The shell model code ANTOINE

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Lecture 3

Joint ICTP-IAEA Workshop on Nuclear Structure and Decay Data

The Shell Model code ANTOINE

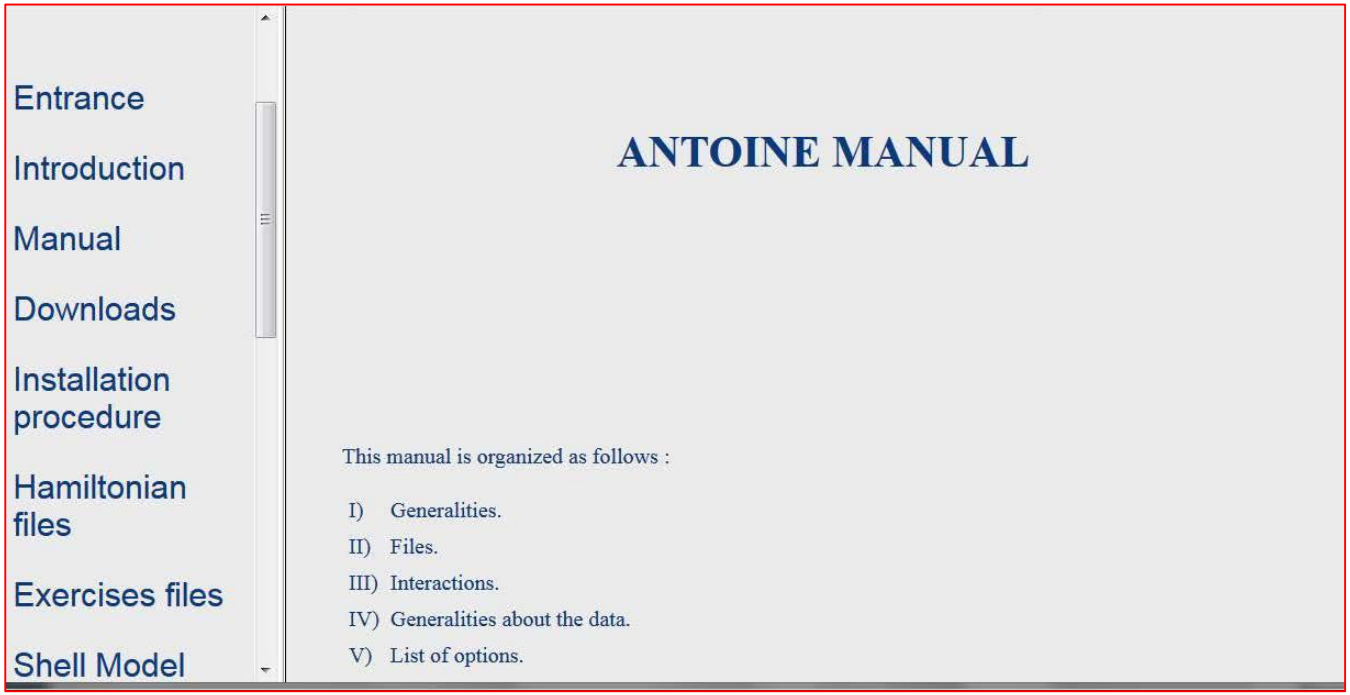
http://www.iphc.cnrs.fr/nutheo/code_antoine/menu.html

Created and maintained by E. Caurier and F. Nowacki, IPHC, Strasbourg

Antoine web page

You can find:

- the manual
- instructions to download
- hamiltonians
- lectures
- exercises



The Lanczos method

It creates a three-diagonal matrix and calculates the lowest states for each spin and parity

Start with a pivot state |1>

$$|\zeta_2\rangle = \hat{H}|1\rangle - H_{11}|1\rangle$$
$$H_{11} = \langle 1|\hat{H}|1\rangle, \quad \langle \zeta_2|1\rangle = 0$$
$$|2\rangle = |\zeta_2\rangle / H_{21}, \quad H_{21} = \langle \zeta_2|\zeta_2\rangle^{1/2}$$
$$H_{21} = \langle 2|\zeta_2\rangle = \langle 2|\hat{H}|1\rangle - H_{11}\langle 2|1\rangle = \langle 2|\hat{H}|1\rangle$$
$$|\zeta_3\rangle = \hat{H}|2\rangle - H_{22}|2\rangle - H_{21}|1\rangle$$
$$|3\rangle = |\zeta_3\rangle / H_{32}, \quad H_{32} = \langle \zeta_3|\zeta_3\rangle^{1/2} = \langle 3|\hat{H}|2\rangle$$
$$\ldots$$

We construct a 3x3 matrix

$$\begin{pmatrix} H_{11} & H_{12} & 0 \\ H_{21} & H_{22} & H_{23} \\ 0 & H_{32} & H_{33} \end{pmatrix}$$

$$H_{13} = H_{31} = 0$$

And find the first eigenvectors and eigenvalues with the same J and parity than |1>

The Lanczos method (2)

Now we proceed iterating at at each step we obtain a new vector:

$$\left|\zeta_{n+1}\right\rangle = \hat{H}\left|n\right\rangle - \sum_{i=1}^{n} H_{in}\left|i\right\rangle$$

$$\begin{pmatrix} H_{11} & H_{12} & 0 & 0 \\ H_{21} & H_{22} & H_{23} & 0 \\ 0 & H_{32} & H_{33} & H_{34} \\ 0 & 0 & H_{43} & H_{44} \end{pmatrix} \Rightarrow \dots$$

The determinant of such a matrix can be obtained iteratively

The process stops when the dimension of the space is reached.
One can decide to stop it when the energy of the states of interest is converged

It may need only a few iterations to get the lowest state of a 10^3 x 10^3 matrix converged!

Antoine Shell Model Code

Works in the m-scheme mode

Basis defined by:

- number of particles in Fluid 1, number and name of valence shells of Fluid 1
- number of particles in Fluid 2, number and name of valence shells of Fluid 2
- Total J projection M, parity of the states (0=positive, 1=negative

(All angular momentum quantum numbers are multiplied by 2)

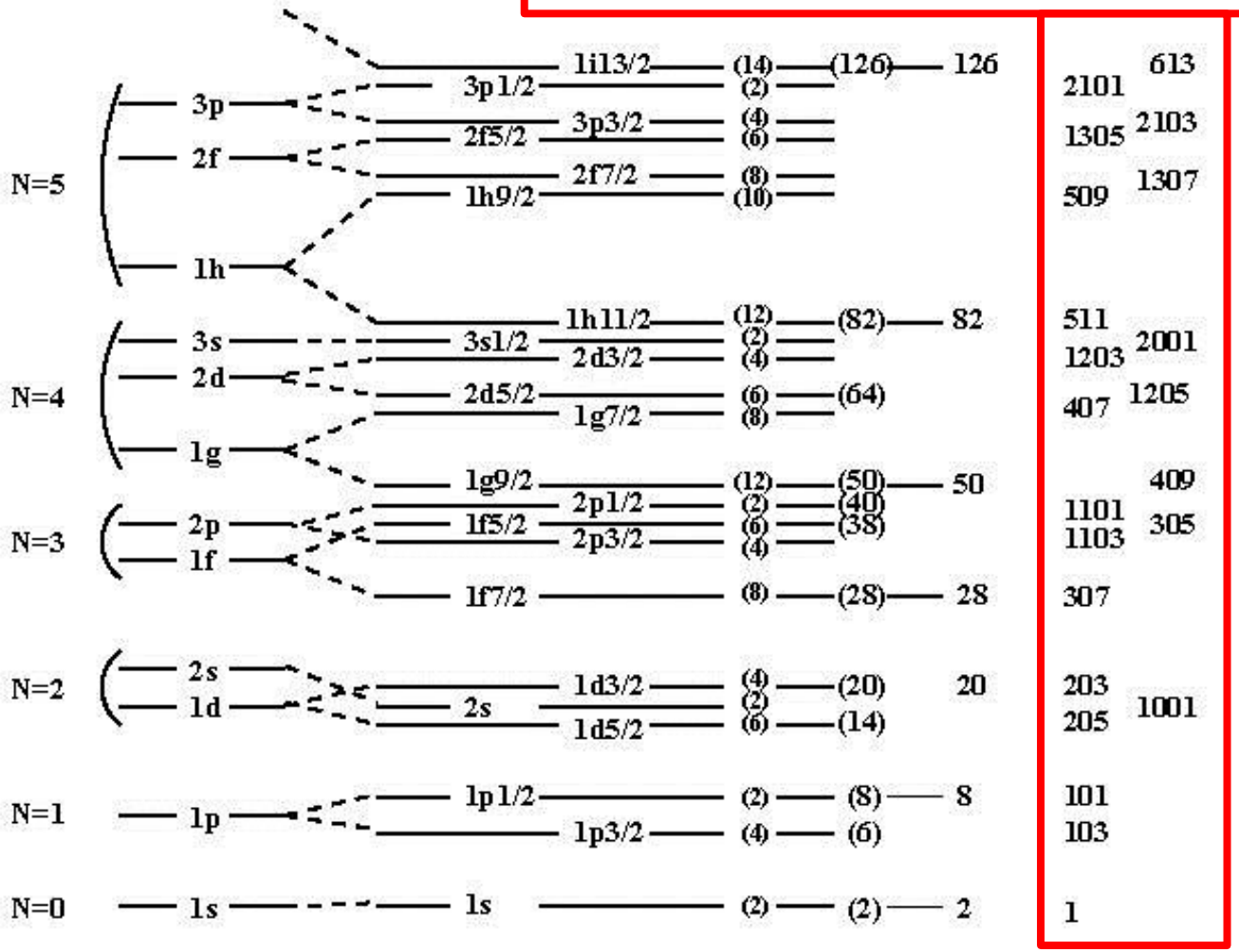
Notation used for the shells

- each shell is denoted by a single number, $1000 \times n + 100 \times l + 2 \times j$:

1	stands for	$0s_{\frac{1}{2}}$	305	stands for	$0f_{\frac{5}{2}}$
101	"	$0p_{\frac{1}{2}}$	307	"	$0f_{\frac{7}{2}}$
103	"	$0p_{\frac{3}{2}}$	2001	"	$2s_{\frac{1}{2}}$
1001	"	$1s_{\frac{1}{2}}$	1203	"	$1d_{\frac{3}{2}}$
203	"	$0d_{\frac{3}{2}}$	1205	"	$1d_{\frac{5}{2}}$
205	"	$0d_{\frac{5}{2}}$	407	"	$0g_{\frac{7}{2}}$
1101	"	$1p_{\frac{1}{2}}$	409	"	$0g_{\frac{9}{2}}$
1103	"	$1p_{\frac{3}{2}}$	511	"	$0h_{\frac{11}{2}}$

