

# Large-scale Shell Model: application to studies of nuclear spectroscopy and gamma transitions

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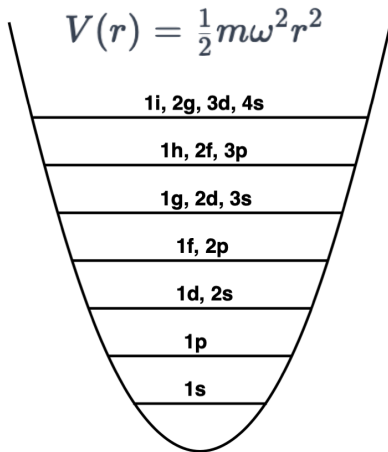
9<sup>th</sup> May 2023



- Introduction
- Properties of the Shell model
- Applications of the Shell model
- Large-scale shell model
- Code Antoine
- Nuclear deformation

# Properties of the Shell model

- The independent particle model (IPM)
- Harmonic oscillator potential



# Properties of the Shell model

$$V_{SO} = \alpha \vec{L} \cdot \vec{S}$$

The model can be improved by adding Spin-Orbit Coupling.

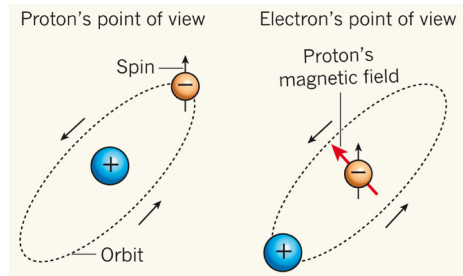
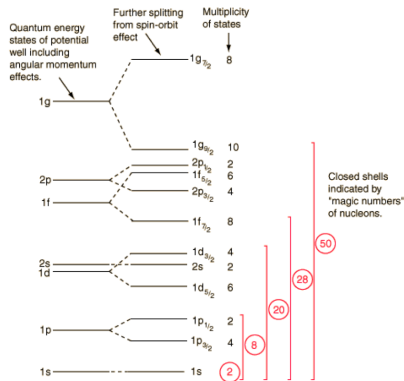


Figure: Spin-Orbit Coupling

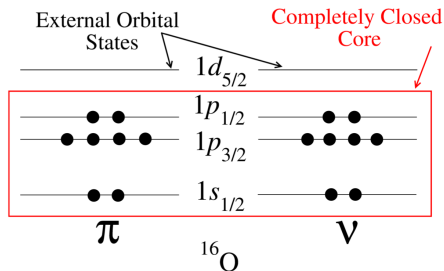
# Properties of the Shell model

- Based on experimental observations of nuclear binding energies and the properties of excited nuclear states.
- Magic numbers



# Properties of the Shell model

Nucleons are positioned in the lowest shells and that allow us to determine the angular momentum and the parity of the state  $J^\pi$ .



# Properties of the Shell model

①  $^{15}_8\text{O}_7$ : The last neutron  $\rightarrow 1p_{1/2}$

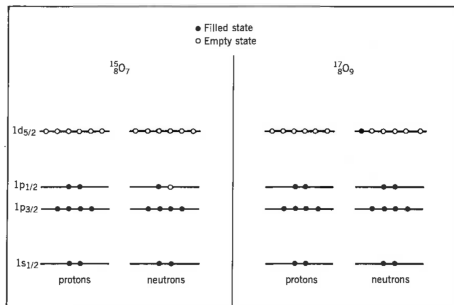
- $j = \frac{1}{2}$
- $\ell = 1$  (from  $p$  orbital)  
 $\Rightarrow$  parity:  $\pi = (-1)^\ell = -$

•  $\therefore J^\pi_{\text{gs}}(^{15}\text{O}) = \frac{1}{2}^-$

②  $^{17}_8\text{O}_9$ : The last neutron  $\rightarrow 1d_{5/2}$

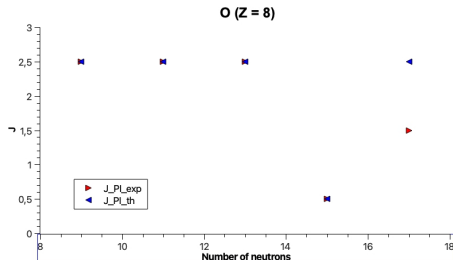
- $j = \frac{5}{2}$
- $\ell = 2$  (from  $d$  orbital)  
 $\Rightarrow$  parity:  $\pi = (-1)^\ell = +$

