



Int. Workshop on Shapes and Symmetries in Nuclei:
From Experiment to Theory (SSNET' 2016)

Gif sur Yvette

November 8 (7-11), 2016

Shell evolution, shape transition and shape coexistence
with realistic nuclear forces

Takaharu Otsuka *University of Tokyo / MSU / KU Leuven*

Yusuke Tsunoda (CNS, Tokyo)

Tomoaki Togashi (CNS, Tokyo)

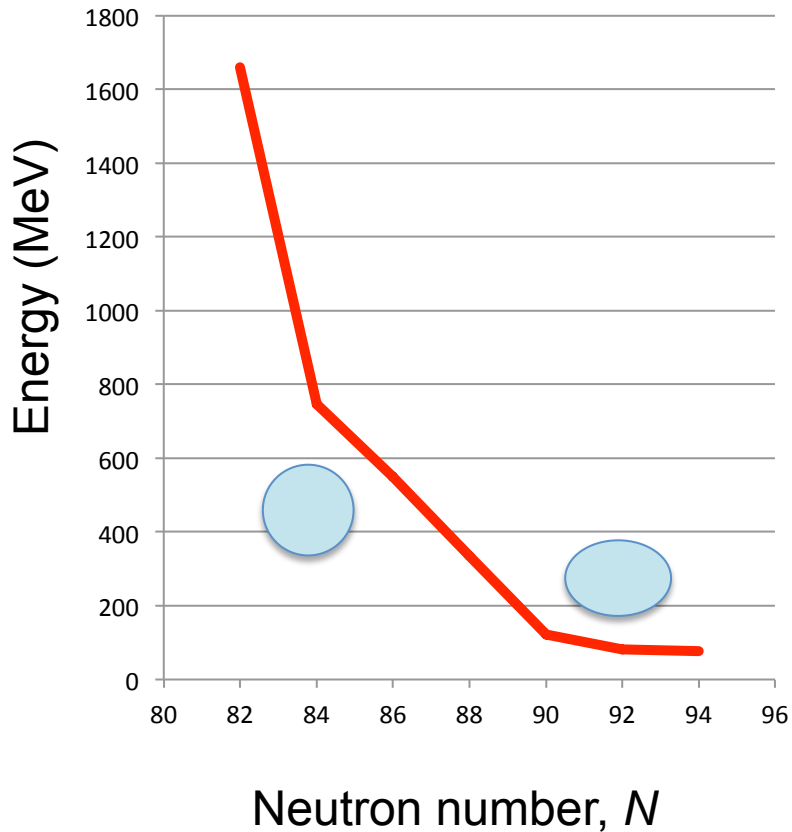
Noritaka Shimuzu (CNS, Tokyo)

Outline

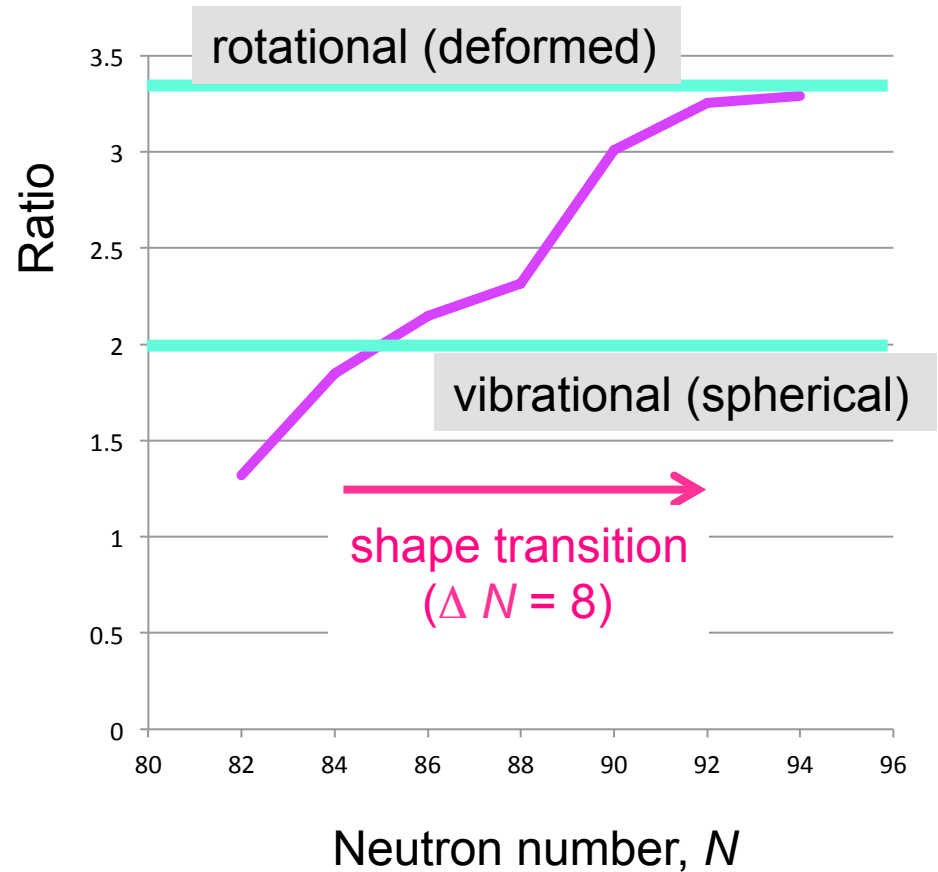
- Introduction
 - shapes and phase transition
- Computational background : advanced Monte Carlo shell model (MCSM)
 - intrinsic shapes of shell-model wave functions (T-plot)
- Shape transition in Zr isotopes and Quantum Phase Transition
- Summary and Perspectives
 - Are symmetries in shapes favored in atomic nuclei ?*

2⁺ and 4⁺ level properties of Sm isotopes

Ex (2⁺) :
excitation energy of first 2⁺ state



$$R_{4/2} = \text{Ex}(4^+) / \text{Ex}(2^+)$$



Can this be a kind of *Phase Transition* ?

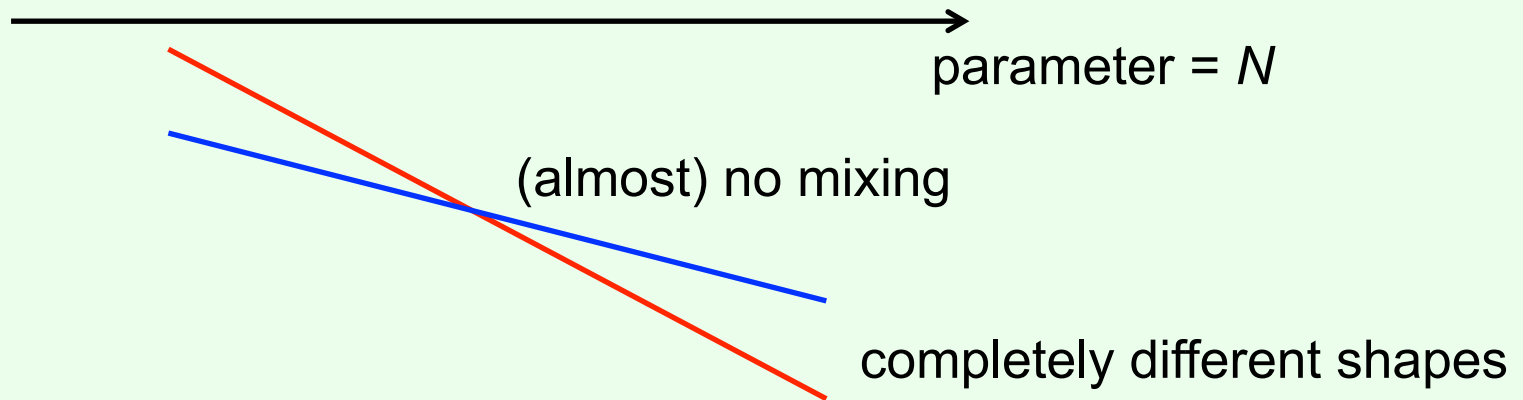
Can the **shape transition** be a “**Quantum Phase Transition**” ?

The shape transition occurs rather gradually.

The **definition** of Quantum Phase Transition :

an **abrupt change** in the **ground state** of a many-body system by varying a **physical parameter** at zero temperature

possible scenario



The usual shape transition may not fulfill the condition being *abrupt*.
Where can we see it ?

If it occurs in atomic nuclei, what is the underlying mechanism ?

Note that sizable mixing occurs usually in finite quantum systems.

Outline

- Introduction
 - shapes and phase transition
- Computational background : advanced Monte Carlo shell model (MCSM)
 - intrinsic shapes of shell-model wave functions (T-plot)
- Shape transition in Zr isotopes and Quantum Phase Transition
- Summary and Perspectives

Advanced Monte Carlo shell model (MCSM)

Superposition of the projected Slater determinants
+ Extrapolation by energy variance

$$|\Psi\rangle = \sum_{k=1}^{N_{MCSM}} f_k P^{J,\pi} |\phi_k\rangle \quad |\phi_k\rangle = \prod_{\alpha=1}^N \left(\sum_{i=1}^{N_{sp}} c_i^\dagger D_{i\alpha}^{(k)} \right) |-\rangle$$

MCSM basis, deformed Slater det.

>10¹⁰ basis vectors

$$\mathbf{H} = \begin{pmatrix} * & * & * & * & * & \dots \\ * & * & * & * & \dots & \dots \\ * & * & * & \dots & \dots & \dots \\ * & * & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix} \xrightarrow{\text{diagonalization}} \begin{pmatrix} \varepsilon_1 & & & & & 0 \\ & \varepsilon_2 & & & & \\ & & \varepsilon_3 & & & \\ & & & \dots & & \\ & & & & \dots & \\ 0 & & & & & \dots \end{pmatrix}$$

Conventional Shell Model
all Slater determinants

$$\mathbf{H} \approx \begin{pmatrix} * & * & * & \dots \\ * & * & * & \dots \\ * & * & \dots & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \xrightarrow{\text{diagonalization}} \begin{pmatrix} \varepsilon'_1 & & 0 \\ & \varepsilon'_2 & \\ 0 & & \dots \end{pmatrix}$$

Monte Carlo Shell Model
bases important for a specific eigenstate

~10² basis vectors

Step 1

- **Select D** stochastically from many candidates generated by the auxiliary-field Monte Carlo technique

