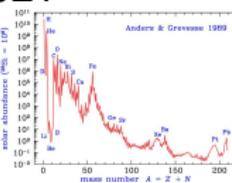
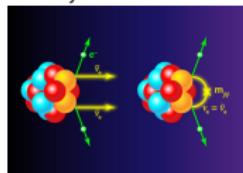
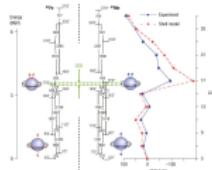


# DESCRIPTION OF HEAVY NUCLEI WITHIN THE SHELL MODEL

Dao Duy Duc and Frédéric Nowacki  
(IPHC-Strasbourg)

Ecole Thématique PhyNuBe

Aussois, December 07th, 2021

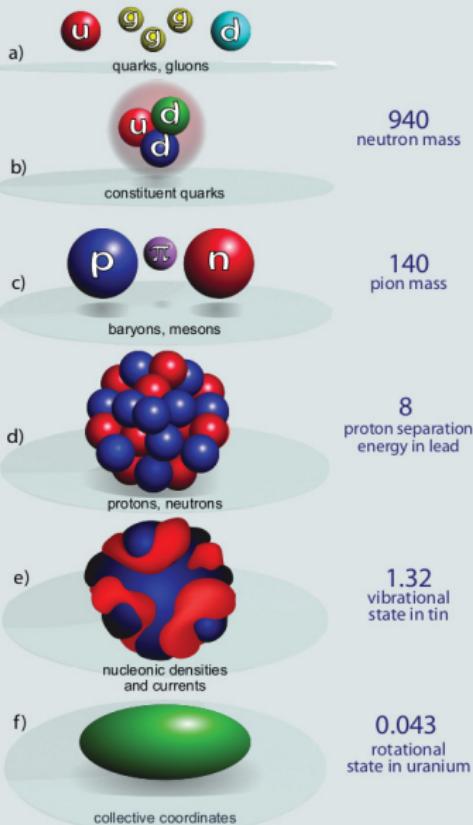


# 1 Nuclear Structure

## Physics of Hadrons

### Degrees of Freedom

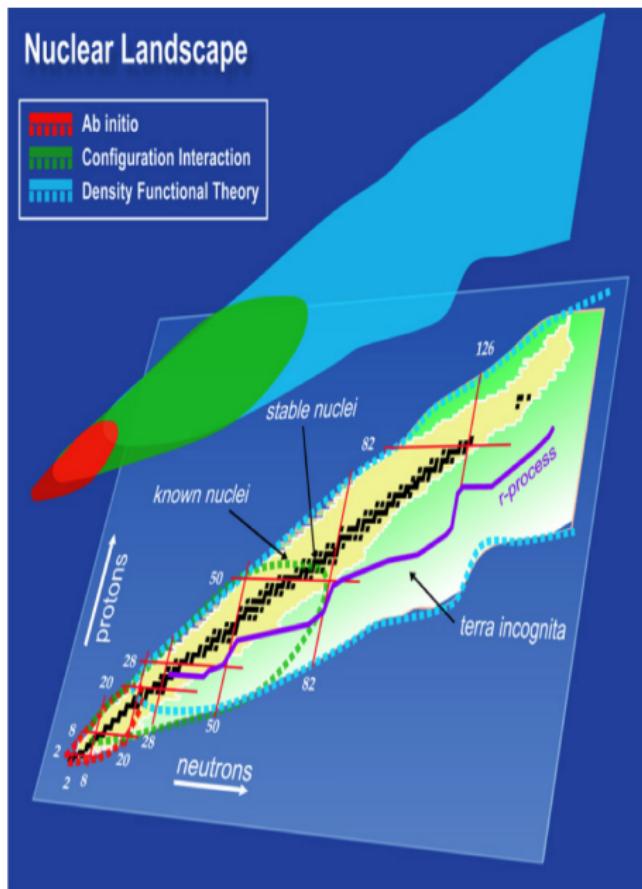
### Energy (MeV)



## Structure of the atomic nucleus

- The atomic nucleus is composed of neutrons and protons which interact mutually by exchange of mesons ( $10^{-15}$  m)
- The nucleons themselves are composed of quarks interacting by gluons exchange ( $10^{-18}$  m)
- The atomic nucleus is a many-body system of great complexity
- At low excitation energies, regularities emerge such as shell structures and collective behaviors (rotation and vibration)

## 2 The Nuclear Many-Body Problem



### Many-body approaches

$$H |\Psi\rangle = E |\Psi\rangle$$

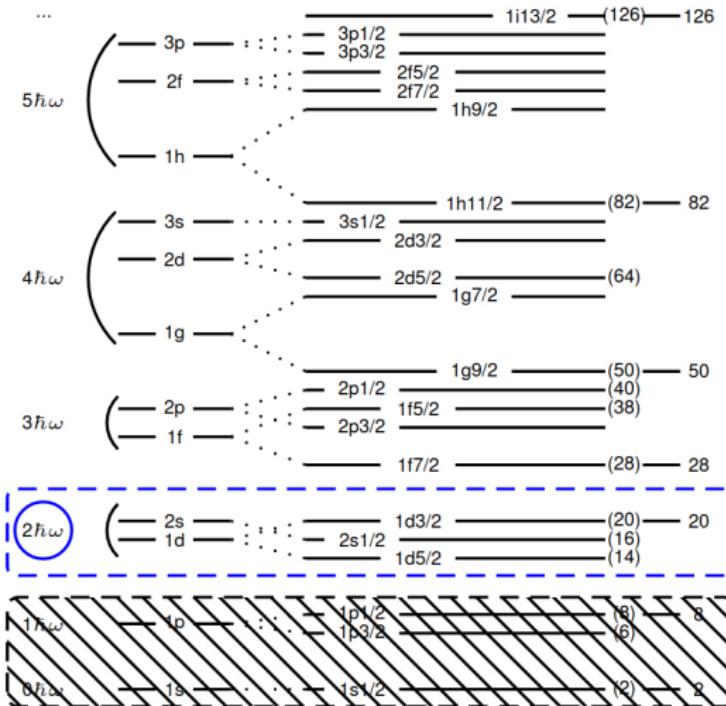
- “ab-initio” approaches
- Interacting Shell Model
- Mean field and beyond mean field methods

### Interacting Shell Model

$$\mathcal{H}_{\text{eff}} |\Psi_{\text{eff}}\rangle = E |\Psi_{\text{eff}}\rangle$$

$$\langle \Psi | \mathcal{O} | \Psi \rangle = \langle \Psi_{\text{eff}} | \mathcal{O}_{\text{eff}} | \Psi_{\text{eff}} \rangle$$

### 3 Interacting Shell Model

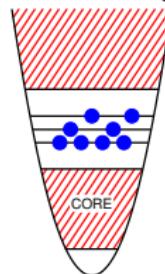


### Secular problem

$$\mathcal{H}_{\text{eff}}|\Psi_{\text{eff}}\rangle = E|\Psi_{\text{eff}}\rangle$$

#### Valence space

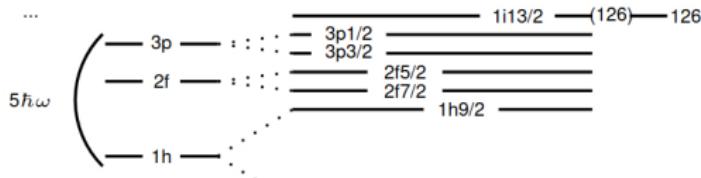
- single-particle orbitals
- closed core at magic numbers



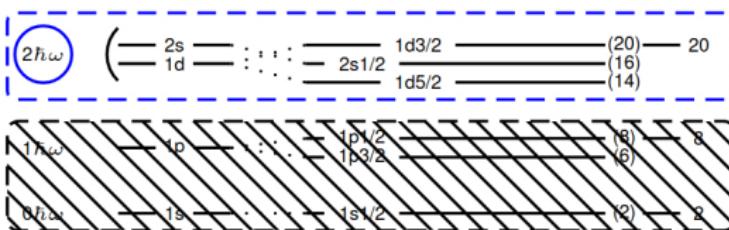
#### Effective interaction

#### Resolution techniques

### 3 Interacting Shell Model



- Light nuclei from  $^{16}\text{O}$  to  $^{40}\text{Ca}$
- Interactions: e.g. USD types (USDA, USDB)  
(A. B. Brown, Phys. Rev. C74, 034315 (2006))

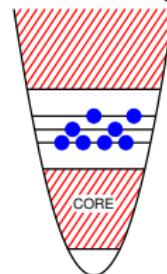


### Secular problem

$$\mathcal{H}_{\text{eff}}|\Psi_{\text{eff}}\rangle = E|\Psi_{\text{eff}}\rangle$$

#### ▷ Valence space

- ◊ single-particle orbitals
- ◊ closed core at magic numbers



#### ▷ Effective interaction

#### ▷ Resolution techniques

## 4 Interacting Shell Model

- Free NN interaction:

$$V(r) = V_0(r) + V_\sigma \sigma_1 \cdot \sigma_2 + V_\tau \tau_1 \cdot \tau_2$$

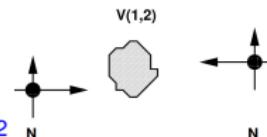
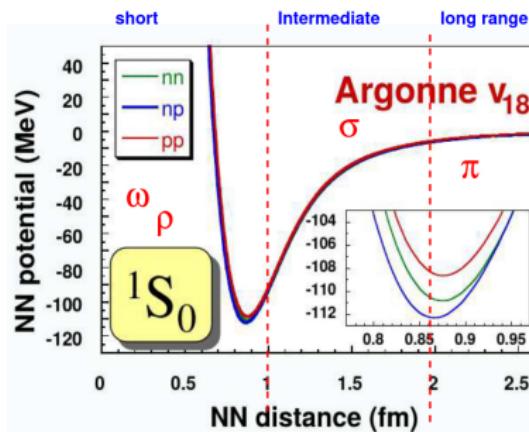
+  $V_{\sigma\tau} (\sigma_1 \cdot \sigma_2)(\tau_1 \cdot \tau_2)$  central

+  $V_{LS} \mathbf{L} \cdot \mathbf{S} + V_{LS}^\tau (\mathbf{L} \cdot \mathbf{S})(\tau_1 \cdot \tau_2)$  spin-orbit

+  $V_T \mathbf{S}_{12} + V_T^\tau \mathbf{S}_{12} (\tau_1 \cdot \tau_2)$  tensor

+ ...

