

Collectivity above ^{78}Ni and ^{132}Sn cores

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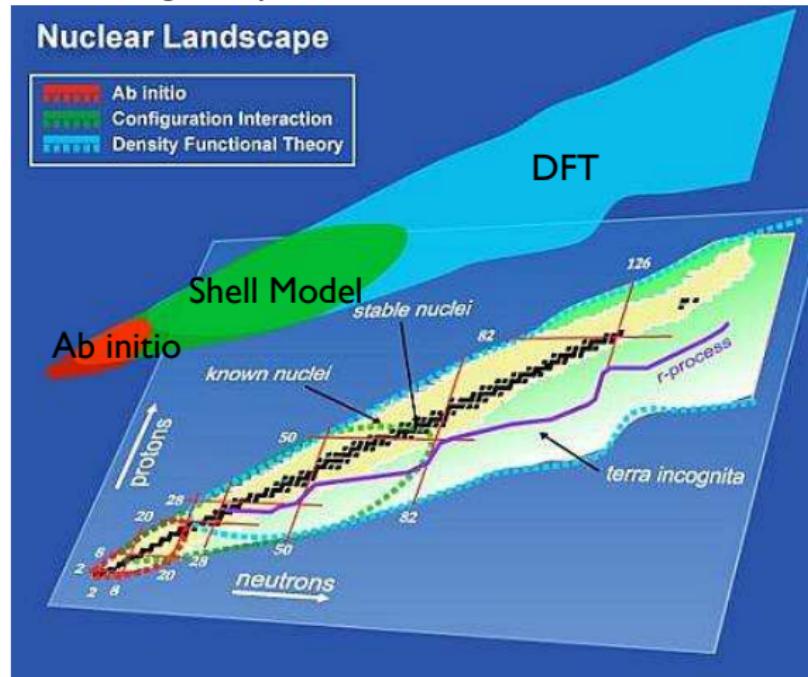
Warszawa, 19.01.2017

Plan

- Generalities about modern shell model approach
- Collectivity above ^{78}Ni core
- Collectivity above ^{132}Sn core
- Radiative strength from shell model

Nuclear many-body problem

The number of nucleons in nuclei is too large for an exact solution of A-body Schrödinger equation. Still, it is much too small for statistical methods.



- Nuclear Shell Model (SM), known as well as Configuration Interaction (CI)

- Density Functional Theory (DFT):

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \iff \mathcal{E}_{EDF}[\rho]$$

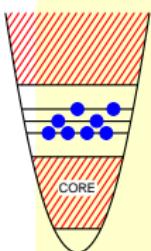
$$\rho_{ij} = \langle \phi | a_j^\dagger a_i^\dagger | \phi \rangle \iff |\phi\rangle = \prod a_i^\dagger |-\rangle.$$

- Macroscopic-microscopic models

Shell model approach

Calculations Ab Initio

- Realistic NN interactions
- Diagonalization in $N\hbar\omega$ h.o.space



- define valence space
- $H_{\text{eff}} \Psi_{\text{eff}} = E \Psi_{\text{eff}}$
- \rightsquigarrow INTERACTIONS
- build and diagonalize Hamiltonian matrix
- \rightsquigarrow CODES

Weak processes:

- β decays
- $\beta\beta$ decays

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

■[ASTROPHYSICS](#)

■[PARTICLE PHYSICS](#)

Collective excitations:

- deformation, superdeformation
- superfluidity
- symmetries

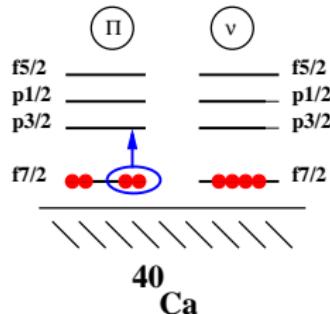
Shell evolution far from stability:

- Shell quenching
- New magic numbers

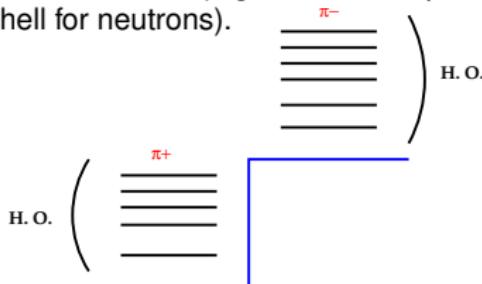
■[ASTROPHYSICS](#)

Model spaces

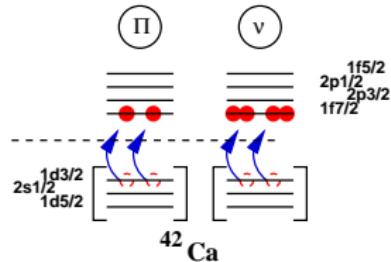
- Classical $0\hbar\omega$ model spaces (e.g. sd -shell, pf -shell) are successful for the description of a low lying states of nuclei, their transition rates and weak-decays.



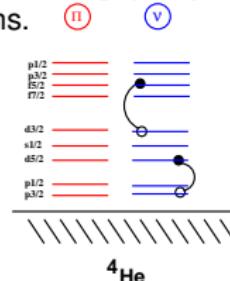
- Neutron rich nuclei require different active proton and neutron shells (e.g. sd -shell for protons, pf -shell for neutrons).



- Deformed nuclei and deformed bands in spherical nuclei are due to many-particle many-hole excitations across the gaps. At least $2\hbar\omega$ spaces are necessary e.g. sd - pf for both neutrons and protons).



- In simple shell-model nuclei, certain observables require going beyond $0\hbar\omega$ model space, e.g. parity changing transitions.



Shell Model: giant computations

- Problem dimension in the m-scheme:

$$D \sim \left(\begin{array}{c} d_\pi \\ p \end{array} \right) \cdot \left(\begin{array}{c} d_\nu \\ n \end{array} \right)$$

In the pf -shell ($1f_{7/2}, 2p_{3/2}, 1f_{5/2}, 2p_{1/2}$):

^{48}Cr 1,963,461

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

- Current diagonalization limit in m-scheme
 10^{10}

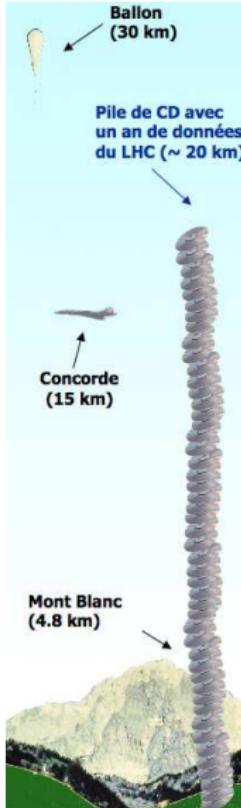
- The largest SM diagonalization up to date has been achieved by the Strasbourg group (using very modest computing resources):

Phys. Rev. C82 (2010) 054301, ibidem 064304

- m scheme CODE ANTOINE
- coupled scheme CODE NATHAN

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

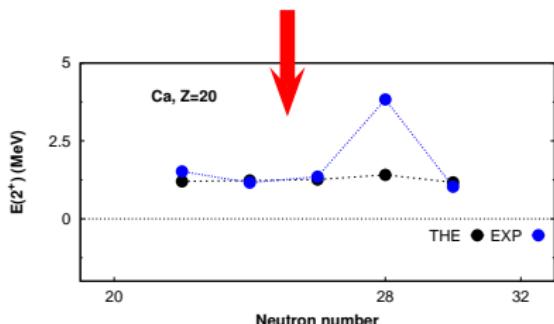
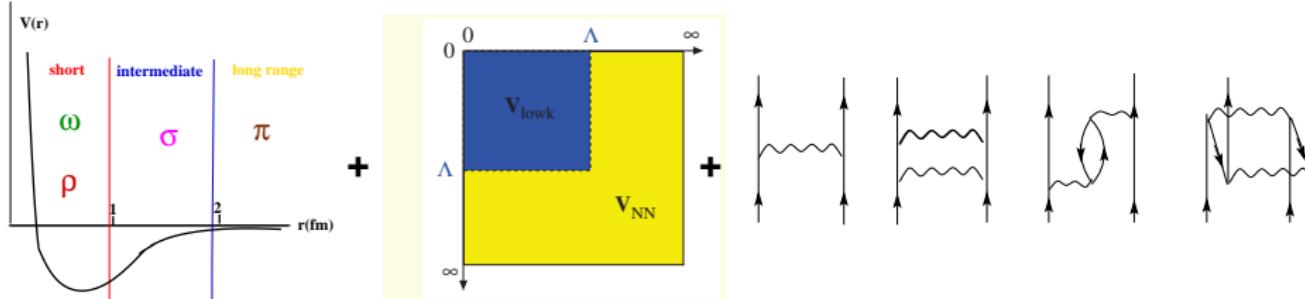
ANTOINE website



Largest SM matrices we treat contain $\sim 10^{14}$ non-zero matrix elements. They can not be stored on a hard drive. It would take 100,000 DVDs to store one matrix!

