SAMMY Workshop Part 4.1d

Dr. Nancy M. Larson
Oak Ridge National Laboratory

Part 4.1d. Spin group assignments

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OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

Spin groups

- Two different channels can lead to the same compound nucleus if they have the same compound-nucleus quantum numbers
  - mass $m+M$
  - charge $z+Z$
  - spin and parity J^{π}
- SAMMY notation: a "spin group" consists of all those channels contributing to the same compound nucleus
  - Channels have different quantum numbers but the same J^{π}

SAMMY's philosophy re spin groups

- Responsibility for defining the spin groups belongs to the SAMMY user
  - NOT to the SAMMY author
- Why?
  - Evaluators require flexibility
    - Sometimes you want to see the cross section for individual spin groups, for example
  - Some spin groups (or some channels for some spin groups) may have negligible contribution to the cross section

SAMMY's philosophy, cont.

- Suggestion has been made that SAMMY should require the user to *always* use *all* spin groups
  - Person who made suggestion was not an evaluator
  - He wanted to prevent a recurrence of a mistake someone made in an ENDF file 20 or 30 years ago

SAMMY's philosophy, cont.

- My response: No.
  - What does *all* mean?
    - For every l, require all possible J ?
    - For every J, require all possible l ?
  - No sense in spending CPU time to calculate zero
    - Negligible channels might as well be omitted
  - The only person competent to judge which channels and spin groups are important is the evaluator
    - NOT the author of the SAMMY code
    - Certainly NOT the author of the processor code

SAMMY's philosophy, cont.

- SAMMY user must therefore be careful to include all possible channels for all possible spin groups
  - Drop only those which are truly negligible
  - SAMMY and SAMQUA will provide guidance
    - SAMQUA ➔ provide QUAntum numbers for SAMmy
    - Completely rewritten in collaboration with Cadarache colleagues (Bouland and Babut)
    - Code is distributed with SAMMY code

SAMQUA

- Generates quantum numbers for spin groups and associated channels
- Treats all types of nuclides, charged particles, inelastic channels, reaction channels, etc.
- Produces output in SAMMY input Particle-Pair format
- Also provides values of penetrabilities and of hard-sphere cross sections

SAMQUA, cont.

- **Documentation:**
  - **"SAMQUA - A Program for Generating All Possible Combinations of Quantum Numbers Leading to the Same Compound Nucleus State in the Framework of the R-matrix Code SAMMY,"**
    - **Olivier Bouland, Richard Babut (Laboratoire d'Etudes de Physique, CEA/Cadarache, France), and Nancy M. Larson (ORNL)**
    - **JEFDOC 929 OECD/NEA Publications and ENDF-363 (October 2003)**
  - **Paper by same title at ND2004 in Santa Fe**

How to generate spin groups

- Do use SAMQUA to be sure you haven't neglected important details
- Do not rely solely on SAMQUA – learn to understand how spin groups are found
- Next: a tutorial re how to determine all the relevant channels and spin groups for any particular incident channel
  - Implicit assumption: the analyst has included all relevant particle-pairs for exit channels

Notation

- **Incident channels:**
  - **incident particle: spin i and parity π**
  - **target particle: spin I and parity Π**
  - **possible channel spins are $|I - i| \leq s \leq I + i$**
  - **orbital angular momentum is l**
- **Exit channels:**
  - **first particle: spin i' and parity π'**
  - **target particle: spin I' and parity Π'**
  - **possible channel spins are $|I' - i'| \leq s' \leq I' + i'$**
  - **orbital angular momentum is l'**
- **For each l and l',**
  - **figure possible *J-parity* values for incident channels**
  - **figure possible *J-parity* values for exit channels**
- **Channels with same *J-parity* are in same spin group**

Example: spin groups for $^{14}N(\alpha,n)^{17}F$

α: $i\ \pi = 0+$
^{14}N: $I\ \Pi = 1+$

n: $i\ \pi = 1/2+$
^{17}F: $I\ \Pi = 5/2+$

Step 1: tabulate all possible channels (for a given max l), perhaps on a spread sheet

	i	I	s	l	J
1	0+	1+	1+	0+	1+
2				1-	0-
3					1-
4					2-
5				2+	1+
6					2+
7					3+
8	1/2+	5/2+	2+	0+	2+
9				1-	1-
10					2-
11					3-
12				2+	0+
13					1+
14					2+
15					3+
16					4+
17			3+	0+	3+
18				1-	2-
19					3-
20					4-
21				2+	1+
22					2+
23					3+
24					4+
25					5+

