



ESNT Workshop “Shape coexistence and electric monopole transitions in atomic nuclei”  
Oct. 24 (23-27), 2017  
CEA-Saclay b703 Orme des Merisiers

*Shape coexistence and quantum phase transition  
in the Monte-Carlo Shell Model*

Takaharu Otsuka

*RIKEN / University of Tokyo / KU Leuven / MSU*

Yusuke Tsunoda (CNS, Tokyo), Tomoaki Togashi (CNS, Tokyo)

Noritaka Shimizu (CNS, Tokyo), Takashi Abe (Tokyo)



東京大学  
THE UNIVERSITY OF TOKYO

**KU LEUVEN**



This work has been supported by MEXT and JICFuS as a priority issue (Elucidation of the fundamental laws and evolution of the universe) to be tackled by using Post ‘K’ Computer

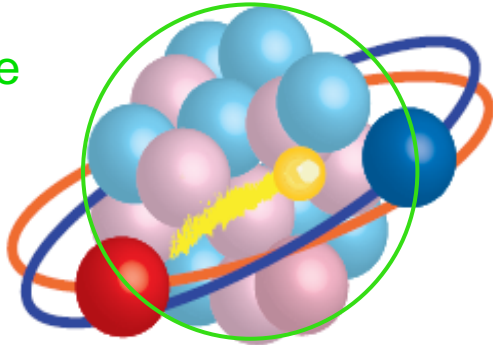
# *Outline*

- I Introduction
- II Presently used numerical methodology of many-body problems
- III First application of MCSM to shape coexistence: Ni isotopes
- IV An example from Quantum Phase Transition in Zr isotopes
- V Basic mechanism
- VI Shape coexistence and/or critical phenomena in Hg/Pb isotopes
- VII Remarks

Collective modes : various types → in the case of the quadrupole deformation

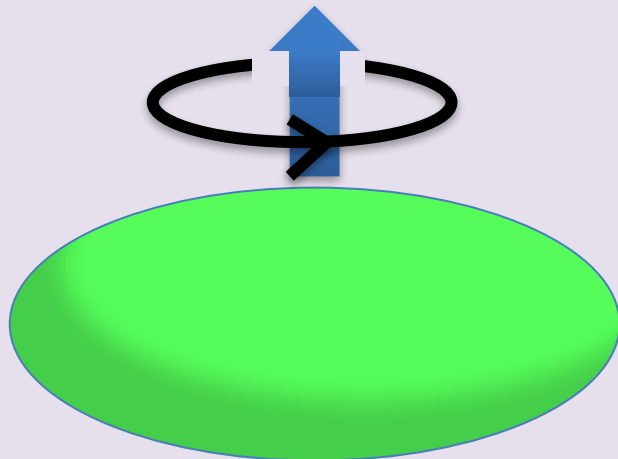
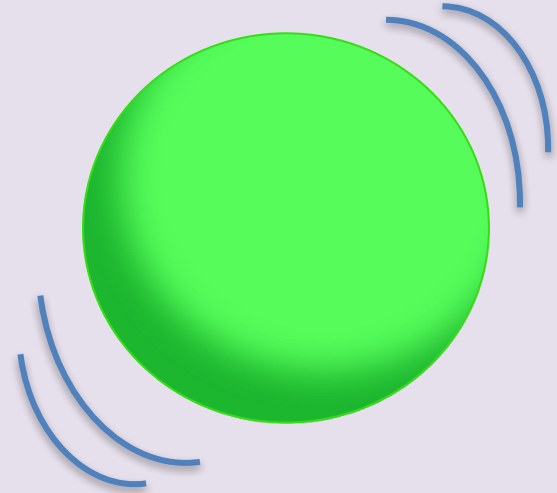
Assembly of  
protons and neutrons

surface



collective  
motion

Vibration between  
sphere and ellipsoid

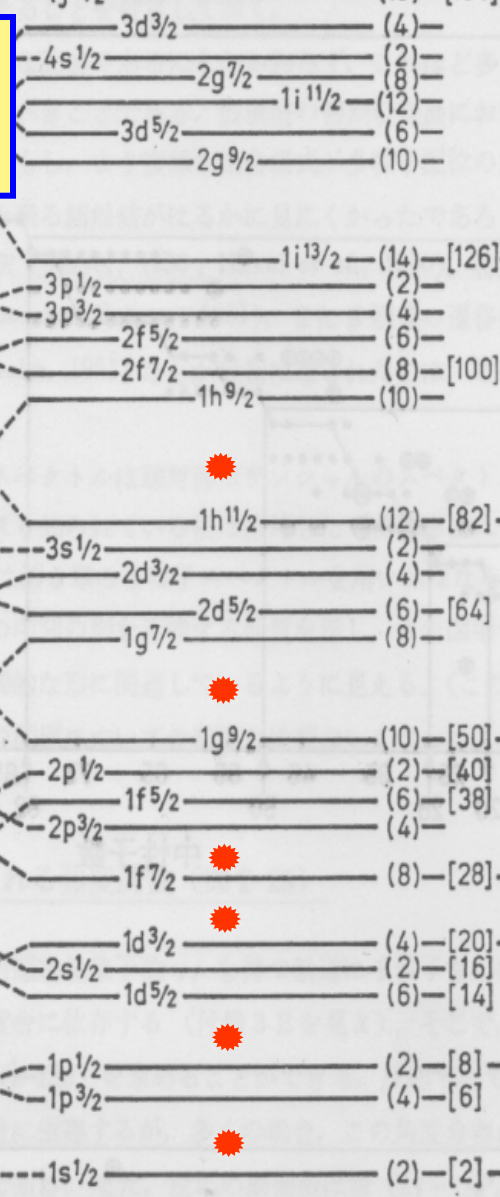


Rigid Ellipsoidal  
Deformation  
and its Rotation

Single-particle states : shell structure and magic numbers due to a "potential"

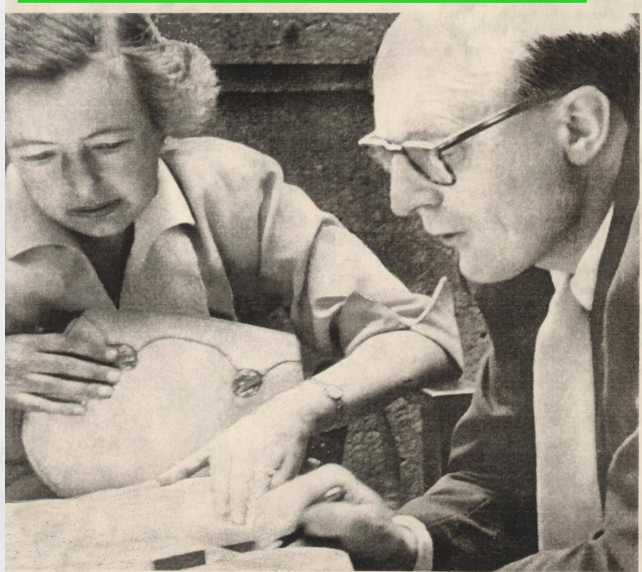
Eigenvalues of HO potential

5ħω  
4ħω  
3ħω  
2ħω  
1ħω  
0



126  
82  
50  
28  
20  
8  
2

Magic numbers by Mayer and Jensen (1949)

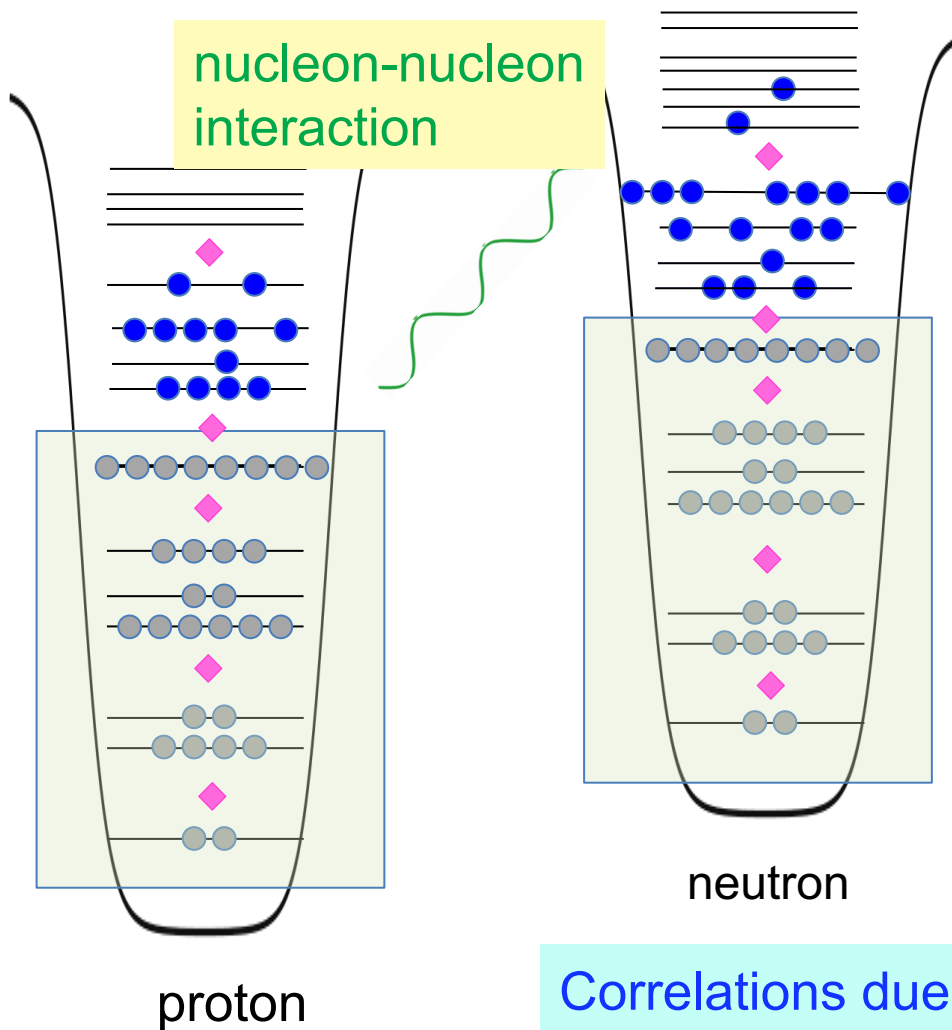


R SHELL MODEL

図 2-23 1 粒子軌道の順序。図は M. G. Mayer and J. H. D. Jensen, *Elementary Theory of Nuclear Shell Structure*, p. 58, Wiley, New York, 1955 からとった。



# single-particle states and correlations



◆ shell gap

Protons and neutrons are orbiting in the mean potential like a “vase”

→ **single-particle states**

Lower orbits form the **inert core** (or closed shell)  
(*shaded parts in the figure*)

Upper orbits are partially occupied and nucleons are active  
(**valence orbits and nucleons**).

