The Nuclear Shell Model

Computer session

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CEN Bordeaux-Gradignan, France

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The Nuclear Shell Model

We will attribute you a rank: X
First, log on the local computer.

Then use “putty” or “SSH Secure Shell Client” Desktop icon to log as wshopX on the calculation server sbgpcs25.in2p3.fr

```
ssh wshopX@sbgpcs25.in2p3.fr
password: bmint2017
```

Then, according to the following table, log again on the working machines:

<table>
<thead>
<tr>
<th>X</th>
<th>machine YY</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>sbgvsrv41</td>
</tr>
<tr>
<td>2</td>
<td>sbgvsrv42</td>
</tr>
<tr>
<td>3</td>
<td>sbgvsrv43</td>
</tr>
<tr>
<td>4</td>
<td>sbgvsrv44</td>
</tr>
<tr>
<td>5</td>
<td>sbgvsrv45</td>
</tr>
<tr>
<td>6</td>
<td>sbgvsrv45</td>
</tr>
</tbody>
</table>

```
ssh wshopX@sbgvsrvYY.in2p3.fr
```

Once you are logged, change to folder bmint: `cd bmint`
and get ready for Exercises.
http://www.iphc.cnrs.fr/nutheo/code_antoine/menu.html

SHELL MODEL CODE ANTOINE
by Etienne CAURIER

THE USE OF THIS CODE IS AUTHORIZED UPON ACKNOWLEDGEMENT
OF THE INTELLECTUAL PROPERTY
BY QUOTING THE FOLLOWING REFERENCES:

E. CAURIER, shell model code ANTOINE,
IRES, STRASBOURG 1989-2004

E. CAURIER, F. NOWACKI

E. CAURIER, G. MARTINEZ-PINEDO, F. NOWACKI, A. POVES, A. P. ZUKER
Reviews of Modern Physics 77, No 2, April 2005
ANTOINE shell-model code

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

- m-scheme code

- basis defined with:
  - number of particles in Fluid 1, shells of Fluid 1
  - number of particles in Fluid 2, shells of Fluid 2
  - a given total $J_z = M$ of the wave function
  - a given parity $\Pi$

- each quantity which can be half-integer has to be doubled
Notations of orbitals

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

<table>
<thead>
<tr>
<th></th>
<th>stands for</th>
<th></th>
<th>stands for</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0s_{1/2}</td>
<td>305</td>
<td>0f_{5/2}</td>
</tr>
<tr>
<td>101</td>
<td></td>
<td>307</td>
<td></td>
</tr>
<tr>
<td>103</td>
<td></td>
<td>2001</td>
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</tr>
<tr>
<td>1001</td>
<td></td>
<td>1203</td>
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<td>203</td>
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<td>1205</td>
<td></td>
</tr>
<tr>
<td>205</td>
<td></td>
<td>407</td>
<td></td>
</tr>
<tr>
<td>1101</td>
<td></td>
<td>409</td>
<td></td>
</tr>
<tr>
<td>1103</td>
<td></td>
<td>511</td>
<td></td>
</tr>
</tbody>
</table>

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

- Inert core: orbits that are always full.

- Valence space: orbits that contain the physical degrees of freedom relevant to a given property. The distribution of the valence particles among these orbitals is governed by the interaction.

- External space: all the remaining orbits that are always empty.

Examples of valence spaces:
- \(0p_{3/2}0p_{1/2}\) orbits beyond \(^4\)He core (\(p\) shell).
- \(0d_{5/2}1s_{1/2}0d_{3/2}\) orbits beyond \(^{16}\)O core (\(sd\) shell).
- \(0f_{7/2}1p_{3/2}1p_{1/2}0f_{5/2}\) orbits beyond \(^{40}\)Ca core (\(pf\) shell).
- each “task” correspond to an option number
- options can performed successively:
  - diagonalization, configurations, electromagnetic transitions ...
- list of essential options we will use:

<table>
<thead>
<tr>
<th>Option Number</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CALCULATE DIMENSIONS OF THE SPACE</td>
</tr>
<tr>
<td>2</td>
<td>NON-ZERO OF THE MATRIX</td>
</tr>
<tr>
<td>4</td>
<td>USUAL LANCZOS PIVOT RANDOM</td>
</tr>
<tr>
<td>5</td>
<td>USUAL LANCZOS PIVOT=E(MINI)</td>
</tr>
<tr>
<td>6</td>
<td>LANCZOS WITH PROJECTED PIVOTS</td>
</tr>
<tr>
<td>7</td>
<td>LANCZOS VECTORS PROJECTED ON J**2</td>
</tr>
<tr>
<td>11</td>
<td>CALCULATION OF OCCUPATION OF SHELLS</td>
</tr>
<tr>
<td>12</td>
<td>TRANSITIONS</td>
</tr>
<tr>
<td>21</td>
<td>SUM RULE OF A TRANSITION OPERATOR</td>
</tr>
<tr>
<td>23</td>
<td>CHANGE TZ</td>
</tr>
<tr>
<td>24</td>
<td>GAMOW-TELLER</td>
</tr>
<tr>
<td>26</td>
<td>SPECTROSCOPIC FACTOR</td>
</tr>
<tr>
<td>31</td>
<td>CHANGE TRUNCATION</td>
</tr>
<tr>
<td>32</td>
<td>CHANGE THE BASIS</td>
</tr>
<tr>
<td>33</td>
<td>CHANGE JZ</td>
</tr>
</tbody>
</table>
Option 1: Calculate Dimensions of the basis

<p>| | | | | | | | | | |</p>
<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>*****</td>
<td>Option 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>205</td>
<td>203</td>
<td>1001</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>3</td>
<td>205</td>
<td>203</td>
<td>1001</td>
<td>0</td>
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<td>10</td>
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<td>0</td>
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</tr>
</tbody>
</table>

Basis definition:
for each fluid (proton or neutrons),
- number of particles
- number of shells
- denomination of shells
- shell class $c_i$
- $t_{max}$ in each fluid
- total $J_z$ value
- total parity
- total $t_{max}$
Option 2: Compute number of non-zero terms in the matrix

\[
\begin{align*}
2 & \quad 0 & \quad 0 & \quad ***** & \quad \text{Option 2} \\
4 & \quad 3 & \quad 205 & \quad 203 & \quad 1001 & \quad 0 & \quad 0 & \quad 0 & \quad 10 \\
6 & \quad 3 & \quad 205 & \quad 203 & \quad 1001 & \quad 0 & \quad 0 & \quad 0 & \quad 10 \\
0 & \quad 0 & \quad 0 & \quad & & & & & \\
\end{align*}
\]

Basis definition:
for each fluid (proton or neutrons),
- number of particles
- number of shells
- denomination of of shells
- shell class \( c_i \)
- \( t_{\text{max}} \) in each fluid
- total \( J_z \) value
- total parity
- total \( t_{\text{max}} \)
Exercises

Exercise 1:
Estimate of all the possible Angular Momentum Couplings of two particles

\[ |j_1 m_1 \rangle |j_2 m_2 \rangle \]_M^J \text{ in } j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2} \text{ orbitals. Distinguish the two cases:}

- two particles are identical
- one particle is a proton, one particle is a neutron

Exercise 2:
Enumerate all the \(|M = m_1 + m_2\rangle\) states build with two particles in \(j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}\). Starting from \(|M_{\text{max}}\rangle\), determine all the distinct \(|JM\rangle\) states. Verify with the code, the basis dimensions of \(^{18}\text{O}\) and \(^{18}\text{F}\)

Exercise 3:
Calculate the basis dimensions of all even-even N=Z nuclei from \(^{20}\text{Ne}\) to \(^{36}\text{Ar}\). Predict the nucleus with the largest dimension. Observe the evolution of number of basis states with increasing Z,N numbers

For even nucleus an "effective dimension" is printed. It is the dimension of the matrix at \(J_z = 0\) taking in account the time reversal symmetry. For odd-odd nucleus it is exactly half \(\text{dim}(J_z = 0)\) for even-even it is a little bit larger

