Beyond-mean-field approach to shape coexistence phenomena in neutron-rich nuclei

A. PETROVICI

Horia Hulubei National Institute for Physics and Nuclear Engineering, Bucharest, Romania

Outline

- *complex* **EXCITED VAMPIR** ***beyond-mean-field variational*** **model**

  - **shape coexistence and first-forbidden β^- decay of ^{92}Rb (N=55) to ^{92}Sr (N=54)**

    - first-forbidden β^- decay of 0^-_{gs} of ^{92}Rb to 0^+_{gs} and 2^+ states in ^{92}Sr

  - **shape coexistence and first-forbidden β^- decay of ^{98}Y (N=59) to ^{98}Zr (N=58)**

    - low-lying isomeric states in ^{98}Y

    - exotic structure and dynamics of low-spin states in ^{98}Zr

    - first-forbidden β^- decay of 0^-_{gs} of ^{98}Y to 0^+ and 2^+ states in ^{98}Zr

Neutron-rich A~100 nuclei manifest dramatic evolution in structure and dynamics :

- *shape transition, shape coexistence, shape mixing*
- *drastic changes in structure with particle number, spin, and excitation energy*
- *particular variations and even "sudden" changes correlated with the onset of deformation around N=58 in Sr and Zr isotopic chains, but a more gradual evolution in the Kr chain*

Challenges for theory

- *beyond-mean-field methods*
- *realistic effective Hamiltonians in adequate large model spaces*

aiming at

- *unitary description of structure and β-decay properties*
- *comprehensive understanding of multifaceted impact of shape coexistence and mixing*

complex EXCITED VAMPIR model

- ***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***

  (include unnatural-parity two-body correlations and T=1 and T=0 neutron-proton pairing correlations already at the mean-field level)

- ***the broken symmetries (s=N, Z, I, p) are restored by projection before variation***

*∗ **The model allows to use rather large model spaces and realistic effective interactions***

complex EXCITED VAMPIR model - *beyond-mean-field variational approach*

VAMPIR

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

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

Θ^s_{00} - symmetry projector

$|F^s_1>$ - HFB vacuum

EXCITED VAMPIR

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

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

Allows to identify in a small energy interval spherical, oblate, prolate deformed orthogonal configurations of a given symmetry.

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

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

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

Projected configurations significantly correlated could become strongly mixed by the final diagonalization.

$$|\Psi_\alpha^{(n)}; sM > = \sum_{i=1}^{n} |\psi_i; sM > f_{i\alpha}^{(n)}, \qquad \alpha = 1, ..., n$$

Neutron-rich nuclei in the A=100 mass region

^{40}Ca - core

model space for both protons and neutrons :

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

Effective interaction - renormalized G-matrix (Bonn CD potential)

- ***pairing properties enhanced by short range Gaussians for:***

  T = 1 pp, nn channels

  T = 0 and 1 np channels

- ***onset of deformation influenced by monopole shifts:***

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

$$\langle 0f_{5/2}\ 1d;\ T=0\ |G|\ 0f_{5/2}\ 1d; T=0\rangle$$

$$\langle 0g_{9/2}\ 0h_{11/2};\ T=0\ |G|\ 0g_{9/2}\ 0h_{11/2}; T=0\rangle$$

- ***Coulomb interaction between valence protons added***

First-forbidden beta decay formalism

$$\frac{1}{t_{1/2}} = \frac{f}{K} \qquad f = \int_1^{W_0} C(W)W(W^2-1)^{1/2}(W_0-W)^2F(Z,W)dW,$$

first-forbidden $\quad 0^- \rightarrow 0^+ \qquad C(W) = k + kb/W$

$$O(0^-) = \sum_{ab} o^{(0)}(0^-)(ab)\langle \xi_f J_f||[c_a^\dagger \tilde{c}_b]_0||\xi_i J_i\rangle$$

$$w = -g_A\sqrt{3}\langle a||r[\boldsymbol{C}_1 \times \boldsymbol{\sigma}]^{(0)}||b\rangle$$

$$w' = -g_A\sqrt{3}\langle a||\frac{2}{3}rI(1,1,1,1,r)[\boldsymbol{C}_1 \times \boldsymbol{\sigma}]^{(0)}||b\rangle$$

$$v = \frac{\epsilon_{mec} g_A \sqrt{3}}{M}\langle a||[\boldsymbol{\sigma} \times \boldsymbol{\nabla}]^{(0)}||b\rangle$$

first-forbidden $\quad 0^- \rightarrow 2^+ \qquad C(W) = k + kaW + kcW^2$

$$O(0^-) = \sum_{ab} o^{(2)}(0^-)(ab)\langle \xi_f J_f||[c_a^+ \tilde{c}_b]_2||\xi_i J_i\rangle$$