Step 2

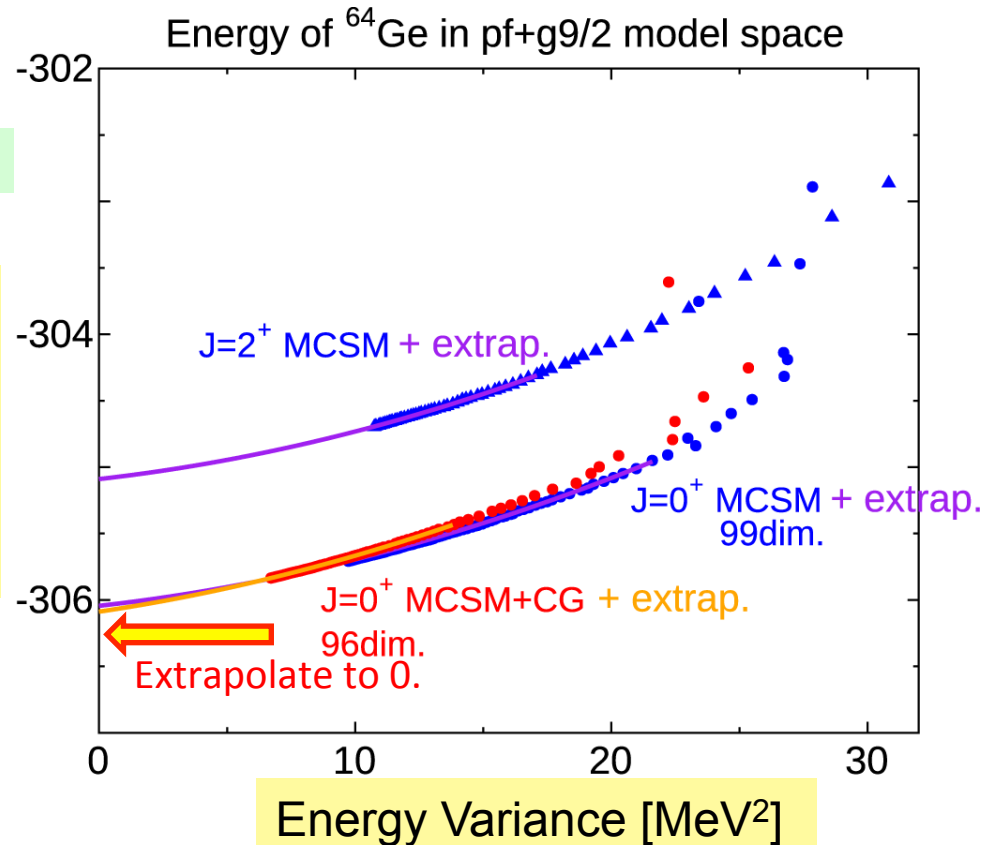
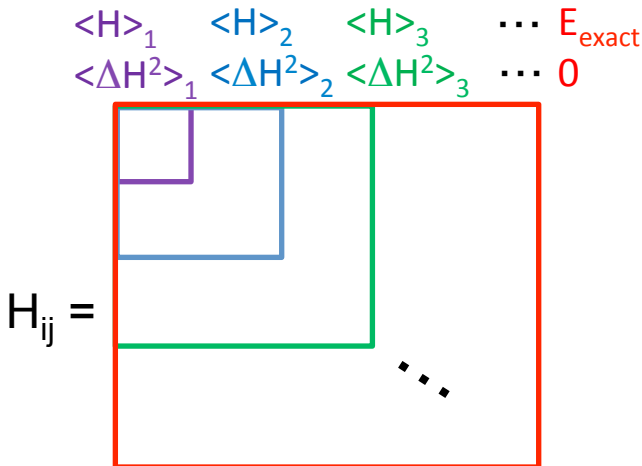
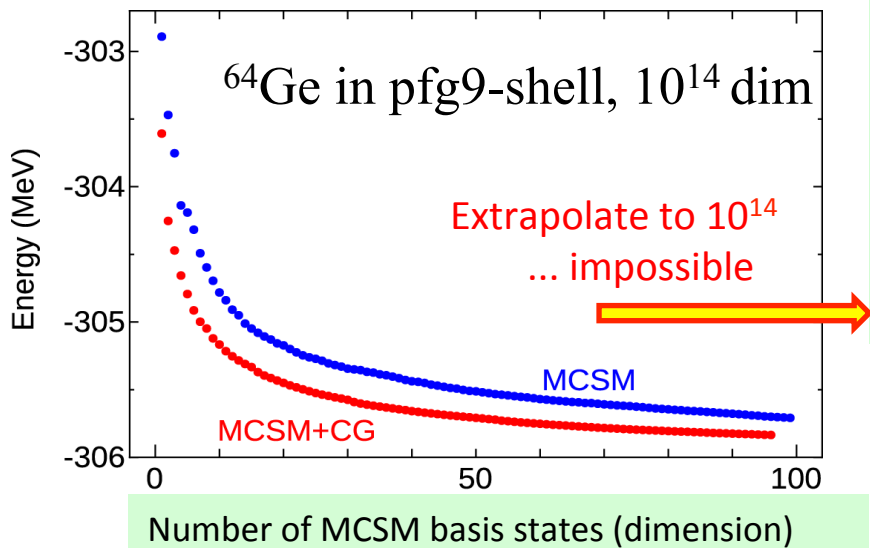
- **optimize D** variationally by the conjugate gradient method so as to minimize the energy eigenvalue of this small matrix

Step 3: Energy variance extrapolation

$$\text{Energy variance: } \langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$$

As the number of basis vectors increases, the approximated w.f. approaches the exact one and the energy variance approaches zero.

$$\text{Extrapolate towards } \langle \Delta H^2 \rangle \rightarrow 0$$



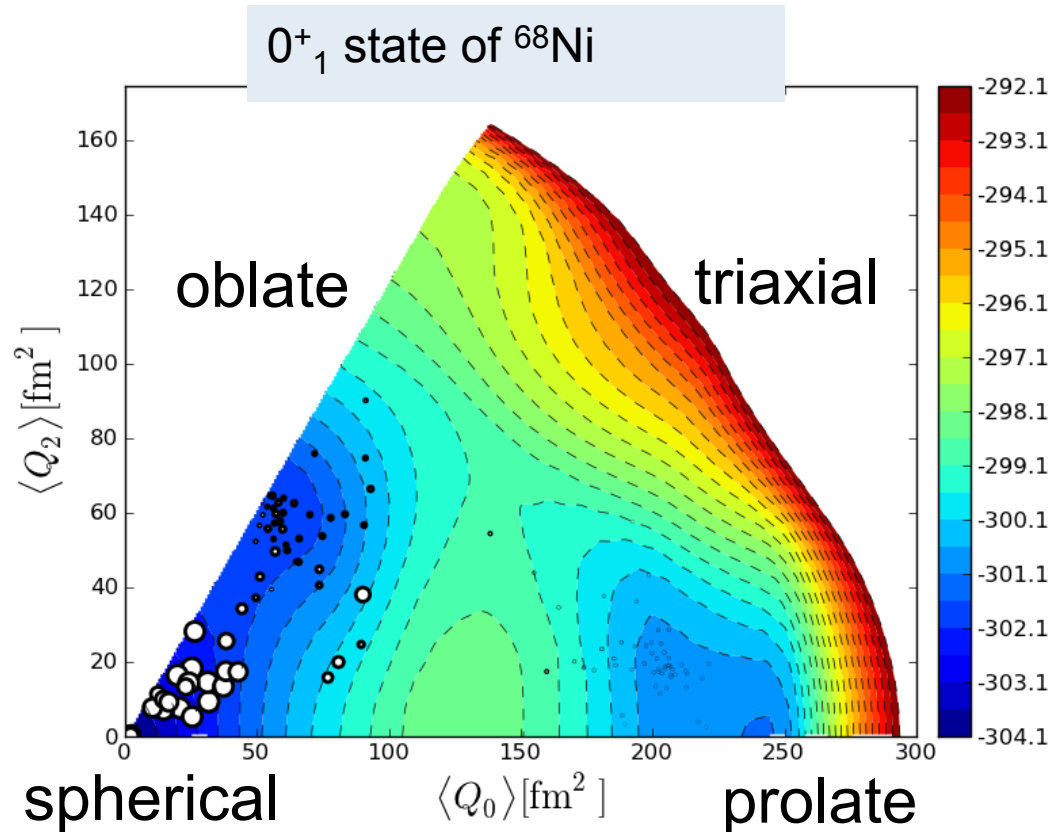
MCSM basis vectors on Potential Energy Surface (*T-plot*)

eigenstate

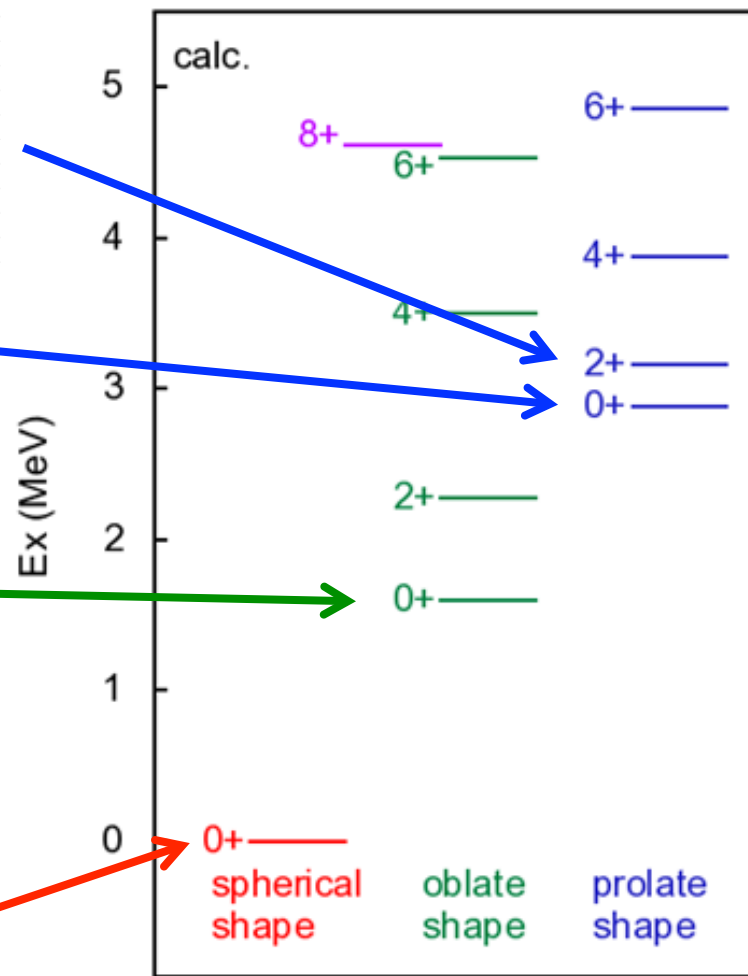
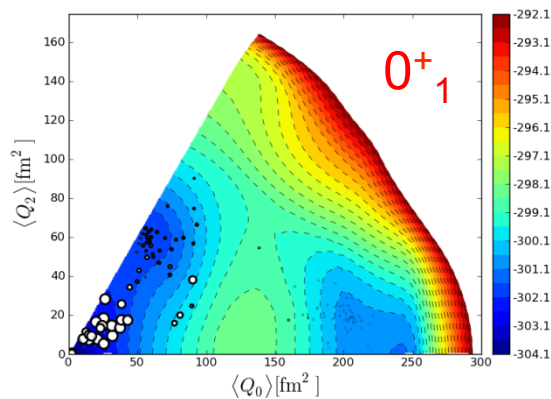
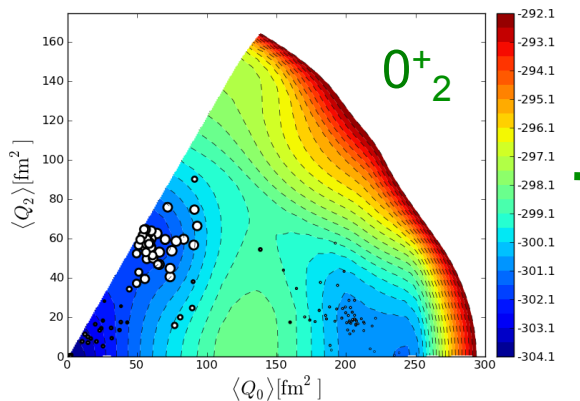
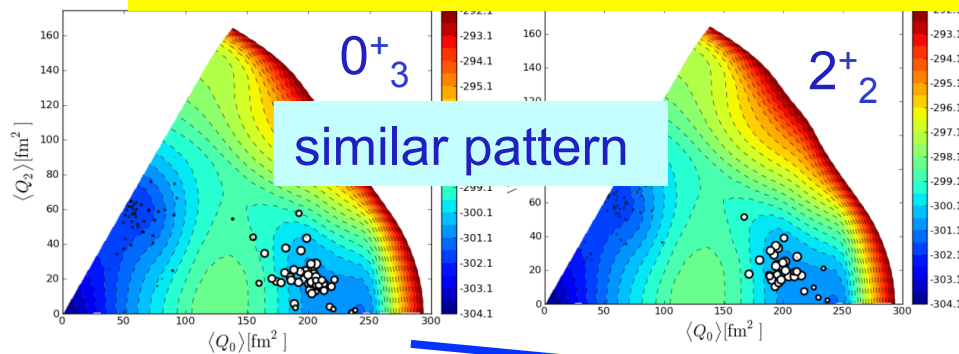
$$\Psi = \sum_i c_i P[J^\pi] \Phi_i$$

