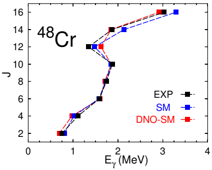
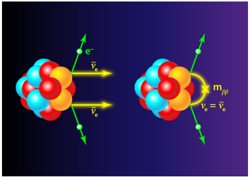
Extended Discrete Non-Orthogonal Shell Model for heavy deformed nuclei

Duy-Duc Dao, F. Nowacki

(IPHC-Strasbourg)

Astranucap Workshop, November 18th, 2024





cnrs IN2P3 Les deux infinis

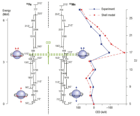
IPHC Institut Pluridisciplinaire Hubert CURIEN STRASBOURG

UNIVERSITÉ DE STRASBOURG

SM-CI approaches through the nuclear chart

Fundamental interactions and collectives excitations

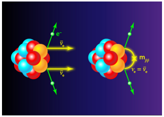
- Deformation, Superdeformation, Dipole/M1 resonances
- Superfluidity, Symmetries
- Isospin symmetry breaking

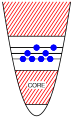


Weak processes

- β decay $\Longleftrightarrow$ fundamental interactions
- $\beta\beta$ decay $\Longleftrightarrow$ nature of neutrinos

$$[T^{0\nu}_{1/2}(0^+ \to 0^+)]^{-1} = G_{0\nu}|M^{0\nu}|^2\langle m_\nu\rangle^2$$





- $\mathcal{H}_{\text{exact}}\Psi_{\text{exact}} = E\Psi_{\text{exact}}$

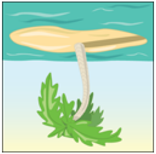
$$\Updownarrow$$

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

Treat Many-Body problem
Treat Effective Interaction

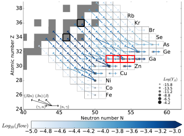
Nuclear structure far from stability

- New magic numbers
- Vanishing of shell closures



Astrophysics and nucleosynthesis

- rp process
- r process



Effective Hamiltonian

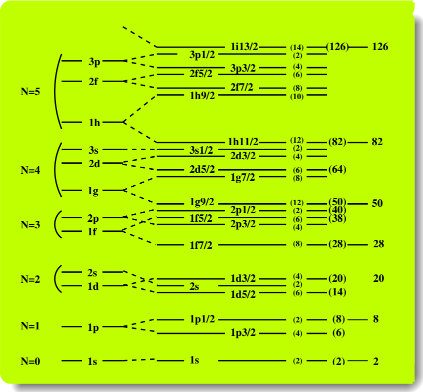
Monopole and multipole

Multipole expansion : $\mathcal{H} = \color{red}{\mathcal{H}_{monopole}} + \color{blue}{\mathcal{H}_{Multipole}}$

$\color{red}{\mathcal{H}_{monopole}}$:

- *Spherical mean-field*
- *Evolution of the spherical single particle levels*

A. Poves and A. Zuker (Phys. Report 70, 235 (1981))



$\color{blue}{\mathcal{H}_{multipole}}$:

- *Correlations*
- *Energy gains*

- *Pairing (SU2)* semi-magic (n-n) (p-p)
- *Quadrupole (SU3/pSU3/qSU3)* p-n in H.O. or Δj = 2

M. Dufour and A. Zuker (PRC 54 1996 1641)

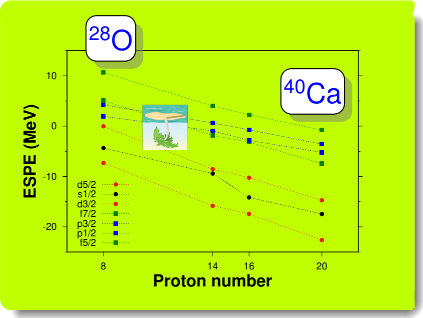
Effective Hamiltonian

Monopole and multipole

Multipole expansion : $\mathcal{H} = \mathcal{H}_{monopole} + \mathcal{H}_{Multipole}$

$\mathcal{H}_{monopole}$:
- *Spherical mean-field*
- *Evolution of the spherical single particle levels*

A. Poves and A. Zuker (Phys. Report 70, 235 (1981))



$\mathcal{H}_{multipole}$:
- *Correlations*
- *Energy gains*

- *Pairing (SU2)* semi-magic (n-n) (p-p)
- *Quadrupole (SU3/pSU3/qSU3)* p-n in H.O. or Δj = 2

M. Dufour and A. Zuker (PRC 54 1996 1641)

Effective Hamiltonian

Monopole and multipole

M

$\mathcal{H}_{mo}$

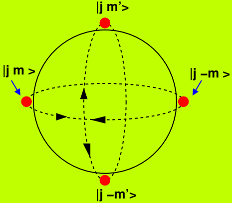
$\mathcal{H}_{mu}$

- **Pairing regime: spherical nuclei**

  ground state = pairs of like-particles coupled at J=0 (seniority v=0)