Shell gaps in nuclei & realistic 2-body interactions

M. Hjorth-Jensen et al., Phys. Rep. 42, 37 (1994) & M. Hjorth-Jensen website

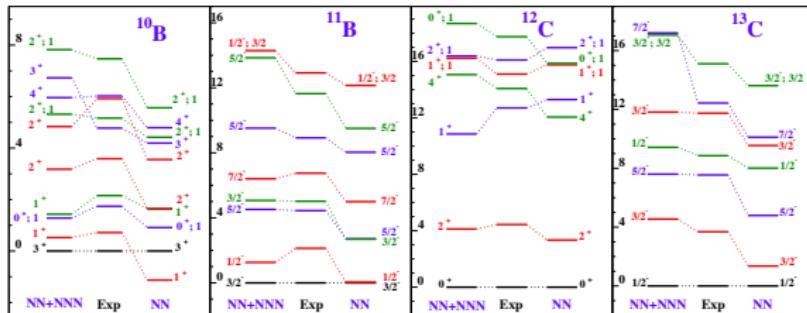
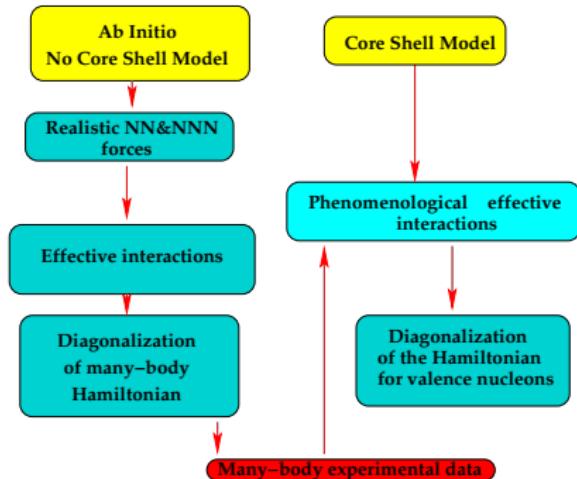


- Realistic 2N potentials produce strong h.o. closures but no spin-orbit ones...

Shell Model & 3N forces

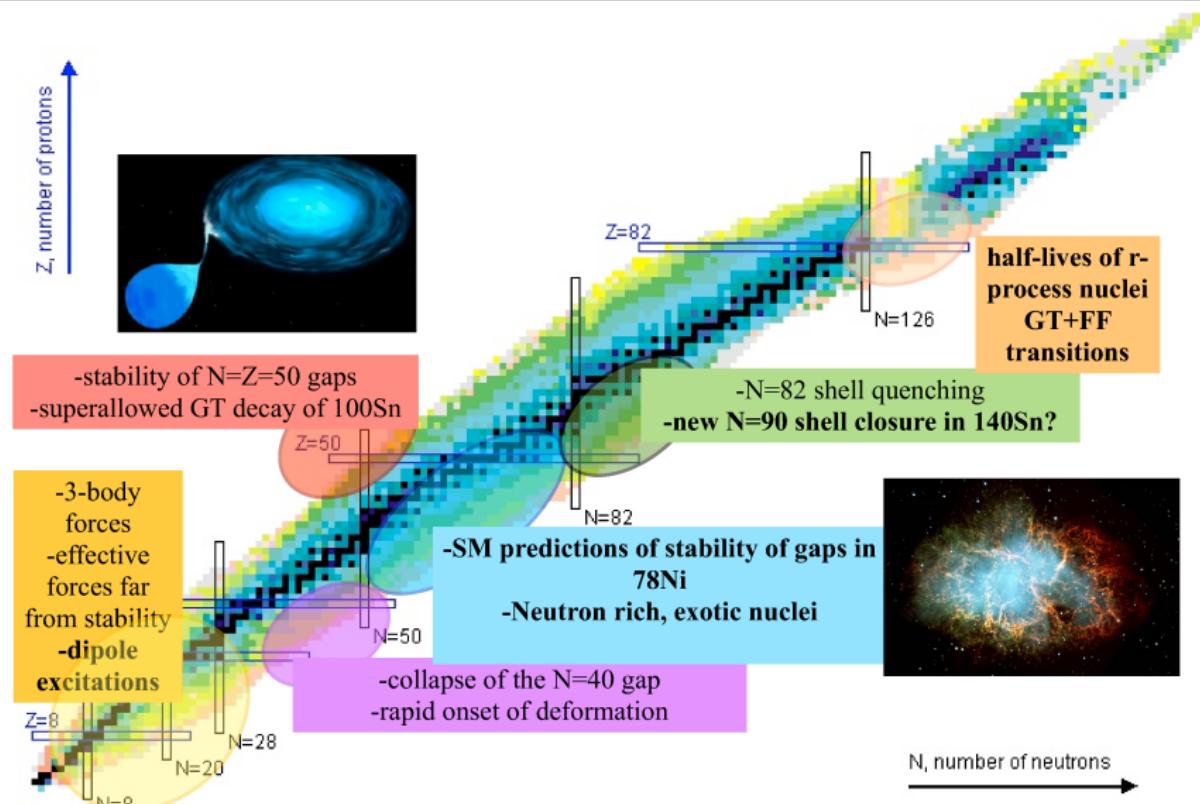
- No-core shell model calculations with 3N forces possible for light systems ($A \sim 12$).
- In core-shell model for heavier nuclei, 3N contribution taken into account empirically.

A. Cortes and A.P. Zuker, "Self-consistency and many-body monopole forces in shell model calculations" Phys. Lett. B84 (1979) 25

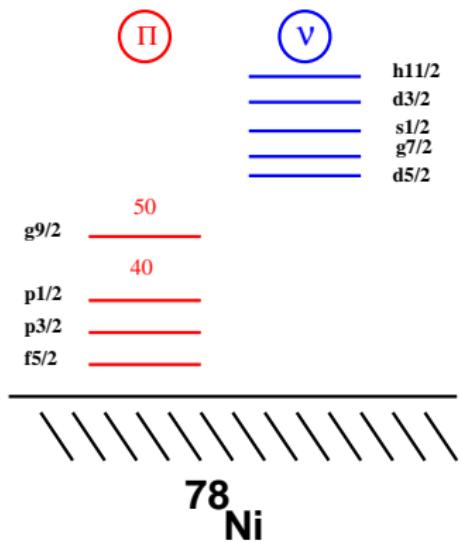


Excitation energies in light nuclei in NCSM with chiral EFT interactions. P. Navratil et al., Phys. Rev. Lett. 99 (2007) 042501.