Entrance channels

Exit channels

Example, continued

Step 2: fill in the blanks on the spread sheet

	i	*I*	*s*	*l*	*J*
1	0+	1+	1+	0+	1+
2	0+	1+	1+	1-	0-
3	0+	1+	1+	1-	1-
4	0+	1+	1+	1-	2-
5	0+	1+	1+	2+	1+
6	0+	1+	1+	2+	2+
7	0+	1+	1+	2+	3+
8	1/2+	5/2+	2+	0+	2+
9	1/2+	5/2+	2+	1-	1-
10	1/2+	5/2+	2+	1-	2-
11	1/2+	5/2+	2+	1-	3-
12	1/2+	5/2+	2+	2+	0+
13	1/2+	5/2+	2+	2+	1+
14	1/2+	5/2+	2+	2+	2+
15	1/2+	5/2+	2+	2+	3+
16	1/2+	5/2+	2+	2+	4+
17	1/2+	5/2+	3+	0+	3+
18	1/2+	5/2+	3+	1-	2-
19	1/2+	5/2+	3+	1-	3-
20	1/2+	5/2+	3+	1-	4-
21	1/2+	5/2+	3+	2+	1+
22	1/2+	5/2+	3+	2+	2+
23	1/2+	5/2+	3+	2+	3+
24	1/2+	5/2+	3+	2+	4+
25	1/2+	5/2+	3+	2+	5+

Example, continued

Step 3: Reorder by $J\,\pi$; assign spin-group numbers and channel numbers

Question: Why are some states not assigned to a spin group?

α: $i\,\pi = 0+$

^{14}N: $I\;\Pi = 1+$

n: $i\,\pi = 1/2+$

^{17}F: $I\;\Pi = 5/2+$

	i	I	s	l	J	sg#	ch#
2	0+	1+	1+	1-	0-	1	1
12	1/2+	5/2+	2+	2+	0+		
3	0+	1+	1+	1-	1-	2	1
9	1/2+	5/2+	2+	1-	1-	2	2
1	0+	1+	1+	0+	1+	3	1
5	0+	1+	1+	2+	1+	3	2
13	1/2+	5/2+	2+	2+	1+	3	3
21	1/2+	5/2+	3+	2+	1+	3	4
4	0+	1+	1+	1-	2-	4	1
10	1/2+	5/2+	2+	1-	2-	4	2
18	1/2+	5/2+	3+	1-	2-	4	3
6	0+	1+	1+	2+	2+	5	1
8	1/2+	5/2+	2+	0+	2+	5	2
14	1/2+	5/2+	2+	2+	2+	5	3
22	1/2+	5/2+	3+	2+	2+	5	4
11	1/2+	5/2+	2+	1-	3-		
19	1/2+	5/2+	3+	1-	3-		
7	0+	1+	1+	2+	3+	6	1
15	1/2+	5/2+	2+	2+	3+	6	2
17	1/2+	5/2+	3+	0+	3+	6	3
23	1/2+	5/2+	3+	2+	3+	6	4
20	1/2+	5/2+	3+	1-	4-		
16	1/2+	5/2+	2+	2+	4+		
24	1/2+	5/2+	3+	2+	4+		
25	1/2+	5/2+	3+	2+	5+		

Example, continued

Step 4: Construct the SAMMY INPut file

Legend:

a = spin group number
b = how many entrance channels
c = how many exit channels
d = channel number
e = 1 if penetrabilities are non-unity
f = 1 if shift factor is non-zero

πJ = parity, spin
z = charge for smaller particle
Z = charge for larger particle
L = orbital angular momentum
s = channel spin

a		b		c		πJ	
	d	z	e	Z	f	L	s
1			1		0	-0.0	
	1	2	1	7	0	1	+1.0
2			1		1	-1.0	
	1	2	1	7	0	1	+1.0
	2		1		0	1	+2.0
3			2		2	+1.0	
	1	2	1	7	0	0	+1.0
	2	2	1	7	0	2	+1.0
	3		1		0	2	+2.0
	4		1		0	2	+3.0
4			1		2	-2.0	
	1	2	1	7	0	1	+1.0
	2		1		0	1	+2.0
	3		1		0	1	+3.0
5			1		3	+2.0	
	1	2	1	7	0	2	+1.0
	2		1		0	0	+2.0
	3		1		0	2	+2.0
	4		1		0	2	+3.0
6			1		3	+3.0	
	1	2	1	7	0	2	+1.0
	2		1		0	0	+3.0
	3		1		0	2	+2.0
	4		1		0	2	+3.0