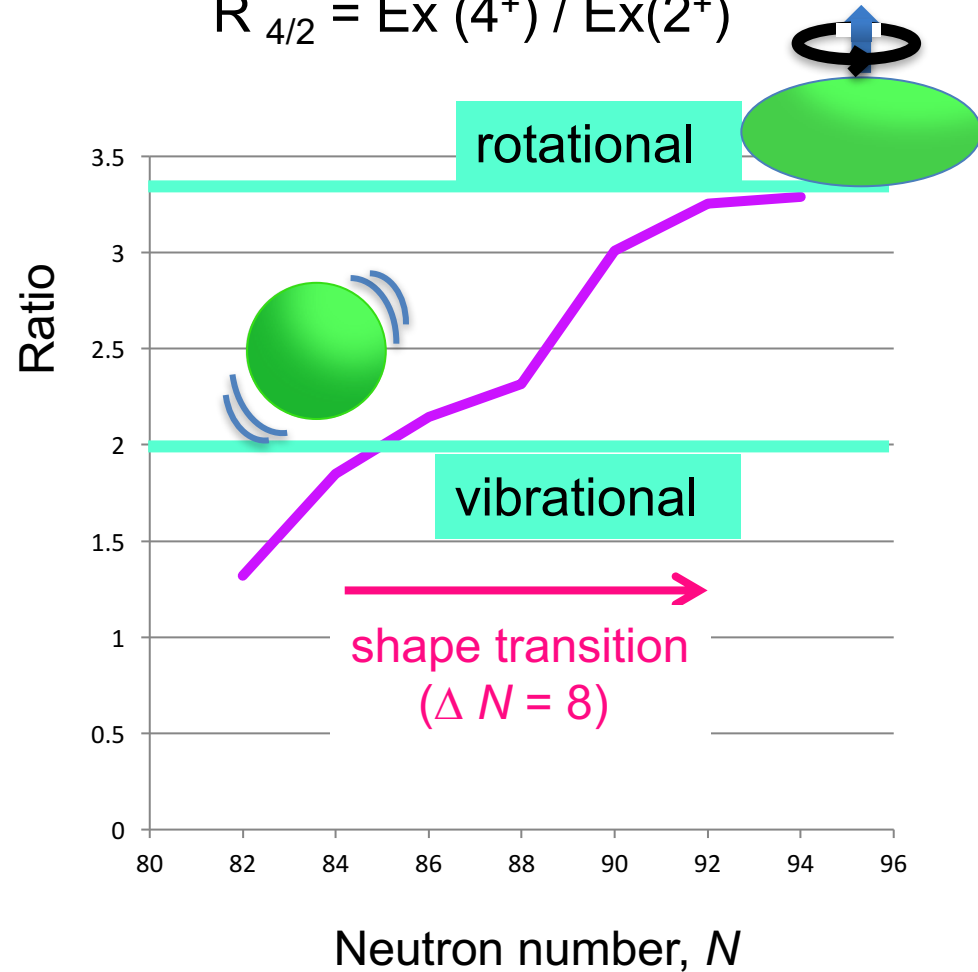
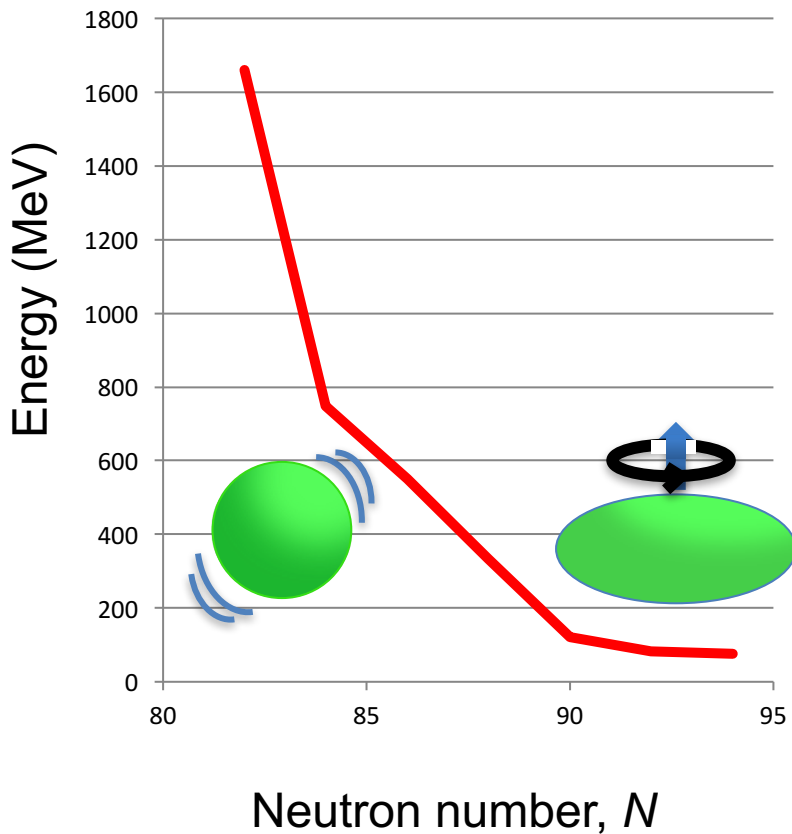
Correlations due to nucleon-nucleon interaction produce the mixing of various configurations of single-particle states.

Various shapes appear as a function of  $N$  (or  $Z$ ) : How can we describe it ?

$2^+$  and  $4^+$  level properties of Sm ( $Z=62$ ) isotopes

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

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



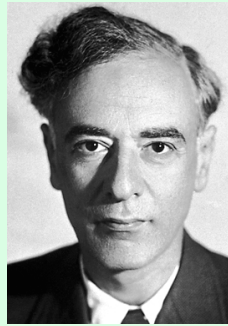
## starting point of the microscopic description

*Atomic nucleus is a quantum*

*Fermi liquid :*

*The nucleus is composed of almost **free nucleons** interacting weakly via residual forces*

*in a (solid) (mean) potential like a **solid “vase”**.*



Landau

*The shape of atomic nucleus can be described by the deformation of the “vase”, a la Nilsson model.*



A. Bohr

Mottelson

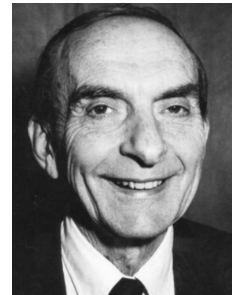
Nilsson

open question

T. Schaefer, Fermi Liquid theory: A brief survey in memory of Gerald E. Brown, NPA 2014)

One of Gerry's main scientific pursuits was to understand the nuclear few and many-body problem in terms of microscopic theories based on the measured two and three-nucleon forces. One of the challenges of this program is to understand how the observed single-particle aspects of finite nuclei, in particular shell structure and the presence of excited levels which carry the quantum numbers of single particle states, can be reconciled with the strong nucleon-nucleon force, and **how single particle states can coexist with collective modes**. A natural framework for addressing these questions is the **Landau theory of Fermi liquids**. **Landau Fermi liquid theory**

G.E. Brown



# Additional deformed field : Nilsson model

## 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),

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

quadrupole deformed field

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

spherical field

constant within a region

Figure	Region	$-v_{IS}$	$-v_{II}$
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	}	(l · s)
A=100	1.12		
A=186	0.91		



## Main subject of this talk

This effect becomes stronger as the nucleus moves away from the closed shell.

*Intuitively speaking, the quadrupole deformation is determined by*

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

resistance power ← For instance, pairing force.

What else ?

- The **quadrupole force** is a part of nuclear forces :  
quadrupole-quadrupole component in the spin-tensor decomposition.
- Driving force for the rotational spectrum, for instance, in Elliott's SU(3)
- Its mean-field effect → Nilsson model
- Pairing + QQ interaction model

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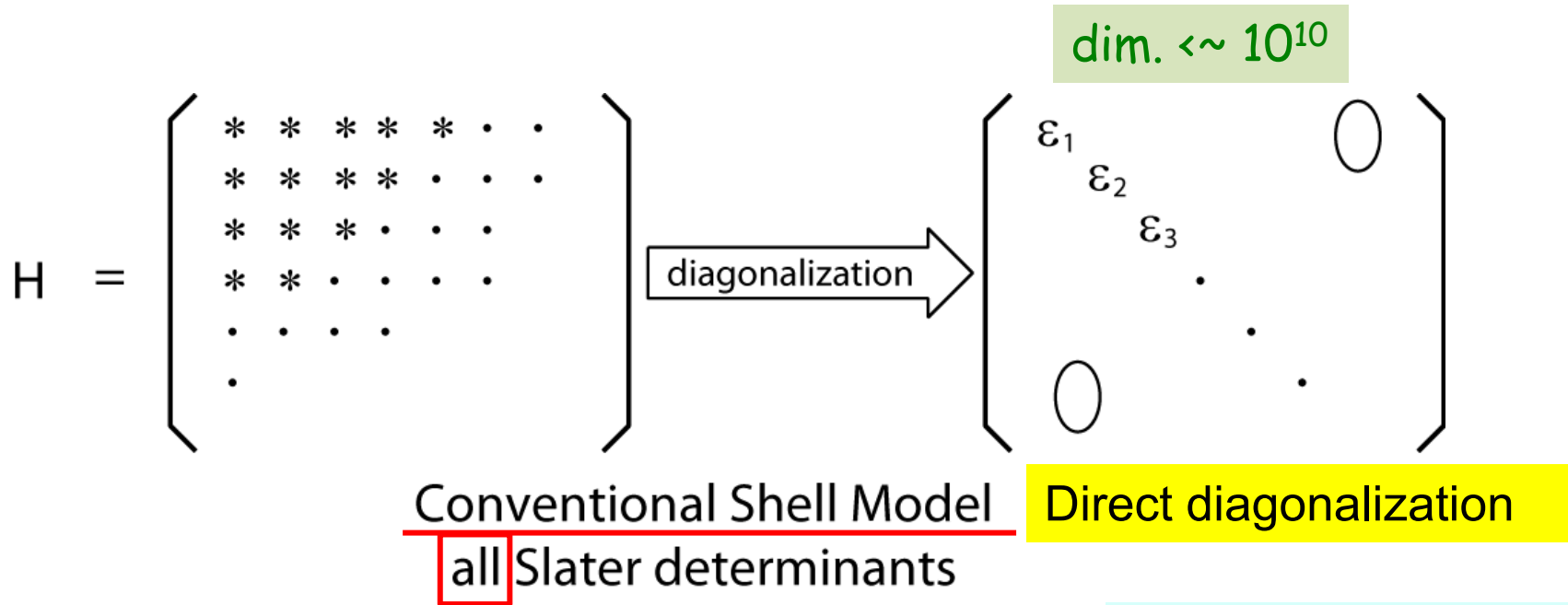
IV An example from Quantum Phase Transition in Zr isotopes

V Basic mechanism

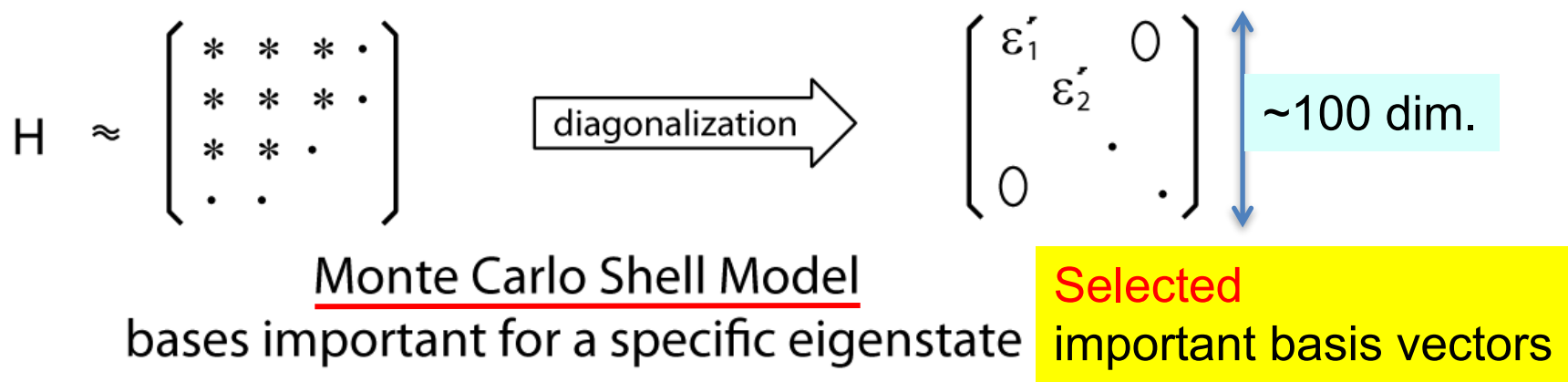
VI Shape coexistence and/or critical phenomena in Hg/Pb isotopes

