and 6j coefficients in eqs. (1a), (2a) and (3a) are divided in two non-classical domains separated by a classical domain. In the non-classical domains at the boundaries $j_{1\,\text{min}}$ and $j_{1\,\text{max}}$ ($m_{2\,\text{min}}$ and $m_{2\,\text{max}}$) the coupling coefficients decay exponentially to zero. In the intermediate classical domain the values of the coupling coefficients oscillate rapidly. This behaviour is somewhat reminiscent of the behaviour of bound state wave functions to the Hamilton operator. Indeed, the recursion equations of $3j$ and $6j$ coefficients given below follow directly from eigenvalue problems which define the coupling coefficients. They are also solved in a way similar to the integration of bound state Schrödinger equations. The recursion equations for the coupling coefficients in eqs. (1a), (2a) and (3a) are

$$j_1 A(j_1+1)\begin{pmatrix} j_1+1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} + B(j_1)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} + (j_1+1)A(j_1)\begin{pmatrix} j_1-1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = 0\,, \quad (1b)$$

where

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

$$B(j_1) = -(2j_1+1)[j_2(j_2+1)m_1-j_3(j_3+1)m_1-j_1(j_1+1)(m_3-m_2)]\,, \quad (1d)$$

and

$$C(m_2+1)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2+1 & m_3-1 \end{pmatrix} + D(m_2)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} + C(m_2)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2-1 & m_3+1 \end{pmatrix} = 0\,, \quad (2b)$$

where

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

$$D(m_2) = j_2(j_2+1)+j_3(j_3+1)-j_1(j_1+1)+2m_2m_3\,, \quad (2d)$$

and

$$j_1 E(j_1+1)\begin{Bmatrix} j_1+1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} + F(j_1)\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} + (j_1+1)E(j_1)\begin{Bmatrix} j_1-1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = 0 \quad (3b)$$

where

$$E(j_1) = \{[j_1^2-(j_2-j_3)^2][(j_2+j_3+1)^2-j_1^2][j_1^2-(l_2-l_3)^2][(l_2+l_3+1)^2-j_1^2]\}^{1/2}\,, \quad (3c)$$

$$F(j_1) = (2j_1+1)\{j_1(j_1+1)[-j_1(j_1+1)+j_2(j_2+1)+j_3(j_3+1)] + l_2(l_2+1)[j_1(j_1+1)+j_2(j_2+1)-j_3(j_3+1)]$$
$$+ l_3(l_3+1)[j_1(j_1+1)-j_2(j_2+1)+j_3(j_3+1)]-2j_1(j_1+1)l_1(l_1+1)\}\,. \quad (3d)$$

These linear recursion equations determine the coupling coefficients except for an overall constant factor which can be obtained from the following unitary properties and phase conventions:

$$\sum_{j_1}(2j_1+1)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}^2 = 1\,, \qquad \mathrm{sign}\left[\begin{pmatrix} j_{1\,\max} & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}\right] = (-1)^{j_2-j_3-m_1}\,, \quad (1e,f)$$

and

$$\sum_{m_2}(2j_1+1)\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix}^2 = 1\,, \qquad \mathrm{sign}\left[\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_{2\,\max} & -m_1-m_{2\,\max} \end{pmatrix}\right] = (-1)^{j_2-j_3-m_1}\,, \quad (2e,f)$$

and

$$\sum_{j_1}(2j_1+1)(2l_1+1)\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}^2 = 1\,, \qquad \operatorname{sign}\left[\begin{Bmatrix} j_{1\,\max} & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}\right] = (-1)^{j_2+j_3+l_2+l_3}\,. \qquad \text{(3e,f)}$$

2. Method of solution

The linear three-term recursion equations (1b), (2b) and (3b) reduce to two terms at the boundaries $j_{1\,\min}$ and $j_{1\,\max}$ ($m_{2\,\min}$ and $m_{2\,\max}$). Hence, the recursion process can be started with a single starting value $F(j_{1\,\min})$ [$G(m_{2\,\min})$, $H(j_{1\,\min})$] for the forward direction or $F(j_{1\,\max})$ [$G(m_{2\,\max})$, $H(j_{1\,\max})$] for the backward direction. Due to the linear character of the recursion equations these starting values can be chosen arbitrarily leaving the generated recursion series $\{F(j_1)\}$, $\{G(m_2)\}$ or $\{H(j_1)\}$ multiplied by a constant factor.

$$F(j_1) = c_1 f(j_1)\,, \quad \text{for all } j_1\,; \qquad G(m_2) = c_2 g(m_2)\,, \quad \text{for all } m_2\,; \qquad H(j_1) = c_3 h(j_1)\,, \quad \text{for all } j_1\,. \qquad \text{(1g, 2g, 3g)}$$

