APR 15 1964

LAAC-6300

81691

MASTER

IRREDUCIBLE REPRESENTATIONS*

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* This work was performed under the auspices of the United States Atomic Energy Commission.

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procedure out;

comment In problems dealing with electron spins, it is frequently useful to know the irreducible representations for the permutation group on n elements corresponding to a Young Tableaux of one or two rows. These representations are conveniently indexed by $\underline{k} = 0, \dots, [\underline{n}/2]$, the number of items in the second row of the Young Tableaux. As all the irreducible representations of the simple permutations of the form $(\underline{i}, \underline{i}+1)$ can be formed as a direct sum of the irreducible representations of the form $(\underline{n}-1, \underline{n})$ we have written an algorithm, irreducible, to produce the $(\underline{n}, \underline{k})$ irreducible representation of the $(\underline{n}-1, \underline{n})$ permutation and an algorithm, LOW, to assemble the $(\underline{i}, \underline{i}+1)$ $1 \leq \underline{i} \leq \underline{n} - 2$ permutations. As any permutation can, if desired, be factored into a product of $(\underline{i}, \underline{i}+1)$ permutations, the relevant group theory is exhausted by these algorithms;

integer n, n, k, i, j, BDB;

integer array F, Dbar [1: nmax, 0: kmax];

real array M [1: Mmax], B [0: nmax, -2: nmax];

comment This procedure contains all the output statements. For values of nmax, kmax, mmax, and Mmax see the table in the comment in LOW;

begin LOW (F, Dbar, M, B);

write ('binomial coefficients' for i: = 0 step 1 until nmax do

begin comment Double space to a new line; for j: = -2 step 1 until nmax do B [i, j] end);

comment The first nmax + 1 lines of the table of binomial coefficients will be listed as below:

0	0	1	0	0	0	0	0	0	0
0	0	1	1	0	0	0	0	0	0
0	0	1	2	1	0	0	0	0	0
0	0	1	3	3	1	0	0	0	0
0	0	1	4	6	4	1	0	0	0
0	0	1	5	10	10	5	1	0	0
0	0	1	6	15	20	15	6	1	0
0	0	1	7	21	35	35	21	7	1

for n := 2 step 1 until nmax do

for k := 0 step 1 until n ÷ 2 do

for BDB := 1 step 1 until n - 1 do begin

comment For a description of the use of F and Dbar see the comment
in procedure LOW;

write (comment Start a new page; 'n' = 'n', 'k' = 'k', 'permutation ('BDB', 'BDB + 1')

for i := 1 step 1 until Dbar [n,k] do begin comment Double space to a new

line; for j := 1 + F [n,k] + (BDB-1) × Dbar [n,k] ↑ 2 step Dbar [n,k] until

F [n,k] + Dbar [n,k] ↑ 2 do M [j] end); end;

comment A sample of the output, for $\underline{n} = 5$, follows:

$\underline{n} = 5$ $\underline{k} = 0$ permutation (1,2)

1

$\underline{n} = 5$ $\underline{k} = 0$ permutation (2,3)/

1

$\underline{n} = 5$ $\underline{k} = 0$ permutation (3,4)

1

$\underline{n} = 5$ $\underline{k} = 0$ permutation (4,5)

1

$\underline{n} = 5$ $\underline{k} = 1$ permutation (1,2)

-1 0 0 0

0 1 0 0

0 0 1 0

0 0 0 1

$\underline{n} = 5$ $\underline{k} = 1$ permutation (2,3)

$1/2$ $\sqrt{3}/2$ 0 0

$\sqrt{3}/2$ $-1/2$ 0 0

0 0 1 0

0 0 0 1

$\underline{n} = 5$ $\underline{k} = 1$ permutation (3,4)

1 0 0 0

0 $1/3$ $2\sqrt{2}/3$ 0

0 $2\sqrt{2}/3$ $-1/3$ 0

0 0 0 1

n = 5 k = 1 permutation (4,5)

1	0	0	00
0	1	0	0
0	0	1/4	$\sqrt{15}/4$
0	0	$\sqrt{15}/4$	-1/4

n = 5 k = 2 permutation (1,2)

-1	0	0	0	0
0	1	0	0	0
0	0	-1	0	0
0	0	0	1	0
0	0	0	0	1

n = 5 k = 2 permutation (2,3)

