

SHELL MODEL DEVELOPMENTS TOWARD HEAVY NUCLEI

Duy-Duc Dao, F. Nowacki
(IPHC-Strasbourg)

*Plenary meeting of the french low energy nuclear physics
community*

Strasbourg, November 3-7th, 2025



1. THE NUCLEAR SHELL MODEL (SM)

2. VARIATIONAL APPROACH FOR THE SHELL MODEL

- VARIATION AFTER PROJECTION THEORY FOR SLATER AND QUASI-SLATER DETERMINANTS
- EXACT SOLUTIONS OF SHELL-MODEL HAMILTONIANS

3. APPLICATIONS TO HEAVY DEFORMED NUCLEI

- PROTON-RICH NUCLEI AT THE $N=Z$ LINE: $^{84,86}\text{Mo}$
- SPECTROSCOPY STUDY OF TRANS-ACTINIDES: ^{254}No
- PRELIMINARY CALCULATIONS FOR DIPOLE EXCITATIONS IN ^{242}Pu
- PRELIMINARY CALCULATIONS IN THE RARE-EARTH REGION: ^{168}Dy

The Nuclear Shell Model

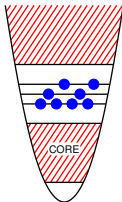
SM-CI approaches through the nuclear chart

◇ Nuclear Shell Model (SM):

$$H_{\text{exact}}|\psi_{\text{exact}}\rangle = E|\psi_{\text{exact}}\rangle$$



$$H_{\text{eff}}|\psi_{\text{eff}}\rangle = E|\psi_{\text{eff}}\rangle$$



◇ Three Pillars of the Shell Model:

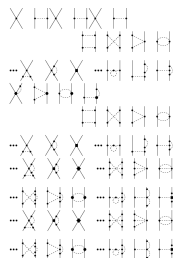
- A good valence space
- An associated effective interaction
- A “shell-model” code

(E. Caurier et al. Rev. Mod. Phys. 77, 427 (2005))

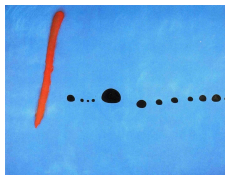
A Complex View, Epelbaum Physics



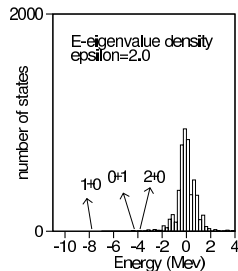
P. Klee, Art



A Simple View, Zuker Physics

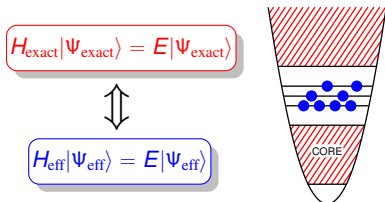


J. Miro, Art



SM-CI approaches through the nuclear chart

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◇ Nuclear structure far from stability

- Deformation, Superdeformation
- Superfluidity, Dipole resonances
- Emergence of magic numbers
- Vanishing of shell closures

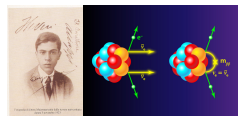


◇ Weak processes

- β decay
- double $\beta\beta$ decay

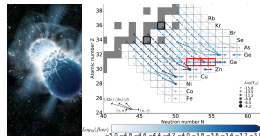
$$[T_{1/2}^{0\nu}(0^+ \rightarrow 0^+)]^{-1} = G_{0\nu} |M^{0\nu}|^2 \langle m_\nu \rangle^2$$

(nature of neutrinos)



◇ Astrophysics and nucleosynthesis

- rp-process
- r-process



Diagonalization versus Variational Methods

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 :

^{48}Cr 1,963,461

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

In *pf-sd*g space :

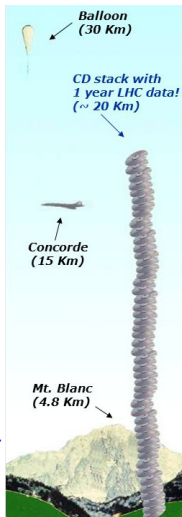
^{78}Ni 210,046,691,518

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 computational resources:

E. Caurier et al., Rev. Mod. Phys. 77 (2005) 427

- m-scheme ANTOINE code
BIGSTICK
KHELL
- coupled scheme NATHAN code



Variational Approximation

$$\mathcal{H}_{\text{eff}} |\Psi_\alpha^{JM}\rangle = E_\alpha^{(J)} |\Psi_\alpha^{JM}\rangle \rightarrow \delta \frac{\langle \Psi_\alpha^{JM} | \mathcal{H}_{\text{eff}} | \Psi_\alpha^{JM} \rangle}{\langle \Psi_\alpha^{JM} | \Psi_\alpha^{JM} \rangle} = 0$$

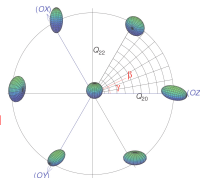
Mixing of shapes:

$$|\Psi_{\text{eff}}\rangle = |\text{shape 1}\rangle + |\text{shape 2}\rangle + \dots$$

Restoration of the rotational symmetry

Degree of freedom

- Multipole: $\beta, \gamma, Q_{30}, \dots$
- Cranking: J_x, J_z
- Pairing constraints
- Variation-After-Projection



Different implementations

- MCSM/QVSM Tokyo group
- DNO-SM Strasbourg group
- PGCM Madrid group

Diagonalization versus Variational Methods

Shell Model Exact Diagonalization

- Exponential growth of basis dimensions:

- *Weak entanglement approximation for nuclear structure*

O. C. Gorton, C. W. Johnson, Phys. Rev. C 110, 034305 (2024), J. Sub. Part. Cos. 3, 100061 (2025).

- *Nuclear shell-model simulation in digital quantum computer*

A. Pérez-Obiol, A.M. Romero, J. Menéndez et al., Sci. Rep. 13, 12291 (2023)

- *Nuclear structure study using a hybrid approach of Shell Model and Gogny-type density functionals*

K. Yoshinaga, N. Shimizu, T. Nakatsukasa, MDPI Particles 8, 2:61 (2025).

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- **Different implementations**

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Variational Approach for the Shell Model

Variation after Projection (VAP) Theory:

◇ **Ritz variational principle:** $H|\psi\rangle = E|\psi\rangle \iff \frac{\delta E}{\delta \psi} = 0, \quad E[\psi] = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$

- Symmetries/Quantum Numbers:

Angular Momentum, Parity (J, π), Neutron, Proton numbers (N, Z), Isospin (T, T_z)

- Restoration of symmetries:

$$|\psi_\alpha^{\pi J N Z}\rangle = \sum_{q,K} f_\alpha^{\pi J N Z}(q; K) \mathcal{P}_{MK}^{\pi J N Z} |\Phi_q\rangle$$

$$|\Phi\rangle = \mathcal{N}_0 e^{\frac{1}{2} \sum_{ij} Z_{ij} \beta_i^\dagger \beta_j^\dagger} |\Phi_0\rangle \text{ (Thouless Theorem)}$$

- Intrinsic states:

► $|\Phi\rangle = \prod_k c_k^\dagger |-\rangle$ (Slater determinant)

► $|\Phi\rangle = \prod_k \beta_k |-\rangle$ (Bogoliubov state)

$$\beta_k^\dagger = \sum_l U_{lk} c_l^\dagger + V_{lk} c_l \text{ (Bogoliubov transformation)}$$

- ◇ **Coupled variational equations:**

$$(H^{\pi J N Z} - E^{\pi J N Z} N^{\pi J N Z}) f_\alpha^{\pi J} = 0 \text{ (Hill-Wheeler)}$$

$$\sum_q \frac{\partial E^{\pi J N Z}}{\partial Z_{ij}^{(q)*}} = \sum_{q', K', q, K} f_\alpha^{\pi J N Z*}(q; K) f_\alpha^{\pi J N Z}(q'; K') \times$$

$$\langle \Phi_q | \beta_j \beta_i (H - E^{\pi J N Z}) \mathcal{P}_{KK'}^{\pi J N Z} | \Phi_{q'} \rangle = 0$$

(Stationary Brillouin conditions)

A bit of history:

► Mainly advocated by the VAMPIR school in 1970s,

1980s (K.W. Schmid and collaborators)

► Fully **Triaxial** too complicated, only **Axial** available

at the times

► **Resonating Hartree-Fock in Quantum Chemistry**

theory developed by H. Fukutome for fermionic systems

K. W. Schmid et al., Phys. Rev. C 29 (1984) 291, ibid. PRC 29, 308.

K. W. Schmid et al., Ann. Phys. 180, 1 (1987).

H. Fukutome, S. Nishiyama, Prog. Theo. Phys. 80, 417 (1988), ibid. 85, 1121 (1991)

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$$\langle \Phi_q | \beta_j \beta_i (H - E^{\pi J N Z}) \mathcal{P}_{KK'}^{\pi J N Z} | \Phi_{q'} \rangle = 0$$

(Stationary Brillouin conditions)

Today: Fully Triaxial VAP with Bogoliubov ansatz for heavy systems becomes possible recently

► Tokyo Group (Quasi-Vacua Shell Model)

Phys. Rev. C 103, 014312 (2021).