Exercise 4:
Calculate the number of non-zero ME of all even-even N=Z nuclei from \(^{20}\text{Ne}\) to \(^{36}\text{Ar}\). Observe the evolution of number of non-zero ME with increasing Z,N numbers

Estimate the ratio of diagonalization time between \(^{20}\text{Ne}\) and \(^{28}\text{Si}\)
USD INT. (SD SHELL)
1 3 203 205 1001
1.64658 -3.94780 -3.16354
1 8 8 0.300000 0.000000
0 1 203 203 203 203 0 3
 0.00000 -1.41510 0.00000 -2.88420
-2.18450 0.00000 -0.06650 0.00000
0 1 205 203 203 203 1 3
 0.56470 0.00000 2.03370
 0.00000 -0.61490 0.00000
0 1 205 203 205 203 1 4
-6.50580 -3.82530 -0.53770 -4.50620
 1.03340 -0.32480 0.58940 -1.44970
Option 4: diagonalization from random initial pivot

4 0 0 ***** Option 4
50 0 2 output file, initialization, number of J matrices
4 3 205 203 1001 0 0 0 10
6 3 205 203 1001 0 0 0 10
0 0 0
93 0 interaction file, COUL
0 4 J values of the 2 matrices
1 1 number of states for each J
60 0.0005 0 0 it max, energy conv., ortho, older iterations

COUL=0 no Coulomb, COUL=1,2 space for protons
Option 5: diagonalization from minimal energy pivot

5 0 0 ***** Option 5
50 0 2 output file, initialization, number of J matrices
4 3 205 203 1001 0 0 0 10
6 3 205 203 1001 0 0 0 10
0 0 0
93 0 interaction file, COUL
0 4 J values of the 2 matrices
1 1 number of states for each J
60 0.0005 0 0 it max, energy conv., ortho, older iterations

COUL=0 no Coulomb, COUL=1,2 space for protons
Exercices

Exercise 5:
Compute the energy spectrum of $^{18}_8O$ and $^{18}_8F$: $J^\pi = 0^+, 1_{1,2}^+, 2^+, 3^+, 4^+, 6^+$. Check the energies of $1_{1,2}^+$ state in $^{18}_8O$ using the USD Hamiltonian.

Exercise 6:
Compute the energy spectrum of $^{28}_{14}Si$: $J^\pi = 0^+, 2^+, 4^+, 6^+$

Exercise 7:
Compute now the energy spectrum of $^{28}_{14}Si$: $J^\pi = 0^+, 2^+_{1,2,3,4,5,6}, 4^+_{1,6}$
Compare the Lanczos matrices, spectra with those from Exercise 5. Try to find the explanation for differences. Fix the problem by orthogonalization to previous calculated states.

Exercise 8:
Compute all the $1^+ T = 0$ states in $^{38}_{19}K$, starting:

- from random pivot (option 4)
- from minimal energy pivot (option 5)

Observe the Lanczos matrices, spectra in both cases. Try to find the explanation for differences.
Option 12: E(L) and M(L) transitions. Parity unchanged.

12 0 0 ***** Option 12
50 0 0 input file, initialization, nb of vectors
4 3 205 203 1001 0 0 0 10
6 3 205 203 1001 0 0 0 10
0 0 0 0
2 0 8 8 1.5 0.5

Multipolarity of the transition \((L = 2)\)
No change of parity \((\Pi = 0)\)
number of core nucleons of FL1
number of core nucleons of FL1
effective charge FL1
effective charge FL2
# Option 12: E(L) and M(L) transitions. Parity unchanged.

```
12 0 0 ***** Option 12
50 0 0      input file, initialization, nb of vectors
4 3  205 203 1001  0 0 0 10
6 3  205 203 1001  0 0 0 10
 0 0 0 0
1 0 8 8 5.586 1.0 -3.826 0.0
```

Multipolarity of the transition \( (L = 1) \)

No change of parity \( (\pi = 0) \)

- number of core nucleons of FL1
- number of core nucleons of FL1
- (effective) spin and orbital g-factors FL1
- (effective) spin and orbital g-factors FL2
Exercise 9:
Compute the energy spectrum of $^{25}_{12}Mg$: $J^\pi = 1/2^+, 3/2^+, 5/2^+, 7/2^+$. Compute $E2$ and $M1$ transitions and moments.