VII Remarks

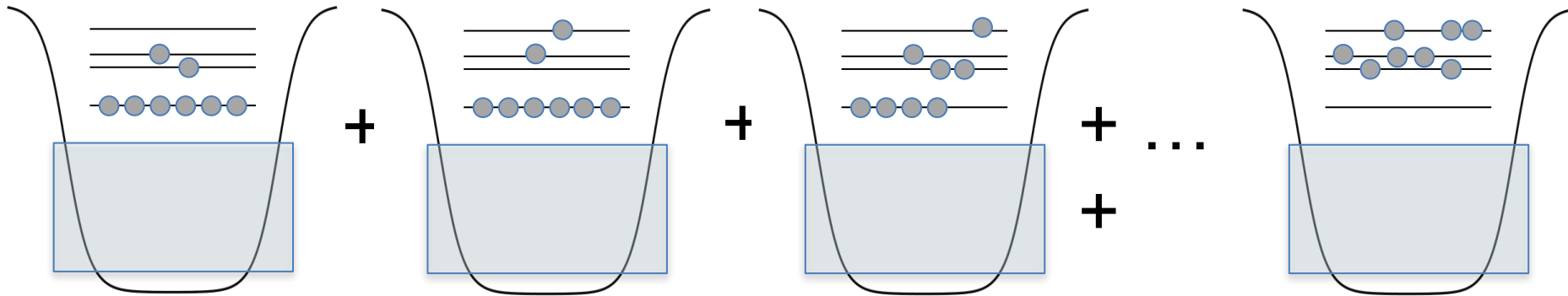
# Two types of shell-model calculations



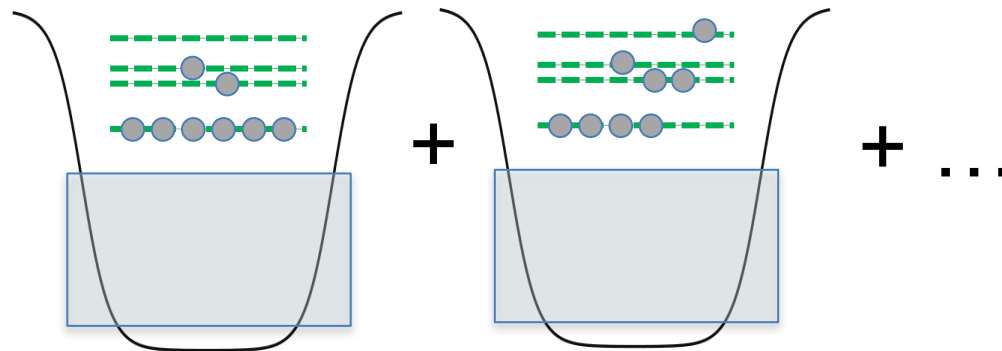
For even bigger problem,



Possible configurations:  $10^{23}$  ways at maximum for Zr isotopes to be discussed



Superposition of original orbits => Select most important  $\sim 100$  ones





# Advanced Monte Carlo Shell Model

$N_B$  : number of basis vectors (dimension)

$N_p$  : number of (active) particles

$N_{sp}$  : number of single-particle states

$$|\Psi(D)\rangle = \sum_{n=1}^{N_B} c_n P^{J,\Pi} |\phi(D^{(n)})\rangle$$

amplitude

Projection op.

$$|\phi(D^{(n)})\rangle = \prod_{\alpha=1}^{N_p} \left( \sum_{i=1}^{N_{sp}} a_i^\dagger D_{i\alpha}^{(n)} \right) |-\rangle$$

$n$ -th basis vector  
(Slater determinant)

Deformed single-particle state

$$E(D) = \langle \Psi(D) | H | \Psi(D) \rangle$$

Minimize  $E(D)$  as a function of  $D$  utilizing qMC and conjugate gradient methods

Step 1 : quantum Monte Carlo type method

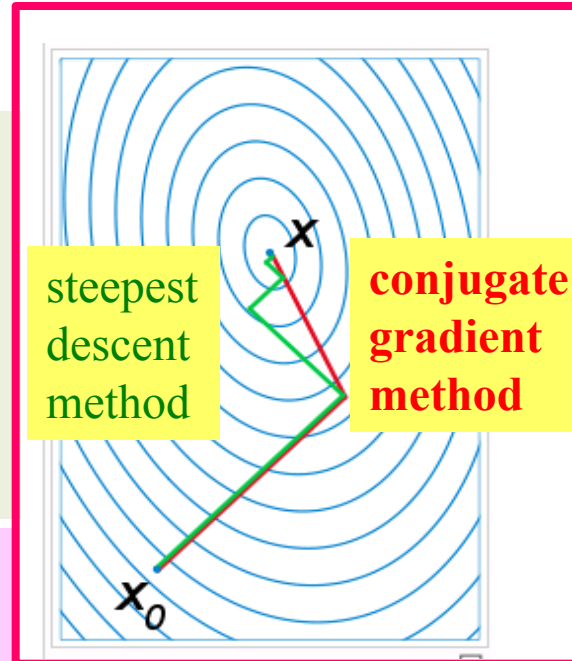
→ candidates of  $n$ -th basis vector ( $\sigma$  : set of random numbers)

$$|\phi(\sigma)\rangle = \prod e^{\Delta\beta \cdot h(\sigma)} \cdot |\phi^{(0)}\rangle$$

“ $\sigma$ ” can be represented by matrix  $D$

Select the one producing the lowest  $E(D)$  (rate < 0.1 %)

Step 2 : polish  $D$  by means of the conjugate gradient method “variationally”.

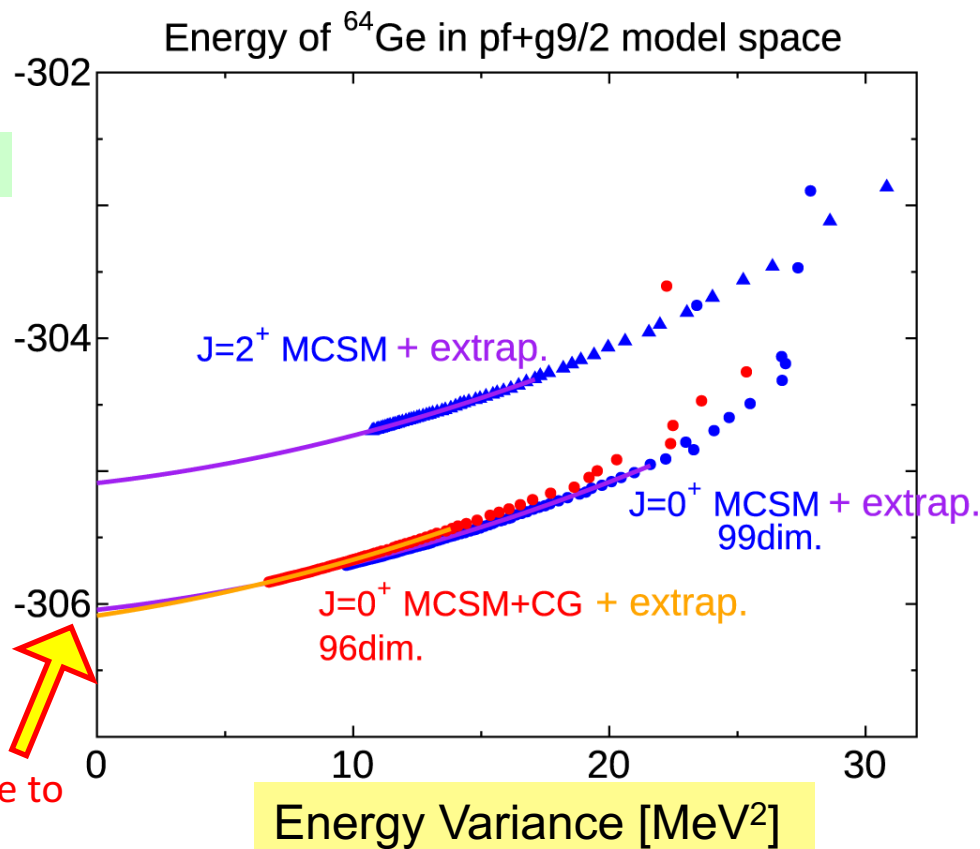
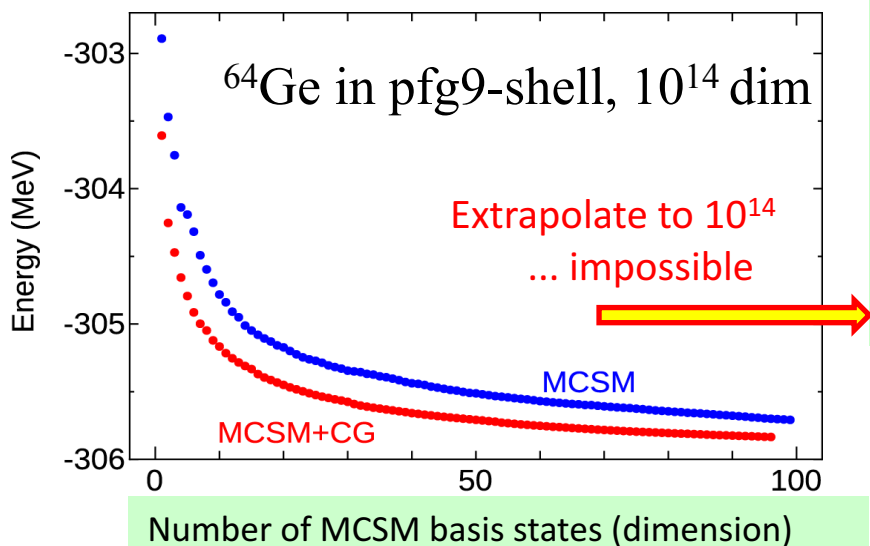


# Step 3: Energy variance extrapolation

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

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

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



$$\begin{matrix} \langle H \rangle_1 & \langle H \rangle_2 & \langle H \rangle_3 & \dots & E_{\text{exact}} \\ \langle \Delta H^2 \rangle_1 & \langle \Delta H^2 \rangle_2 & \langle \Delta H^2 \rangle_3 & \dots & 0 \end{matrix}$$

$$H_{ij} = \begin{matrix} \begin{matrix} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{matrix} \\ \begin{matrix} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{matrix} \\ \begin{matrix} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{matrix} \\ \dots \end{matrix}$$

Extrapolate to Variance 0

## MCSM (Monte Carlo Shell Model -Advanced version-)

1. Selection of important many-body basis vectors  
by **quantum Monte-Carlo** + diagonalization methods  
*basis vectors : about 100 selected Slater determinants  
composed of "deformed" single-particle states*
2. **Variational** refinement of basis vectors  
*conjugate gradient method*
3. Variance **extrapolation** method -> **exact** eigenvalues

+ innovations in algorithm and code (=> now moving to GPU)



