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## ALGORITHM 260

### 6-J SYMBOLS [Z]

J. H. GUNN (Recd. 13 Nov. 1964)

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```
real procedure SJS (J1, J2, J3, L1, L2, L3, factorial);
  value J1, J2, J3, L1, L2, L3;
  integer J1, J2, J3, L1, L2, L3;
  array factorial;
comment SJS calculates the 6-j symbols defined by the following formula

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = \frac{\Delta(j_1, j_2, j_3)\Delta(j_1, l_2, l_3)\Delta(l_1, j_2, l_3)\Delta(l_1, l_2, j_3)}{\times \sum_z (-1)^z (z+1)! / ((z-j_1-j_2-j_3)!(z-j_1-l_2-l_3)!(z-l_1-j_2-l_3)!(z-l_1-l_2-j_3)!(j_1+j_2+l_1+l_2-z)!(j_2+j_3+l_2+l_3-z)!(j_3+j_1+l_3+l_1-z)!)}$$

```

where

$$\Delta(a, b, c) = \left[ \frac{(a+b-c)!(a-b+c)!(-a+b+c)!}{(a+b+c+1)!} \right]^{1/2}$$

and where  $j_1 = J_1/2$ ,  $j_2 = J_2/2$ ,  $j_3 = J_3/2$ ,  $l_1 = L_1/2$ ,  $l_2 = L_2/2$ ,  $l_3 = L_3/2$ . [Reference formula 6.3.7 page 99 of EDMONDS, A. R. Angular momentum in quantum mechanics. In *Investigations in Physics*, 4, Princeton U. Press, 1957]. The parameters of the procedure  $J_1, J_2, J_3, L_1, L_2, L_3$  are interpreted as being twice their physical value, so that actual parameters may be inserted as integers. Thus to calculate the 6-j symbol

$$\begin{Bmatrix} 2 & 2 & 0 \\ 2 & 2 & 0 \end{Bmatrix}$$

the call would be  $SJS(4, 4, 0, 4, 4, 0, factorial)$ . The procedure checks that the triangle conditions for the existence of a coefficient are satisfied and that  $j_1 + j_2 + j_3$ ,  $j_1 + l_2 + l_3$ ,  $l_1 + j_2 + l_3$  and  $l_1 + l_2 + j_3$  are integral. If the conditions are not satisfied the value of the procedure is zero. The parameter *factorial* is an array containing the factorials from 0 up to at least  $1 + \text{largest of } j_1 + j_2 + j_3, j_1 + l_2 + l_3, l_1 + j_2 + l_3$  and  $l_1 + l_2 + j_3$ . Since in actual calculations the procedure *SJS* will be called many times it is more economical to have the factorials in a global array rather than compute them on every

entry to the procedure. The notation is consistent with that used in the procedure for calculating Vector-coupling coefficients. See Algorithm 252, Vector Coupling or Clebsch-Gordan Coefficients [*Comm. ACM* 8 (Apr. 1965), 217];

```
begin integer w, wmin, wmax;
real omega;
real procedure delta (a, b, c);
  value a, b, c;
  integer a, b, c;
begin delta := sqrt (factorial [(a+b-c)÷2]
  × factorial [(a-b+c)÷2]
  × factorial [(-a+b+c)÷2]/factorial [(a+b+c+2)÷2])
end delta;
if J1 + J2 < J3 ∨ abs(J1 - J2) > J3 ∨ J1 + J2 + J3 ≠ 2 ×
  2 × ((J1+J2+J3)÷2)
  ∨ J1 + L2 < L3 ∨ abs(J1-L2) > L3 ∨ J1 + L2 + L3 ≠ 2 ×
  ((J1+L2+L3)÷2)
  ∨ L1 + J2 < L3 ∨ abs(L1-J2) > L3 ∨ L1 + J2 + L3 ≠ 2 ×
  ((L1+J2+L3)÷2)
  ∨ L1 + L2 < J3 ∨ abs(L1-L2) > J3 ∨ L1 + L2 + J3 ≠ 2 ×
  ((L1+L2+J3)÷2)
then SJS := 0 else
begin
  omega := 0;
  wmin := J1 + J2 + J3;
  if wmin < J1 + L2 + L3 then wmin := J1 + L2 + L3;
  if wmin < L1 + J2 + L3 then wmin := L1 + J2 + L3;
  if wmin < L1 + L2 + J3 then wmin := L1 + L2 + J3;
  wmax := J1 + J2 + L1 + L2;
  if wmax > J2 + J3 + L2 + L3 then wmax := J2 + J3 +
    L2 + L3;
  if wmax > J3 + J1 + L3 + L1 then wmax := J3 + J1 +
    L3 + L1;
  for w := wmin step 2 until wmax do
    omega := omega + (if w=4×(w÷4) then 1 else -1)
    × factorial [w÷2+1]/(factorial [(w-J1-J2-J3)÷2]
    × factorial [(w-J1-L2-L3)÷2]
    × factorial [(w-L1-J2-L3)÷2]
    × factorial [(w-L1-L2-J3)÷2]
    × factorial [(J1+J2+L1+L2-w)÷2]
    × factorial [(J2+J3+L2+L3-w)÷2]
    × factorial [(J3+J1+L3+L1-w)÷2]);
  SJS := delta (J1, J2, J3) × delta (J1, L2, L3)
    × delta (L1, J2, L3) × delta (L1, L2, J3) × omega;
end
end SJS
```

## ALGORITHM 261

### 9-J SYMBOLS [Z]

J. H. GUNN (Recd. 13 Nov. 1964)

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```
real procedure NJS(J11, J12, J13, J21, J22, J23, J31, J32, J33,
  factorial);
  value J11, J12, J13, J21, J22, J23, J31, J32, J33;
  integer J11, J12, J13, J21, J22, J23, J31, J32, J33;
  array factorial;
comment NJS calculates the 9-j symbols defined by the following formula
```