The unknown constants c_1, c_2 or c_3 can be determined through

$$c_1 = (-1)^{j_2-j_3-m_1}\operatorname{sign}[F(j_{1\,\max})]/\left[\sum_{j_1}(2j_1+1)F(j_1)^2\right]^{1/2}, \qquad \text{(1f)}$$

$$c_2 = (-1)^{j_2-j_3-m_1}\operatorname{sign}[G(m_{2\,\max})]/\left[\sum_{m_2}(2j_1+1)G(m_2)^2\right]^{1/2}, \qquad \text{(2f)}$$

$$c_3 = (-1)^{j_2+j_3+l_2+l_3}\operatorname{sign}[H(j_{1\,\max})]/\left[\sum_{j_1}(2j_1+1)(2l_1+1)H(j_1)^2\right]^{1/2}. \qquad \text{(3f)}$$

The signs follow from Wigner's phase convention (1f), (2f) and (3f), the absolute magnitudes from the normalization conditions (1e), (2e) and (3e).

The recursion procedure is stable only in the direction of increasing coupling coefficients. From the semiclassical expressions one observes that large quantum number $3j$ and $6j$ coefficients increase exponentially in the non-classical regions at both ends of the recursion domain [4]. Hence, the recursion must proceed simultaneously forward and backward from the two non-classical domains towards the intermediate classical domain of large coupling coefficients.

Let us take in the following the recursion of the $3j$ coefficients in eq. (1a) as an example to illustrate the numerical procedure. What will be said applies equally to the $3j$ and $6j$ coefficients in (2a) and (3a), respectively. One needs to generate the forward and backward recursion series

$$\vec{F}(j_{\min}), \vec{F}(j_{1\,\min}+1), \ldots, \vec{F}(j_{1\,\mathrm{int}})\,, \qquad \overleftarrow{F}(j_{1\,\max}), \overleftarrow{F}(j_{1\,\max}-1), \ldots, \overleftarrow{F}(j_{1\,\mathrm{int}})\,,$$

each started with arbitrary values. These series have to be matched at an intermediate j_1 value $j_{1\,\mathrm{int}}$. For this purpose one may rescale either the forward or the backward recursion series such that $\vec{F}(j_{\mathrm{int}}) = \overleftarrow{F}(j_{1\,\mathrm{int}})$. If one chooses to rescale the forward recursion series, the scaling factor is

$$\lambda = \overleftarrow{F}(j_{1\,\mathrm{int}})/\vec{F}(j_{1\,\mathrm{int}})\,. \qquad (4')$$

This expression is not suitable numerically since $\vec{F}(j_{1\,\mathrm{int}})$ and $\overleftarrow{F}(j_{1\,\mathrm{int}})$ may be small, perhaps zero, and connected with large relative errors. It is advantageous to match forward and backward recursion at three contiguous j_1 values simultaneously by a least squares fit. The scaling factor λ is then determined such that

$$[\lambda\vec{F}(j_{1\,\mathrm{int}}+1)-\overleftarrow{F}(j_{1\,\mathrm{int}}+1)]^2 + [\lambda\vec{F}(j_{1\,\mathrm{int}})-\overleftarrow{F}(j_{1\,\mathrm{int}})]^2 + [\lambda\vec{F}(j_{1\,\mathrm{int}}-1)-\overleftarrow{F}(j_{1\,\mathrm{int}}-1)]^2$$

takes on its minimum value, i.e.

$$\lambda = \frac{\vec{F}(j_{1\,\mathrm{int}}+1)\,\overleftarrow{F}(j_{1\,\mathrm{int}}+1) + \vec{F}(j_{1\,\mathrm{int}})\,\overleftarrow{F}(j_{1\,\mathrm{int}}) + \vec{F}(j_{\mathrm{int}}-1)\,\overleftarrow{F}(j_{\mathrm{int}}-1)}{\vec{F}(j_{1\,\mathrm{int}}+1)^2 + \vec{F}(j_{1\,\mathrm{int}})^2 + \vec{F}(j_{1\,\mathrm{int}}-1)^2}\,, \tag{4}$$

where $j_{1\,\mathrm{int}}$ must be chosen to lie within the classical domain where no three contiguous coupling coefficients are small. Recursion equation (1b) [and similarly eqs. (2b) and (3b)] enter the recursion program in the form

$$f(j_1+1) = \alpha(j_1) f(j_1) + \beta(j_1) f(j_1-1)\,, \tag{5}$$

where $|\beta(j_1)| \approx 1$. The semiclassical theory of angular momentum coupling which is applicable for moderate and large quantum numbers [4] reveals that $|\alpha(j_1)|$ takes on its minimum value in the classical domain and varies monotonically in the non-classical domains. Hence, by monitoring the variation of $|\alpha(j_1)|$ in the forward recursion step a suitable point for forward and backward recursion can be found.