*K computer (in Kobe) 10 peta flops machine*

⇒ *Projection of basis vectors*

Rotation with three Euler angles  
with about 50,000 mesh points

Example :  $8^+ \text{ } ^{68}\text{Ni}$  7680 core x 14 h

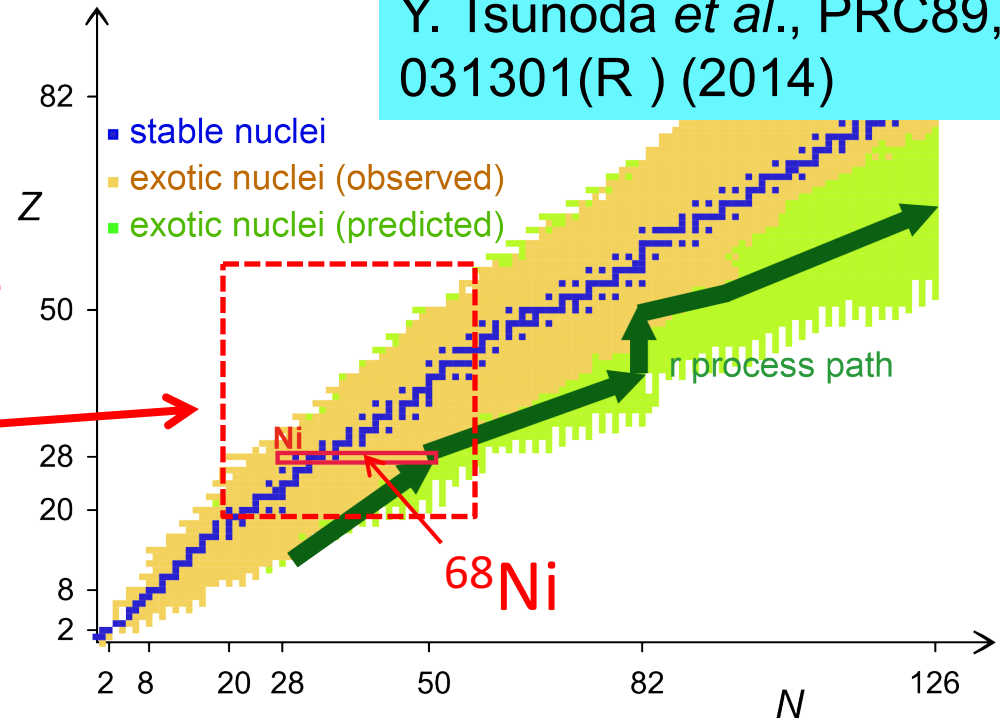
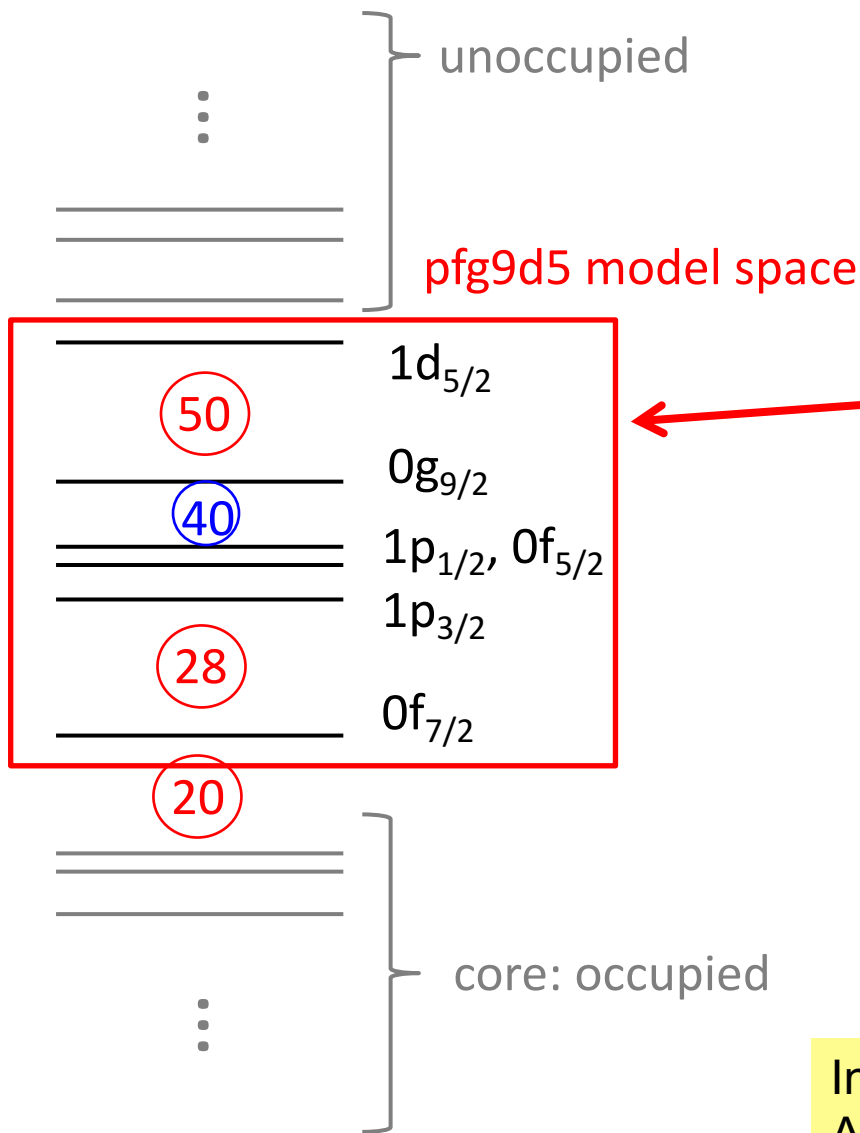
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# Monte Carlo Shell Model (MCSM) calculation on Ni isotopes

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



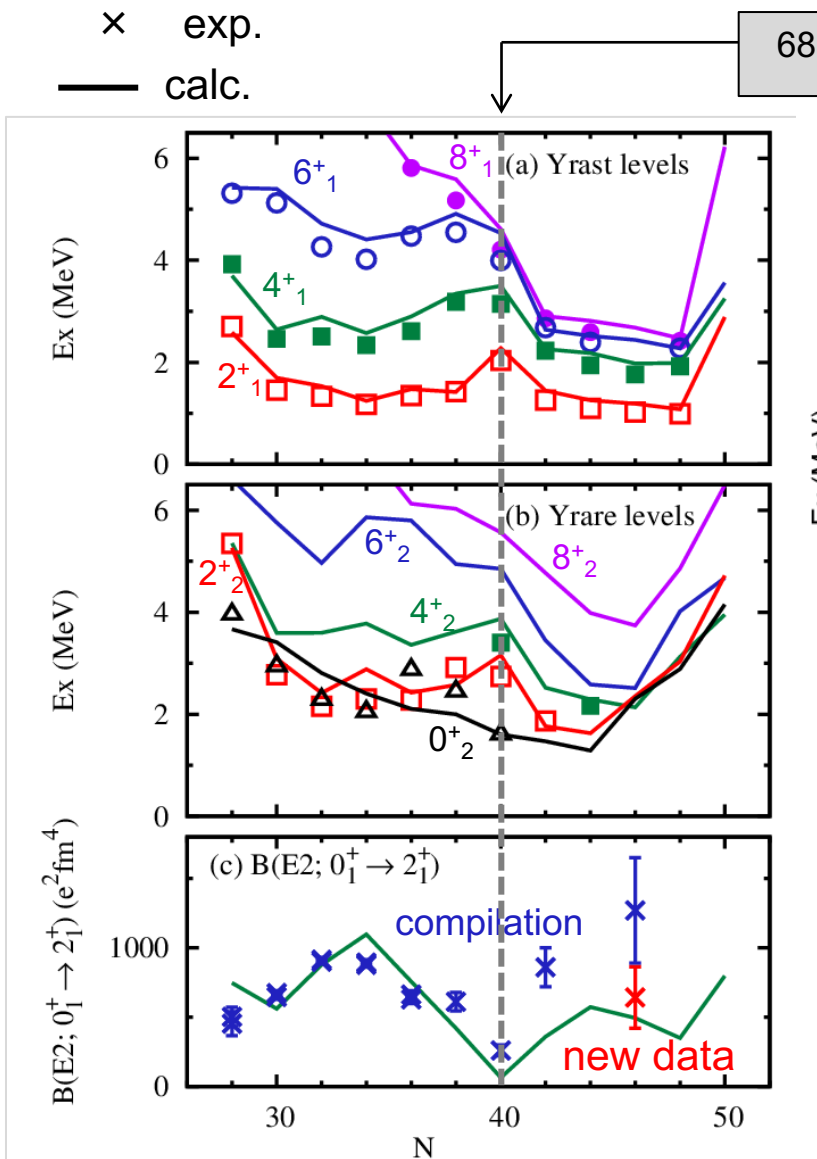
This model space is wide enough to discuss how **magic numbers 28, 50** and **semi-magic number 40** are visible or smeared out.

Interaction:  
A3DA interaction is used with minor corrections

# Energy levels and B(E2) values of Ni isotopes

Description by the same Hamiltonian

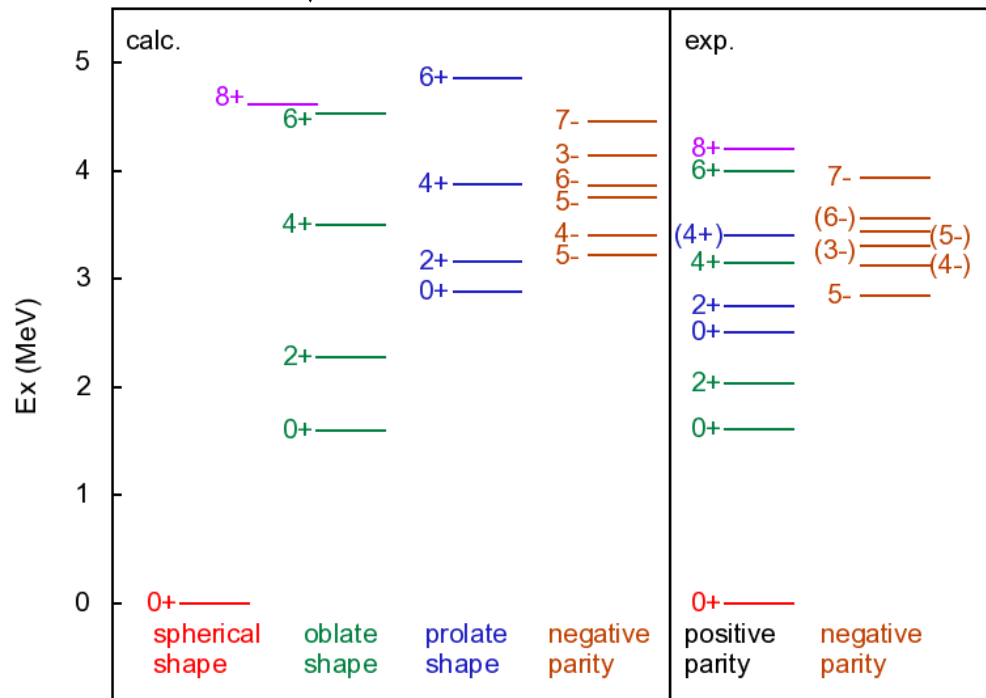
Shape coexistence in  $^{68}\text{Ni}$



$^{68}\text{Ni}$

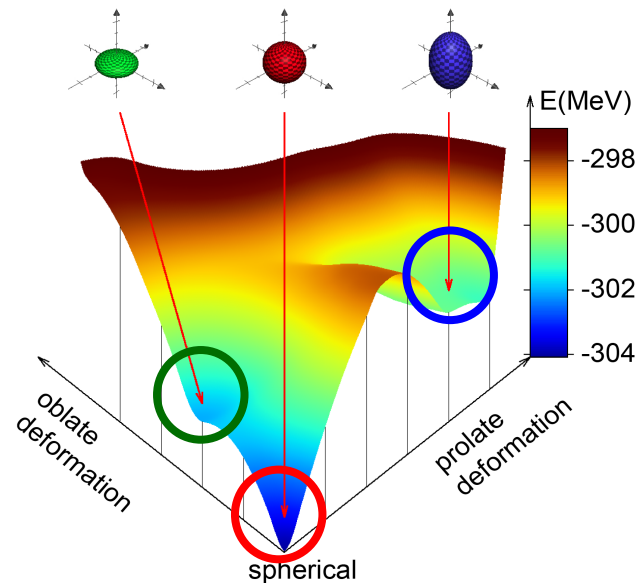
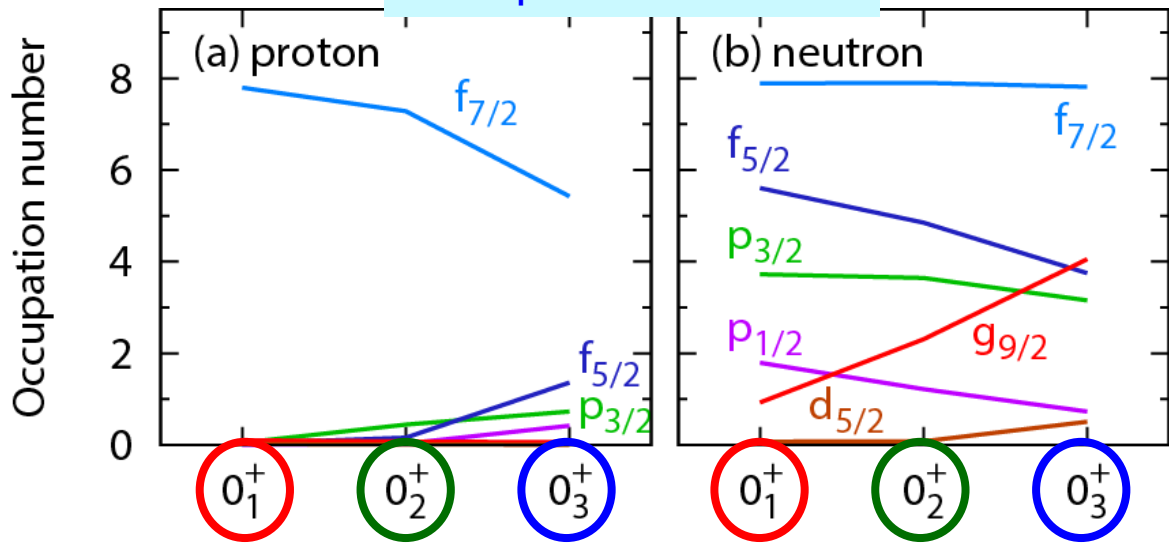
calc.

exp.