- the same notation holds for shells in the Hamiltonian file of TBME

Notation used for the shells



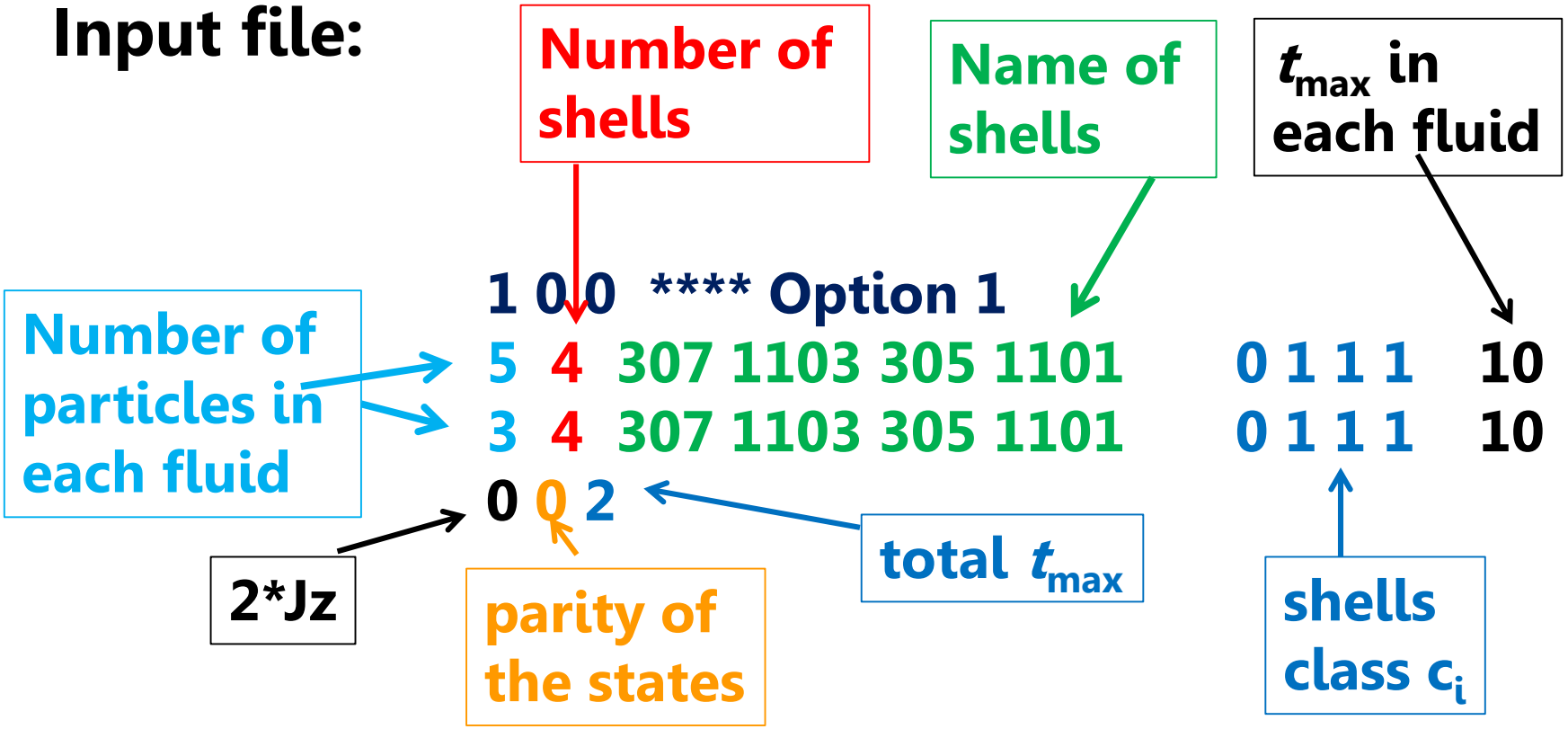
The program options

You can use Antoine to calculate **different useful and interesting nuclear properties** and observables.

In this lectures we will solve Schroedinger equations (**wavefunctions, energy levels**), and calculate **nuclear moments and electromagnetic transition probabilities**.

Option 1: Calculate the dimension of the basis

Input file:



The number of the option determines the type of calculation

Output file: ^{48}V

********** **CAS= 1** **********

CALCULATE DIMENSIONS OF THE SPACE

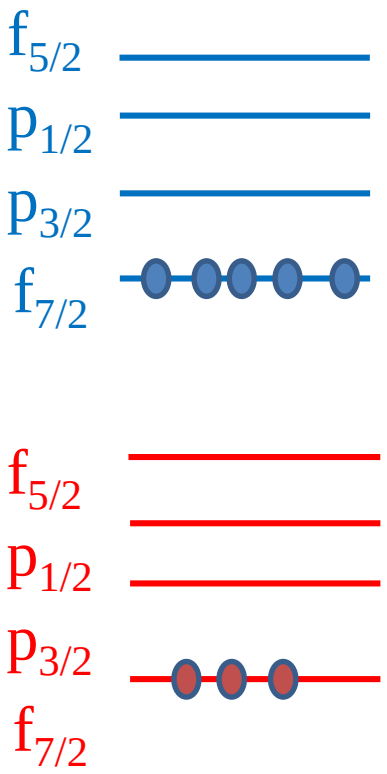
***** **FLUID=1 5 PARTICLES JUMP MAX= 2**

SHELL	N=0	L= 3	2*J= 7	CLAS= 0
SHELL	N=1	L= 1	2*J= 3	CLAS= 1
SHELL	N=0	L= 3	2*J= 5	CLAS= 1
SHELL	N=1	L= 1	2*J= 1	CLAS= 1

***** **FLUID=2 3 PARTICLES JUMP MAX= 2**

SHELL	N=0	L= 3	2*J= 7	CLAS= 0
SHELL	N=1	L= 1	2*J= 3	CLAS= 1
SHELL	N=0	L= 3	2*J= 5	CLAS= 1
SHELL	N=1	L= 1	2*J= 1	CLAS= 1

M= 0 PARITY=0 JUMP MAX= 2



Output file:

2*M= 0	DIM=	45778	DIM 2*J=	825
2*M= 2	DIM=	44953	DIM 2*J=	2380
2*M= 4	DIM=	42573	DIM 2*J=	3713
2*M= 6	DIM=	38860	DIM 2*J=	4689
2*M= 8	DIM=	34171	DIM 2*J=	5258
2*M= 10	DIM=	28913	DIM 2*J=	5400
2*M= 12	DIM=	23513	DIM 2*J=	5170
2*M= 14	DIM=	18343	DIM 2*J=	4645
2*M= 16	DIM=	13698	DIM 2*J=	3933
2*M= 18	DIM=	9765	DIM 2*J=	3146
2*M= 20	DIM=	6619	DIM 2*J=	2370
2*M= 22	DIM=	4249	DIM 2*J=	1684
2*M= 24	DIM=	2565	DIM 2*J=	1118
2*M= 26	DIM=	1447	DIM 2*J=	695
2*M= 28	DIM=	752	DIM 2*J=	395
2*M= 30	DIM=	357	DIM 2*J=	208
2*M= 32	DIM=	149	DIM 2*J=	95
2*M= 34	DIM=	54	DIM 2*J=	39
2*M= 36	DIM=	15	DIM 2*J=	12
2*M= 38	DIM=	3	DIM 2*J=	3

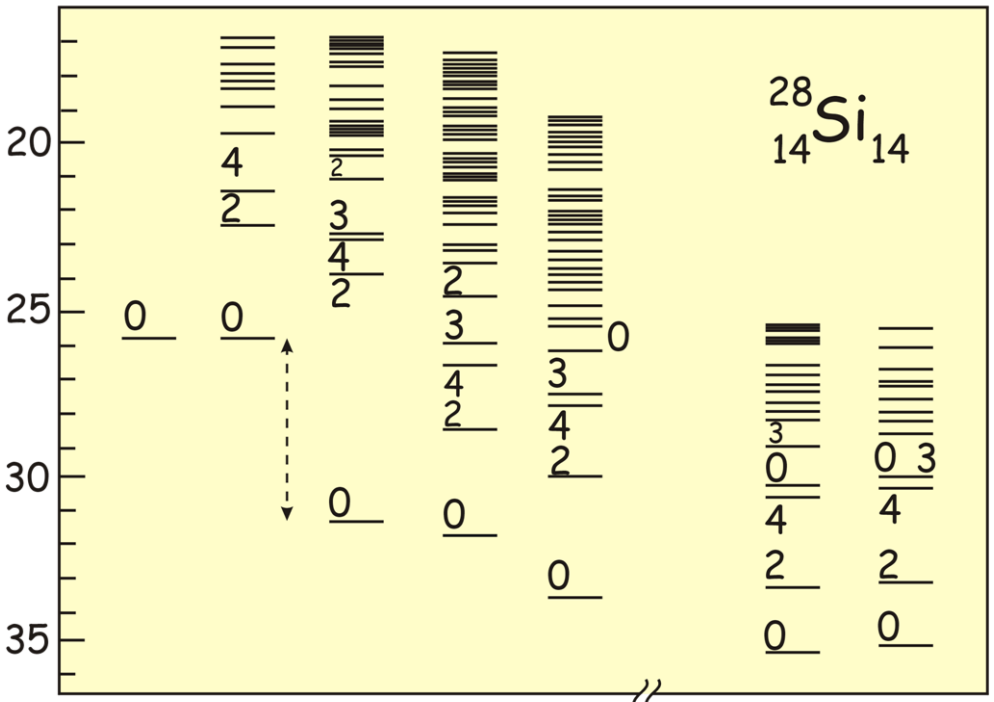
EFFECTIVE DIMENSION = 0 22889

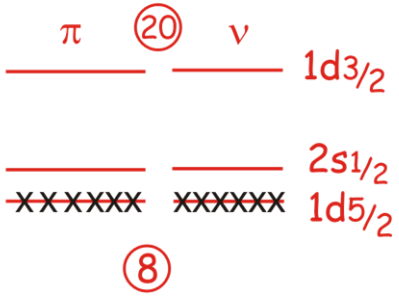
MAXI DIM (M,PI) = 0 6578

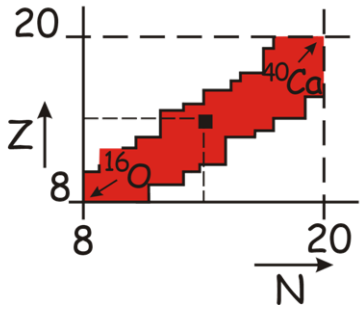
MAXI DIM (M,PI,T) = 0 3740

An example

sd MODEL SPACE







Increasing the dimensions

```
1 0 0
5   4  307 1103 305 1101      0 1 1 1    3
3   4  307 1103 305 1101      0 1 1 1    3
0 0 4
```

********** CAS= 1 ********************

Output file: ^{48}V

CALCULATE DIMENSIONS OF THE SPACE

***** FLUID=1 5 PARTICLES JUMP **MAX= 3**

SHELL N=0 L= 3 2*J= 7 CLAS= 0
SHELL N=1 L= 1 2*J= 3 CLAS= 1
SHELL N=0 L= 3 2*J= 5 CLAS= 1
SHELL N=1 L= 1 2*J= 1 CLAS= 1

EFFECTIVE DIMENSION = 270256

***** FLUID=2 3 PARTICLES JUMP **MAX= 3**

SHELL N=0 L= 3 2*J= 7 CLAS= 0
SHELL N=1 L= 1 2*J= 3 CLAS= 1
SHELL N=0 L= 3 2*J= 5 CLAS= 1
SHELL N=1 L= 1 2*J= 1 CLAS= 1

M= 0 PARITY=0 **JUMP MAX= 4**

Still increasing the dimensions

```
1 0 0
5   4  307 1103 305 1101      0 1 1 1    5
3   4  307 1103 305 1101      0 1 1 1    5
0 0 8
```