  2^+ state (break of pair; v=2) at high energy

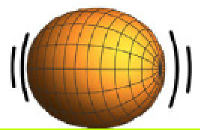
  superfluid nucleus:



  Typical example: **semi-magic Tin isotopes**

- **Quadrupole regime: deformed nuclei**

  prolate nucleus:



  Typical example: **open shell N=Z nuclei**

M. Dufour and A. Zuker (PRC 54 1996 1641)

Effective Hamiltonian

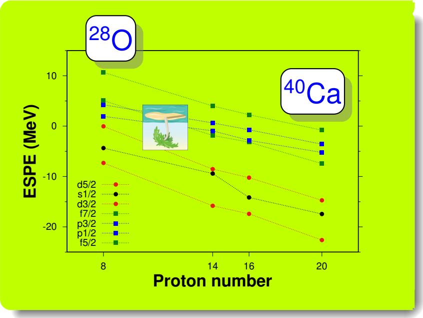
Monopole and multipole

Multipole expansion : $\mathcal{H} = \mathcal{H}_{monopole} + \mathcal{H}_{\mathcal{PP}} + \mathcal{H}_{\mathcal{QQ}}$

$\mathcal{H}_{monopole}$:

- *Spherical mean-field*
- *Evolution of the spherical single particle levels*

A. Poves and A. Zuker (Phys. Report 70, 235 (1981))



$\mathcal{H}_{multipole}$:

- *Correlations*
- *Energy gains*

- *Pairing (SU2)* semi-magic (n-n) (p-p)
- *Quadrupole (SU3/pSU3/qSU3)* p-n in H.O. or Δj = 2

M. Dufour and A. Zuker (PRC 54 1996 1641)

Spherical versus Deformed Description of Nuclei

Shell Model Exact Diagonalization

- Exponential growth of basis dimensions :

$$D \sim \begin{pmatrix} d_\pi \\ p \end{pmatrix} \cdot \begin{pmatrix} d_\nu \\ n \end{pmatrix}$$

In *pf* shell :

^{56}Ni **1,087,455,228**

In *pf*-*sdg* space :

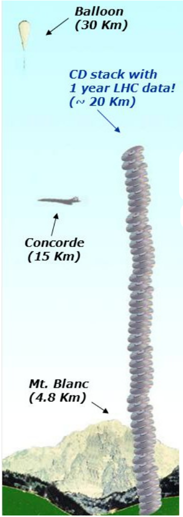
^{78}Ni **210,046,691,518**

ANTOINE CODE (1989)

- Actual limits in giant diagonalizations :
  $\sim 10^{12}$, $\sim 10^{15}$ $\neq 0$ **matrix elements**

- Some of the largest diagonalizations ever are performed in Strasbourg with relatively modest computationnal ressources :
  E. Caurier et al., Rev. Mod. Phys. 77 (2005) 427

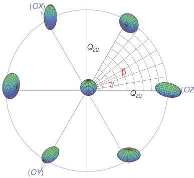
- m-scheme — ANTOINE code, BIGSTICK, KSHELL
- coupled scheme — NATHAN code



Shell Model in non-spherical basis

$$\mathcal{H}_{\rm eff}\,|\Psi^{JM}_\alpha\rangle = E^{(J)}_\alpha\,|\Psi^{JM}_\alpha\rangle \;\rightarrow\; \delta\,\frac{\langle\Psi^{JM}_\alpha|\mathcal{H}_{\rm eff}|\Psi^{JM}_\alpha\rangle}{\langle\Psi^{JM}_\alpha|\Psi^{JM}_\alpha\rangle} = 0$$

- **Mixing of shapes:**



- **Restoration of the rotational symmetry**

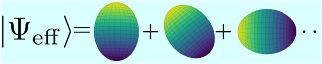
- **Degree of freedom**
  - Multipole: $\beta, \gamma, Q_{30}, \ldots$
  - Cranking: J_x, J_z
  - Pairing constraints
  - Variation-After-Projection

- **Different implementations**
  - MCSM — Tokyo group
  - DNO-SM — Strasbourg group
  - Taurus code — Madrid group

Discrete Non-Orthogonal Shell Model (DNO-SM)

◇ Configuration mixing via the generator coordinate method:

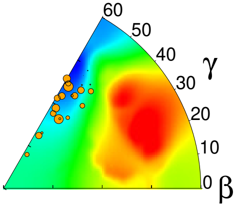
- $\langle J_z \rangle$, $(q_{20}, q_{22}) \equiv (\beta, \gamma)$ (cranking, axial and triaxial)
- Contribution of $q = (\beta, \gamma)$ in the correlated state J_α
- Caurier minimization technique

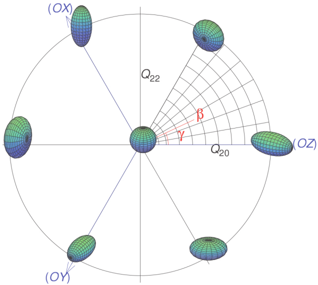


$$|\Psi_{\text{eff}}\rangle = \cdots$$

$$\boxed{P_\alpha^{(J)}(q) = \sum_K |M_\alpha^{(J)}(q,K)|^2}$$

(D.D. Dao and F. Nowacki, PRC 105, 054314 (2022))