•  $\therefore J^\pi_{\text{gs}}(^{17}\text{O}) = \frac{5}{2}^+$



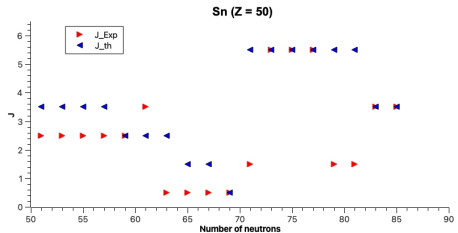
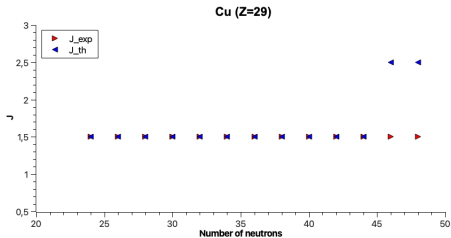
# Applications of the Shell model

comparison of the angular momentum predicted by our model with experimental results for different isotopes of O, Cu and Sn



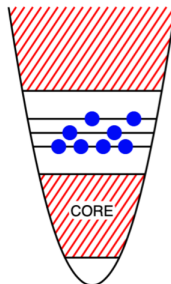


# Applications of the Shell model



# Large-scale 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 (limit of calculation)



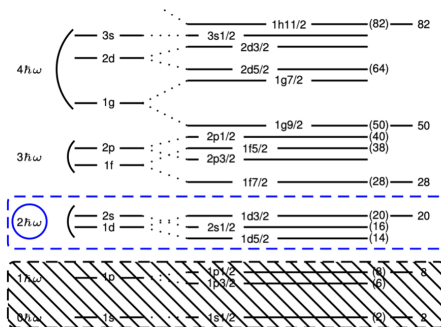
- Define a valence space
- Derive an effective interaction  
 $H\psi = E\psi \longrightarrow H_{eff}\psi = E_{eff}\psi$
- Build and diagonalize the Hamiltonian matrix.

$$\Psi = \frac{1}{\sqrt{n!}} \sum_p (-1)^p P \begin{pmatrix} \phi_1(1) & \cdots & \phi_n(1) \\ \vdots & \ddots & \vdots \\ \phi_1(n) & \cdots & \phi_n(n) \end{pmatrix}$$

# Large-scale shell model

Valence space :

- 4 A 16 : Cohen-Kurath interaction
- 16 A 40 : sd shell USD interaction
- 40 A 80 : KB3 interactions



# Antoine Code

- Computer program used to perform shell model calculations in nuclear physics.
- Based on the large-scale shell model and allows for the calculation of nuclear properties, such as excitation energies, magnetic moments, and decay rates.
- Diagonalisation of large Hamiltonian matrices for solving the nuclear many-body problem.



- option 1 : Calculate Dimensions of the basis
- option 2 : Compute number of non-zero terms in the matrix
- option 4 : Diagonalization from random initial pivot
- option 12 : Wave-function Quadrupole moment
- option 31 : Change truncation basis