********** CAS= 1 **********

Output file: ^{48}V

CALCULATE DIMENSIONS OF THE SPACE

***** FLUID=1 5 PARTICLES JUMP **MAX= 5**

SHELL N=0 L= 3 2*J= 7 CLAS= 0
SHELL N=1 L= 1 2*J= 3 CLAS= 1
SHELL N=0 L= 3 2*J= 5 CLAS= 1
SHELL N=1 L= 1 2*J= 1 CLAS= 1

EFFECTIVE DIMENSION = 744584

(Full space dimension)

***** FLUID=2 3 PARTICLES JUMP **MAX= 5**

SHELL N=0 L= 3 2*J= 7 CLAS= 0
SHELL N=1 L= 1 2*J= 3 CLAS= 1
SHELL N=0 L= 3 2*J= 5 CLAS= 1
SHELL N=1 L= 1 2*J= 1 CLAS= 1

M= 0 PARITY=0 **JUMP MAX= 8**

Full space dimension

```
1 0 0
5   4  307 1103 305 1101      0 0 0 0    0
3   4  307 1103 305 1101      0 0 0 0    0
0 0 0
```

********** CAS= 1 **********

Output file: ^{48}V

CALCULATE DIMENSIONS OF THE SPACE

***** FLUID=1 5 PARTICLES JUMP **MAX= 0**

SHELL N=0 L= 3 2*J= 7 CLAS= 0
SHELL N=1 L= 1 2*J= 3 CLAS= 0
SHELL N=0 L= 3 2*J= 5 CLAS= 0
SHELL N=1 L= 1 2*J= 1 CLAS= 0

EFFECTIVE DIMENSION = 744584

***** FLUID=2 3 PARTICLES JUMP **MAX= 0**

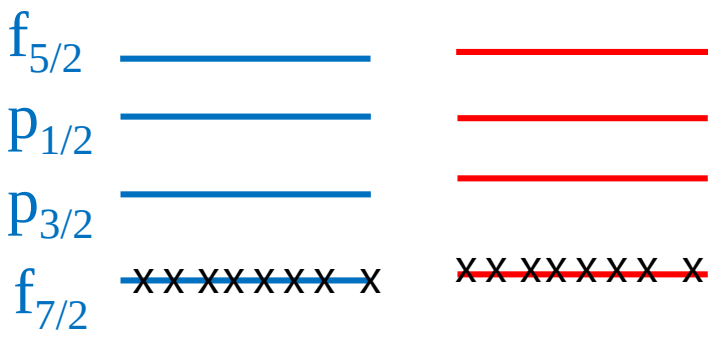
SHELL N=0 L= 3 2*J= 7 CLAS= 0
SHELL N=1 L= 1 2*J= 3 CLAS= 0
SHELL N=0 L= 3 2*J= 5 CLAS= 0
SHELL N=1 L= 1 2*J= 1 CLAS= 0

M= 0 PARITY=0 **JUMP MAX= 0**

Identical and different particles

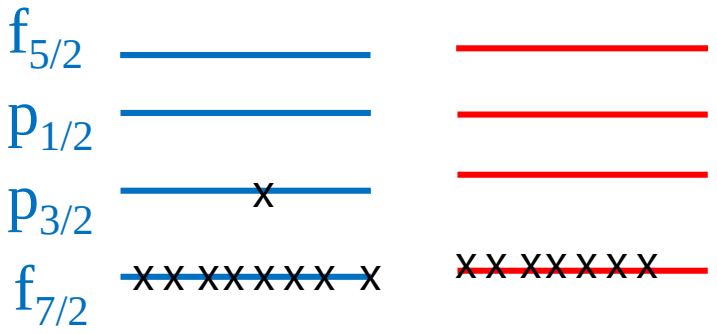
```
1 0 0
8  4 307 1103 305 1101      0 0 0 0     0
8  4 307 1103 305 1101      0 0 0 0     0
0 0 0
```

EFFECTIVE DIMENSION = 615 991856




```
1 0 0
9  4 307 1103 305 1101      0 0 0 0     0
7  4 307 1103 305 1101      0 0 0 0     0
0 0 0
```

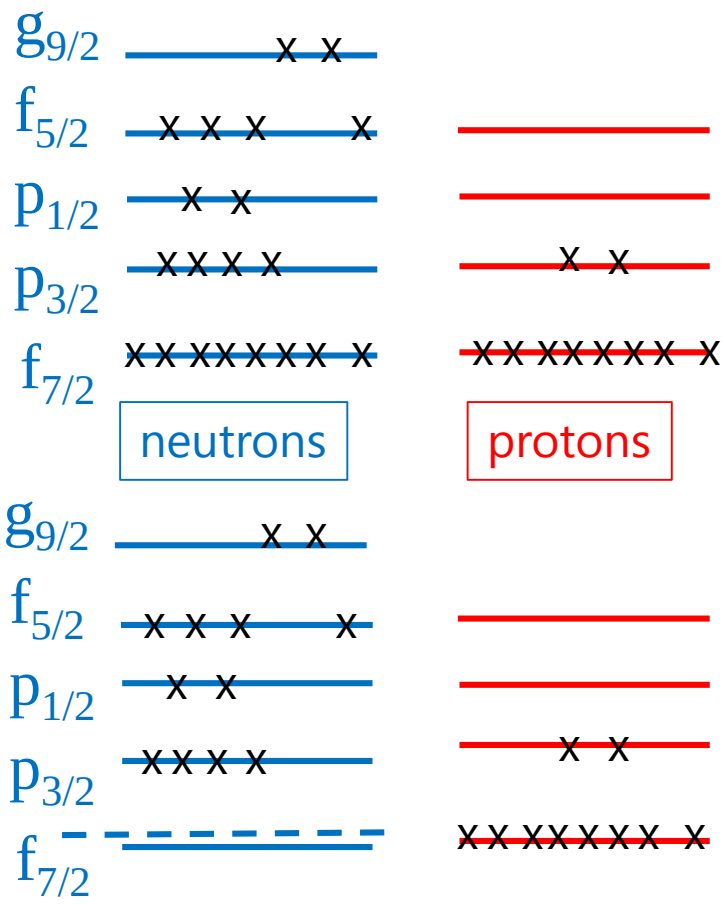
EFFECTIVE DIMENSION = 448 435431



different inputs but identical goal

```
1 0 0
20  5  307  1103  305  1101  409    0 7 7 7 8    10
10  4  307  1103  305  1101          0 1 1 1     10
0 0 6
```

```
1 0 0
12  4        1103   305  1101   409      0 0 0 1    10
10  4   307  1103   305  1101            0 1 1 1    10
0 0 6
```



dimensions will be identical

Interaction file

Contains the single-particle energies and two-body matrix elements of the hamiltonian in a specific valence space.

Example: USD interaction for the sd shell (isospin symmetric and independent)

just the first lines

USD Interaction (sd shell) text line

1 3 205 1001 203 **type of part., number of shells, list of shells**

-3.94780 -3.16354 1.64658 **single-particle energies**

1 8 8 0.300000 0.000000 **mass dep., core, scaling factor**

0 1 203 203 203 203 0 3 **t_{min} t_{max}, sh1 sh2 sh3 sh4, J_{min} J_{max}**

0.00000 -1.41510 0.00000 -2.88420 V_{1234} **($J_{min} \leq J \leq J_{max}$) (T=0)**

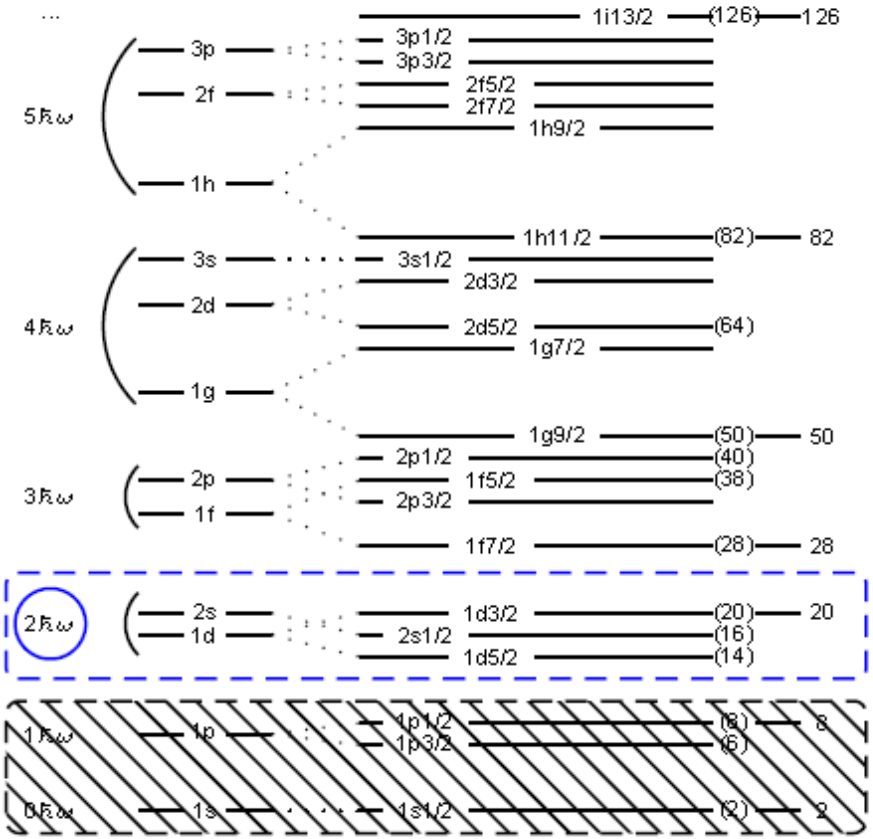
-2.18450 0.00000 -0.06650 0.00000 V_{1234} **($J_{min} \leq J \leq J_{max}$) (T=1)**

0 1 205 203 203 203 1 3

0.56470 0.00000 2.03370

0.00000 -0.61490 0.00000

The model space (1)



Valence space

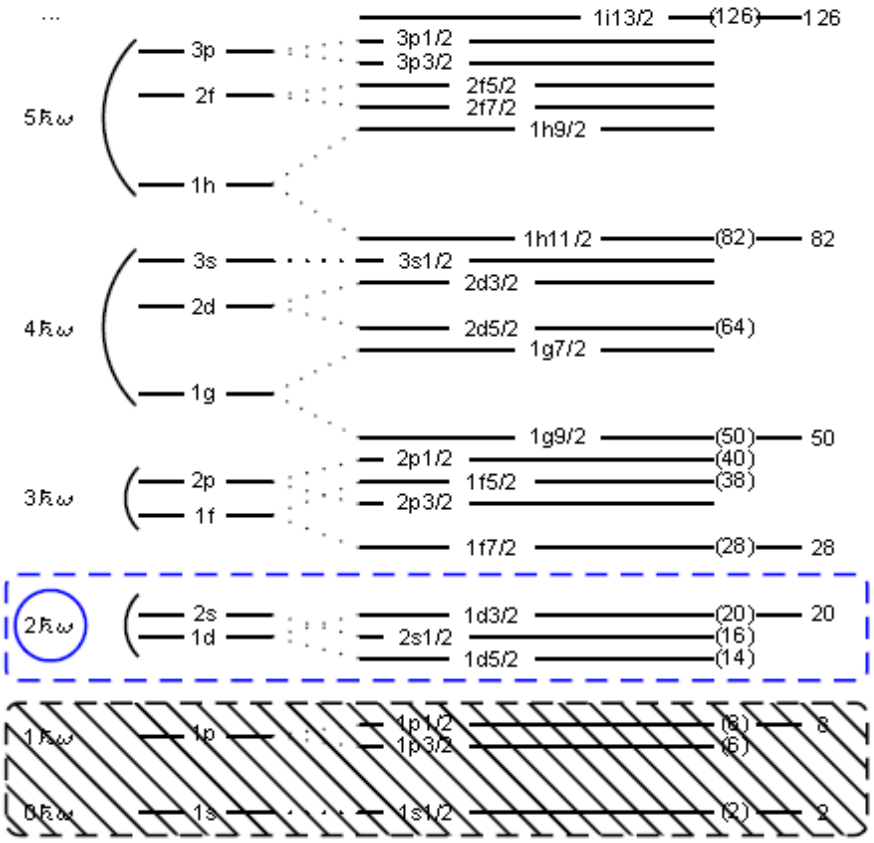
- $4 \leq A \leq 16$ p shell

  Cohen-Kurath interaction

- $16 \leq A \leq 40$ sd shell

  USD interaction

The model space (2)



