Shell-model : Recent advances from mid-mass to superheavy elements

Duy-Duc Dao, F. Nowacki

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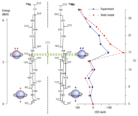
SM-CI approaches through the nuclear chart

Fundamental interactions and collectives excitations

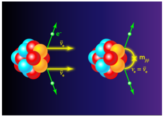
- Deformation Dipole/M1 resonances
- Superfluidity, Symmetries
- Isospin symmetry breaking

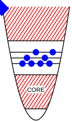


Weak processes

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

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

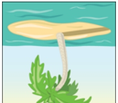





- define effective interaction
- $\mathcal{H}_{\text{eff}}\Psi_{\text{eff}} = E\Psi_{\text{eff}}$
- build and diagonalize energy matrix

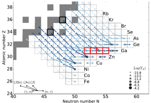
Nuclear structure far from stability

- New magic numbers
- Vanishing of shell closures



Astrophysics and nucleosynthesis

- rp process
- r process

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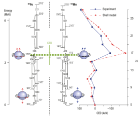
- Superfluidity, Symmetries
- Isospin symmetry breaking
- **Superformation, Superheavy nuclei**



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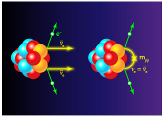

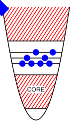

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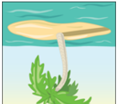

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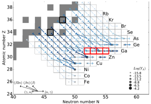


Diagonalization versus Variational Methods

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*-*sdg* space :

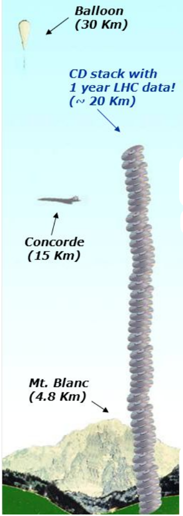
^{78}Ni **210,046,691,518**

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

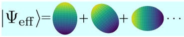
- m-scheme — ANTOINE code, BIGSTICK, KSHELL
- coupled scheme — NATHAN code

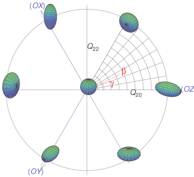


Variational Approximation

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

- **Mixing of shapes :**





- **Restoration of the rotational symmetry**

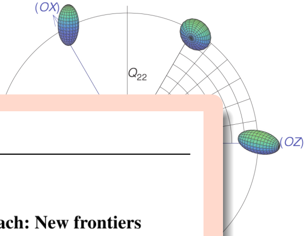
- **Degree of freedom**
  - Multipole: β, γ, Q_{30}, ...
  - Cranking: J_x, J_z
  - Pairing constraints
  - Variation-After-Projection

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

Discrete Non-Orthogonal Shell Model (DNO-SM)

◇ Generator coordinate method :

- Deformed Hartree-Fock Slater determinants
- Contribution of $q = (\beta, \gamma)$ in the correlated state J_α
- Rotational symmetry restoration



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

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

D. D. Dao and F. Nowacki

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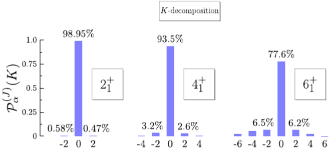
(Received 8 March 2022; accepted 6 May 2022; published 23 May 2022)

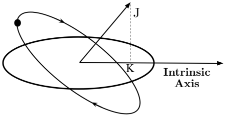
(D.D

◇ K

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

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





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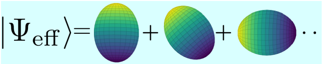
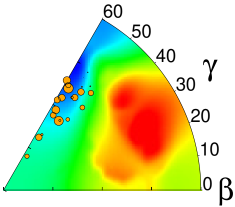
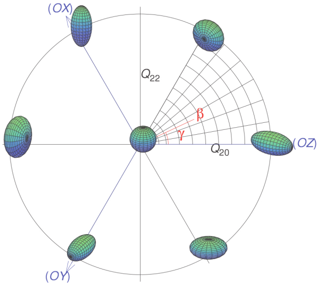


$$P_\alpha^{(J)}(q) = \sum_K |M_\alpha^{(J)}(q, K)|^2$$

(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
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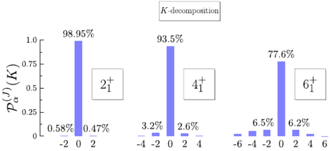

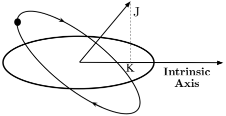

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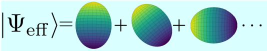
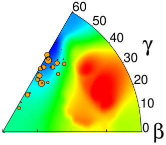




$$P_{\alpha}^{(J)}(q) = \sum_{K} |M_{\alpha}^{(J)}(q, K)|^2$$

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

◇ Problems :

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

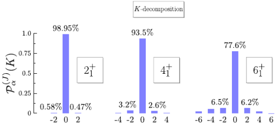
LNPS effective interaction

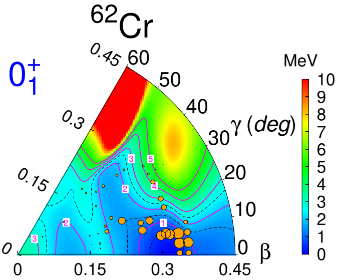
^{62}Cr	DNO-SM(β, γ)	SM
E(0_1^+) (MeV)	−212.426	−214.138
B(E2,$2_1^+ \to 0_1^+$) (e^2fm^4)	458	362

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

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

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





Variation After Projection = Incorporation of NpNh excitations

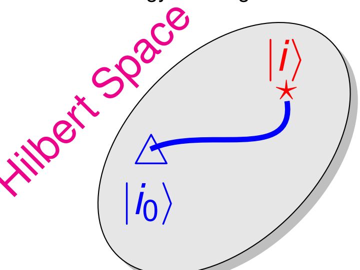
◇ Trial symmetry-projected Slater determinants :

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

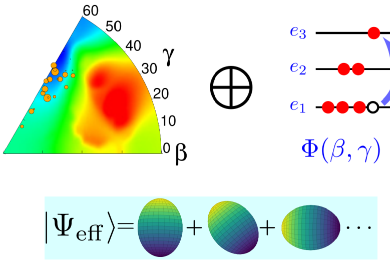
Double variation AFTER Angular Momentum Projection : Mixing coefficient Slater state

◇ DNO-SM(VAP)

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



◇ DNO-SM(PAV) : (β,γ) + NpNh



Variation After Projection = Incorporation of NpNh excitations

◇ Trial symmetry-projected Slater determinants :

$\langle \Psi^{JM} | \mathcal{H} ... | \Psi^{JM} \rangle$ ... $P^J_{MK} |\Phi(q)\rangle$

Do ... Slater state

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

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

arXiv :2507.09073

◇ DN... NpNh

- $q = 1, 2, 3, \ldots$
- $J_\alpha = 0_1, \ldots$
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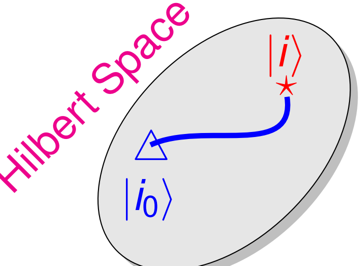
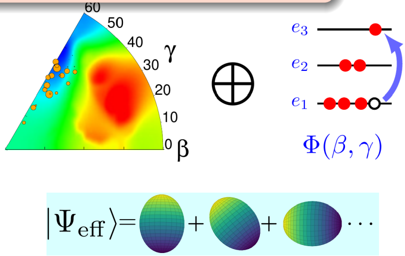
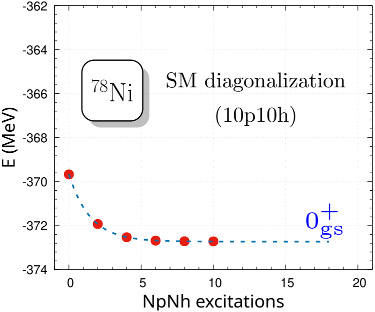




Coexistence in ^{78}Ni

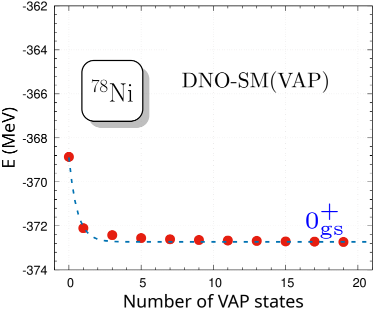


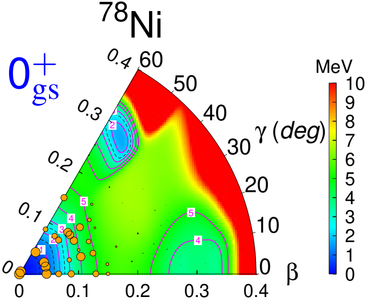
(D.D. Dao, F. Nowacki, in preparation)

PFSDG-U effective interaction

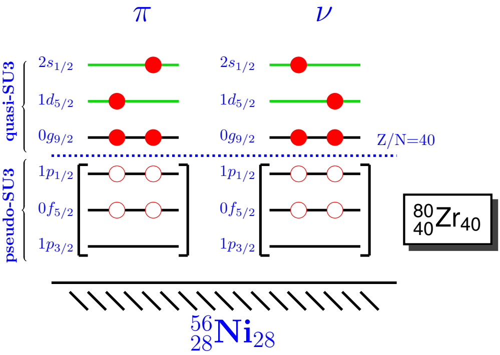
Ground State Energy in MeV

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





N=40 at N=Z



- p shell : ^{16}O spherical/doubly magic
  PRL 21 (1968) 39

ZBM1

- sd shell : ^{40}Ca spherical/doubly magic
  PLB 522 (2001) 240

ZBM2

- pf shell : ^{80}Zr deformed nucleus
  ...

