

Coexistence phenomena in neutron-rich $A \sim 100$ nuclei within beyond-mean-field approach

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Outline

- *complex EXCITED VAMPIR beyond-mean-field model*
- *neutron-rich $A \sim 100$ nuclei*
 - *triple shape coexistence and shape evolution in the $N=58$ Sr and Zr isotopes*
 - *shape evolution in even-even Zr nuclei*
 - *Gamow-Teller β -decay relevant for :*
 - *r -process ($^{104,106}\text{Zr}$)*
 - *reactor decay heat ($^{102,104}\text{Tc}$)*

Characteristic features of neutron-rich $A \sim 100$ nuclei

- *shape transition, shape coexistence, shape mixing*
- *drastic changes in structure with particle number, spin, excitation energy*

Open problems for theoretical models

- *realistic effective Hamiltonians and adequate large model spaces*
- *beyond-mean-field models*

Goals

- *unitary description of evolution in structure at low and high spins*
- *unitary treatment of structure and β -decay properties*

complex VAMPIR model family

- the **model space** is defined by a finite dimensional set of **spherical single particle states**
 - the effective many-body **Hamiltonian** is represented as a sum of **one- and two-body terms**
 - the basic **building blocks** are Hartree-Fock-Bogoliubov (**HFB**) vacua
 - the HFB transformations are **essentially complex** and allow for **proton-neutron, parity and angular momentum mixing** being restricted by time-reversal and axial symmetry
 - the broken symmetries (**s=N, Z, I, p**) are restored by **projection before variation**
- * The models allow to use rather large model spaces and realistic effective interactions*

Beyond-mean-field variational procedure: complex EXCITED VAMPIR model

Vampir

$$E^s[F_1^s] = \frac{\langle F_1^s | \hat{H} \hat{\Theta}_{00}^s | F_1^s \rangle}{\langle F_1^s | \hat{\Theta}_{00}^s | F_1^s \rangle}$$

Θ_{00}^s - symmetry projector

$|F_1^s\rangle$ - HFB vacuum

$$|\psi(F_1^s); sM\rangle = \frac{\Theta_{M0}^s |F_1^s\rangle}{\sqrt{\langle F_1^s | \hat{\Theta}_{00}^s | F_1^s \rangle}}$$

Excited Vampir

$$|\psi(F_i^s); sM\rangle = \sum_{j=1}^i |\phi(F_j^s)\rangle \alpha_j^i \quad \text{for } i = 1, \dots, n-1$$

$$|\phi(F_i^s); sM\rangle = \Theta_{M0}^s |F_i^s\rangle$$

$$|\psi(F_n^s); sM\rangle = \sum_{j=1}^{n-1} |\phi(F_j^s)\rangle \alpha_j^n + |\phi(F_n^s)\rangle \alpha_n^n$$

$$(H - E^{(n)}N)f^n = 0$$

$$(f^{(n)})^+ N f^{(n)} = 1$$

$$|\Psi_\alpha^{(n)}; sM\rangle = \sum_{i=1}^n |\psi_i; sM\rangle f_{i\alpha}^{(n)}, \quad \alpha = 1, \dots, n$$

A~100 mass region

^{40}Ca - core

model space for both protons and neutrons :

$1p_{1/2}$ $1p_{3/2}$ $0f_{5/2}$ $0f_{7/2}$ $2s_{1/2}$ $1d_{3/2}$ $1d_{5/2}$ $0g_{7/2}$ $0g_{9/2}$ $0h_{11/2}$

(single-particle energies adjusted within complex MONSTER (VAMPIR))

renormalized G-matrix (OBEP, Bonn A)

- pairing properties enhanced by short range Gaussians for:*

T = 1 pp, np, nn channels

T = 0, S = 0 and S = 1 channels

- onset of deformation influenced by monopole shifts:*

$$\langle 0g_{9/2} \ 0f; T=0 | G | 0g_{9/2} \ 0f; T=0 \rangle$$

- Coulomb interaction between valence protons added*

Triple shape coexistence and shape evolution in the N=58 Sr and Zr isotopes

A. Petrovici, Phys. Rev. C85 (2012) 034337

Neutron-rich Sr and Zr isotopes: - rapid transition from spherical to deformed shapes
- sudden onset of quadrupole deformation for $N > 58$

Positive parity states up to spin 20^+ in ^{96}Sr and ^{98}Zr (12-dimensional EXVAM many-nucleon bases)

The amount of mixing for the lowest 0^+ states of ^{96}Sr .

$I[\hbar]$	spherical	prolate	oblate
0_1^+	36%	20%	44%
0_2^+	57%	18%	25%
0_3^+		69%	31%
0_4^+	4%	6%	90%

• maximum oblate-prolate mixing for 2^+ and 4^+ states

$$\Delta E (2_{\text{oblate}}^+ - 2_{\text{prolate}}^+) = 24 \text{ keV}$$

$$\Delta E (4_{\text{prolate}}^+ - 4_{\text{oblate}}^+) = 154 \text{ keV}$$

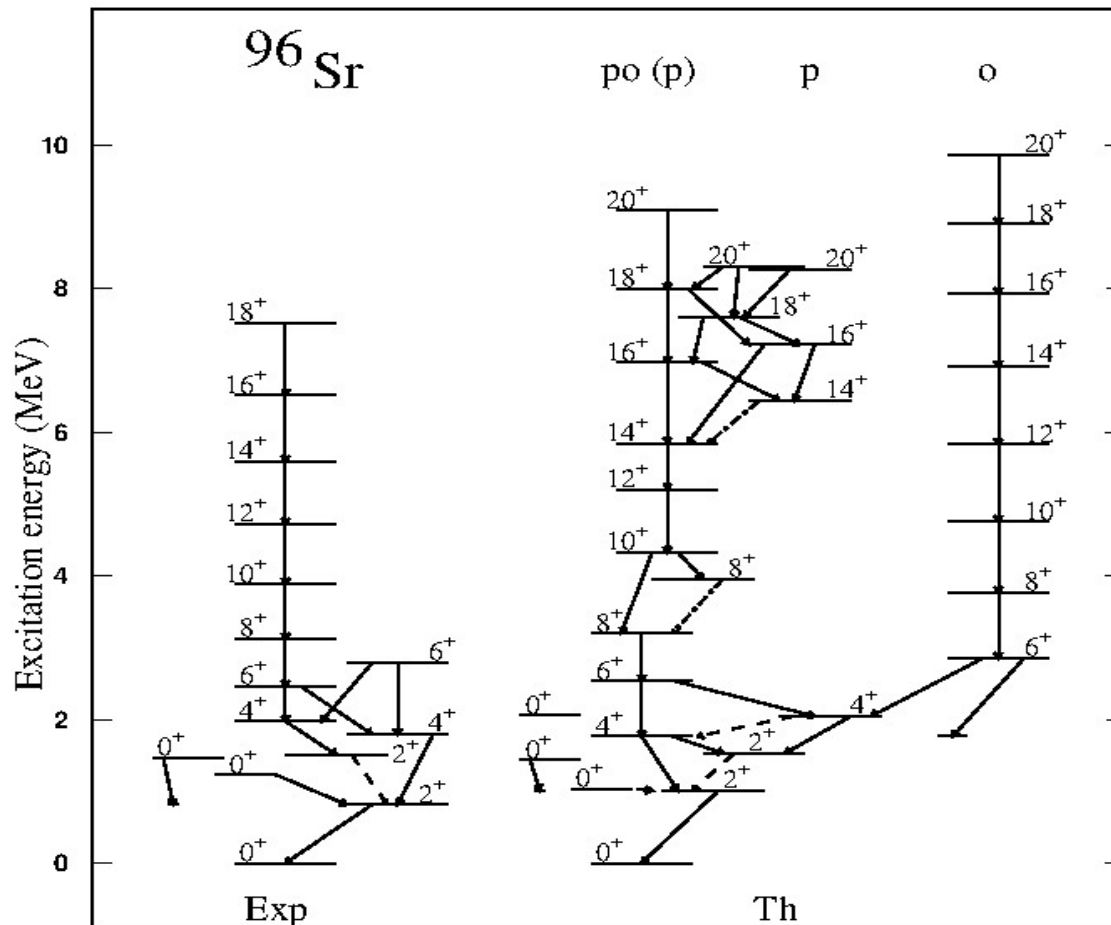
• spherical EXVAM configurations for spins 2^+ and 4^+ not found up to 4 MeV excitation energy

Particular case for 0^+ states

- the lowest 0^+ VAMPIR configuration is spherical
- the 3-lowest 0^+ orthogonal EXVAM configurations (s , o , p) are situated in an energy interval of 375 keV

The mixing for the 2^+ and 4^+ states.