- Realistic potentials: Paris, Argonne, CD-Bonn, Hamada-Johnston



## Secular problem

$$\mathcal{H}_{\text{eff}} |\Psi_{\text{eff}}\rangle = E |\Psi_{\text{eff}}\rangle$$

- ▷ Valence space

- ▷ Effective interaction

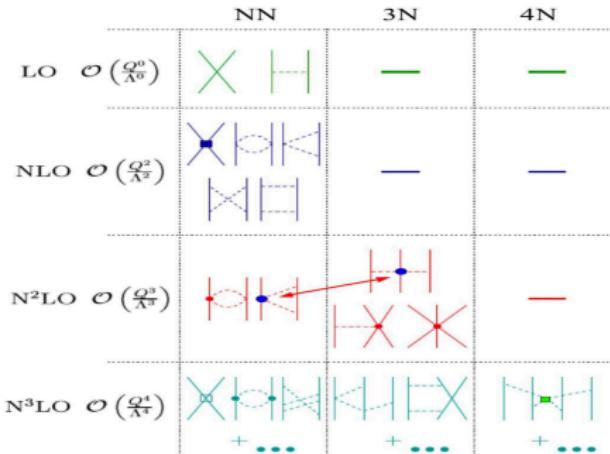
- ◊ Regularization of short-range repulsion: e.g.  $V_{low\ k}$ , G-matrix, SRG

- ◊ Adapted to the valence space by many-body perturbation theory

- ◊ Monopole corrected NN interactions: Empirical or three-body forces

- ▷ Resolution techniques

# 5 Interacting Shell Model



## Modern chiral forces

- Nuclear interaction: Pion exchanges + contact
- Perturbative expansion with “Power Counting”:  $(\frac{Q}{\Lambda_\chi})^\nu$  with  $Q \sim m_\pi$  (140 MeV) and  $\Lambda_\chi \sim 700$  MeV (chiral breakdown scale)
- Many-body forces:  $V_{NN} > V_{NNN} > \dots$   
(E. Epelbaum et al. Rev. Mod. Phys. 81 (2009) 1773)

## Secular problem

$$\mathcal{H}_{\text{eff}} |\Psi_{\text{eff}}\rangle = E |\Psi_{\text{eff}}\rangle$$

- ▷ Valence space
- ▷ Effective interaction

- ◊ Regularization of short-range repulsion: e.g.  $V_{low\ k}$ , G-matrix, SRG
- ◊ Adapted to the valence space by many-body perturbation theory

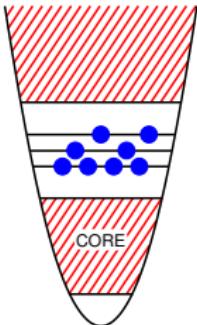
- ◊ Monopole corrected NN interactions: Empirical or three-body forces

( $\Rightarrow$  see more in Zhen Li's talk (CENBG) on Wednesday)

- ▷ Resolution techniques

## 6 Interacting Shell Model

- Exact diagonalization



- $|\Psi_{\text{eff}}\rangle = \sum_i c_i |\phi_i\rangle$
- $H_{ij} = \langle \phi_i | \mathcal{H} | \phi_j \rangle$
- $\dim\{|\phi_m\rangle\} \sim \binom{d_\pi}{p} \cdot \binom{d_\nu}{n}$   
(Strasbourg codes  
ANTOINE, NATHAN)

### Secular problem

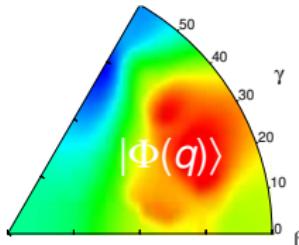
$$\mathcal{H}_{\text{eff}} |\Psi_{\text{eff}}\rangle = E |\Psi_{\text{eff}}\rangle$$

- Valence space
- Effective interaction

- Projected Hartree–Fock + GCM



- $\{|\Phi(q)\rangle\}$  non-orthogonal
- $|\Psi_{\text{eff}}\rangle = \sum f(q) \mathcal{P}_{MK}^J |\Phi(q)\rangle$
- $H_{K'K}^J(q', q) = \langle \Phi(q') | \mathcal{H} \mathcal{P}_{K'K}^J | \Phi(q) \rangle$



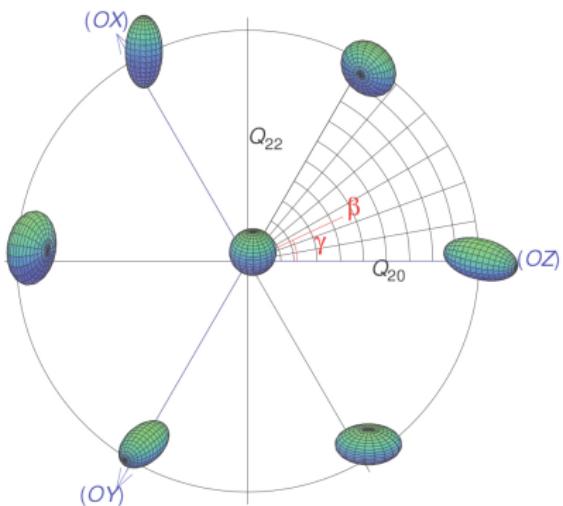
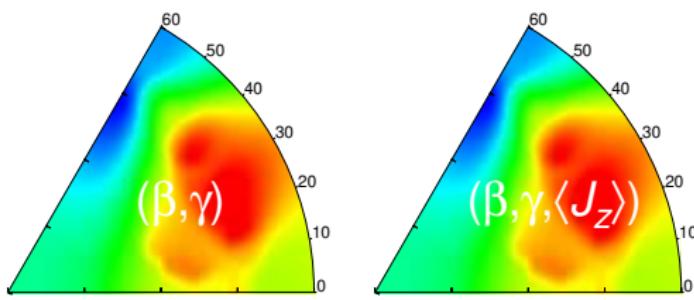
selection of relevant deformed HF state:  
Caurier's minimization technique

## 7 Minimization technique

### Selection of relevant deformed states: Minimization Technique

"The first point is the one such that it minimizes the energy. The second point is chosen in such a way that the energy obtained from diagonalizing the Hamiltonian in the 2-dimensional space be a minimum. One proceeds in the same way to determine the third basis vector etc..." (E. Caurier, Proc. on GCM, BLG report **484** (1975), Bouten, M., Van Leuven, P. (ed.))

- ▷ Choice of constraining coordinate(s)  $q$ :  
 $q_{\lambda\mu} = \langle \Phi | Q_{\lambda\mu} + (-)^{\mu} Q_{\lambda-\mu} | \Phi \rangle$ ,  $\langle J_{x,z} \rangle$ ,  $\langle \mathbf{J}^2 \rangle$ . In practice,  $(q_{20}, q_{22}) \iff (\beta, \gamma)$
- ▷ Organization of the minimization:  
 $\beta, \gamma, \langle J_z \rangle = \Omega_1, \Omega_2, \Omega_3, \dots$



## 7 Minimization technique

### Selection of relevant deformed states: Minimization Technique

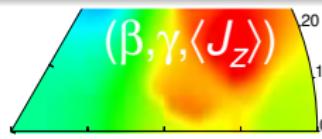
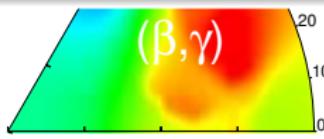
"The first point is the one such that it minimizes the energy. The second point is chosen in such a way that the energy obtained from diagonalizing the Hamiltonian in the 2-dimensional space be a minimum. One proceeds in the same way to deter-

#### ◊ Procedure:

- Fix a state  $E_{\alpha}^{(J)}$  to be minimized
- Define a searching region of the coordinate(s)  $q$
- Start from a first point which can be the HF minimum
- Diagonalize the Hamiltonian matrix  $\langle \Phi(q') | \mathcal{H} \mathcal{P}_{K'K}^J | \Phi(q) \rangle$  over the whole searching region to find the second state etc... until the convergence of  $E_{\alpha}^{(J)}$

#### ◊ Generalization: One lets the Hamiltonian to choose not only the coordinate(s) $q$ but also to decide which state $J_{\alpha}$ to be minimized.