$$z = 2g_A\langle a||r[\mathbf{C_1} \times \boldsymbol{\sigma}]^2||b\rangle$$

Shape coexistence and first-forbidden β^- decay of ^{92}Rb to ^{92}Sr

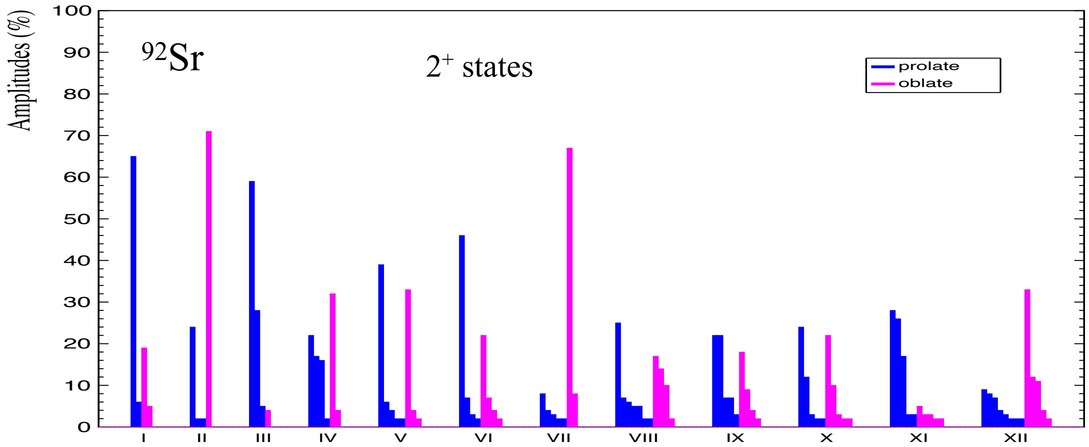
A. Petrovici, Phys. Rev. C 109, 024303 (2024)

***^{92}Rb : 0^-_{gs} - spherical** configuration*

(spherical occupation $(d^{\nu}_{5/2})^{4.81}$)

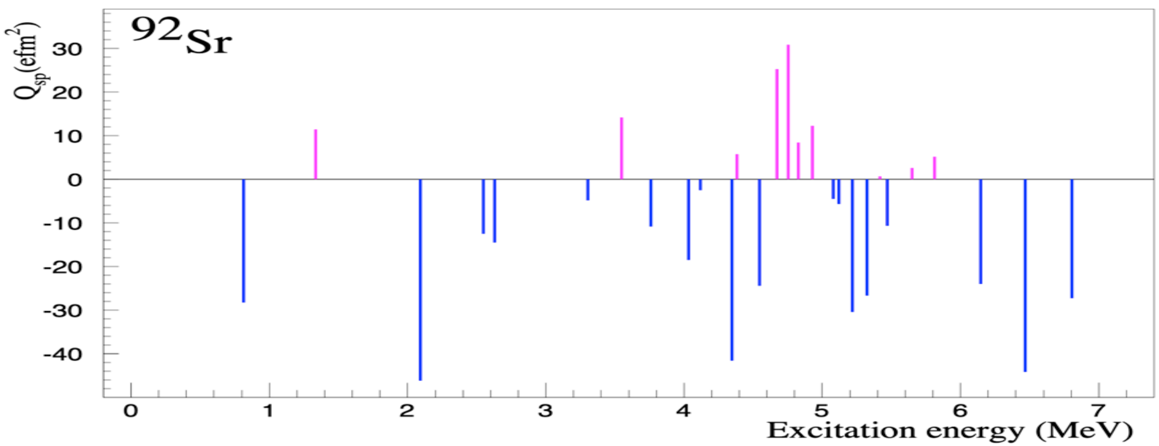
^{92}Sr : 0^+_{gs} - multiple shape coexistence : spherical (57%),

***prolate (28%), oblate (15%)** configurations*



β_2= 0.06 ÷ 0.31

β_2= - 0.18 ÷ - 0.25



$B^{EXP}(E2;2^+_1 \rightarrow 0^+_{gs})$=197(74) e^2fm^4

$B^{EXVAM}(E2;2^+_1 \rightarrow 0^+_{gs})$=277 e^2fm^4

First-forbidden β⁻ decay of the 0⁻ ground state of ^{92}Rb to 0⁺ ground state of ^{92}Sr

$$v = \frac{\epsilon_{mec} g_A \sqrt{3}}{M} \langle a || [\boldsymbol{\sigma} \times \boldsymbol{\nabla}]^{(0)} || b \rangle$$