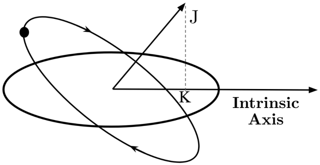




◇ K-mixing contents of the wave functions in the instrinsic frame

- K: Projection of total angular momentum J onto the intrinsic axis
- Contribution of K-components in the correlated state J_α

$$\boxed{P_\alpha^{(J)}(K) = \sum_q |M_\alpha^{(J)}(q,K)|^2}$$



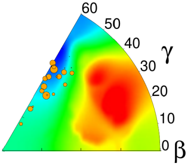
Extented Discrete Non-Orthogonal Shell Model : deformed *N*p*N*h & Variation After Projection

◇ Variation-After-Projection DNO-SM approach

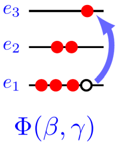
$$\mathcal{H}_{\rm eff}|\Psi_\alpha^{JM}\rangle = E_\alpha^{(J)}|\Psi_\alpha^{JM}\rangle \Longrightarrow \delta\frac{\langle\Psi_\alpha^{JM}|\mathcal{H}_{\rm eff}|\Psi_\alpha^{JM}\rangle}{\langle\Psi_\alpha^{JM}|\Psi_\alpha^{JM}\rangle} = 0, \quad |\Psi_\alpha^{JM}\rangle = \sum_{q,K}\boxed{f_\alpha^{(J)}(q,K)}\,\mathcal{P}^J_{MK}\boxed{|\Phi(q)\rangle}$$

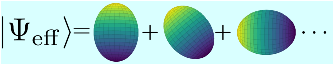
Double variation AFTER Angular Momentum Projection: Mixing coefficient Slater state

◇ DNO-SM(PAV): (β,γ) + *N*p*N*h



$\bigoplus$

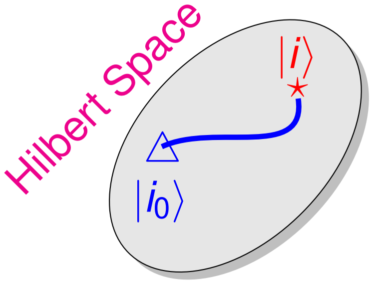




(D.D. Dao and F. Nowacki, in preparation (2024))

◇ DNO-SM(VAP)

- $q = 1, 2, 3, ...$
- $J_\alpha = 0_1, \ldots$
- Best energy-favoring Slater states



Extented Discrete Non-Orthogonal Shell Model : deformed NpNh & Variation After Projection

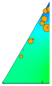
◇ Variation-After-Projection DNO-SM approach

$$\mathcal{H}_{\rm eff}|\Psi^{JM}_\alpha\rangle = E^{(J)}_\alpha|\Psi^{JM}_\alpha\rangle \Longrightarrow \delta \frac{\langle\Psi^{JM}_\alpha|\mathcal{H}_{\rm eff}|\Psi^{JM}_\alpha\rangle}{\langle\Psi^{JM}_\alpha|\Psi^{JM}_\alpha\rangle} = 0, \quad |\Psi^{JM}_\alpha\rangle = \sum \boxed{f^{(J)}_\alpha(q,K)}\,\mathcal{P}^J_{MK}\boxed{|\Phi(q)\rangle}$$

Double

er state

◇ DN



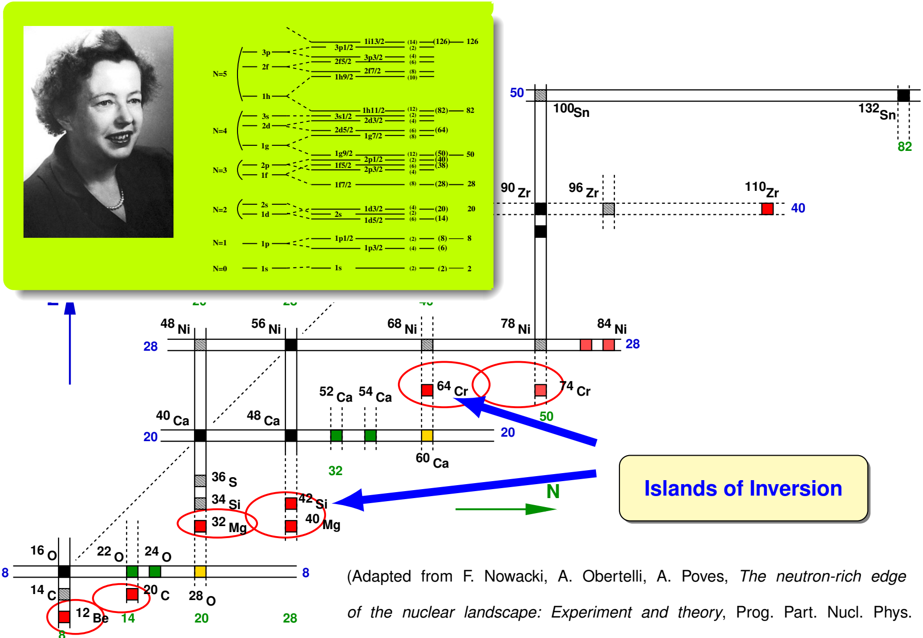
s

(D.