Large quantum number 3*j* and 6*j* coefficients may vary over many orders of magnitude. To prevent 'overflow' in the recursion step and 'underflow' in the normalization step the recursion series $\vec{F}(j_1)$ and $\overleftarrow{F}(j_1)$ are rescaled such that the largest $\vec{F}(j_1)$–[$\overleftarrow{F}(j_1)$–] values does not exceed SHRUGE = $[\mathrm{HUGE}]^{1/2}$ where HUGE is the largest number representable on the computer.

Those $\vec{F}(j_1)[\overleftarrow{F}(j_1)]$ which fall then below TINY, the smallest value representable on the computer, are set to zero. Thus, the recursion program evaluates the relative magnitudes of contiguous coupling coefficients exactly but may set the smallest 3*j* and 6*j* coefficients to zero.

3. Program structure

The recursive evaluation of the coupling coefficients in (1a), (2a) and (3a) is carried out in subroutines REC3JJ, REC3JM and REC6J, respectively. The subroutines are driven by test routines which read in the test data and determine the partition of recursion domains in non-classical and classical domains. The recursion routines are documented by comment cards which together with what has been said above allow the program steps to be easily followed.

3.1. Input

(a) For the generation of 3*j* coefficients

$$f(L_1) = \begin{pmatrix} L_1 & L_2 & L_3 \\ -M_2-M_3 & M_2 & M_3 \end{pmatrix}, \quad \text{as in eq. (1a),}$$

Card 1ff. FORMAT (4F10.1) L_2, L_3, M_2, M_3.

(b) For the generation of 3*j* coefficients

$$g(M_2) = \begin{pmatrix} L_1 & L_2 & L_3 \\ M_1 & M_2 & -M_1-M_2 \end{pmatrix}, \text{ as in eq. (2a),}$$

Card 1ff. FORMAT (4F10.1) L_1, L_2, L_3, M_1.

(c) For the generation of 6*j* coefficients

$$h(L_1) = \begin{Bmatrix} L_1 & L_2 & L_3 \\ L_4 & L_5 & L_6 \end{Bmatrix}, \quad \text{as in eq. (3a),}$$

Card 1ff. FORMAT (5F10.1) L_2, L_3, L_4, L_5, L_6.

3.2. Output

The string of 3*j* and 6*j* coefficients

$$\begin{pmatrix} L_1 & 100 & 60 \\ -10 & 60 & -50 \end{pmatrix} \quad 40 \leqslant L_1 \leqslant 160\,, \tag{1a}$$

$$\begin{pmatrix} 120 & 60 & 70 \\ -10 & M_2 & 10-M_2 \end{pmatrix} \quad -60 \leqslant M_2 \leqslant 60\,, \tag{2a}$$

$$\begin{Bmatrix} L_1 & 80 & 150 \\ 190 & 230 & 120 \end{Bmatrix} \quad 110 \leqslant L_1 \leqslant 230\,, \tag{3a}$$

are calculated assuming for test purposes that TINY = 10^{-10} and HUGE = 10^{10}. The test driving programs give the classical regions $47.1 < L_1 < 114.6$ for (1a), $-21.0 < M_2 < 30.1$ for (2a), and $131.7 < L_1 < 189.9$ for (3a). Outside the classical regions the exponential decay of the coupling coefficients can be observed, inside the classical region the values of the coupling coefficients oscillate rapidly exhibiting ten nodes for the examples chosen. The matching point of forward and backward recursions lie well within the classical domain: $L_1 = 69$ for (1a), $M_2 = 5$ for (2a), and $L_1 = 159$ for (3a). The recursion series have been rescaled twice (1a), six times (2a) and four times (3a). All coupling coefficients with absolute values below TINY = 10^{-10} have been set to zero. We have also added results for 3*j* and 6*j* coefficients with small quantum numbers.

Acknowledgement

The authors would like to thank the Gesellschaft für wissenschaftliche Datenverarbeitung mbH Göttingen for excellent facilities and assistance.