Slater determinant
 → intrinsic deformation

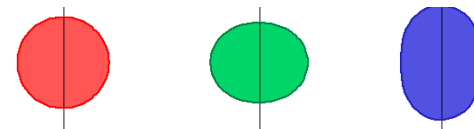
- PES is calculated by CHF
- Location of circle : quadrupole deformation of unprojected MCSM basis vectors
- Area of circle : overlap probability between each projected basis and eigen wave function



T-plot analysis of band structure of ^{68}Ni



Shape coexistence



Y. Tsunoda *et al.*, PRC89, 031301(R) (2014)

Outline

- **Introduction**
 - shapes and phase transition
- **Computational background** : advanced Monte Carlo shell model (MCSM)
 - intrinsic shapes of shell-model wave functions (T-plot)
- **Shape transition in Zr isotopes and Quantum Phase Transition**
- Summary and Perspectives

Present work : model space and effective interaction

- Effective interaction:

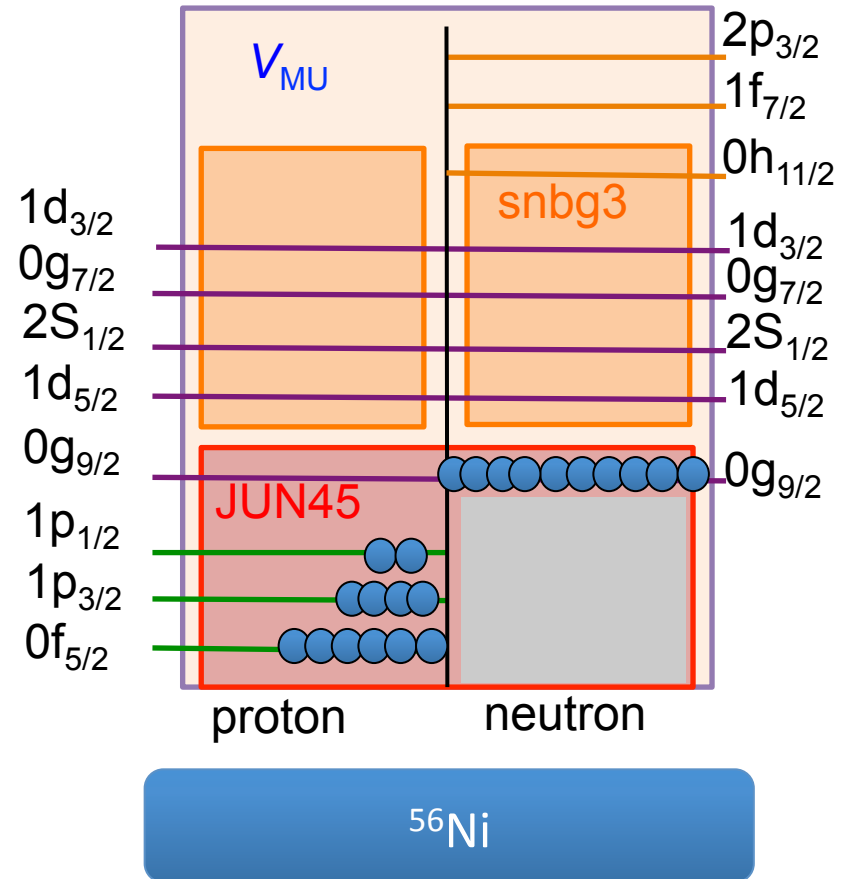
$$\text{JUN45} + \text{snbg3} + V_{\text{MU}}$$

known effective interactions

+ minor fit for a part of
T=1 TBME's

Nucleons are excited fully
within this model space
(no truncation)

We performed **Monte Carlo Shell Model (MCSM)** calculations, where the largest case corresponds to the diagonalization of 3.7×10^{23} **dimension** matrix.



Togashi, Tsunoda, TO *et al.* PRL
117, 172502 (2016)

From earlier shell-model works ...

PHYSICAL REVIEW C

VOLUME 20, NUMBER 2

AUGUST 1979

Unified shell-model description of nuclear deformation

P. Federman

Instituto de Física, Universidad Nacional Autónoma de México, Apartado Postal 20-364, México 20, D. F.

S. Pittel

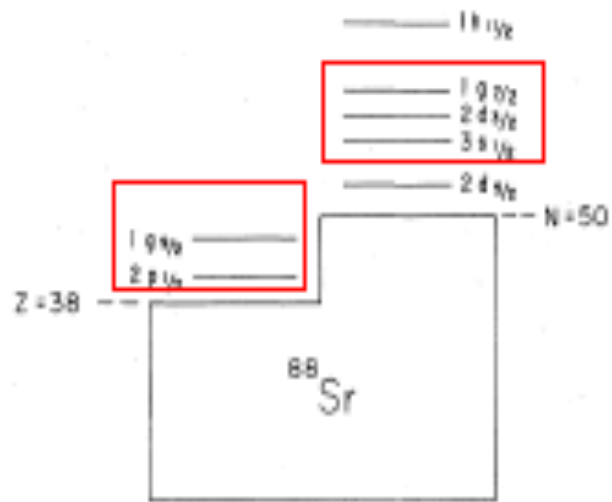


FIG. 3. Single-particle levels appropriate to a description of nuclei in the Zr-Mo region. An ^{88}Sr core is assumed.

PHYSICAL REVIEW C 79, 064310 (2009)

Shell model description of zirconium isotopes

K. Sieja,^{1,2} F. Nowacki,³ K. Langanke,^{2,4} and G. Martínez-Pinedo¹

In this paper, we perform for the first time a SM study of Zr isotopes in an extended model space ($1f_{5/2}$, $2p_{1/2}$, $2p_{3/2}$, $1g_{9/2}$) for protons and ($2d_{5/2}$, $3s_{1/2}$, $2d_{3/2}$, $1g_{7/2}$, $1h_{11/2}$) for neutrons, dubbed hereafter $\pi(r3 - g)$, $\nu(r4 - h)$.