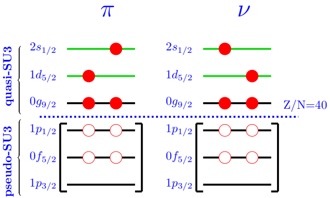
ZBM3

- Low-lying states in H.O. N=Z=8 : **CS** , 4p4h, 8p8h
- Low-lying states in H.O. N=Z=20 : **CS** , 4p4h,8p8h
- Low-lying states in H.O. N=Z=40 : 4p4h ? 8p8h ? 12p12h ?

Island of Inversion at the N=Z line

◇ Strongly deformed states 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



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

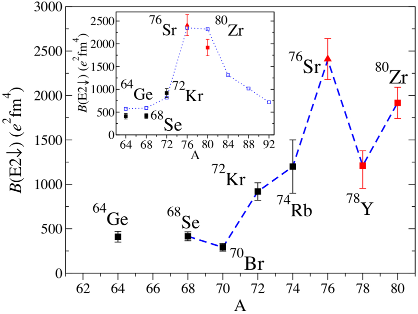


FIG. 3. Schematics of the $B(E2\downarrow)$ values for the $N = Z$ nuclei

- 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 (lnl) interaction
- SM + DNO-SM for most deformed cases

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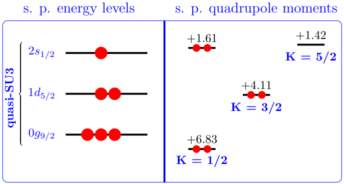

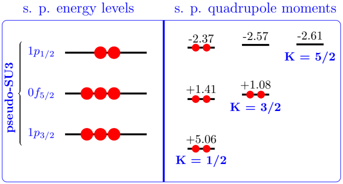

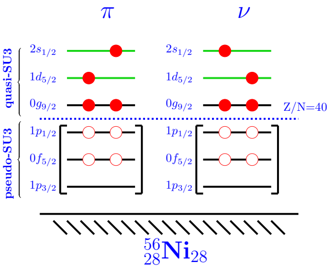

				B(E2)(e^2.fm^4)		
nucleus	Np-Nh*	ZRP	PHF	Exp.	DNO-SM*	SM
^{84}Mo	4p-4h	1104	1193	**1740^{+580}_{-430}**	1512	-
	8p-8h	1891	1732			
^{86}Mo	0p-0h	542	196	**707(71)**	893	731
	2p-2h	1030	871			
	4p-4h	1416	1179			
	6p-6h	1858	1655			

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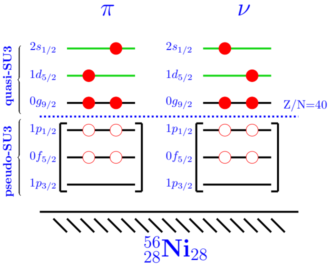

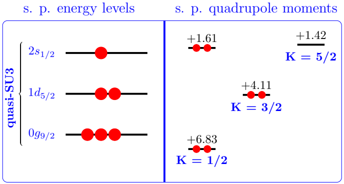

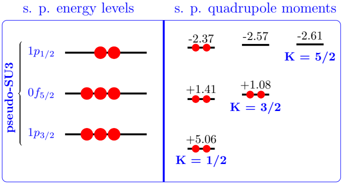

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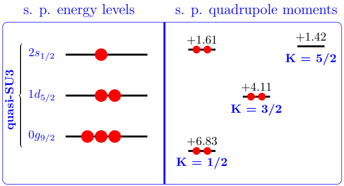

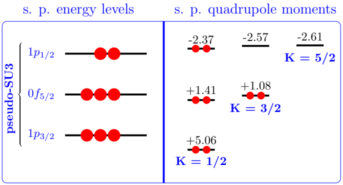

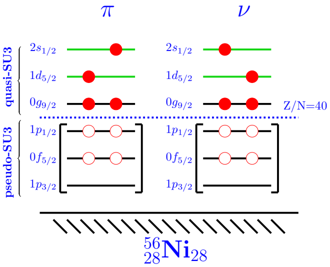

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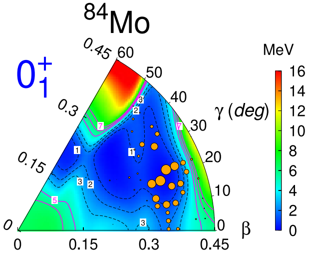
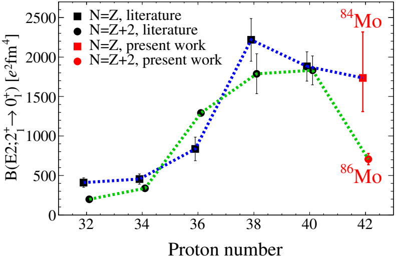
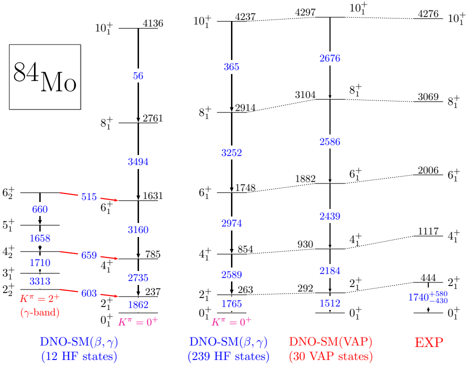


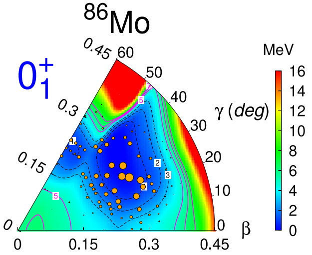


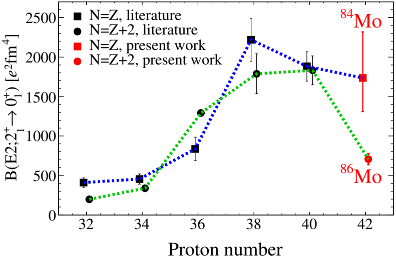


Island of Inversion at the N=Z line

◇ Strongly deformed states at $N = Z$

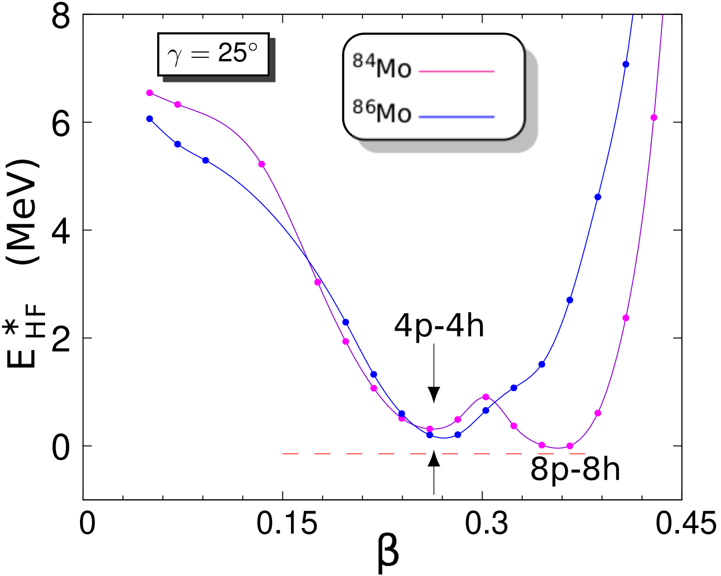
- Configuration mixing in ^{72}Kr
- Most deformed cases for ^{76}Sr, ^{80}Zr
- New spectroscopy for ^{84}Mo and ^{86}Mo
  NSCL/GRETINA Experiment



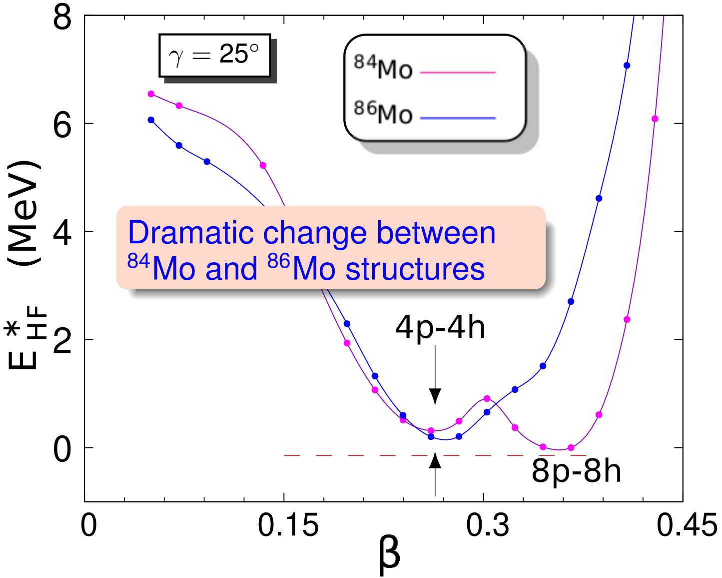


				B(E2)(e^2.fm^4)		
nucleus	Np-Nh*	ZRP	PHF	Exp.	DNO-SM*	SM
^{84}Mo	4p-4h 8p-8h	1104 1891	1193 1732	**1740$^{+580}_{-430}$**	1512	-
^{86}Mo	0p-0h 2p-2h 4p-4h 6p-6h	542 1030 1416 1858	196 871 1179 1655	**707(71)**	893	731