Exercises for the student

- Assume you need higher *l* values for the α + ^{14}N case described above. Generate the spin group information in this situation.
- What are the appropriate spin groups and channels for n + ^{16}O, assuming your measurements go above the (n,α) threshold?
- Extend to include inelastic channels.

New format options for INPut file

- **Problem**: formats for INPut file are becoming unwieldy due to options not originally available
  - outgoing channel particles have different masses and quantum numbers from incident channel particles
  - charge must be specified
  - threshold and radii must be given
- **Solution**: reorganize and simplify
  - specify the two particles (charge, spin, mass, threshold) independent of spin group definition; provide a label to pair
  - channel definition gives l and s plus pair-label

Example: t100a.inp – the “old” version

```
17O(alpha,n)20Ne fit (R. BABUT 03-13-2001) vs BAIR data (Phys. Rev. C 7,4,1973)
O17       16.99913   2000000.0 5500000.0         2  100
csisrs
spin of incident particle is +0.0
use new spin group format
cm coulomb excitation energies
cm non coulomb excitation energies
broadening is not wanted

   5.00000   1.000
REACTION CROSS SECTION
       2.5
  1      1    1 -0.5  1.000   2.5          17O
    1  2 1  8 0    3  2.5     0.0               0  5.00 5.00  16.99913 4.0026
    2    1    0    1  0.5     0.0         -588708. 3.8003.800 19.992436 1.0086649
  2      1    1  0.5  1.000   2.5          17O
    1  2 1  8 0    2  2.5     0.0               0  5.00 5.00  16.99913 4.0026
    2    1    0    0  0.5     0.0         -588708. 3.8003.800 19.992436 1.0086649
  3      2    1 -1.5  1.000   2.5          17O
    1  2 1  8 0    1  2.5     0.0               0  5.00 5.00  16.99913 4.0026
    2  2 1  8 0    3  2.5     0.0               0  5.00 5.00  16.99913 4.0026
    3    1    0    1  0.5     0.0         -588708. 3.8003.800 19.992436 1.0086649
  4      2    1  1.5  1.000   2.5          17O
    1  2 1  8 0    2  2.5     0.0               0  5.00 5.00  16.99913 4.0026
...
```

```
...
    2  2 1  8 0    4  2.5     0.0              0  5.00 5.00  16.99913 4.0026
    3    1    0    2  0.5     0.0        -588708. 3.8003.800 19.992436 1.0086649
  5      3    1 -2.5  1.000   2.5         17O
    1  2 1  8 0    1  2.5     0.0              0  5.00 5.00  16.99913 4.0026
    2  2 1  8 0    3  2.5     0.0              0  5.00 5.00  16.99913 4.0026
    3  2 1  8 0    5  2.5     0.0              0  5.00 5.00  16.99913 4.0026
    4    1    0    3  0.5     0.0        -588708. 3.8003.800 19.992436 1.0086649
  6      3    1  2.5  1.000   2.5         17O
    1  2 1  8 0    0  2.5     0.0              0  5.00 5.00  16.99913 4.0026
    2  2 1  8 0    2  2.5     0.0              0  5.00 5.00  16.99913 4.0026
    3  2 1  8 0    4  2.5     0.0              0  5.00 5.00  16.99913 4.0026
    4    1    0    2  0.5     0.0        -588708. 3.8003.800 19.992436 1.0086649
  7      3    1 -3.5  1.000   2.5         17O
    1  2 1  8 0    1  2.5     0.0              0  5.00 5.00  16.99913 4.0026
    2  2 1  8 0    3  2.5     0.0              0  5.00 5.00  16.99913 4.0026
    3  2 1  8 0    5  2.5     0.0              0  5.00 5.00  16.99913 4.0026
    4    1    0    3  0.5     0.0        -588708. 3.8003.800 19.992436 1.0086649

... [incomplete]
```