SM with empirical interactions: regions of activity



Nuclei above ^{78}Ni



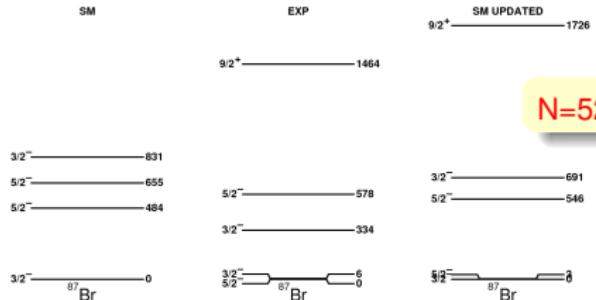
- Knowing s.p. structure of ^{79}Ni will be useful to validate the model assumptions

Interaction: $\pi\pi$ fit of Lisetskiy & Brown, $\nu\nu$ GCN5082, $\pi\nu$ monopole corrected G-matrix. Proven successful and predictive in a large number of applications:

- Structure, mixed symmetry states in Zr isotopes, shell evolution between ^{91}Zr and ^{101}Sn
K. Sieja et al., Phys. Rev. C79 (2009) 064310
- Isomers and medium-spin structures of ^{95}Y , $^{91-95}\text{Rb}$, $^{92-96}\text{Sr}$
PRC85 (2012) 014329, PRC79 (2009) 024319, PRC82 (2010) 024302, PRC79 (2009) 044304
- Collectivity and $j-1$ anomaly of ^{87}Se
PRC88 (2013) 034302
- β -decays of Ga nuclei and structure of $N = 52, 54$ isotones
PRC88 (2013) 047301, PRC88 (2013) 044330, PRC88 (2013) 044314
- Magnetic moments of ^{86}Kr , ^{88}Sr ,
PRC 80 (2014) 064305
- Collectivity of $N = 52, 54$ nuclei
PRC88 (2013) 034327

Nuclei above ^{78}Ni : new developments

- New estimate of proton $f_{5/2}-p_{3/2}$ splitting in the core from studies of neutron-rich copper isotopes



- New fit of proton-proton interaction for N=50 isotones, using some new data e.g. ^{83}As from EXILL

P. Baczyk et al., Phys. Rev. C 91, 047302 (2015)

- Ni78-II interaction:

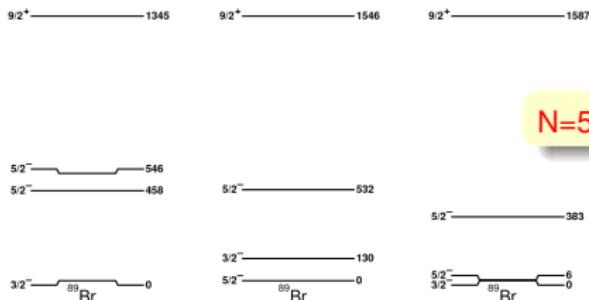
W. Urban et al., Phys. Rev. C 94, 044328 (2016)

M. Czerwinski et al., Phys. Rev. C 93, 034318 (2016)

J. Litzinger et al., Phys. Rev. C 92, 064322 (2015)

T. Materna et al., Phys. Rev. C 94, 034305 (2015)

M. Czerwinski et al., Phys. Rev. C 94, 014328 (2015)

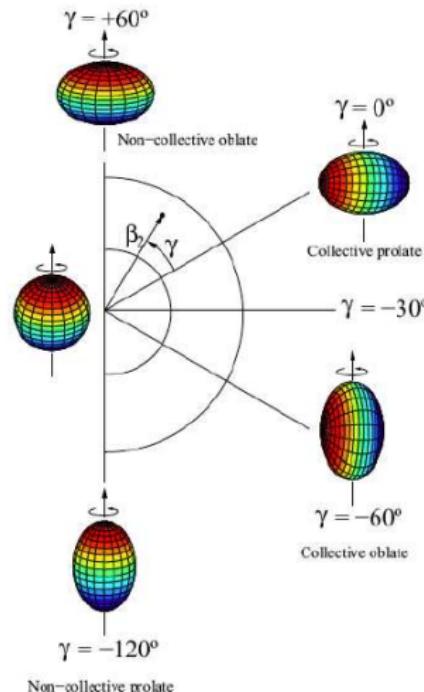


N=52

N=54

Nuclear deformation

The nuclear shape can be characterized by the Bohr parameters (β, γ) which describe the quadrupole shape of the nuclear surface. The most used model is the rigid axial rotor of Bohr Mottelson and its generalization to a triaxial shape by Davidov and Filipov.



$$\begin{aligned} R_\lambda &= R \left(1 + \beta \sqrt{\frac{5}{4\pi}} \cos(\gamma - \frac{2\pi}{3}\lambda) \right) \\ \lambda &= 1, 2, 3 \\ Q_0 &= \frac{3ZR^2\beta}{\sqrt{5\pi}} \\ R &= R_0 A^{1/3} \end{aligned}$$

Collectivity and triaxiality

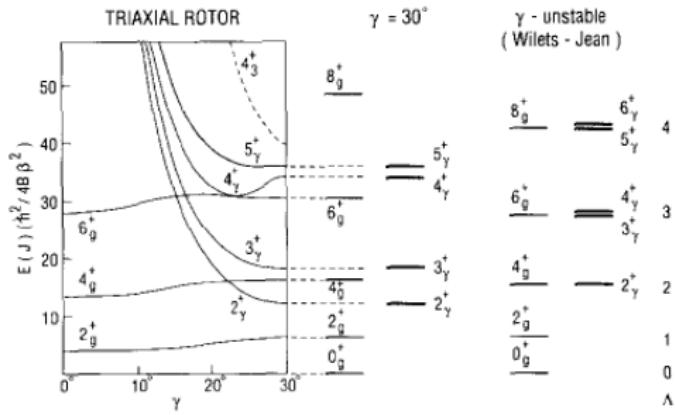


Fig. 1. Comparison of triaxial (or Davydov [6]) rigid γ rotor and γ -soft models. The Davydov results for $\gamma=30^\circ$ are shown explicitly in the middle for comparison with the γ -unstable, or Wilets-Jean [7], model. (The γ -band levels are shown as thicker lines.)



$S(4,3,2) > 0$
for a rigid triaxial rotor (+1.67)

$S(4,3,2) < 0$
for γ -independent potential (-2)

N.V. Zamfir and R. Casten, Phys. Lett. B260, 265 (1991)

stagerring of the γ band:

$$S(J, J-1, J-2) = \frac{[E(J) - E(J-1)] - [E(J-1) - E(J-2)]}{E(2_1^+)}$$

Quadrupole shape invariants

K. Kumar, Phys. Rev. Lett. 28 (1972) 249

$$Q_{int}(s) = \sqrt{\frac{16\pi}{5}} p_s^{(2)} \quad \cos 3\gamma(s) = -\sqrt{7/2} p_s^{(3)} \left(p_s^{(2)}\right)^{-3/2}$$

$$p_s^{(2)} = (2I_s + 1)^{-1} \sum_r M_{sr}^2 = \frac{5(I_s + 1)(2I_s + 3)}{16\pi I_s(2I_s - 1)} Q_{spec}^2(s) + \sum_{r \neq s} B(E2; s \rightarrow r),$$

M_{sr} = reduced $E2$ matrix elements

$$p_s^{(3)} = -\sqrt{5}(2I_s + 1)^{-1}(-1)^{2I_s} \sum_{rt} \left\{ \begin{array}{ccc} 2 & 2 & 2 \\ I_s & I_r & I_t \end{array} \right\} M_{sr} M_{rt} M_{ts},$$

For the rigid triaxial rotor the parameters p_2 and p_3 are directly related to the (β, γ) deformation parameters and nuclear radius R_0 .

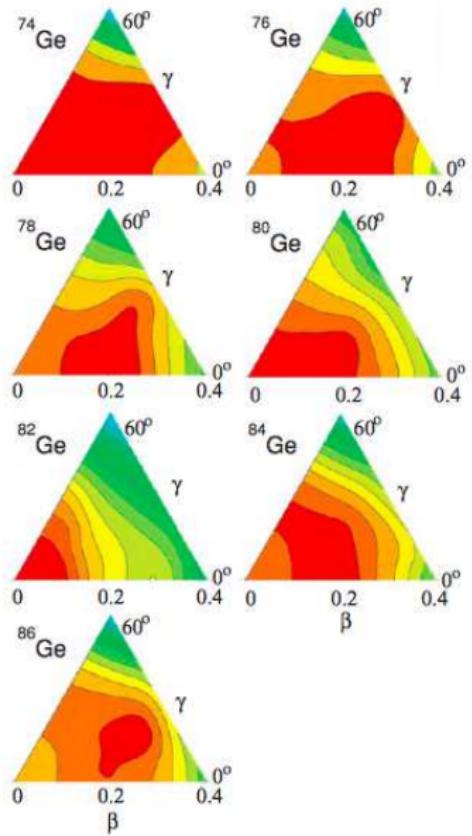
$$p_2 = e^2 Q_0^2 \beta^2$$

$$p_3 = e^3 Q_0^3 \beta^3 \cos(3\gamma) = p_2^{3/2} \cos(3\gamma)$$

where $Q_0 = 3ZR_0^2/(4\pi)$

p_2 and p_3 can be obtained from multipole sums of $E2$ matrix elements
(Cline Flaum sum rule)