◇ Ground state correlations captured in PAV and VAP calculations: (D.D. Dao and F. Nowacki, in preparation (2024))

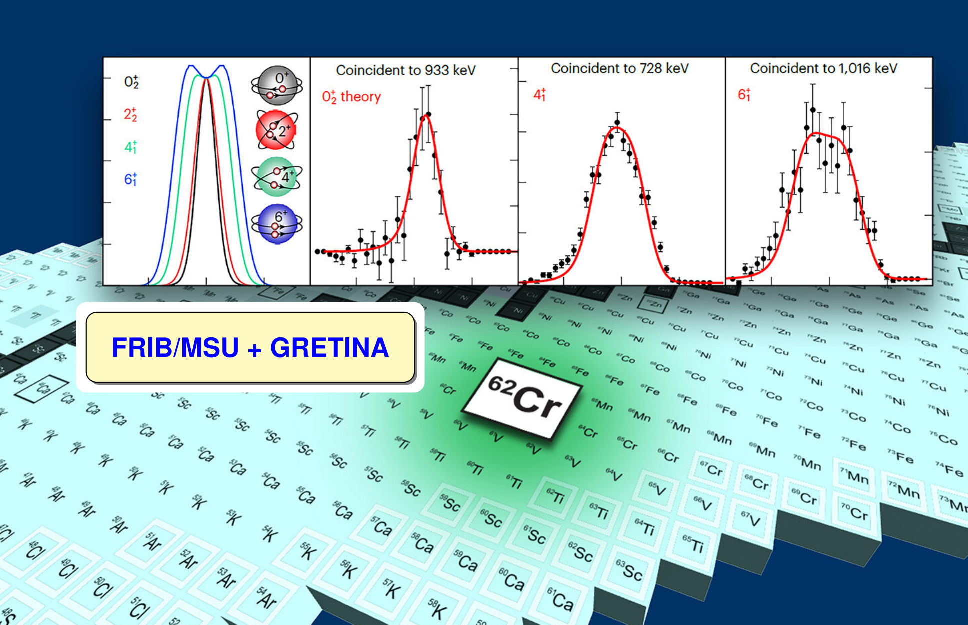
	DNO-SM(PAV)		DNO-SM(VAP)	Exact SM
	(β,γ)	(β,γ)+NpNh		
^{20}Ne	−40.35736	−40.47233	−40.47231	−40.47233
	7	51	3	640
^{24}Mg	−86.73278	−87.10428	−87.10305	−87.10445
	16	975	10	28503
^{28}Si	−135.21742	−135.85891	−135.85364	−135.86073
	27	4255	13	93710
^{26}Al	–	–	−105.72564	−105.74934
	–	–	9	26914

Landscape of medium mass nuclei



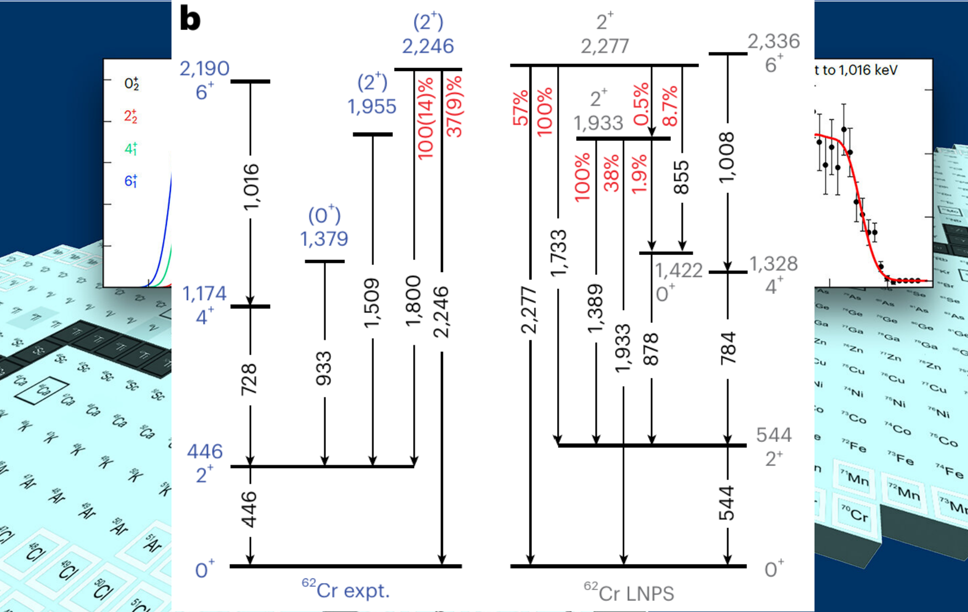
(Adapted from F. Nowacki, A. Obertelli, A. Poves, *The neutron-rich edge of the nuclear landscape: Experiment and theory*, Prog. Part. Nucl. Phys.