Log *ft values for the decay of 0^-_{gs} of ^{92}Rb to 0^+_{gs} of ^{92}Sr*

$\epsilon_{\rm mec} = 1.3$	$\epsilon_{\rm mec} = 1.4$	$\epsilon_{\rm mec} = 1.5$	Expt.
5.92	5.78	5.66	5.75

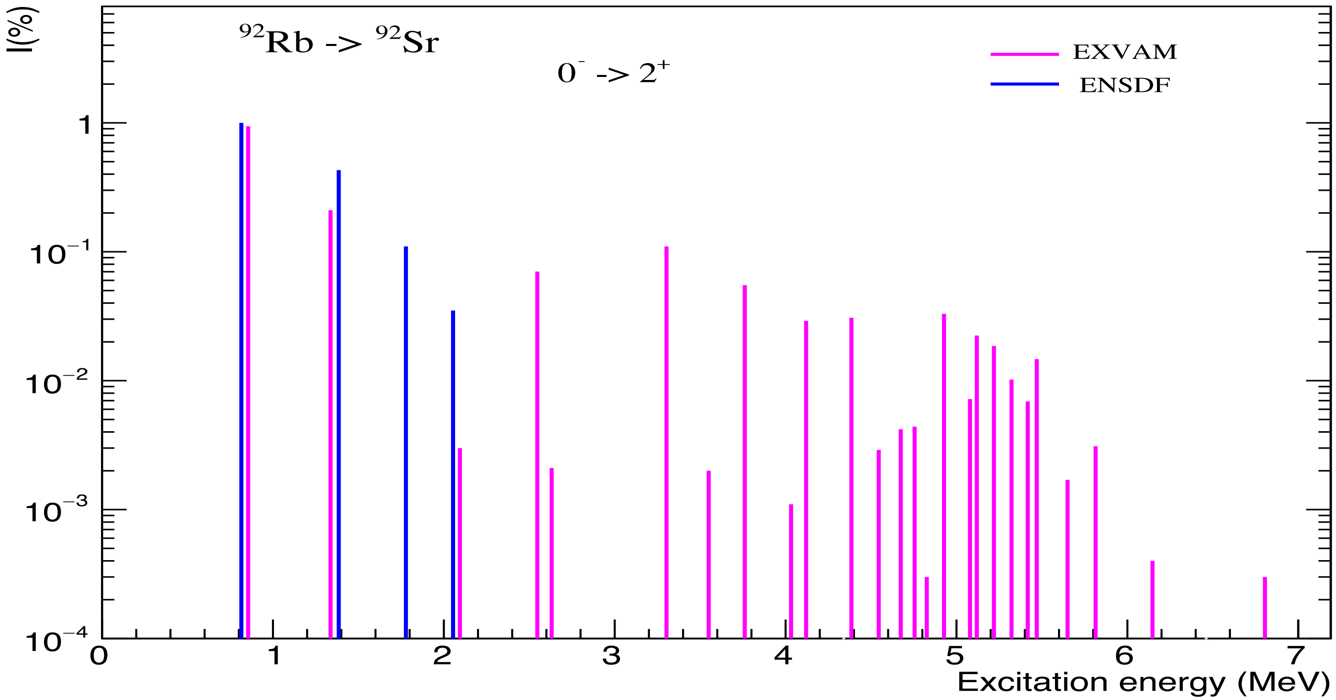
Contributions: - main : $d^{\nu}_{5/2} f^{\pi}_{5/2}$ matrix elements

- very small effects: $s^{\nu}_{1/2} p^{\pi}_{1/2}$, $d^{\nu}_{3/2} p^{\pi}_{3/2}$, $g^{\nu}_{7/2} f^{\pi}_{7/2}$ matrix elements

Log *ft values for the decay of 0^-_{gs} of ^{92}Rb to 0^+_{gs} of ^{92}Sr constraining the final state to 100% spherical, prolate or oblate content*

	$\epsilon_{\rm mec} = 1.3$	$\epsilon_{\rm mec} = 1.4$	$\epsilon_{\rm mec} = 1.5$
$0^+_{\rm spherical}$	5.62	5.49	5.37
$0^+_{\rm prolate}$	7.57	7.45	7.34
$0^+_{\rm oblate}$	9.15	9.06	9.02

First-forbidden β^- decay of 0^- ground state of ^{92}Rb to 2^+ states in ^{92}Sr