$I[\hbar]$	prolate	oblate
2_1^+	34(2)%	58(5)%
2_2^+	65%	33(2)%
4_1^+	56(1)%	36(6)%
4_2^+	43%	52(5)%



po(p)-band - strong prolate-oblate mixing at low spins
 - variable prolate mixing at higher spins

almost pure o-band feeds the second 4^+ (maximum o-p mixing)

- the 3-lowest 0^+ EXVAM configurations (s , p , o) are separated by 323 keV

The amount of mixing for the lowest 0^+ states of ^{98}Zr .

$I[\hbar]$	spherical	prolate	oblate
0_1^+	12%	43%	45%
0_2^+	84%	12%	4%
0_3^+	1%	57%	42%
0_4^+	2%	10%	88%

- strong prolate-oblate mixing

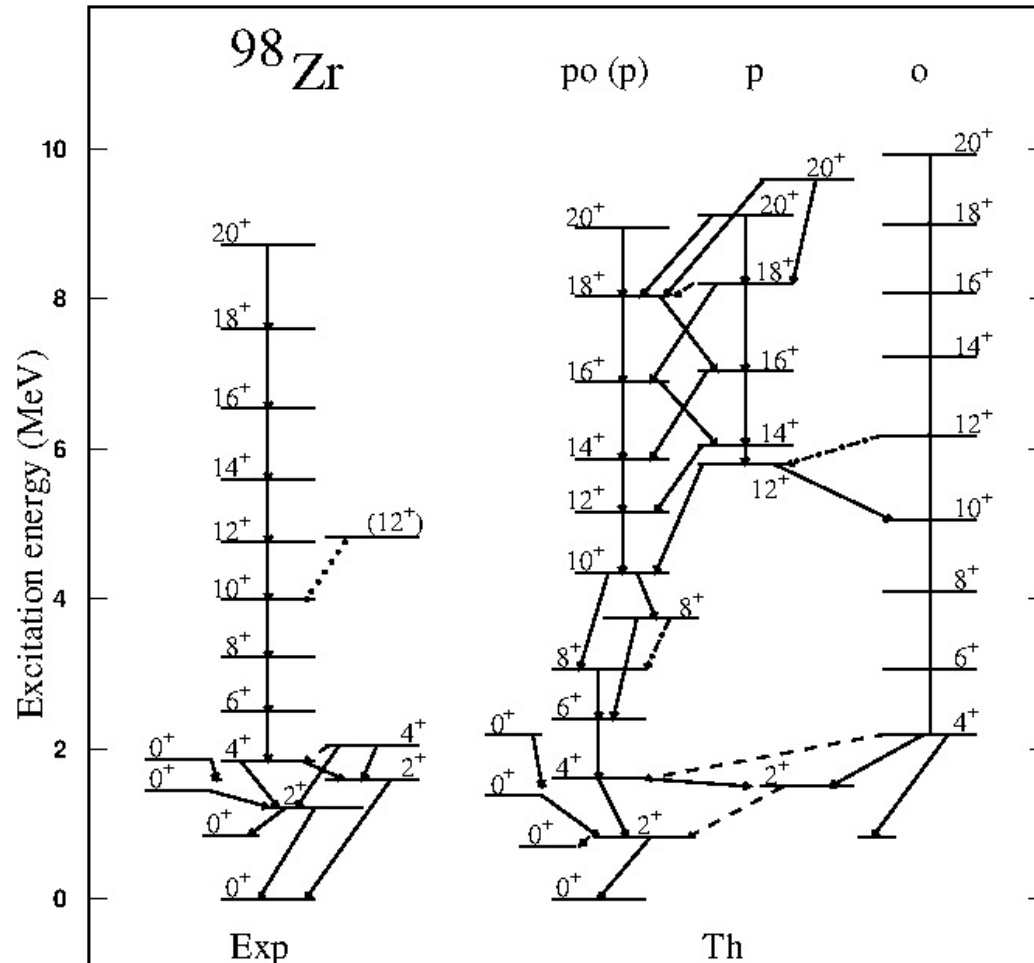
$$\Delta E(2^+_{\text{prolate}} - 2^+_{\text{oblate}}) = 206 \text{ keV}$$

$$\Delta E(4^+_{\text{prolate}} - 4^+_{\text{oblate}}) = 431 \text{ keV}$$

The mixing for the 2^+ and 4^+ states.

$I[\hbar]$	prolate	oblate
2_1^+	60(8)%	31%
2_2^+	36%	63(1)%
4_1^+	83(7)%	10%
4_2^+	13(1)%	85(1)%

- spherical EXVAM configurations for spins 2^+ and 4^+ not found up to 4 MeV excitation energy



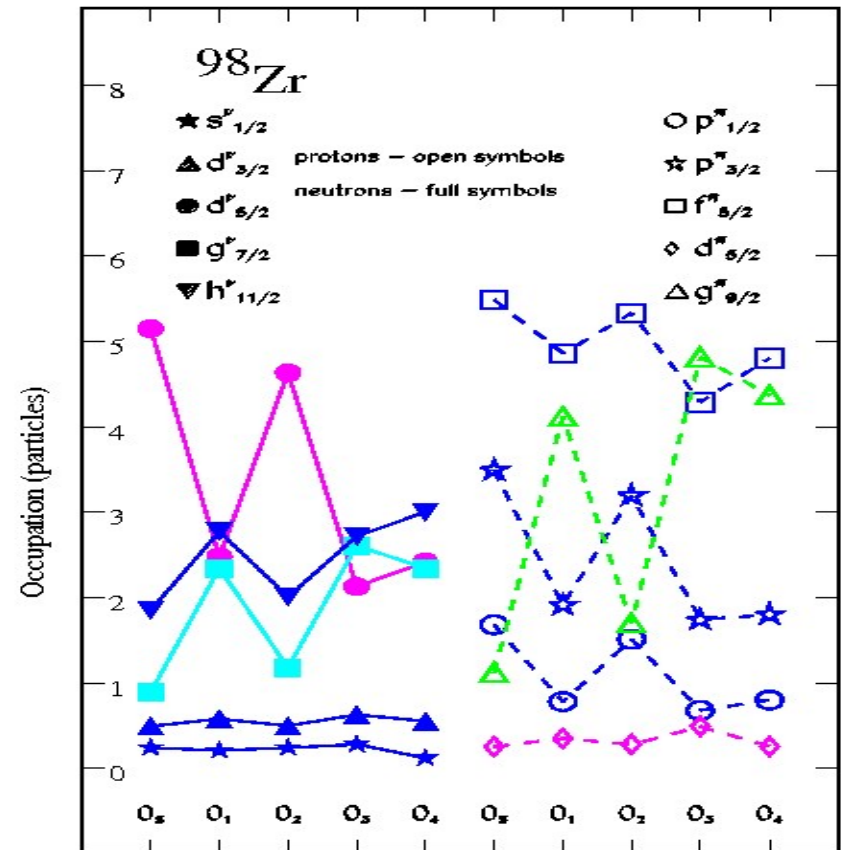
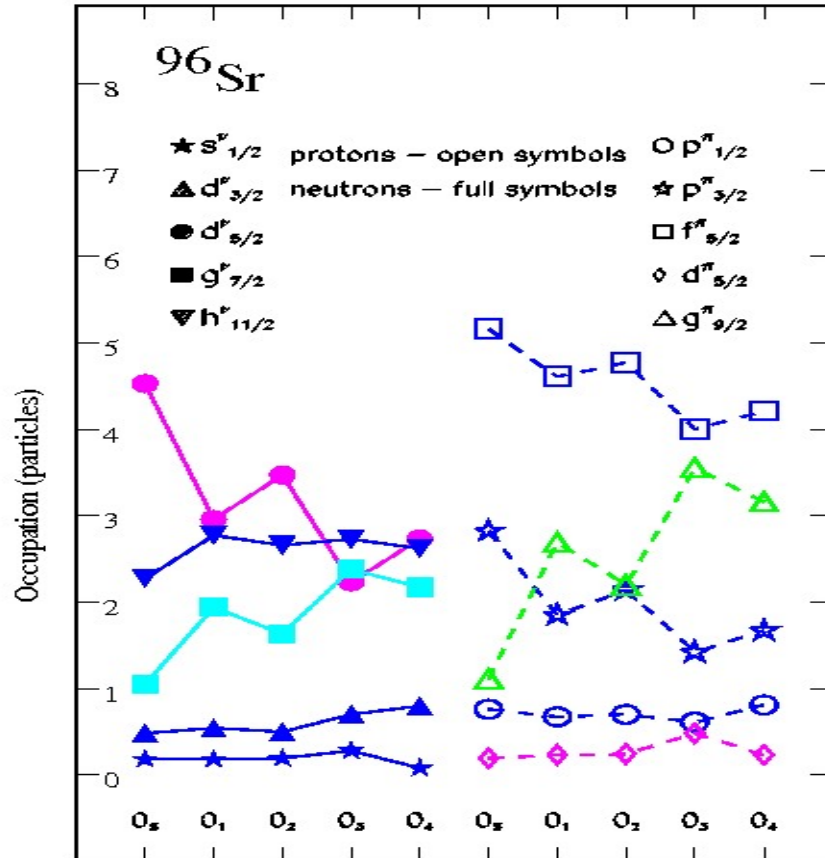
po(p)-band - strong prolate-oblate mixing at low spins
 - variable prolate mixing at higher spins