Valence space

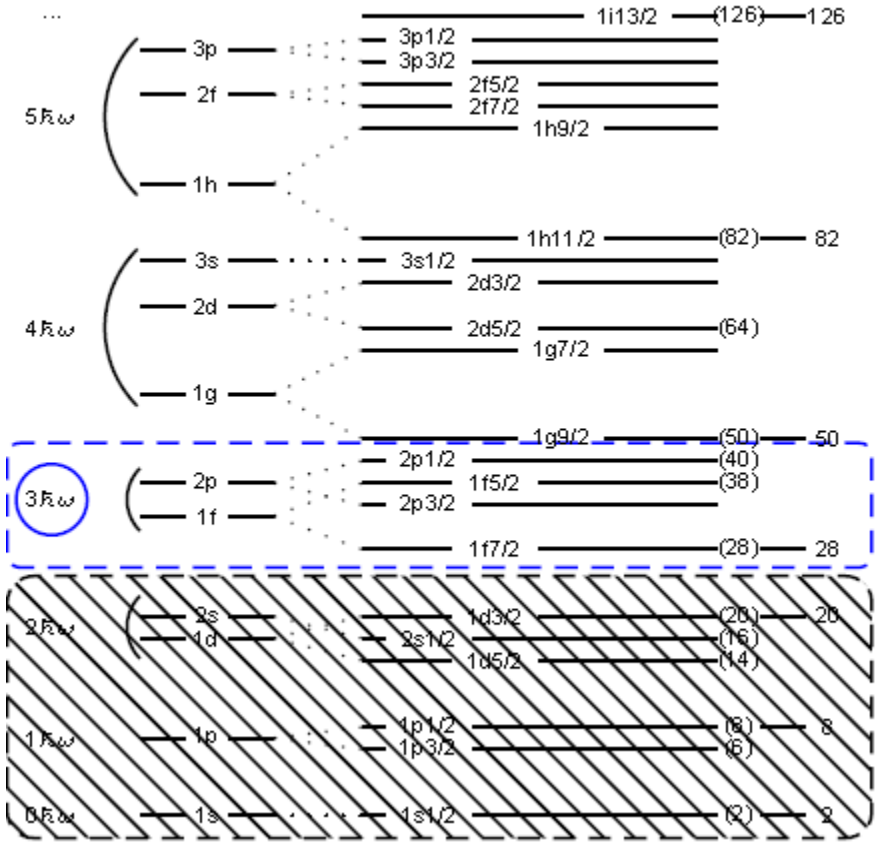
- $4 \leq A \leq 16$ p shell

  Cohen-Kurath interaction

- $16 \leq A \leq 40$ sd shell

  USD interaction

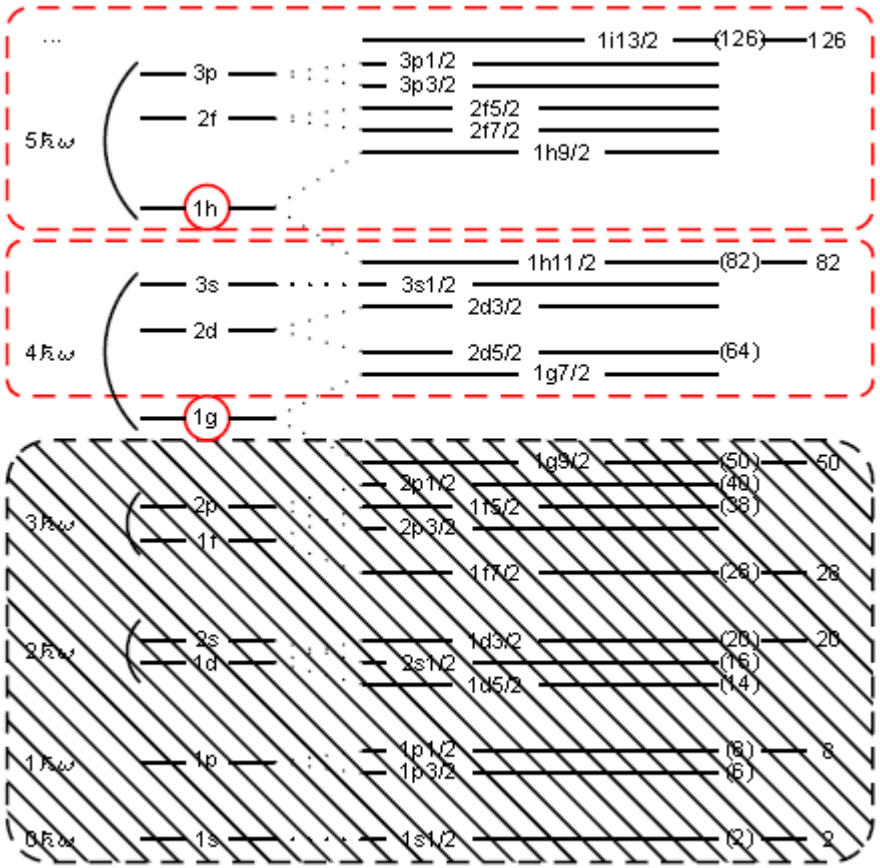
The model space (3)



Valence space

- $4 \leq A \leq 16$ p shell
  Cohen-Kurath interaction
- $16 \leq A \leq 40$ sd shell
  USD interaction
- $40 \leq A \leq 80$ pf shell
  KB3, GXPF1 interactions

The model space (4)



Valence space

- $4 \leq A \leq 16$ p shell

  Cohen-Kurath interaction

- $16 \leq A \leq 40$ sd shell

  USD interaction

- $40 \leq A \leq 80$ pf shell

  KB3, GXPF1 interactions

- **Heavier nuclei :**
  Spin-orbite shell closures

  28, 50, 82, 126

  Transition between ^{40}Ca and ^{100}Sn

Interaction file

Example: USD + Coulomb interaction for the sd shell (charge asymmetric Vpp≠Vnn)

USD Interaction (sd shell) + Coulomb text line — just the first lines

2 3 205 1001 203 — type of part., number of shells, list of shells

-3.94780 -3.16354 1.64658 single-particle energies

-3.94780 -3.16354 1.64658 single-particle energies

1 8 8 0.300000 0.000000 mass dep., core, scaling factor

0 2 203 203 203 203 0 3 t_{min} t_{max}, sh1 sh2 sh3 sh4, J_{min} J_{max}

0.00000 -1.41510 0.00000 -2.88420 V_{1234} ($J_{min} \le J \le J_{max}$) (T=0)

-2.18450 0.00000 -0.06650 0.00000 V_{1234} ($J_{min} \le J \le J_{max}$) (T=1 nn=pn)

-1.72181 0.000000 0.31656 0.00000 V_{1234} ($J_{min} \le J \le J_{max}$) (T=1 pp)

Note: single-particle energies may be different for protons and neutrons

Interaction file

Example: USD + Coulomb interaction for the sd shell
(charge asymmetric and charge dependent Vpp≠Vnn≠Vpn)

USD Interaction (sd shell) + Coulomb + charge dependence **text line**

2 3 205 1001 203 **type of part., number of shells, list of shells**

-3.94780 -3.16354 1.64658 **single-particle energies**

-3.94780 -3.16354 1.64658 **single-particle energies**

1 8 8 0.300000 0.000000 **mass dep., core, scaling factor**

0 3 203 203 203 203 0 3 **t_{min} t_{max}, sh1 sh2 sh3 sh4, J_{min} J_{max}**

0.00000 -1.41510 0.00000 -2.88420 V_{1234} **($J_{min} \le J \le J_{max}$) (T=0 pn)**

-2.08450 0.00000 -0.05650 0.00000 V_{1234} **($J_{min} \le J \le J_{max}$) (T=1 pn)**

-2.18450 0.00000 -0.06650 0.00000 V_{1234} **($J_{min} \le J \le J_{max}$) (T=1 nn)**

-1.72181 0.000000 0.31656 0.00000 V_{1234} **($J_{min} \le J \le J_{max}$) (T=1 pp)**

Note: single-particle energies may be different for protons and neutrons

Diagonalization of the matrix

Option 4: Diagonalization from random initial pivot

```
4  0  0 *** Option 4
50  0  3    output file   initialization  number of  J  states
4   4  307  1103  305  1101      0 0 0 0      0
2   4  307  1103  305  1101      0 0 0 0      0
0  0  0
 90  0      interaction file   COUL
0  4   8     2*J values
1  2  1      number of states for each J
60  0.0005  0   max. number of iterations,  en. conv. in keV,  orthog.
```