Q_{gg} = 8.095 MeV

Significant first-forbidden unique transitions in the high-energy region –

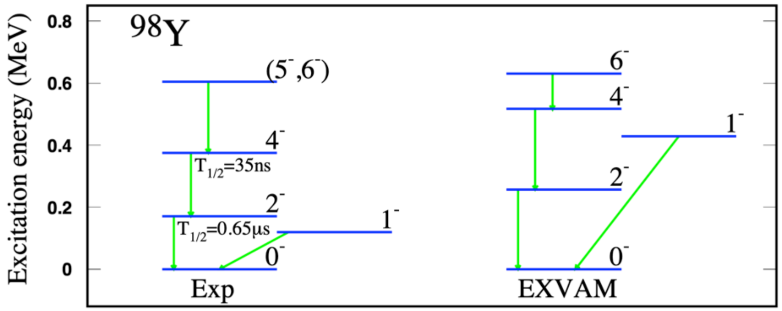
relevant input for the investigation of the reactor antineutrino spectra

Contributions: - main : $d^{\nu}_{5/2} f^{\pi}_{5/2}$ matrix elements

- small effects: $d^{\nu}_{5/2} p^{\pi}_{1/2}$, $d^{\nu}_{5/2} p^{\pi}_{3/2}$, $g^{\nu}_{7/2} f^{\pi}_{5/2}$ matrix elements