o-band feeds the second 2^+ (maximum o-p mixing)

Occupation of valence single-particle orbitals for 0^+ states – sensitive to intrinsic deformation

$d^v_{5/2}$ occupation – essential for spherical 0^+ EXVAM configuration

$g^\pi_{9/2}$ occupation – significantly changing from intrinsically oblate to prolate deformed 0^+ EXVAM configurations



Strong $E0$ transitions support mixing of differently deformed configurations in 0^+ wave functions

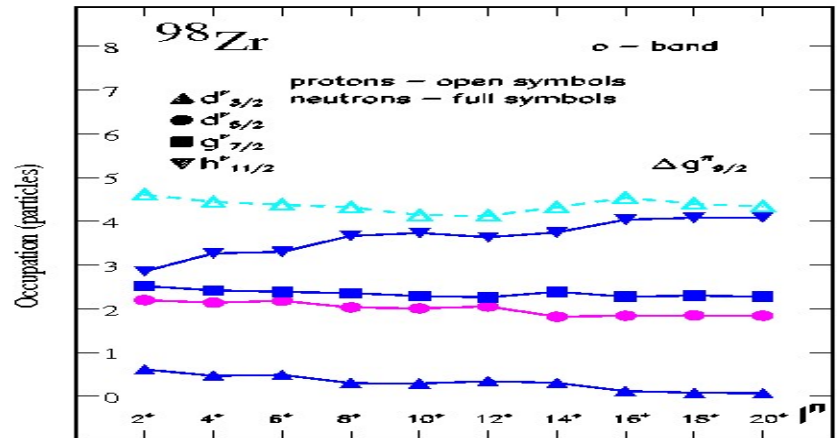
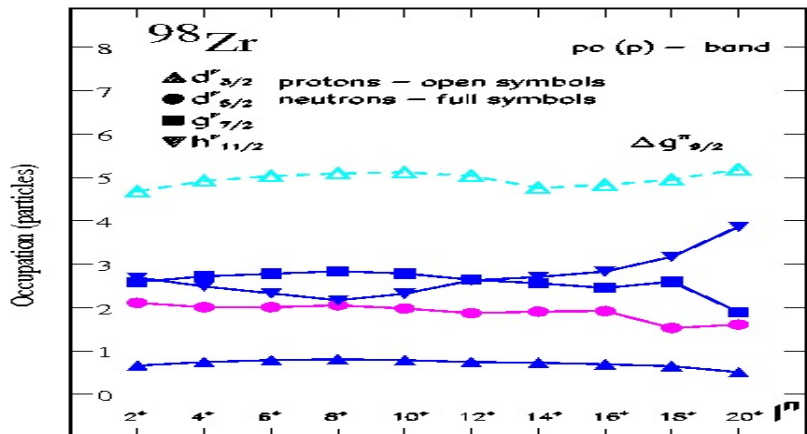
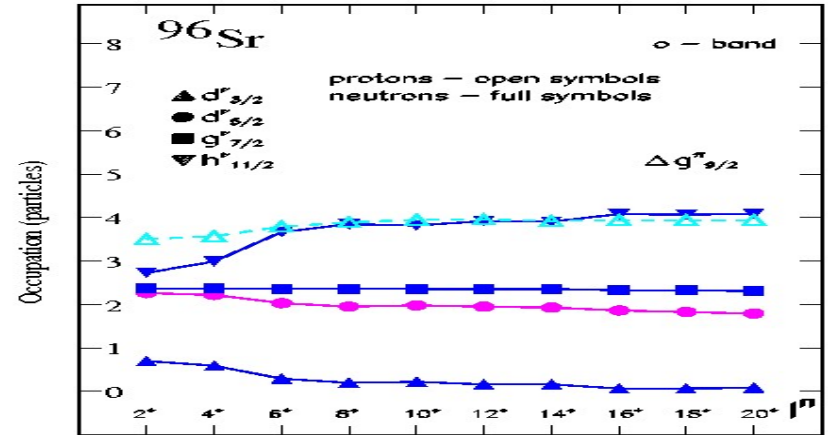
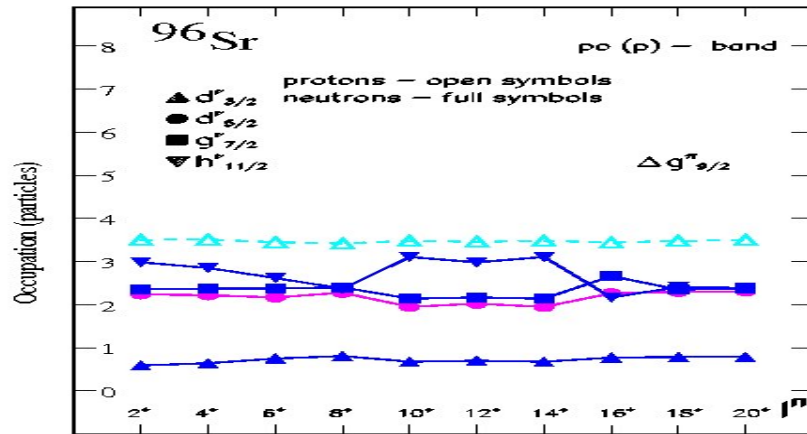
$$\rho^2{}^{\text{exp}}_{\text{max}}(E0; 0^+_3 \rightarrow 0^+_2) = 0.180$$