COUL = 0 Vpp=Vnn
COUL = 1 protons in fluid1
COUL = 2 protons in fluid2

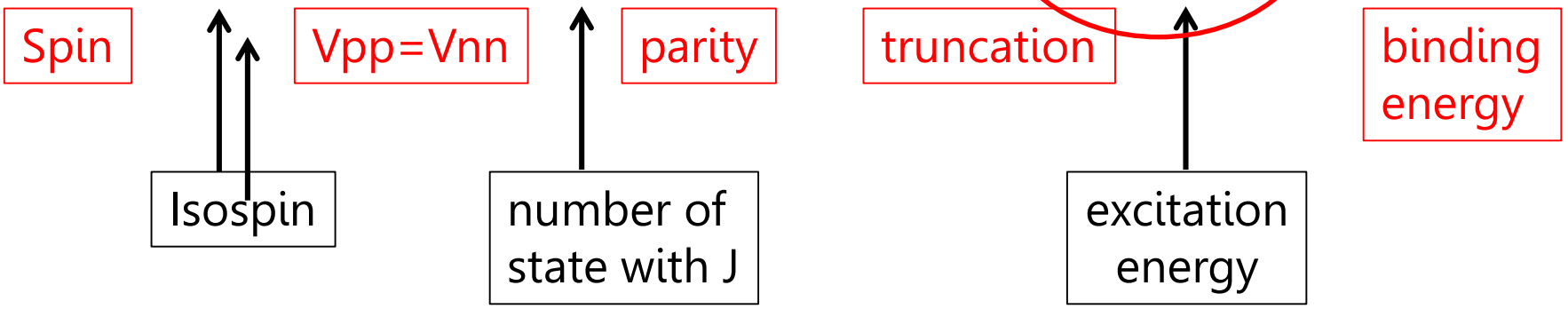
Output file:

```
 STATE 2*J=  0    LANCZOS UNTIL CONVERGENCE OF THE EIGENVALUE N=  1

 ITER=  1    DIA=    12.627658    NONDIA=    10.592916
 ITER=  2    DIA=    14.519892    NONDIA=    13.169668
 ITER=  3    DIA=    12.091361    NONDIA=    13.488098
        3
  -3.528856   12.417493   30.350274
 CONVERGENCE DELTA E= 16.156514

 ITER=  4    DIA=     9.573934    NONDIA=    13.856208
 ITER=  5    DIA=     7.868243    NONDIA=    14.632639
 ITER=  6    DIA=     8.565486    NONDIA=    15.225399
        6
 -14.459636   -4.567652    5.799751   16.428004   26.993335   35.052772
 CONVERGENCE DELTA E= 10.930781
.....
 ITER= 19    DIA=    10.338945    NONDIA=    13.221777
 ITER= 20    DIA=    10.918592    NONDIA=    12.666825
 ITER= 21    DIA=    10.175517    NONDIA=    12.310465
       21
 -19.620982  -15.269020  -14.216000  -12.037258   -9.089115   -6.728591
  -3.338916    0.024160    3.333789    6.888502   10.617373   14.060224
 CONVERGENCE DELTA E=  0.000033
.....
 STORE IN FILE          60
      E=  -19.620982                PIVOT RANDOM T=TZ
 D= 51880  A=  4  2   2*M= 0   P=0   RVT= 1  2*J=0  T-TZ= 0 COUL=0   N= 1  JUMP= 0
```

Energy levels in 46Ti

GROUND-STATE (AMONG THE READ STATES) ENERGY= -19.62098 (in MeV)

2*J= 0 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 0.00000 E= -19.62098
2*J= 4 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 0.95913 E= -18.66185
2*J= 8 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 1.81918 E= -17.80180



Adopted values:

0+	g.s.
2+	889 keV
4+	2009.8 keV

Try another interaction

Just change the number of the interaction file in the input file

GXPF1A

GROUND-STATE (AMONG THE READ STATES) ENERGY= -70.51574

```
2*J=  0 T-TZ= 0 COUL=0 N=  1 P=0 2*M= 0 C= 0  EXC=   0.00000 E=   -70.51574
2*J=  4 T-TZ= 0 COUL=0 N=  1 P=0 2*M= 0 C= 0  EXC=   1.00515 E=   -69.51059
2*J=  8 T-TZ= 0 COUL=0 N=  1 P=0 2*M= 0 C= 0  EXC=   1.83559 E=   -68.68015
```

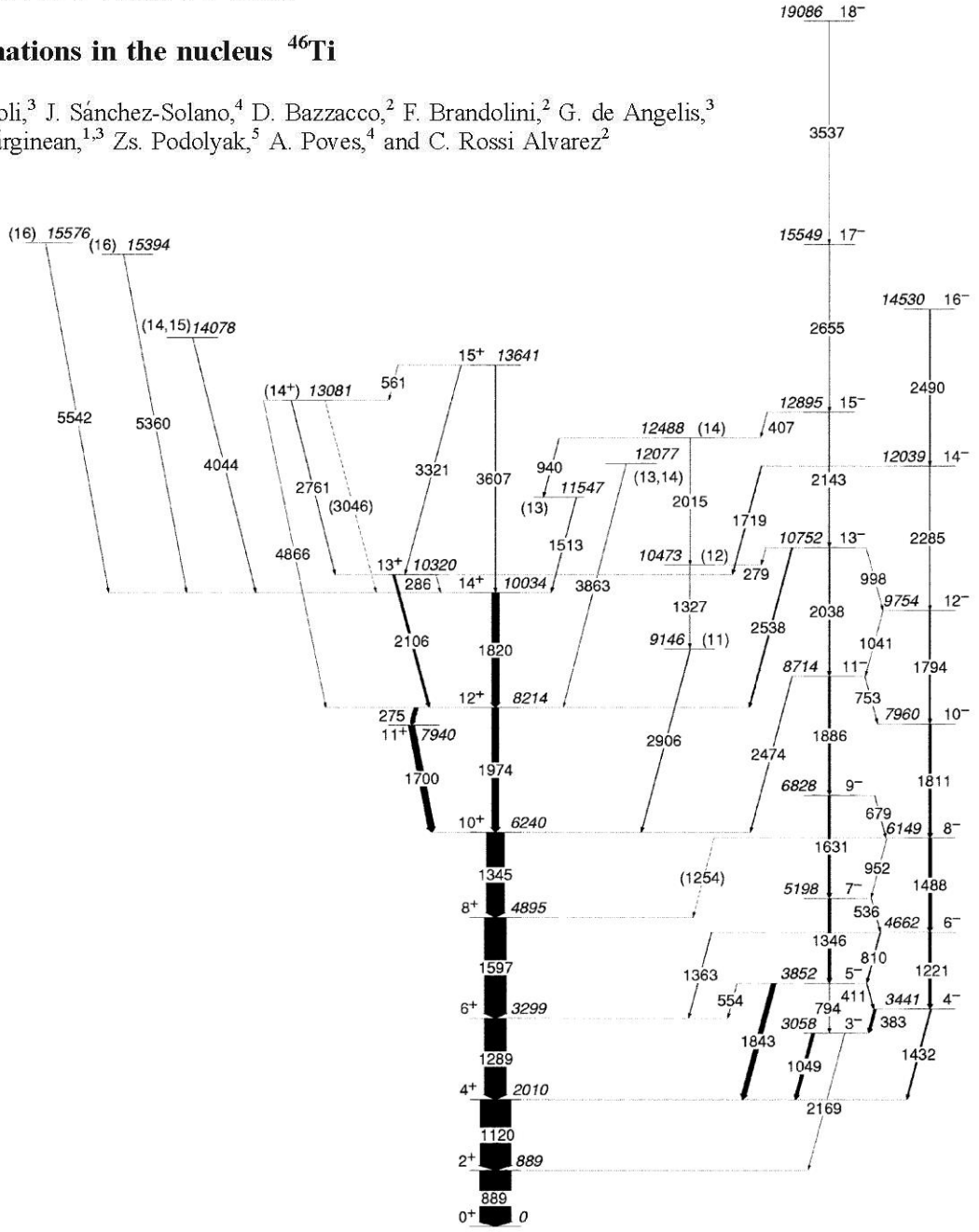
Adopted values:

0+	g.s.
2+	889 keV
4+	2009.8 keV

a little worst

Band terminations in the nucleus ^{46}Ti

D. Bucurescu,[1] C. A. Ur,[1,2] S. M. Lenzi,[2] D. R. Napoli,[3] J. Sánchez-Solano,[4] D. Bazzacco,[2] F. Brandolini,[2] G. de Angelis,[3] E. Farnea,[2] A. Gadea,[3] S. Lunardi,[2] N. Mărginean,[1,3] Zs. Podolyak,[5] A. Poves,[4] and C. Rossi Alvarez[2]



Excited states in ^{46}Ti

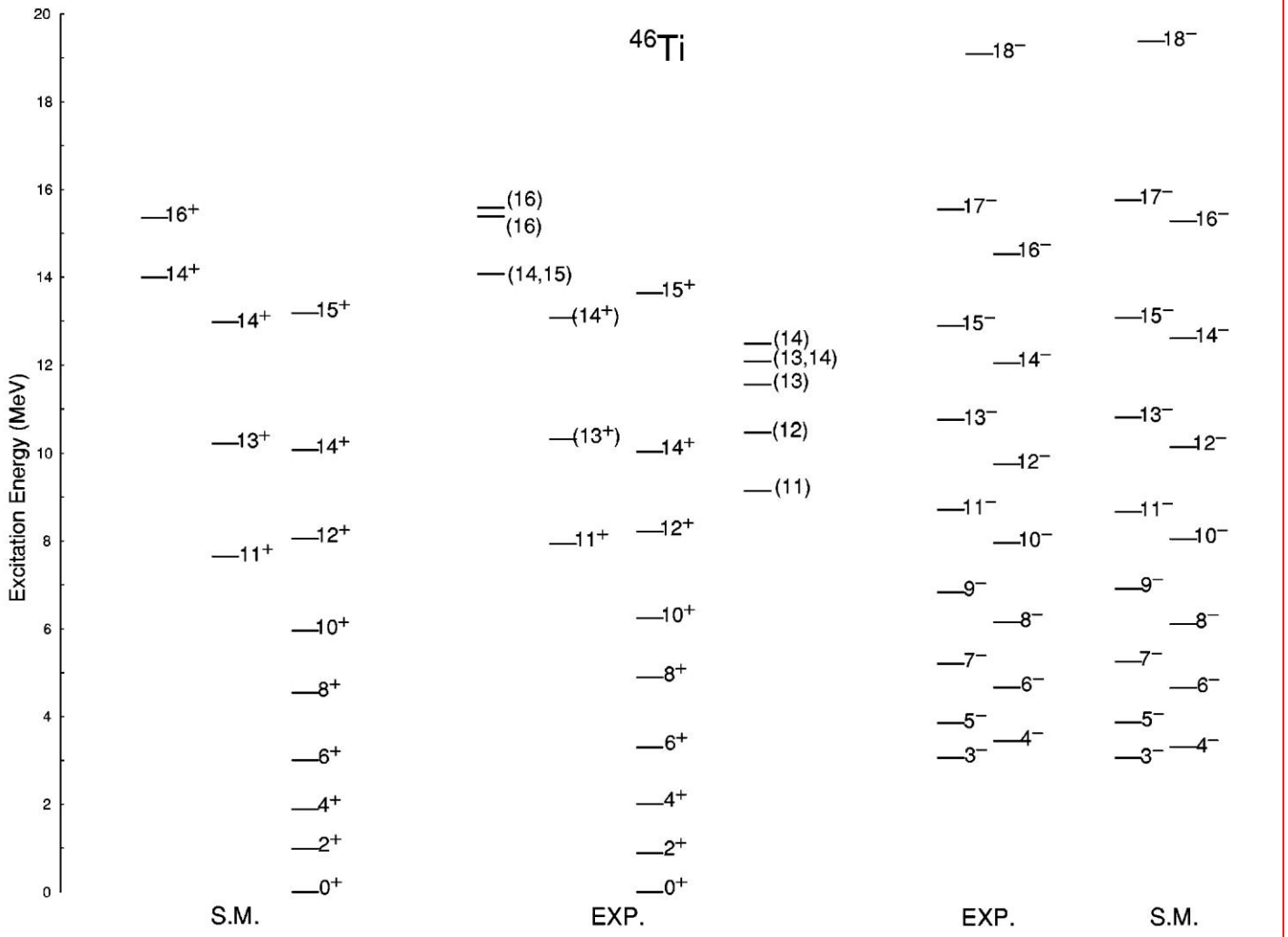


FIG. 3. Comparison between the experimental level scheme of ^{46}Ti and the one calculated with the shell model (code ANTOINE), in the full *pf* shell. For the experimental levels without parity assignment, no possible theoretical counterparts are shown.

calculate more than 1 state per J

```
 4  0  0
 60  0  3
 4    4   307 1103 305 1101          0  0  0  0      0
 2    4   307 1103 305 1101          0  0  0  0      0
 0  0   0
 92   0
0  4  8
2  2  1
60   0.0005   0  0
```