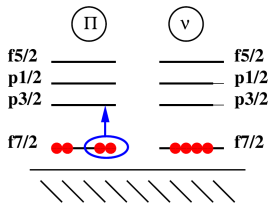
► Strasbourg Group (treatment of Bogoliubov states)

... done two weeks ago.

Broeckhove-Deumens Theorem:

- Theorem for non-orthogonal states: Z. Phys. A292, 243 (1979)

Given a separable Hilbert space $\mathcal{H}$ spanned by a continuous family of states $\Gamma = \{\psi(\alpha) | \alpha \in \mathbf{R}\}$, there exists a countable subset $\Gamma_0 = \{\phi(\alpha_i) | i \in \mathbf{N}\} \subset \Gamma$ with the property $\mathcal{H} = \overline{\text{span} \Gamma_0}$, i.e. Γ_0 is a skew or non-orthogonal basis in $\mathcal{H}$.



$$\psi = c_1 \phi_1 + c_2 \phi_2 + \dots + c_i \phi_i + \dots$$

IMPLICATIONS:

- Non-Orthogonal Slater Determinants spans the full shell-model space
- The number of such Slater Determinants is FINITE
- "Labels" for eigenstates: $|\alpha, J^\pi M, T T_z\rangle$
 - symmetries: $(J, \pi, \dots)$
 - intrinsic label: α related to the dynamics of the Hamiltonian
- Caurier minimization technique justified: Reconciliation of formal problems related to the integral Hill-Wheeler representation $\psi = \int d\alpha f(\alpha) \phi(\alpha)$

Discrete Non-Orthogonal Shell Model (DNO-SM)

◇ Hill-Wheeler-Griffin Generator Coordinate Method:

- $\langle J_z \rangle, (\beta, \gamma)$ (cranking, axial and triaxial)

◇ Problems:

- Underbinding energies
- Compressed spectra, large BE2

PHYSICAL REVIEW C **105**, 054314 (2022)

Nuclear structure within a discrete nonorthogonal shell model approach: New frontiers

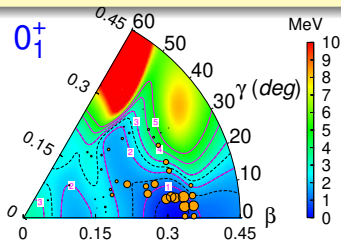
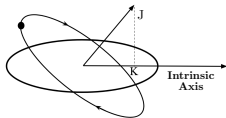
D. D. Dao  and F. Nowacki 

Université de Strasbourg, CNRS, IPHC UMR7178, 23 rue du Loess, F-67000 Strasbourg, France

◇ functions in the intrinsic frame

- K : Intrinsic quantum number
- Contribution of K -mixing

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



Discrete Non-Orthogonal Shell Model (DNO-SM)

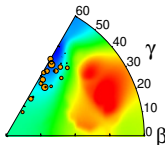
◇ Hill-Wheeler-Griffin Generator Coordinate Method:

- $\langle J_z \rangle$, (β, γ) (cranking, axial and triaxial)
- Selection of (β, γ) : Courier technique
- Rotational symmetry restoration

$$|\Psi_{\text{eff}}\rangle = |\text{shape 1}\rangle + |\text{shape 2}\rangle + |\text{shape 3}\rangle + \dots$$

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

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



◇ Problems:

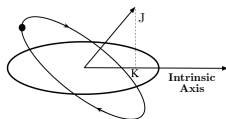
- Underbinding energies
- Compressed spectra, large BE2
- Missing correlations

LNPS effective interaction

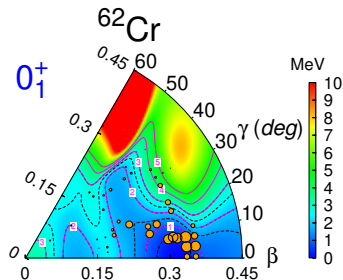
⁶² Cr	(β, γ)	SM
$E(0_1^+)$ (MeV)	-212.426	-214.138
$B(E2, 2_1^+ \rightarrow 0_1^+)$ (e ² fm ⁴)	458	362

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

- K : Intrinsic quantum number
- Contribution of K -mixing



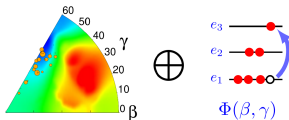
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Discrete Non-Orthogonal Shell Model (DNO-SM)

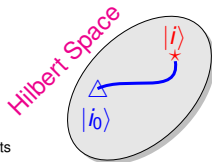
◇ Hill-Wheeler-Griffin Generator Coordinate Method: (PAV scheme)

- Triaxial mixing $q = (\beta, \gamma) + \text{NpNh excitations}$
- Caurier minimization technique



◇ Variation after Projection:

- $q = 1, 2, 3, \dots$: Resonating Hartree-Fock
- $J_\alpha = 0_1, \dots$
- Intrinsic states dynamically generated



USDB effective interaction^a with non-orthogonal Slater Determinants

(^a B.A. Brown, W. A. Richter, PRC74, 034315 (2006))

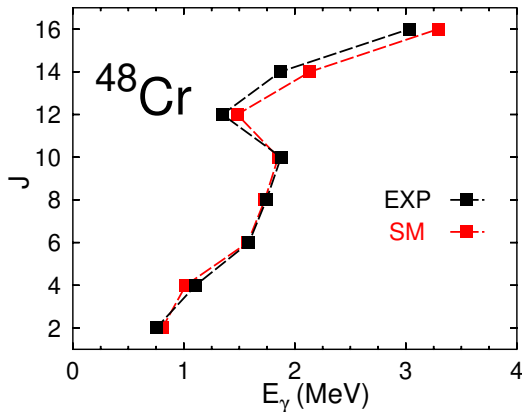
	PAV		VAP	Exact SM
	(β, γ)	$(\beta, \gamma) + \text{NpNh}$		
²⁰ Ne	-40.35736	-40.47233	-40.47231	-40.47233
	7	51	3	640
²⁴ Mg	-86.73278	-87.10428	-87.10405	-87.10445
	16	975	16	28503
²⁸ Si	-135.21742	-135.85891	-135.86003	-135.86073
	27	4255	45	93710
²⁶ Al	—	—	-105.74901	-105.74934
	—	—	22	26914

Backbending in ^{48}Cr with KB3 interaction

	DNO-SM(β, γ)	DNO-SM(VAP)	Exact SM
dimension	22	50	1 963 461
$E(0_{gs}^+)$ (MeV)	-31.873	-32.953	-32.953

Approaches:

- Textbook Shell-Model Description of pairing correlations effects on the rotational band



E. Caurier et al., Phys. Rev. Lett. **75**, 2466 (1995)

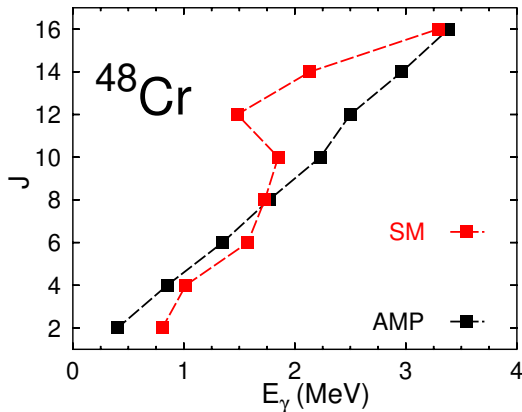
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Approaches:

● AMP Projected Hartree-Fock:

~ Pure Rotor $J(J+1)$ law

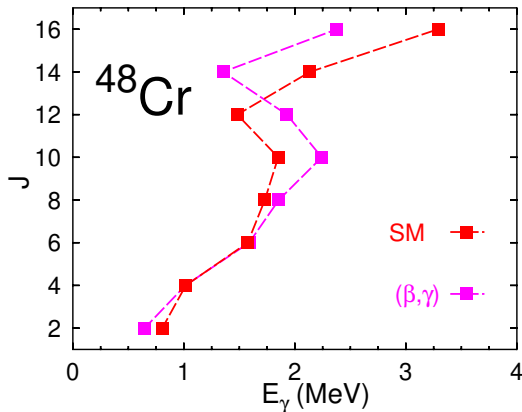


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- Triaxial Configuration Mixing:
~ Partially capturing pairing