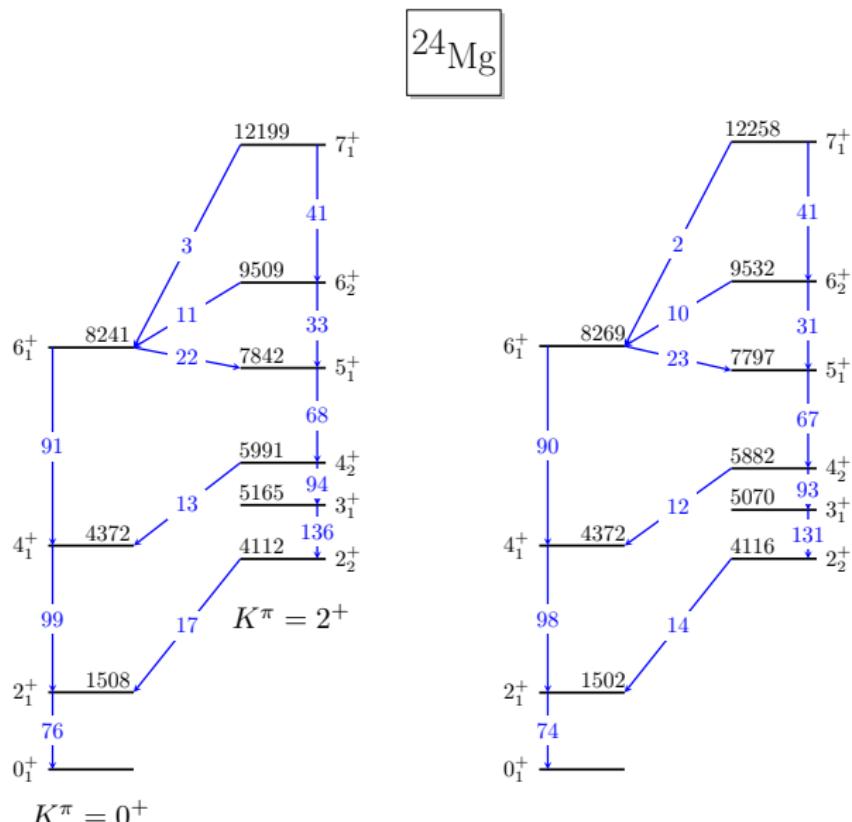
⇒ minimization of many states at the same time



# 8 Illustration in sd nuclei

- ▷ Effective interaction: USDB
- ▷ Equidistant mesh:
  - 7 points  $\beta \in [0.1, 0.54]$
  - 9 points  $\gamma \in [5^\circ, 60^\circ]$
- ▷ Cranked component:
 
$$\langle J_z \rangle = -2, -3, -4, -5, -6$$
- ▷ Ground state energy:
 
$$E_{gcm} = -86.86 \text{ MeV}$$

$$E_{sm} = -87.10 \text{ MeV.}$$

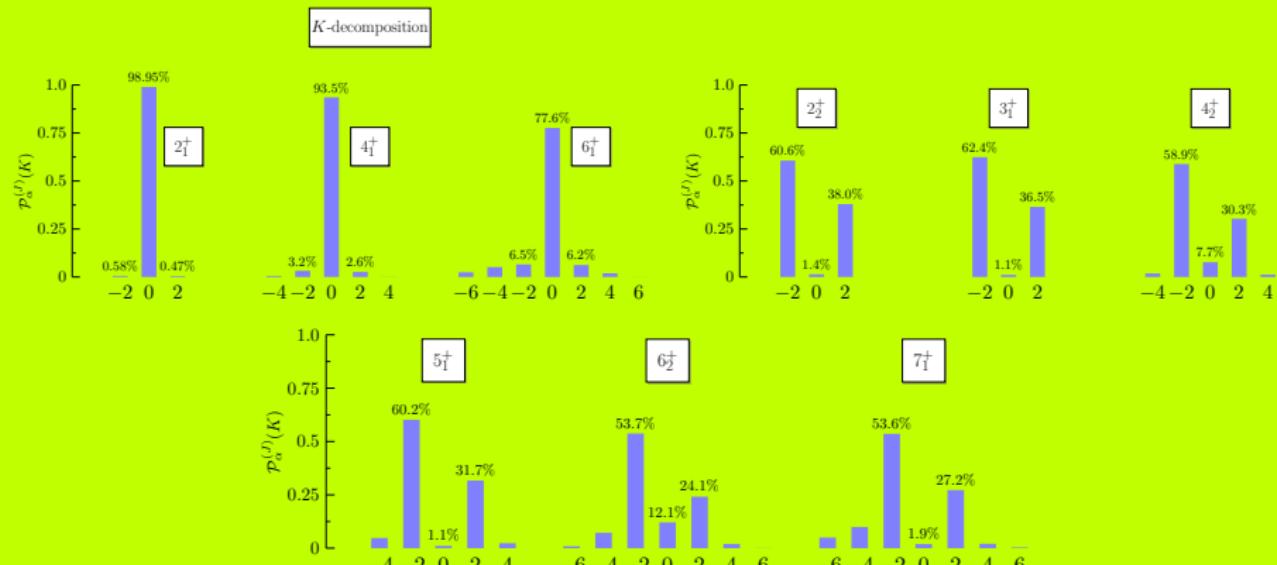
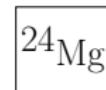


GCM (with 55 states)

Classic SM

# 8 Illustration in sd nuclei

- Effective interaction: USDB
- Equidistant mesh:



$$\begin{aligned}
 p_\alpha^{(J)}(K) &= \sum_q |\mathcal{M}_\alpha^{(J)}(q; K)|^2, \quad \mathcal{M}_\alpha^{(J)}(q; K) = \sum_{q', K'} [\mathcal{N}^{1/2}]_{KK'}^{(J)}(q, q') f_\alpha^{(J)}(q'; K') \\
 \mathcal{N}_{KK'}^{(J)}(q, q') &= \langle \Phi(q) | \mathcal{P}_{KK'}^J | \Phi(q') \rangle
 \end{aligned}$$

# 9 Illustration in sd nuclei

► Effective interaction: USDB

► Equidistant mesh:

7 points  $\beta \in [0.1, 0.51]$

8 points  $\gamma \in [1.5^\circ, 60^\circ]$

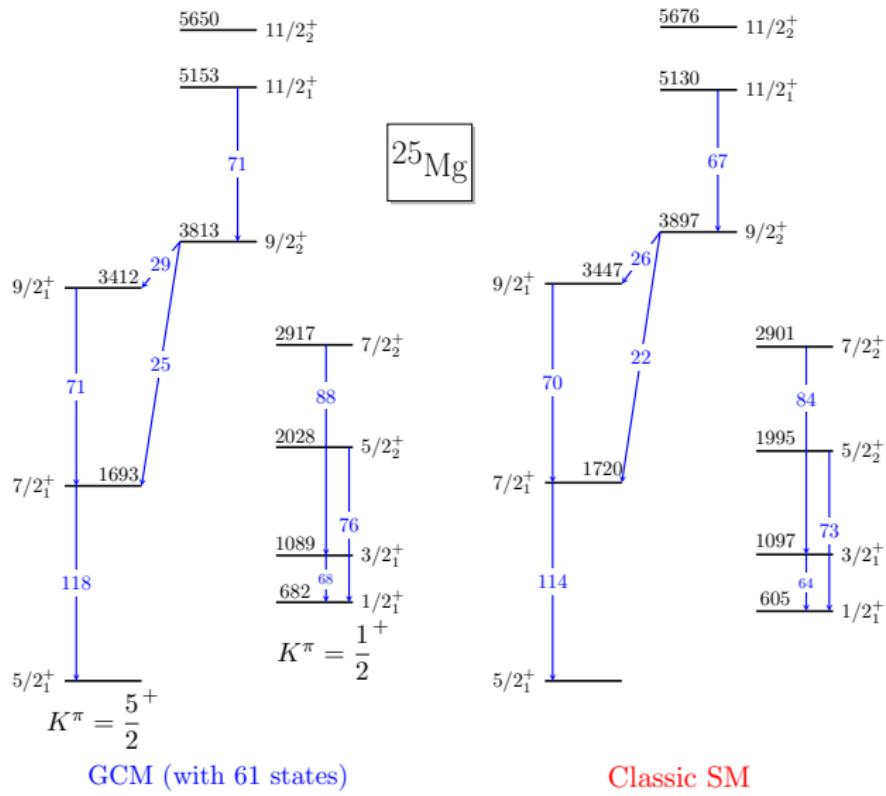
► Cranked component:

$$\langle J_z \rangle = -1/2, -3/2, -5/2, -7/2, -9/2$$

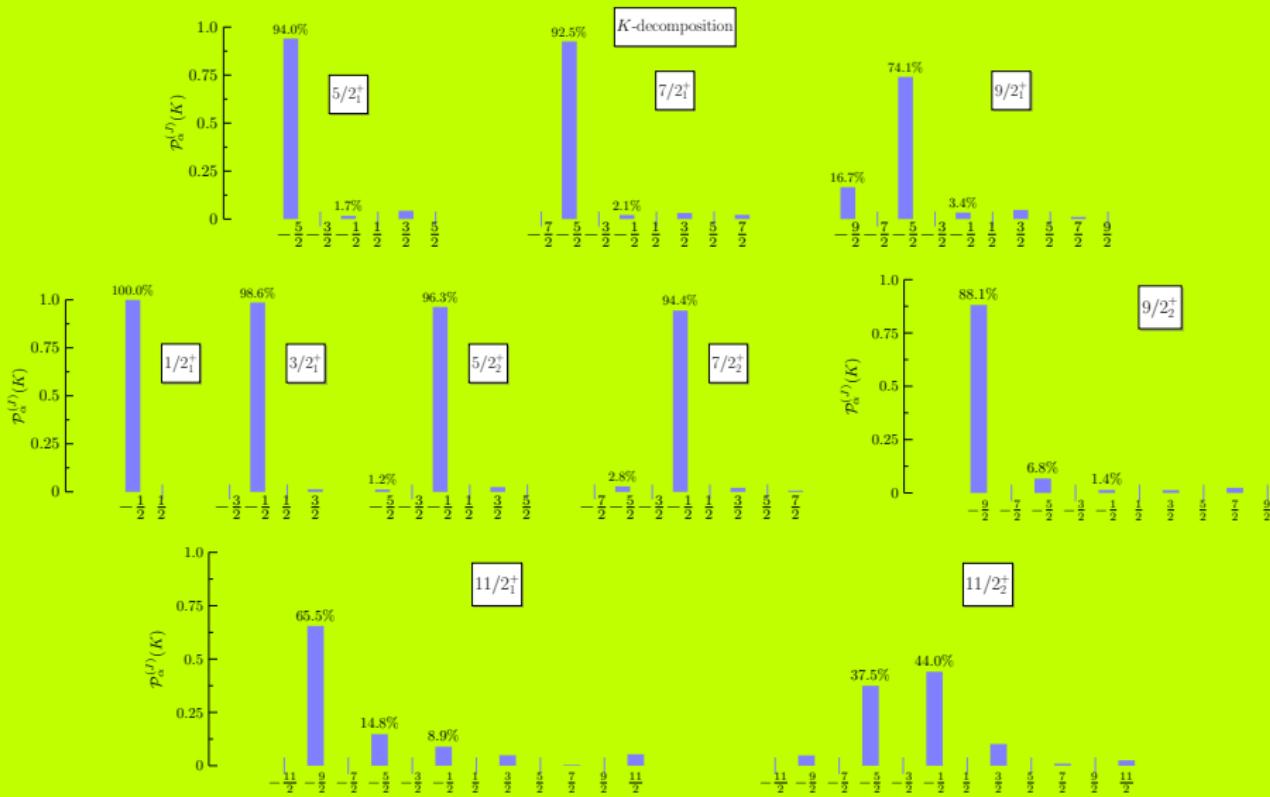
► Ground state energy:

$$E_{gcm} = -93.89 \text{ MeV}$$

$$E_{sm} = -94.40 \text{ MeV.}$$

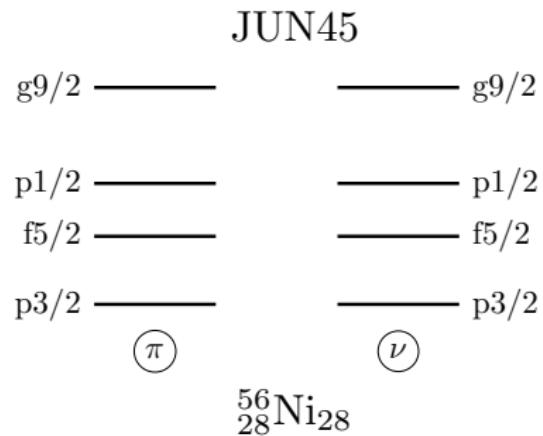
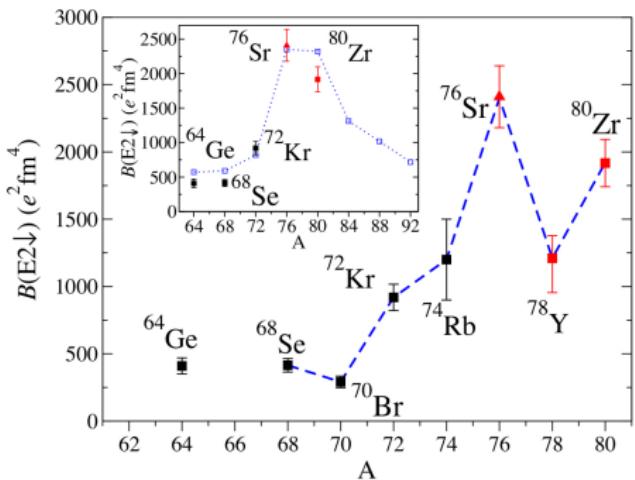


# 9 Illustration in sd nuclei



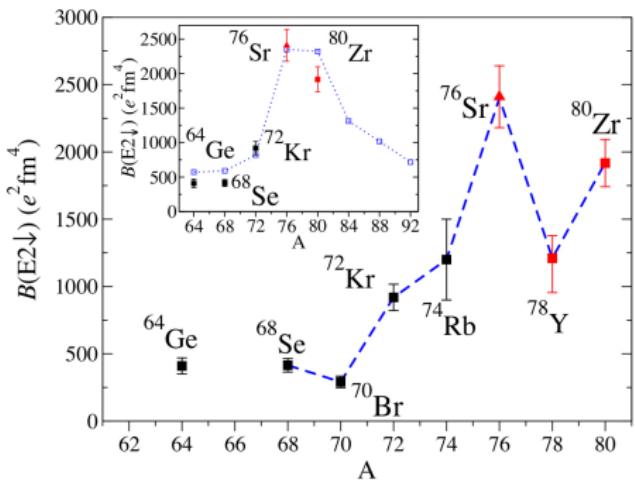
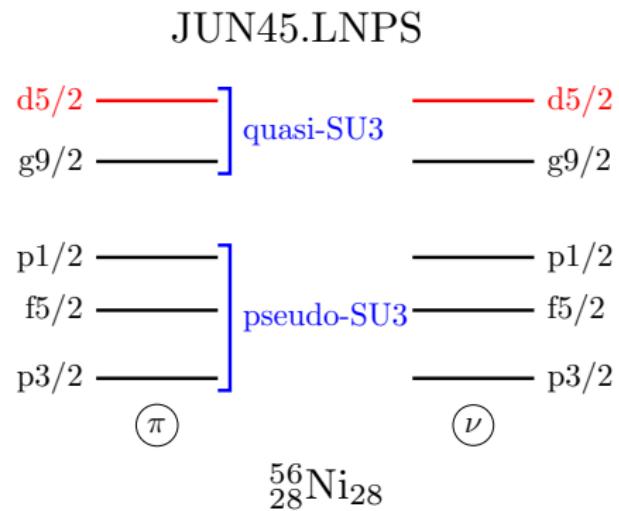
Establishing the Maximum Collectivity in Highly Deformed  $N = Z$  Nuclei

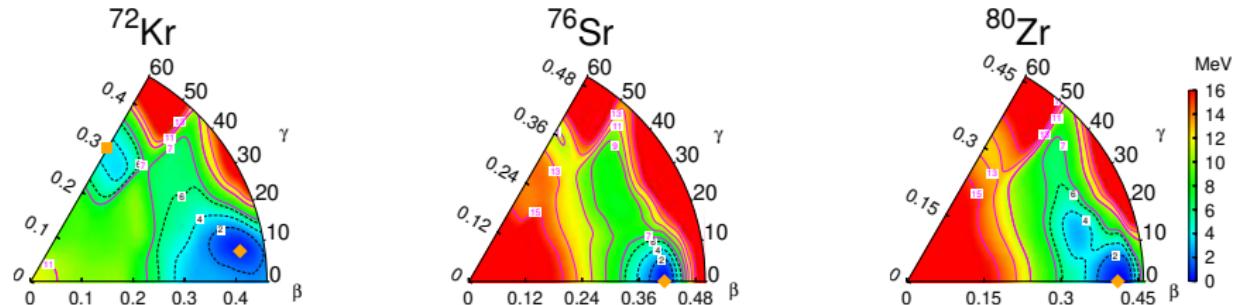
R. D. O. Llewellyn,<sup>1,\*</sup> M. A. Bentley,<sup>1</sup> R. Wadsworth,<sup>1,†</sup> H. Iwasaki,<sup>2,3</sup> J. Dobaczewski,<sup>1,4</sup> G. de Angelis,<sup>5</sup> J. Ash,<sup>2,3</sup> D. Bazin,<sup>2,3</sup> P. C. Bender,<sup>2,‡</sup> B. Cederwall,<sup>6</sup> B. P. Crider,<sup>2,§</sup> M. Doncel,<sup>7</sup> R. Elder,<sup>2,3</sup> B. Elman,<sup>2,3</sup> A. Gade,<sup>2,3</sup> M. Grinder,<sup>2,3</sup> T. Haylett,<sup>1</sup> D. G. Jenkins,<sup>1</sup> I. Y. Lee,<sup>8</sup> B. Longfellow,<sup>2,3</sup> E. Lunderberg,<sup>2,3</sup> T. Mijatović,<sup>2,||</sup> S. A. Milne,<sup>1</sup> D. Muir,<sup>1</sup> A. Pastore,<sup>1</sup> D. Rhodes,<sup>2,3</sup> and D. Weisshaar<sup>2</sup>

FIG. 3. Schematics of the  $B(E2\downarrow)$  values for the  $N = Z$  nuclei

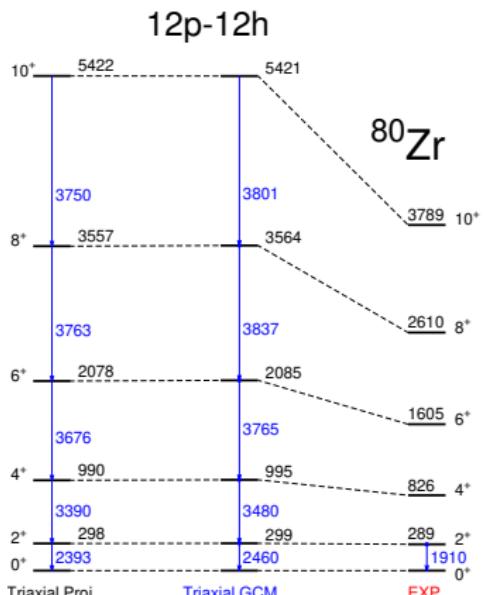
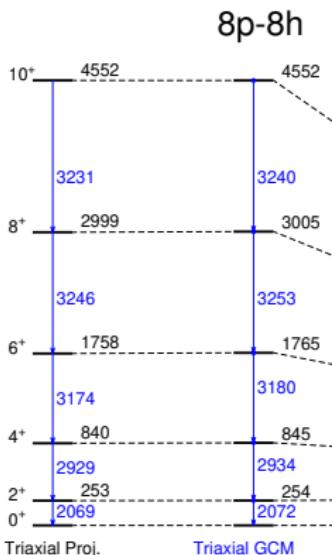
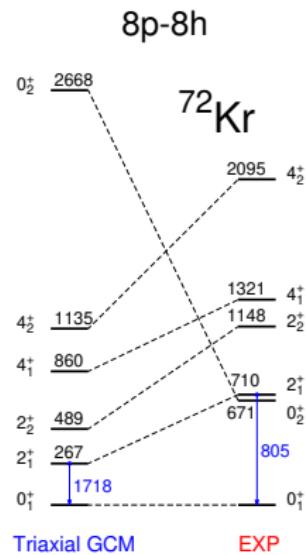
Establishing the Maximum Collectivity in Highly Deformed  $N = Z$  Nuclei