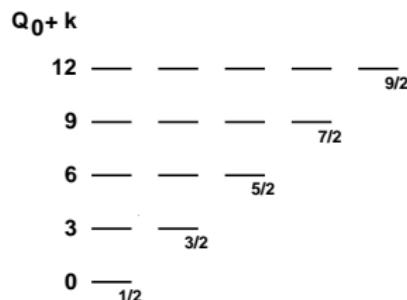
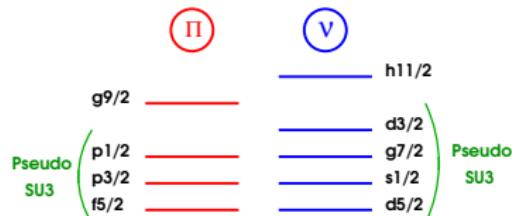
Collectivity and triaxiality in Ge isotopes



- Experimental hint for collectivity in ^{84}Ge
M. Lebois et al., Phys. Rev. C 80, 044308 (2009)
- Experimental signs of rigid collectivity in the g.s. claimed in ^{76}Ge :
 $S(4) = 0.09$
Y. Toh et al., Phys. Rev. C 87, 041304R (2013)
- It is known from SM and experimental studies that proton $p_{3/2}$ and $f_{5/2}$ orbits remain close in the ^{78}Ni region. SM extrapolation gives degenerate neutron $d_{5/2}$ and $s_{1/2}$ orbits. These are perfect conditions for quadrupole collectivity to develop.

Collectivity and triaxiality above ^{78}Ni

Simple perspective: predictions of the pseudo-SU(3) scheme



Predictions of pseudo-SU(3) model for N=52,54:

Nucleus	Q_0	$B(E2; 2^+ \rightarrow 0^+)$
^{82}Zn	114	258
^{84}Ge	131	342
^{86}Se	148	436
^{88}Kr	117	272
^{84}Zn	135	362
^{86}Ge	151	454
^{88}Se	168	561
^{90}Kr	137	373

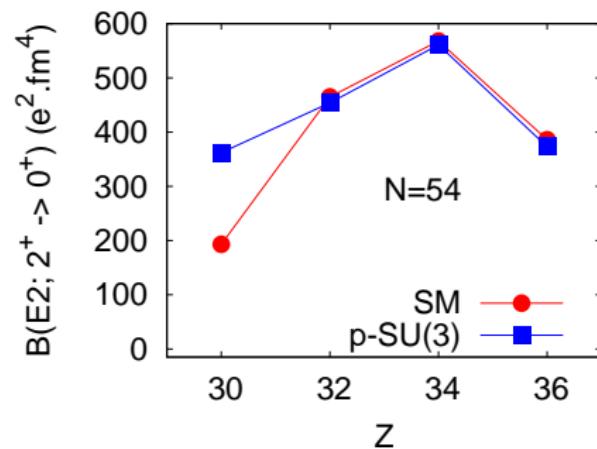
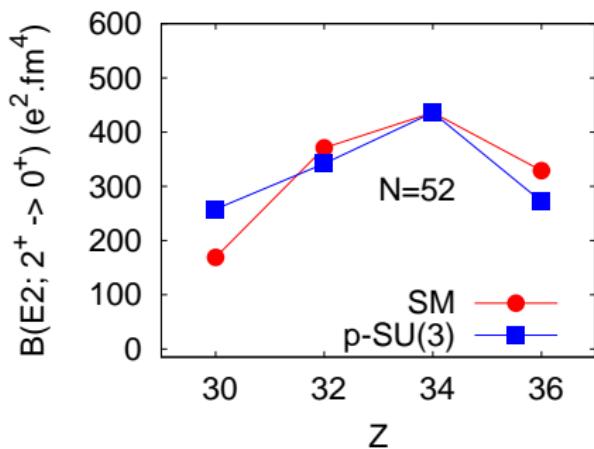
- maximal prolate deformation in ^{88}Se
- possible triaxiality in ^{86}Ge (degeneracy of $K = 0$ and $K = 2$ configurations)

$$q_0(n, \chi, k) = (2n - 3\chi)b^2$$

$$\chi = 0, \dots, n \quad k = \pm \left(\frac{1}{2}, \dots, \frac{1}{2} + \chi \right)$$

A. P. Zuker et al., Nilsson-SU3 selfconsistency: Quadrupole dominance in heavy N=Z nuclei, <http://arxiv.org/abs/1404.0224>

Predictions of the pseudo-SU(3) model vs SM diagonalization



- pseudo-SU(3) is a good approximation for the proton mid-shell
 - maximal prolate deformation in ^{88}Se
 - possible triaxiality in ^{86}Ge

Intrinsic shape parameters of shell model states

(Yrast)	State	Q_0	β	γ (deg.)
^{86}Ge	0_{gs}^+	165	0.238	19
	2_1^+	161	0.232	8
	4_1^+	152	0.218	12
	6_1^+	118	0.172	10
^{88}Se	0_{gs}^+	174	0.250	9
	2_1^+	169	0.243	12
	4_1^+	159	0.229	15
	6_1^+	118	0.173	14
(Excited)	State	Q_0	β	γ (deg.)
^{86}Ge	2_2^+	152	0.219	28
	3_1^+	148	0.213	32
	4_2^+	116	0.169	41
	5_1^+	105	0.154	33
^{88}Se	2_2^+	152	0.219	35
	3_1^+	143	0.207	36
	4_2^+	114	0.166	40
	5_1^+	100	0.146	36

$$Q_{int}(s) = \sqrt{\frac{16\pi}{5}} p_s^{(2)}$$

$$\cos 3\gamma(s) = -\sqrt{7/2} p_s^{(3)} \left(p_s^{(2)}\right)^{-3/2}$$

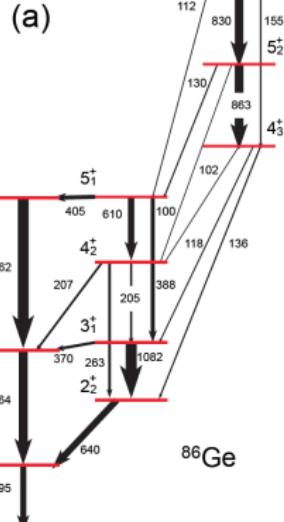
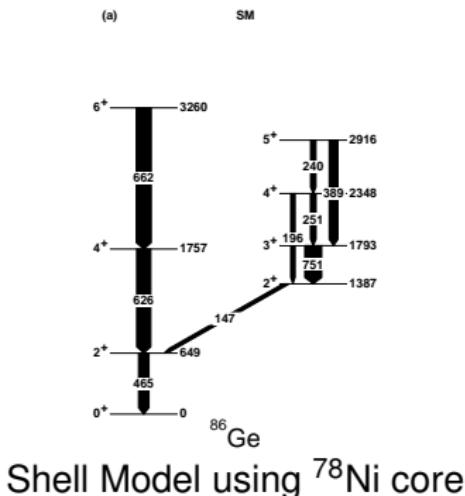
$$\begin{aligned} p_s^{(2)} &= (2I_s + 1)^{-1} \sum_r M_{sr}^2 \\ &= \frac{5(I_s + 1)(2I_s + 3)}{16\pi I_s(2I_s - 1)} Q_{spec}^2(s) \\ &+ \sum_{r \neq s} B(E2; s \rightarrow r), \end{aligned}$$

M_{sr} = reduced $E2$ matrix elements

$$\begin{aligned} p_s^{(3)} &= -\sqrt{5}(2I_s + 1)^{-1} (-1)^{2I_s} \\ &\sum_{rt} \left\{ \begin{array}{ccc} 2 & 2 & 2 \\ I_s & I_r & I_t \end{array} \right\} M_{sr} M_{rt} M_{ts}, \end{aligned}$$

K. Kumar, Phys. Rev. Lett. 28 (1972) 249

Triaxiality above ^{78}Ni ?