KB3G interaction

STATE 2*J= 0 LANCZOS UNTIL CONVERGENCE OF THE EIGENVALUE N= 2

```
 ITER=  1    DIA=    12.627658    NONDIA=    10.592916
 ITER=  2    DIA=    14.519892    NONDIA=    13.169668
 ITER=  3    DIA=    12.091361    NONDIA=    13.488098
       3
  -3.528856   12.417493   30.350274
 ITER=  4    DIA=     9.573934    NONDIA=    13.856208
 ITER=  5    DIA=     7.868243    NONDIA=    14.632639
 ITER=  6    DIA=     8.565486    NONDIA=    15.225399
       6
 -14.459636   -4.567652    5.799751   16.428004   26.993335   35.052772
```

CONVERGENCE DELTA E= 10.930781 16.985144

calculate more than 1 state per J

GROUND-STATE (AMONG THE READ STATES) ENERGY= -19.62098

2*J= 0 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 0.00000 E= -19.62098
2*J= 4 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 0.95912 E= -18.66187
2*J= 8 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 1.81918 E= -17.80180
2*J= 4 T-TZ= 0 COUL=0 N= 2 P=0 2*M= 0 C= 0 EXC= 2.70789 E= -16.91309
2*J= 0 T-TZ= 0 COUL=0 N= 2 P=0 2*M= 0 C= 0 EXC= 4.27990 E= -15.34108

Adopted values:

0+	g.s.
2+	889 keV
4+	2009.8 keV
0+	2611 keV
2+	2961 kev

→ not in the pure fp valence space

Increasing the precision

Instead of case 4, that uses a random pivot to start the iterations, one can use option 5 (minimal energy pivot). The input is the same, just changing "4" by "5" in the first row.

When the dimension of the matrix becomes very large, it is better to start with a less precise (truncated calculation) and use the eigenstates of this preliminary calculation as pivot for a more precise one.

input

```
5 0 0  **** Option 5  Lanczos calculation minim. en. pivot (Option 4 also possible)
50  0  3
 6   4  307 1103 305 1101       0 1 1 1     10
 2   4  307 1103 305 1101       0 1 1 1     10
 0 0 2   only 2 particles can be excited from the f7/2 shell
   90   0
 0  4  8  the 2*J is given only the first time
 1  1  1  the number of states is repeated in option 6
45  0.0005   0

 31   0   0  **** Option 31 Change truncation
 51  50  0 0 3 reads in file 50 and writes in file 51, 3 vectors
 6  4 307 1103 305 1101       0 1 1 1     10
 2  4 307 1103 305 1101       0 1 1 1     10
 0 0 4  allows 4 particles can be excited from the f7/2 shell

 6 0 0   ****   Lanczos  (Option 7 with projected pivots also possible)
 50  51  0  0  3   reads in file 51 and writes in file 50, 3 vectors
 6  4 307 1103 305 1101       0 1 1 1     10
 2  4 307 1103 305 1101       0 1 1 1     10
 0 0 4
 90  0
 1  1  1
 0  45  0.0005  0
```

Increasing precision

You can continue increasing the precision in this way.
This method saves time. You can add the following to the previous input:

31 0 0 ** Option 31 Change truncation**
51 50 0 0 3
6 4 307 1103 305 1101 0 1 1 1 10
2 4 307 1103 305 1101 0 1 1 1 10
0 0 6 allows 6 particles to be excited from the $f_{7/2}$ shell

6 0 0 ** Lanczos (Option 7 with projected pivots in J^2 also possible)**
50 51 0 0 3 reads in file 51 and writes in file 50, only 1 vector per spin
6 4 307 1103 305 1101 0 1 1 1 10
2 4 307 1103 305 1101 0 1 1 1 10
0 0 6
90 0
1 1 1
0 45 0.0005 0 0

etc, etc.....

Calculate ^{48}Cr up to the 16^{+} state

```
 4  0  0
-60  0   4  we calculate  the first 4 states store in unit 60 (not rewind)
 4     4    307 1103 305 1101        0  0  0  0        0
 4     4    307 1103 305 1101        0  0  0  0        0
 0  0   0
       93  0
0  4  8  12
1  1  1  1
60   0.00005   0

  4  0  0
60  0   5  and afterwards we calculate the other 5 states
 4     4    307 1103 305 1101        0  0  0  0        0
 4     4    307 1103 305 1101        0  0  0  0        0
 16  0    0  we use a different Jz to help convergence
       93  0
16  20  24  28  32
1  1  1  1  1
60 0.00005   0
```

Output

GROUND-STATE (AMONG THE READ STATES) ENERGY= -99.57789

2*J= 0 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 0.00000 E= -99.57789
2*J= 4 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 0.78845 E= -98.78944
2*J= 8 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 1.71686 E= -97.86103
2*J= 12 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 3.22890 E= -96.34899

GROUND-STATE (AMONG THE READ STATES) ENERGY= -94.82482

2*J= 16 T-TZ= 0 COUL=0 N= 1 P=0 2*M=16 C= 0 EXC= 0.00000 E= -94.82482
2*J= 20 T-TZ= 0 COUL=0 N= 1 P=0 2*M=16 C= 0 EXC= 1.67633 E= -93.14849
2*J= 24 T-TZ= 0 COUL=0 N= 1 P=0 2*M=16 C= 0 EXC= 2.96908 E= -91.85575
2*J= 28 T-TZ= 0 COUL=0 N= 1 P=0 2*M=16 C= 0 EXC= 4.94764 E= -89.87719
2*J= 32 T-TZ= 0 COUL=0 N= 1 P=0 2*M=16 C= 0 EXC= 8.05249 E= -86.77234

How to recover the Jz

We run case 33

```
33  0  0  ***  Option 33 Change Jz
61  60  0  0   0
 4    4   307 1103 305 1101       0  0  0  0       0
 4    4   307 1103 305 1101       0  0  0  0       0
```

0 0 0 we then change Jz to have all states in the same file (61) with Jz-0

This is needed to obtain the transition probabilities (see later)

Look at the wave functions

To have all vectors in the same file we used option 33.
Now we will read the vectors from file 61 and analyze the composition of the wavefunctions.
For this purpose we will use Option 11

Input

```
11  0  0  **** Option 11 Calculation of shell occupations
61  0  0*
 4   4  307 1103 305 1101        0 0 0 0     0
 4   4  307 1103 305 1101        0 0 0 0     0
 0 0  0
```

* It is not necessary to indicate the number of states if we want to look at all of them

Analysis of the wave functions

The output file will give us the information on the configuration of the states:

The full hamiltonian is: $H = H_0 + H_{res}$

$$H\left|\Psi_p\right\rangle = E_p\left|\Psi_p\right\rangle$$

If the basis set (configurations) is defined as $\left|\psi_k^0\right\rangle (k = 1,\ldots,n)$ solutions of $H_0\left|\psi_k^0\right\rangle = E_k^0\left|\psi_k^0\right\rangle$

$$\psi_k^0(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_A) = \frac{1}{\sqrt{A!}}\det\begin{pmatrix} \varphi_1(\vec{r}_1) & \varphi_1(\vec{r}_1) & \cdots & \varphi_1(\vec{r}_A) \\ \vdots & \ddots & & \vdots \\ \varphi_A(\vec{r}_1) & \varphi_A(\vec{r}_1) & \cdots & \varphi_A(\vec{r}_A) \end{pmatrix}$$

$$E_k^0 = \sum_{i=1}^{A} \varepsilon_i$$

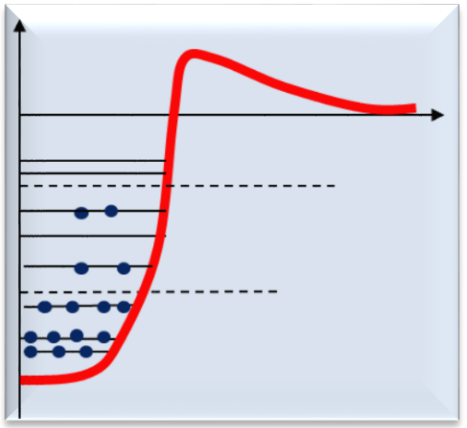
The total wave function can be expanded as:

$$\left|\Psi_p\right\rangle = \sum_{k=1}^{n} a_{kp}\left|\psi_k^0\right\rangle$$

Analysis of the wave functions

$$E_k^0 = \sum_{i=1}^{A} \varepsilon_i$$

is the sum of the s.p. energies and depends on the occupation of the s.p. states



The **square of the amplitudes** in the expansion of the wave function that is the eigenstate of the full hamiltonian are the probability of the particular configuration *k* in the wave function

$$\left|\Psi_p\right\rangle = \sum_{k=1}^{n} a_{kp} \left|\psi_k^0\right\rangle$$

Output file

```
********** CAS= 11  ********************

CALCULATION OF OCCUPATION OF SHELLS

***** FLUID=1    4 PARTICLES  JUMP     MAX=  0

     SHELL    N=0    L= 3    2*J= 7    CLAS= 0
     SHELL    N=1    L= 1    2*J= 3    CLAS= 0
     SHELL    N=0    L= 3    2*J= 5    CLAS= 0
     SHELL    N=1    L= 1    2*J= 1    CLAS= 0

***** FLUID=2    4 PARTICLES  JUMP     MAX=  0

     SHELL    N=0    L= 3    2*J= 7    CLAS= 0
     SHELL    N=1    L= 1    2*J= 3    CLAS= 0
     SHELL    N=0    L= 3    2*J= 5    CLAS= 0
     SHELL    N=1    L= 1    2*J= 1    CLAS= 0

          M=  0     PARITY=0     JUMP MAX=  0
WE TAKE ALL THE VECTORS ON THE FILE
```

Wavefunction of the g.s. in 48Cr

Output

E= -99.577889 PIVOT RANDOM T=TZ

D= 1141343 A= 4 4 2*M= 0 P=0 RVT= 1 2*J= 0 T-TZ= 0 COUL=0 N= 1 JUMP= 0

0.40867630	4 0 0 0 4 0 0 0
0.06509183	4 0 0 0 3 1 0 0
0.04656886	4 0 0 0 3 0 1 0
0.02381536	4 0 0 0 2 2 0 0
0.01123589	4 0 0 0 2 1 1 0
0.01675142	4 0 0 0 2 0 2 0
0.06509183	3 1 0 0 4 0 0 0
0.05193021	3 1 0 0 3 1 0 0
0.04656886	3 0 1 0 4 0 0 0
0.02266685	3 0 1 0 3 0 1 0
0.02381536	2 2 0 0 4 0 0 0
0.01123589	2 1 1 0 4 0 0 0
0.01675142	2 0 2 0 4 0 0 0

this means that the probability that the 4 protons and the 4 neutrons are in the $f_{7/2}$ shell is 40.87 %

6.5 % probability that 1 neutron is excited to the p3/2

Only configurations with more than 1% probability are listed

FLUID 1 NI=	3.43835	0.30914	0.20411	0.04840
FLUID 2 NI=	3.43835	0.30914	0.20411	0.04840
	$f_{7/2}$	$p_{3/2}$	$f_{5/2}$	$p_{1/2}$

average occupation of the shells (in number of particles) for the two fluids (in the N=Z are the same)