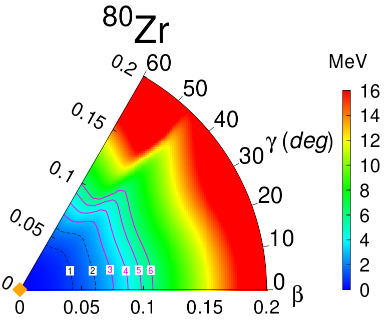
3N forces in light nuclei

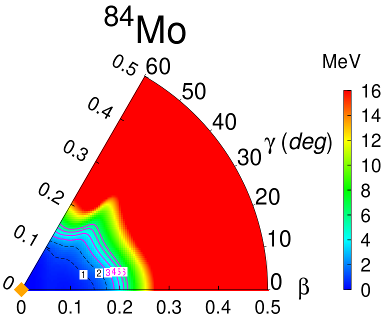


3N forces in light nuclei



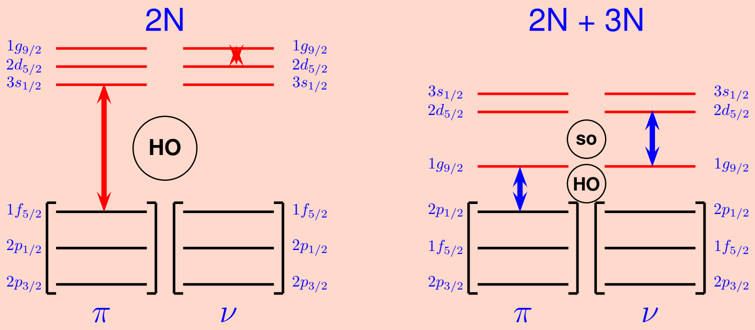
N3LO NN calculations





				B(E2)(e^2.fm^4)		
nucleus	NpNh*	ZRP	PHF	**Exp.**	DNO-SM	N3LO
^{80}Zr	4p-4h	587	637			
	8p-8h	1713	1509	**1910(180)**	2325	0.03
	12p-12h	2663	2396			
^{84}Mo	4p-4h	1104	1193	**1740^{+580}_{-430}**	1740	174
	8p-8h	1891	1732			

N3LO NN calculations



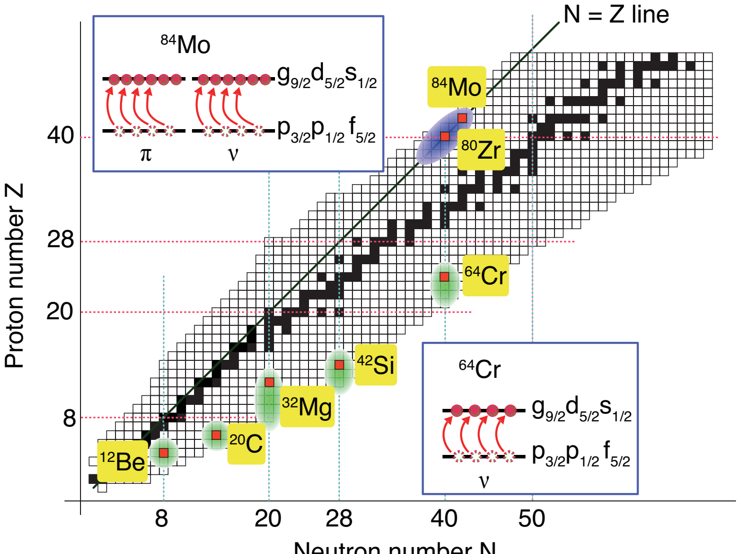
Three body forces and persistence of spin-orbit shell gaps in medium-mass nuclei : Towards the doubly magic ^{78}Ni,

K. Sieja, F. Nowacki

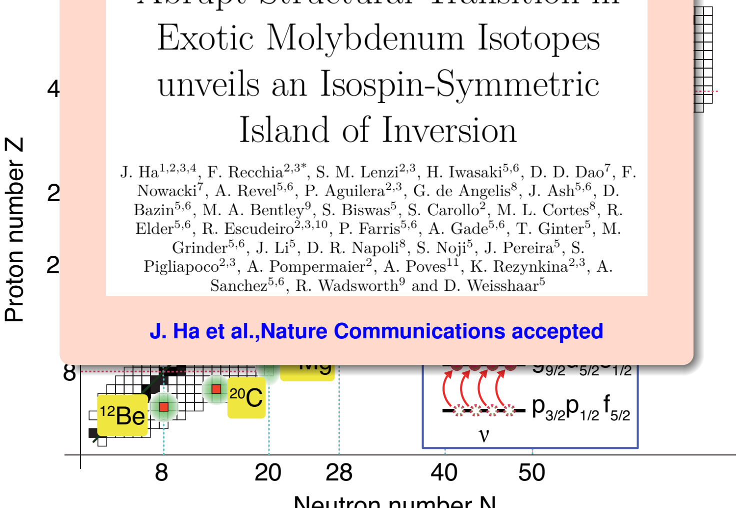
Phys. Rev. **C85**, 051301(R) (2012)

^{80}Zr	4p-4h	587	637			
	8p-8h	1713	1509	**1910(180)**	2325	0.03
	12p-12h	2663	2396			
^{84}Mo	4p-4h	1104	1193	**1740^{+580}_{-430}**	1740	174
	8p-8h	1891	1732			

Isospin Symmetric Island of Inversion



Isospin Symmetric Island of Inversion

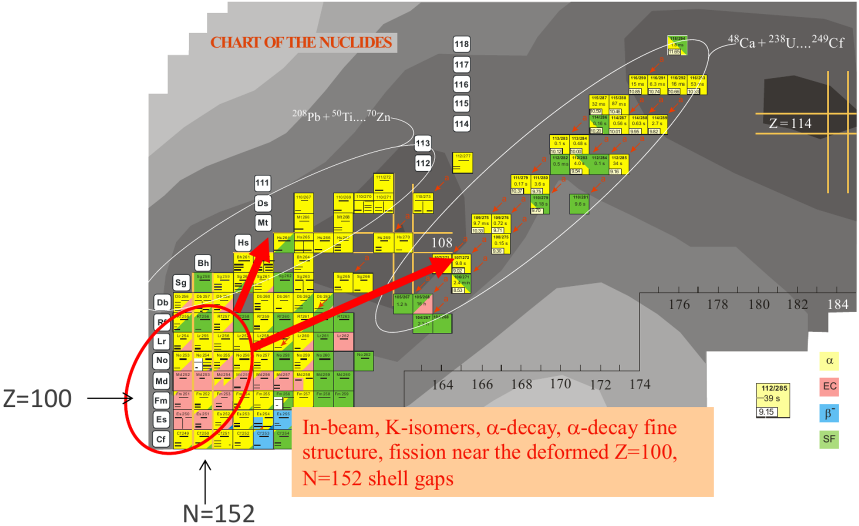


Abrupt Structural Transition in Exotic Molybdenum Isotopes unveils an Isospin-Symmetric Island of Inversion

J. Ha[1,2,3,4], F. Recchia[2,3*], S. M. Lenzi[2,3], H. Iwasaki[5,6], D. D. Dao[7], F. Nowacki[7], A. Revel[5,6], P. Aguilera[2,3], G. de Angelis[8], J. Ash[5,6], D. Bazin[5,6], M. A. Bentley[9], S. Biswas[5], S. Carollo[2], M. L. Cortes[8], R. Elder[5,6], R. Escudeiro[2,3,10], P. Farris[5,6], A. Gade[5,6], T. Ginter[5], M. Grinder[5,6], J. Li[5], D. R. Napoli[8], S. Noji[5], J. Pereira[5], S. Pigliapoco[2,3], A. Pompermaier[2], A. Poves[11], K. Rezynkina[2,3], A. Sanchez[5,6], R. Wadsworth[9] and D. Weisshaar[5]

J. Ha et al.,Nature Communications accepted

Landscape of superheavy nuclei



(From Seweryniak (SSNET 2024))

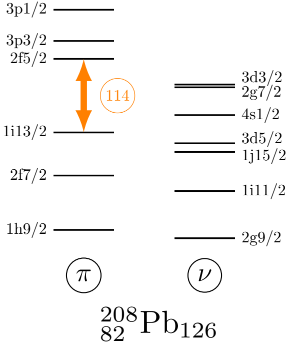
Applications to superheavy nuclei

Kuo-Herling interaction :

- $^{208}_{82}Pb_{126}$ 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*

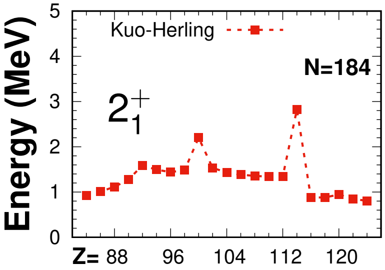


Calculations : NATHAN & CARINA codes

◇ Diagonalization within the seniority scheme along the chains of $N = 126$ and $N = 184$

◇ Variation After Projection calculations : ^{253,254,255}Es, ^{249,251,253}Cf, ^{253,254}No, ^{256}Fm