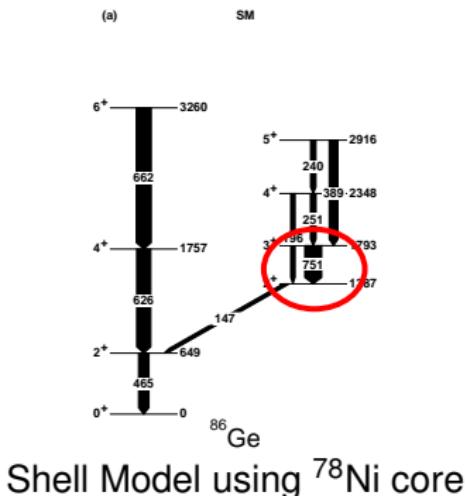


Agreement of excitation energies for the 1st excited band **within keV!**

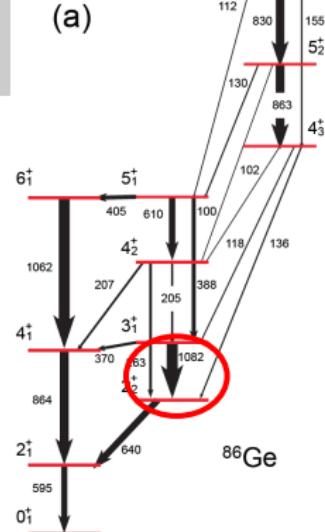
- matrices dimension 10^6
- feasible on a laptop
- typical time of calculations:
5min to 4h on one processor

- symmetry conserved (particle number and angular momentum)
- cluster of 140 CPUs
- typical time of calculations: 1 month

Triaxiality above ^{78}Ni ?



Shell Model using ^{78}Ni core



GCM-Gogny

Agreement of excitation energies for the 1st excited band **within keV!**

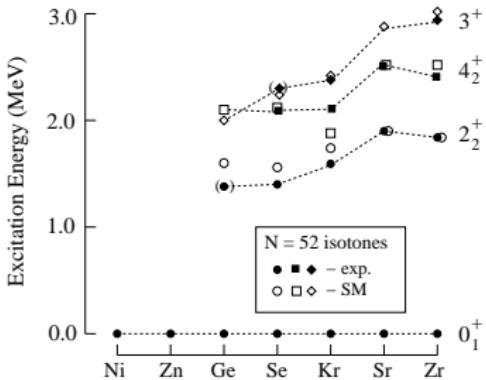
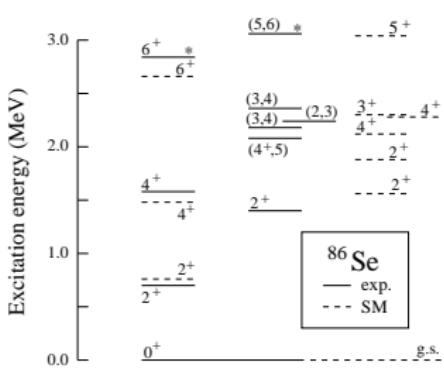
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- symmetry conserved (particle number and angular momentum)
- cluster of 140 CPUs
- typical time of calculations: 1 month

K. Sieja, T.R. Rodriguez, K. Kolos and D. Verney, Phys. Rev. C88 (2013) 034327

Some experimental results at N=52

T. Materna et al., Phys. Rev. C 94, 034305 (2015)

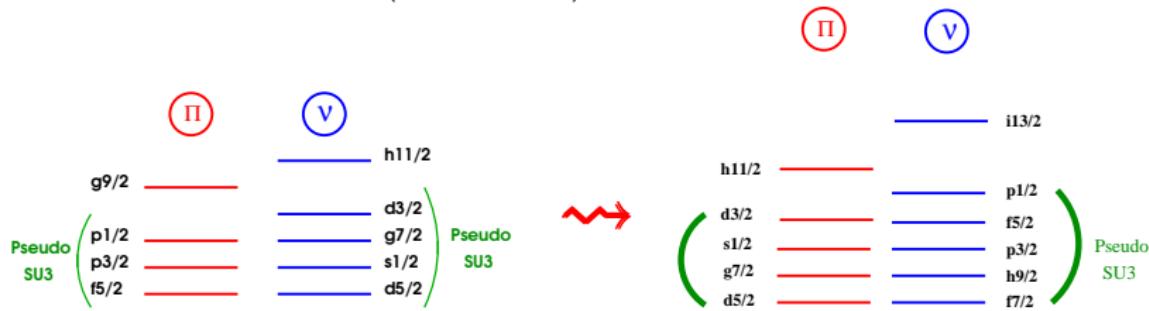


- Second excited state in ^{84}Ge is 2₂⁺, in agreement with predictions of 5DCH-D1S Gogny model, which gives a γ -soft ground state. SM supports the Gogny predictions with 2₂⁺ being a head of a quasi- γ band.
K. Kolos et al., Phys. Rev. C88 (2013) 047301 A. Korgul et al., Phys. Rev. C88 (2013) 044330
- ^{86}Se appears little deformed ($\beta \sim 0.1$) but γ -soft from analysis of n-body quadrupole moments.
- Recent B(E2) from lifetimes (Cologne) in ^{86}Se in good agreement with the SM ones!
J. Litzinger et al., Phys. Rev. C92 (2015) 064322

Outlook: Collectivity above ^{132}Sn core

pseudo-SU(3) predictions

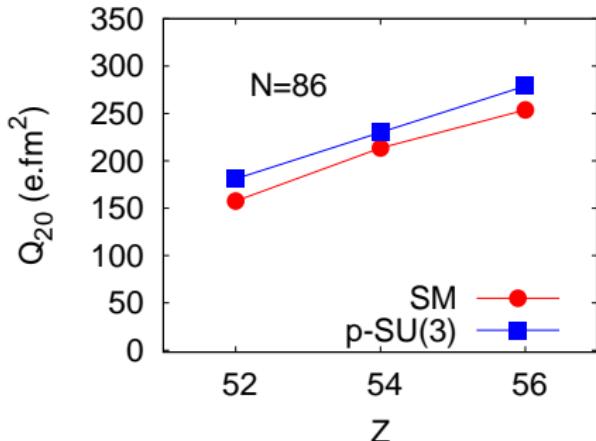
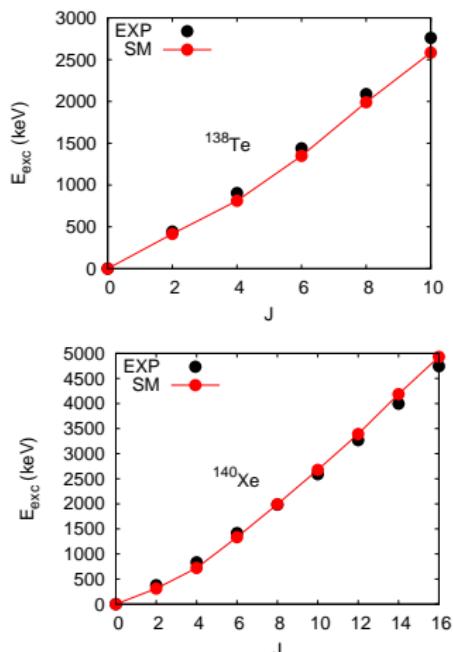
In analogy to what we have seen above the ^{78}Ni , collectivity should also thrive for the open-shell nuclei above the ^{132}Sn core ($N=54 \rightarrow N=86$)



Some K-mixing should be possible in realistic calculations leading to triaxially deformed shapes

Collectivity above ^{132}Sn core

- Diagonalization in proton gds -neutron hfp model space, interaction based on N3LO, empirically corrected
- SM results in good agreement with experiment in ^{138}Te and ^{140}Xe



Nucleus	$B(E2; 3^+ \rightarrow 2^+_2)$	$Q_{\text{spec}}(3^+)$
^{138}Te	18 W.u.	$-3.5 \text{ e} \cdot \text{fm}^2$
^{140}Xe	44 W.u.	$-2.2 \text{ e} \cdot \text{fm}^2$
^{142}Ba	37 W.u.	$-4.1 \text{ e} \cdot \text{fm}^2$