References

[1] K. Schulten and R.G. Gordon, J. Math. Phys. 16 (1975) 1961–1970.
[2] E.U. Condon and G.H. Shortley, The Theory of Atomic Spectra (Cambridge University Press, Cambridge, 1935). p. 67.
[3] M.E. Rose, Elementary Theory of Angular Momentum (John Wiley and Sons, New York. 1957), pp. 42–45.
[4] K. Schulten and R.G. Gordon, J. Math. Phys. 16 (1975) 1971–1988.

TEST RUN OUTPUT FROM J1-RECURSION OF 3J-COEFFICIENTS

```
TABLE OF 3J-COEFFICIENTS       L1 100.0  60.0      L1-DOMAIN (QU. MECH.)   40.0 --  160.0     RECURSIONS MATCHED AT
   (RESCALED    2 TIMES)     -10.0  60.0 -50.0               (CLASSICAL)   47.1 --  114.6              69.0

  .4998748398-004 L1= 40.0     .2107509508-003 L1= 41.0     .6217978400-003 L1= 42.0     .1479014117-002 L1= 43.0
  .3000050929-002 L1= 44.0     .5341679723-002 L1= 45.0     .8484716148-002 L1= 46.0     .1212489103-001 L1= 47.0
  .1562646903-001 L1= 48.0     .1809236427-001 L1= 49.0     .1857229118-001 L1= 50.0     .1637459581-001 L1= 51.0
  .1138785780-001 L1= 52.0     .4283413034-002 L1= 53.0    -.3516327256-002 L1= 54.0    -.1015005103-001 L1= 55.0
 -.1385106534-001 L1= 56.0    -.1354067655-001 L1= 57.0    -.9266653885-002 L1= 58.0    -.2295386211-002 L1= 59.0
  .5193111132-002 L1= 60.0     .1081563934-001 L1= 61.0     .1274480694-001 L1= 62.0     .1037160043-001 L1= 63.0
  .4541798196-002 L1= 64.0    -.2713186713-002 L1= 65.0    -.8874838045-002 L1= 66.0    -.1182087354-001 L1= 67.0
 -.1057355132-001 L1= 68.0    -.5638688730-002 L1= 69.0     .1188456078-002 L1= 70.0     .7476742063-002 L1= 71.0
  .1102984883-001 L1= 72.0     .1065613928-001 L1= 73.0     .6563667621-002 L1= 74.0     .2500662640-003 L1= 75.0
 -.6056575983-002 L1= 76.0    -.1019148491-001 L1= 77.0    -.1079382267-001 L1= 78.0    -.7739713718-002 L1= 79.0
 -.2134712702-002 L1= 80.0     .4107036658-002 L1= 81.0     .8930291919-002 L1= 82.0     .1081468733-001 L1= 83.0
  .9236301203-002 L1= 84.0     .4780704358-002 L1= 85.0    -.1101614624-002 L1= 86.0    -.6590891942-002 L1= 87.0
 -.1006906998-001 L1= 88.0    -.1058480457-001 L1= 89.0    -.8083163283-002 L1= 90.0    -.3356302954-002 L1= 91.0
  .2240634483-002 L1= 92.0     .7201299032-002 L1= 93.0     .1027801824-001 L1= 94.0     .1077860557-001 L1= 95.0
  .8686083408-002 L1= 96.0     .4594763019-002 L1= 97.0    -.4943153179-003 L1= 98.0    -.5446330380-002 L1= 99.0
 -.9256992877-002 L1=100.0    -.1124732934-001 L1=101.0    -.1115646464-001 L1=102.0    -.9130574592-002 L1=103.0
 -.5630672056-002 L1=104.0    -.1295456321-002 L1=105.0     .3202669654-002 L1=106.0     .7277730157-002 L1=107.0
  .1050805001-001 L1=108.0     .1266764387-001 L1=109.0     .1371605519-001 L1=110.0     .1376024421-001 L1=111.0
  .1300249638-001 L1=112.0     .1168759074-001 L1=113.0     .1005848383-001 L1=114.0     .8325364939-002 L1=115.0
  .6648978061-002 L1=116.0     .5136281403-002 L1=117.0     .3845015697-002 L1=118.0     .2793416658-002 L1=119.0
  .1971783341-002 L1=120.0     .1353509582-002 L1=121.0     .9041732893-003 L1=122.0     .5881279833-003 L1=123.0
  .3726549027-003 L1=124.0     .2300876618-003 L1=125.0     .1384604907-003 L1=126.0     .8121972081-004 L1=127.0
  .4644331039-004 L1=128.0     .2588822247-004 L1=129.0     .1406565956-004 L1=130.0     .7447822595-005 L1=131.0
  .3842501662-005 L1=132.0     .1931034748-005 L1=133.0     .9449400413-006 L1=134.0     .4500632065-006 L1=135.0
  .2085371458-006 L1=136.0     .9394769735-007 L1=137.0     .4112422660-007 L1=138.0     .1747812932-007 L1=139.0
  .7206277022-008 L1=140.0     .2879587775-008 L1=141.0     .1113993490-008 L1=142.0     .4167107929-009 L1=143.0
  .1505153696-009 L1=144.0     .0000000000     L1=145.0     .0000000000     L1=146.0     .0000000000     L1=147.0
  .0000000000     L1=148.0     .0000000000     L1=149.0     .0000000000     L1=150.0     .0000000000     L1=151.0
  .0000000000     L1=152.0     .0000000000     L1=153.0     .0000000000     L1=154.0     .0000000000     L1=155.0
  .0000000000     L1=156.0     .0000000000     L1=157.0     .0000000000     L1=158.0     .0000000000     L1=159.0
  .0000000000     L1=160.0

TIME NEEDED (IN MILLISECONDS)      48.0


TABLE OF 3J-COEFFICIENTS       L1    4.5   3.5     L1-DOMAIN (QU. MECH.)    1.0 --    8.0     RECURSIONS MATCHED AT
   (RESCALED    0 TIMES)      1.0  -3.5   2.5                (CLASSICAL)     .6 --    6.3              2.0

  .2788866755+000 L1=  1.0    -.9534625892-001 L1=  2.0    -.6741998625-001 L1=  3.0     .1533110352+000 L1=  4.0
 -.1564465547+000 L1=  5.0     .1099450412+000 L1=  6.0    -.5536235693-001 L1=  7.0     .1799835451-001 L1=  8.0

TIME NEEDED (IN MILLISECONDS)      3.0


TABLE OF 3J-COEFFICIENTS       L1    9.0   7.0     L1-DOMAIN (QU. MECH.)    2.0 --   16.0     RECURSIONS MATCHED AT
   (RESCALED    0 TIMES)      2.0  -7.0   5.0                (CLASSICAL)    1.7 --   11.6              3.0

  .1769286567+000 L1=  2.0    -.2114701923-001 L1=  3.0    -.8063217712-001 L1=  4.0     .1068133566+000 L1=  5.0
 -.6994607055-001 L1=  6.0     .3797663080-002 L1=  7.0     .5645859113-001 L1=  8.0    -.8545877055-001 L1=  9.0
  .9202994825-001 L1= 10.0    -.7391557565-001 L1= 11.0     .4866975616-001 L1= 12.0    -.2651448662-001 L1= 13.0
  .1176741060-001 L1= 14.0    -.4054268739-002 L1= 15.0     .9460155046-003 L1= 16.0

TIME NEEDED (IN MILLISECONDS)      6.0
```