◇ Comparison of spectra and electromagnetic moments



Yrast systematics : odd-even $^{251}_{98}Cf_{153}$

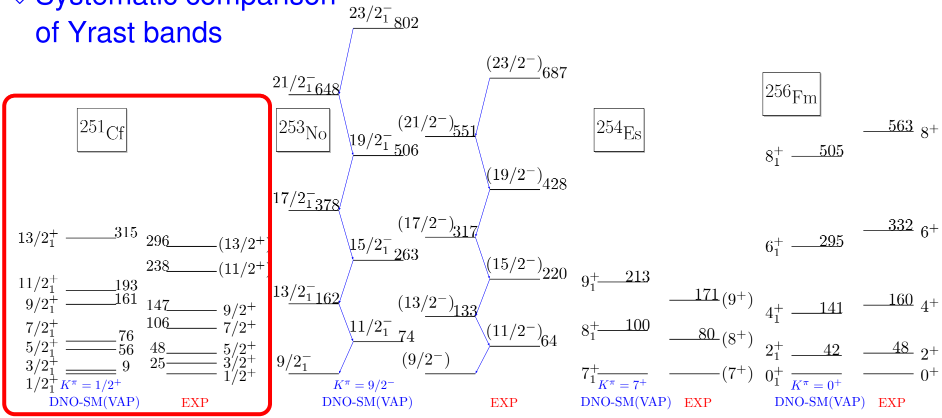
First complete description of low-lying spectroscopy in ^{254}No

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

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

◇ Systematic comparison of Yrast bands

arXiv :2409.08210



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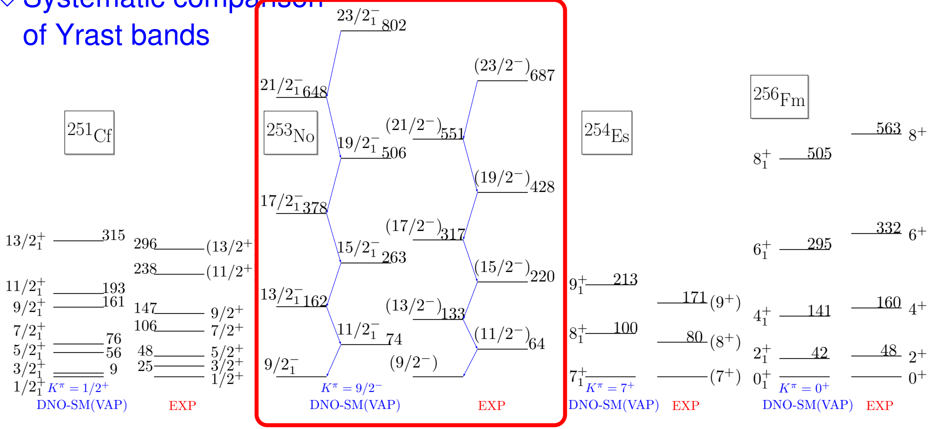
- ◇ Systematic comparison of Yrast bands



Yrast systematics : odd-odd $^{254}_{99}Es_{155}$

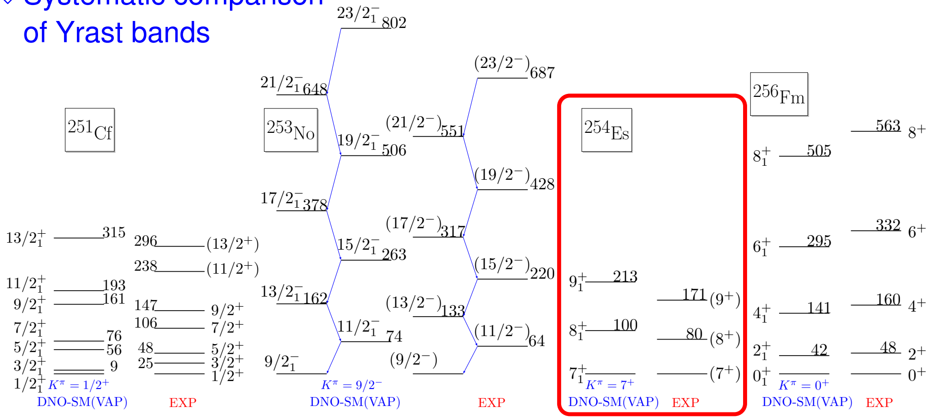
First complete description of low-lying spectroscopy in ^{254}No

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

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

arXiv :2409.08210

◇ Systematic comparison of Yrast bands



Yrast systematics : even-even $^{256}_{100}Fm_{156}$

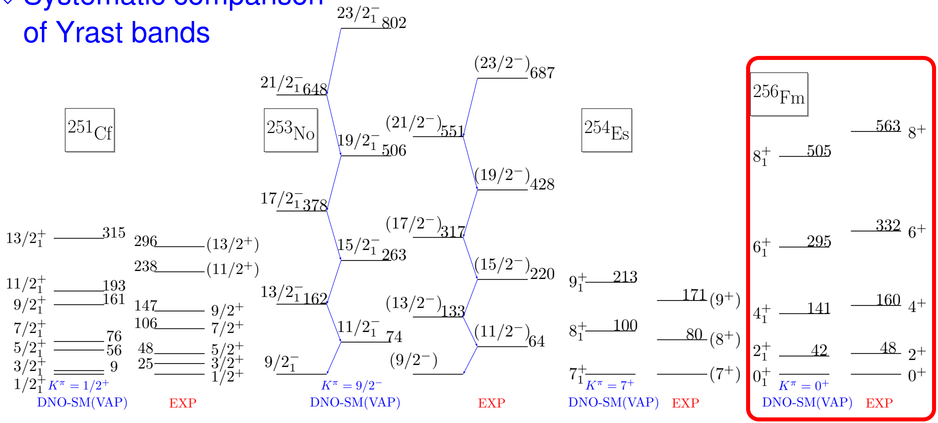
First complete description of low-lying spectroscopy in ^{254}No

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

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

arXiv :2409.08210

◇ Systematic comparison of Yrast bands



Applications to superheavy nuclei : Electromagnetic moments

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

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

[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^{π}_{gs}		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	-

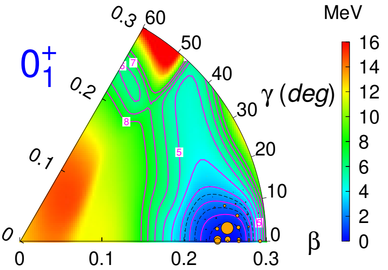
Applications to superheavy nuclei : $^{254}_{102}\mathrm{No}_{152}$

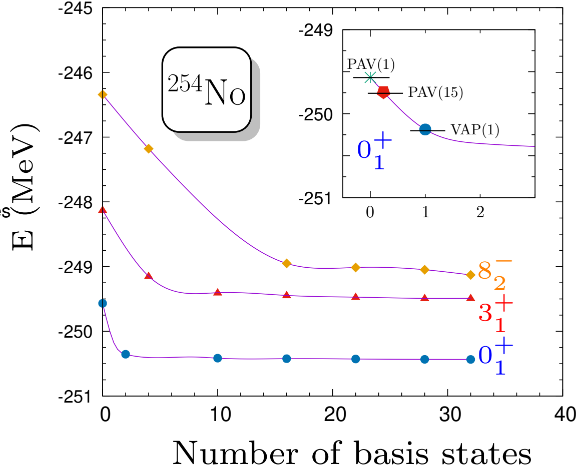
Known spectrospcopy :

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

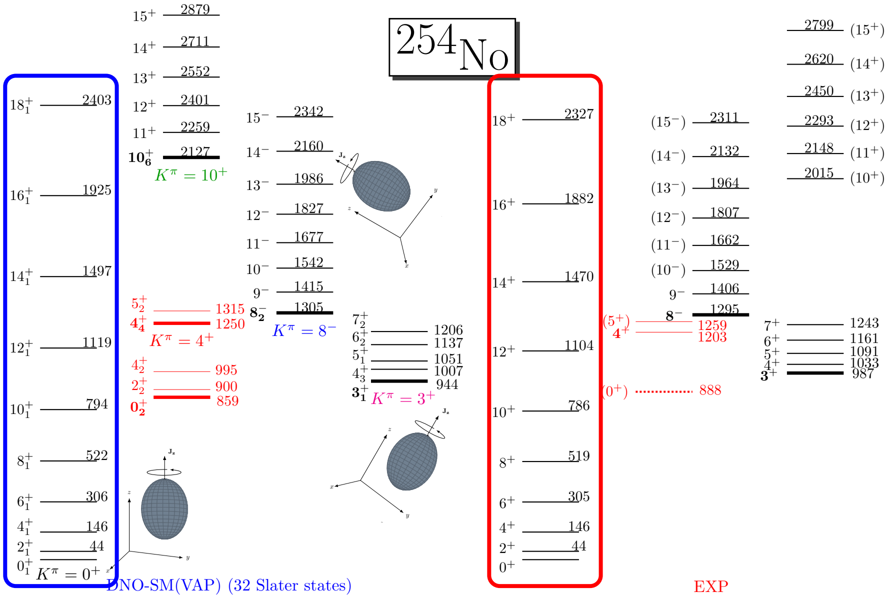
Calculations :