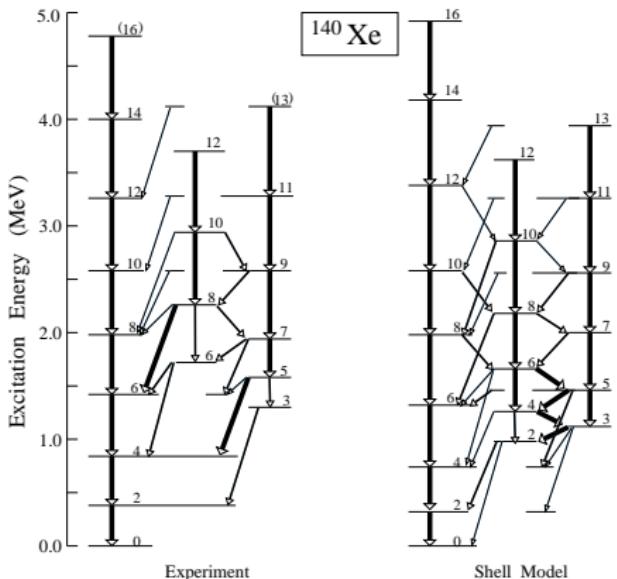
K. Sieja, Acta Phys. Pol. B47 (2016) 883

Collectivity above the ^{132}Sn core

PHYSICAL REVIEW C 93, 034326 (2016)

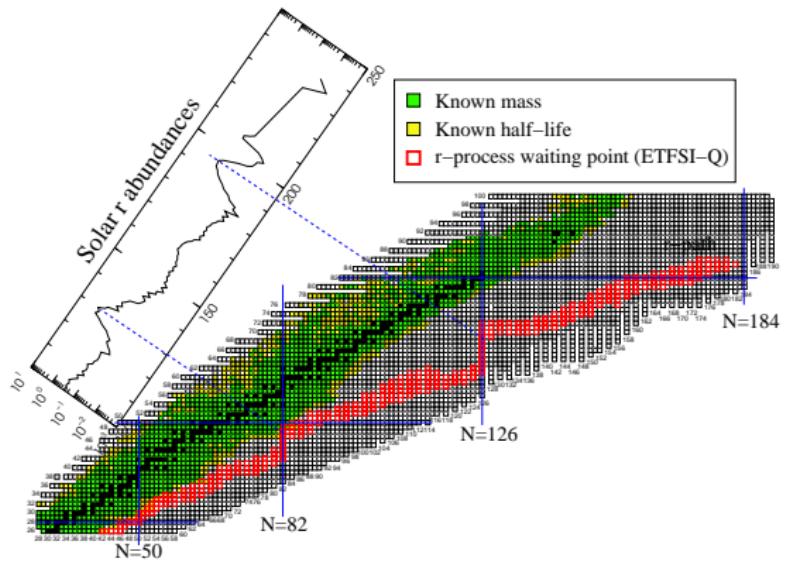
First evidence of γ collectivity close to the doubly magic core ^{132}Sn

W. Urban,¹ K. Sieja,^{2,3} T. Rząca-Urban,¹ M. Czerwiński,¹ H. Naïdja,^{2,3,4,5} F. Nowacki,^{2,3} A. G. Smith,⁶ and I. Ahmad⁷



- good agreement between experimental and SM spectra
- (β, γ) from SM $E2$ are $0.15, 16^\circ$ in the g.s. of ^{140}Xe

Astrophysics aspects



Nuclear input for astrophysics models:

- β strength function (GT, FF)
← masses, wave-functions

PRC87 (2013) 025803

- (n, γ) rates
← level densities, γ strength functions
EPJ A (2012)
-fission properties

Neutron capture cross sections

$$\sigma_{(n,\gamma)}^{\mu\nu}(E_i, n) = \frac{\pi\hbar^2}{2M_{i,n}E_{i,n}} \frac{1}{(2J_i^\mu + 1)(2J_n + 1)} \sum_{J,\pi} (2J+1) \frac{T_n^\mu T_\gamma^\nu}{T_{tot}},$$

where:

$E_{i,n}, M_{i,n}$ - center-of-mass energy, reduced mass of the system

$J_n = 1/2$ -neutron spin

transmission coefficients:

$$T_n^\mu = T_n(E, J, \pi; E_i^\mu, J_i^\mu, \pi_i^\mu) \quad T_\gamma^\nu = T_\gamma(E, J, \pi; E_m^\nu, J_m^\nu, \pi_m^\nu)$$

For a given multipolarity

$$T_{XL}(E, J, \pi, E^\nu, J^\nu, \pi^\nu) = 2^{2L+1} f_{XL}(E, E_\gamma)$$

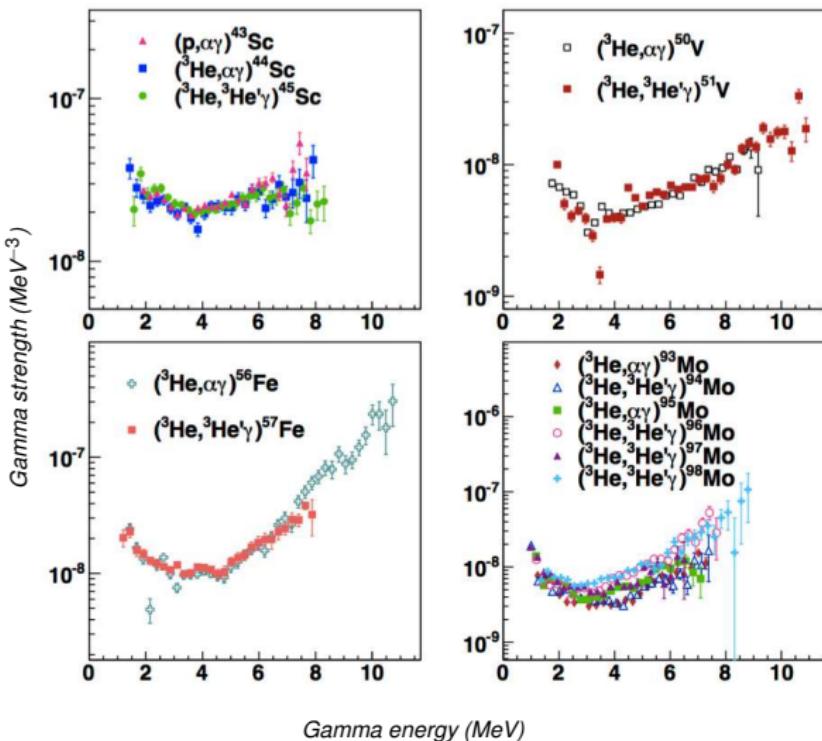
Key ingredients in Hauser-Feshbach calculations:

- description of gamma emission spectra of a compound nucleus
- Brink-Axel hypothesis

Overview & Motivation

Low energy enhancement of the γ -strength function

Data from Oslo group



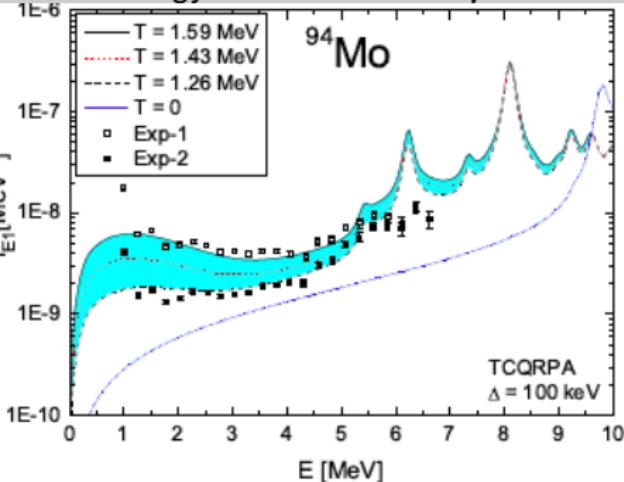
- Microscopic strength functions are different from global parametrizations
- Low energy enhancement of γ -strength observed in different regions of nuclei
- It can influence the (n, γ) rates of the r-process by a factor of 10!
- Evidence for the dipole nature of low energy enhancement in ^{56}Fe