Multiple shape coexistence in ^{98}Zr by first-forbidden β^- decay of ^{98}Y

Low-lying isomeric states in ^{98}Y



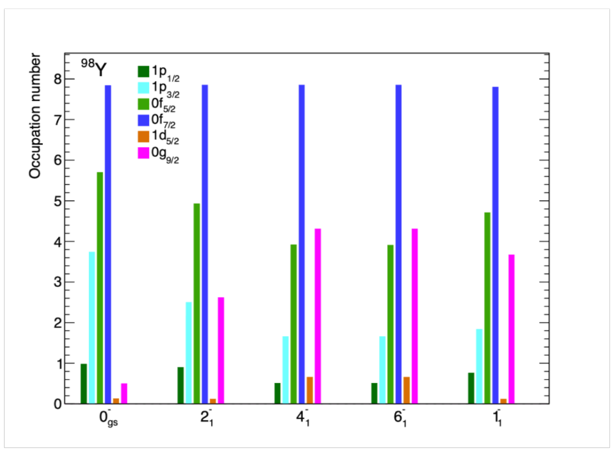
0^-_{gs} : spherical configuration

2^-_1 : mixing of oblate deformed configurations

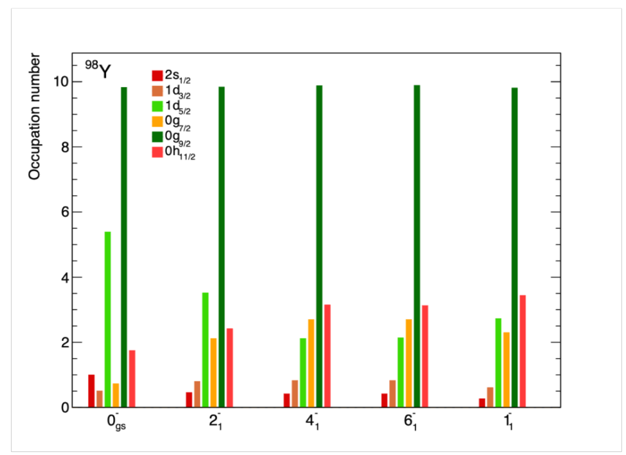
4^-_1 : prolate deformed configuration

6^-_1 : prolate deformed configuration

1^-_1 : mixing of oblate deformed configurations



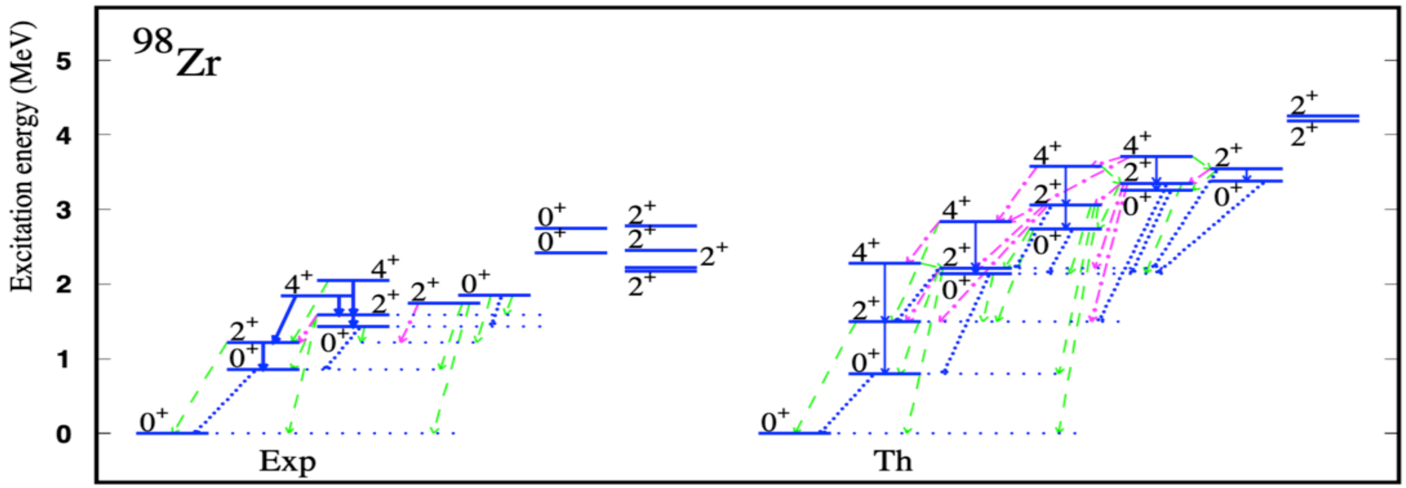
Proton occupation of valence spherical orbitals



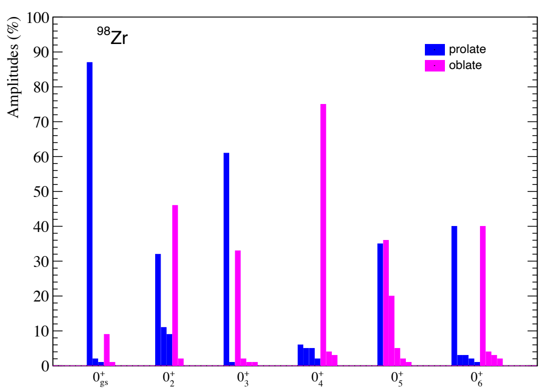
Neutron occupation of valence spherical orbitals

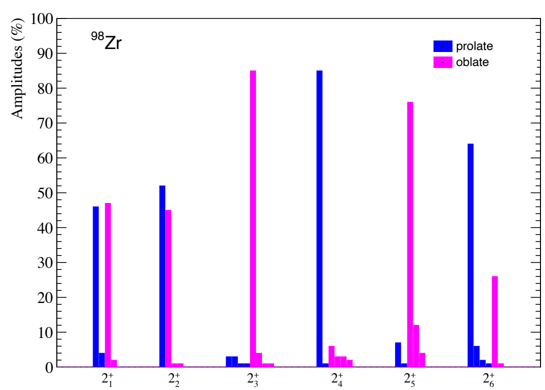
Multifaceted impact of shape coexistence at low-spins in ^{98}Zr

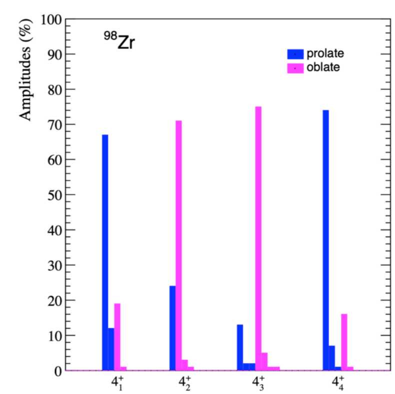
Spectrum of ^{98}Zr populated by β^- decay of ^{98}Y