TEST RUN OUTPUT FROM M2-RECURSION OF 3J-COEFFICIENTS

```
TABLE OF 3J-COEFFICIENTS   120.0  60.0   70.0     M2-DOMAIN (QU. MECH.)  -60.0 --   60.0    RECURSIONS MATCHED AT
   (RESCALED   6 TIMES)    -10.0    M2 -M1-M2               (CLASSICAL)  -21.0 --   30.1                5.0

  .0000000000     M2= -60.0    .0000000000     M2= -59.0    .0000000000     M2= -58.0    .0000000000     M2= -57.0
  .0000000000     M2= -56.0    .0000000000     M2= -55.0    .0000000000     M2= -54.0    .0000000000     M2= -53.0
  .0000000000     M2= -52.0    .0000000000     M2= -51.0    .0000000000     M2= -50.0    .0000000000     M2= -49.0
  .0000000000     M2= -48.0    .0000000000     M2= -47.0    .0000000000     M2= -46.0    .0000000000     M2= -45.0
  .0000000000     M2= -44.0    .0000000000     M2= -43.0    .0000000000     M2= -42.0    .1253032414-009 M2= -41.0
  .5449698580-009 M2= -40.0    .2222497237-008 M2= -39.0    .8514316697-008 M2= -38.0    .3068838908-007 M2= -37.0
  .1042061344-006 M2= -36.0    .3337306747-006 M2= -35.0    .1008985823-005 M2= -34.0    .2881896280-005 M2= -33.0
  .7780544987-005 M2= -32.0    .1986221329-004 M2= -31.0    .4794986264-004 M2= -30.0    .1094575548-003 M2= -29.0
  .2361822525-003 M2= -28.0    .4814000393-003 M2= -27.0    .9259333216-003 M2= -26.0    .1678146191-002 M2= -25.0
  .2859990117-002 M2= -24.0    .4570349345-002 M2= -23.0    .6821254570-002 M2= -22.0    .9455001629-002 M2= -21.0
  .1207055316-001 M2= -20.0    .1400881572-001 M2= -19.0    .1445350820-001 M2= -18.0    .1267910187-001 M2= -17.0
  .8410372678-002 M2= -16.0    .2164712627-002 M2= -15.0   -.4623839992-002 M2= -14.0   -.9884601319-002 M2= -13.0
 -.1163247551-001 M2= -12.0   -.8917690905-002 M2= -11.0   -.2551554991-002 M2= -10.0    .4885099674-002 M2=  -9.0
  .1001178061-001 M2=  -8.0    .1022709594-001 M2=  -7.0    .5245117330-002 M2=  -6.0   -.2476875351-002 M2=  -5.0
 -.8815448672-002 M2=  -4.0   -.1019315174-001 M2=  -3.0   -.5720017720-002 M2=  -2.0    .2088387633-002 M2=  -1.0
  .8632929278-002 M2=    .0    .9947486248-002 M2=   1.0    .5180245447-002 M2=   2.0   -.2775314101-002 M2=   3.0
 -.9005000314-002 M2=   4.0   -.9630995556-002 M2=   5.0   -.4260405857-002 M2=   6.0    .3762578063-002 M2=   7.0
  .9468266994-002 M2=   8.0    .9367761663-002 M2=   9.0    .3568793148-002 M2=  10.0   -.4389801563-002 M2=  11.0
 -.9779660620-002 M2=  12.0   -.9517481180-002 M2=  13.0   -.3856236424-002 M2=  14.0    .3962976839-002 M2=  15.0
  .9700502363-002 M2=  16.0    .1045238975-001 M2=  17.0    .6013968645-002 M2=  18.0   -.1309687434-002 M2=  19.0
 -.8099935516-002 M2=  20.0   -.1151885077-001 M2=  21.0   -.1043001198-001 M2=  22.0   -.5551312300-002 M2=  23.0
  .1198798470-002 M2=  24.0    .7672304307-002 M2=  25.0    .1228889837-001 M2=  26.0    .1439352998-001 M2=  27.0