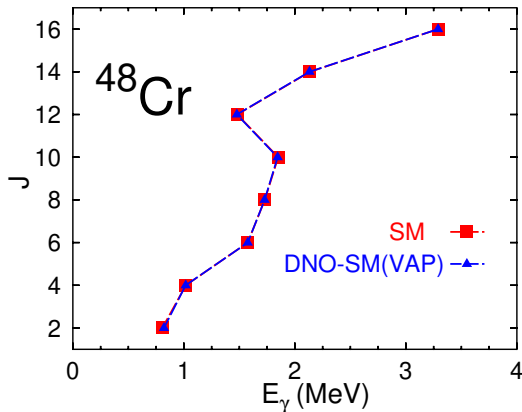


Backbending in ^{48}Cr with KB3 interaction

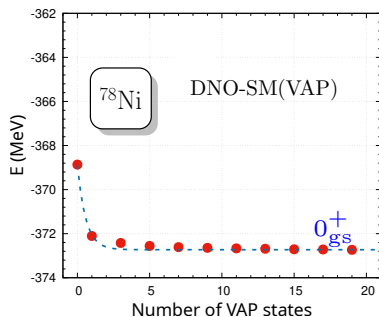
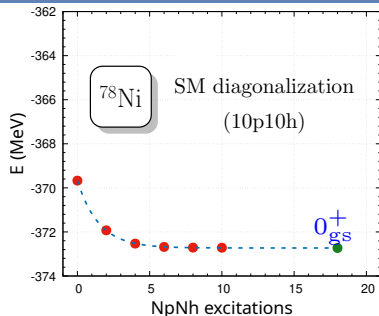
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~ Pure Rotor $J(J+1)$ law
- Triaxial Configuration Mixing:
~ Partially capturing pairing
- Variation After Projection:
~ Fully capturing pairing



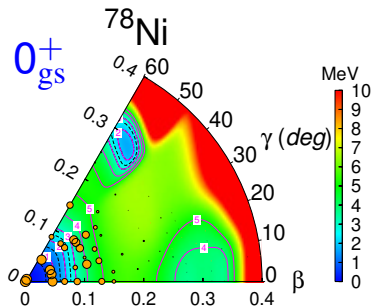
Coexistence in ^{78}Ni



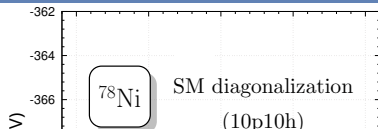
(D.D. Dao, F. Nowacki, in preparation)

PFSDG-U effective interaction
Ground State Energy in MeV

(β, γ)	VAP	SM (10p-10h)
81	19	$\sim 2 \times 10^{12}$
-370.630	-372.733	-372.717
	extrapolated	-372.729(7)



Coexistence in ^{78}Ni



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

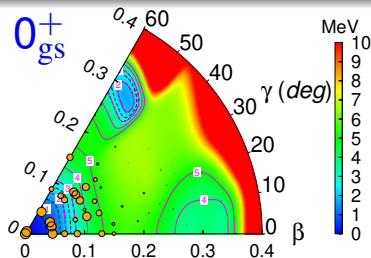
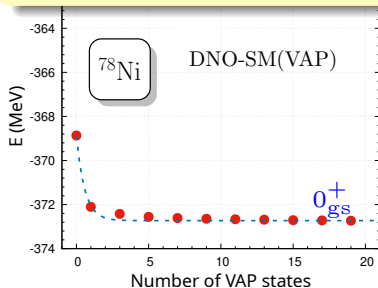
PFSDG-U effective interaction
Ground State Energy in MeV

Exact solutions of the nuclear shell-model secular problem: Discrete Non-Orthogonal Shell Model within a Variation After Projection approach

Duy-Duc Dao^a, Frédéric Nowacki^a

^a Université de Strasbourg, CNRS, IPHC UMR7178, 23 rue du Loess, F-67000 Strasbourg, France

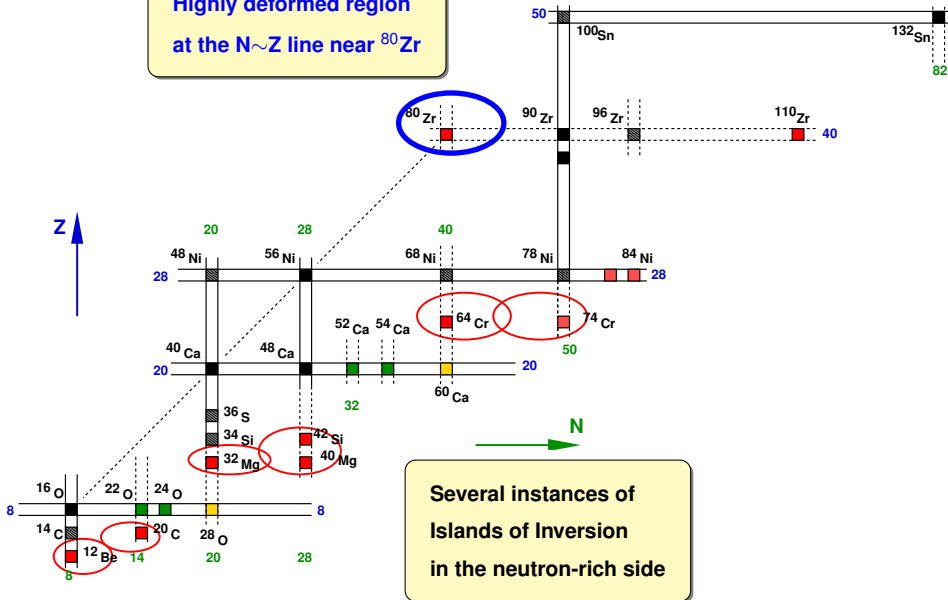
ArXiv:2507.09073 [nucl-th] (2025)



Applications to heavy deformed nuclei

Landscape of medium mass nuclei

Highly deformed region
at the $N \sim Z$ line near ^{80}Zr

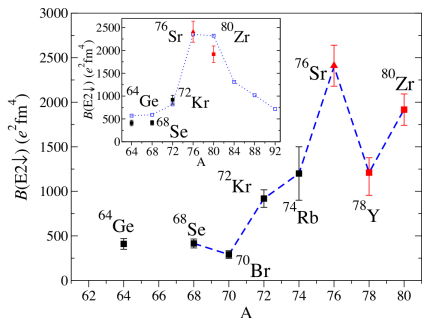
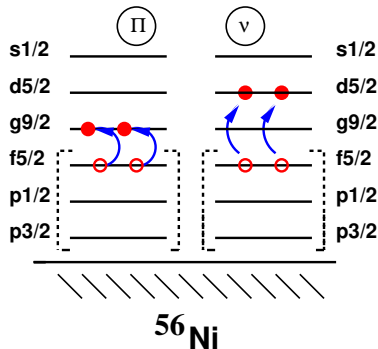


Island of Inversion at the $N=Z$ line

Highly deformed nuclei at $N = Z$:

- Configuration mixing in ^{72}Kr
- Most deformed cases for ^{76}Sr , ^{80}Zr
- New spectroscopy for ^{84}Mo and ^{86}Mo
NSCL/GRETINA Experiment

Valence Space and Interactions:



R.D.O. Llewellyn *et al.*, PRL **124**, 152501 (2020)

- ZBM3 valence space:
extension of JUN45
to pseudo-SU3 + Quasi-SU3
- New effective interactions:
 - Realistic TBME + Monopole “3N” constraints”
 - ab-initio N3LO (2N) interaction
 - ongoing ab-initio N3LO (2N) + 3N (Inl) interaction
- SM + DNO-SM for most **deformed cases**

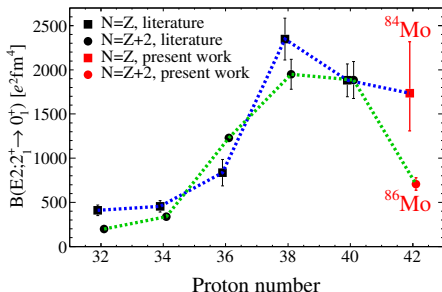
Structural transition in $^{84,86}\text{Mo}$

◇ Collapse of collectivity:

● New spectroscopy for ^{84}Mo and ^{86}Mo

NSCL/GRETINA Experiment

(F. Recchia et al., Nat. Comms, accepted (2025))