Spherical, prolate, oblate mixing in the structure of the wave functions



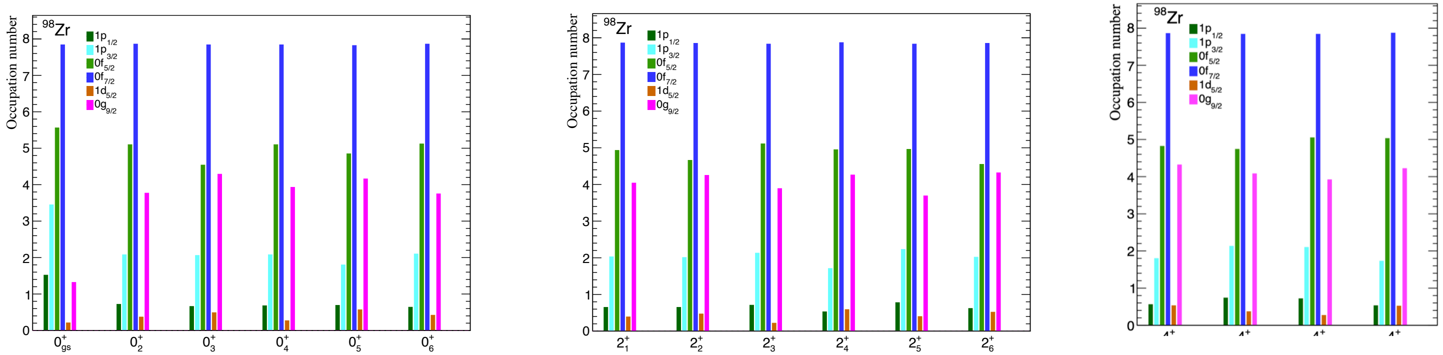




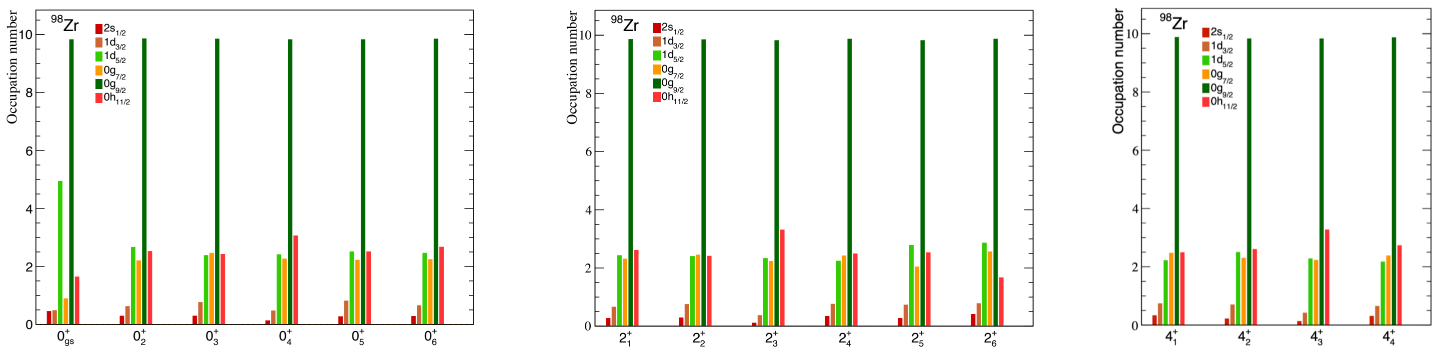
β_2= 0.03 ÷ 0.36 *β_2= - 0.24 ÷ - 0.34*

Occupation of valence spherical orbitals

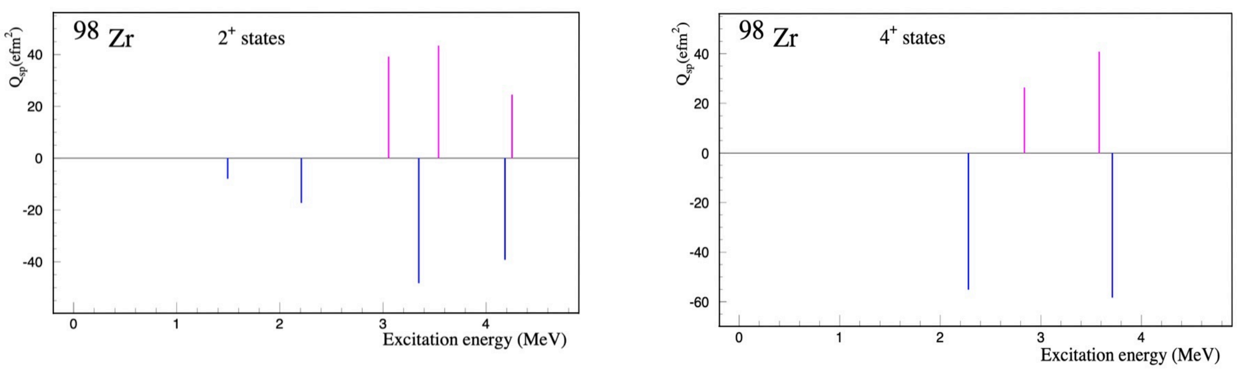
Protons



Neutrons



Spectroscopic quadrupole moments



$g(2^+_1) = 0.48 \quad g(2^+_2) = 0.48 \quad g(2^+_3) = 0.435$

$g(4^+_1) = 0.49 \quad g(4^+_2) = 0.43 \quad g(4^+_3) = 0.33$

E0 transitions

$\rho^2(E0)$ values for the lowest six 0^+ states in ^{98}Zr

$I[\hbar]$	EXVAM 0_2^+	EXP 0_2^+	EXVAM 0_3^+	EXP 0_3^+	EXVAM 0_4^+	EXP 0_4^+	EXVAM 0_5^+	EXVAM 0_6^+
0_1^+	0.033	0.0112(12)						
0_2^+			0.020	0.076(6)			0.005	0.007
0_3^+					0.022	0.061(8)	0.013	0.011
0_4^+								0.006