1/2	$\sqrt{3}/2$	0	0	0
$\sqrt{3}/2$	-1/2	0	0	0
0	0	1/2	$\sqrt{3}/2$	0
0	0	$\sqrt{3}/2$	-1/2	0
0	0	0	0	1

n = 5 k = 2 permutation (3,4)

-1	0	0	0	0
0	1	0	0	0
0	0	1	0	0
0	0	0	1/3	$2\sqrt{2}/3$
0	0	0	$2\sqrt{2}/3$	1/3

<u>n</u> = 5	<u>k</u> = 2	<u>permutation</u> (4,5)		
1/2	0	$\sqrt{3}/2$	0	00
0	1/2	0	$\sqrt{3}/2$	0
$\sqrt{3}/2$	0	-1/2	0	0
0	$\sqrt{3}/2$	0	-1/2	0
0	0	0	0	1 ;

end procedure out

procedure LOW (F, Dbar, M, B);

integer n, k, m, i, j, Loc, BDB, mtilde;

integer array F, Dbar [1:mmax, 0:kmax];

real array M[1:Mmax], I[1:mmax, 1:mmax], B[0:mmax, -2:mmax];

comment A single irreducible representation for a type (n-1,n) permutation is generated and stored in temporary storage array I by irreducible and then transferred by LOW to M for permanent storage. Permutations of the type (i, i+1) with $1 \leq i \leq n-2$ are assembled from the M array using the irreducible representations for n-1.

Dbar[n,k] contains m the size of the square matrix for the (n,k) irreducible representations. M[F[n,k] + 1] is where the first word of the first permutation for (n,k) is stored. The permutations are stored in the order (1,2), (2,3), (3,4), ..., (n-1,n). The first word of the (i,i+1) permutation is in M[F[n,k] + (i-1) × Dbar [n,k]² + 1]. B contains a table of binomial coefficients.

These procedures were written in COLASL for an IBM 7030 computer as part of a larger program. Using disk storage all irreducible representations for permutations of the types $(\underline{1}, \underline{1}+1)$ and $(\underline{1}, \underline{1}+1)$ $1 \leq \underline{1} \leq \underline{n} - 1$ with $2 \leq \underline{n} \leq 11$, $0 \leq \underline{k} \leq \underline{n} \div 2$ have been generated and tested. Matrices corresponding to $2 \leq \underline{n} \leq 9$, $0 \leq \underline{k} \leq \underline{n} \div 2$ have been checked with those given by Katsura.¹ For values $2 \leq \underline{n} \leq 5$, $0 \leq \underline{k} \leq \underline{n} \div 2$ the matrices agree with those given by Hamermesh,² except for $\underline{n} = 5$, $\underline{k} = 2$ which, as Katsura¹ pointed out, is erroneous. The convention used by Katsura¹ and Hamermesh² is to give the transpose about the secondary diagonal of our resulting matrices.

All array lengths are determined by the maximum value of $\underline{n}$. The table below indicates the necessary array lengths for values of maximum $\underline{n}$:

<u>nmax</u>	<u>kmax</u>	<u>mmax</u>	<u>Mmax</u>
2	1	1	2
3	1	2	12
4	2	3	54
5	2	5	222
6	3	9	882
7	3	14	3456
8	4	28	13466
9	4	48	52362
10	5	90	203526
11	5	165	791386;

¹ S. Katsura, J. Chem. Phys. 38, 3033 (1963). Doc. No. 7567 with ADI Auxiliary Pub. Project.

² M. Hamermesh, Group Theory and Its Application to Physical Problems (Addison-Wesley, Reading, Mass. 1962) p. 224-228.