$$\rho^2{}^{\text{EXVAM}}_{\text{max}}(E0; 0^+_2 \rightarrow 0^+_1) = 0.066$$

$$\rho^2{}^{\text{exp}}_{\text{max}}(E0; 0^+_3 \rightarrow 0^+_2) = 0.075(8)$$

$$\rho^2{}^{\text{EXVAM}}_{\text{max}}(E0; 0^+_2 \rightarrow 0^+_1) = 0.060$$

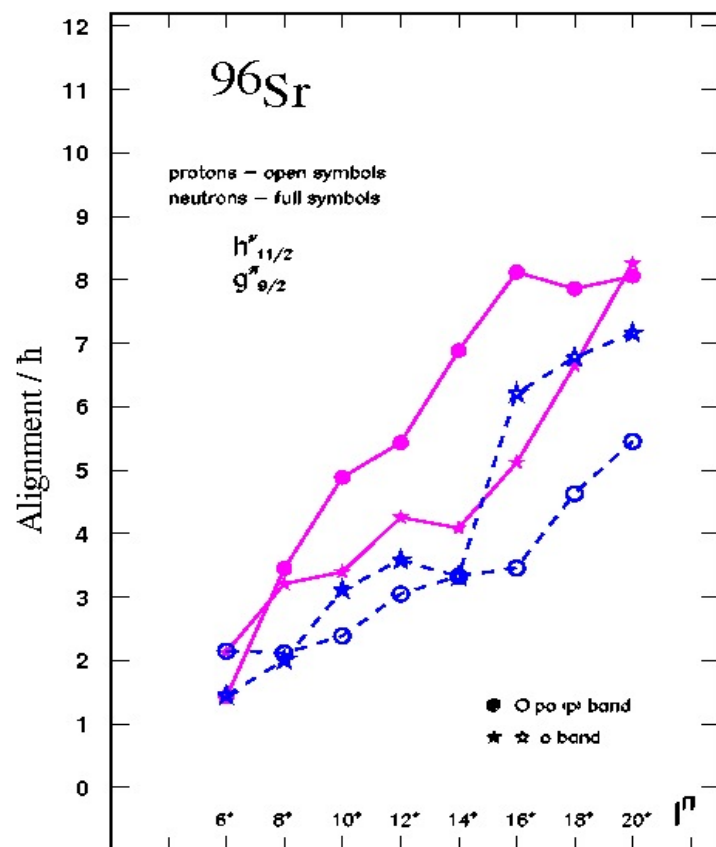
Evolution in structure with spin and excitation energy revealed by relevant spherical occupations



changes in structure corroborated with underlying shapes and evolution of shape mixing

Changes in structure revealed by angular momentum alignment and magnetic properties

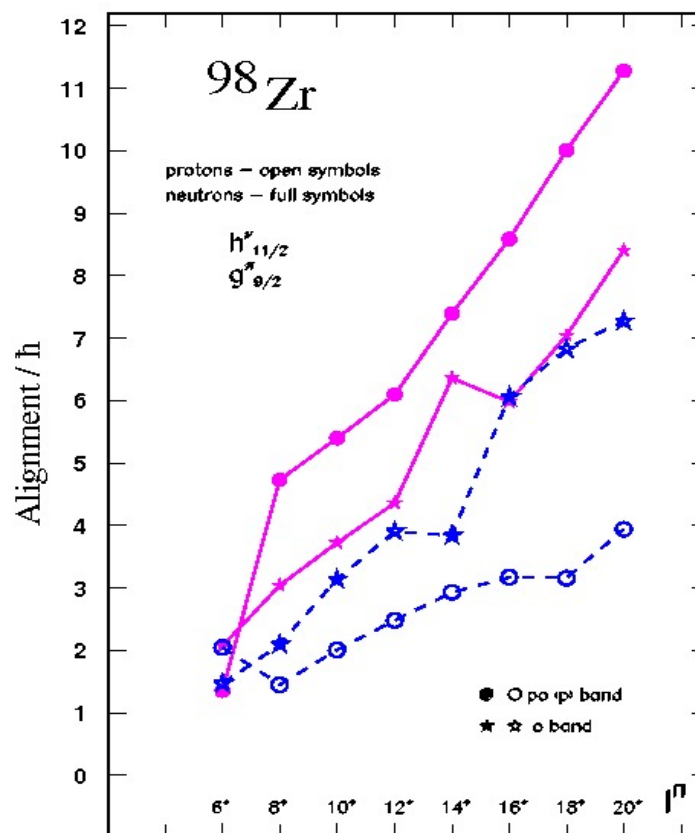
dominant contribution from ν - $h_{11/2}$ and π - $g_{9/2}$ alignment



• g -factor : $\cong 0.24$ ($I^{\pi} \geq 8^{+}$) (po(p)-band)

* g -factor : $\cong 0.50$ ($I^{\pi} \geq 10^{+}$) (o-band)

$$B(M1; 8^{+}_3 \rightarrow 8^{+}_1) = 1.29 \mu_N^2$$



• g -factor : $\cong 0.14$ ($I^{\pi} \geq 8^{+}$) (po(p)-band)

* g -factor : $\cong 0.44$ ($I^{\pi} \geq 10^{+}$) (o-band)

$$B(M1; 8^{+}_2 \rightarrow 8^{+}_1) = 1.60 \mu_N^2$$

$B(E2; \Delta I = 2)$ strengths $\rightarrow$ fragmentation $\leftrightarrow$ mixing

$B(E2; I \rightarrow I - 2)$ values (in $e^2 fm^4$) for the lowest bands of ^{96}Sr (EXVAM) (effective charges $e_p = 1.3$, $e_n = 0.3$).

$I[\hbar]$	$\rho o(p)$ -band	α -band
2 ⁺	795 340(209) (old) 580 (preliminary-Isolde)	
4 ⁺	1770 (187)	1901 (12)
6 ⁺	1911 (560)	1484 (215) (89)
8 ⁺	2127 (361)(122)	1436 (159) (121) (99)
10 ⁺	819 (1329) (168)	1514 (231)
12 ⁺	2332 (142)	1760
14 ⁺	2354 (57) (44)	1392
16 ⁺	238 (2237) (160)	1590
18 ⁺	753 (1374) (248)	1459
20 ⁺	2183 (97)	1359

$B(E2; I \rightarrow I - 2)$ values (in $e^2 fm^4$) for the lowest bands of ^{98}Zr (EXVAM) (effective charges $e_p = 1.3$, $e_n = 0.3$).

$I[\hbar]$	$\rho o(p)$ -band	p -band	α -band
2 ⁺	1140 (198)(161)		1305 (28) (18) (15)
4 ⁺	2072 (620)		1593 (56)
6 ⁺	2558 (101)		1662
8 ⁺	1802 (942)(153)		1572 (123)
10 ⁺	719 (1430)		1314 (119) (100)
12 ⁺	2300 (216)	731 (345) (212)	663 (621) (307)
14 ⁺	2428 (123)	1840 (392)	1094 (494)
16 ⁺	1360 (832) (190)	548 (246) (1421)	602 (250) (195)
18 ⁺	863 (207) (1416)	1347 (713) (808)	1115
20 ⁺	409 (1958)	347 (185) (1972)	1313

Experimental lifetimes for intermediate spin states: simultaneous fit to several levels suggests deformation

$$Q_{exp_0}^{(12^+ \rightarrow 10^+ \rightarrow 8^+)} = 220 (15) \text{ efm}^2$$

$$Q_{exp_0}^{(12^+ \rightarrow 10^+ \rightarrow 8^+ \rightarrow 6^+)} = 200 (10) \text{ efm}^2$$

Spectroscopic quadrupole moments $\rightarrow$ deformation and mixing

Q_2^{sp} (in efm^2) for the lowest bands of ^{96}Sr
(effective charges $e_p = 1.3$, $e_n = 0.3$).

$I[\hbar]$	$po(p)$	o
2 ⁺	9.5	0 (preliminary-Isolde)
4 ⁺	-23.9	1.4
6 ⁺	-100.3	75.5
8 ⁺	-120.1	77.3
10 ⁺	-120.7	94.4
12 ⁺	-124.1	94.6
14 ⁺	-124.5	90.5
16 ⁺	-130.0	85.4
18 ⁺	-126.2	80.1
20 ⁺	-124.4	68.1

Q_2^{sp} (in efm^2) for the lowest bands of ^{98}Zr
(effective charges $e_p = 1.3$, $e_n = 0.3$).