Wavefunction of the 2+ state

Output

```
E=  -98.789438                    PIVOT RANDOM T=TZ
D=  1141343   A=  4  4    2*M= 0  P=0   RVT= 1 2*J=  4 T-TZ= 0 COUL=0    N=  1 JUMP= 0
  0.33507674   4 0 0 0 4 0 0 0
  0.10215638   4 0 0 0 3 1 0 0
  0.03897654   4 0 0 0 3 0 1 0
  0.02137056   4 0 0 0 2 2 0 0
  0.01549685   4 0 0 0 2 1 1 0
  0.01011773   4 0 0 0 2 0 2 0
  0.10215638   3 1 0 0 4 0 0 0
  0.04997149   3 1 0 0 3 1 0 0
  0.01422874   3 1 0 0 3 0 1 0
  0.01284526   3 1 0 0 2 2 0 0
  0.03897654   3 0 1 0 4 0 0 0
  0.01422874   3 0 1 0 3 1 0 0
  0.01457791   3 0 1 0 3 0 1 0
  0.02137056   2 2 0 0 4 0 0 0
  0.01284526   2 2 0 0 3 1 0 0
  0.01549685   2 1 1 0 4 0 0 0
  0.01011773   2 0 2 0 4 0 0 0
 FLUID 1  NI=   3.38232   0.37804   0.18710   0.05255
 FLUID 2  NI=   3.38232   0.37804   0.18710   0.05255
 ********************************
```

Wavefunction of the 16+ state

Output

E= -86.772339 PIVOT RANDOM T=TZ

D= 1141343 A= 4 4 2*M= 0 P=0 RVT= 1 2*J= 32 T-TZ= 0 COUL=0 N= 1 JUMP= 0

0.93023765 4 0 0 0 4 0 0 0

0.01178401 4 0 0 0 3 1 0 0

0.01147750 4 0 0 0 3 0 1 0

0.01178401 3 1 0 0 4 0 0 0

0.01147750 3 0 1 0 4 0 0 0

FLUID 1 NI= 3.95229 0.02651 0.02010 0.00111

FLUID 2 NI= 3.95229 0.02651 0.02010 0.00111

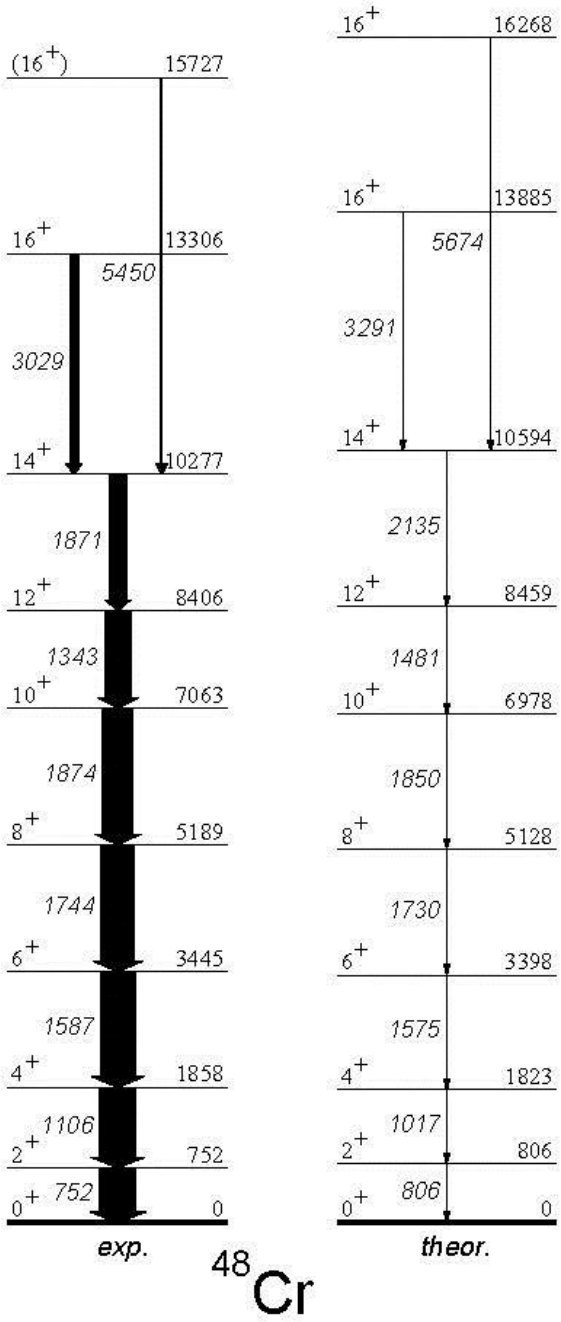
****

Energy spectrum

Output

```
GROUND-STATE (AMONG THE READ STATES) ENERGY=   -99.57789

2*J=  0 T-TZ= 0 COUL=0 N=  1 P=0 2*M= 0  C= 0  EXC=   0.00000 E=   -99.57789
2*J=  4 T-TZ= 0 COUL=0 N=  1 P=0 2*M= 0  C= 0  EXC=   0.78845 E=   -98.78944
2*J=  8 T-TZ= 0 COUL=0 N=  1 P=0 2*M= 0  C= 0  EXC=   1.71686 E=   -97.86103
2*J= 12 T-TZ= 0 COUL=0 N=  1 P=0 2*M= 0 C= 0  EXC=   3.22890 E=   -96.34899
2*J= 16 T-TZ= 0 COUL=0 N=  1 P=0 2*M= 0 C= 0  EXC=   4.75306 E=   -94.82482
2*J= 20 T-TZ= 0 COUL=0 N=  1 P=0 2*M= 0 C= 0  EXC=   6.42940 E=   -93.14849
2*J= 24 T-TZ= 0 COUL=0 N=  1 P=0 2*M= 0 C= 0  EXC=   7.72214 E=   -91.85575
2*J= 28 T-TZ= 0 COUL=0 N=  1 P=0 2*M= 0 C= 0  EXC=   9.70070 E=   -89.87719
2*J= 32 T-TZ= 0 COUL=0 N=  1 P=0 2*M= 0 C= 0  EXC=  12.80555 E=   -86.77234
```

Rotational motion and band termination in ^{48}Cr



Shell model can reproduce collective phenomena and in particular rotational spectra if the number of particles and the valence space are small enough to allow the diagonalization but large enough to include the relevant (quadrupole) degrees of freedom

Nuclear moments and Transition probabilities

Quadrupole moments and transition

Spectroscopic Quadrupole moments are obtained in the laboratory frame.

$$\widehat{Q}^{\text{int}}_{\lambda\mu} = \sum_{\mu'} D^{\lambda}_{\mu\mu'} \widehat{Q}^{lab}_{\lambda\mu}$$

Since Q^{int} does not depend on the Euler angles, the reduced matrix elements are

$$< I_1 K_1 \| \widehat{Q}^{lab}_{\lambda\mu} \| I_2 K_2 >= \sum_{\mu'} \widehat{Q}^{\text{int}}_{\lambda\mu} (-1)^{I_1 - K_1} ((2I_1+1)(2I_2+1))^{1/2} \begin{pmatrix} I_1 & \lambda & I_2 \\ K_1 & \mu' & K_2 \end{pmatrix}$$

If we restrict to a pure K band, the E2 matrix Q elements are:

$$< I_2 K n_\beta n_\gamma \| \widehat{Q}^{lab}_2 \| I_2 K n_\beta n_\gamma >=$$

$$= \sqrt{\frac{5}{16\pi}} Q_0(n_\beta, n_\gamma) \sqrt{(2I_1+1)(2I_2+1)} (-1)^{I_1 - K} \begin{pmatrix} I_1 & 2 & I_2 \\ -K & 0 & K \end{pmatrix}$$

where Q_0 is the intrinsic quadrupole moment that depends on the quantum numbers that characterize the band (vibrations, s.particle)

Quadrupole moments and transitions

For fixed β and $\gamma = 0$:

$$Q_0 = \sqrt{\frac{16\pi}{5}} \frac{3}{4\pi} ZeR_0^2 \beta$$

The spectroscopic quadrupole moment is given by:

$$Q_2 = \sqrt{\frac{16\pi}{5}} < IIK \,||\, \hat{Q}_2^{lab} \,||\, IIK >= Q_0 \frac{3K^2 - I(I+1)}{(2I+3)(I+1)}$$

The reduced transition probability is given by:

$$B(E2, I_1 \rightarrow I_2) = \frac{1}{2I_1 + 1} |< I_2 K \,||\, \hat{Q}_2 \,||\, I_1 K >|^2$$

For K = 0:

$$B(E2, I+2 \rightarrow I) = Q_0^2 \frac{5}{16\pi} \frac{3}{2} \frac{(I+1)(I+2)}{(2I+3)(2I+5)}$$

Quadrupole moments and B(E2)

4 0 0 ** Option 4 Lanczos**

```
50   0   4
4   4  307 1103 305 1101        0 0 0 0     0
4   4  307 1103 305 1101        0 0 0 0     0
0  0  0
     93 0
0  4  8  12
1  1  1  1
60  0.0005  0
```

12 0 0 ** Option 12 Transition probabilities and nuclear moments**

```
50  0  0
 4   4  307 1103 305 1101        0 0 0 0     0
 4   4  307 1103 305 1101        0 0 0 0     0
 0  0  0
```

2 0 20 20 0.5 1.5 multipolarity, parity, core, eff. ch. fluid1, eff. ch. fluid2

We prefer to use the effective charges $e_n = 0.46$ $e_p = 1.31$

Output

INITIAL STATE P= 0 2*J= 4 N= 1
Q(L=2)= -30.687894 (in efm^2)
P= 0 2*J= 0 N= 1 DE= 0.788 BE(L)= 249.7653 (in e^{2}fm^4) $2^+ \rightarrow 0^+$

INITIAL STATE P= 0 2*J= 8 N= 1
Q(L=2)= -40.727252
P= 0 2*J= 4 N= 1 DE= 0.928 BE(L)= 337.0700 **$4^+ \rightarrow 2^+$**

INITIAL STATE P= 0 2*J=12 N= 1
Q(L=2)= -40.291805
P= 0 2*J= 8 N= 1 DE= 1.512 BE(L)= 335.8291 **$6^+ \rightarrow 2^+$**

GROUND-STATE (AMONG THE READ STATES) ENERGY= -99.57789

2*J= 0 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 0.00000 E= -99.57789
2*J= 4 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 0.78845 E= -98.78944
2*J= 8 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 1.71686 E= -97.86103
2*J= 12 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 3.22890 E= -96.34899

Quadrupole transitions (odd-J states)

4 0 0 ** Option 4 Lanczos**

```
50   0   4
4   4  307 1103 305 1101        0 0 0 0     0
2   4  307 1103 305 1101        0 0 0 0     0
0  0  0
     93 0
0  4  6  8
1  1  1  1
60  0.0005  0
```

12 0 0 ** Option 12 Transition probabilities and nuclear moments**

```
50  0  0
4   4  307 1103 305 1101        0 0 0 0     0
2   4  307 1103 305 1101        0 0 0 0     0
0  0  0
```