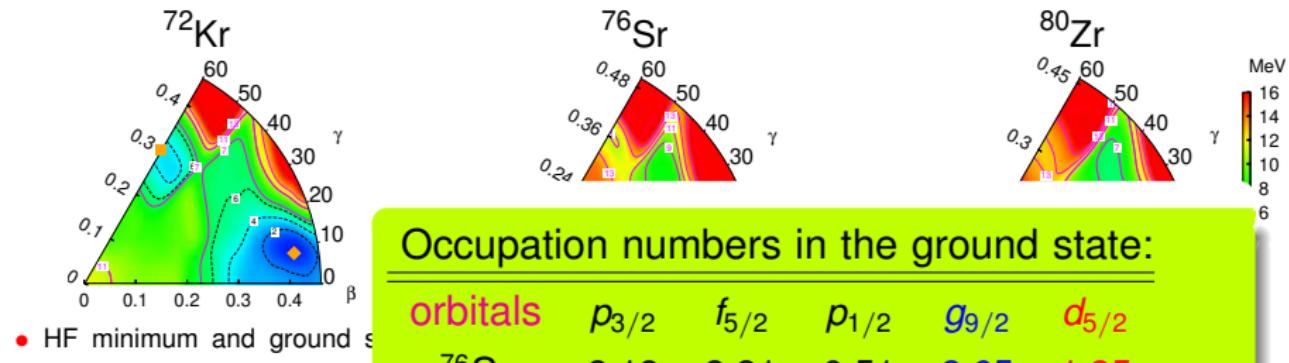
R. D. O. Llewellyn,<sup>1,\*</sup> M. A. Bentley,<sup>1</sup> R. Wadsworth,<sup>1,†</sup> H. Iwasaki,<sup>2,3</sup> J. Dobaczewski,<sup>1,4</sup> G. de Angelis,<sup>5</sup> J. Ash,<sup>2,3</sup> D. Bazin,<sup>2,3</sup> P. C. Bender,<sup>2,‡</sup> B. Cederwall,<sup>6</sup> B. P. Crider,<sup>2,§</sup> M. Doncel,<sup>7</sup> R. Elder,<sup>2,3</sup> B. Elman,<sup>2,3</sup> A. Gade,<sup>2,3</sup> M. Grinder,<sup>2,3</sup> T. Haylett,<sup>1</sup> D. G. Jenkins,<sup>1</sup> I. Y. Lee,<sup>8</sup> B. Longfellow,<sup>2,3</sup> E. Lunderberg,<sup>2,3</sup> T. Mijatović,<sup>2,||</sup> S. A. Milne,<sup>1</sup> D. Muir,<sup>1</sup> A. Pastore,<sup>1</sup> D. Rhodes,<sup>2,3</sup> and D. Weisshaar<sup>2</sup>

FIG. 3. Schematics of the  $B(E2\downarrow)$  values for the  $N = Z$  nuclei

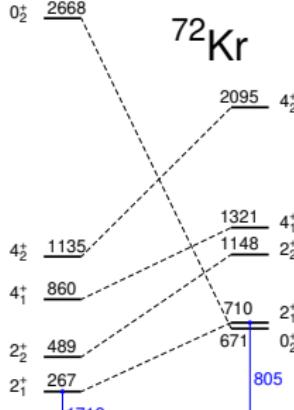


- HF minimum and ground state structures:





$0_2^+$  2668



Occupation numbers in the ground state:

| orbitals         | $p_{3/2}$ | $f_{5/2}$ | $p_{1/2}$ | $g_{9/2}$ | $d_{5/2}$ |
|------------------|-----------|-----------|-----------|-----------|-----------|
| $^{76}\text{Sr}$ | 2.18      | 3.31      | 0.51      | 2.65      | 1.35      |
| $^{80}\text{Zr}$ | 2.03      | 3.47      | 0.51      | 4.62      | 1.37      |

Space dimension

GCM

Shell Model

Actual limit

$^{76}\text{Sr}$

30

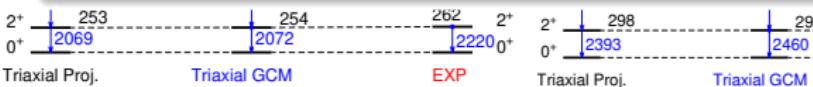
$10^{15}$

$10^{11}$

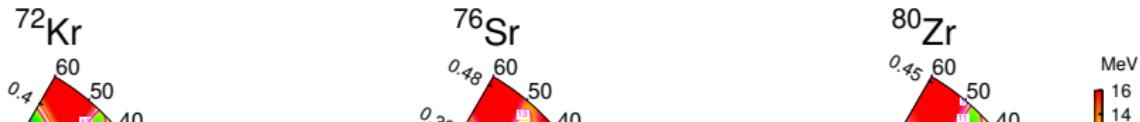
$^{80}\text{Zr}$

30

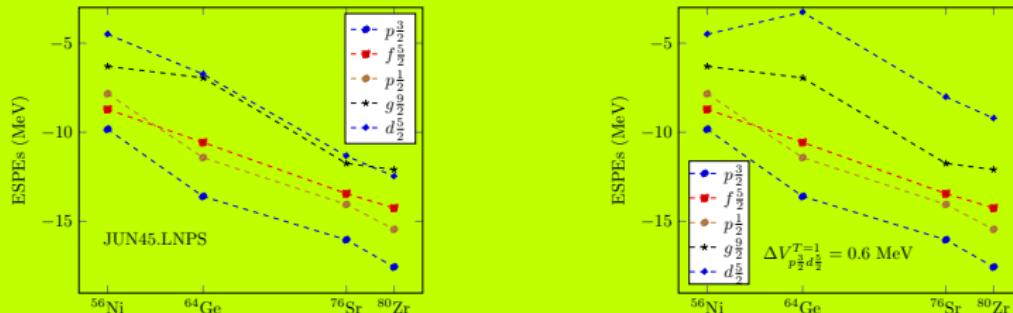
$10^{16}$



# 11 Collectivity in heavy $N = Z$ nuclei



- Effective Single Particle Energies (ESPEs)



- Work under progress...

- First calculations of heavy  $N = Z$  nuclei within the Shell Model
- Good description in the case of  $^{76}\text{Sr}$ ,  $^{80}\text{Zr}$
- Location of the  $d_{5/2}^5$  orbit (systematics of second excited states  $0_2^+$  where JUN45 becomes inadapted)



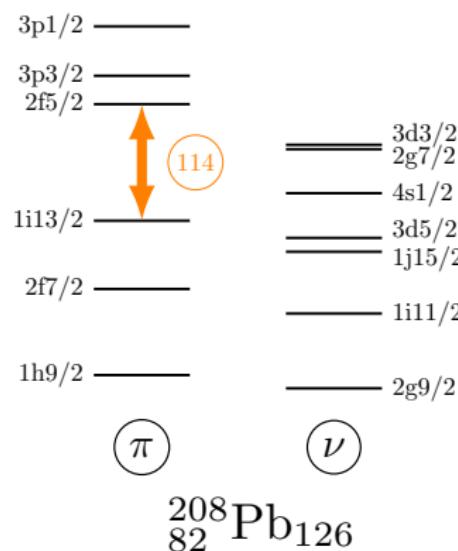
# 12 Shell Model calculations in Nobelium isotopes

## Kuo-Herling interaction:

- $^{208}_{82}\text{Pb}_{126}$  core, realistic TBMEs
- $82 \leq Z \leq 126$  shells for proton and  $126 \leq N \leq 184$  for neutrons
- monopole corrections (3N force)

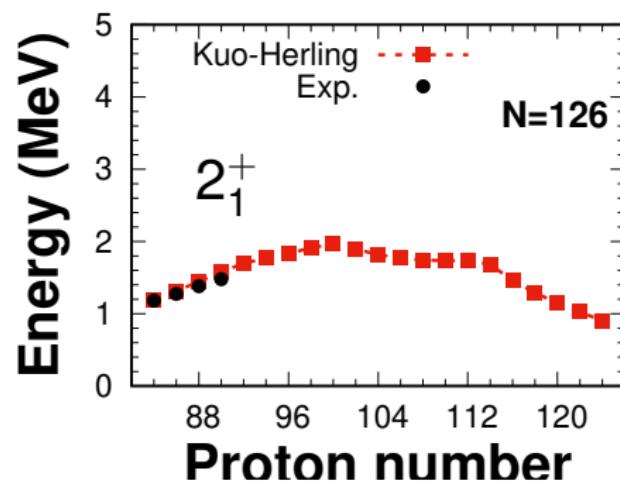
*E. Caurier and F. Nowacki,*

PRL 87 (2001), 072501



## Calculations: NATHAN & DFSM

- ◊ Diagonalization within the seniority scheme along the chains of  $N = 126$  and  $N = 184$
- ◊ Deformed Hartree-Fock and Angular momentum projection plus shapes mixing through the GCM:  $^{252,253,254}\text{No}$



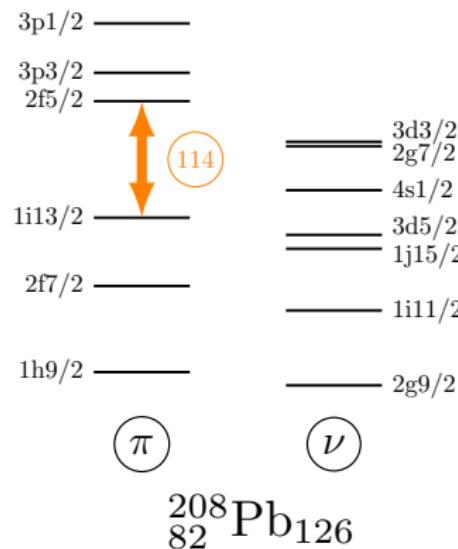
# 12 Shell Model calculations in Nobelium isotopes