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

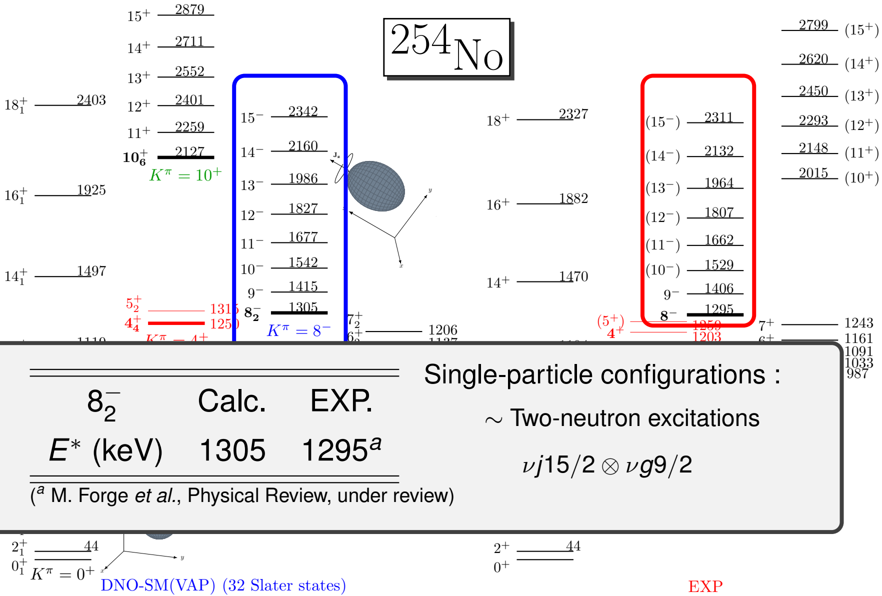




Reproduction of spectra : Yrast rotational band



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



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

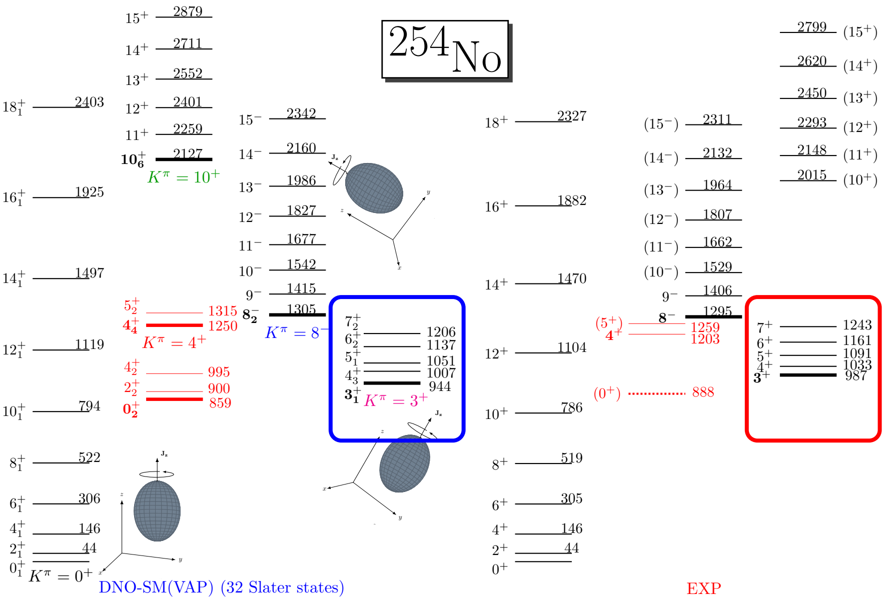
([a] M. Forge *et al.*, Physical Review, under review)

Single-particle configurations :

$\sim$ Two-neutron excitations

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

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



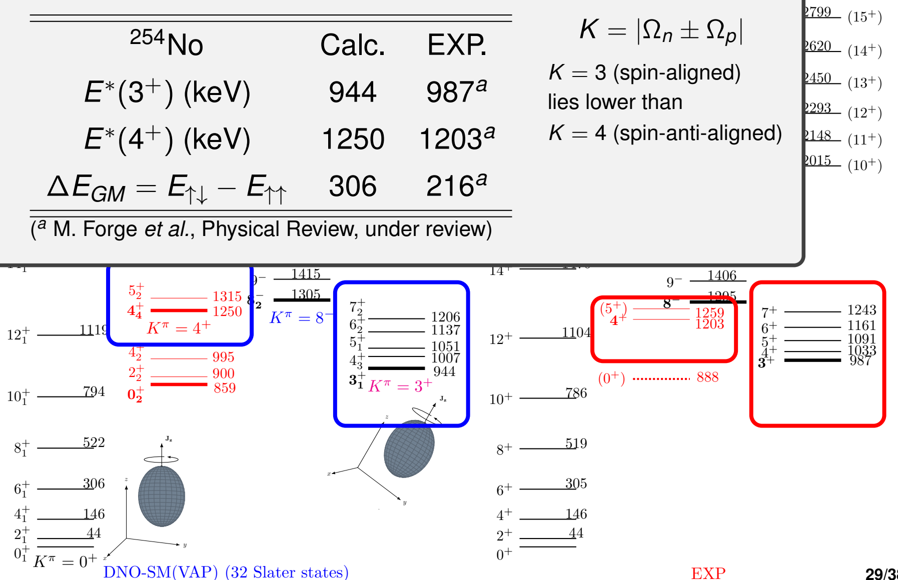
Isomeric $3^+(K=3)$ band : Gallagher-Moszkowski partner $4^+(K=4)$

^{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)



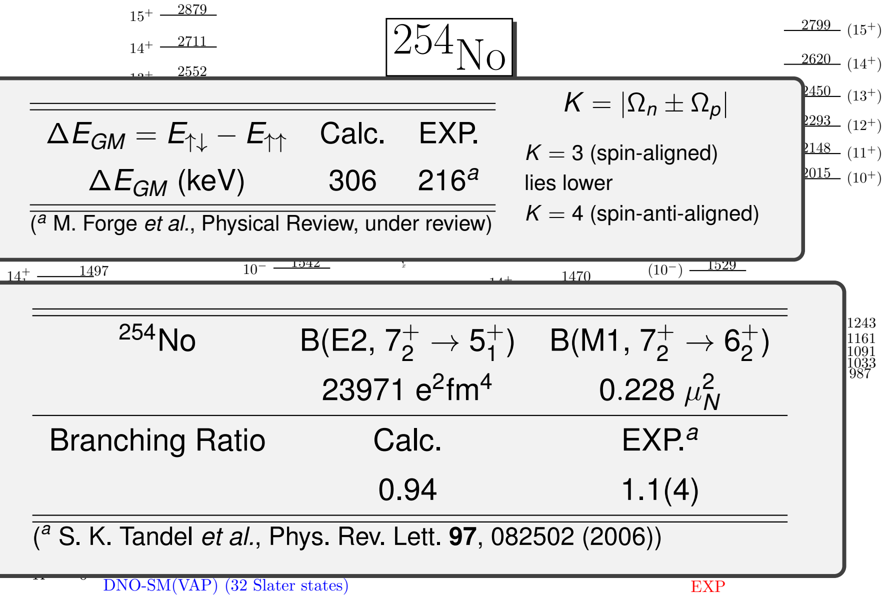
Single-particle Occupations : $3^+(K=3)$, $4^+(K=4)$

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

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

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



$\Delta E_{GM} = E_{\uparrow\downarrow} - E_{\uparrow\uparrow}$	Calc.	EXP.
ΔE_{GM} (keV)	306	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)

^{254}No	$B(E2, 7_2^+ \to 5_1^+)$	$B(M1, 7_2^+ \to 6_2^+)$
	23971 e^2fm^4	0.228 μ_N^2
Branching Ratio	Calc.	EXP.[a]
	0.94	1.1(4)

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

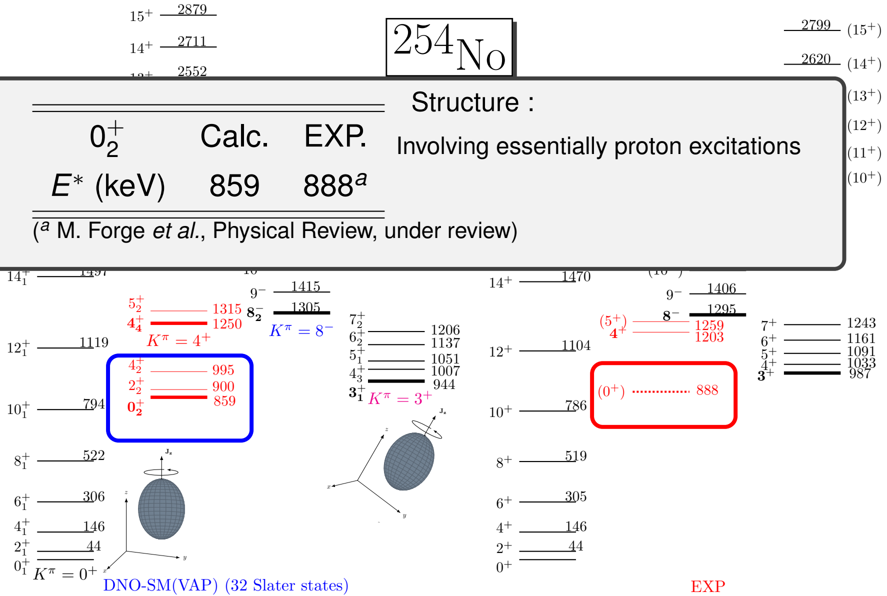
Low-lying excited 0_2^+ state

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

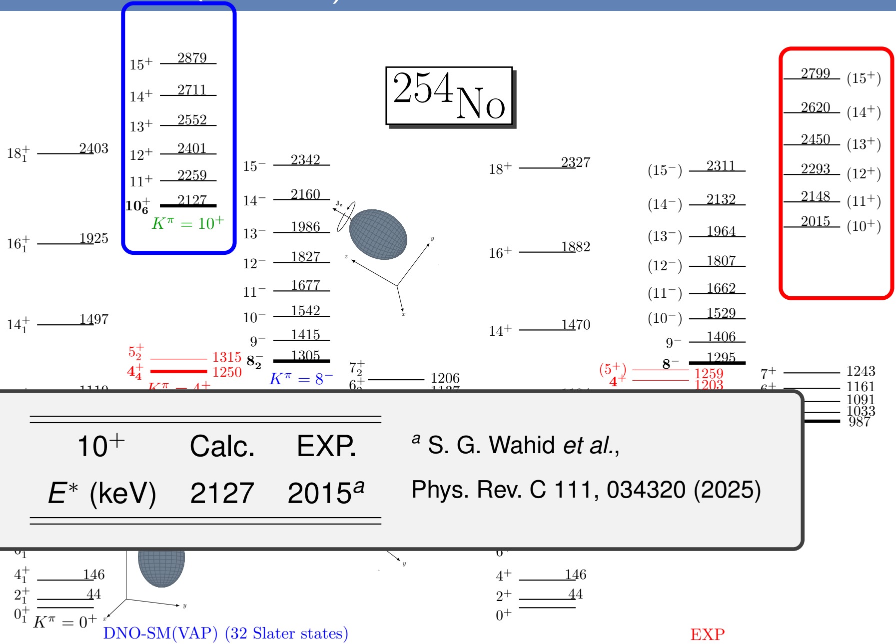
([a] M. Forge *et al.*, Physical Review, under review)