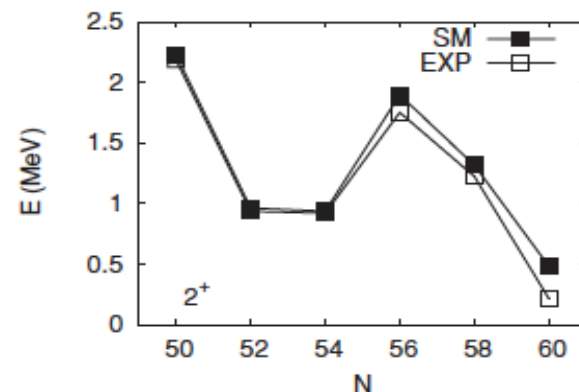
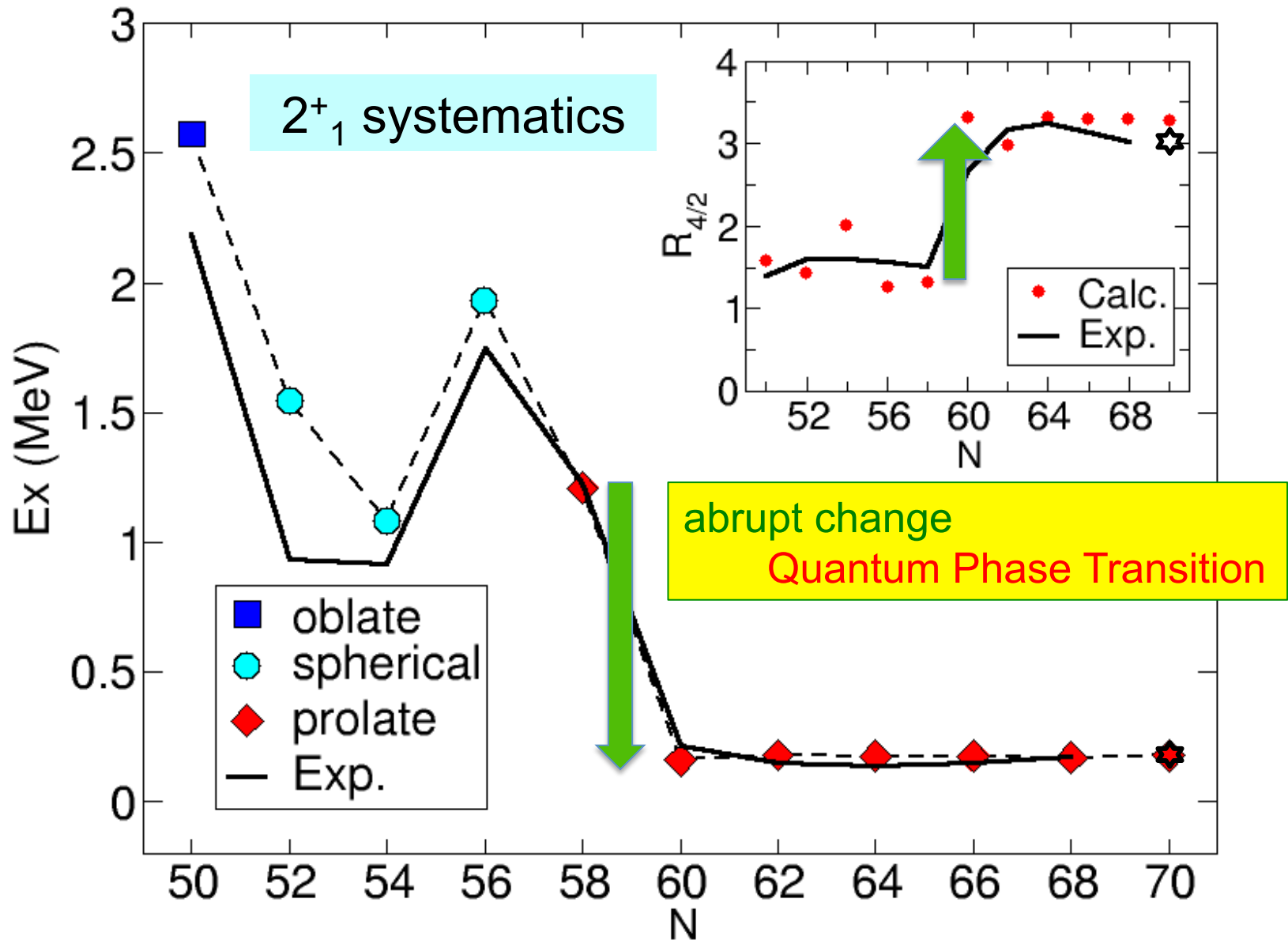
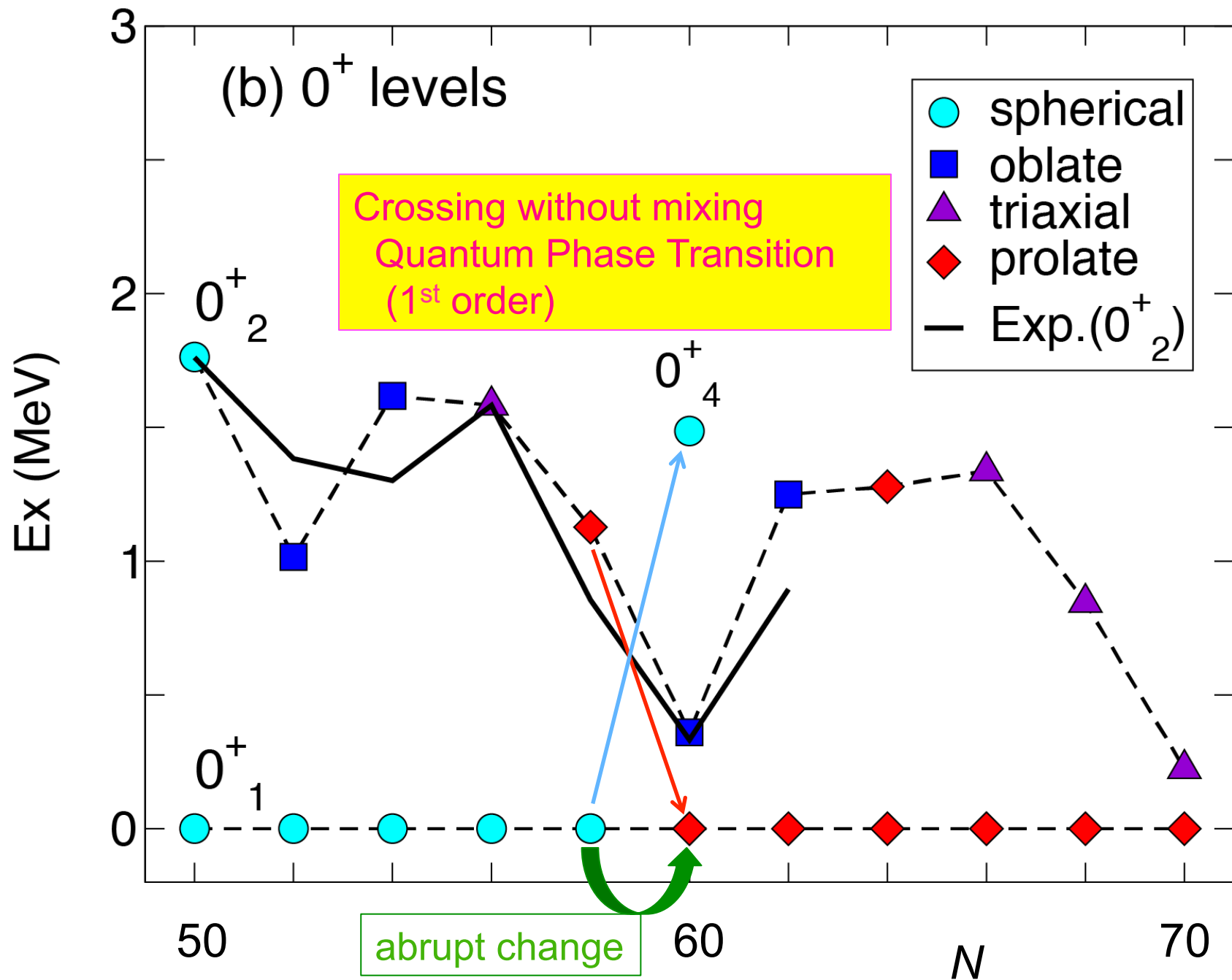
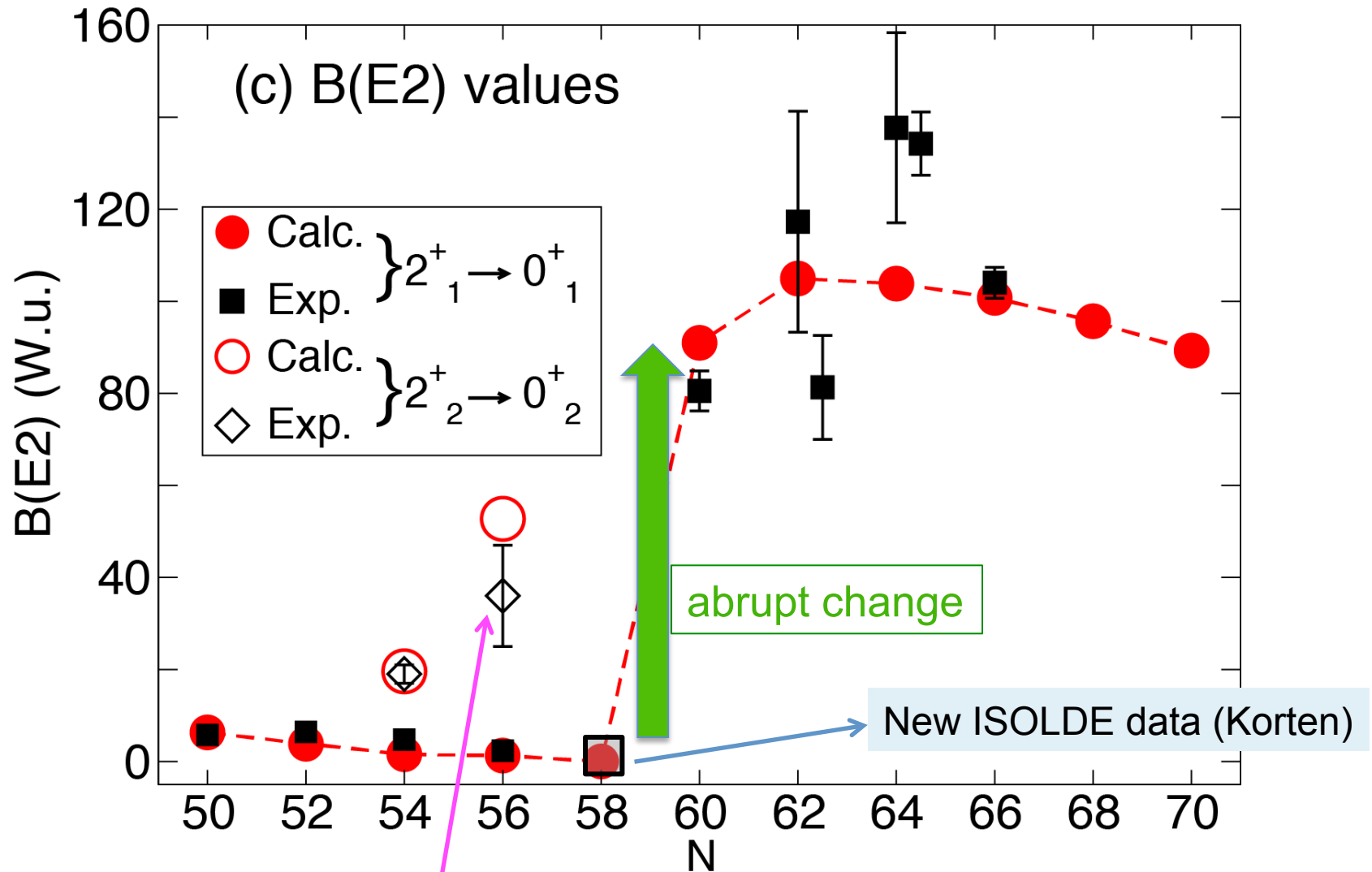


FIG. 12. Systematics of the experimental and theoretical first excited 2^+ states along the zirconium chain.