$I[\hbar]$	$po(p)$	p	o
2 ⁺	-36.6		7.1
4 ⁺	-89.6		54.7
6 ⁺	-115.5		76.7
8 ⁺	-126.7		70.7
10 ⁺	-130.1		58.2
12 ⁺	-129.1	-98.5	55.6
14 ⁺	-126.1	-121.2	30.5
16 ⁺	-126.6	-123.0	60.8
18 ⁺	-124.2	-134.4	74.9
20 ⁺	-125.6	-135.4	68.9

$po(p)$ -band: $\beta_2^{EXVAM} (8^+/10^+/12^+) \cong 0.3$

o -band: $\beta_2^{EXVAM} (8^+/10^+/12^+) \cong -0.19 \div -0.23$

o -band: $\beta_2^{EXVAM} (8^+/10^+/12^+) \cong -0.17 \div -0.13$

Gamow-Teller β decay of ^{102}Tc and ^{104}Tc (reactor decay heat)

M.D. Jordan, A. Algorta A. Petrovici et al., Phys. Rev. C87 (2013) 044318



$$Q_{\beta} = 4.532 \pm 0.009 \text{ MeV}$$

$$Q_{\beta} = 5.516 \pm 0.006 \text{ MeV}$$

$$1_{gs}^{+} \rightarrow 0^{+} / 1^{+} / 2^{+}$$

$$3_{gs}^{+} \rightarrow 2^{+} / 3^{+} / 4^{+}$$

$$T_{1/2} = 5.28(15) \text{ s}$$

$$T_{1/2} = 1098(18) \text{ s}$$

complex EXCITED VAMPIR wave functions

$$1_{gs}^{+} \rightarrow \text{53\% oblate} / \text{47\% prolate} \\ (\text{7 EXVAM components})$$

$$3_{gs}^{+} \rightarrow > \text{99\% prolate} \\ (\text{7 EXVAM components})$$

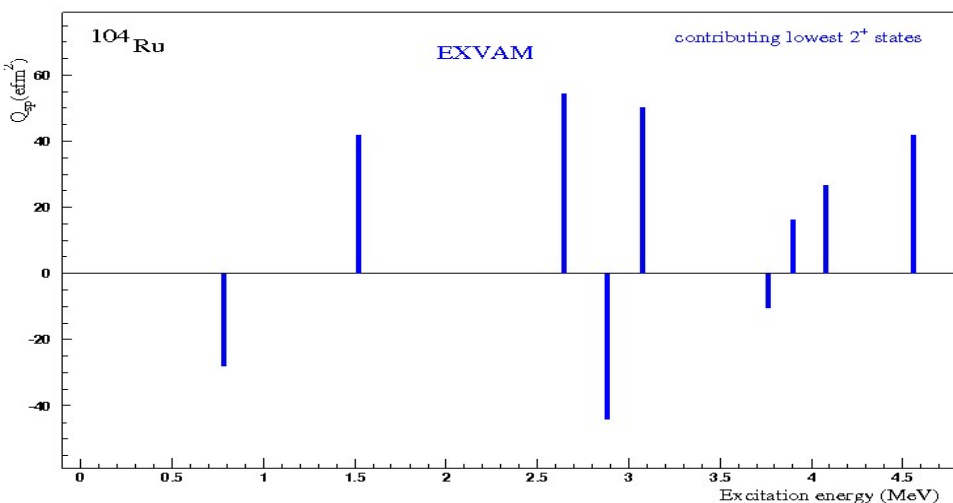
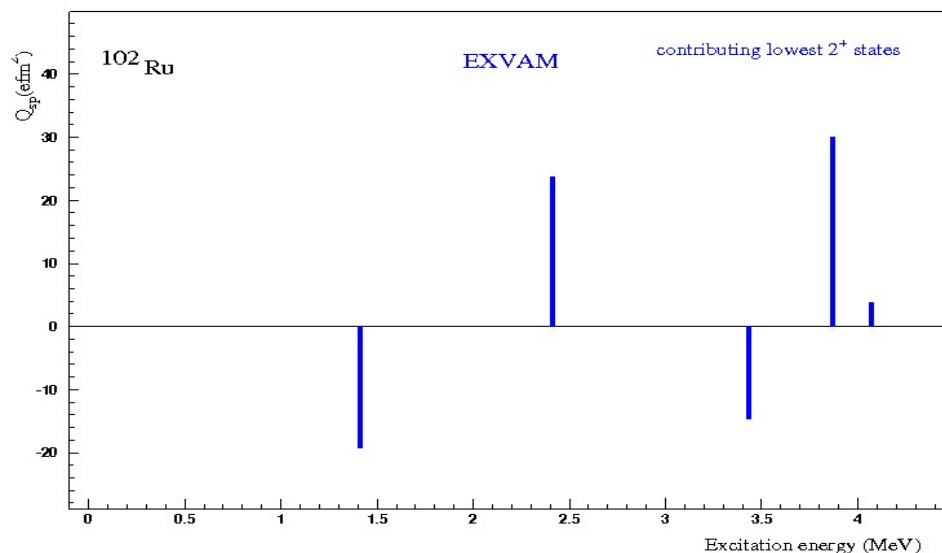
$^{102}\text{Ru}_{58}$

*complex EXCITED VAMPIR bases:
26 orthogonal projected configurations
for the spins 0^+ , 1^+ , 2^+*

Gamow-Teller contributing states

0^+ : from 85% to 26% prolate components
including almost spherical ones

2^+ : from 78% to 26% prolate components



$^{104}\text{Ru}_{60}$

*complex EXCITED VAMPIR bases:
25 orthogonal projected configurations
for the spins 2^+ , 3^+ , 4^+*

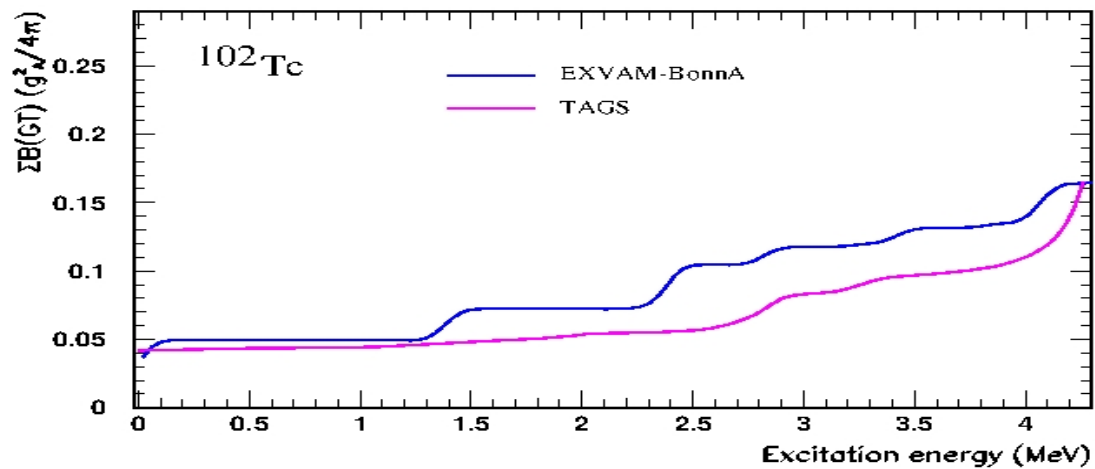
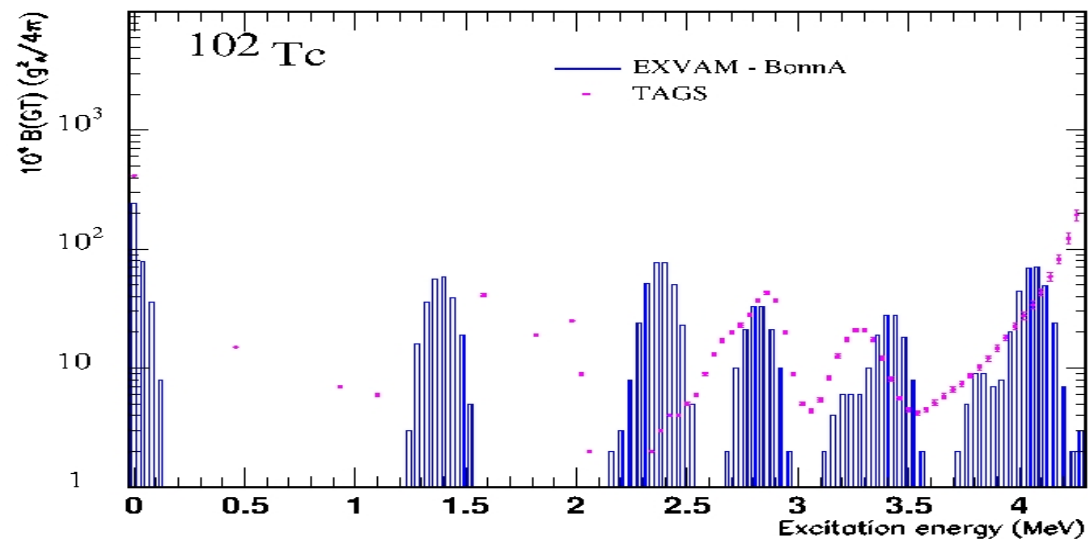
Gamow-Teller contributing states