## Kuo-Herling interaction:

- $^{208}_{82}\text{Pb}_{126}$  core, realistic TBMEs
- $82 \leq Z \leq 126$  shells for proton and  $126 \leq N \leq 184$  for neutrons
- monopole corrections (3N force)

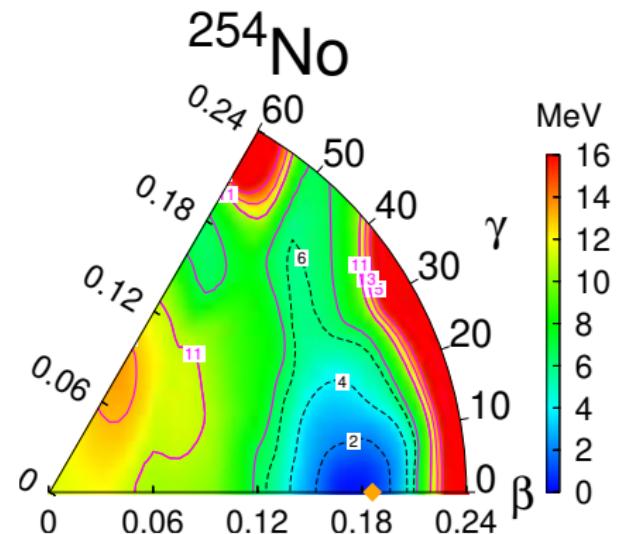
*E. Caurier and F. Nowacki,*

PRL 87 (2001), 072501

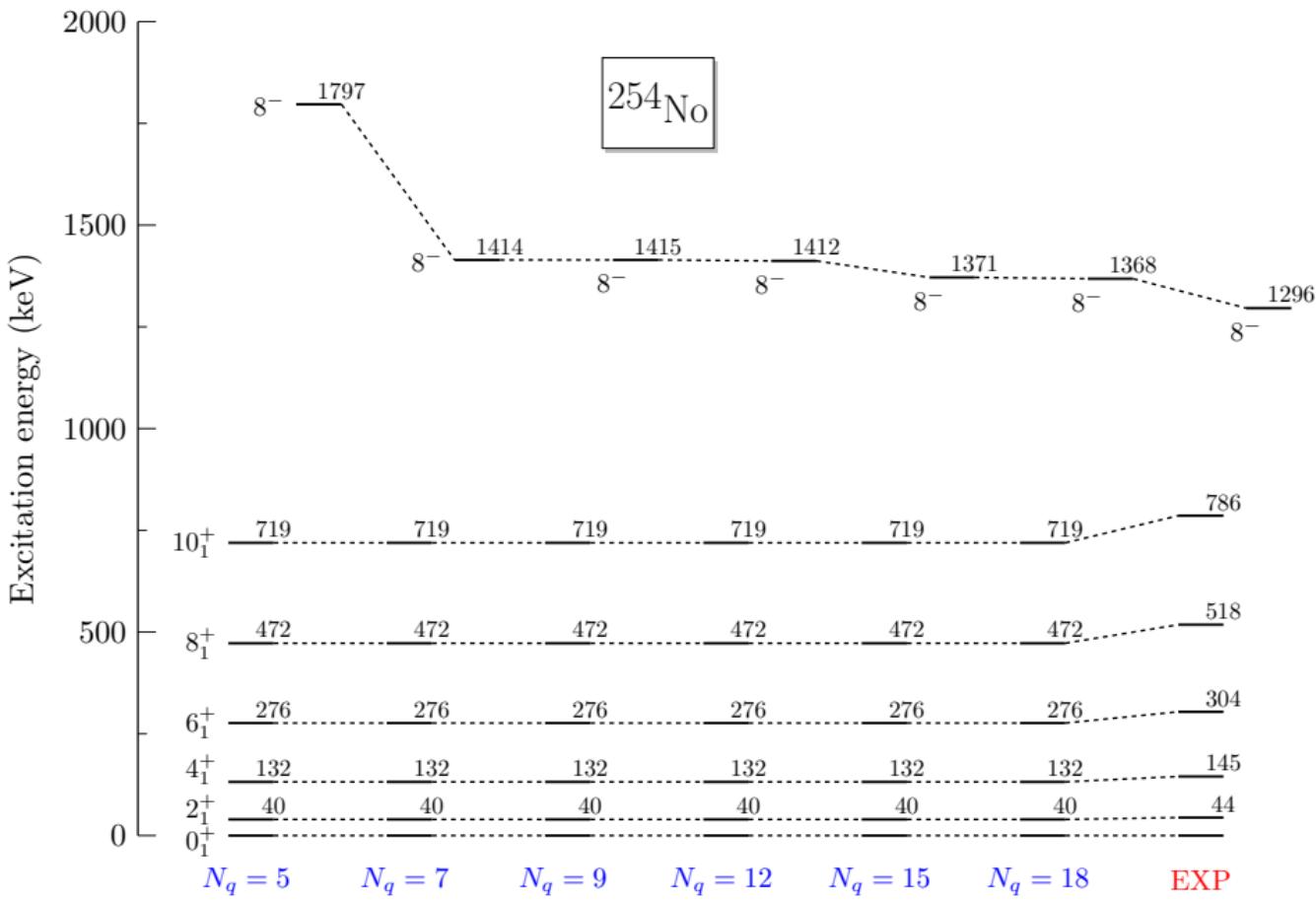


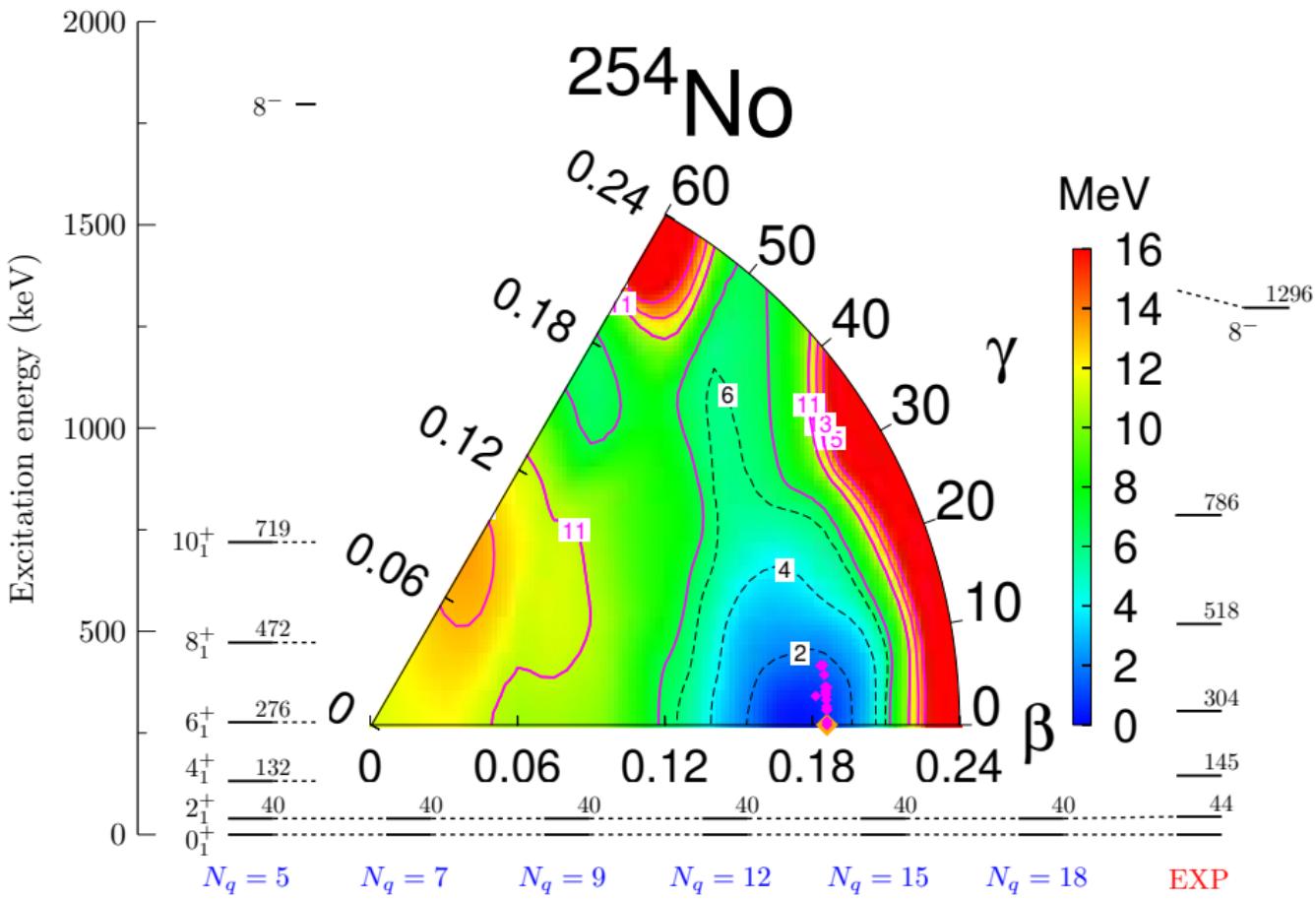
## Calculations: NATHAN & DFSM

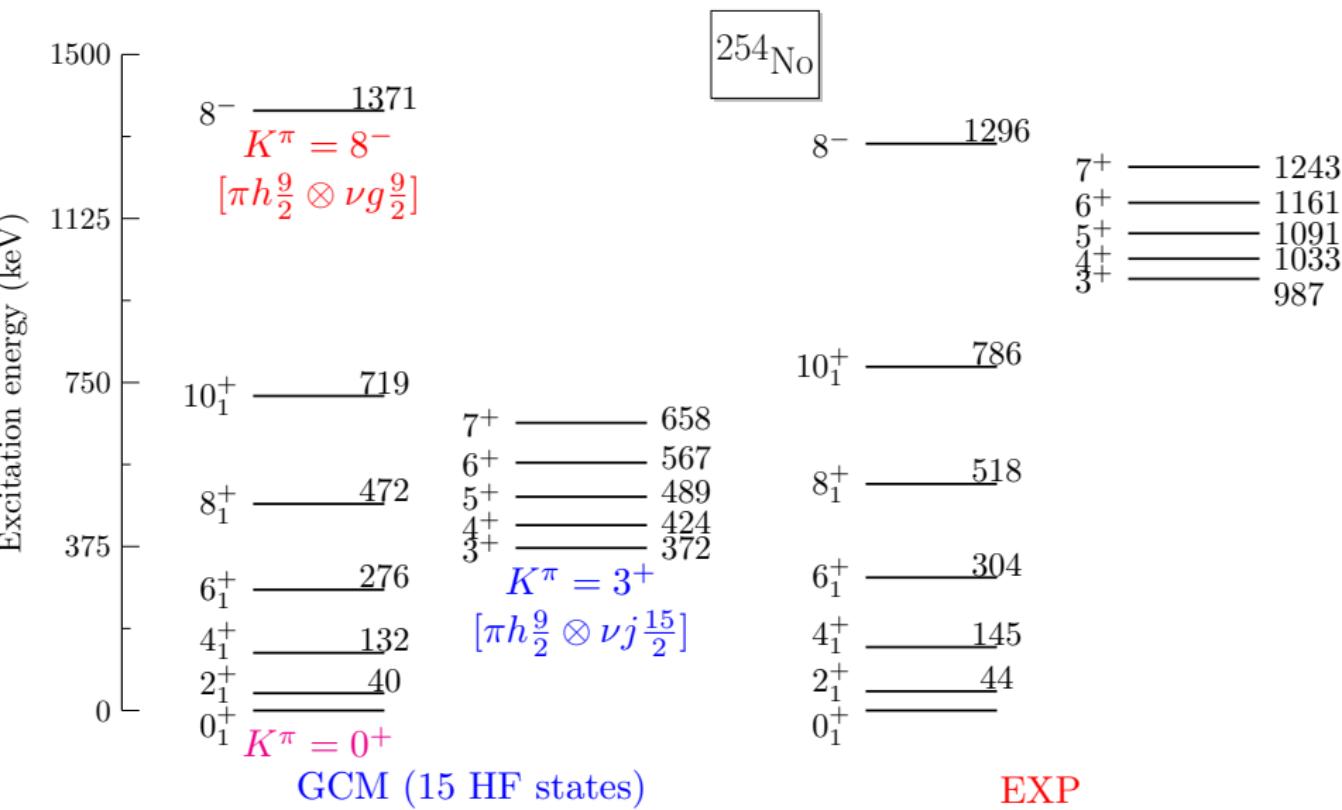
- ◊ Diagonalization within the seniority scheme along the chains of  $N = 126$  and  $N = 184$
- ◊ Deformed Hartree-Fock and Angular momentum projection plus shapes mixing through the GCM:  $^{252,253,254}\text{No}$

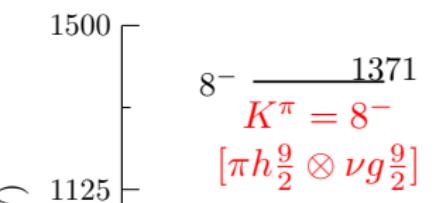