Structure :

Involving essentially proton excitations



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



10^+	Calc.	EXP.
E^* (keV)	2127	2015[a]

[a] S. G. Wahid *et al.*, Phys. Rev. C 111, 034320 (2025)

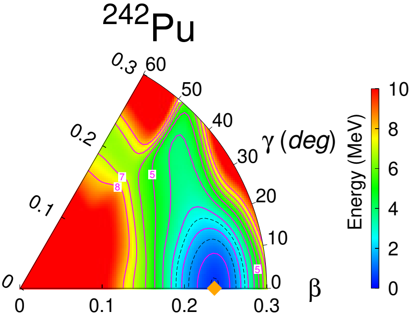
Dipole excitations in $^{242}_{94}\mathrm{Pu}_{148}$

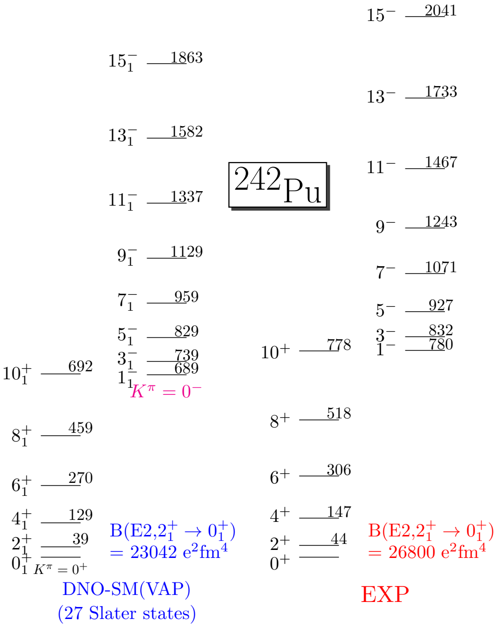
Known spectrospcopy :

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

Calculations :

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

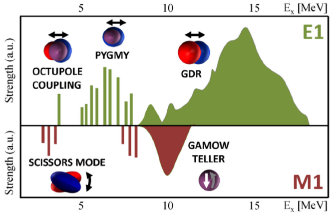




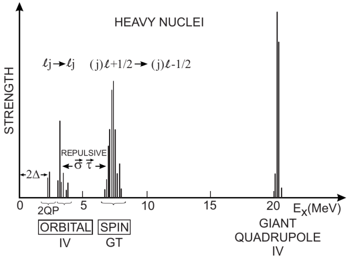
Dipole excitations in $^{242}_{94}Pu_{148}$

◇ Strength function description of *M*1, *E*1 :

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



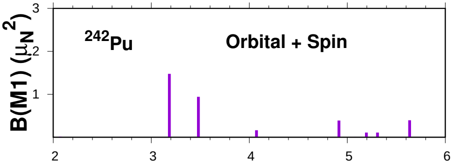
D. Budker *et al.*, Ann. Phys. **2022**, 534, 2100284.



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

◇ Open problems :

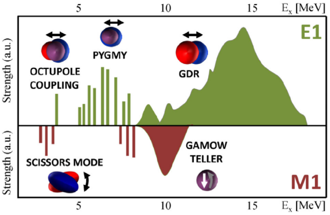
- Generate easily structure function for many final states
- E1 transitions forbidden in the natural valence space
  ⟶ add QSU3 higher orbitals



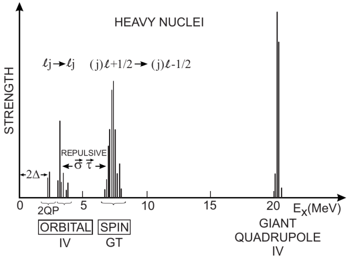
Dipole excitations in $^{242}_{94}\mathrm{Pu}_{148}$

◇ 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 :

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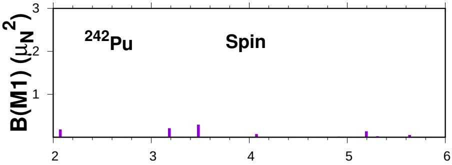
  $\longrightarrow$ add QSU3 higher orbitals



Summary

- Non-Orthogonal Multi-Slater Determinants give an exact representation of shell-model wave functions
- Pairing correlations are fully captured by the variation after projection where the rotational symmetry is consistently restored
- Isospin symmetric Island of Inversion around A$\sim$ 80
- First shell-model description of superheavy nuclei : ^{253,254,255}Es, ^{249,251,253}Cf, ^{253,254}No, ^{256}Fm
- Complete reproduction of known spectroscopy of ^{254}No : yrast and excited isomeric structures
- Ongoing study of dipole excitations in ^{242}Pu

Summary

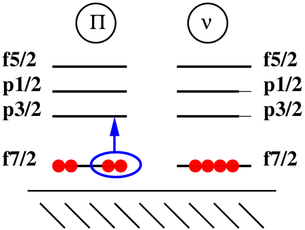
Special thanks to :

- G. Martinez-Pinedo, A. Poves, S. Lenzi
- A. Gade, O. Sorlin, A. Obertelli

Discrete Non-Orthogonal Shell Model (DNO-SM)

- Broeckhove-Deumens Theorem : Z. Phys. A**292**, 243 (1979)

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



$$\psi = c_1\phi_1 + c_2\phi_2 + \cdots + c_i\phi_i + \ldots$$

IMPLICATIONS :

- Non-Orthogonal Slater Determinants spans the full shell-model space
- The number of Slater Determinants is FINITE
- "Labels" for eigenstates : $|\alpha, J^\pi M, TT_z\rangle$
  - symmetries : $(J, \pi, \ldots)$
  - intrinsic label : α related to the dynamics of the Hamiltonian

- VARIATIONAL PROJECTED SLATER DETERMINANT SOLVES THE SHELL-MODEL DIAGONALIZATION PROBLEM

Variation After Projection : DNO-SM(VAP)

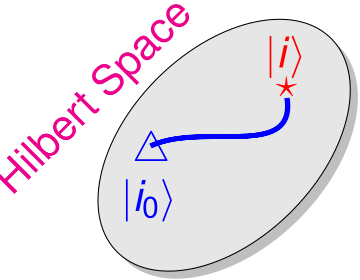
◇ Trial symmetry-projected Slater determinants :

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

Double variation AFTER Angular Momentum Projection : Mixing coefficient Slater state

◇ DNO-SM(VAP)

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



◇ Energy Minimization :

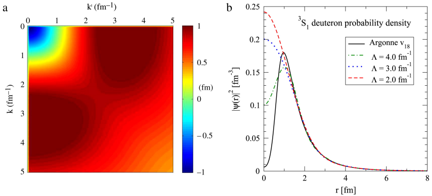
$$|\Phi\rangle = e^{\sum_{ij} Z_{ij} c_i^\dagger c_j}|\Phi_0\rangle$$

$$\frac{\partial E_\alpha^{(J)}}{\partial Z}, \; |\Phi\rangle = |\Phi_0\rangle + \eta\frac{\partial E_\alpha^{(J)}}{\partial Z}$$

$$(\mathcal{H}^{(J)} - E_\alpha^{(J)}\mathcal{N}^{(J)})f_\alpha^{(J)} = 0, \; \{E_\alpha^{(J)}, |\Psi_\alpha^{JM}\rangle\}$$

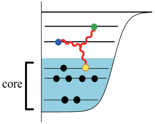
Monopole-corrected effective interactions

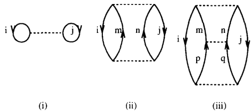
△ V-low k derived from NN interactions



(S.K. Bogner et al., Prog. Part. Nucl. Phys. **65**, 1 (2010) 94-147)

△ Valence-space MBPT renormalization



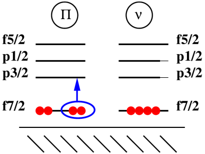


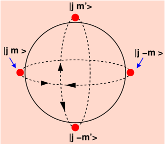
(H.-W. Hammer *et al.* RMP **85**, 197 (2013)) (M. Hjorth-Jensen *et al.* Phys. Rep. **261** (1995) 125-270)

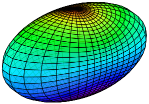
△ Multipole decomposition

$$H = H_{monopole} + H_{multipole}$$

(M. Dufour, A. P. Zuker, Phys. Rev. C **54**, 1641 (1996))







$H_{monopole}$: *spherical mean-field*

☞responsible for the global saturation properties and for the evolution of the spherical single particle levels.