2^+ : from 82% to 9% prolate components

4^+ : from 96% to 8% prolate components

Spectroscopic quadrupole moments:

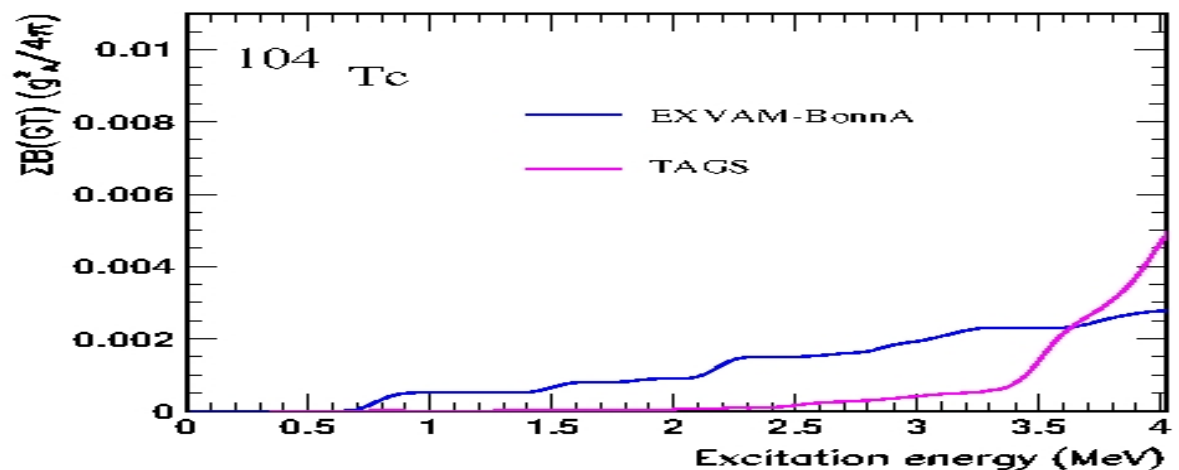
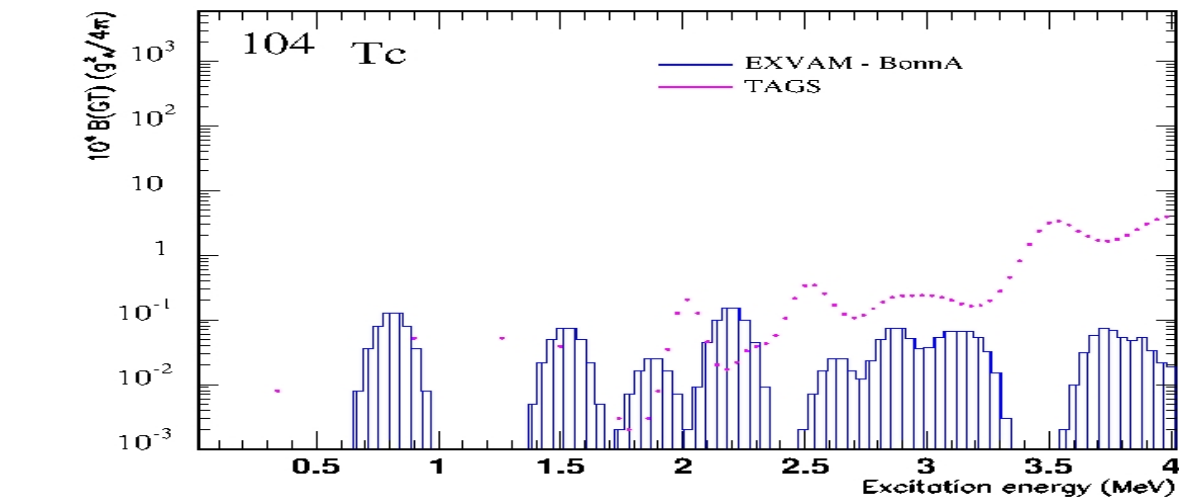
larger deformation for the $N=60$ states with respect to the $N=58$ ones



$$T_{1/2}^{\text{exp}} = 5.3 \text{ s}$$

$$T_{1/2}^{\text{EXVAM}} = 6.6 \text{ s}$$

Essential contribution from $g^{\pi}_{9/2} g^{\nu}_{7/2}$, $d^{\pi}_{5/2} d^{\nu}_{3/2}$, and $d^{\pi}_{5/2} d^{\nu}_{5/2}$ matrix elements



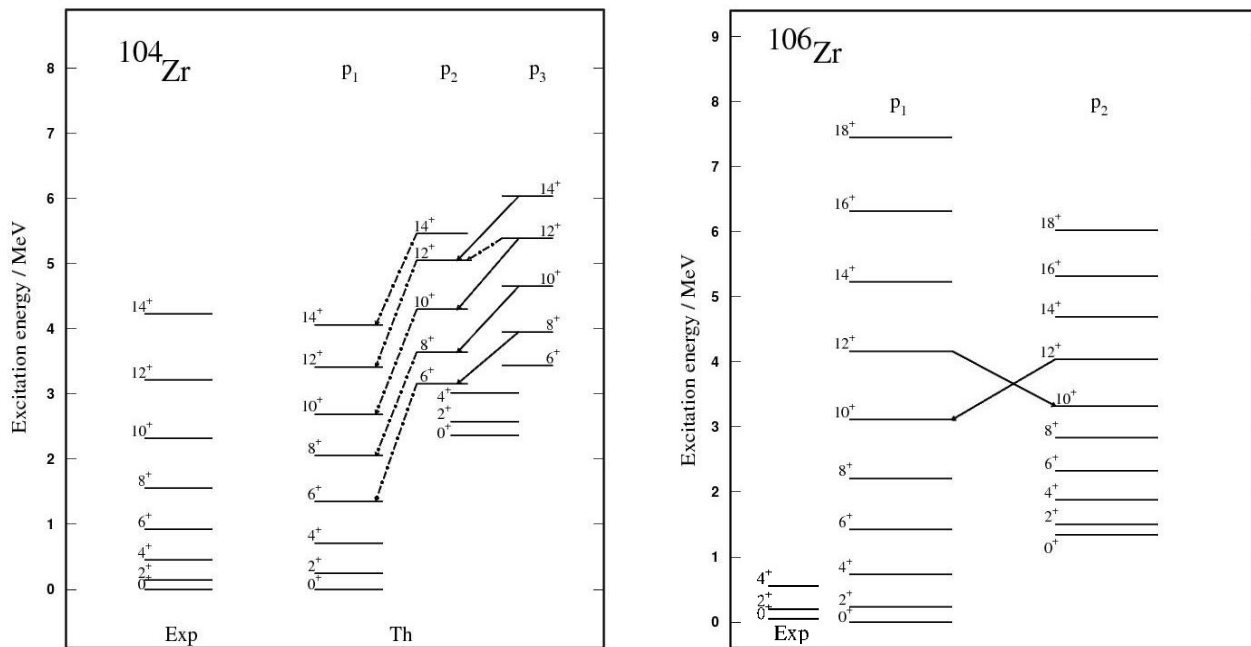
$$T_{1/2}^{\text{exp}} = 1098 \text{ s}$$

$$T_{1/2}^{\text{EXVAM}} = 385 \text{ s}$$

Contributions from $g^{\pi}_{9/2}g^{\nu}_{7/2}$, $d^{\pi}_{5/2}d^{\nu}_{3/2}$, $d^{\pi}_{5/2}d^{\nu}_{5/2}$, $p^{\pi}_{1/2}p^{\nu}_{3/2}$, $p^{\pi}_{3/2}p^{\nu}_{1/2}$ matrix elements, all small, manifesting also cancellation effect