# 12 Shell Model calculations in Nobelium isotopes





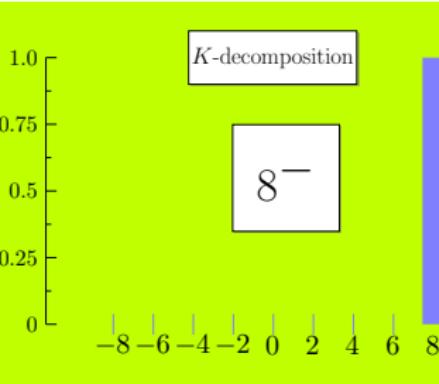




$^{254}\text{No}$

$8^- \quad 1296$

|       |      |
|-------|------|
| $7^+$ | 1243 |
| $6^+$ | 1161 |
| $5^+$ | 1091 |
| $4^+$ | 1033 |
| $3^+$ | 987  |



$7^+ \quad 658$   
 $6^+ \quad 567$   
 $5^+ \quad 489$   
 $4^+ \quad 424$   
 $3^+ \quad 372$   
 $K^\pi = 3^+$   
 $[\pi h\frac{9}{2} \otimes \nu j\frac{15}{2}]$

$10_1^+ \quad 786$

$8_1^+ \quad 518$

$6_1^+ \quad 304$

$4_1^+ \quad 145$

$2_1^+ \quad 44$

$0_1^+$

$2_1^+ \quad 40$   
 $0_1^+ \quad K^\pi = 0^+$

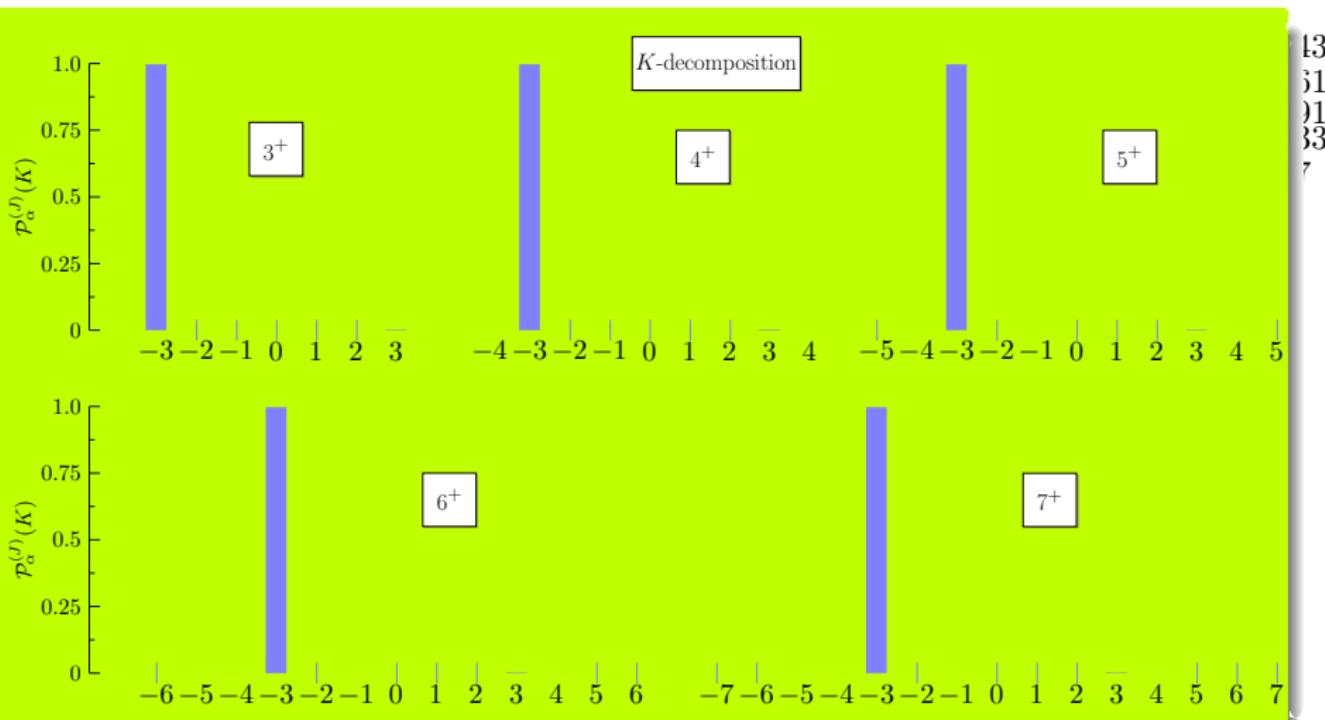
GCM (15 HF states)

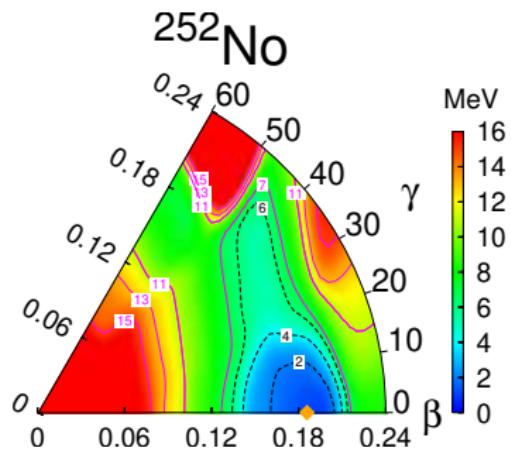
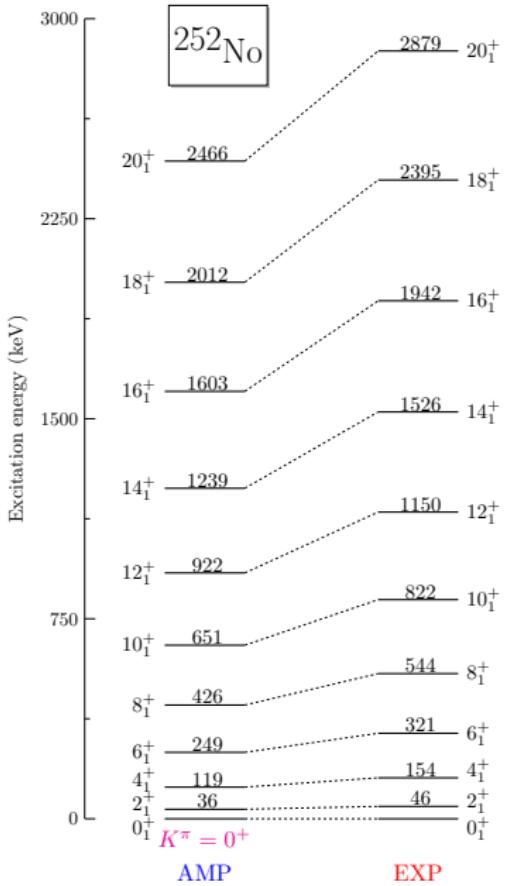
EXP