$H_{multipole}$: *correlator*

☞ pairing, quadrupole, octupole...

3N forces in light nuclei

PRL **105,** 032501 (2010) PHYSICAL REVIEW LETTERS week ending 16 JULY 2010

Three-Body Forces and the Limit of Oxygen Isotopes

Takaharu Otsuka,[1,2,3] Toshio Suzuki,[4] Jason D. Holt,[5] Achim Schwenk,[5] and Yoshinori Akaishi[6]

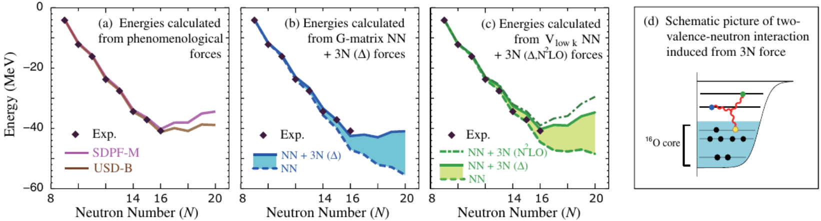


FIG. 4 (color online). Ground-state energies of oxygen isotopes measured from ^{16}O, including experimental values of the bound 16–24 O. Energies obtained from (a) phenomenological forces SDPF-M [13] and USD-B [14], (b) a G matrix and including FM $3N$ forces due to Δ excitations, and (c) from low-momentum interactions $V_{\text{low }k}$ and including chiral EFT $3N$ interactions at N^{2}LO as well as only due to Δ excitations [25]. The changes due to $3N$ forces based on Δ excitations are highlighted by the shaded areas. (d) Schematic illustration of a two-valence-neutron interaction generated by $3N$ forces with a nucleon in the ^{16}O core.

3N forces in light nuclei

PRL **109,** 032502 (2012) PHYSICAL REVIEW LETTERS week ending 20 JULY 2012

Evolution of Shell Structure in Neutron-Rich Calcium Isotopes

G. Hagen,[1,2] M. Hjorth-Jensen,[3,4] G. R. Jansen,[3] R. Machleidt,[5] and T. Papenbrock[1,2]
[1]*Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
[2]*Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA*
[3]*Department of Physics and Center of Mathematics for Applications, University of Oslo, N-0316 Oslo, Norway*
[4]*National Superconducting Cyclotron Laboratory and Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA*
[5]*Department of Physics, University of Idaho, Moscow, Idaho 83844, USA*
(Received 16 April 2012; published 17 July 2012)

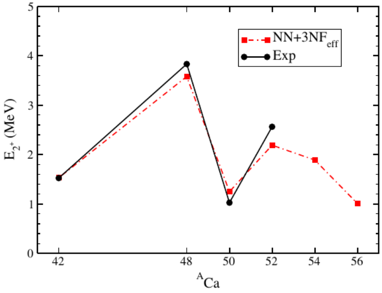


FIG. 2 (color online). (Excitation energies of $J^\pi = 2^+$ states in the isotopes ^{42,48,50,52,54,56}Ca (experiment: black circles,

3N forces in light nuclei

PHYSICAL REVIEW C **100**, 034324 (2019)

Contribution of chiral three-body forces to the monopole component of the effective shell-model Hamiltonian

Y. Z. Ma,[1] L. Coraggio,[2] L. De Angelis,[2] T. Fukui,[2] A. Gargano,[2] N. Itaco,[2,3] and F. R. Xu[1]

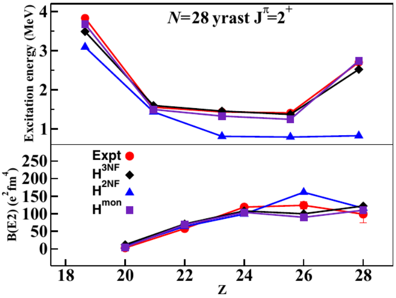


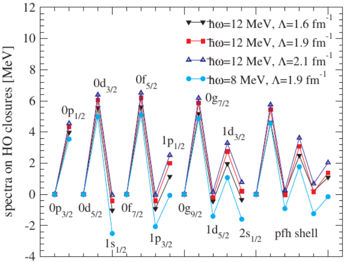
FIG. 22. Experimental and calculated excitation energies of the yrast $J^\pi = 2^+$ states and $B(E2; 2_1^+ \to 0_1^+)$ transition rates for the $N = 28$ isotones. See text for details.

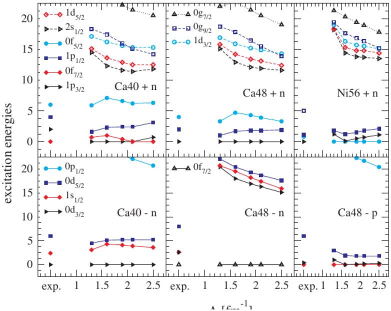
Shell closures and 2N forces only

PHYSICAL REVIEW C **74**, 061302(R) (2006)

Shell-model phenomenology of low-momentum interactions

Achim Schwenk[1,*] and Andrés P. Zuker[2,†]
[1]Nuclear Theory Center, Indiana University, 2401 Milo B. Sampson Lane, Bloomington, Indiana 47408, USA
[2]Institut de Recherches Subatomiques, IN2P3-CNRS, Université Louis Pasteur, F-67037 Strasbourg, France
(Received 14 January 2005; revised manuscript received 20 September 2006; published 12 December 2006)





- no Spin-orbite shell closures in ^{12}C, ^{22}O, ^{48}Ca, ^{56}Ni
- too strong H. O. shell closures ^{16}O, ^{40}Ca, ... and ^{80}Zr !!!

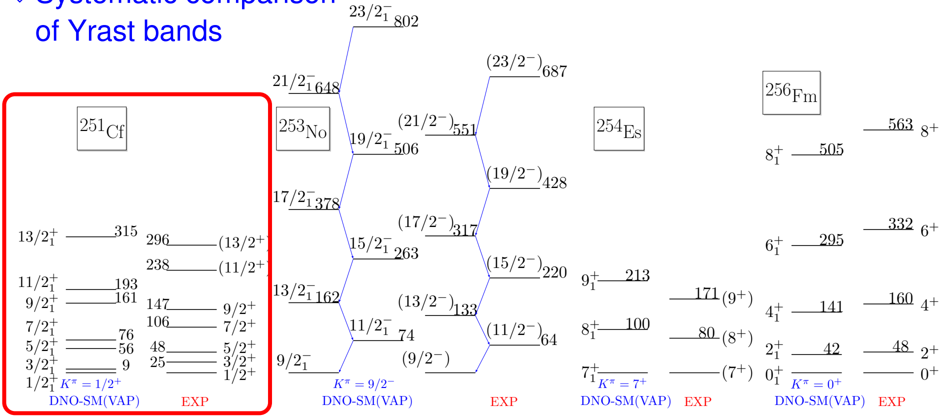
Yrast systematics : odd-even $^{251}_{98}Cf_{153}$

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

Duy Duc Dao[1] and Frédéric Nowacki[1]
[1] *Université de Strasbourg, CNRS, IPHC UMR7178, 23 rue du Loess, F-67000 Strasbourg, France*

arXiv :2409.08210

◇ Systematic comparison of Yrast bands



Yrast systematics : odd-even $^{253}_{102}No_{151}$

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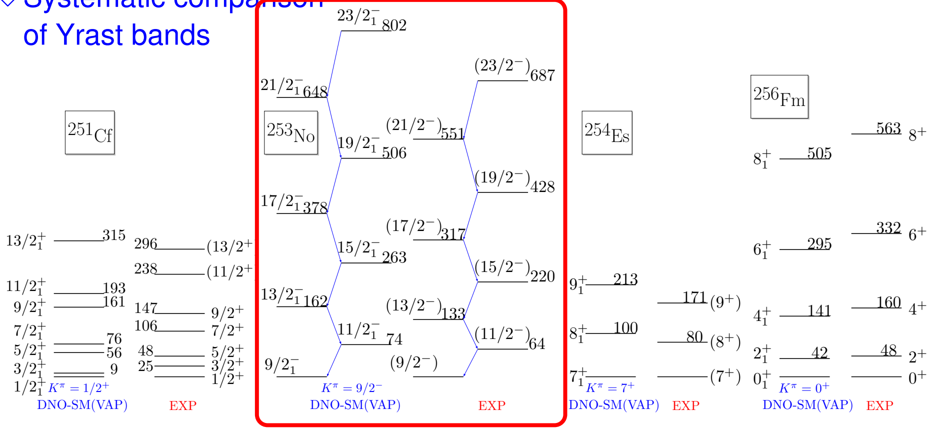

Yrast systematics : odd-odd $^{254}_{99}Es_{155}$

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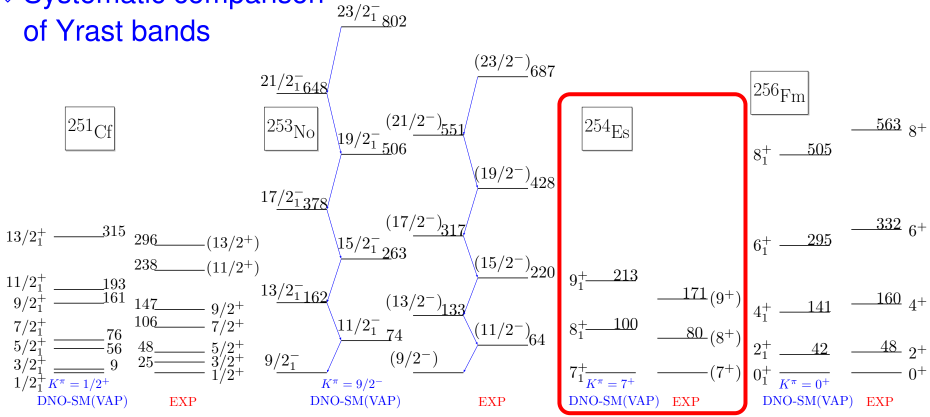