Option 1: Calculate Dimensions of the basis

Option 2: Compute number of non-zero terms in the matrix

1 0 0 \*\*\*\*\* Option 1

4 3 205 203 1001 0 0 0 10

6 3 205 203 1001 0 0 0 10

0 0 0

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  $t_{max}$

# Antoine Code

```
INITIAL STATE P= 0 2*J= 4 N= 1
Q(L=2)= -16.339347
P= 0 2*J= 0 N= 1 DE= 1.509 BE(L)= 69.47740369

INITIAL STATE P= 0 2*J= 4 N= 2
Q(L=2)= 16.578464
P= 0 2*J= 4 N= 1 DE= 2.613 BE(L)= 15.15699610
P= 0 2*J= 0 N= 1 DE= 4.122 BE(L)= 6.20638656

INITIAL STATE P= 0 2*J= 8 N= 1
Q(L=2)= -19.857931
P= 0 2*J= 4 N= 2 DE= 0.256 BE(L)= 0.46933800
P= 0 2*J= 4 N= 1 DE= 2.869 BE(L)= 92.35718046

INITIAL STATE P= 0 2*J= 8 N= 2
Q(L=2)= -9.085790
P= 0 2*J= 8 N= 1 DE= 1.556 BE(L)= 12.63539846
P= 0 2*J= 4 N= 2 DE= 1.812 BE(L)= 35.30633272
P= 0 2*J= 4 N= 1 DE= 4.425 BE(L)= 3.11890756

INITIAL STATE P= 0 2*J=12 N= 1
Q(L=2)= -16.733946
P= 0 2*J= 8 N= 2 DE= 2.328 BE(L)= 7.26175402
P= 0 2*J= 8 N= 1 DE= 3.885 BE(L)= 87.48414172

INITIAL STATE P= 0 2*J=12 N= 2
Q(L=2)= -20.484379
P= 0 2*J=12 N= 1 DE= 1.322 BE(L)= 9.25116535
P= 0 2*J= 8 N= 2 DE= 3.650 BE(L)= 45.96907524
P= 0 2*J= 8 N= 1 DE= 5.207 BE(L)= 0.15884931

INITIAL STATE P= 0 2*J=16 N= 1
Q(L=2)= 15.147648
P= 0 2*J=12 N= 2 DE= 2.503 BE(L)= 0.65399637
P= 0 2*J=12 N= 1 DE= 3.825 BE(L)= 10.94581083
```

```
GROUND-STATE (AMONG THE READ STATES) ENERGY= -87.08958

2*J= 0 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 0.00000 E= -87.08958
2*J= 4 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 1.50907 E= -85.50051
2*J= 4 T-TZ= 0 COUL=0 N= 2 P=0 2*M= 0 C= 0 EXC= 4.12220 E= -82.96738
2*J= 8 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 4.37828 E= -82.71130
2*J= 6 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 5.09658 E= -81.99300
2*J= 8 T-TZ= 0 COUL=0 N= 2 P=0 2*M= 0 C= 0 EXC= 5.93446 E= -81.15512
2*J= 10 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 7.88347 E= -79.28611
2*J= 12 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 8.26295 E= -78.82663
2*J= 12 T-TZ= 0 COUL=0 N= 2 P=0 2*M= 0 C= 0 EXC= 9.58485 E= -77.50473
2*J= 16 T-TZ= 0 COUL=0 N= 1 P=0 2*M= 0 C= 0 EXC= 12.08806 E= -75.00152
2*J= 16 T-TZ= 0 COUL=0 N= 2 P=0 2*M= 0 C= 0 EXC= 13.16017 E= -73.92941

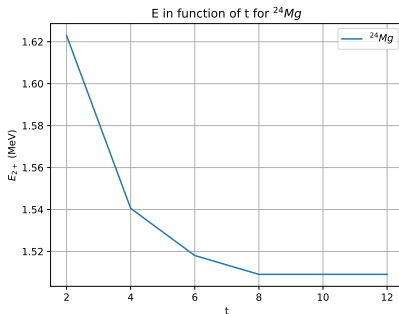
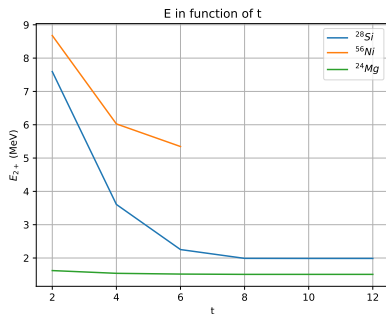
REWIND FILE 50

TIME FOR THIS OPTION= 0.180
*****
NORMAL END OF THE JOB
```