Shape coexistence in N=40 Island of Inversion : ^{62}Cr

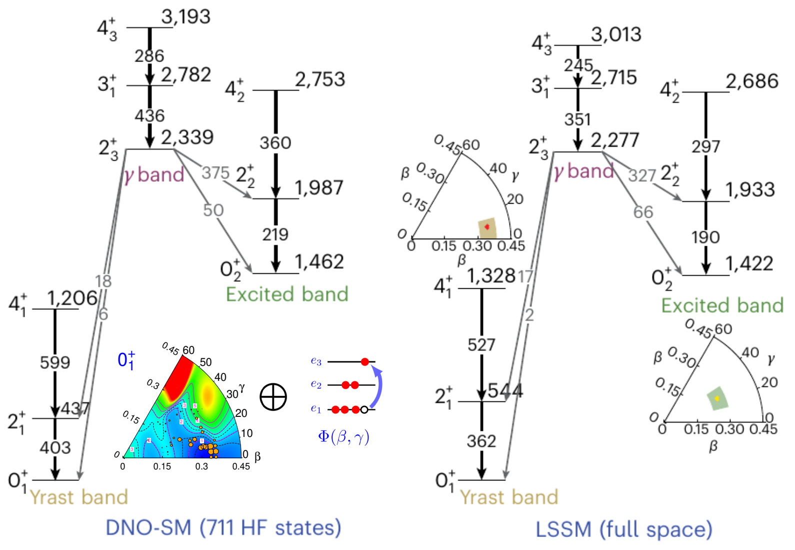


FRIB/MSU + GRETINA

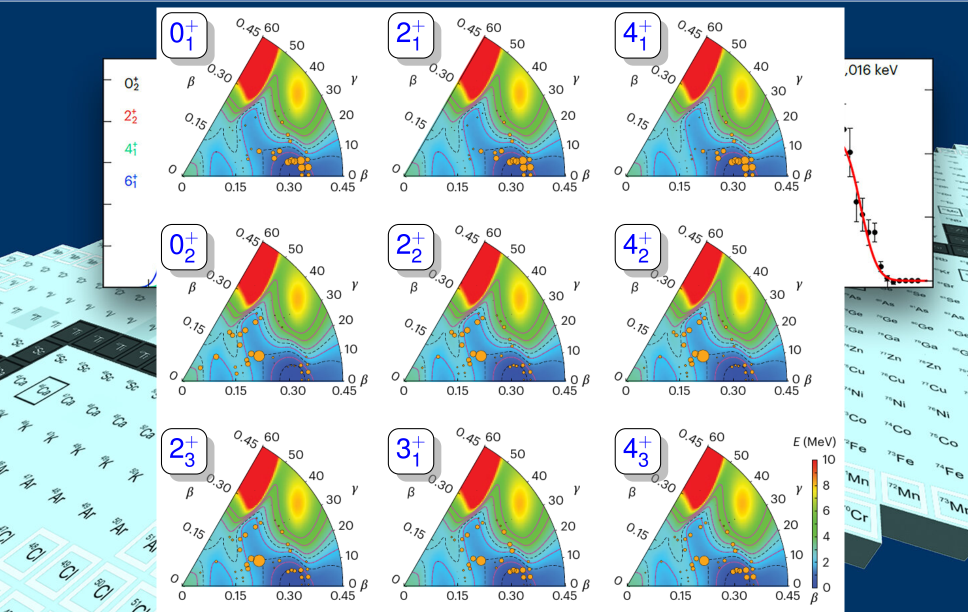
Shape coexistence in N=40 Island of Inversion : ^{62}Cr



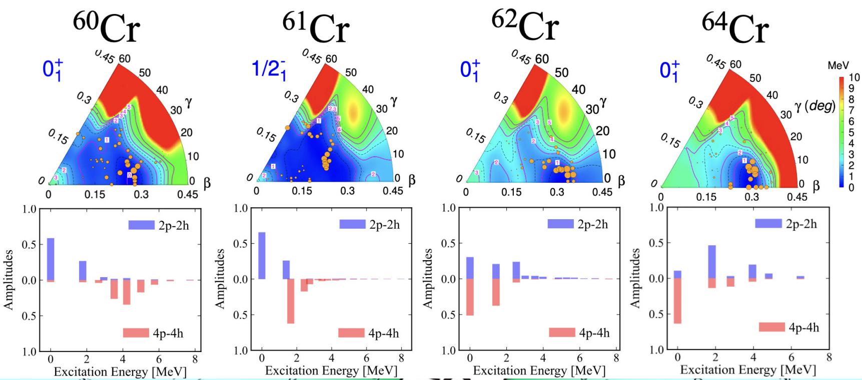
Shape coexistence in N=40 Island of Inversion : ^{62}Cr