$\rho^2(E0)$ values for 2^+ and 4^+ states in ^{98}Zr

Transition	EXVAM	Transition	EXVAM
$2_2^+ \to 2_1^+$	0.013	$4_2^+ \to 4_1^+$	0.009
$2_3^+ \to 2_1^+$	0.004	$4_4^+ \to 4_1^+$	0.016
$2_4^+ \to 2_1^+$	0.012	$4_3^+ \to 4_2^+$	0.008
$2_5^+ \to 2_1^+$	0.006		
$2_3^+ \to 2_2^+$	0.011		
$2_4^+ \to 2_2^+$	0.006		
$2_5^+ \to 2_2^+$	0.020		
$2_5^+ \to 2_3^+$	0.005		
$2_7^+ \to 2_5^+$	0.012		

E2 transition strengths

$B(E2;\Delta I=2)$ (W.u.) in ^{98}Zr

Transition	EXVAM	Cologne(2020)	ENSDF
$2_1^+ \to 0_1^+$	3.5	1.1 *+0.3-0.2*	2.9 *+8-5*
$2_1^+ \to 0_2^+$	28.1	11 *+3-2*	29 *+8-6*
$0_3^+ \to 2_1^+$	3.7		58 *8*
$0_4^+ \to 2_1^+$	0.45		0.103 *8*
$2_2^+ \to 0_1^+$	0.04	0.26 *+0.20-0.08*	
$2_2^+ \to 0_2^+$	1.24	1.8 *+1.4-0.6*	
$2_2^+ \to 0_3^+$	34.6	40 *18*^{Triumf}	
$0_4^+ \to 2_2^+$	0.75		42 *3*
$2_3^+ \to 0_1^+$	0.13	0.14 *+0.12-0.04*	
$2_3^+ \to 0_2^+$	0.25	1.7 *+1.5-0.5*	
$2_3^+ \to 0_3^+$	0.25		
$2_3^+ \to 0_4^+$	23.8		
$2_4^+ \to 0_3^+$	2.3		
$2_4^+ \to 0_4^+$	0.64		
$2_4^+ \to 0_5^+$	24.9		
$0_6^+ \to 2_4^+$	53.5		
$2_5^+ \to 0_5^+$	6.9		
$2_5^+ \to 0_6^+$	18.7		
$4_1^+ \to 2_1^+$	43.6	25 *+15-7*	42 *+10-7*
$4_1^+ \to 2_2^+$	10.6	38 *+26-13*	54 *+18-16*
$4_2^+ \to 2_1^+$	1.56	0.6 *+0.17-0.12*	
$4_2^+ \to 2_2^+$	40.4	4.6 *+1.7-1.3*	
$4_3^+ \to 2_3^+$	30.7		
$4_3^+ \to 2_4^+$	4.7		
$4_4^+ \to 2_4^+$	47.7		
$4_4^+ \to 2_5^+$	3.9		

$B(E2;\Delta I=0)$ (W.u.) in ^{98}Zr

Transition	EXVAM	Cologne(2020)	Triumf(2023)
$2_2^+ \to 2_1^+$	41.6	46 *+35-14*	33 *17*
$2_3^+ \to 2_1^+$	0.3	7.6 *+6.5-2.3*	
$2_3^+ \to 2_2^+$	0.5		
$2_4^+ \to 2_1^+$	2.3		
$2_4^+ \to 2_2^+$	5.9		
$2_4^+ \to 2_3^+$	4.6		
$2_5^+ \to 2_3^+$	0.4		
$2_5^+ \to 2_4^+$	13		
$2_6^+ \to 2_3^+$	4.6		
$4_2^+ \to 4_1^+$	28.2		
$4_3^+ \to 4_2^+$	1.2		
$4_4^+ \to 4_2^+$	5.5		
$4_4^+ \to 4_3^+$	16.8		

First-forbidden β⁻ decay of 0⁻ ground state of ^{98}Y to 0^+ states in ^{98}Zr

^{98}Y : 0^-_{gs} - **spherical** configuration

0^-_{gs} : $(s^{\nu}_{1/2})^1\,(d^{\nu}_{5/2})^{5.39}$

^{98}Zr : 0^+_{gs} : **spherical (87%), prolate (3%), oblate (10%)** configurations