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begin

for i: = 1 step 1 until mmax do

for j: = 0 step 1 until kmax do

F[i,j]: = Dbar[i,j]: = 0;

for i: = 1 step 1 until Mmax do M[i]: = 0;

binomial (B);

Loc: = 0; n: = 2; k: = 0;

first: irreducible (n, k, I, m, B);

comment The (n - 1, n) permutation is now stored in the array I. If n = 2,
the permutation will be stored in M. If n ≠ 2, the (i, i+1), 1 ≤ i < n - 2,
permutations will be assembled from M and stored before I is stored;

Dbar[n,k]: = m; F[n,k]: = Loc; if n = 2 then go to LJ; BDB: = 1;

if n - 1 < 2 × k then go to kone;

D1: mtilde = Dbar [n-1,k]; Kone: = F[n-1,k] + (BDB-1) × mtilde ↑ 2;

for i: = 1 step 1 until mtilde do
for j: = 1 step 1 until mtilde do
M[(j-1) × m + i + Loc]: = M[(j-1) × mtilde + i + Kone];

kone: if k < 1 then go to Loc1; mtilde: = Dbar [n-1,k-1];

Kone: = F[n-1,k-1] + (BDB-1) × mtilde ↑ 2;

for i: = 1 step 1 until mtilde do
for j: = 1 step 1 until mtilde do M[(D[1,0] + j-1) × m+1+D[1,0] + Loc]
: = M[(j-1) × mtilde + i + Kone];

Loc1: Loc = Loc + m ↑ 2; if BDB < n-2 then begin BDB: = BDB + 1; go to D1 end;

LJ: for i: = 1 step 1 until m do for j: = 1 step 1 until m do
M[(j-1) × m + i + Loc]: = I[i,j]; Loc: = Loc + m ↑ 2;

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k: = k + 1; if n ≥ 2 × k then go to first; k: = 0; n: = n + 1;

if n < nmax + 1 then go to first;

end procedure LOW

procedure irreducible (n, k, I, m, B);

real oddiag, onon;

integer n, k, m, i, j

real array I[1:mmax, 1:mmax], B[0:mmax, -2:mmax];

comment I is the name of the array where this procedure will store
the irreducible representation matrix of size m rows by m
columns;

integer array D[0:2, 0:2];

begin

for i: = 1 step 1 until mmax do

for j: = 1 step 1 until mmax do I[i, j] = 0;

if k = 0 then begin m: = 1; I[1,1]: = 1; go to return; end;

D[0,0]: = B[n,k] - B[n,k-1]; if n - 1 < 2 × k then

begin D[1,0]: = D[1,1]: = D[1,2]: = 0; go to two; end;

D[1,0]: = B[n-1,k] - B[n-1,k-1]; if n - 2 < 2 × k then begin

D[1,1]: = 0; go to next; end; D[1,1]: = B[n-2,k] - B[n-2,k-1];

next:

if k = 1 then begin D[1,2]: = D[2,0]: = D[2,1]: = 1; D[2,2] = 0; go to

check; end;

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D[1,2]: = B[n-2,k-1] - B[n-2,k-2];

two:   D[2,0]: = B[n-1,k-1] - B[n-1,k-2];
       D[2,1]: = B[n-2,k-1] - B[n-2,k-2];
       D[2,2]: = B[n-2,k-2] - B[n-2,k-3];

check: m = D[0,0];
       for i: = 1 step 1 until D[1,1] do I[i,i]: = 1;
       for i: = D[1,0] + D[2,1] + 1 step 1 until D[0,0] do I[i,i]: = 1;
       if D[1,2] = 0 then go to three;
       odiag: = 1/(n-2 x k+1); onon: = (1-odiag ↑2) ↑.5;
       for i: = D[1,1] + 1 step 1 until D[1,0] do I[i,i]: = odiag;
       for i: = D[1,0] + 1 step 1 until D[1,0] + D[2,1] do I[i,i] = - odiag;
       for i: = 1 step 1 until D[1,2] do I[D[1,1] + i, D[1,0] + i]: = I[D[1,0]
           + i, D[1,1] + i]: = onon; go to return;

three: for i: = D[1,0] + 1 step 1 until D[1,0] + D[2,1] do I[i,i]: = - 1;

return: end procedure irreducible

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procedure binomial (B);

real array B[0:nmax, -2:nmax];

integer i, j;

comment This procedure generates and stores the binomial coefficients
        in the array B;

begin

for i := 0 step 1 until nmax do

for j := -2 step 1 until nmax do

B[i, j] := if j = 0 and i = j then 1 else 0;

for j := 1 step 1 until nmax do

for i := j+1 step 1 until nmax do B[i, j] := B[i-1, j-1] + B[i-1, j];

end procedure binomial

```