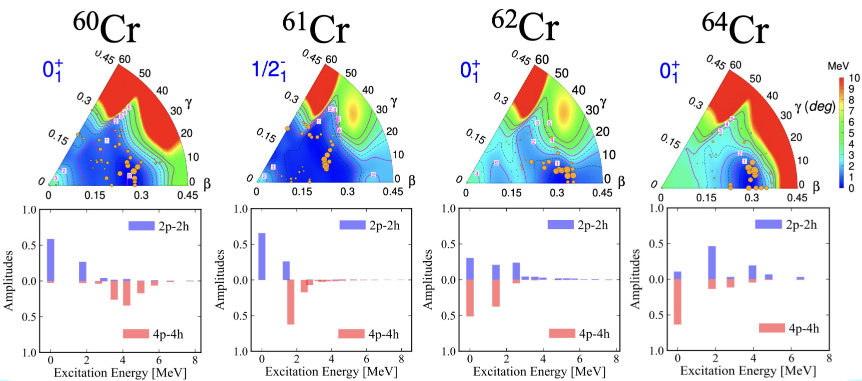
Shape coexistence in N=40 Island of Inversion : ^{62}Cr



Shape coexistence in N=40 Island of Inversion : ^{62}Cr



Shape coexistence in N=40 Island of Inversion : ^{62}Cr



- ^{62}Cr appears as the portal to the $N = 40$ Island of Inversion of 4p4h regime, exhibiting a competing shape coexistence structure
- Excited 0_2^+ state: interpreted as the remnant of the 2p2h excitations
- Observation of the γ-band $K = 2$ associated to the excited 0_2^+

Shape coexistence in N=40 Island of Inversion : ^{62}Cr

nature physics

Article

https://doi.org/10.1038/s41567-024-02680-0

In-beam spectroscopy reveals competing nuclear shapes in the rare isotope ^{62}Cr

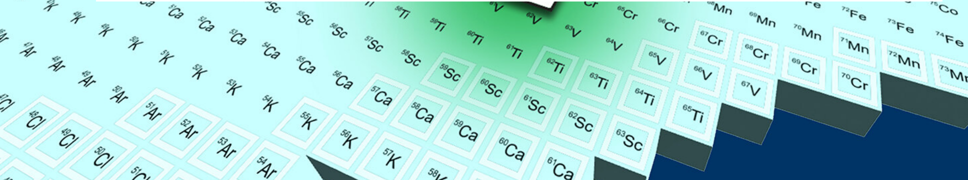
Received: 17 March 2024

Accepted: 24 September 2024

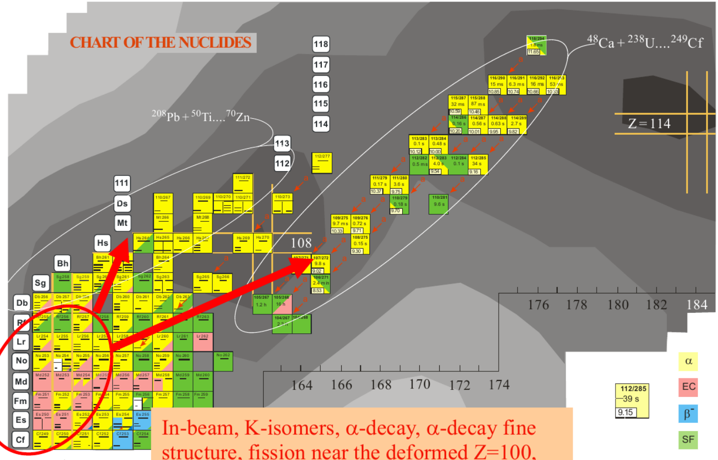
Published online: 18 October 2024

Check for updates

Alexandra Gade[1,2] ✉, Brenden Longfellow[3], Robert V. F. Janssens[4,5], Duc D. Dao[6], Frédéric Nowacki[6], Jeffrey A. Tostevin[7], Akaa D. Ayangeakaa[4,5], Marshall J. Basson[1,2], Christopher M. Campbell[8], Michael P. Carpenter[9], Joseph Chung-Jung[1,2], Heather L. Crawford[8], Benjamin P. Crider[10], Peter Farris[1,2], Stephen Gillespie[1], Ava M. Hill[1,2], Silvia M. Lenzi[11], Shumpei Noji[1], Jorge Pereira[1], Carlotta Porzio[8], Alfredo Poves[12], Elizabeth Rubino[1] & Dirk Weisshaar[1]



Landscape of superheavy nuclei



Z=100

N=152

In-beam, K-isomers, α-decay, α-decay fine structure, fission near the deformed Z=100, N=152 shell gaps

(From Seweryniak talk at SSNET 2024)

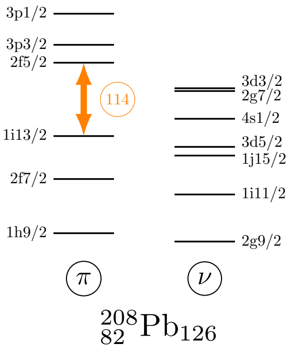
New frontiers for shell-model description of superheavy nuclei

Kuo-Herling interaction:

- ${}^{208}_{82}\mathrm{Pb}_{126}$ 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),072511*