t100b.inp – the "new" version

```
17O(alpha,n)20Ne fit (R. BABUT 03-13-2001) vs BAIR data (Phys. Rev. C 7,4,1973)
O17        16.99913   2000000.0 5500000.0          2  100
csisrs
spin of incident particle is +0.0
cm coulomb excitation energies
cm non coulomb excitation energies
broadening is not wanted
particle-pair definitions are given
-----------------------------------------------------------------------------
a = default for incident, b = def for target
u = Lpent (1 or 0), v = Ishift (0 or 1)
name      a b   z   Zuv    i    I          m          M Threshold      Reff      Rtru
-----------------------------------------------------------------------------

alf+17O        2  810   0.0   2.5 4.0026000 16.999130            5.0000000 5.0000000
n+20Ne    n    0 1010   0.5   0.0 1.        19.992436 -588708.0 3.8000000 3.8000000

   5.00000   1.000
REACTION CROSS SECTION
  1       1    1 -0.5  1.000   2.5          17O
    1  alf+17O      3  2.5
    2  n+20Ne       1  0.5
  2       1    1  0.5  1.000   2.5          17O
    1  alf+17O      2  2.5
    2  n+20Ne       0  0.5
  3       2    1 -1.5  1.000   2.5          17O
...
```

Comments (between lines)

Information about the two particle pair sets

Spin groups then refer to particle-pair information

```
...
 1  alf+17O     1  2.5
    2  alf+17O     3  2.5
    3  n+20Ne      1  0.5
  4      2    1  1.5  1.000   2.5         17O
    1  alf+17O     2  2.5
    2  alf+17O     4  2.5
    3  n+20Ne      2  0.5
  5      3    1 -2.5  1.000   2.5         17O
    1  alf+17O     1  2.5
    2  alf+17O     3  2.5
    3  alf+17O     5  2.5
    4  n+20Ne      3  0.5
  6      3    1  2.5  1.000   2.5         17O
    1  alf+17O     0  2.5
    2  alf+17O     2  2.5
    3  alf+17O     4  2.5
    4  n+20Ne      2  0.5
  7      3    1 -3.5  1.000   2.5         17O
    1  alf+17O     1  2.5
    2  alf+17O     3  2.5
    3  alf+17O     5  2.5
    4  n+20Ne      3  0.5

[... incomplete]
```

t100by.inp – the "newest" version

```
17O(alpha,n)20Ne fit (R. BABUT 03-13-2001) vs BAIR data (Phys. Rev. C 7,4,1973)
O17        16.99913   2000000.0 5500000.0          2  100
csisrs
cm coulomb excitation energies
cm non coulomb excitation energies
broadening is not wanted
key-word particle-pair definitions are given

Name = alf+17O
   Pa = alpha      Pb=17O     Zb=8    Sb=2.5        Mb=16.999130
   Mass a = 4.0026000000
Name = n+20Ne
   pa=n  particle b = 20Ne  Zb=10  Mass b = 19.992436
   Q=588708.0

   5.00000   1.000
REACTION CROSS SECTION
  1       1     1 -0.5  1.000
    1  alf+17O      3  2.5
    2  n+20Ne       1  0.5
  2       1     1  0.5  1.000
    1  alf+17O      2  2.5
    2  n+20Ne       0  0.5
  3       2     1 -1.5  1.000
    1  alf+17O      1  2.5
    2  alf+17O      3  2.5
    3  n+20Ne       1  0.5 ...
```

Key word particle pair definitions

```
...
 4       2     1  1.5  1.000
    1  alf+17O      2  2.5
    2  alf+17O      4  2.5
    3  n+20Ne       2  0.5
 5       3     1 -2.5  1.000
    1  alf+17O      1  2.5
    2  alf+17O      3  2.5
    3  alf+17O      5  2.5
    4  n+20Ne       3  0.5
```

```
...
 6       3     1  2.5  1.000
    1  alf+17O      0  2.5
    2  alf+17O      2  2.5
    3  alf+17O      4  2.5
    4  n+20Ne       2  0.5
 7       3     1 -3.5  1.000
    1  alf+17O      1  2.5
    2  alf+17O      3  2.5
    3  alf+17O      5  2.5
    4  n+20Ne       3  0.5

[... incomplete]
```