Gamow-Teller β -decay half-lives and β -delayed neutron emission probabilities of Zr isotopes relevant for the r-process $A = 104, 106$

$98 - {}^{110}\text{Zr}$ chain : *rapid transition* $\rightarrow$ from spherical to deformed shape
shape coexistence $\rightarrow$ competing prolate, oblate, and spherical shapes



- variable mixing of prolate deformed EXVAM configurations at intermediate and high spins
- ground state dominated (99%) by a strongly deformed EXVAM configuration

$^{104}\text{Zr} \rightarrow ^{104}\text{Nb}$

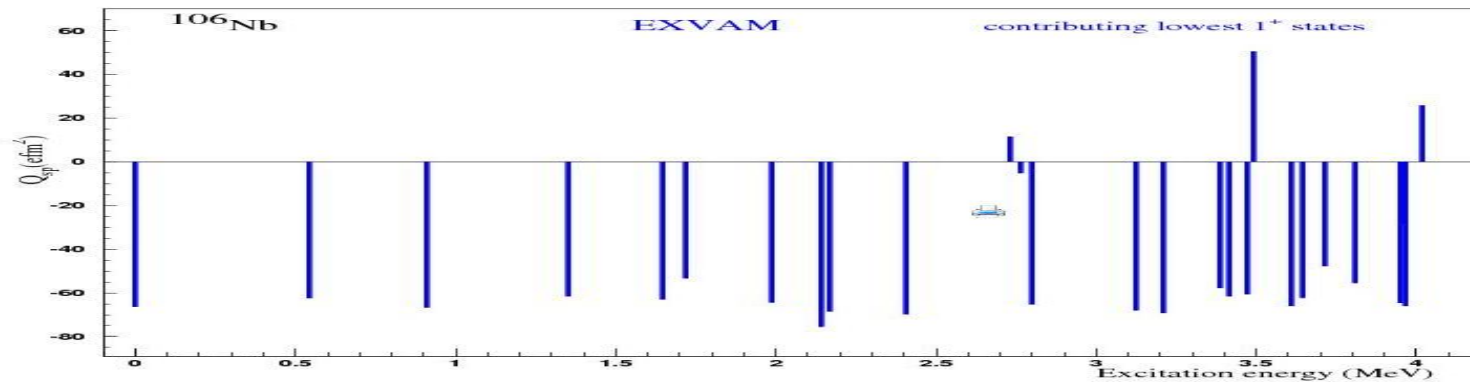
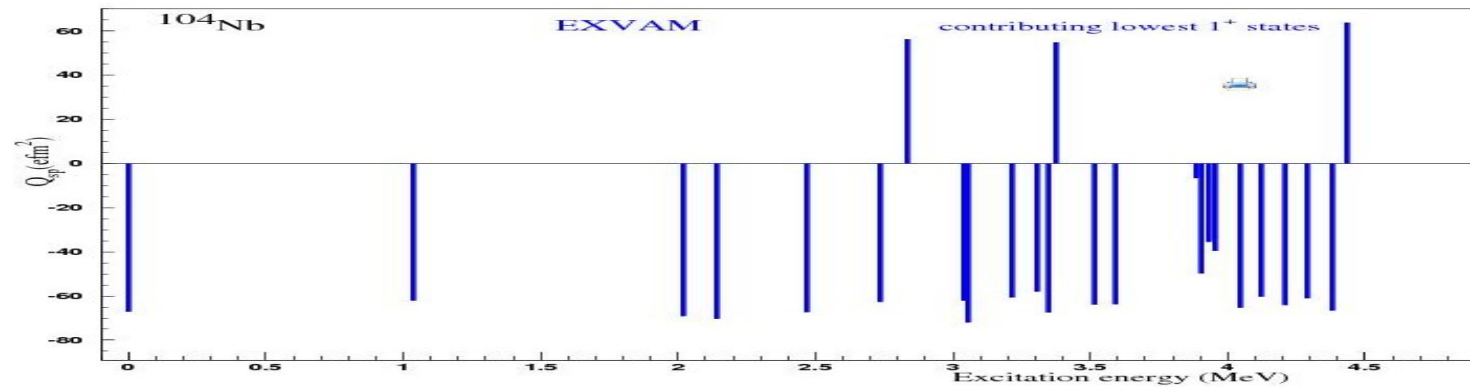
$^{106}\text{Zr} \rightarrow ^{106}\text{Nb}$

NCSL-MSU / J. Pereira et al., Phys. Rev. C79 (2009) 035801

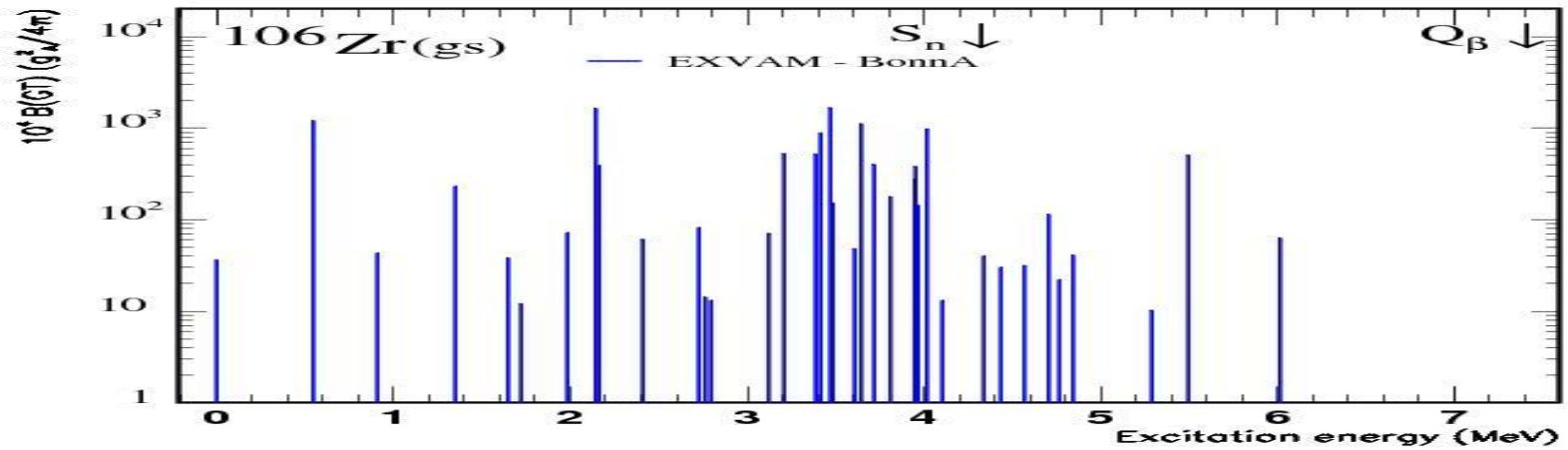
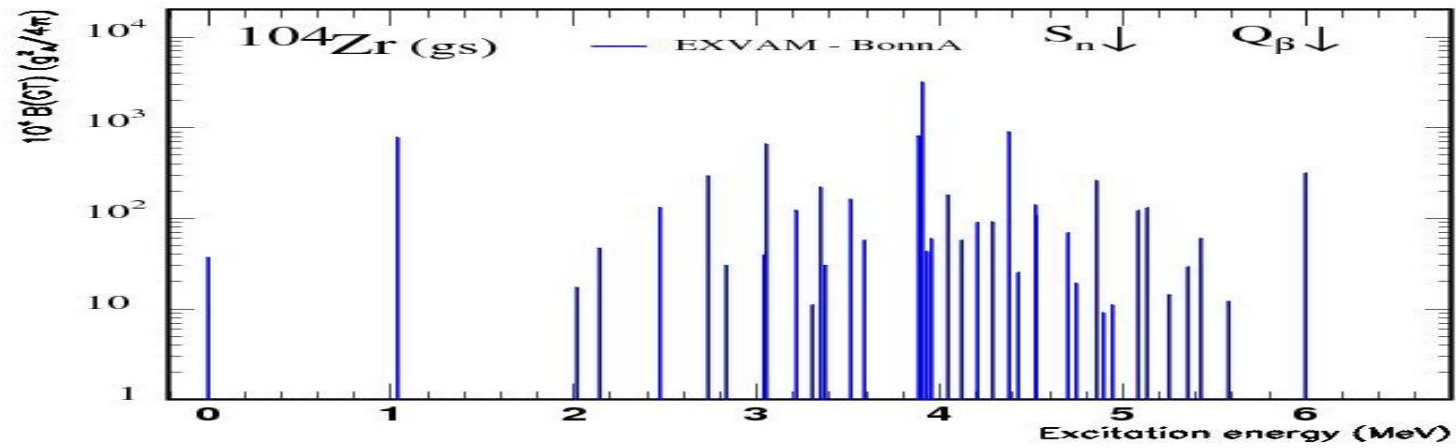
A. Petrovici et al., Prog. Part. Nucl. Phys. 66 (2011) 287