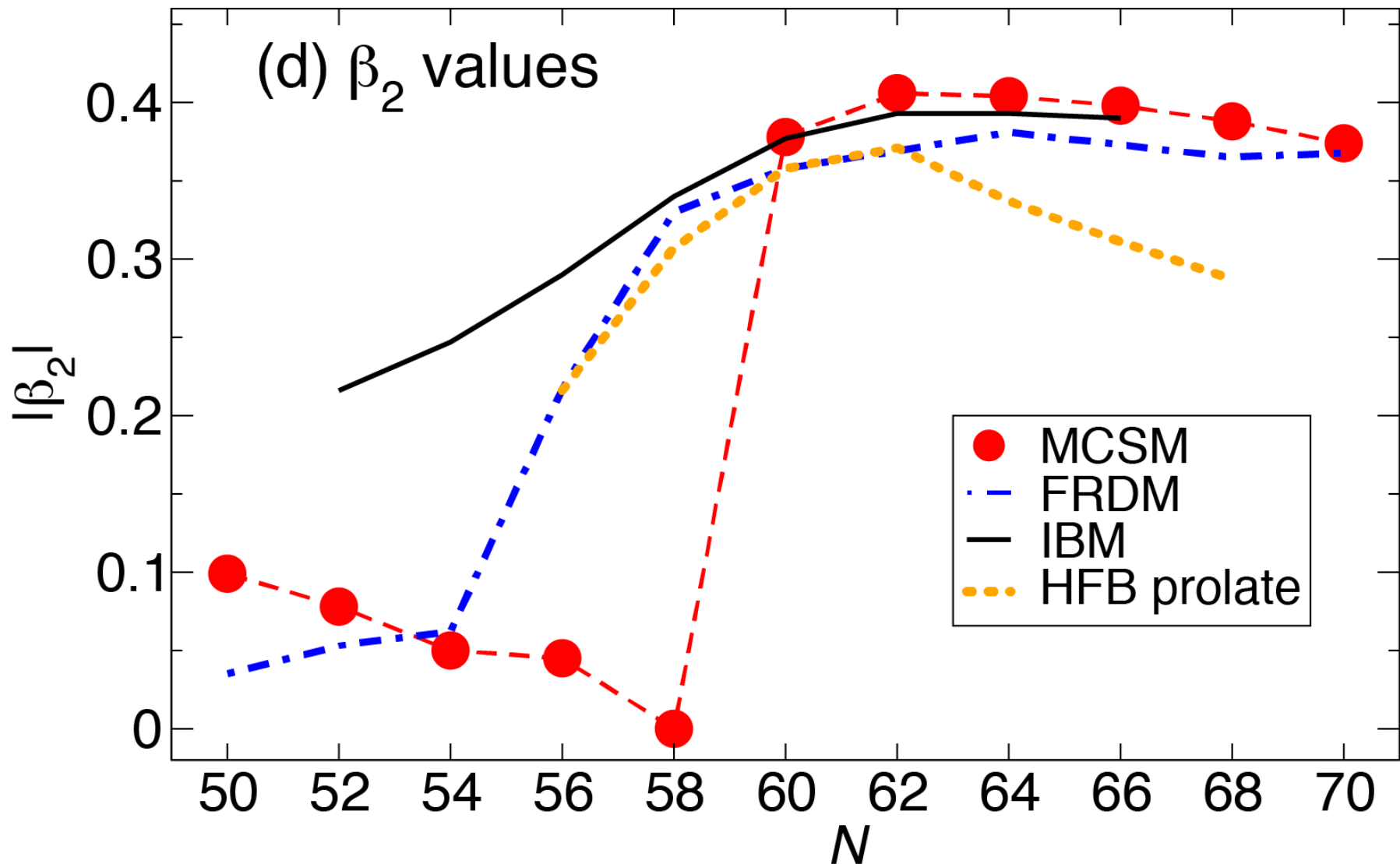




B(E2; 2⁺ → 0⁺) systematics



New data from Darmstadt, Kremer *et al.* PRL 117, 172503 (2016)

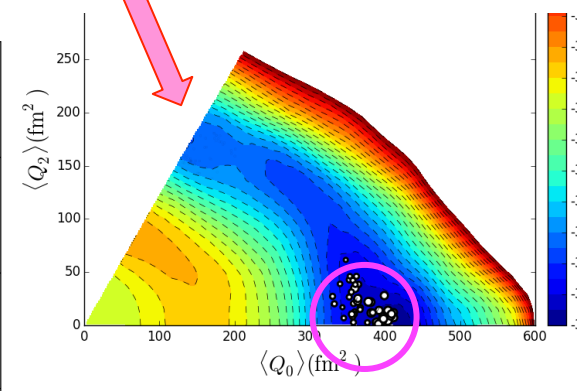
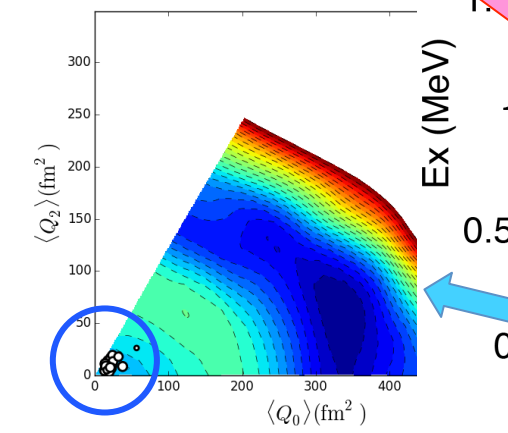
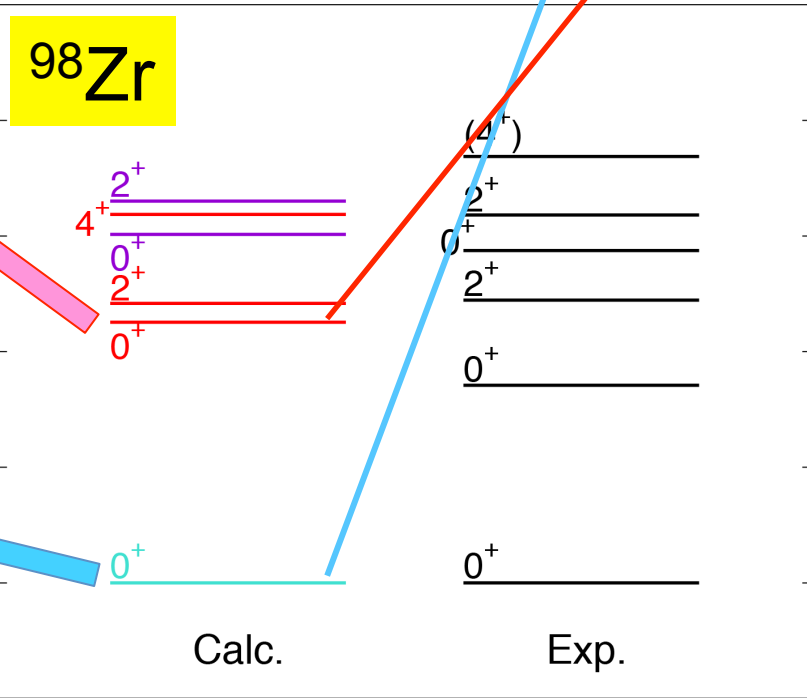
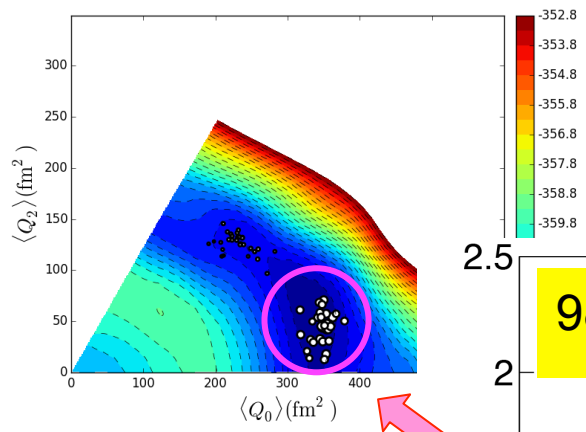
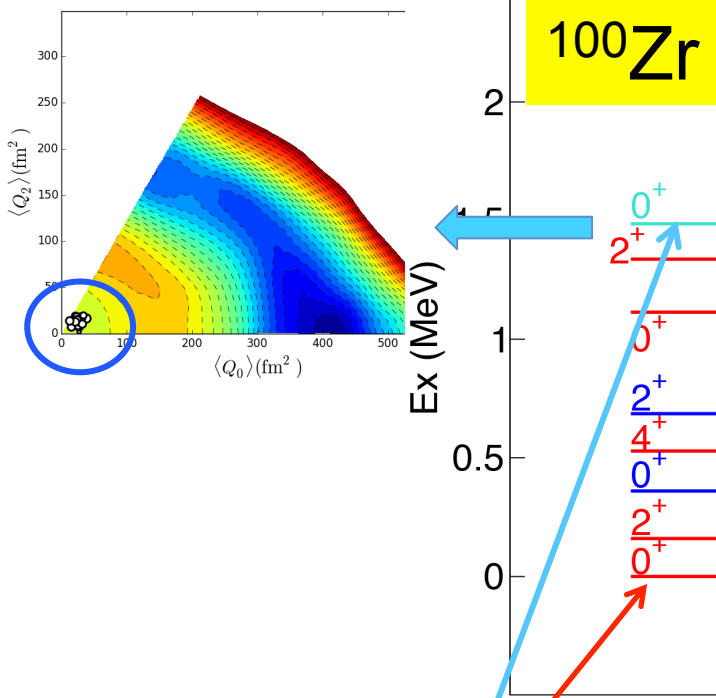


FRDM: S. Moeller et al. At. Data Nucl. Data Tables 59, 185 (1995).

IBM: M. Boyukata et al. J. Phys. G 37, 105102 (2010).

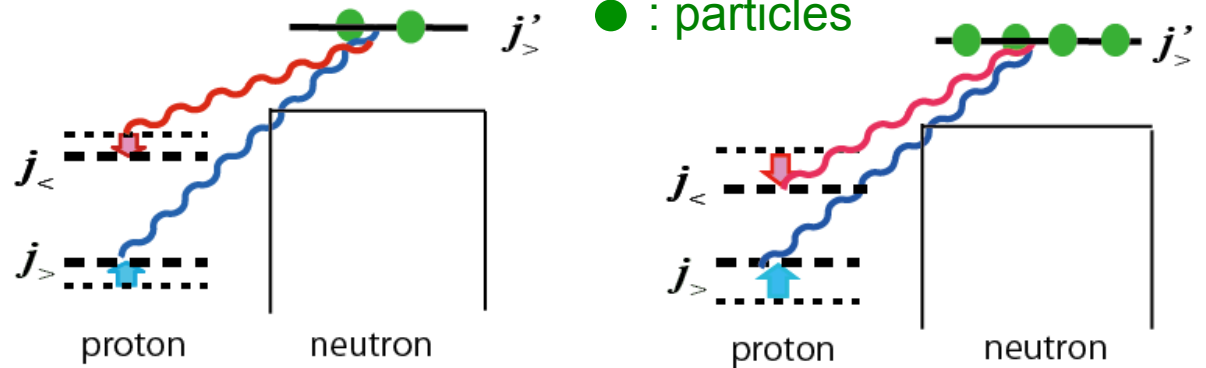
HFB: R. Rodriguez-Guzman et al. Phys. Lett. B 691, 202 (2010).