  .1417845281-001 M2=  28.0    .1234847108-001 M2=  29.0    .9742912980-002 M2=  30.0    .7061454194-002 M2=  31.0
  .4742702599-002 M2=  32.0    .2969052270-002 M2=  33.0    .1739490695-002 M2=  34.0    .9564677824-003 M2=  35.0
  .4945681514-003 M2=  36.0    .2408123671-003 M2=  37.0    .1105103747-003 M2=  38.0    .4781874822-004 M2=  39.0
  .1951252127-004 M2=  40.0    .7506952807-005 M2=  41.0    .2721693638-005 M2=  42.0    .9291994028-006 M2=  43.0
  .2984140207-006 M2=  44.0    .9003026796-007 M2=  45.0    .2547397020-007 M2=  46.0    .6746343785-008 M2=  47.0
  .1668211411-008 M2=  48.0    .3840443052-009 M2=  49.0    .0000000000     M2=  50.0    .0000000000     M2=  51.0
  .0000000000     M2=  52.0    .0000000000     M2=  53.0    .0000000000     M2=  54.0    .0000000000     M2=  55.0
  .0000000000     M2=  56.0    .0000000000     M2=  57.0    .0000000000     M2=  58.0    .0000000000     M2=  59.0
  .0000000000     M2=  60.0

TIME NEEDED (IN MILLISECONDS)     40.0


TABLE OF 3J-COEFFICIENTS     8.0   7.5    6.5     M2-DOMAIN (QU. MECH.)   -7.5 --    5.5    RECURSIONS MATCHED AT
   (RESCALED   0 TIMES)      1.0    M2 -M1-M2               (CLASSICAL)   -6.7 --    5.5               -3.5

  .2091589733-001 M2=  -7.5    .8537565553-001 M2=  -6.5    .9082953709-001 M2=  -5.5   -.3890543778-001 M2=  -4.5
 -.6637349702-001 M2=  -3.5    .6495240405-001 M2=  -2.5    .2158943106-001 M2=  -1.5   -.7789127118-001 M2=   -.5
  .3597643711-001 M2=    .5    .5473015000-001 M2=   1.5   -.7596786660-001 M2=   2.5   -.2192244455-001 M2=   3.5
  .1012677443+000 M2=   4.5    .7348257262-001 M2=   5.5

TIME NEEDED (IN MILLISECONDS)      6.0


TABLE OF 3J-COEFFICIENTS    16.0  15.0   13.0     M2-DOMAIN (QU. MECH.)  -15.0 --   11.0    RECURSIONS MATCHED AT
   (RESCALED   0 TIMES)      2.0    M2 -M1-M2               (CLASSICAL)  -13.0 --   10.5               -9.0

  .1366359996-002 M2= -15.0    .1174164859-001 M2= -14.0    .3984625091-001 M2= -13.0    .6155138764-001 M2= -12.0
  .2448674585-001 M2= -11.0   -.4147799593-001 M2= -10.0   -.2431652050-001 M2=  -9.0    .4098711034-001 M2=  -8.0
  .9064619371-002 M2=  -7.0   -.4232161016-001 M2=  -6.0    .1425472725-001 M2=  -5.0    .3194459674-001 M2=  -4.0
 -.3497590789-001 M2=  -3.0   -.6953148830-002 M2=  -2.0    .3969202661-001 M2=  -1.0   -.2206471170-001 M2=    .0
 -.2403676824-001 M2=   1.0    .3975265704-001 M2=   2.0   -.2526654930-002 M2=   3.0   -.3994722080-001 M2=   4.0
  .2589747152-001 M2=   5.0    .3036247798-001 M2=   6.0   -.3965425198-001 M2=   7.0   -.2712528653-001 M2=   8.0
  .4444433389-001 M2=   9.0    .5908159616-001 M2=  10.0    .2525641247-001 M2=  11.0

TIME NEEDED (IN MILLISECONDS)      9.0
```