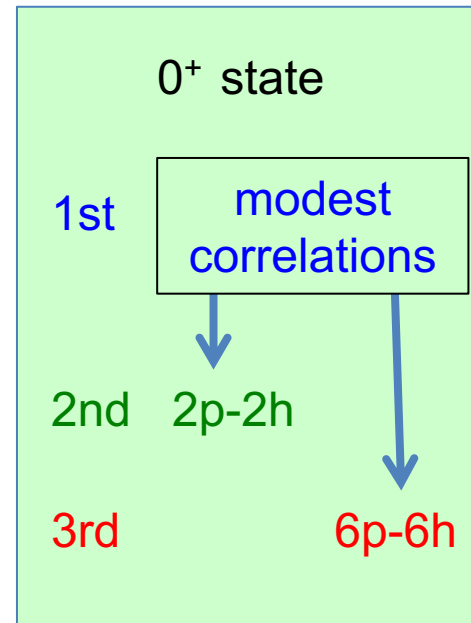
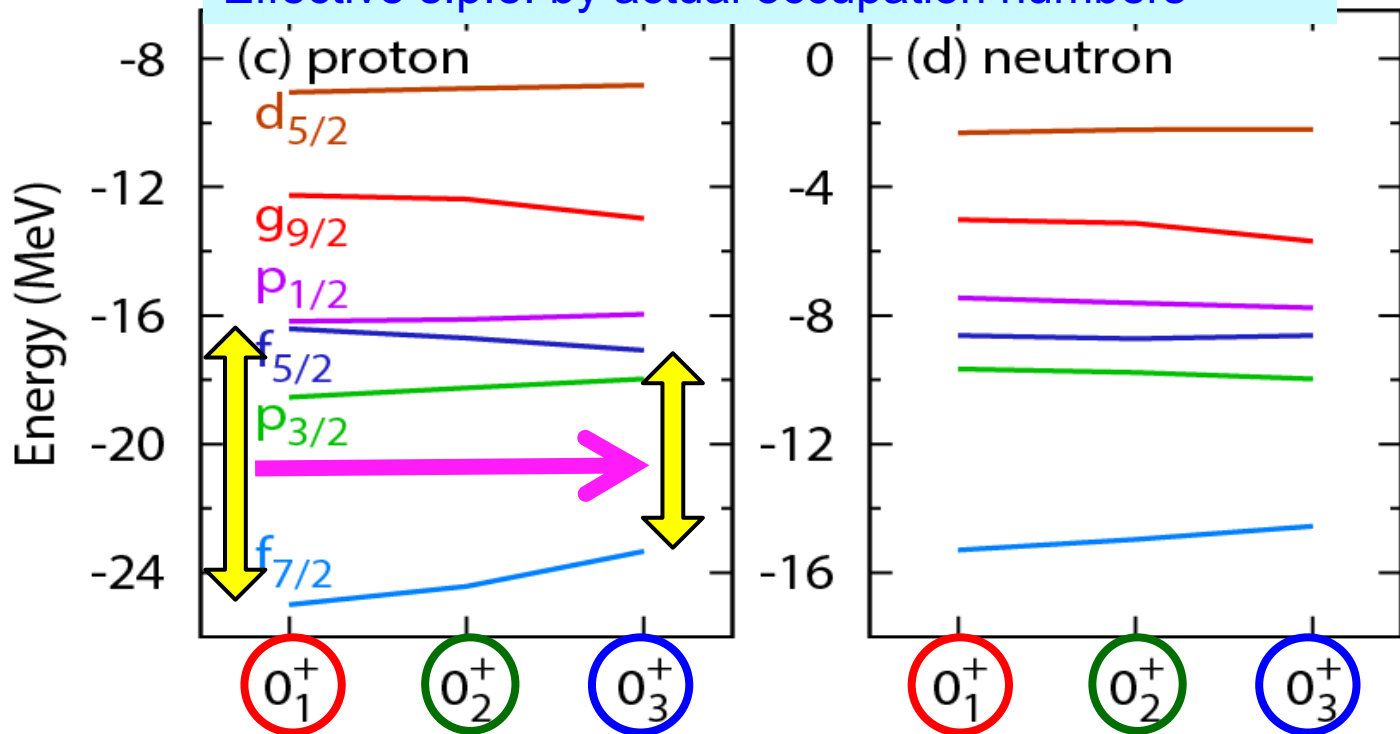


Y. Tsunoda, TO, Shimizu, Honma and Utsuno, PRC 89, 031301 (R) (2014)

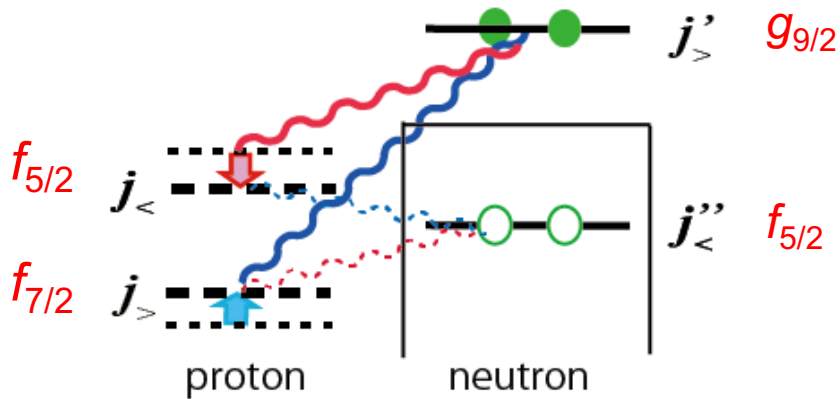
## Occupation numbers



## Effective s.p.e. by actual occupation numbers



# Type II Shell Evolution in $^{68}\text{Ni}$ ( $Z=28, N=40$ )

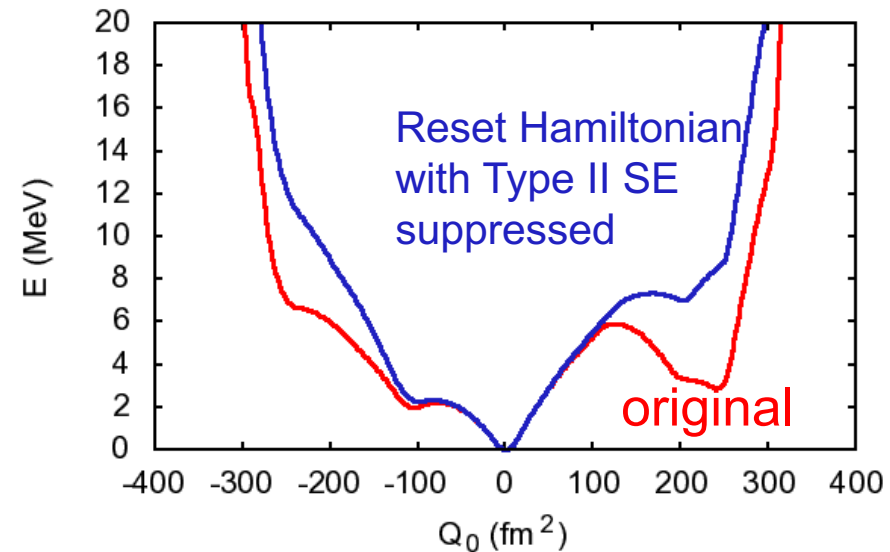


Spin-orbit splitting works against quadrupole deformation (cf. Elliott's  $SU(3)$ ).

weakening of spin-orbit splitting  
**Type II shell evolution**

stronger deformation of protons  
 → more neutron p-h excitation

PES along axially symmetric shape



Type II shell evolution is suppressed by **resetting monopole interactions** as

$$\pi f_{7/2} - \nu g_{9/2} = \pi f_{5/2} - \nu g_{9/2}$$

$$\pi f_{7/2} - \nu f_{5/2} = \pi f_{5/2} - \nu f_{5/2}$$

The local minima become much less pronounced.

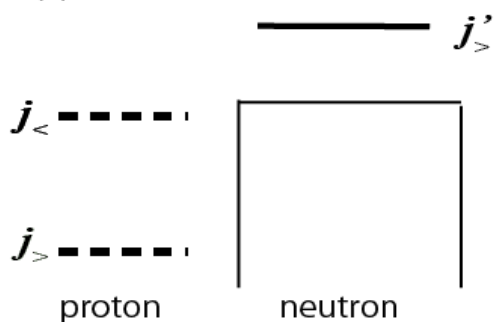
**Shape coexistence** is enhanced by **type II shell evolution** because the same quadrupole interaction can work more efficiently.

# Underlying mechanism of the appearance of low-lying deformed states : Type II Shell Evolution

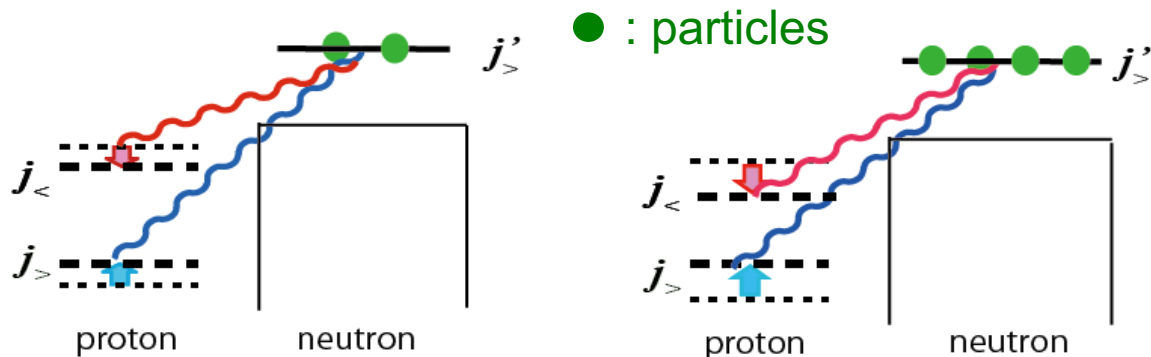
TO and Y. Tsunoda, J. Phys. G: Nucl. Part. Phys. 43 (2016) 024009

Monopole effects on the shell structure from the tensor interaction

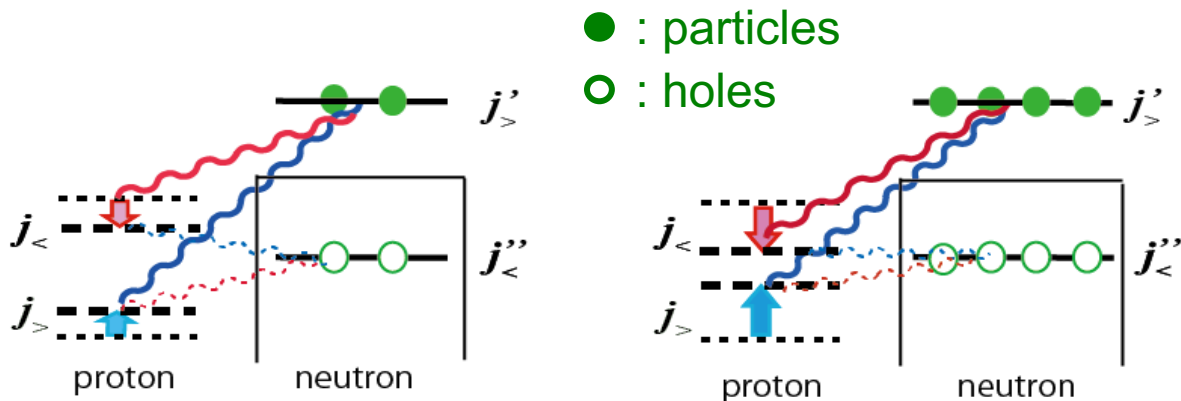
(a)