complex Excited Vampir many-nucleon basis: 50 projected 1^+ configurations in ^{104}Nb and ^{106}Nb

Gamow-Teller contributing states: large variety of spectroscopic quadrupole moments above 2 MeV excitation energy



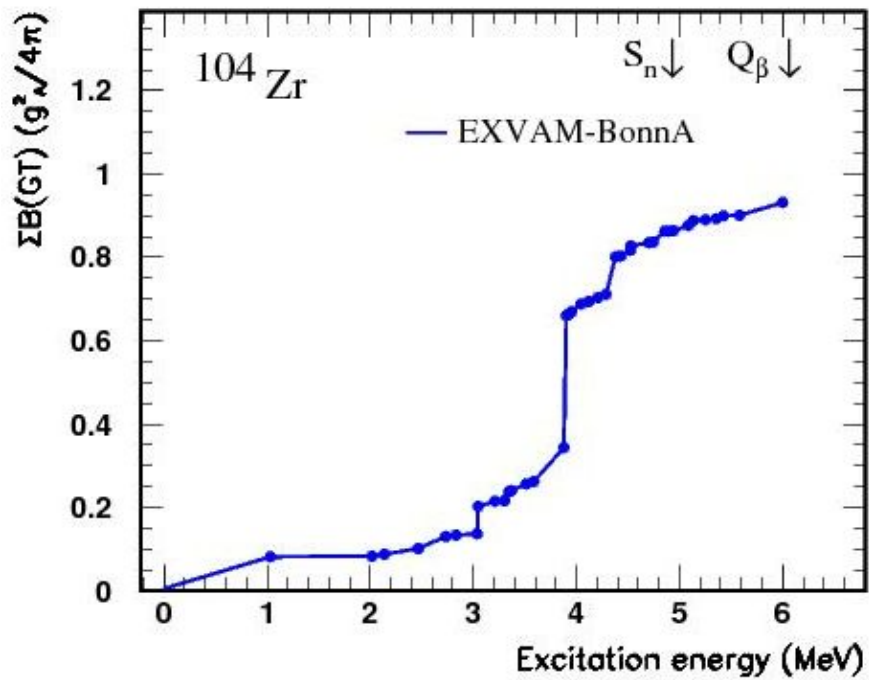
Gamow-Teller strength distribution specific for each isotope



Essential contribution from $g^{\pi_{9/2}} g^{\nu_{7/2}}$, $d^{\pi_{5/2}} d^{\nu_{3/2}}$, and $d^{\pi_{5/2}} d^{\nu_{5/2}}$ GT matrix elements

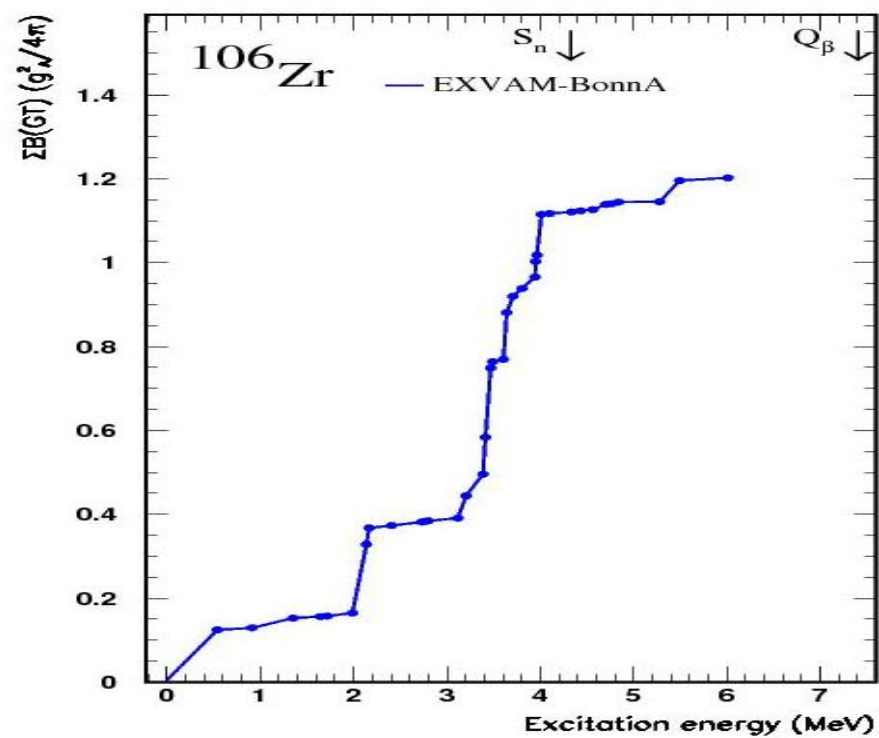
Gamow-Teller accumulated strengths, half-lives, β -delayed ν -emission probabilities

$$P_n = \frac{\frac{Q_\beta}{S_n} \sum f(Z, Q_\beta - E_{ex}) B(GT, E_{ex})}{\sum_0 f(Z, Q_\beta - E_{ex}) B(GT, E_{ex})}$$



$T_{1/2}^{exp} = 870(50)$
 $(30) \text{ ms (MSU 2009)}$
 $1200(300) \text{ ms (Mainz 1980)}$
 $P_n^{exp} < 1 \text{ \% (MSU 2009)}$

$T_{1/2}^{EXVAM} = 2040 \text{ ms}$
 $(50 \text{ } 1^+ \text{ states in } ^{104}\text{Nb})$
 $P_n^{EXVAM} \sim 1 \text{ \%}$



$T_{1/2}^{exp} = 260(20)$
 $(30) \text{ ms (MSU 2009)}$
 $P_n^{exp} < 7 \text{ \% (MSU 2009)}$

$T_{1/2}^{EXVAM} = 230 \text{ ms}$
 $(50 \text{ } 1^+ \text{ states in } ^{106}\text{Nb})$
 $P_n^{EXVAM} \sim 2 \text{ \%}$

Summary and outlook

complex EXCITED VAMPIR model explains self-consistently

- experimental trends in the N=58 Sr and Zr isotopes manifesting shape coexistence and mixing :
 - triple coexistence of spherical, prolate, and oblate configurations in the structure of lowest 4 0^+ states
 - multifaceted yrast structure specific for ^{96}Sr and ^{98}Zr
- large prolate deformation in ^{104}Zr and ^{106}Zr
- Gamow-Teller β -decay and β -delayed neutron-emission for $^{104,106}\text{Zr}$
- remarkable difference in the Gamow-Teller β -decay of ^{102}Tc and ^{104}Tc revealed by TAGS data

The effective interaction for the $A\sim 100$ region is currently improved starting from a G-matrix based on Bonn CD potential