◇ Calculations/Experiments

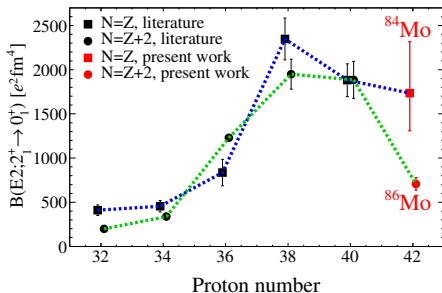
nucleus	Np-Nh*	ZRP	PHF	B(E2)(e ² .fm ⁴)		
				Exp.	DNO-SM*	SM
^{84}Mo	4p-4h	1104	1193	1740⁺⁵⁸⁰₋₄₃₀	1512	-
	8p-8h	1891	1732			
^{86}Mo	0p-0h	542	196	707(71)	893	731
	2p-2h	1030	871			
	4p-4h	1416	1179			
	6p-6h	1858	1655			

Structural transition in $^{84,86}\text{Mo}$

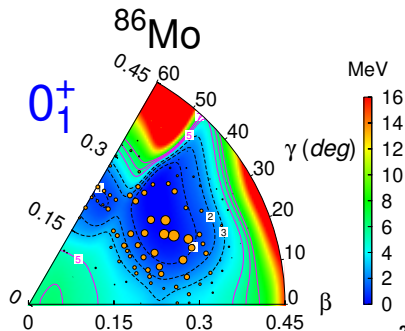
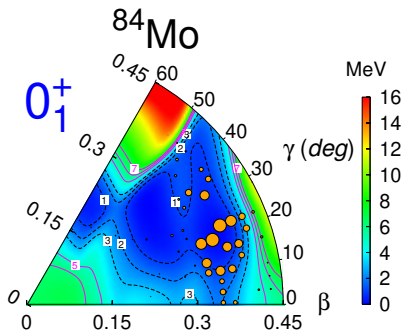
◇ Collapse of collectivity:

- New spectroscopy for ^{84}Mo and ^{86}Mo
NSCL/GRETINA Experiment

(F. Recchia et al., Nat. Comms, accepted (2025))



◇ Ground state configuration mixing

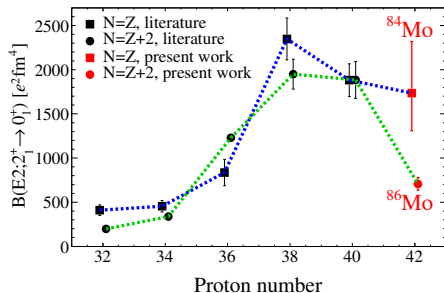


Structural transition in $^{84,86}\text{Mo}$

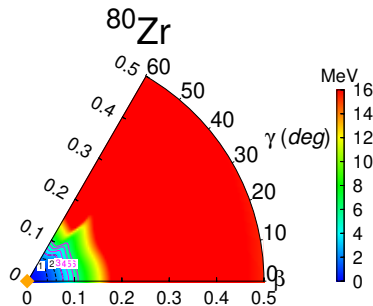
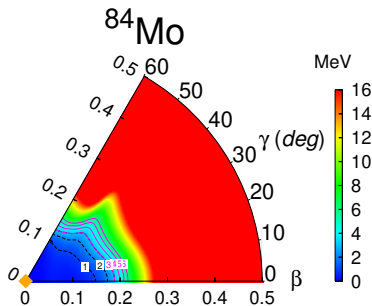
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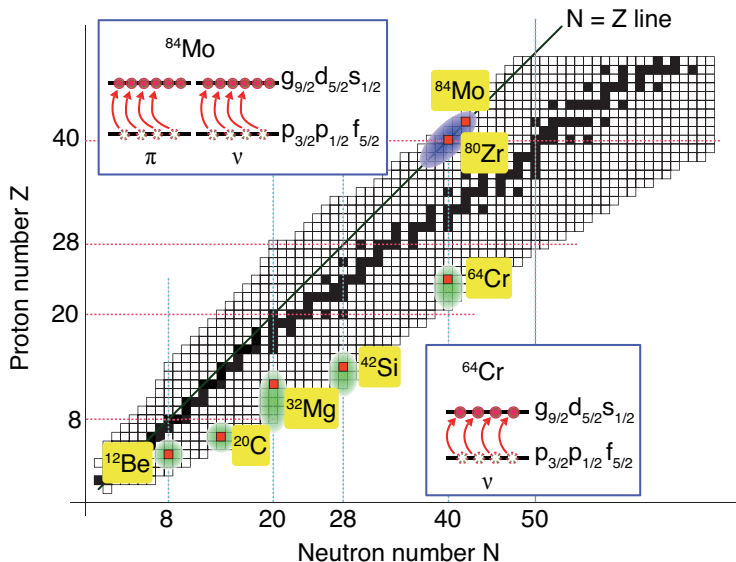
(F. Recchia et al., Nat. Comms, accepted (2025))



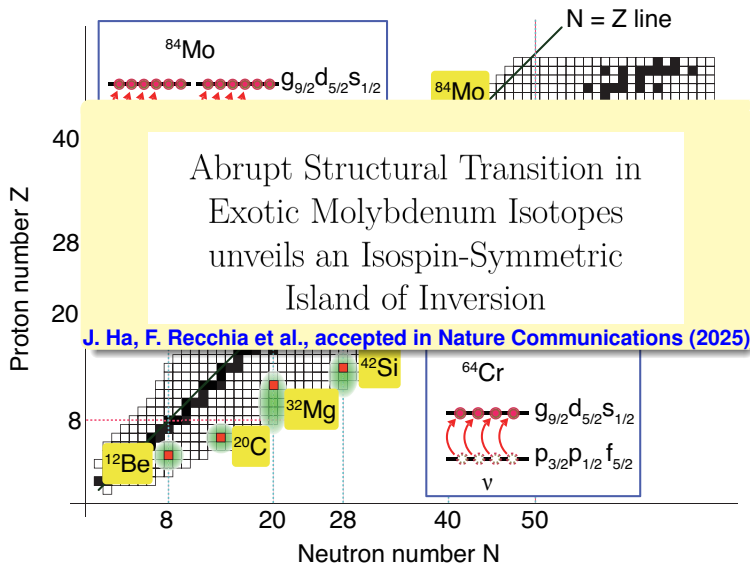
◇ No intruder effects with N3LO-2N V-low k interaction



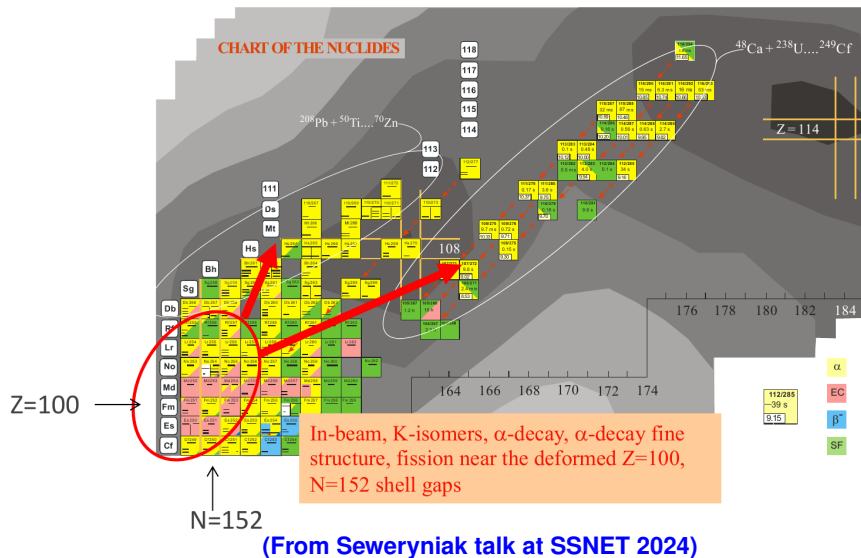
Isospin Symmetric Island of Inversion



Isospin Symmetric Island of Inversion



Landscape of superheavy nuclei



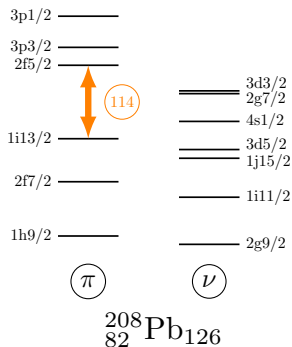
Spectroscopy study of trans-actinides

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)