$$\begin{Bmatrix} j_{11} & j_{12} & j_{13} \\ j_{21} & j_{22} & j_{23} \\ j_{31} & j_{32} & j_{33} \end{Bmatrix} = \sum_k (-1)^{2k} (2k+1) \begin{Bmatrix} j_{11} & j_{21} & j_{31} \\ j_{32} & j_{33} & k \end{Bmatrix} \begin{Bmatrix} j_{12} & j_{22} & j_{32} \\ j_{21} & k & j_{23} \\ j_{32} & j_{33} & k \end{Bmatrix}$$

where  $j_{11} = J_{11}/2$ ,  $j_{12} = J_{12}/2$ ,  $j_{13} = J_{13}/2$ ,  $j_{21} = J_{21}/2$ ,

$j22 = J22/2$ ,  $j23 = J23/2$ ,  $j31 = J31/2$ ,  $j32 = J32/2$ ,  $j33 = J33/2$  [Reference formula 6.4.3 page 101 of EDMONDS, A. R. Angular momentum in quantum mechanics. In *Investigations in Physics*, 4, Princeton U. Press, 1957]. The parameters of the procedure  $J11, J12, J13, J21, J22, J23, J31, J32, J33$  are interpreted as being twice their physical value, so that actual parameters may be inserted as integers. Thus to calculate the 9-j symbol

$$\begin{Bmatrix} 2 & 2 & 0 \\ 2 & 2 & 0 \\ 0 & 0 & 0 \end{Bmatrix}$$

the call would be  $NJS(4, 4, 0, 4, 4, 0, 0, 0, 0, factorial)$ . The procedure checks that the triangle conditions for the existence of a coefficient are satisfied and that  $j11 + j21 + j31$ ,  $j21 + j22 + j23$ ,  $j31 + j32 + j33$ ,  $j11 + j12 + j13$ ,  $j12 + j22 + j32$ ,  $j13 + j23 + j33$  are integral. If the conditions are not satisfied the value of the procedure is zero. The parameter *factorial* is an array containing the factorials from 0 up to at least  $1 + \text{largest of } j11 + j21 + j31, j21 + j22 + j23, j31 + j32 + j33, j11 + j12 + j13, j12 + j22 + j32, j13 + j23 + j33$ . The procedure makes use of the procedure *SJS* [Algorithm 260, 6-j symbols, *Comm. ACM* 8 (Aug. 1965), 492], for calculating 6-j symbols;

```

begin integer k, kmin, kmax;
real NJ;
if J11 + J21 < J31 ∨ abs(J11-J21) > J31 ∨ J11 + J21 +
   J31 ≠ 2 × ((J11+J21+J31)÷2)
   √ J21 + J22 < J23 ∨ abs(J21-J22) > J23 ∨ J21 + J22 +
   J23 ≠ 2 × ((J21+J22+J23)÷2)
   √ J31 + J32 < J33 ∨ abs(J31-J32) > J33 ∨ J31 + J32 +
   J33 ≠ 2 × ((J31+J32+J33)÷2)
   √ J11 + J12 < J13 ∨ abs(J11-J12) > J13 ∨ J11 + J12 +
   J13 ≠ 2 × ((J11+J12+J13)÷2)
   √ J12 + J22 < J32 ∨ abs(J12-J22) > J32 ∨ J12 + J22 +
   J32 ≠ 2 × ((J12+J22+J32)÷2)
   √ J13 + J23 < J33 ∨ abs(J13-J23) > J33 ∨ J13 + J23 +
   J33 ≠ 2 × ((J13+J23+J33)÷2)
then NJS := 0 else
begin NJ := 0;
kmin := abs(J21-J32);
if kmin < abs(J11-J33) then kmin := abs(J11-J33);
if kmin < abs(J12-J23) then kmin := abs(J12-J23);
kmax := J21 + J32;
if kmax > J11 + J33 then kmax := J11 + J33;
if kmax > J12 + J23 then kmax := J12 + J23;
for k := kmin step 2 until kmax do
NJ := NJ + (if k=2×(k÷2) then 1 else -1) × (k+1) ×
   SJS(J11, J21, J31, J32, J33, k, factorial) ×
   SJS(J12, J22, J32, J21, k, J23, factorial) ×
   SJS(J13, J23, J33, k, J11, J12, factorial);
NJS := NJ
end
end NJS