Figure: Data from Antoine code

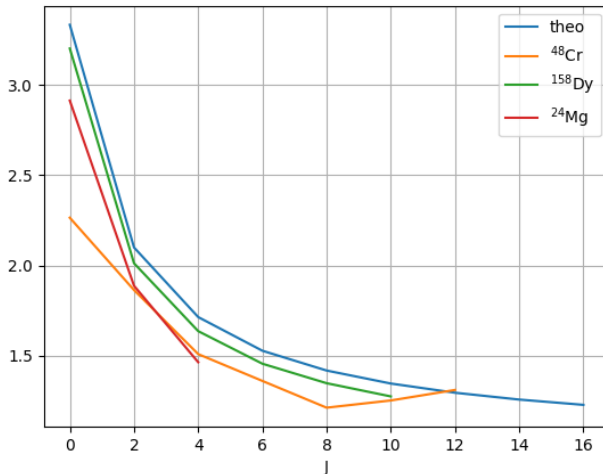
Figure: Data from Antoine code

# Results of numerical calculation



Evolution of the excitation energy of the  $2^+$  state as a function of the truncation

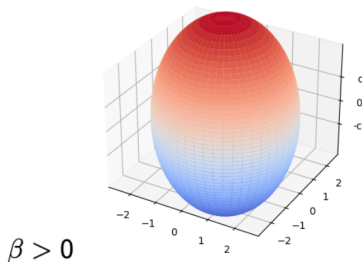
## Rotational limit



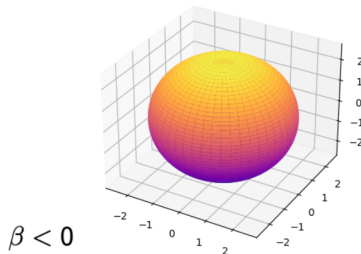


# Nuclear deformation

Shape of the prolate nucleus



Shape of the oblate nucleus



$$R(\theta, \phi) = R_0 \left( 1 + \beta \sqrt{\frac{5}{16\pi}} (\cos\gamma (3\cos^2\theta - 1) + \sqrt{3}\sin\gamma \sin^2\theta \cos 2\phi) \right)$$

# Nuclear deformation

- Quadrupole deformation :

$$\beta = \frac{4\pi}{3} \frac{Q}{ZR^2}$$

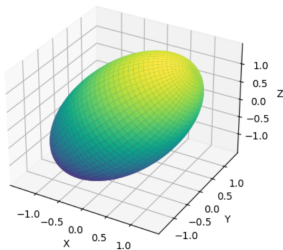
- Quadrupole moment

$$Q = \int \rho(\vec{r})(3Z^2 - r^2)d^3r$$

- Core radius

$$R = r_0 A^{1/3}$$

Shape of the triaxial core



$$\gamma = \frac{2}{3} \frac{\beta}{R} \sqrt{\frac{5\pi}{16\pi - 3}}$$

- Quadrupole moment :

$$Q = Q_0 \frac{3K^2 - I(I+1)}{(2I+3)(I+1)}$$

- Transition probability :

$$B(E2; K I_1 \longrightarrow K I_2) = \frac{5}{16\pi} e^2 Q_0^2 \langle I_1 K 20 | I_2 K \rangle^2$$

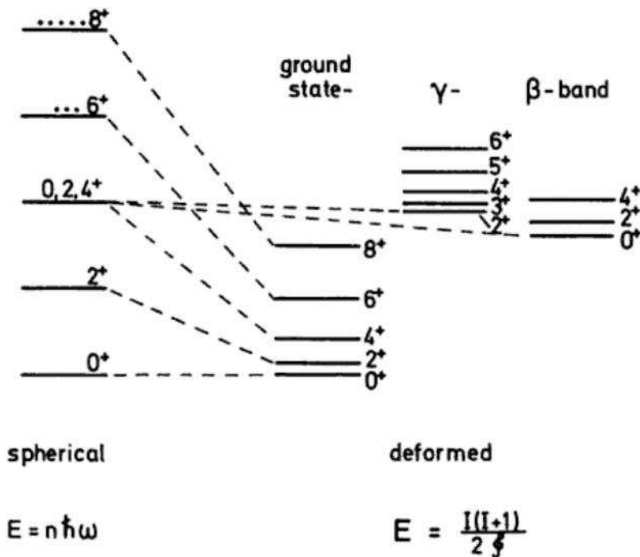
# Nuclear deformation

States	$Q_0 \text{ exp}$	$Q_0 \text{ from BE2}$	$Q_0 \text{ from } Q$	$\beta$
2+	121,7	113,2	109,4	0,317
4+	100,2	110,9	114,2	0,330
6+	97,4	105,4	105,1	0,304
8+	87,6	98,6	98,2	0,284
10+	76,2	82,1	55,8	0,161
12+	79,5	68,9	13,1	0,038
14+	64,9	60,7	13,2	0,038
16+	35,9	43,7	15,7	0,046