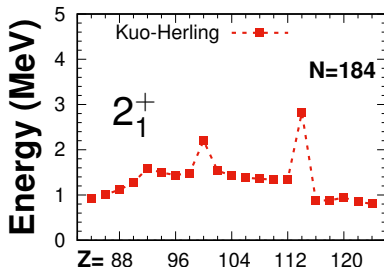
E. Caurier and F. Nowacki,

PRL 87 (2001),072511



Calculations: NATHAN & CARINA codes

- ◊ Diagonalization within the seniority scheme along the chains of $N = 126$ and $N = 184$
- ◊ Variation After Projection calculations: $^{253,254,255}\text{Es}$, $^{249,251,253}\text{Cf}$, $^{253,254}\text{No}$, ^{256}Fm
- ◊ Comparison of spectra and electromagnetic moments



Yrast systematics: odd-even $^{251}_{98}\text{Cf}_{153}$

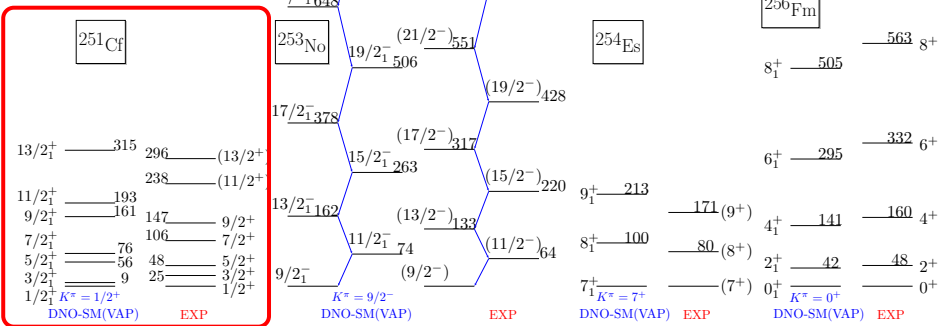
First complete description of low-lying spectroscopy in ^{254}No

Duy Duc Dao¹ and Frédéric Nowacki¹

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

Systematic comparison of Yrast bands

arXiv:2409.08210



Yrast systematics: odd-even $^{253}_{102}\text{No}$

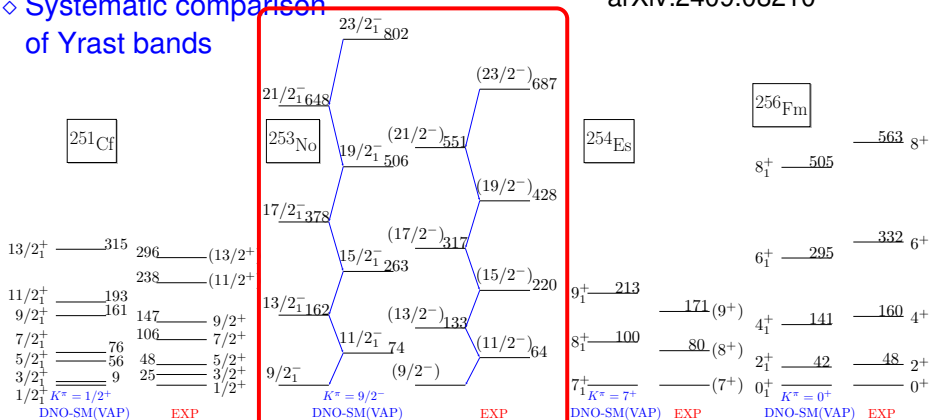
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Systematic comparison of Yrast bands

arXiv:2409.08210



Yrast systematics: odd-odd $^{254}_{99}\text{Es}_{155}$

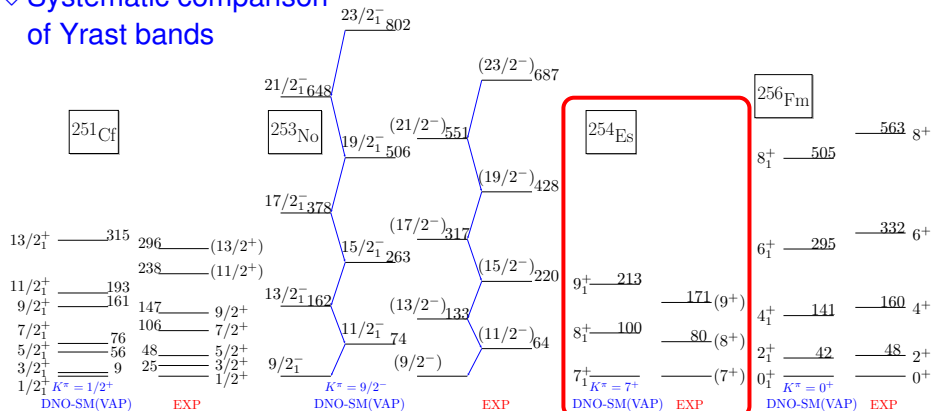
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Systematic comparison of Yrast bands

arXiv:2409.08210



Yrast systematics: even-even $^{256}_{100}\text{Fm}_{156}$

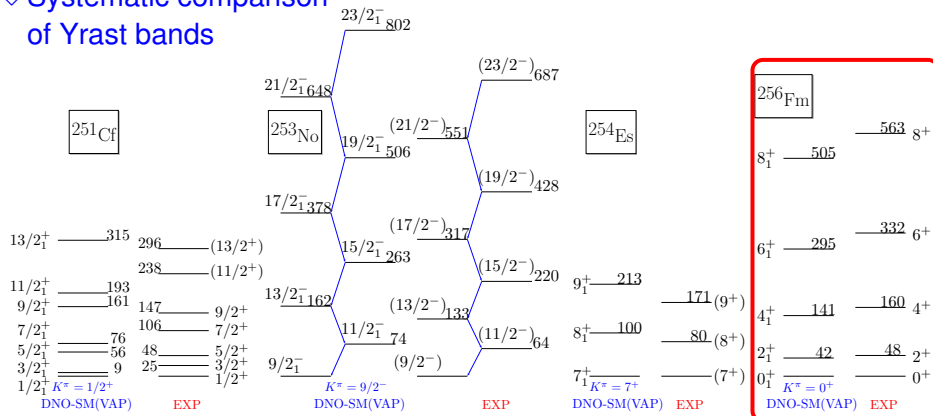
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Systematic comparison of Yrast bands



Systematics of electromagnetic observables

First complete description of low-lying spectroscopy in ^{254}No

Duy Duc Dao¹ and Frédéric Nowacki¹

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

arXiv:2409.08210

◇ Comparison of magnetic and quadrupole moments

Effective charges: $e_p = 1.72$, $e_n = 0.75$

J_{gs}^π	E (MeV)			$\mu(\mu_N)$			Q_s (eb)		
		PHF	VAP	PHF	VAP	EXP	PHF	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	-

Systematics of electromagnetic observables

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arXiv:2409.08210

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Systematics of electromagnetic observables

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arXiv:2409.08210

◇ Comparison of magnetic and quadrupole moments

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^{253}No	PHF	VAP	EXP
$J^\pi = 9/2^-$	+0.591	-0.493	-0.527(33)(75)
$K = 9/2$	100.0%	99.6%	
$K = 7/2$	0.0 %	0.4 %	

- K-mixing is necessary to reproduce the magnetic moment.

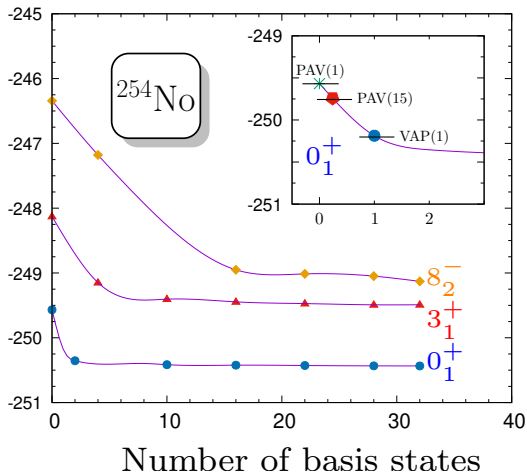
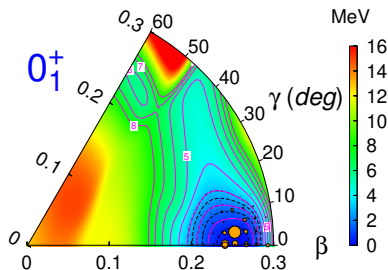
Applications to superheavy nuclei: $^{254}_{102}\text{No}_{152}$

Known spectroscopy:

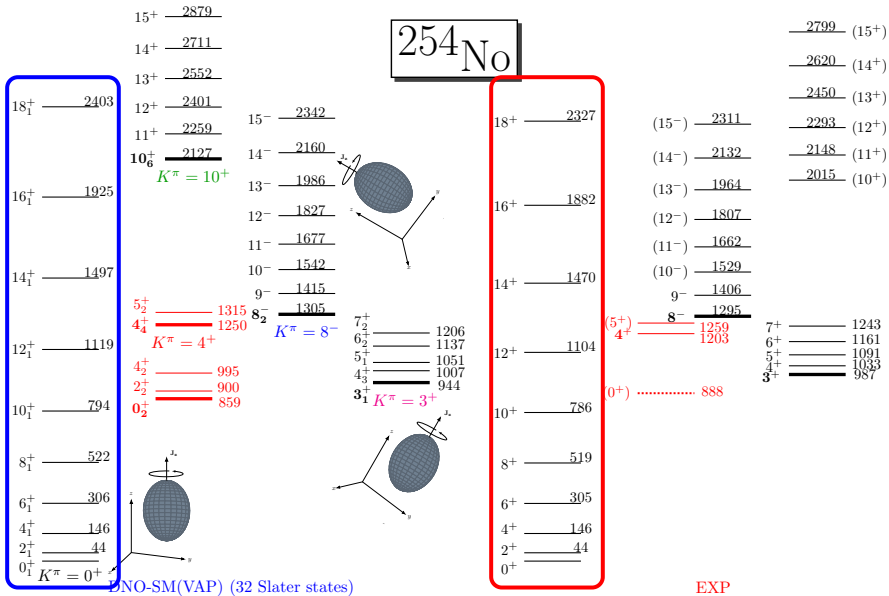
- Axially well-deformed nucleus
- Ground-state rotational band
- Several isomeric states (8^- , 3^+ , 10^+)

Calculations:

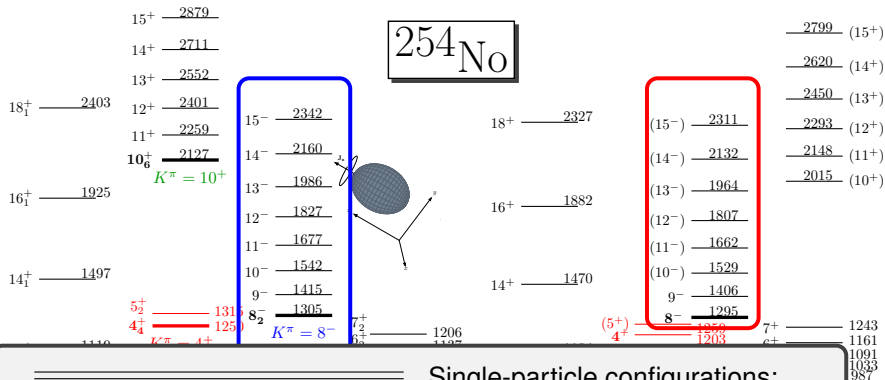
- Deformed Axial Minimum at $\beta = 0.25$
- Mixing of triaxial configurations (β, γ) (PAV(15))
- VAP calculations for band-head structures



Reproduction of spectra: Yrast rotational band



Isomeric $8^- (K = 8)$ band



8_2^-	Calc.	EXP.
E^* (keV)	1305	1295 ^a

(^a M. Forge *et al.*, Physical Review, under review)

Single-particle configurations:

~ Two-neutron excitations

$$\nu j15/2 \otimes \nu g9/2$$

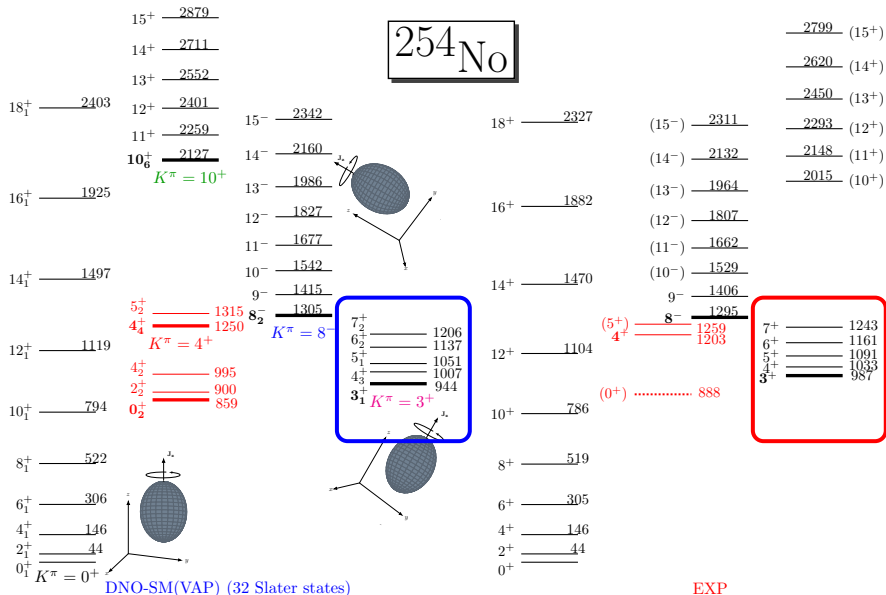
2_1^+ 44
 0_1^+ $K^\pi = 0^+$

DNO-SM(VAP) (32 Slater states)

2^+ 44
 0^+

EXP

Isomeric $3^+(K=3)$ band



Isomeric $3^+(K=3)$ band: Gallagher-Moszkowski partner $4^+(K=4)$

^{254}No	Calc.	EXP.
$E^*(3^+)$ (keV)	944	987 ^a
$E^*(4^+)$ (keV)	1250	1203 ^a
$\Delta E_{GM} = E_{\uparrow\downarrow} - E_{\uparrow\uparrow}$	306	216 ^a

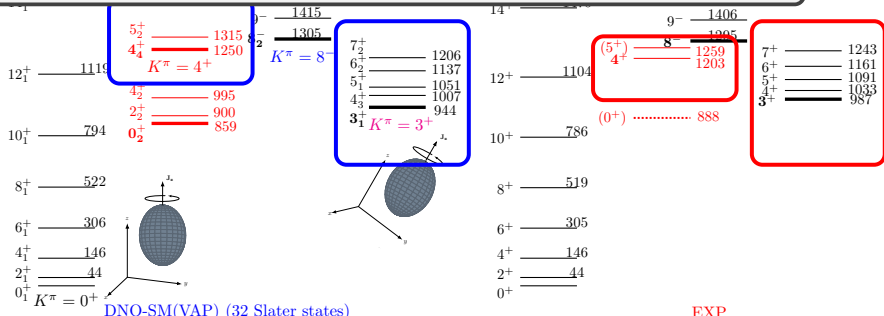
(^a M. Forge *et al.*, Physical Review, under review)

$$K = |\Omega_n \pm \Omega_p|$$

$K=3$ (spin-aligned)

lies lower than

$K=4$ (spin-anti-aligned)



Single-particle Occupations: $3^+(K=3)$, $4^+(K=4)$

Ground- and excited-states occupations

Proton orbits	$0h_{9/2}$	$0i_{13/2}$	$1f_{7/2}$	$1f_{5/2}$	$2p_{3/2}$	$2p_{1/2}$	
0_1^+	6.03	7.75	3.43	1.49	0.77	0.52	
0_2^+	7.08	7.91	3.23	0.89	0.69	0.21	
$3_1^+(K=3)$	6.47	7.98	3.34	1.15	0.72	0.34	
$4_4^+(K=4)$	6.50	7.83	3.41	1.18	0.72	0.36	
$8_2^-(K=8)$	6.48	7.90	3.36	1.19	0.70	0.37	
$10_6^+(K=10)$	6.55	7.03	3.48	1.56	0.79	0.58	
Neutron orbits	$0i_{11/2}$	$0j_{15/2}$	$1g_{9/2}$	$1g_{7/2}$	$2d_{5/2}$	$2d_{3/2}$	$3s_{1/2}$
0_1^+	7.30	9.91	5.43	1.00	1.09	0.84	0.43
0_2^+	7.36	9.95	5.45	0.96	1.05	0.80	0.42
$3_1^+(K=3)$	7.32	9.94	5.46	0.97	1.07	0.81	0.42
$4_4^+(K=4)$	7.34	9.79	5.48	1.03	1.11	0.81	0.44
$8_2^-(K=8)$	7.42	9.00	6.30	0.98	1.06	0.81	0.43
$10_6^+(K=10)$	7.23	8.89	5.72	1.40	1.34	0.97	0.45

- $3_1^+, 4_4^+$: similar structure
involving a $\pi h9/2$
recoupled with others orbitals

Branching Ratio: $3^+(K=3)$ band

15+ — 2879

14+ — 2711

13+ — 2552

^{254}No

— 2799 (15+)

— 2620 (14+)

— 2450 (13+)

— 2293 (12+)

— 2148 (11+)

— 2015 (10+)

$$\Delta E_{GM} = E_{\uparrow\downarrow} - E_{\uparrow\uparrow} \quad \text{Calc.} \quad \text{EXP.}$$

$$\Delta E_{GM} \text{ (keV)} \quad 306 \quad 216^a$$

(^a M. Forge *et al.*, Physical Review, under review)

$$K = |\Omega_n \pm \Omega_p|$$

$K = 3$ (spin-aligned)

lies lower

$K = 4$ (spin-anti-aligned)

14+ — 1497

10- — 1342

1470

(10-) — 1529

^{254}No

$$B(E2, 7_2^+ \rightarrow 5_1^+)$$

$$23971 \text{ e}^2\text{fm}^4$$

$$B(M1, 7_2^+ \rightarrow 6_2^+)$$

$$0.228 \mu_N^2$$

Branching Ratio

Calc.