```

## ALGORITHM 262

### NUMBER OF RESTRICTED PARTITIONS OF N [A1]

J. K. S. MCKAY (Recd. 7 Dec. 1964 and 9 Mar. 1965)  
Computer Unit, University of Edinburgh, Scotland

```

procedure set(p, N); integer N; integer array p;
comment The number of partitions of n with parts less than
or equal to m is set in p[n, m] for all n, m such that N ≥ n ≥
m ≥ 0.

```

#### REFERENCES:

- GUPTA, H., GWYTHOR, C. E., AND MILLER, J. C. P. Tables of

partitions. In *Royal Society Mathematical Tables*, vol. 4, Cambridge U. Press, 1958.

2. HARDY, G. H., AND WRIGHT, E. M. *The Theory of Numbers*. Ch. 19, 4th ed., Clarendon Press, Oxford, 1960;

```

begin integer m, n;
p[0, 0] := 1;
for n := 1 step 1 until N do
begin p[n, 0] := 0;
  for m := 1 step 1 until n do
    p[n, m] := p[n, m-1] +
      p[n-m, if n-m < m then n-m else m]
  end
end set

```

## ALGORITHM 263

### PARTITION GENERATOR [A1]

J. K. S. MCKAY (Recd. 7 Dec. 1964 and 9 Mar. 1965)  
Computer Unit, University of Edinburgh, Scotland.

```

procedure generate(p, N, position, ptn, length);
integer array p, ptn; integer N, length, position;
comment The partitions of N may be mapped in their natural
order, 1 – 1, onto the consecutive integers from 0 to P(N) – 1
where P(N) (= p[N, N]) is the number of unrestricted partitions
of N. The array p is set by the procedure set [Algorithm 262,
Number of Restricted Partitions of N, Comm. ACM 8 (Aug.
1965), 493]. On entry position contains the integer into which
the partition is mapped. On exit length contains the number of
parts and ptn[1: length] contains the parts of the partition in
descending order.

```

#### REFERENCE:

- LITTLEWOOD, D. E. *The Theory of Group Characters*. Ch. 5, 2nd ed., Clarendon Press, Oxford, 1958;

```

begin integer m, n, psn;
n := N; psn := position; length := 0;
A: length := length + 1; m := 1;
B: if p[n, m] < psn then begin m := m + 1; go to B end else
  if p[n, m] > psn then
C: begin
  ptn[length] := m; psn := psn - p[n, m-1]; n := n - m;
  if n ≠ 0 then go to A; go to D
end
else m := m + 1; go to C;
D: end generate

```

## ALGORITHM 264

### MAP OF PARTITIONS INTO INTEGERS [A1]

J. K. S. MCKAY (Recd. 7 Dec. 1964 and 9 Mar. 1965)  
Computer Unit, University of Edinburgh, Scotland

```

integer procedure place(p, n, ptn); value n;
integer array p, ptn; integer n;
comment place is the inverse of the procedure generate [Al-
gorithm 263, Partition Generator, Comm. ACM 8 (Aug. 1965),
493]. The array p is set by the procedure set [Algorithm 262,
Number of Restricted Partitions of N, Comm. ACM 8 (Aug.
1965), 493]. The procedure produces the integer into which
the partition of n, stored in descending order of parts in ptn[1]
onwards, is mapped;

```

```

begin integer j, d;
d := 0;
if n = 0 then go to B;
j := 0;
A: j := j + 1; d := p[n, ptn[j]-1] + d; n := n - ptn[j];
  if n ≠ 0 then go to A;
B: place := d
end place

```