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ALGORITHM 260

6-J SYMBOLS [Z]

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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

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

where

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

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 *J1, J2, J3, L1, L2, L3* 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 $1 + \text{largest of } j_1 + j_2 + j_3, j_1 + l_2 + l_3, l_1 + j_2 + l_3 \text{ and } l_1 + l_2 + j_3$. 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 $J_1 + J_2 < J_3 \vee \text{abs}(J_1 - J_2) > J_3 \vee J_1 + J_2 + J_3 \neq 2 \times ((J_1+J_2+J_3) \div 2)$
 $\vee J_1 + L_2 < L_3 \vee \text{abs}(J_1 - L_2) > L_3 \vee J_1 + L_2 + L_3 \neq 2 \times ((J_1+L_2+L_3) \div 2)$
 $\vee L_1 + J_2 < L_3 \vee \text{abs}(L_1 - J_2) > L_3 \vee L_1 + J_2 + L_3 \neq 2 \times ((L_1+J_2+L_3) \div 2)$
 $\vee L_1 + L_2 < J_3 \vee \text{abs}(L_1 - L_2) > J_3 \vee L_1 + L_2 + J_3 \neq 2 \times ((L_1+L_2+J_3) \div 2)$
then *SJS* := 0 **else**
begin
omega := 0;
wmin := $J_1 + J_2 + J_3$;
if *wmin* < $J_1 + L_2 + L_3$ **then** *wmin* := $J_1 + L_2 + L_3$;
if *wmin* < $L_1 + J_2 + L_3$ **then** *wmin* := $L_1 + J_2 + L_3$;
if *wmin* < $L_1 + L_2 + J_3$ **then** *wmin* := $L_1 + L_2 + J_3$;
wmax := $J_1 + J_2 + L_1 + L_2$;
if *wmax* > $J_2 + J_3 + L_2 + L_3$ **then** *wmax* := $J_2 + J_3 + L_2 + L_3$;
if *wmax* > $J_3 + J_1 + L_3 + L_1$ **then** *wmax* := $J_3 + J_1 + L_3 + L_1$;
for *w* := *wmin* **step** 2 **until** *wmax do*
omega := *omega* + (**if** $w=4 \times (w \div 4)$ **then** 1 **else** -1)
× *factorial* [$w \div 2 + 1$]/(*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]

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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

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

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

$j_{22} = J_{22}/2$, $j_{23} = J_{23}/2$, $j_{31} = J_{31}/2$, $j_{32} = J_{32}/2$, $j_{33} = J_{33}/2$ [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 J_{11} , J_{12} , J_{13} , J_{21} , J_{22} , J_{23} , J_{31} , J_{32} , J_{33} are interpreted as being twice their physical value, so that actual parameters may be inserted as integers. Thus to calculate the 9- j symbol

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

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 $j_{11} + j_{21} + j_{31}$, $j_{21} + j_{22} + j_{23}$, $j_{31} + j_{32} + j_{33}$, $j_{11} + j_{12} + j_{13}$, $j_{12} + j_{22} + j_{32}$, $j_{13} + j_{23} + j_{33}$ 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 $1 + \text{largest of } j_{11} + j_{21} + j_{31}, j_{21} + j_{22} + j_{23}, j_{31} + j_{32} + j_{33}, j_{11} + j_{12} + j_{13}, j_{12} + j_{22} + j_{32}, j_{13} + j_{23} + j_{33}$. 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  $J_{11} + J_{21} < J_{31} \vee \text{abs}(J_{11}-J_{21}) > J_{31} \vee J_{11} + J_{21} + J_{31} \neq 2 \times ((J_{11}+J_{21}+J_{31})\div 2)$ 
∨  $J_{21} + J_{22} < J_{23} \vee \text{abs}(J_{21}-J_{22}) > J_{23} \vee J_{21} + J_{22} + J_{23} \neq 2 \times ((J_{21}+J_{22}+J_{23})\div 2)$ 
∨  $J_{31} + J_{32} < J_{33} \vee \text{abs}(J_{31}-J_{32}) > J_{33} \vee J_{31} + J_{32} + J_{33} \neq 2 \times ((J_{31}+J_{32}+J_{33})\div 2)$ 
∨  $J_{11} + J_{12} < J_{13} \vee \text{abs}(J_{11}-J_{12}) > J_{13} \vee J_{11} + J_{12} + J_{13} \neq 2 \times ((J_{11}+J_{12}+J_{13})\div 2)$ 
∨  $J_{12} + J_{22} < J_{32} \vee \text{abs}(J_{12}-J_{22}) > J_{32} \vee J_{12} + J_{22} + J_{32} \neq 2 \times ((J_{12}+J_{22}+J_{32})\div 2)$ 
∨  $J_{13} + J_{23} < J_{33} \vee \text{abs}(J_{13}-J_{23}) > J_{33} \vee J_{13} + J_{23} + J_{33} \neq 2 \times ((J_{13}+J_{23}+J_{33})\div 2)$ 
then  $NJS := 0$  else
begin  $NJ := 0$ ;
   $kmin := \text{abs}(J_{21}-J_{32})$ ;
  if  $kmin < \text{abs}(J_{11}-J_{33})$  then  $kmin := \text{abs}(J_{11}-J_{33})$ ;
  if  $kmin < \text{abs}(J_{12}-J_{23})$  then  $kmin := \text{abs}(J_{12}-J_{23})$ ;
   $kmax := J_{21} + J_{32}$ ;
  if  $kmax > J_{11} + J_{33}$  then  $kmax := J_{11} + J_{33}$ ;
  if  $kmax > J_{12} + J_{23}$  then  $kmax := J_{12} + J_{23}$ ;
  for  $k := kmin$  step 2 until  $kmax$  do
     $NJ := NJ + (\text{if } k=2 \times (k\div 2) \text{ then } 1 \text{ else } -1) \times (k+1) \times$ 
       $SJS(J_{11}, J_{21}, J_{31}, J_{32}, J_{33}, k, factorial) \times$ 
       $SJS(J_{12}, J_{22}, J_{32}, J_{21}, k, J_{23}, factorial) \times$ 
       $SJS(J_{13}, J_{23}, J_{33}, k, J_{11}, J_{12}, factorial)$ ;
   $NJS := NJ$ 
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  $N \geq n \geq m \geq 0$ .

```

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```

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
         $p[n, m] := p[n, m-1] +$ 
           $p[n-m, \text{if } n-m < m \text{ then } n-m \text{ else } m]$ 
      end
    end
end set

```

ALGORITHM 263
PARTITION GENERATOR [A1]
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```

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:

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```

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

```

ALGORITHM 264
MAP OF PARTITIONS INTO INTEGERS [A1]
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```

integer procedure place ( $p, n, ptn$ ); value  $n$ ;
integer array  $p, ptn$ ; integer  $n$ ;
comment place is the inverse of the procedure generate [Algorithm 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  $n \neq 0$  then go to  $A$ ;
   $B: \text{place} := d$ 
end place

```