TEST RUN OUTPUT FROM J1-RECURSION OF 6J-COEFFICIENTS

```
TABLE OF 6J-COEFFICIENTS         L1   80.0 150.0       L1-DOMAIN (QU. MECH.)  110.0 --  230.0    RECURSIONS MATCHED AT
   (RESCALED     4 TIMES)     190.0 230.0 120.0                  (CLASSICAL)  131.7 --  189.9             159.0

  .0000000000      L1=110.0     .0000000000      L1=111.0     .0000000000      L1=112.0     .0000000000      L1=113.0
  .1058795562-009  L1=114.0     .4828865758-009  L1=115.0     .1966822822-008  L1=116.0     .7253982361-008  L1=117.0
  .2446909355-007  L1=118.0     .7605753076-007  L1=119.0     .2191026942-006  L1=120.0     .5875975890-006  L1=121.0
  .1472178685-005  L1=122.0     .3455172977-005  L1=123.0     .7612038468-005  L1=124.0     .1576493451-004  L1=125.0
  .3072145006-004  L1=126.0     .5635179224-004  L1=127.0     .9727265037-004  L1=128.0     .1578681450-003  L1=129.0
  .2404668860-003  L1=130.0     .3427832828-003  L1=131.0     .4552303443-003  L1=132.0     .5592904372-003  L1=133.0
  .6284988075-003  L1=134.0     .6333507807-003  L1=135.0     .5502903011-003  L1=136.0     .3729434444-003  L1=137.0
  .1215792492-003  L1=138.0    -.1544148721-003  L1=139.0    -.3852306519-003  L1=140.0    -.5009258947-003  L1=141.0
 -.4580877141-003  L1=142.0    -.2625819102-003  L1=143.0     .2333705128-004  L1=144.0     .2969599685-003  L1=145.0
  .4519622507-003  L1=146.0     .4230116931-003  L1=147.0     .2182725674-003  L1=148.0    -.7776855348-004  L1=149.0
 -.3366931076-003  L1=150.0    -.4422482278-003  L1=151.0    -.3450857438-003  L1=152.0    -.8896890518-004  L1=153.0
  .2067190344-003  L1=154.0     .4021514617-003  L1=155.0     .4041895851-003  L1=156.0     .2122746465-003  L1=157.0
 -.8052488317-004  L1=158.0    -.3326196210-003  L1=159.0    -.4229585180-003  L1=160.0    -.3095879779-003  L1=161.0
 -.4878702161-004  L1=162.0     .2338756411-003  L1=163.0     .4050519663-003  L1=164.0     .3866995974-003  L1=165.0
  .1934496754-003  L1=166.0    -.9144381050-004  L1=167.0    -.3316116450-003  L1=168.0    -.4260032283-003  L1=169.0
 -.3378096386-003  L1=170.0    -.1087226155-003  L1=171.0     .1640852275-003  L1=172.0     .3716965562-003  L1=173.0
  .4372498648-003  L1=174.0     .3420723227-003  L1=175.0     .1263817636-003  L1=176.0    -.1317563726-003  L1=177.0
 -.3477278611-003  L1=178.0    -.4587580569-003  L1=179.0    -.4400109207-003  L1=180.0    -.3054978568-003  L1=181.0
 -.9688574850-004  L1=182.0     .1333551462-003  L1=183.0     .3378374347-003  L1=184.0     .4846929152-003  L1=185.0
  .5610843260-003  L1=186.0     .5708754571-003  L1=187.0     .5289253410-003  L1=188.0     .4546197001-003  L1=189.0
  .3665542259-003  L1=190.0     .2792733064-003  L1=191.0     .2020790462-003  L1=192.0     .1393823501-003  L1=193.0
  .9189223170-004  L1=194.0     .5802839679-004  L1=195.0     .3515537486-004  L1=196.0     .2045847906-004  L1=197.0