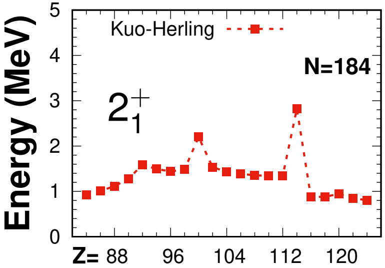


Calculations: NATHAN & CARINA codes

◇ Diagonalization within the seniority scheme along the chains of $N = 126$ and $N = 184$ (in preparation)

◇ Variation After Projection calculations: ${}^{253,254,255}\mathrm{Es}$, ${}^{249,251,253}\mathrm{Cf}$, ${}^{253,254}\mathrm{No}$, ${}^{256}\mathrm{Fm}$ (submitted to Physical Review Letters)

◇ Comparison of spectra and electromagnetic moments



New frontiers for shell-model description of superheavy nuclei : Yrast systematics

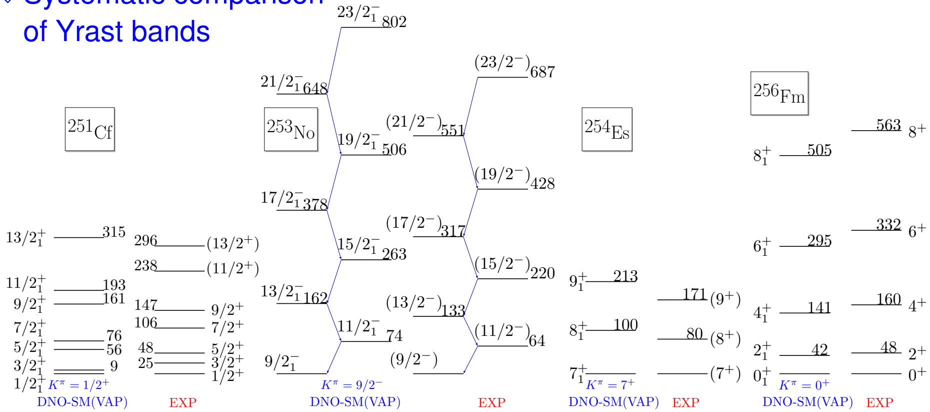
First complete shell-model description of ^{254}No: a new paradigm for superheavy nuclear structure studies

Duy Duc Dao[1] and Frédéric Nowacki[1]

[1] *Université de Strasbourg, CNRS, IPHC UMR7178, 23 rue du Loess, F-67000 Strasbourg, France*

(Dated: September 24, 2024)

- ◇ Systematic comparison of Yrast bands



New frontiers for shell-model description of superheavy nuclei : Electromagnetic moments

First complete shell-model description of ^{254}No: a new paradigm for superheavy nuclear structure studies

Duy Duc Dao[1] and Frédéric Nowacki[1]
[1] *Université de Strasbourg, CNRS, IPHC UMR7178, 23 rue du Loess, F-67000 Strasbourg, France*
(Dated: September 24, 2024)

◇ Comparison of magnetic and quadrupole moments

J^{π}_{gs}		E (MeV)		$\mu(\mu_N)$			Q_s (eb)		
		PAV	VAP	PAV	VAP	EXP	PAV	VAP	EXP
^{253}No	$9/2^-$	-241.818	-242.816	$+0.591$	-0.493	$-0.527(33)(75)$	-3.5	$+7.2$	$+5.9(1.4)(0.9)$
^{253}Cf	$7/2^+$	-253.402	-253.818	-0.677	-0.556	$-0.731(35)$	$+5.77$	$+5.78$	$+5.53(51)$
^{251}Cf	$1/2^+$	-241.321	-241.724	-0.727	-0.610	$-0.571(24)$	-	-	-
^{249}Cf	$9/2^-$	-229.021	-229.381	-0.480	-0.461	$-0.395(17)$	$+6.62$	$+6.63$	$+6.27(33)$
^{255}Es	$7/2^+$	-263.512	-264.695	-1.10	$+3.94$	$+4.14(10)$	$+6.0$	$+5.8$	$+5.1(1.7)$
^{254}Es	7^+	-257.492	-258.441	$+0.778$	$+3.36$	$+3.42(7)$	$+1.8$	$+8.4$	$+9.6(1.2)$
^{253}Es	$7/2^+$	-251.837	-252.280	$+3.63$	$+3.93$	$+4.10(7)$	$+5.87$	$+5.9$	$+6.7(8)$
^{256}Fm	0^+	-268.999	-269.717	$+0.87$	$+0.89$	-	-3.57	-3.60	-
^{254}No	0^+	-249.568	-250.187	$+0.87$	$+0.91$	-	-3.78	-3.75	-

New frontiers for shell-model description of superheavy nuclei : Electromagnetic moments

First complete shell-model description of ^{254}No: a new paradigm for superheavy nuclear structure studies

Duy Duc Dao[1] and Frédéric Nowacki[1]