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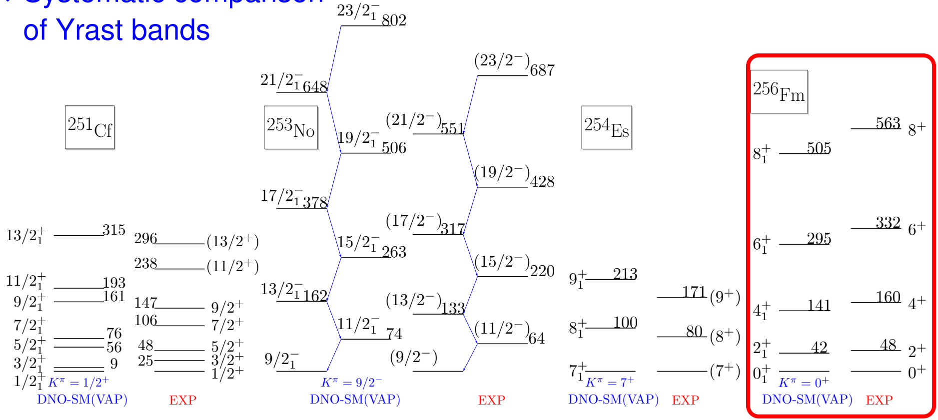

Applications to superheavy nuclei : Electromagnetic moments

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Duy Duc Dao[1] and Frédéric Nowacki[1]
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arXiv :2409.08210

◇ Comparison of magnetic and quadrupole moments

Effective charges : e_p = 1.72, e_n = 0.75

	J^{π}_{gs}	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	-

Applications to superheavy nuclei : Electromagnetic moments

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Applications to superheavy nuclei : Electromagnetic moments

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arXiv :2409.08210

◇ Comparison of magnetic and quadrupole moments

Effective charges : e_p = 1.72, e_n = 0.75

^{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.

Single-particle Occupations : $8^{-}(K = 8)$

Isomeric structures :

- 8^{-}_{2} : two-neutron coupling $\nu j15/2 \otimes \nu g9/2$

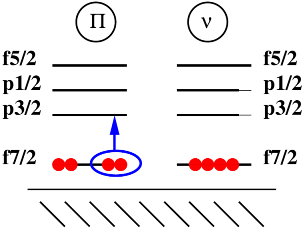
Ground- and excited-states occupations

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

Discrete Non-Orthogonal Shell Model (DNO-SM)

- Broeckhove-Deumens Theorem : Z. Phys. A**292**, 243 (1979)

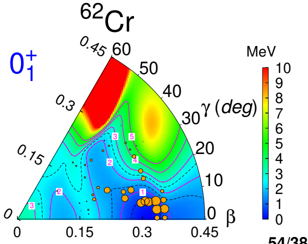
  Given a separable Hilbert space $\mathscr{H}$ spanned by a continuous family of states $\Gamma = \{\psi(\alpha) | \alpha \in \mathbb{R}\}$, there exists a countable subset $\Gamma_0 = \{\phi(\alpha_i) | i \in \mathbb{N}\} \subset \Gamma$ with the property $\mathscr{H} = \overline{\text{span}\Gamma_0}$,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



$$\psi = c_1\phi_1 + c_2\phi_2 + \cdots + c_i\phi_i + \ldots$$

IMPLICATIONS :

- Non-Orthogonal Slater Determinants spans the full shell-model space
- The number of Slater Determinants is FINITE
- Heuristic technique to select triaxial (β, γ) configurations



Isomeric single-particle configurations

Isomeric structures :

- 8_2^- : two-neutron coupling $\nu j15/2 \otimes \nu g9/2$
- $3_1^+, 4_4^+$: involving a $\pi h9/2$

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
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$8_2^-(K=8)$	7.42	9.00	6.30	0.98	1.06	0.81	0.43
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Monopole-corrected effective interactions

Multipole Universality :

△ **Multipole decomposition**

$$H = H_{monopole} + H_{multipole}$$

F. Nowacki et al., Prog. Part. Nucl. Phys. **120**, 103866 (2021)

Table 2
Dominant terms of several effective interactions for the *sd*-shell in MeV (see text). To the left particle–particle channels, isovector, isoscalar and quadrupole pairing, to the right particle–hole channels, quadrupole, hexadecapole, spin, and spin–isospin.

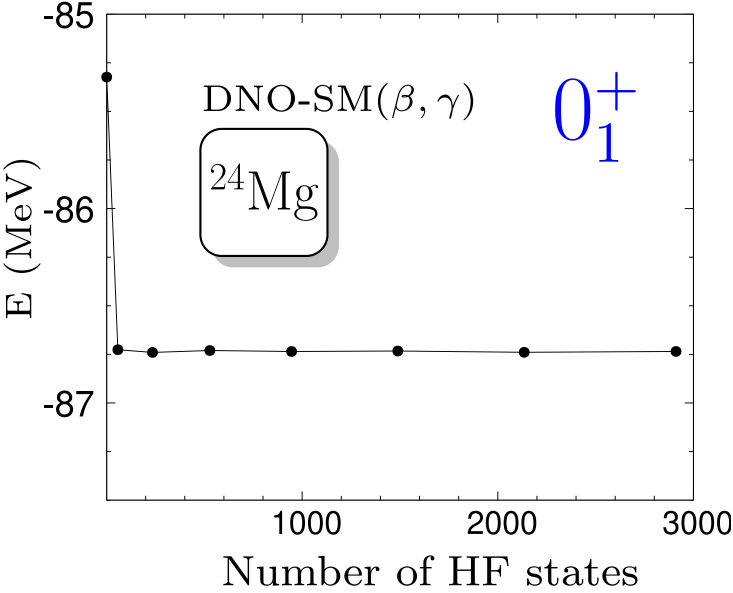
	pp(JT)			ph(λτ)			
	10	01	21	20	40	10	11
KB	−5.83	−4.96	−3.21	−3.53	−1.38	+1.61	+3.00
USD−A	−5.62	−5.50	−3.17	−3.24	−1.60	+1.56	+2.99
CCEI	−6.79	−4.68	−2.93	−3.40	−1.39	+1.21	+2.83
NN+NNN−MBPT	−6.40	−4.36	−2.91	−3.28	−1.23	+1.10	+2.43
NN−MBPT	−6.06	−4.38	−2.92	−3.35	−1.31	+1.03	+2.49

Pairing Components

Quadrupole

Table 3
Strengths of the coherent multipole components of different interactions for the *pf*-shell.

Interaction	particle-particle		particle-hole		
	JT = 01	JT = 10	λτ = 20	λτ = 0	λτ = 1
KB3	−4.75	−4.46	−2.79	−1.39	+2.46
FPD6	−5.06	−5.08	−3.11	−1.67	+3.17
GOGNY	−4.07	−5.74	−3.23	−1.77	+2.46
GXPF1	−4.18	−5.07	−2.92	−1.39	+2.47
BONNC	−4.20	−5.60	−3.33	−1.29	+2.70



DNO-SM(β, γ)
^{24}Mg
0^+_1
-85
-86
-87
E (MeV)
1000
2000
3000
Number of HF states

$J_i^\pi \rightarrow$	J_f^π	$B(E2)$ ($e^2.fm^4$)	$B(M1)$ (μ_N^2)
$2_1^+ \rightarrow$	0_1^+	28666	-
$4_1^+ \rightarrow$	2_1^+	41021	-
$0_2^+ \rightarrow$	2_1^+	98.236	-
$2_2^+ \rightarrow$	0_2^+	25327	-
	4_1^+	60.738	-
	2_1^+	25.227	3.980×10^{-6}
$3_1^+ \rightarrow$	2_2^+	2.5959×10^{-2}	8.020×10^{-6}
	4_1^+	2.7359×10^{-4}	2.957×10^{-7}
	2_1^+	9.6147×10^{-4}	6.050×10^{-6}
$4_2^+ \rightarrow$	2_2^+	36147	-
	3_1^+	5.4204×10^{-1}	4.200×10^{-7}
	4_1^+	23.783	8.360×10^{-6}
	2_1^+	18.569	-
$4_3^+ \rightarrow$	3_1^+	45803	1.3852×10^{-1}
	6_1^+	6.3712×10^{-4}	-
	4_1^+	6.5482×10^{-3}	3.634×10^{-5}
	2_1^+	8.2100×10^{-6}	-
$4_4^+ \rightarrow$	3_1^+	1.1354×10^{3}	1.977×10^{-3}
	4_3^+	9.6847×10^{2}	1.737×10^{-2}
	2_2^+	4.438×10^{-4}	-
	2_1^+	1.398×10^{-4}	-

Pairing correlations in ^{254}No

^{48}Cr	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 :

- AMP Projected Hartree-Fock :
  ∼ Pure Rotor $J(J+1)$ law
- "Well-deformed" heavy/superheavy nuclei :
  Impact of pairing is PERTURBATIVE
- Variation After Projection :
  ∼ Fully capturing pairing
  (Slater Determinants preserving Particle Numbers)