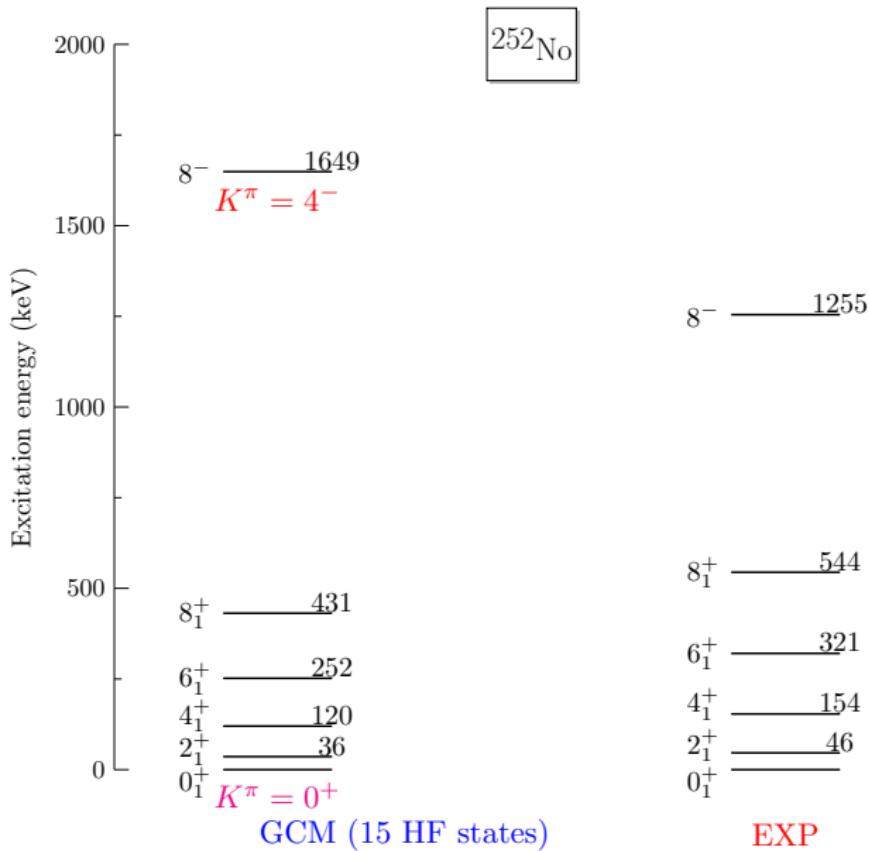
1500

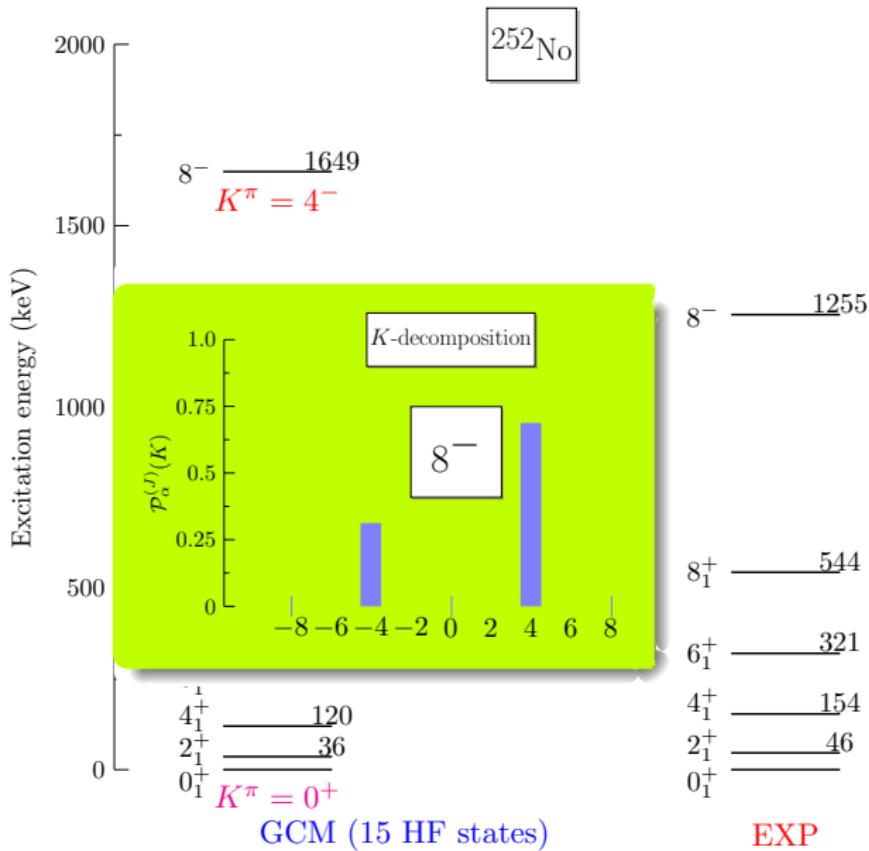
~-

1371

 $^{254}\text{No}$ 

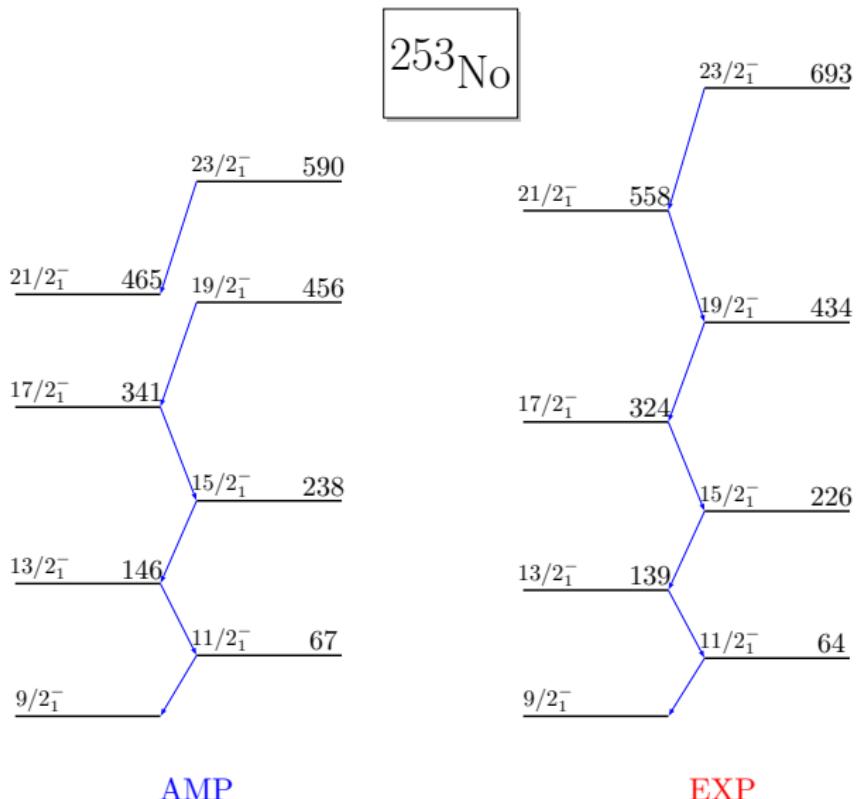






Occupation numbers:

| proton orbits  | $1h_{9/2}$  | $1i_{13/2}$ | $2f_{7/2}$ | $2f_{5/2}$ | $3p_{3/2}$ | $3p_{1/2}$ |
|----------------|-------------|-------------|------------|------------|------------|------------|
| $0^+_1$        | 5.66        | 7.99        | 3.47       | 1.55       | 0.76       | 0.56       |
| $8^-$          | 7.47        | 7.02        | 3.39       | 1.14       | 0.66       | 0.32       |
| neutron orbits | $1i_{11/2}$ | $1j_{15/2}$ | $2g_{9/2}$ | $2g_{7/2}$ | $3d_{5/2}$ | $3d_{3/2}$ |
| $0^+_1$        | 7.17        | 8.00        | 5.48       | 1.00       | 1.07       | 0.84       |
| $8^-$          | 7.27        | 7.99        | 5.61       | 0.92       | 1.02       | 0.76       |
|                |             |             |            |            |            | $4s_{1/2}$ |
|                |             |             |            |            |            | 0.44       |
|                |             |             |            |            |            | 0.43       |



**Kuo-Herling interaction:**

- cranked component  $\langle \hat{J}_z \rangle = -1/2$
- deformation:  $\beta = 0.177$ , axial minimum.

# Conclusion

- ▷ Alternative approach for tackling the diagonalization problem in the Shell Model: efficient minimization technique using the GCM.
- ▷ New frontiers for Shell Model study in very deformed and heavy nuclei.
  - First study of heavy  $N = Z$  nuclei using the Shell Model.
  - First calculations of superheavy nuclei with the Shell Model. Reproduction of both the rotational band AND isomeric states in Nobelium isotopes.
- ▷ Possibility to test effective interactions consistently derived from modern two- and three-body chiral forces.
- ▷ Calculations of nuclear matrix elements:  $0\nu\beta\beta$  decay