A.C. Larsen and S. Goriely, Phys. Rev. C82 (2010) 014318

A. C. Larsen et al., Phys. Rev. Lett. 111 (2013) 242504

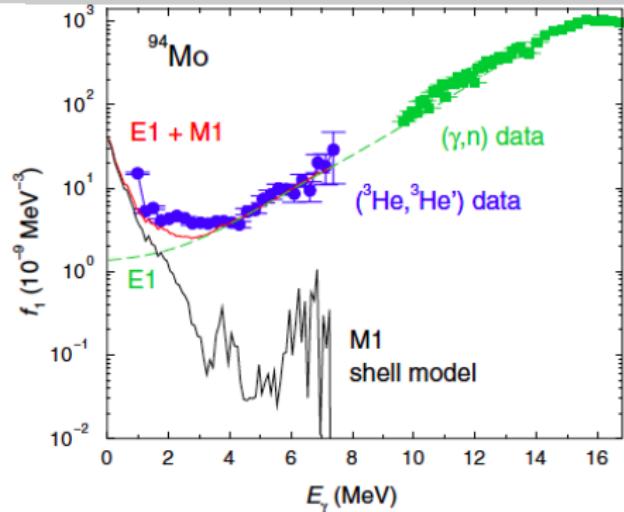
Overview & Motivation

Low energy enhancement of γ -SF



E. Litvinova and N. Belov, Phys. Rev. C88 (2013) 031302R

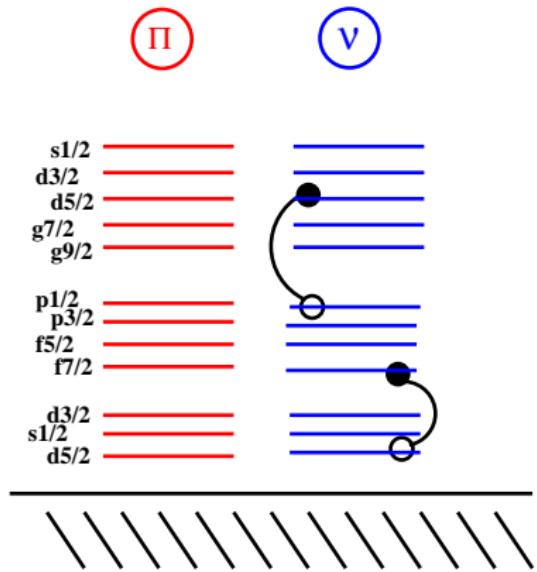
- Thermal continuum QRPA calculations
- Enhancement due to transitions between thermally unblocked s.p. states and the continuum
- Note the difference between $T = 0$ (ground state) and $T > 0$ (excited state) E1 strength distribution



R. Schwengner et al., PRL111 (2013) 232504

- Shell model transitions between a large amount of states
- Enhancement due to the M1 transitions between states in the region near the quasicontinuum
- A general mechanism to be found throughout the nuclear chart

SM calculations in $sd - pf - gds$ valence space



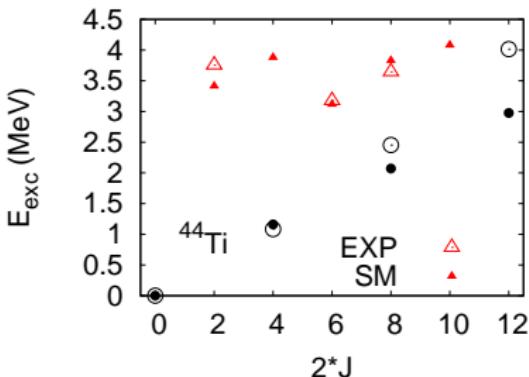
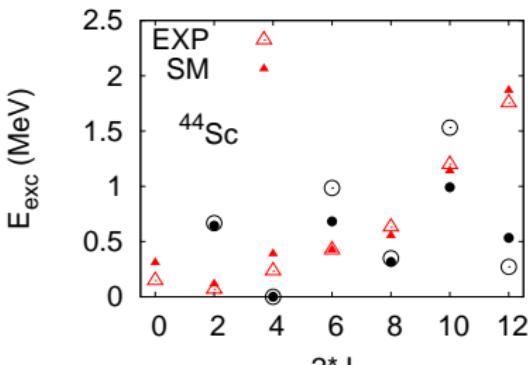
^{16}O

	fp	$1p-1h$
^{48}Cr	1.963.461	165.821.912
^{56}Fe	345.400.174	23.194.461.394

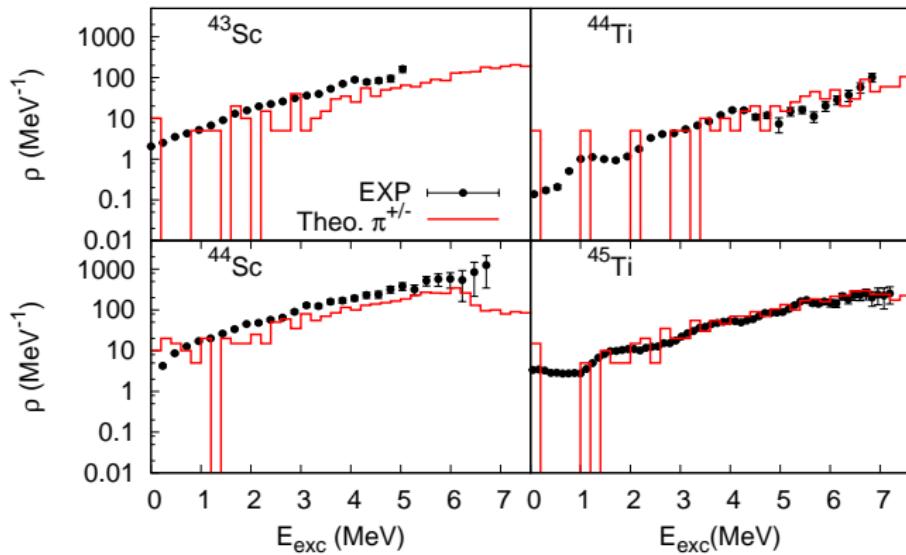
- Full fp -calculations for positive parity states
- Full $1\hbar\omega$ calculations for negative parity states- all 1p-1h excitations from sd and to gds shells
- $H_{SM} = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{i,j,k,l} V_{ijkl} c_i^\dagger c_j^\dagger c_l c_k + ta_{c.m.} H_{c.m.}$
- **60 states per spin and parity**
 $S_{M1/E1} = \langle B(M1/E1) \rangle \rho(E_i)$
(60×5000 iterations...)
- or Lanczos SF method with 500 iterations for upward
 $S_{M1/E1}$

Effective Hamiltonian

- Interaction from V_{lowk} based on the CD-Bonn potential
- Monopole corrections to fix the s.p. and s.h. energies (spectra of ^{39}K , ^{41}Ca) and position of opposite parity states (^{41}Ca , ^{42}Ca , ^{78}Sr)
- Good reproduction of low lying levels in considered nuclei and accurate position of the first 1p-1h states
- Quenching of 0.75 on magnetic spin operator
- Accurate reproduction of known magnetic moments of $f_{7/2}$ -shell nuclei