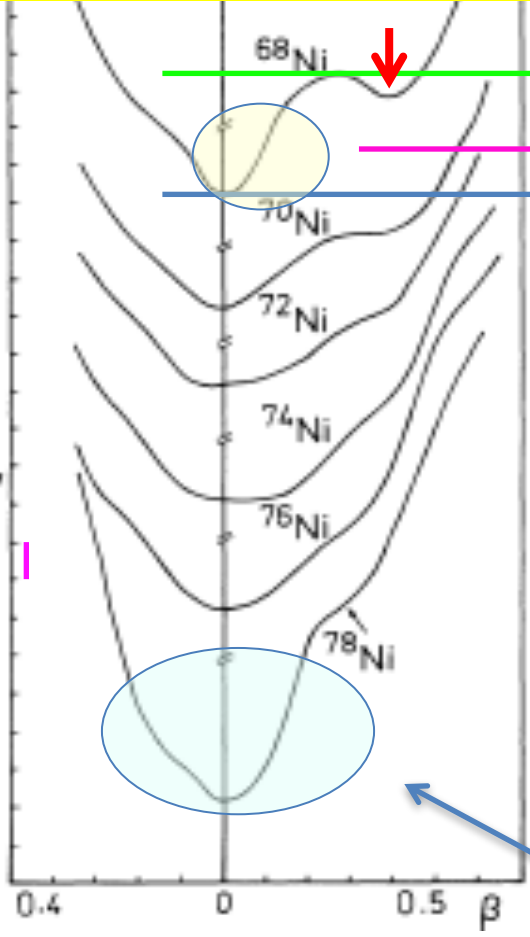
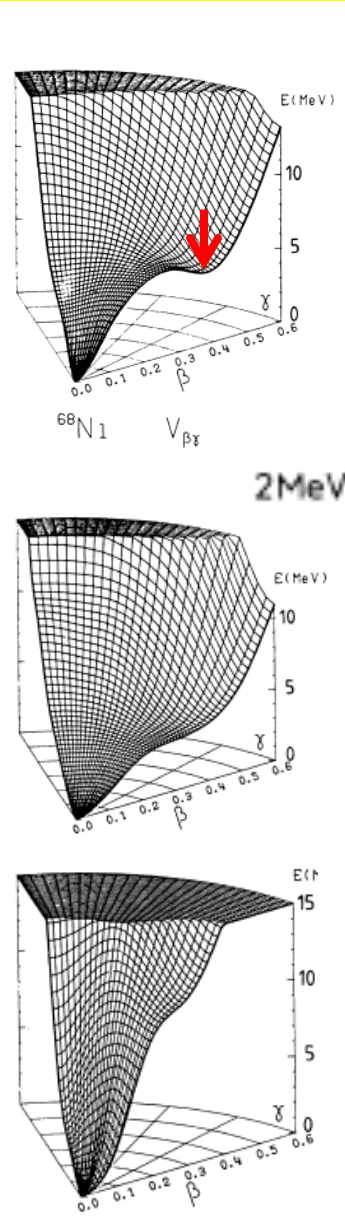
Type I Shell Evolution : different isotopes



Type II Shell Evolution : within the same nucleus

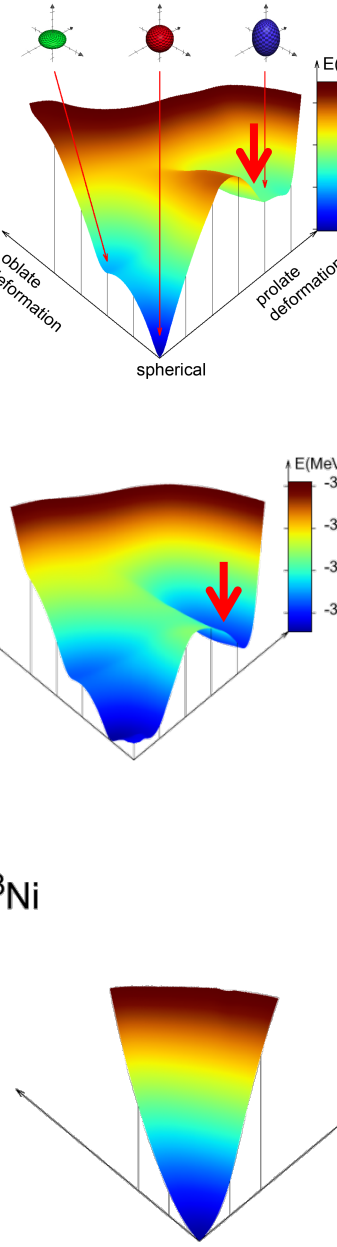
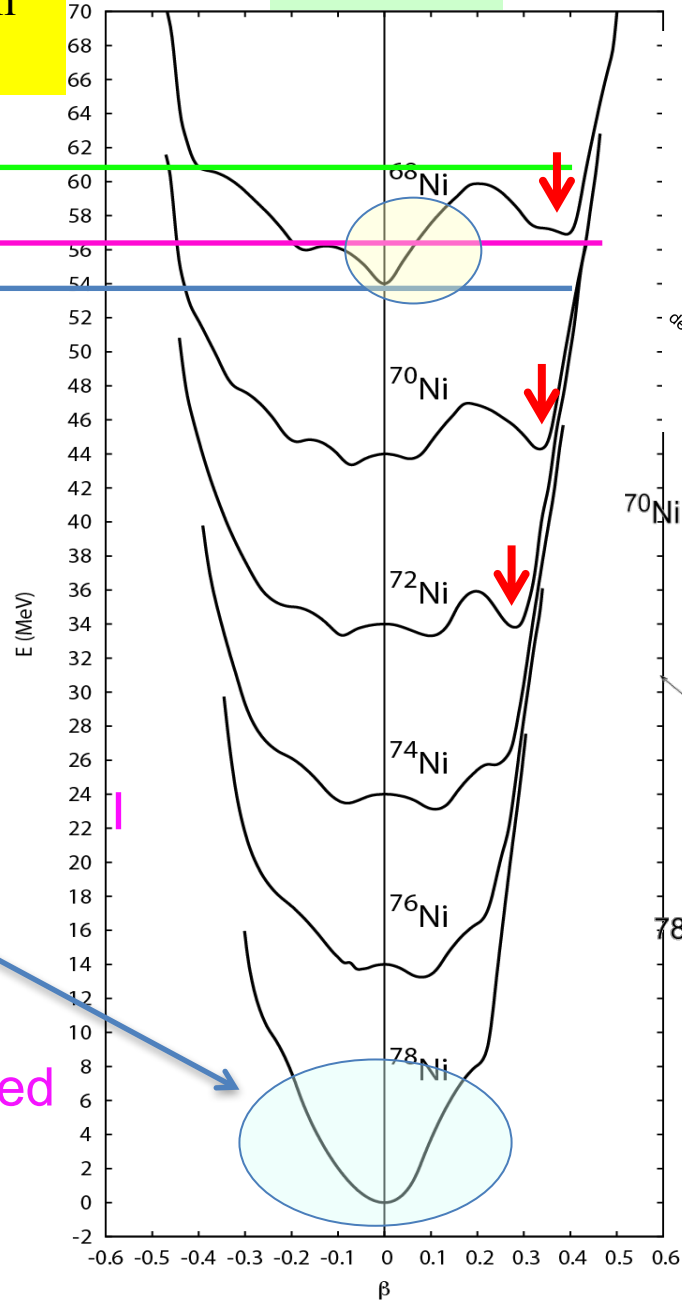


Bohr-model calc. by HFB with **Gogny** force,  
 Girod, Dessagne, Bernes, Langevin, Pougheon  
 and Roussel, PRC 37,2600 (1988)

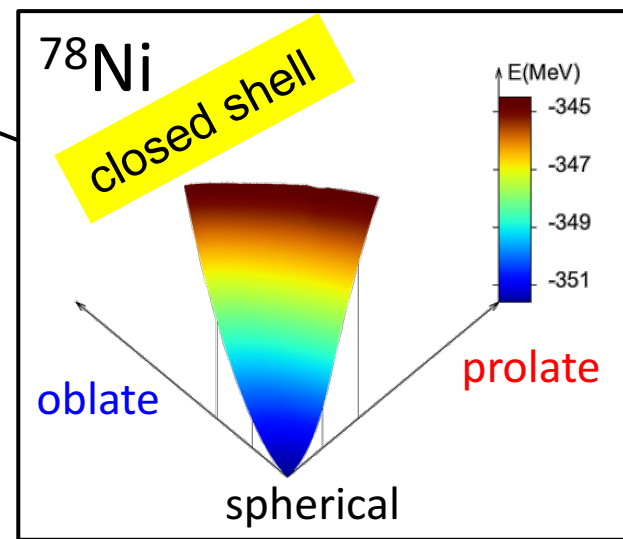
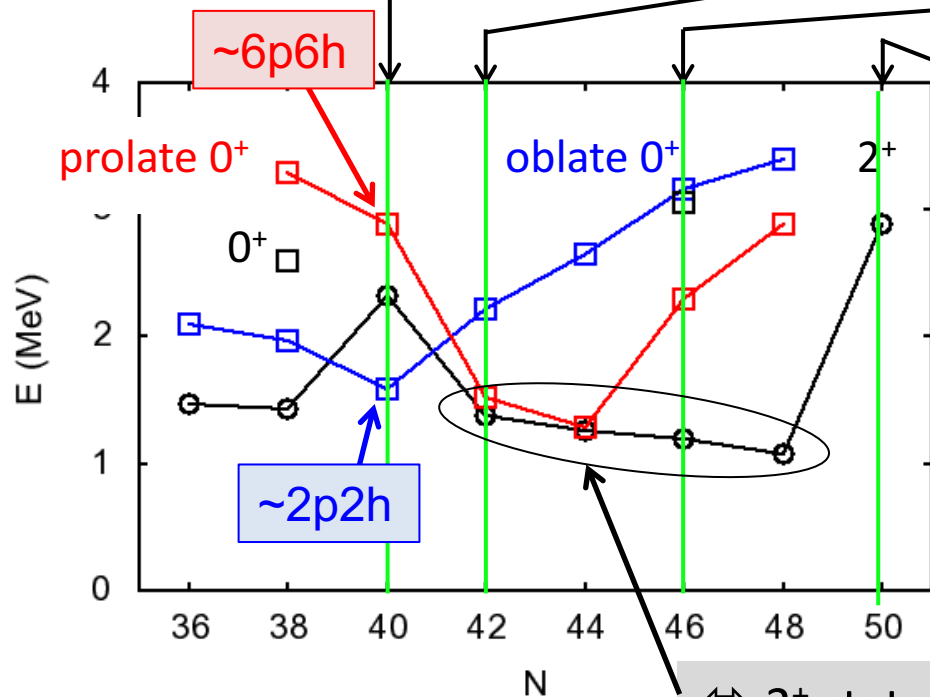
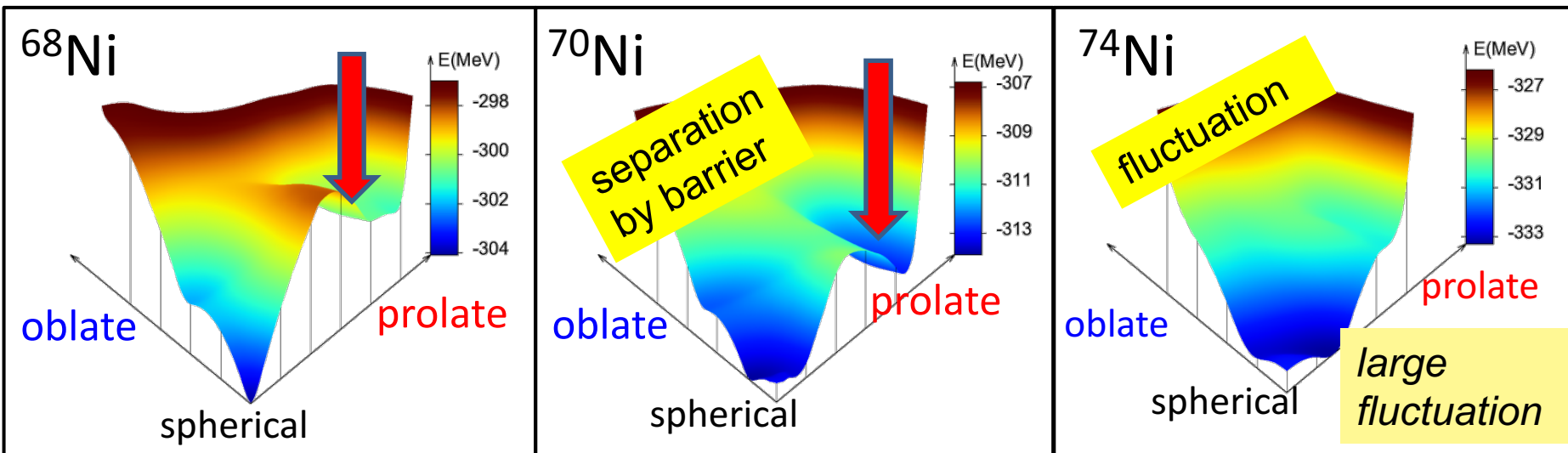


scale adjusted

present



# Shape or structure evolution of Ni isotopes



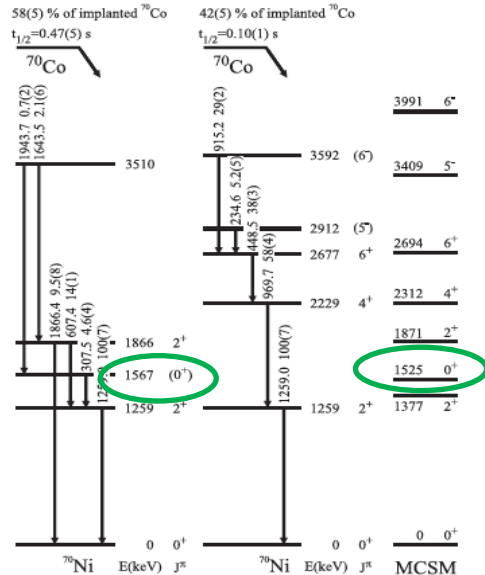
$\Leftrightarrow 2^+$  states in the  $g_{9/2}$  seniority scheme