0^+_{gs} : $(d^{\nu}_{5/2})^{4.94}$

$$v = \frac{\epsilon_{mec} g_A \sqrt{3}}{M} \langle a || [\boldsymbol{\sigma} \times \boldsymbol{\nabla}]^{(0)} || b \rangle$$

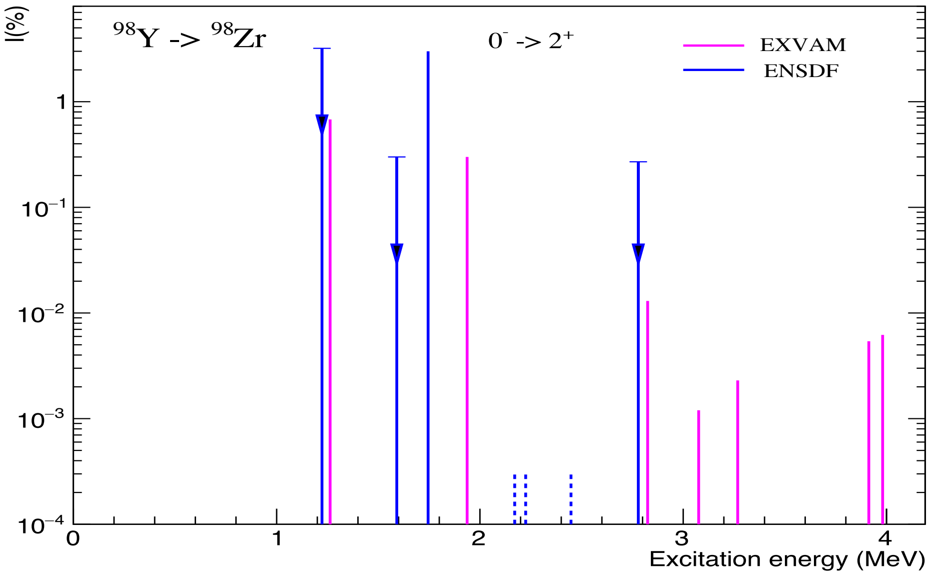
Log *ft values for the decay of* 0^-_{gs} *of* ^{98}Y *to* 0^+ *states in* ^{98}Zr

$I[\hbar]$	EXVAM (ϵ_{mec} =1.15)	Exp.
0^+_{gs}	5.75	5.8 (2)
0^+_2	6.56	$>$ 7.2
0^+_3	7.53	6.0 (1)
0^+_4	7.76	5.6 (1)
0^+_5	7.34	
0^+_6	7.66	

Contributions: - main : $s^{\nu}_{1/2}\,p^{\pi}_{1/2}$ matrix elements

- very small (or cancelling effects): $d^{\nu}_{3/2}\,p^{\pi}_{3/2}$ and $d^{\nu}_{5/2}\,f^{\pi}_{5/2}$ matrix elements

First-forbidden β^- decay of 0^- ground state of ^{98}Y to 2^+ states in ^{98}Zr



Q_{gg} = 8.992 MeV

Contributions: *$s^{\nu}{}_{1/2}\,p^{\pi}{}_{3/2}$, $d^{\nu}{}_{5/2}\,p^{\pi}{}_{1/2}$, and $d^{\nu}{}_{5/2}\,f^{\pi}{}_{5/2}$ matrix elements*

Summary

Comprehensive understanding of multifaceted impact of shape coexistence in neutron-rich nuclei *within* ***complex*** **Excited Vampir** ***beyond-mean field variational model***

- ***Shape coexistence and first-forbidden*** β^- ***decay of*** ^{92}***Rb to*** ^{92}***Sr***

  - ^{92}***Rb*** **-** ***spherical*** **0^- ground state**

  - ^{92}***Sr*** **-** ***spherical-prolate-oblate mixing*** *in* **0^+ ground state**

    - ***complex prolate-oblate mixing*** *in* **2^+ states** (signature - ***spectroscopic quadrupole moments***)

  * ***significant first-forbidden unique transitions in high-energy region -*** *relevant for* ***reactor antineutrino anomalies***

- ***Multiple shape coexistence and first-forbidden*** β^- ***decay of*** ^{98}***Y to*** ^{98}***Zr***

  - ^{98}***Y*** - ***spherical*** **0^- ground state**

    - ***variable mixing of prolate and oblate configurations*** *creates* ***low-spin isomers***

  - ^{98}***Zr*** **-** ***spherical-prolate-oblate mixing*** in **0^+ states** *induces* ***significant E0 transitions***

    - ***variable prolate-oblate mixing*** in **2^+ and 4^+ states** *induces* ***complex decay pattern***

  * ***unitary description of exotic structure and first-forbidden*** β^- ***decay induced by multiple shape coexistence***