EXP.^a

0.94

1.1(4)

(^a S. K. Tandel *et al.*, Phys. Rev. Lett. **97**, 082502 (2006))

1243
1161
1091
1033
987

DNO-SM(VAP) (32 Slater states)

EXP

Low-lying excited 0_2^+ state

15+ — 2879
14+ — 2711
13+ — 2552

^{254}No

— 2799 (15+)
— 2620 (14+)

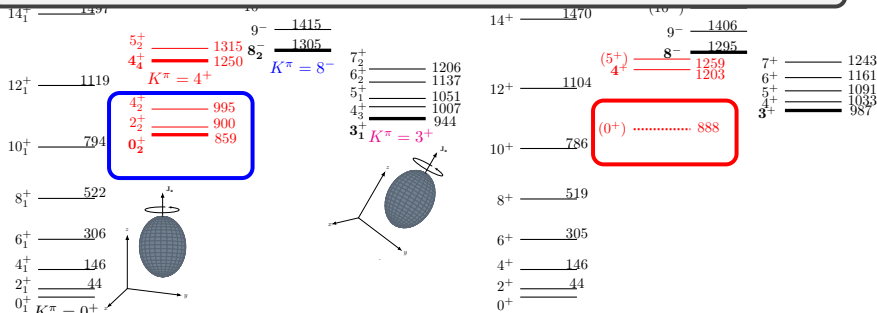
(13+)
(12+)
(11+)
(10+)

Structure:

Involving essentially proton excitations

0_2^+	Calc.	EXP.
E^* (keV)	859	888 ^a

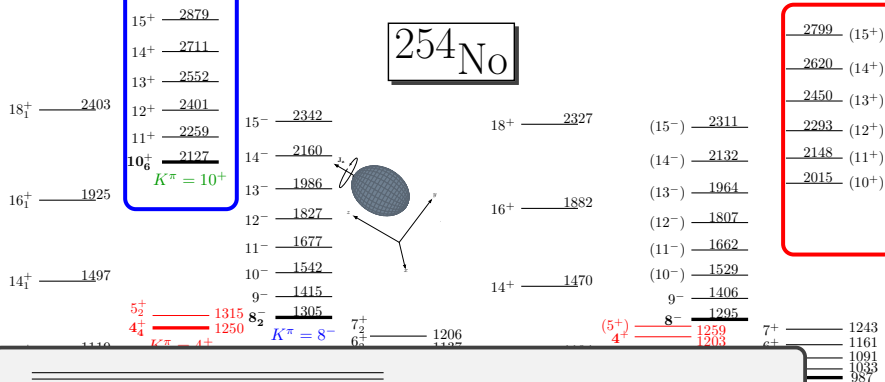
(^a M. Forge *et al.*, Physical Review, under review)



DNO-SM(VAP) (32 Slater states)

EXP

Isomeric $10^+(K=10)$ band



10^+

Calc.

EXP.

^a S. G. Wahid *et al.*,

E^* (keV)

2127

2015^a

Phys. Rev. C 111, 034320 (2025)

4_1^+ — 146
 2_1^+ — 44
 0_1^+ — 44
 $K^\pi = 0^+$

DNO-SM(VAP) (32 Slater states)

4^+ — 146
 2^+ — 44
 0^+ — 44

EXP

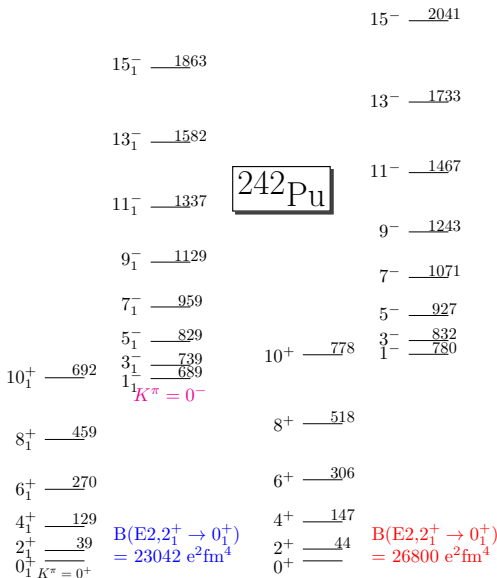
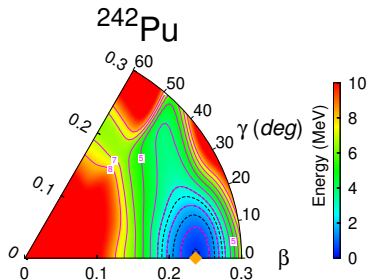
Dipole excitations in $^{242}_{94}\text{Pu}_{148}$

Known spectroscopy:

- Axially well-deformed nucleus
- Ground-state rotational band
- Several side bands:
 $1^- (K=0), 3^- (K=3), 7^-$

Ongoing calculations:

- Deformed Axial Minimum at $\beta = 0.24$
- VAP calculations for band-head structures



DNO-SM
(27 Slater states)

EXP

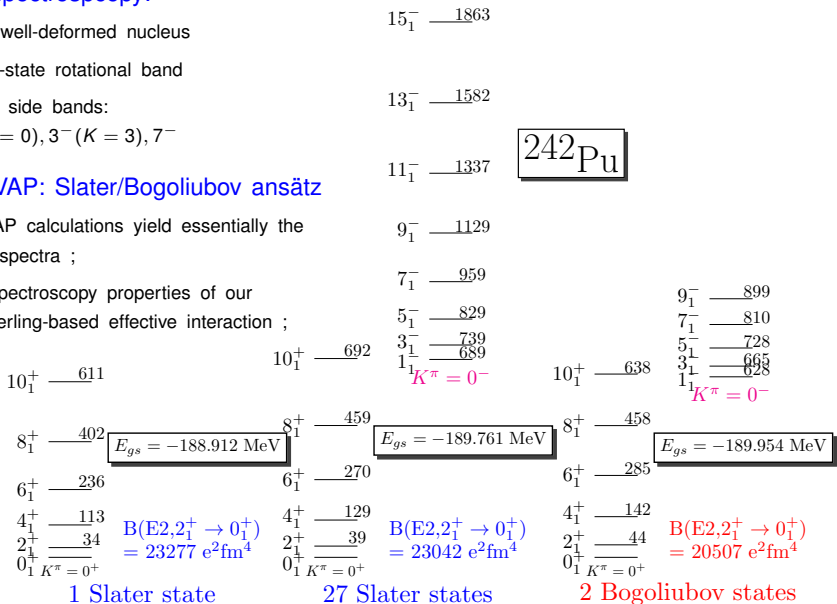
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Triaxial VAP: Slater/Bogoliubov ansatz

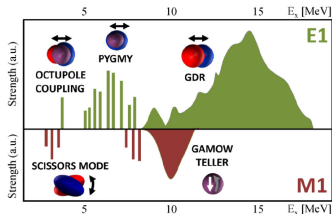
- Both VAP calculations yield essentially the same spectra ;
- Good spectroscopy properties of our Kuo-Herling-based effective interaction ;



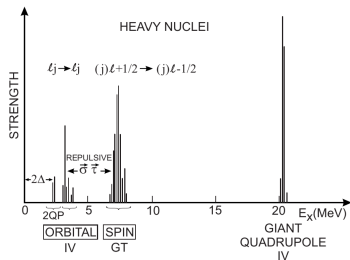
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◇ Strength function description of $M1$, $E1$:

- Scissors mode in deformed nuclei
- DNO-SM(VAP): capture correlations



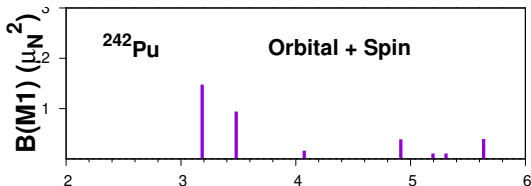
D. Budker *et al.*, Ann. Phys. **2022**, 534, 2100284.