# Low-lying $0^+_2$ in $^{70}\text{Ni}$ : prediction and verification

PHYSICAL REVIEW C 92, 061302(R) (2015)

C. J. Prokop,<sup>1,2,\*</sup> B. P. Crider,<sup>1</sup> S. N. Liddick,<sup>1,2</sup>  
*et al.*



Physics Letters B 763 (2016) 108–113

Shape coexistence from lifetime and branching-ratio measurements in  $^{68,70}\text{Ni}$

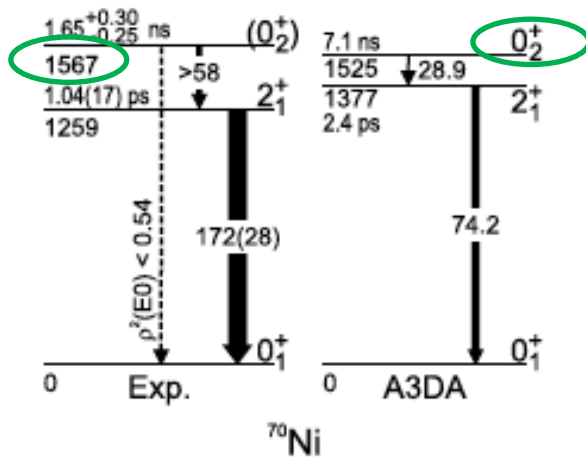
B.P. Crider<sup>a,\*</sup>, C.J. Prokop<sup>a,b</sup>, S.N. Liddick<sup>a,b</sup>, M. Al-Shudifat<sup>c</sup>, A.D. Ayangeakaa<sup>d</sup>, M.P. Carpenter<sup>d</sup>, J.J. Carroll<sup>e</sup>, J. Chen<sup>a</sup>, C.J. Chiara<sup>f</sup>, H.M. David<sup>d,1</sup>, A.C. Dombos<sup>a,g</sup>, S. Go<sup>c</sup>, R. Grzywacz<sup>c,h</sup>, J. Harker<sup>d,i</sup>, R.V.F. Janssens<sup>d</sup>, N. Larson<sup>a,b</sup>, T. Lauritsen<sup>d</sup>, R. Lewis<sup>a,b</sup>, S.J. Quinn<sup>a,g</sup>, F. Recchia<sup>j</sup>, A. Spyrou<sup>a,g</sup>, S. Suchyta<sup>k</sup>, W.B. Walters<sup>i</sup>, S. Zhu<sup>d</sup>

Upon addition of just two neutrons leading to  $^{70}\text{Ni}$ , the expectations for shape coexistence differ. Some models predict spherical-prolate shape coexistence [10,19,16] while others predict no shape coexistence at all [23–25]. The recent observation of a tentative  $0^+$  state at 1567 keV in  $^{70}\text{Ni}$  [11] suggested a drop in excitation energy of the prolate potential minimum, in line with theoretical expectations for the neutron-rich, even-Ni isotopes. The measure-

[10] S. Suchyta, S.N. Liddick, Y. Tsunoda, T. Otsuka, M.B. Bennett, A. Chemey, M. Honma, N. Larson, C.J. Prokop, S.J. Quinn, N. Shimizu, A. Simon, A. Spyrou, V. Tripathi, Y. Utsuno, J.M. VonMoss, Shape coexistence in  $^{68}\text{Ni}$ , Phys. Rev. C 89 (2014) 021301, <http://dx.doi.org/10.1103/PhysRevC.89.021301>.

[19] Y. Tsunoda, T. Otsuka, N. Shimizu, M. Honma, Y. Utsuno, Novel shape evolution in exotic Ni isotopes and configuration-dependent shell structure, Phys. Rev. C 89 (2014) 031301, <http://dx.doi.org/10.1103/PhysRevC.89.031301>.

[16] F. Flavigny, D. Pauwels, D. Radulov, I.J. Darby, H. De Witte, J. Diriken, D.V. Fedorov, V.N. Fedosseev, L.M. Fraile, M. Huyse, V.S. Ivanov, U. Köster, B.A. Marsh, T. Otsuka, L. Popescu, R. Raabe, M.D. Seliverstov, N. Shimizu, A.M. Sjödin, Y. Tsunoda, P. Van den Bergh, P. Van Duppen, J. Van de Walle, M. Venhart, W.B. Walters, K. Wimmer, Characterization of the low-lying  $0^+$  and  $2^+$  states in  $^{68}\text{Ni}$  via  $\beta$  decay of the low-spin  $^{68}\text{Co}$  isomer, Phys. Rev. C 91 (2015) 034310, <http://dx.doi.org/10.1103/PhysRevC.91.034310>.



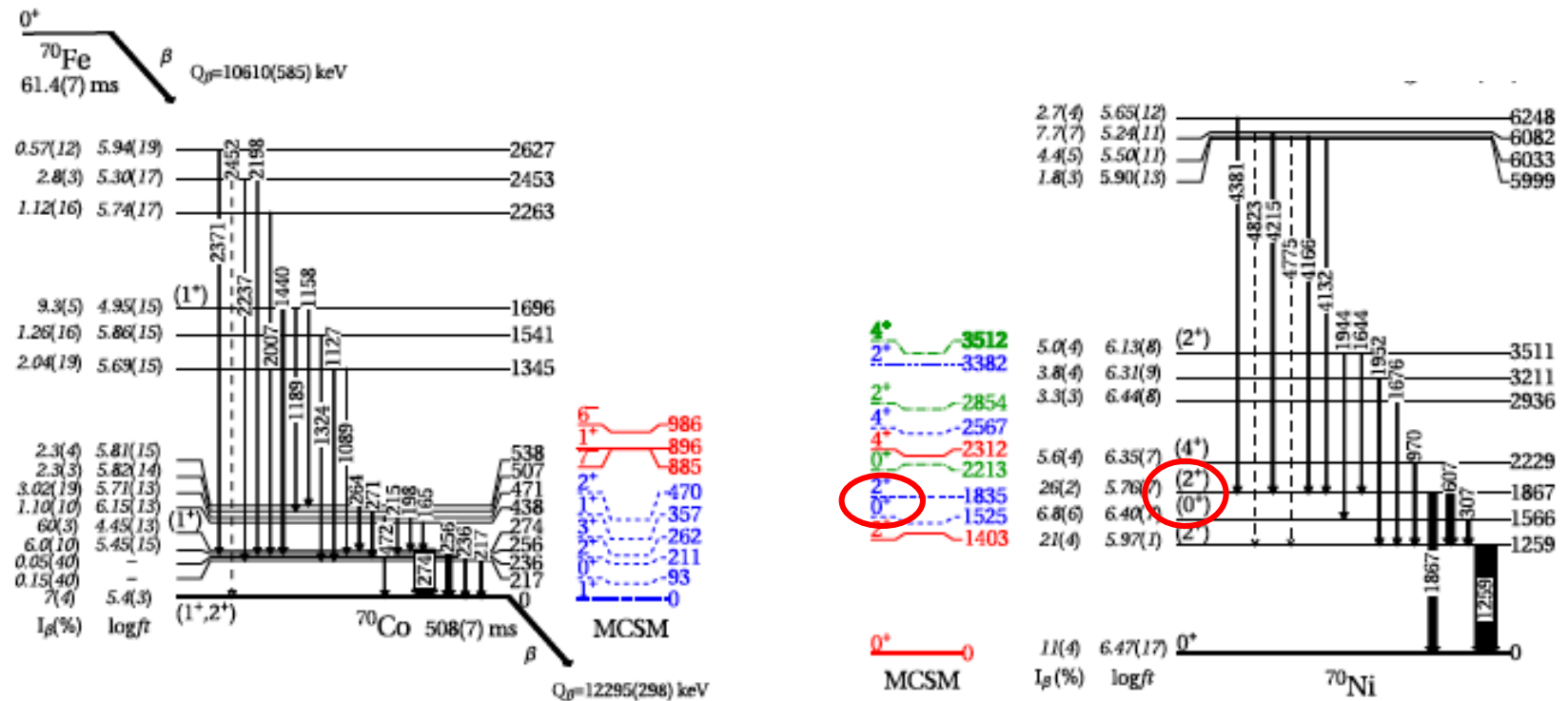


Type II shell evolution in  $A = 70$  isobars from the  $N \geq 40$  island of inversion

A.I. Morales<sup>a,b,\*</sup>, G. Benzoni<sup>a</sup>, H. Watanabe<sup>c,d</sup>, Y. Tsunoda<sup>e</sup>, T. Otsuka<sup>f,g,h</sup>, S. Nishimura<sup>d</sup>, F. Browne<sup>i,d</sup>, R. Daido<sup>j</sup>, P. Doornenbal<sup>d</sup>, Y. Fang<sup>j</sup>, G. Lorusso<sup>d</sup>, Z. Patel<sup>k,d</sup>, S. Rice<sup>k,d</sup>, L. Sinclair<sup>l,d</sup>, P.-A. Söderström<sup>d</sup>, T. Sumikama<sup>m</sup>, J. Wu<sup>d</sup>, Z.Y. Xu<sup>f,d</sup>, A. Yagi<sup>j</sup>, R. Yokoyama<sup>f</sup>, H. Baba<sup>d</sup>, R. Avigo<sup>a,b</sup>, F.L. Bello Garrote<sup>n</sup>, N. Blasi<sup>a</sup>, A. Bracco<sup>a,b</sup>, F. Camera<sup>a,b</sup>, S. Ceruti<sup>a,b</sup>, F.C.L. Crespi<sup>a,b</sup>, G. de Angelis<sup>o</sup>, M.-C. Delattre<sup>p</sup>, Zs. Dombradi<sup>q</sup>, A. Gottardo<sup>o</sup>, T. Isobe<sup>d</sup>, I. Kojouharov<sup>r</sup>, N. Kurz<sup>r</sup>, I. Kuti<sup>q</sup>, K. Matsui<sup>f</sup>, B. Melon<sup>s</sup>, D. Mengoni<sup>t,u</sup>, T. Miyazaki<sup>f</sup>, V. Modamio-Hoybjør<sup>o</sup>, S. Momiyama<sup>f</sup>, D.R. Napoli<sup>o</sup>, M. Niikura<sup>f</sup>, R. Orlandi<sup>h,v</sup>, H. Sakurai<sup>d,f</sup>, E. Sahin<sup>n</sup>, D. Sohler<sup>q</sup>, H. Schaffner<sup>r</sup>, R. Taniuchi<sup>f</sup>, J. Taprogge<sup>w,x</sup>, Zs. Vajta<sup>q</sup>, J.J. Valiente-Dobón<sup>o</sup>, O. Wieland<sup>a</sup>, M. Yalcinkaya<sup>y</sup>

<sup>a</sup> Istituto Nazionale di Fisica Nucleare, Sezione di Milano, Via Celoria 16, 20133 Milano, Italy