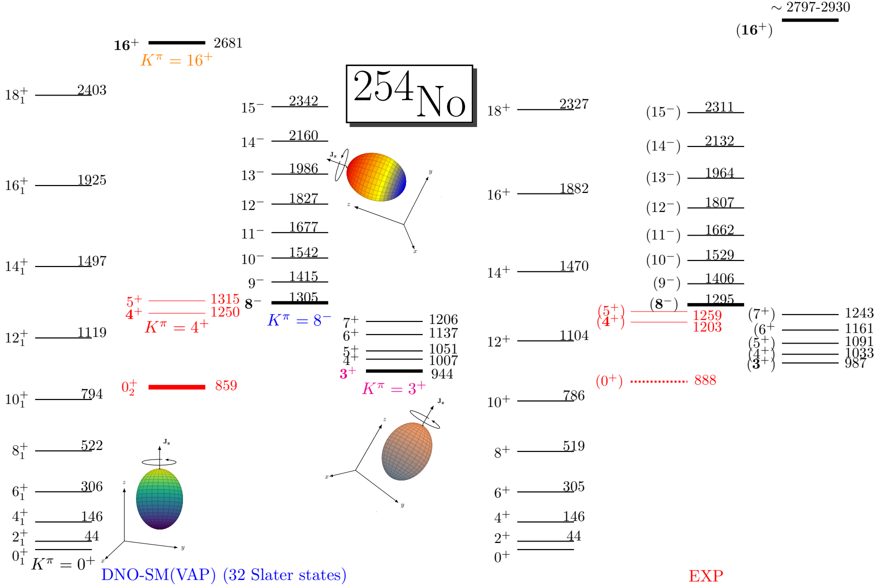
[1] *Université de Strasbourg, CNRS, IPHC UMR7178, 23 rue du Loess, F-67000 Strasbourg, France*

(Dated: September 24, 2024)

◇ Comparison of magnetic and quadrupole moments

J^{π}_{gs}		E (MeV)		$\mu(\mu_N)$			Q_s (eb)		
		PAV	VAP	PAV	VAP	EXP	PAV	VAP	EXP
^{253}No	$9/2^-$	−241.818	−242.816	+0.591	−0.493	−0.527(33)(75)	−3.5	+7.2	+5.9(1.4)(0.9)
^{253}Cf	$7/2^+$	−253.402	−253.818	−0.677	−0.556	−0.731(35)	+5.77	+5.78	+5.53(51)
^{251}Cf	$1/2^+$	−241.321	−241.724	−0.727	−0.610	−0.571(24)	-	-	-
^{249}Cf	$9/2^-$	−229.021	−229.381	−0.480	−0.461	−0.395(17)	+6.62	+6.63	+6.27(33)
^{255}Es	$7/2^+$	−263.512	−264.695	−1.10	+3.94	+4.14(10)	+6.0	+5.8	+5.1(1.7)
^{254}Es	7^+	−257.492	−258.441	+0.778	+3.36	+3.42(7)	+1.8	+8.4	+9.6(1.2)
^{253}Es	$7/2^+$	−251.837	−252.280	+3.63	+3.93	+4.10(7)	+5.87	+5.9	+6.7(8)
^{256}Fm	0^+	−268.999	−269.717	+0.87	+0.89	-	−3.57	−3.60	-
^{254}No	0^+	−249.568	−250.187	+0.87	+0.91	-	−3.78	−3.75	-

New frontiers for shell-model description of superheavy nuclei : ^{254}No

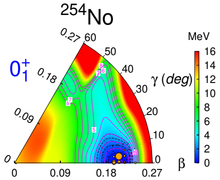


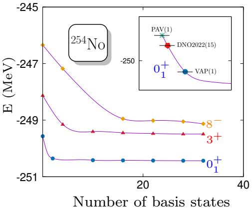
New frontiers for shell-model description of superheavy nuclei : ^{254}No

~ 2797-2930

(16^+)

- Reproduction of the complete spectroscopy in ^{254}No: Yrast band AND various isomeric structures and K bands
- The ground state structure is dominated by essentially axial deformed configurations
- Prediction of a second 0_2^+ state and excited $K = 4$ $(4^+, 5^+)$ structures which agree remarkably well with the new experimental findings





1243
1161
1091
1033
987

(D.D. Dao, F. Nowacki, arXiv:2409.08210, submitted to PRL)

Conclusions

- Extensions of the Discrete Non-Orthogonal Shell Model (DNO-SM)
  - DNO-SM(PAV): Inclusion of both deformed Slater states and its NpNh excitations in the Projection-After-Variation (PAV) scheme
  - DNO-SM(VAP): Development of a fully variational approach with the Variation-After-Projection (VAP) technique and the Restoration of the rotational symmetry
- Reproduction of exact shell-model solutions in the benchmark cases of sd shell
- Laboratory versus Intrinsic interpretations, shape evolution analysis of ^{62}Cr exhibiting a peculiar shape coexistence occurrence prior to the $N = 40$ Island of Inversion
- New frontiers for shell-model description in the superheavy mass region of the nuclear chart
- Ongoing (ASTRANUCAP) studies for Island of Inversion at $A \sim 80$