  .1144729698-004  L1=198.0     .6163087911-005  L1=199.0     .3194438846-005  L1=200.0     .1594615405-005  L1=201.0
  .7668050985-006  L1=202.0     .3552455067-006  L1=203.0     .1585559010-006  L1=204.0     .6817005261-007  L1=205.0
  .2822685420-007  L1=206.0     .1125233355-007  L1=207.0     .4316585295-008  L1=208.0     .1592622990-008  L1=209.0
  .5647626904-009  L1=210.0     .1923308300-009  L1=211.0     .0000000000      L1=212.0     .0000000000      L1=213.0
  .0000000000      L1=214.0     .0000000000      L1=215.0     .0000000000      L1=216.0     .0000000000      L1=217.0
  .0000000000      L1=218.0     .0000000000      L1=219.0     .0000000000      L1=220.0     .0000000000      L1=221.0
  .0000000000      L1=222.0     .0000000000      L1=223.0     .0000000000      L1=224.0     .0000000000      L1=225.0
  .0000000000      L1=226.0     .0000000000      L1=227.0     .0000000000      L1=228.0     .0000000000      L1=229.0
  .0000000000      L1=230.0

TIME NEEDED (IN MILLISECONDS)      61.0


TABLE OF 6J-COEFFICIENTS         L1    8.0   7.0       L1-DOMAIN (QU. MECH.)    1.0 --   15.0    RECURSIONS MATCHED AT
   (RESCALED     0 TIMES)      6.5    7.5   7.5                    (CLASSICAL)     .8 --   13.9             -2.0

  .3490905138-001 L1=  1.0    -.3743025040-001 L1=  2.0     .1890866351-001 L1=  3.0     .7342448255-002 L1=  4.0
 -.2358935185-001 L1=  5.0     .1913476955-001 L1=  6.0     .1288017398-002 L1=  7.0    -.1930018366-001 L1=  8.0
  .1677305949-001 L1=  9.0     .5501147275-002 L1= 10.0    -.2135439791-001 L1= 11.0     .3460364451-002 L1= 12.0
  .2520950055-001 L1= 13.0     .1483990561-001 L1= 14.0    '.2708577681-002 L1= 15.0

TIME NEEDED (IN MILLISECONDS)      8.0


TABLE OF 6J-COEFFICIENTS         L1   16.0  14.0       L1-DOMAIN (QU. MECH.)    2.0 --   30.0    RECURSIONS MATCHED AT
   (RESCALED     0 TIMES)     13.0  15.0  15.0                   (CLASSICAL)    2.0 --   27.4             25.0

  .1218415617-001 L1=  2.0    -.1694202107-001 L1=  3.0     .1330633823-001 L1=  4.0    -.3207657855-002 L1=  5.0
 -.7077433408-002 L1=  6.0     .1110515826-001 L1=  7.0    -.6762397930-002 L1=  8.0    -.2161462351-002 L1=  9.0
  .8663002587-002 L1= 10.0    -.7764070616-002 L1= 11.0     .4658549005-003 L1= 12.0     .6871491561-002 L1= 13.0
 -.7728185493-002 L1= 14.0     .1290388899-002 L1= 15.0     .6275875647-002 L1= 16.0    -.7224302229-002 L1= 17.0
  .2312116715-003 L1= 18.0     .7068295312-002 L1= 19.0    -.5617804543-002 L1= 20.0    -.3487486663-002 L1= 21.0
  .7795024971-002 L1= 22.0     .4217371779-003 L1= 23.0    -.8478601965-002 L1= 24.0    -.5630188629-003 L1= 25.0
  .9406935871-002 L1= 26.0     .8966305627-002 L1= 27.0     .3874713883-002 L1= 28.0     .8469170293-003 L1= 29.0
  .7635839418-004 L1= 30.0

TIME NEEDED (IN MILLISECONDS)      14.0
```