Exercise 10:
Compute the energy spectrum of $^{24}_{12}Mg$: $J^\pi = 0^+, 2_1^+, 4_1^+, 6_1^+$. Compute $E2$ transitions and moments and $M1$ moments.
### Option 33: Change $J_z$

<table>
<thead>
<tr>
<th>Option 33</th>
<th>Change $J_z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>33 0 0 *****</td>
<td>Option 33</td>
</tr>
<tr>
<td>51 50 0 1 0</td>
<td>output file, input file initialization, initialization, nb of vectors</td>
</tr>
<tr>
<td>4 3 205 203 1001</td>
<td>0 0 0 0</td>
</tr>
<tr>
<td>6 3 205 203 1001</td>
<td>0 0 0 0</td>
</tr>
<tr>
<td>2 0 0</td>
<td>final $J_z$</td>
</tr>
</tbody>
</table>
Exercise 10bis:
Compute the energy spectrum of $^{24}_{12}\text{Mg}$: $J^\pi = 0^+, 2^+, 4^+, 6^+$. Compute $E2$ transitions and moments and $M1$ moments.
Option 31: Change truncation basis

31 0 0 ***** Option 31

51 50 0 0 2 output file, input file initialization, initialization, nb of vectors
4 3 205 203 1001 0 1 1 10
6 3 205 203 1001 0 1 1 10
0 0 2 final truncation

Option 32: Change basis

32 0 0 ***** Option 32

51 50 0 0 2
4 3 205 203 1001 0 0 0 10 final basis
6 3 205 203 1001 0 0 0 10
0 0 0
4 3 205 203 1001 0 1 1 10 initial basis
6 3 205 203 1001 0 1 1 10
0 0 2
Option 6: diagonalization from calculated pivot

6 0 0 ***** Option 6
50 51 0 0 2 output file, input file, initialization, initialization, nb of J matrices
4 3 205 203 1001 0 0 0 10
6 3 205 203 1001 0 0 0 10
0 0 0
93 0 interaction file, COUL
1 2 number of Converged states for each J matrix
0 60 0.0005 0 0 KPVT, it max, energy conv., ortho, older iterations

KPVT: determination of the pivot

- KPVT > 0 pivot: linear combination of the KPVT vectors on the initial file
- KPVT = 0 pivot: linear combination of the N vectors on the initial file, N being the number of converge states we need.

In the example we must have on the file 51:
- 1 state of a given $J_1$ followed by
- 2 states of given $J_2$
### Option 7: same with angular momentum projection

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Option 7: same with angular momentum projection</td>
<td>7 0 0</td>
</tr>
<tr>
<td>Output file, input file, initialization</td>
<td>50 51</td>
</tr>
<tr>
<td>nb of J matrices</td>
<td>0 2</td>
</tr>
<tr>
<td>Initialization</td>
<td>0 0 0</td>
</tr>
<tr>
<td>nb of J matrices</td>
<td>0 0 0</td>
</tr>
<tr>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>Interaction file, COUL</td>
<td>93 0</td>
</tr>
<tr>
<td>Number of Converged states for each J matrix</td>
<td>1 2</td>
</tr>
<tr>
<td>KPVT, it max, energy conv., ortho, older iterations</td>
<td>0 60 0.0005 0 0</td>
</tr>
</tbody>
</table>

**KPVT: determination of the pivot**

- **KPVT > 0** pivot: linear combination of the KPVT vectors on the initial file
- **KPVT = 0** pivot: linear combination of the N vectors on the initial file, N being the number of converge states we need.

In the example we must have on the file 51:
- 1 state of a given $J_1$ followed by
- 2 states of given $J_2$
Exercise 11:
Compute the energy spectrum of $^{28}_{14}Si$: $J^\pi = 0^+, 2_1^+, 4_1^+, 6_1^+$ but

- precalculation in $t=2$ space
- with precalculation in successive truncation $t=2$ and $t=4$ spaces

Compare number of iterations, computing time ...