Table: Values of Quadrupole Moment for  $^{48}\text{Cr}$

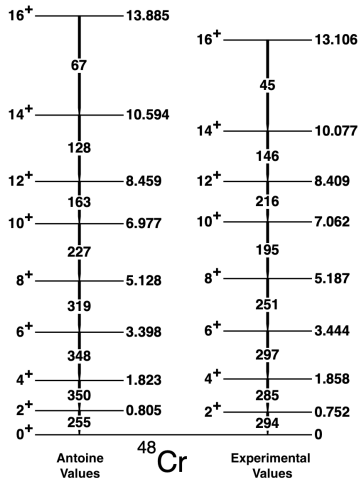
$\beta > 0$  for  $^{48}\text{Cr} \implies$  prolate

# Nuclear deformation



# Nuclear deformation

We observe that values obtain with the code for energy levels and probability of transition are very close to experimental values.



# Nuclear deformation

- $Q(2_1+) = -Q(2_\gamma+)$  and  $Q(3_+)$  is near to 0 : That's the proof of the  $\gamma$  band exist for  $Mg24$
- We can determine  $\gamma = 15$  non-zero and deduce that the Nuclei is triaxial

States	$Q_{spectro}$	$Q_0$ from code	$\beta$
2+	-16,34	57,19	0,525
4+	-19,86	54,61	0,502
6+	-16,73	41,83	0,384
8+	15,15	-35,98	-0,331

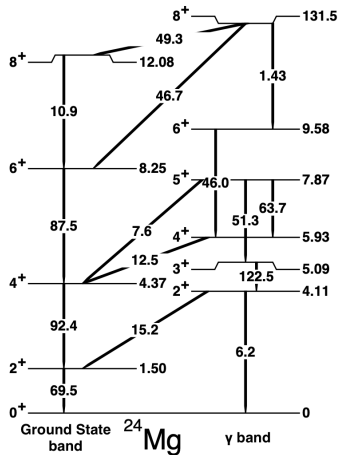
Table: Values from code for  $^{24}Mg$  for ground state band

States	$Q_{spectro}$	$Q_0$ from code	$\beta$
2+	16,58	-58,02	-0,53
3+	-0,05	0,16	0,001
4+	-9,08	62,46	0,573
5+	-13,70	59,35	0,545
6+	-20,48	71,69	0,659

Table: Values from code for  $^{24}Mg$  for  $\gamma$  band

# Nuclear deformation

Then we have built the levels scheme of  $Mg^{24}$  and we can see the  $\gamma$  band next to the ground state band.





# Summary

- Basis of shell model, IPM, adding spin orbit coupling
- Angular momentum coupling for two and three particles
- Fortran code compilation
- We learn how to use the code with exercices ; some examples :
  - Verify with the code, the basis dimensions of  $^{16}\text{O}$  and  $^{18}\text{F}$
  - Calculate the basis dimensions of all even-even  $N=Z$  nuclei from  $^{20}\text{Ne}$  to  $^{36}\text{Ar}$
  - Calculate the number of non-zero matrix element of all even-even  $N=Z$  nuclei from  $^{20}\text{Ne}$  to  $^{36}\text{Ar}$
  - Compute the energy spectrum of  $^{28}\text{Si}$  for  $J^\pi = 0+; 2+; 4+; 6+$
  - Compute the energy spectrum of  $^{22}\text{O}$  ; Compute E2 transitions and moments.

# Summary

- Computing of energy levels and probability transition and Creation of levels scheme with another fortran code.
- Study of general properties of electromagnetic transitions in nuclei, Bohr-Mottelson model . . .
- Study of notion about nuclear deformation and apply to  $^{24}\text{Mg}$  and  $^{48}\text{Cr}$
- Python script to plot in 3D the nuclei form in function of quadrupole moment.