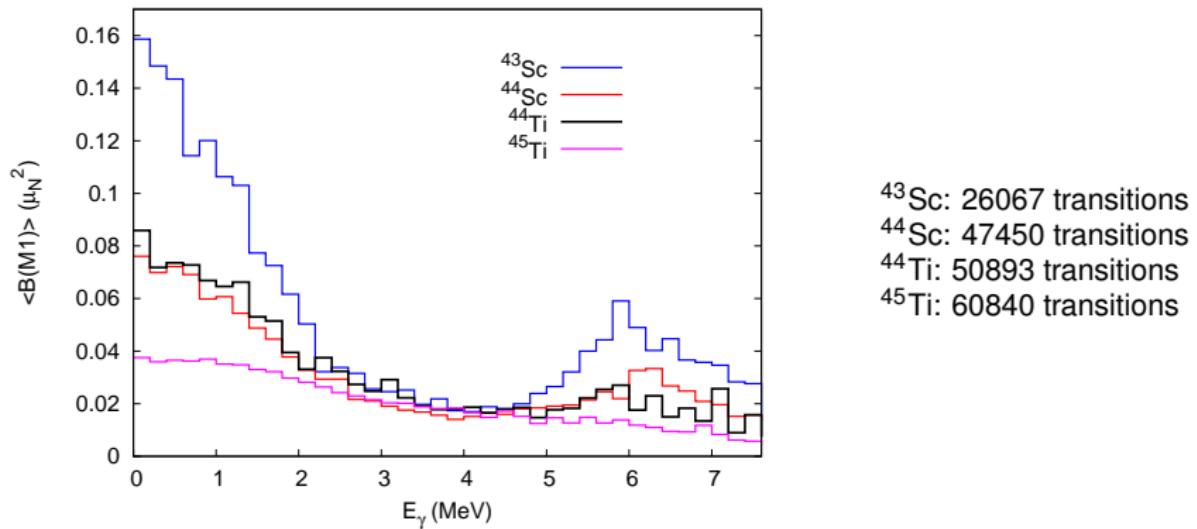


Level densities



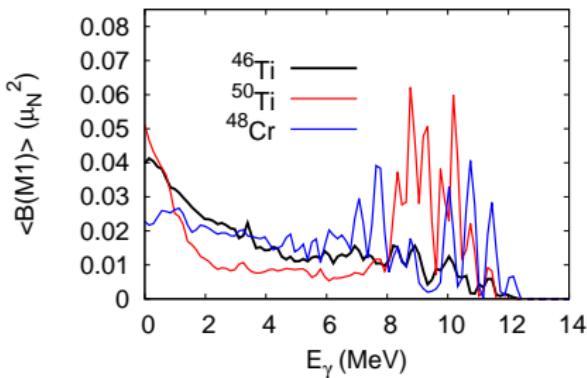
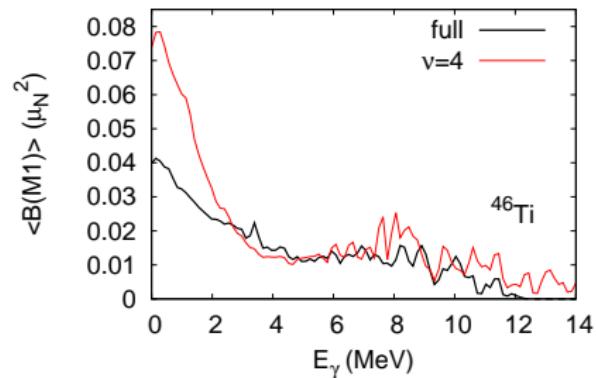
- Good reproduction though not enough natural parity states in Sc nuclei - missing contribution from 2p-2h

M1 calculations: natural parity (pf -shell states)



- Correlation between the magnitude of the enhancement and the complexity of the nucleus (wave functions)

M1 calculations: natural parity (pf -shell states)

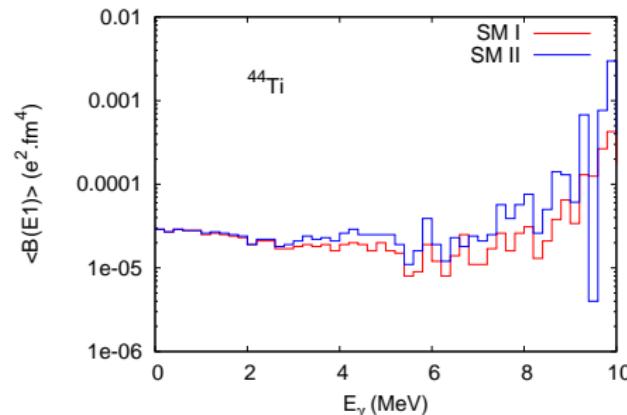
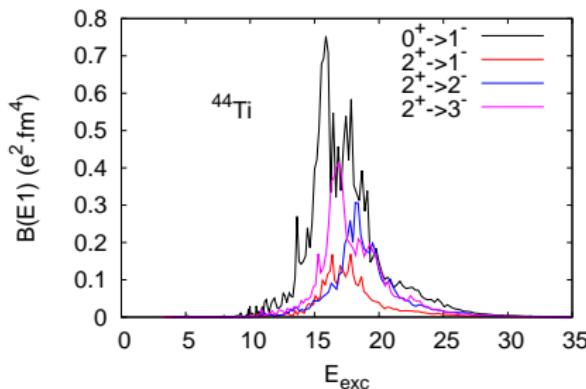
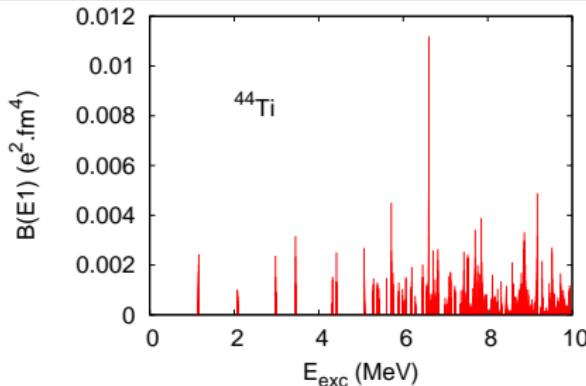


☞ Simpler wave functions → larger upbend

☞ Dependence of the upbend on the nuclear shape

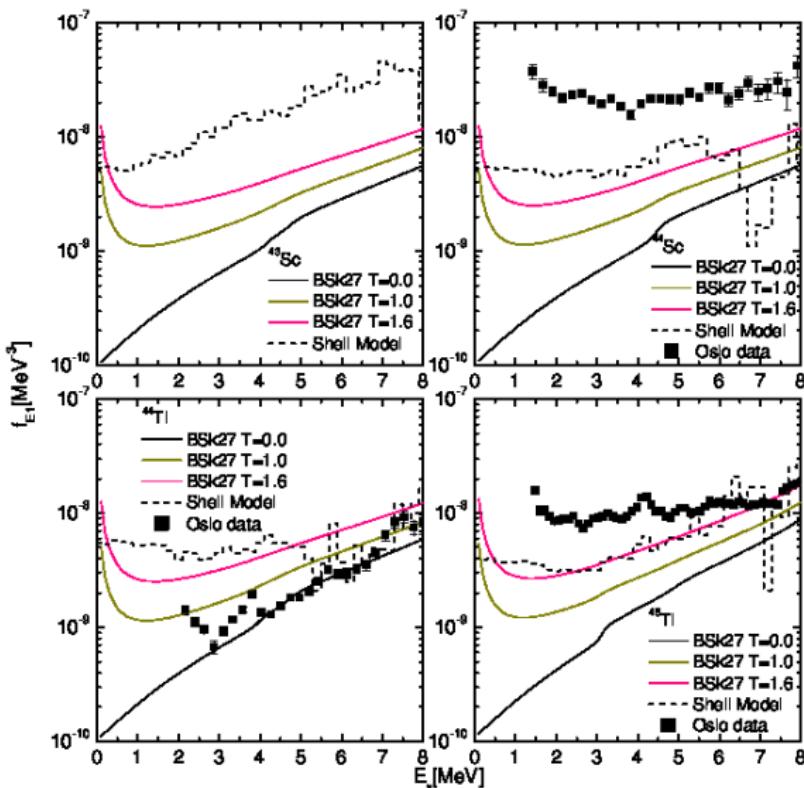
E1 calculations

^{44}Ti



SM I: 60 states of each spin/parity ($J=0-12$)
SM II: + contribution from 300 higher
lying 1^- , 2^- , 3^- states

E1 calculations: low lying strength



- SM probably the most accurate tool for the low lying strength
- Can one build a reliable global RSF model based on SM results?
- 3-years In2p3 project (CEA-DAM, ULB, Oslo, IThemba LABS, ...)

S. Goriely, private comm. & S. Goriely et al., Nucl. Phys. A739, 331 (2004)

Conclusions

- SM with empirical interactions is a powerful tool in the studies of spectroscopy and deformation properties of nuclei.
- Triaxial shapes are predicted to exist above ^{78}Ni and ^{132}Sn cores in $N = 54$ and $N = 86$ isotones
- Available experimental data support theoretical predictions
- New applications of shell model to statistical properties of nuclei are in progress