K. Heyde *et al.*, Rev. Mod. Phys. **104**, 045801 (2021).

◇ Open questions:

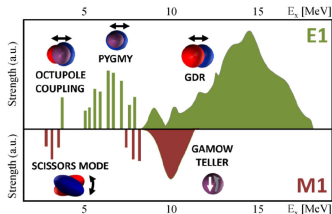
- Generate easily structure function for many final states
- E1 transitions forbidden in the natural valence space
→ add QSU3 higher orbitals



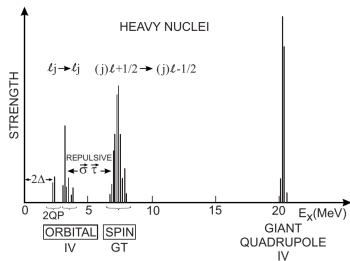
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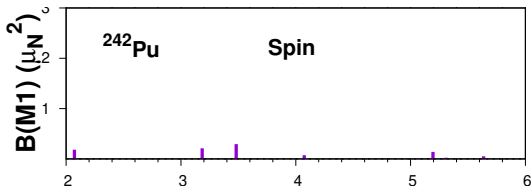
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◇ Open questions:

- Generate easily structure function for many final states
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→ add QSU3 higher orbitals



Spectroscopy in rare-earth region

◊ Few spectroscopy:

- Well-deformed nucleus
- Ground-state rotational band
- few negative parity states bands: 3^- , 4^- ...

◊ Ongoing calculations:

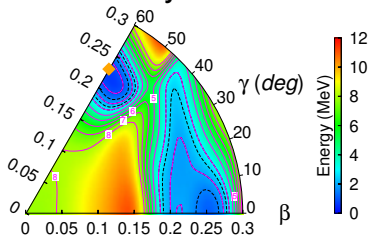
- realistic N3LO interaction for ^{132}Sn core and

$$\begin{array}{c} \pi \quad g_{7/2}^+ d_{5/2}^+ d_{3/2}^+ s_{1/2}^+ h_{11/2}^+ \\ \nu \quad h_{9/2}^- f_{7/2}^- f_{5/2}^- p_{3/2}^- p_{1/2}^- i_{13/2}^- \end{array} \quad \text{orbitals}$$

- Deformed Oblate minimum at $\beta = 0.23$

- VAP calculations for band-head structures

^{168}Dy



$$6_1^- \text{ --- } 1792$$

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$$4_1^- \text{ --- } 1527$$

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$$2_1^- \text{ --- } 1352$$

$$K^\pi = 2^-$$

^{168}Dy

$$6^- \text{ --- } 1378$$

$$5^- \text{ --- } 1246$$

$$4^- \text{ --- } 1141$$

$$3^- \text{ --- } 1055$$

$$2^- \text{ --- } 990$$

$$6_1^+ \text{ --- } 587$$

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$$2_1^+ \text{ --- } 86$$

$$0_1^+ \text{ --- } K^\pi = 0^+$$

DNO-SM(VAP)

$$6^+ \text{ --- } 516$$

$$4^+ \text{ --- } 248$$

$$2^+ \text{ --- } 75$$

$$0^+ \text{ --- }$$

EXP

Octupole excitations in $^{168}_{66}\text{Dy}_{102}$

♦ Few spectroscopy:

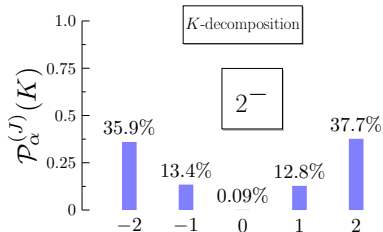
- Well-deformed nucleus
- Ground-state rotational band
- few negative parity states bands: 3^- , 4^- ...

♦ Ongoing calculations:

- realistic N3LO interaction for ^{132}Sn core and

$$\begin{array}{c} \pi \quad g_{7/2}^+ d_{5/2}^+ d_{3/2}^+ s_{1/2}^+ h_{11/2}^+ \\ \nu \quad h_{9/2}^- f_{7/2}^- f_{5/2}^- p_{3/2}^- p_{1/2}^- i_{13/2}^- \end{array} \quad \text{orbitals}$$

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EXP

Conclusions and perspectives

SUMMARY

- Non-Orthogonal Multi-Slater Determinants give an exact representation of shell-model wave functions
- Broeckhove-Deumens Theorem is numerically proved
- Pairing correlations are fully captured by the variation after projection where the rotational symmetry is consistently restored
- Collapse of collectivity at $N \sim Z$ line: Isospin Symmetric Island of Inversion
- First shell-model description of superheavy nuclei: $^{253,254,255}\text{Es}$, $^{249,251,253}\text{Cf}$, $^{253,254}\text{No}$, ^{256}Fm
- Complete reproduction of known spectroscopy of ^{254}No : yrast and excited isomeric structures

PERSPECTIVES

- Tackle larger valence spaces for shell-model studies
- Need of higher Quasi-SU3 orbitals for E1 excitations and intruders
- Neutrinoless double beta decay matrix elements at different levels of approximation:
 - Using shell-model Hamiltonians: Spectroscopy reproduced at the same time
 - Axial β , Triaxial (β, γ) , Variation-after-Projection (Slater/Bogoliubov), full shell-model diagonalization

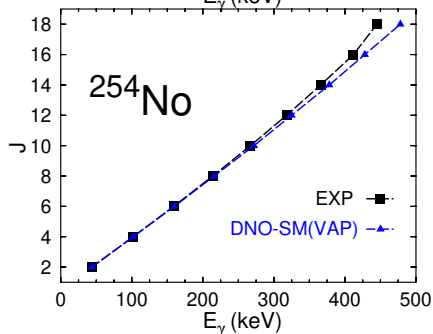
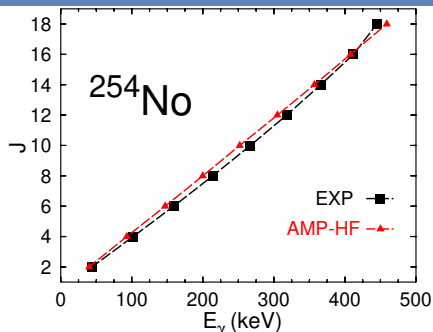
*THANK YOU FOR YOUR
ATTENTION!*

BACKUP

Impact of pairing correlations

◇ Why should it work ?

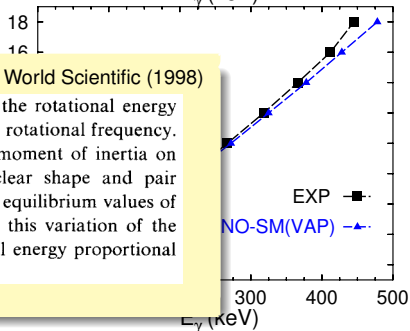
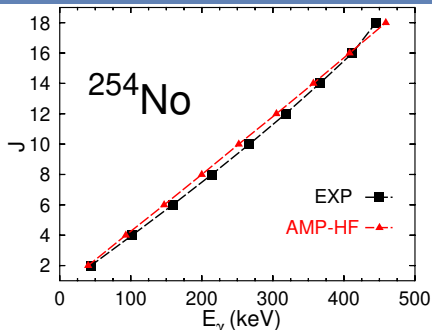
- AMP Projected Hartree-Fock:
~ Pure Rotor $J(J+1)$ law
- “Well-deformed” heavy/superheavy nuclei:
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- Variation After Projection better than Projected Hartree-Fock



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A. Bohr, B. Mottelson, Nuclear Structure, Vol II, p. 30, World Scientific (1998)

The deviations from the $I(I+1)$ dependence of the rotational energy express the variation of the moment of inertia with the rotational frequency. Such a variation arises from the dependence of the moment of inertia on the collective parameters that characterize the nuclear shape and pair correlations. In turn, this dependence implies that the equilibrium values of the parameters have a term proportional to $I(I+1)$; this variation of the equilibrium with I gives rise to a decrease in the total energy proportional to $I^2(I+1)^2$.

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- Hierarchy of nucleon-nucleon forces:
 $3N < 2N$

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