Quantum Phase Transition
(1st order)
due to crossing
without mixing

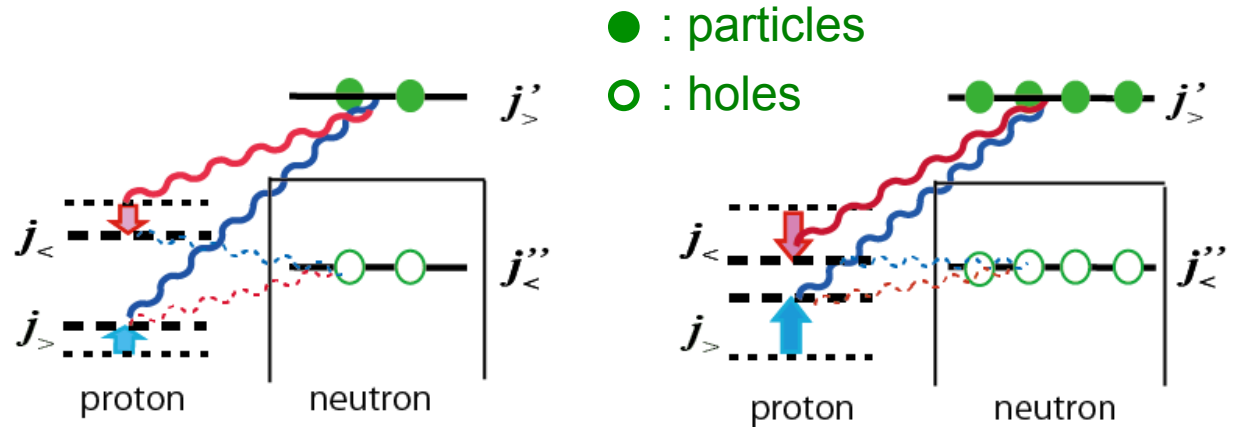


Shell Evolution - from Type I to Type II -

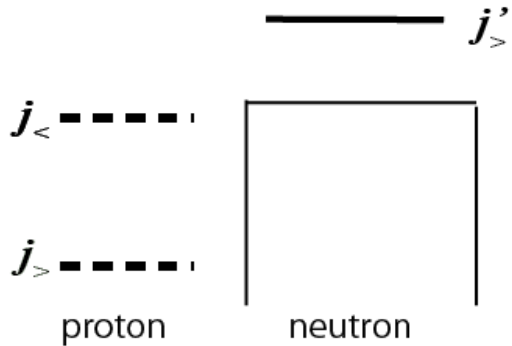
Type I Shell Evolution : different isotopes



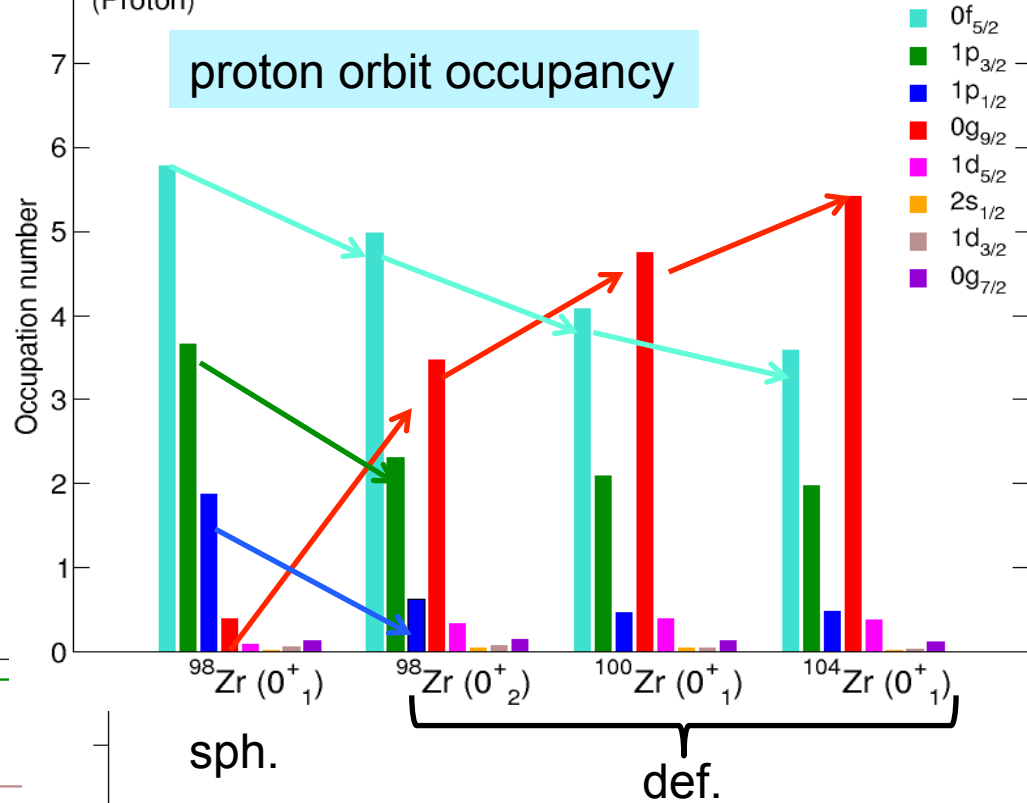
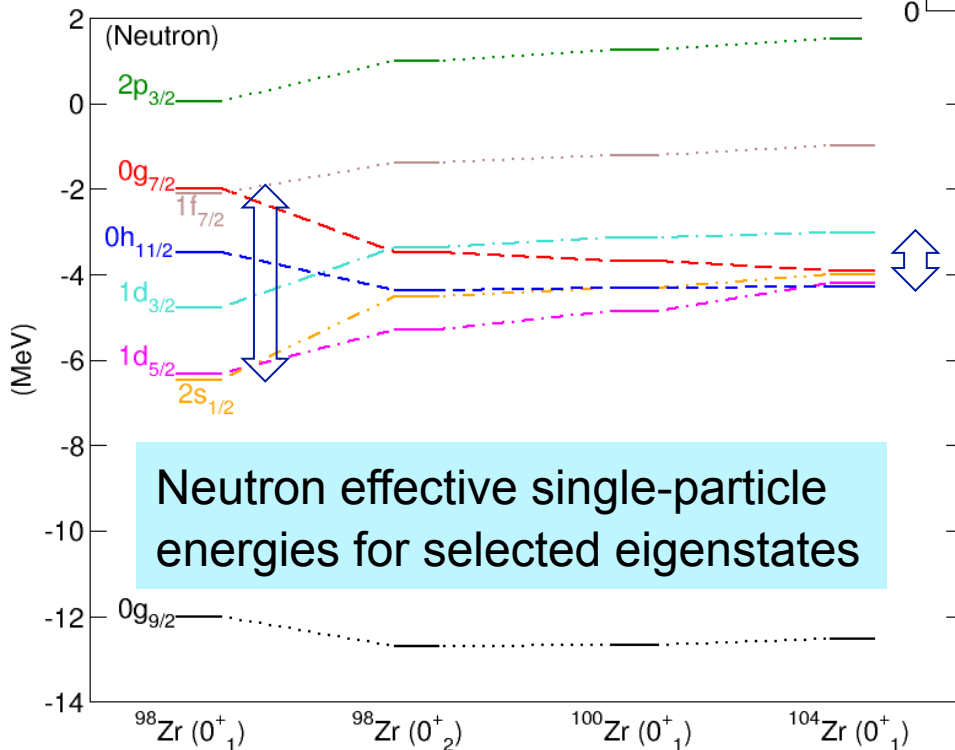
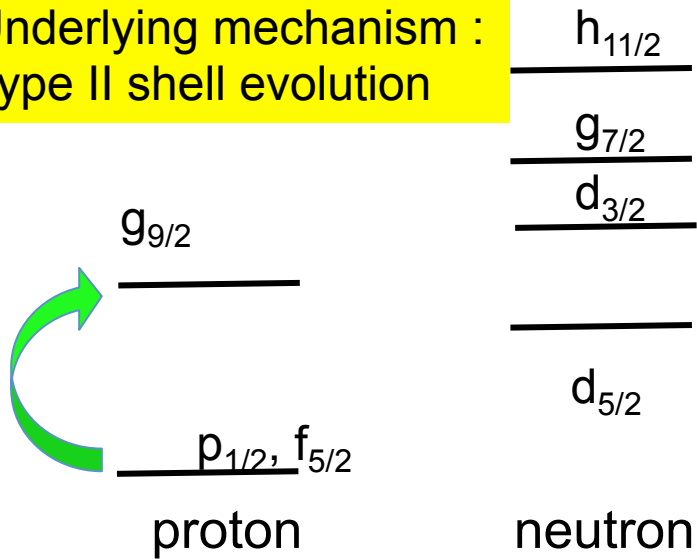
Type II Shell Evolution : within the same nucleus



(a)



Underlying mechanism :
Type II shell evolution



Neutron effective single-particle energies are **self-reorganized** by nuclear forces (tensor and central) and certain configurations, so as to **reduce resistance power against deformation**.

- a case of *type II shell evolution* -

Intuitively speaking,

$$\text{deformation} = \frac{\text{quadrupole force}}{\text{resistance power}}$$

resistance power ← pairing force

↙ single-particle energies

Atomic nuclei can “organize” their single-particle energies by taking particular configurations of protons and neutrons, thanks to orbit-dependences of nuclear forces (e.g., tensor force).

Quantum Self Organization

Note : spherical single-particle energies are often treated being constant

Nilsson model Hamiltonian

“Nuclear structure II” by Bohr and Mottelson

deformed nuclei, is obtained by a simple modification of the harmonic oscillator (Nilsson, 1955; Gustafson *et al.*, 1967),

$$H = \frac{\mathbf{p}^2}{2M} + \frac{1}{2}M(\omega_3^2 x_3^2 + \omega_\perp^2(x_1^2 + x_2^2)) + v_{ll}\hbar\omega_0(l^2 - \langle l^2 \rangle_N) + v_{ls}\hbar\omega_0(\mathbf{l} \cdot \mathbf{s}) \quad (5-10)$$

quadrupole deformed field
spherical field

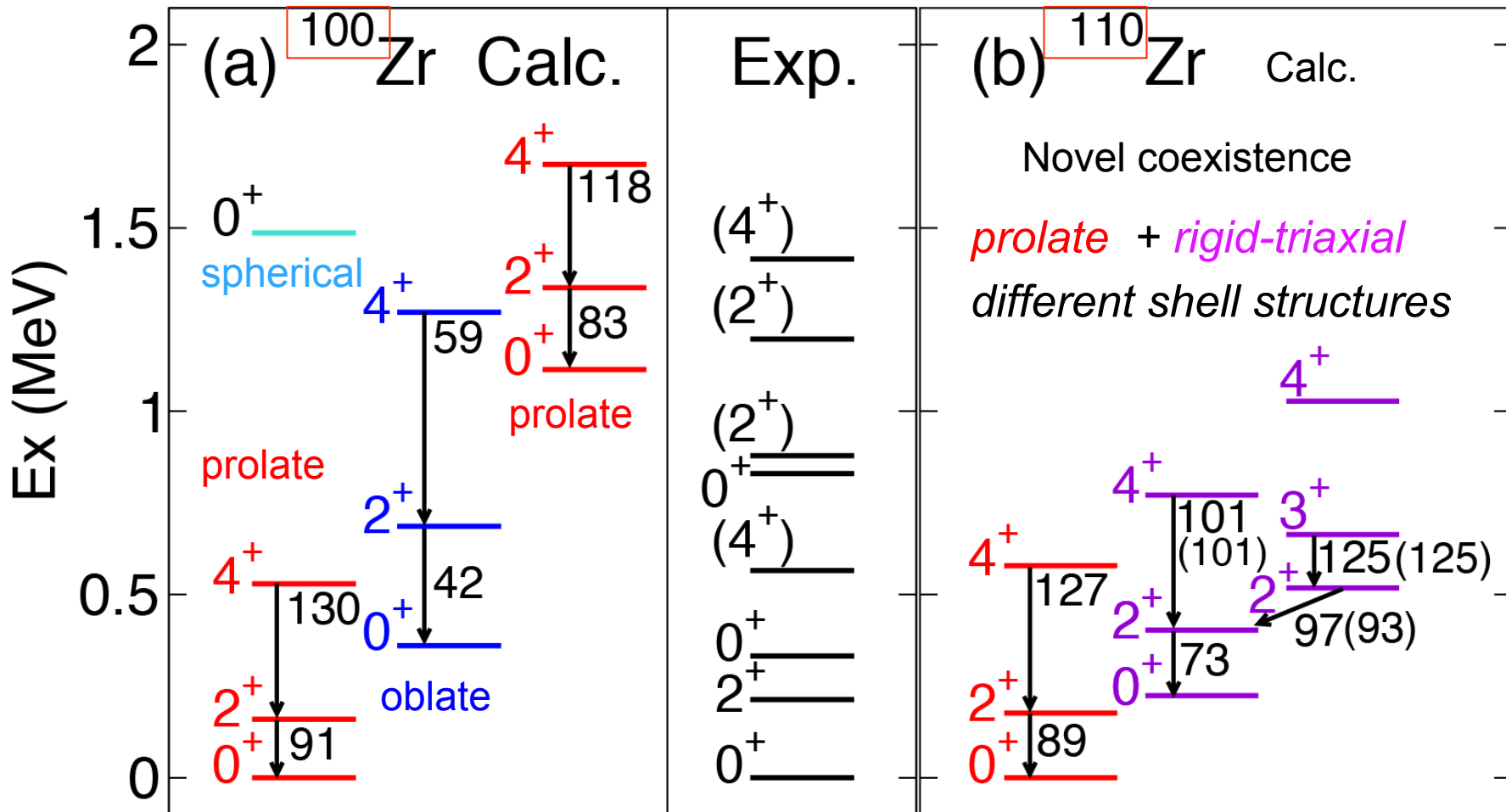
$$\langle l^2 \rangle_N = \frac{1}{2}N(N+3)$$