2 0 20 20 0.5 1.5 multipolarity, parity, core, eff. ch. fluid1, eff. ch. fluid2

Output

INITIAL STATE P= 0 2*J= 4 N= 1
Q(L=2)= -13.640378
P= 0 **2*J= 0** N= 1 DE= 1.005 BE(L)= 124.2363

INITIAL STATE P= 0 **2*J= 8** N= 1
Q(L=2)= -23.509924
P= 0 **2*J= 4** N= 1 DE= 0.830 BE(L)= 158.2068

INITIAL STATE P= 0 **2*J= 6** N= 1 **No transitions in this case**
Q(L=2)= -3.511501

GROUND-STATE (AMONG THE READ STATES) ENERGY= -70.51574

2*J= 0 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 0.00000 E= -70.51574
2*J= 4 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 1.00515 E= -69.51059
2*J= 8 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 1.83559 E= -68.68015
2*J= 6 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 3.75867 E= -66.75707

Important remark

$$\langle J_i 0 \lambda 0 | J_f 0 \rangle = 0$$

if $J_i + \lambda + J_f$ =odd

Therefore, with $J_z = 0$

- no $E2$ transition computed between odd and even J's
- no $M1$ magnetic moment computed

☞need to apply J_+ to wave function

4 0 0 ** Option 4 Lanczos**

50 0 4

4 4 307 1103 305 1101 0 0 0 0 0

2 4 307 1103 305 1101 0 0 0 0 0

0 0 0

93 0

0 4 **6** 8

1 1 1 1

60 0.0005 0

We then change Jz

33 0 0 ****Option 33 Change Jz

51 50 0 0 0

4 4 307 1103 305 1101 0 1 1 1 10

4 4 307 1103 305 1101 0 1 1 1 10

4 0 0

12 0 0 ** Option 12 Transition probabilities and nuclear moments**

51 0 0

4 4 307 1103 305 1101 0 0 0 0 0

2 4 307 1103 305 1101 0 0 0 0 0

4 0 0

2 0 20 20 0.5 1.5

multipolarity, parity, core, eff. ch. fluid1 (n), eff. ch. fluid2 (p)

Output

```
INITIAL STATE  P= 0     2*J= 4   N= 1
   Q(L=2)=    -13.640378

INITIAL STATE  P= 0     2*J= 8   N= 1
   Q(L=2)=    -23.509924
     P= 0     2*J= 4   N=  1 DE=  0.830  BE(L)=      158.2068

INITIAL STATE  P= 0     2*J= 6   N= 1
     P= 0     2*J= 8   N=  1 DE=  1.923  BE(L)=        5.1364
     P= 0     2*J= 4   N=  1 DE=  2.754  BE(L)=        4.1354

 GROUND-STATE (AMONG THE READ STATES) ENERGY=   -69.51059

2*J=  4 T-TZ= 0 COUL=0 N=  1 P=0 2*M= 4 C= 0  EXC=   0.00000 E=   -69.51059
2*J=  8 T-TZ= 0 COUL=0 N=  1 P=0 2*M= 4 C= 0  EXC=   0.83043 E=   -68.68015
2*J=  6 T-TZ= 0 COUL=0 N=  1 P=0 2*M= 4 C= 0  EXC=   2.75352 E=   -66.75707
```

Deducing the quadrupole deformation

The criteria to define a deformed rotor from the spherical shell model results are:

- J(J+1) spectrum
- Q_0 extracted from the BE2 has to be rather constant
- Q_0 extracted from the Q_{spec} has to be constant and equal to the ones deduced from the BE2

TABLE VI. ^{48}Cr; quadrupole properties of the yrast band.

J	$B(E2)_{expt}$	$B(E2)_{theor}$	$Q_0(t)$	$Q_0(s)$	$Q_0(t)[f7/2,p3/2]$
2	321(41)	228	107	103	104
4	330(100)	312	105	108	104
6	300(80)	311	100	99	103
8	220(60)	285	93	93	102
10	185(40)	201	77	52	98
12	170(25)	146	65	12	80
14	100(16)	115	55	13	50
16	37(6)	60	40	15	40

from Caurier et al., RMP 77 (2005) 427

Magnetic moments and transitions

```
 4 0 0 **** Option 4  Lanczos
 50   0   4
 3   4  307 1103 305 1101        0 0 0 0     0
 2   4  307 1103 305 1101        0 0 0 0     0
 1  0  0
     93   0
1  3  5  7
1  1  1  1
60  0.0005  0
```

```
 12 0 0 **** Option 12 Transition probabilities and nuclear moments
50  0  0
 3   4  307 1103 305 1101        0 0 0 0     0
 2   4  307 1103 305 1101        0 0 0 0     0
 1  0  0
 1  0  20 20 -3.826 0.0 5.586 1.0  (bare values)
multipolarity, parity, core, g-factors (spin, orbital) fluid (n), g-factors fluid2 (p)
```

you may use also -2.8695 -0.1 4.1895 1.1 (effective (quenched) values)

Except when the M1 transitions are fully dominated by the spin term, the use of effective g factors does not modify the results very much due to the compensation between the spin and orbital modifications.

Output

INITIAL STATE P= 1 2*J= 1 N= 1
MAGNETIC MOMENT L= 1 -0.07100 (in μ_N)

INITIAL STATE P= 1 2*J= 3 N= 1
MAGNETIC MOMENT L= 1 -0.82413
P= 1 2*J= 1 N= 1 DE= -2.158 **BM1= 0.0080 (in μ_N^2)**

INITIAL STATE P= 1 2*J= 5 N= 1
MAGNETIC MOMENT L= 1 -0.68951
P= 1 2*J= 3 N= 1 DE= -0.339 **BM1= 0.0514**

INITIAL STATE P= 1 2*J= 7 N= 1
MAGNETIC MOMENT L= 1 -1.09361
P= 1 2*J= 5 N= 1 DE= -0.011 **BM1= 0.1088**

GROUND-STATE (AMONG THE READ STATES) ENERGY= -57.71841

2*J= 7 T-TZ= 0 COUL=0 N= 1 P=1 2*M= 1 C= 0 EXC= 0.00000 E= -57.71841
2*J= 5 T-TZ= 0 COUL=0 N= 1 P=1 2*M= 1 C= 0 EXC= 0.01089 E= -57.70752
2*J= 3 T-TZ= 0 COUL=0 N= 1 P=1 2*M= 1 C= 0 EXC= 0.35024 E= -57.36817
2*J= 1 T-TZ= 0 COUL=0 N= 1 P=1 2*M= 1 C= 0 EXC= 2.50779 E= -55.21063

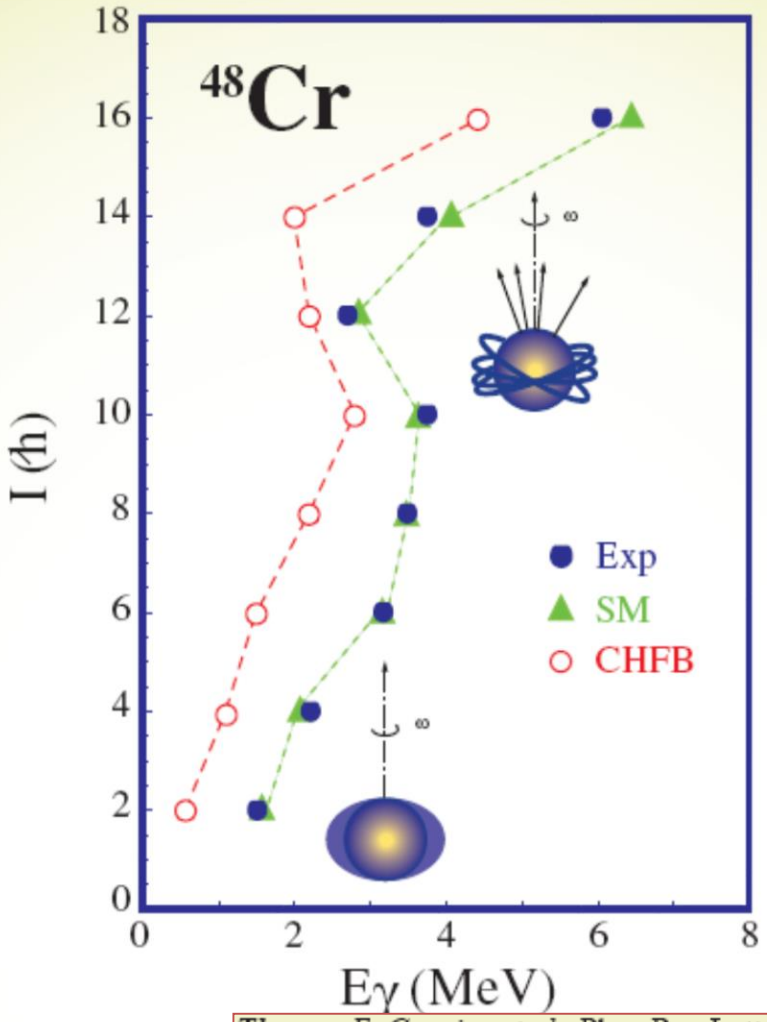
Antoine's transitions

All transitions are calculated from the higher spin towards the lower spin, independent than their excitation energy. The proper transformation has to be taken into account

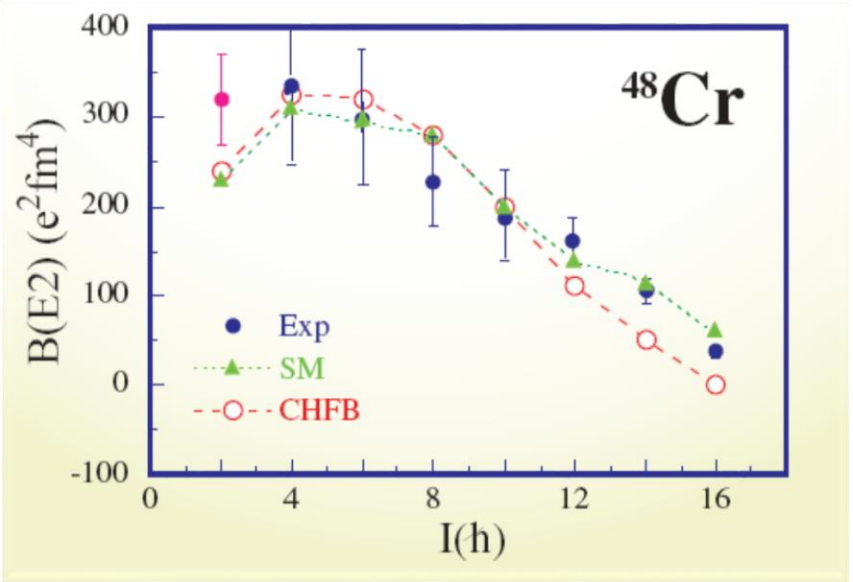
$$(2I_1+1)B(E2, I_1 \rightarrow I_2) = (2I_2+1)B(E2, I_2 \rightarrow I_1)$$

$$(2I_1+1)B(M1, I_1 \rightarrow I_2) = (2I_2+1)B(M1, I_2 \rightarrow I_1)$$

Shell model and collective phenomena



Shell model calculations in the full fp shell give an excellent description of the structure of collective rotations in nuclei of the $f_{7/2}$ shell



Theory: *E. Caurier et al.*, Phys.Rev.Lett.**75**(1995)225
Experiments: *S. M. Lenzi et al.*, Z.Phys.**A354**(1996)117 - *F. Brandolini et al.*, Nucl.Phys.**A642**(1998)387

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Good luck!