Figure	Region	$-v_{ls}$	$-v_{ll}$
5-1	N and $Z < 20$	0.16	0
5-2	$50 < Z < 82$	0.127	0.0382
5-3	$82 < N < 126$	0.127	0.0268
5-4	$82 < Z < 126$	0.115	0.0375
5-5	$126 < N$	0.127	0.0206

Table 5-1 Parameters used in the single-particle potentials of Figs. 5-1 to 5-5.

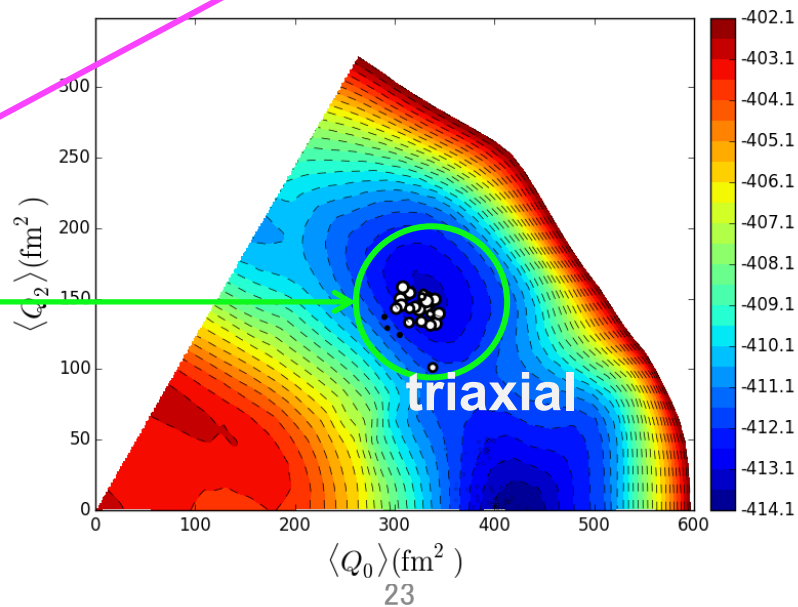
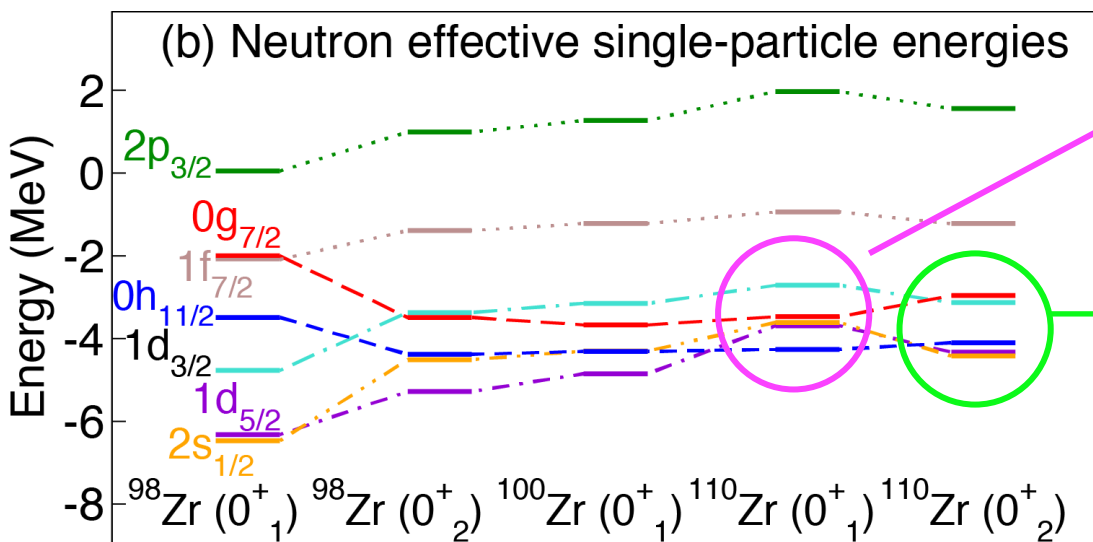
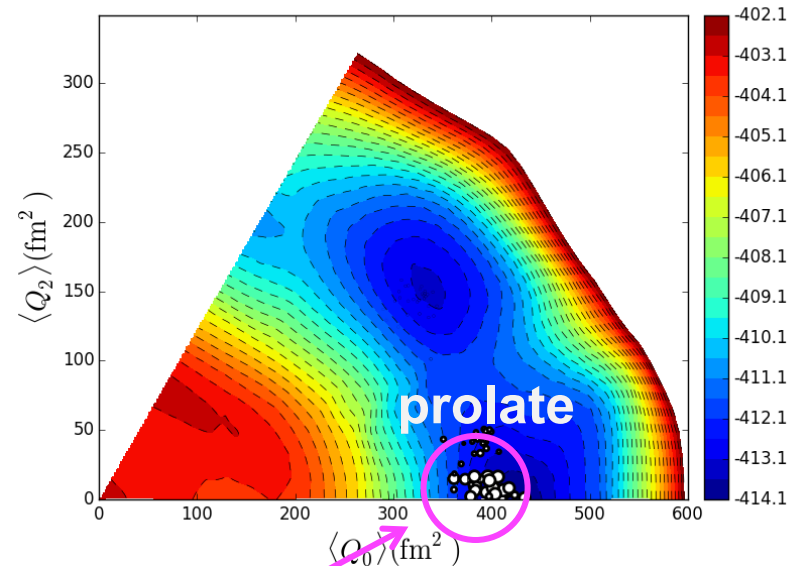
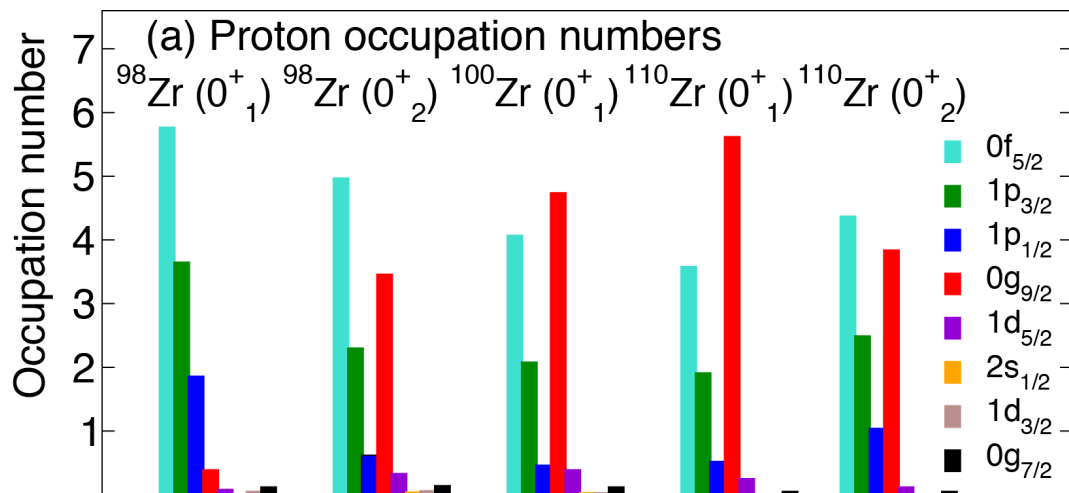
Spin-orbit force		
A= 68	1.28	} $(\mathbf{l} \cdot \mathbf{s})$
A=100	1.12	
A=186	0.91	

Prolate – rigid-triaxial shape coexistence



() : Rigid-triaxial rotor with $\gamma=28$ degrees normalized at $2^+ \rightarrow 0^+$

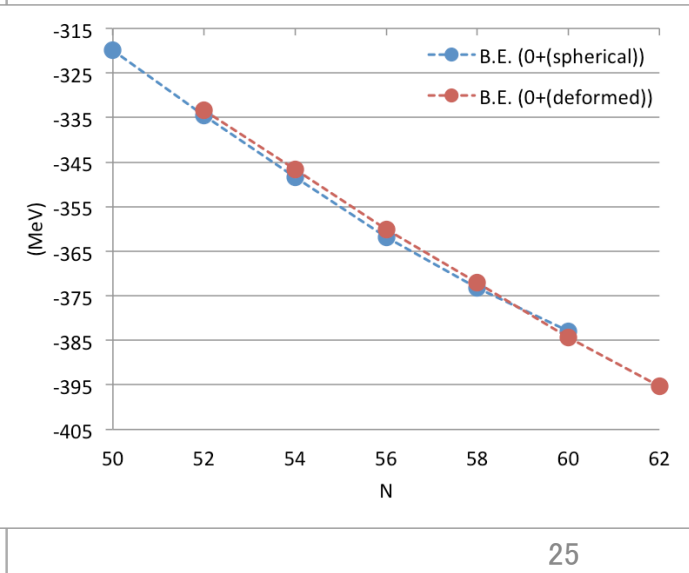
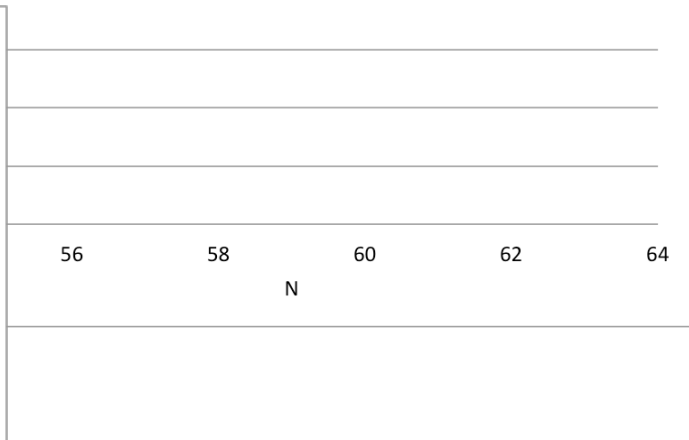
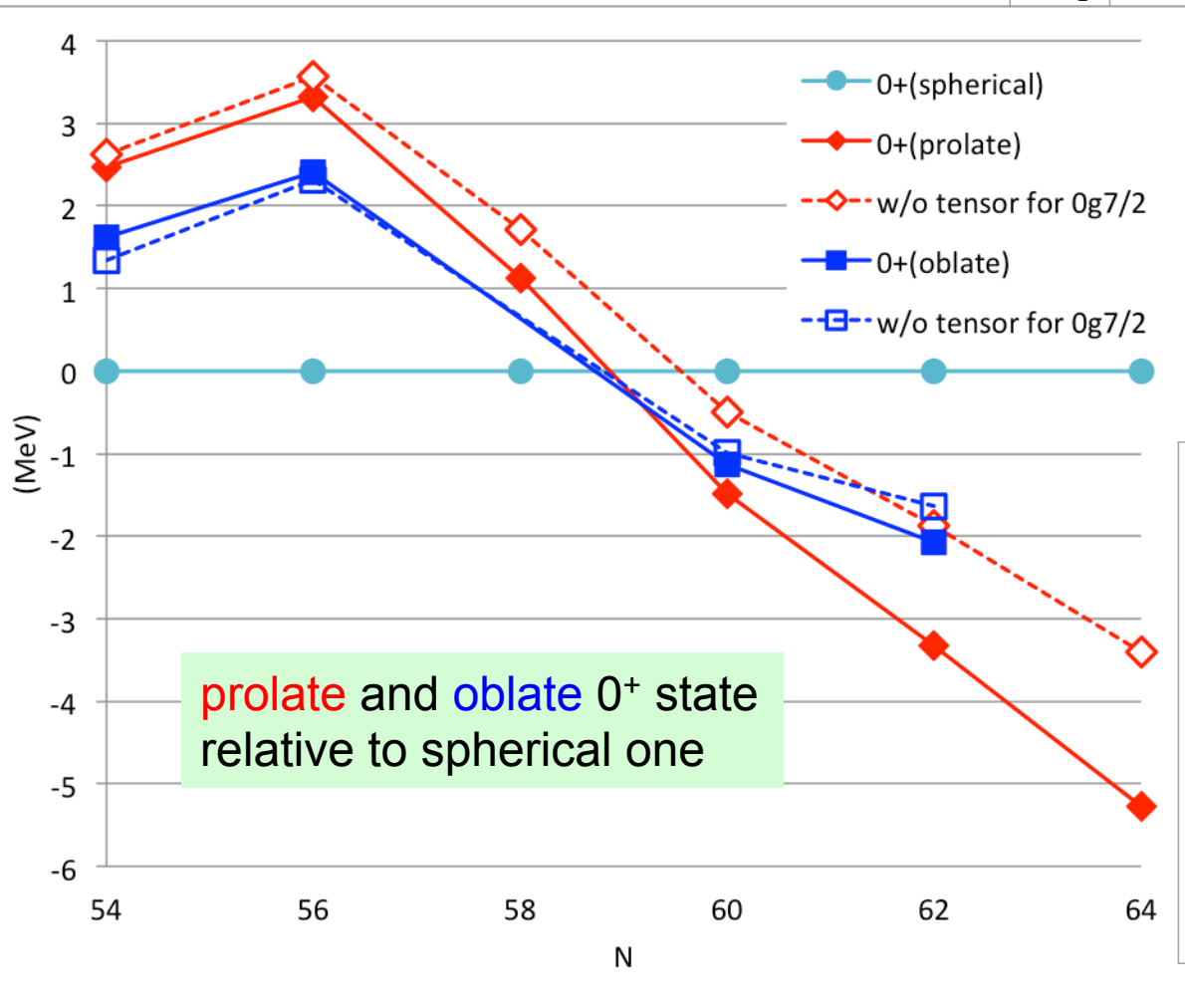
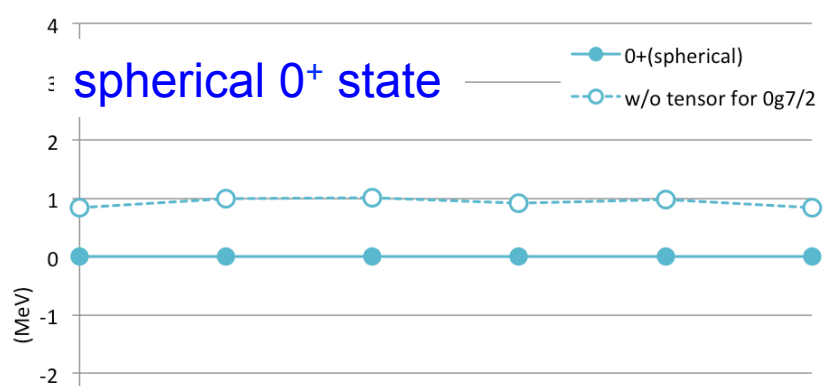
different shell structures ~ like “different nuclei”



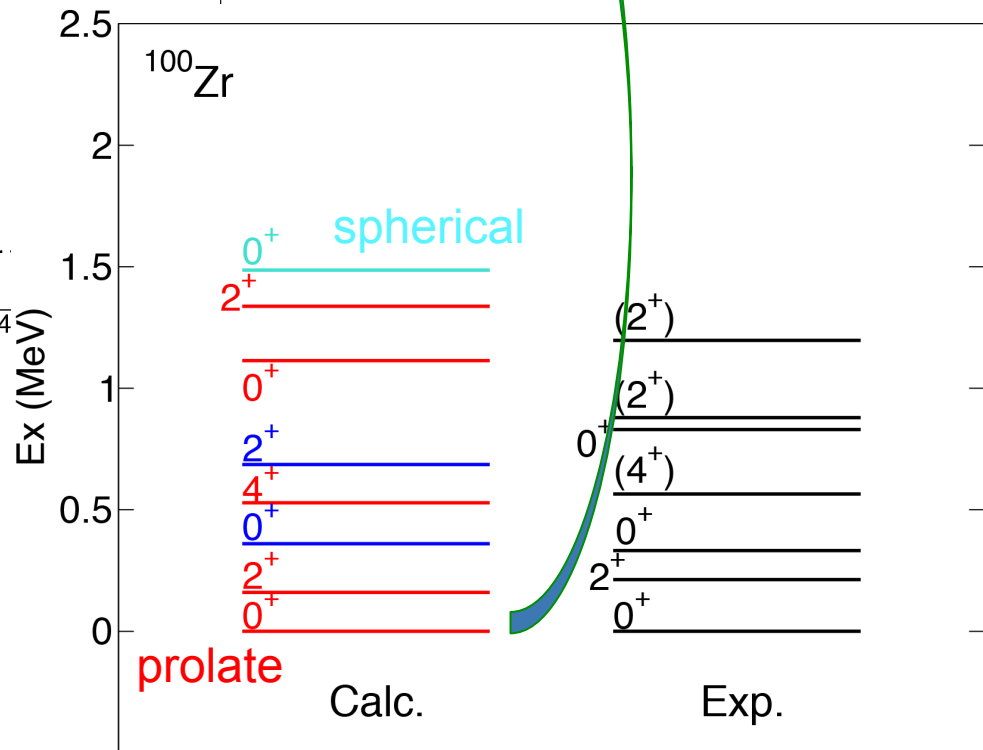
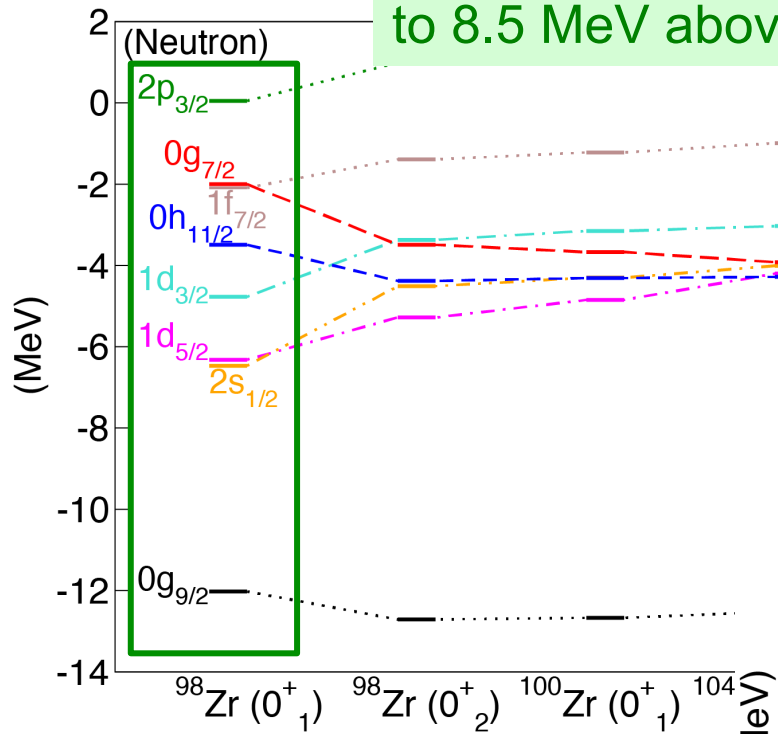
Summary and Perspectives

- The shape transition in Zr is described with a standard SM interaction.
- **The quantum phase transition (QPM) is identified** between ^{98}Zr and ^{100}Zr .
(*abrupt qualitative change in the ground state as a function of N*)
- **Type II shell evolution** reduces, in general, the **resistance against deformation**, with **very different configurations for different shapes**.
→ shape coexistence, QPM in shapes, *super D*, *octupole D*, *fission*, etc.
- The abrupt change (1st order QPM) is a consequence of level crossing with (almost) no mixing due to completely different configurations, despite that the nucleus is a finite quantum system.
- In more general terms, **single particle energies** can be **self-organized** (*quantum self-organization*), with the following condition:
 - (i) **two quantum liquids** (protons and neutrons),
 - (ii) **two major force components** : e.g., **quadrupole** interaction to **drive deformation** and **monopole** interaction to **control resistance**.→ *Nuclei favor more distinct shapes, i.e., enhanced symmetries !*

Effect of tensor force for $g_{7/2}$



If these s.p.e.'s are used and the monopole interaction is eliminated, the prolate 0^+ is raised to 8.5 MeV above the spherical one.



Schematic picture of shape evolution (sphere to ellipsoid)

- monotonic pattern throughout the nuclear chart –
one “shape” per one nucleus in many stable nuclei