<sup>b</sup> Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy



# MCSM basis vectors on Potential Energy Surface

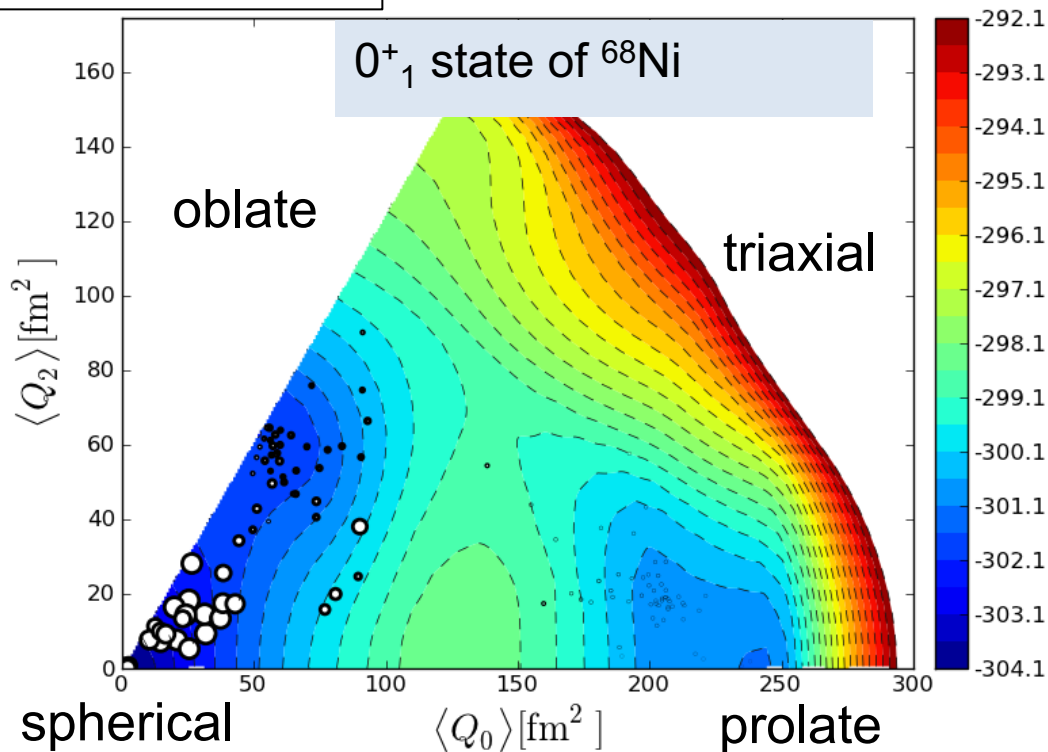
eigenstate  $\Psi = \sum_i c_i P[J^\pi](\Phi_i)$

amplitude  $c_i$

projection onto  $J^\pi$   $P[J^\pi]$

Slater determinant of deformed s. p. states  $\rightarrow$  intrinsic shape  $\Phi_i$

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



Called **T-plot** in reference to Y. Tsunoda, *et al.* PRC 89, 031301 (R) (2014)



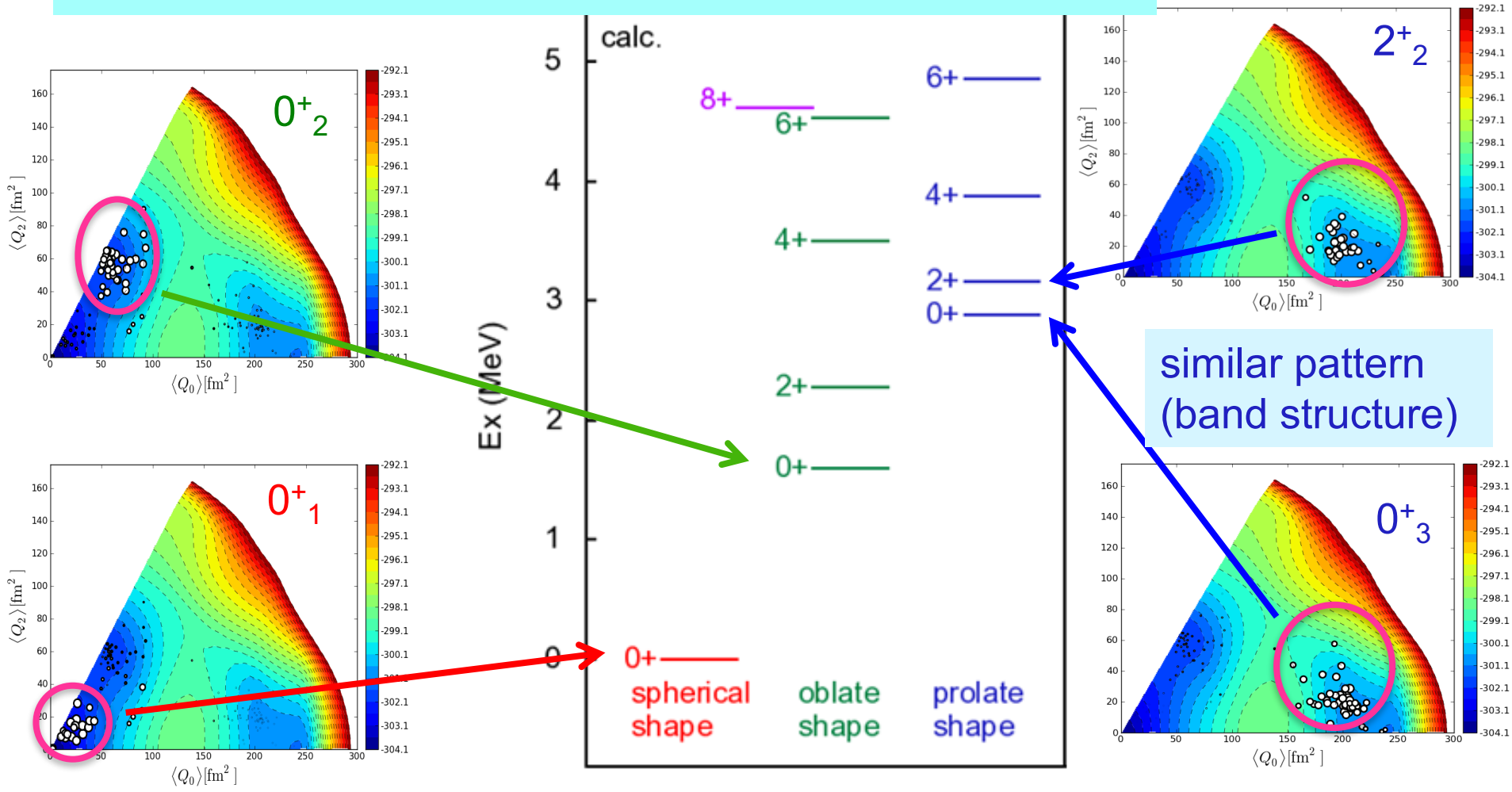
# General properties of T-plot :

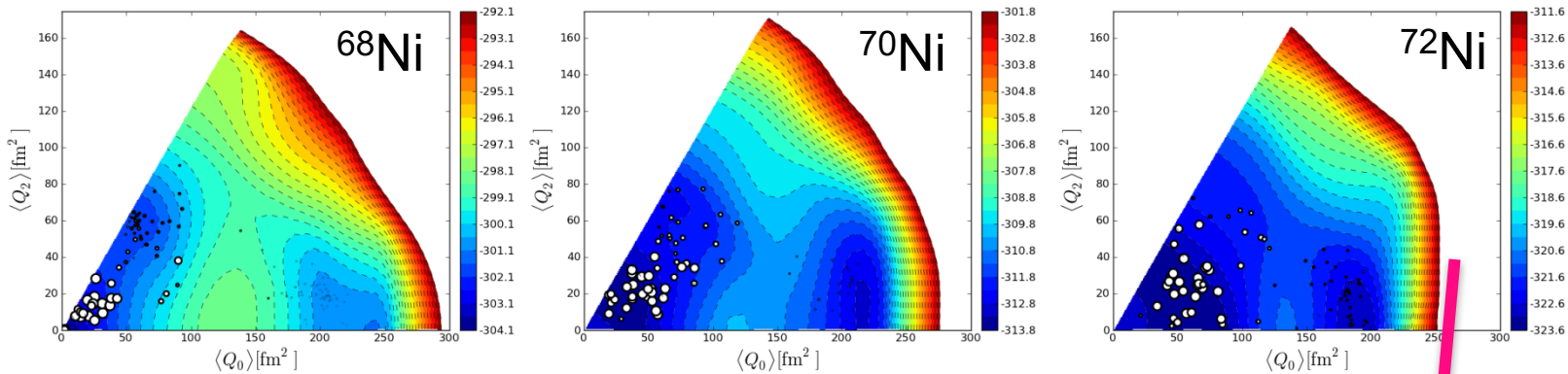
Certain number of large circles in a small region of PES

⇔ pairing correlations

Spreading beyond this can be due to shape fluctuation

## Example : shape assignment to various $0^+$ states of $^{68}\text{Ni}$



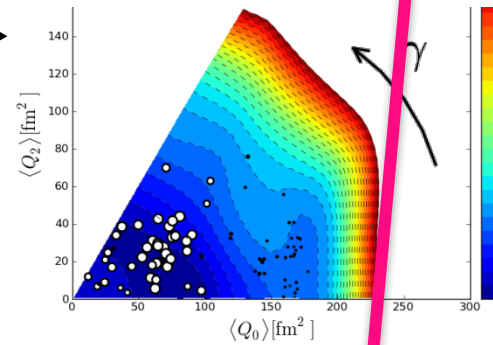


Energy of prolate state comes down.  
Barrier becomes low.

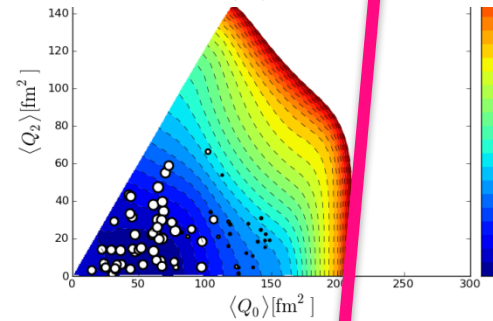
T-plot  
for  $0^+_{1}$  states of  $^{68-78}\text{Ni}$

The ground state is always like  
seniority-zero (BCS-type)  
spherical state.

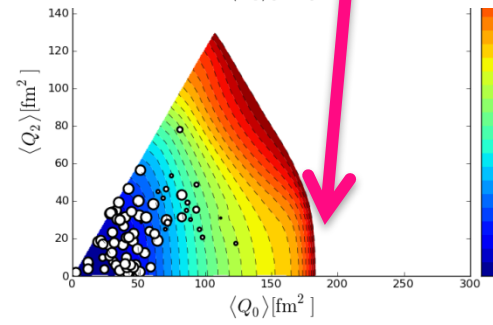
$^{74}\text{Ni}$



$^{76}\text{Ni}$



$^{78}\text{Ni}$



$\gamma$ -soft deformation  
(strong fluctuation in the  $\gamma$  direction)



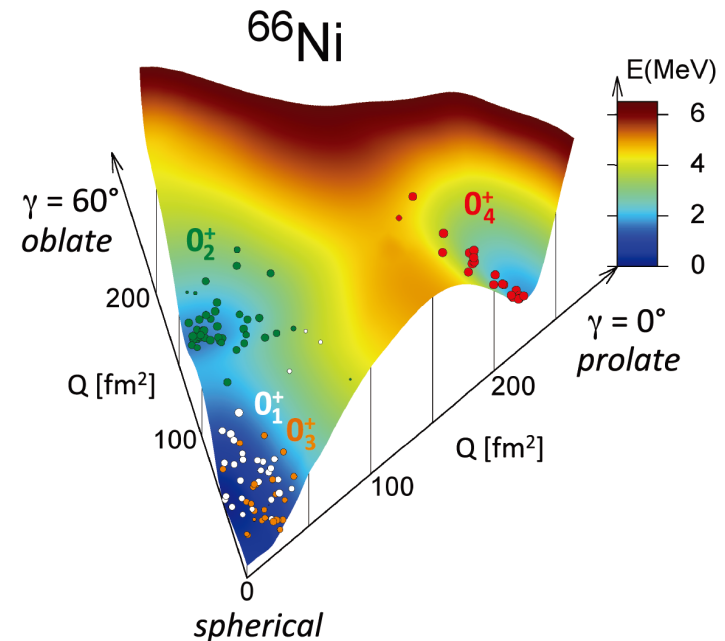
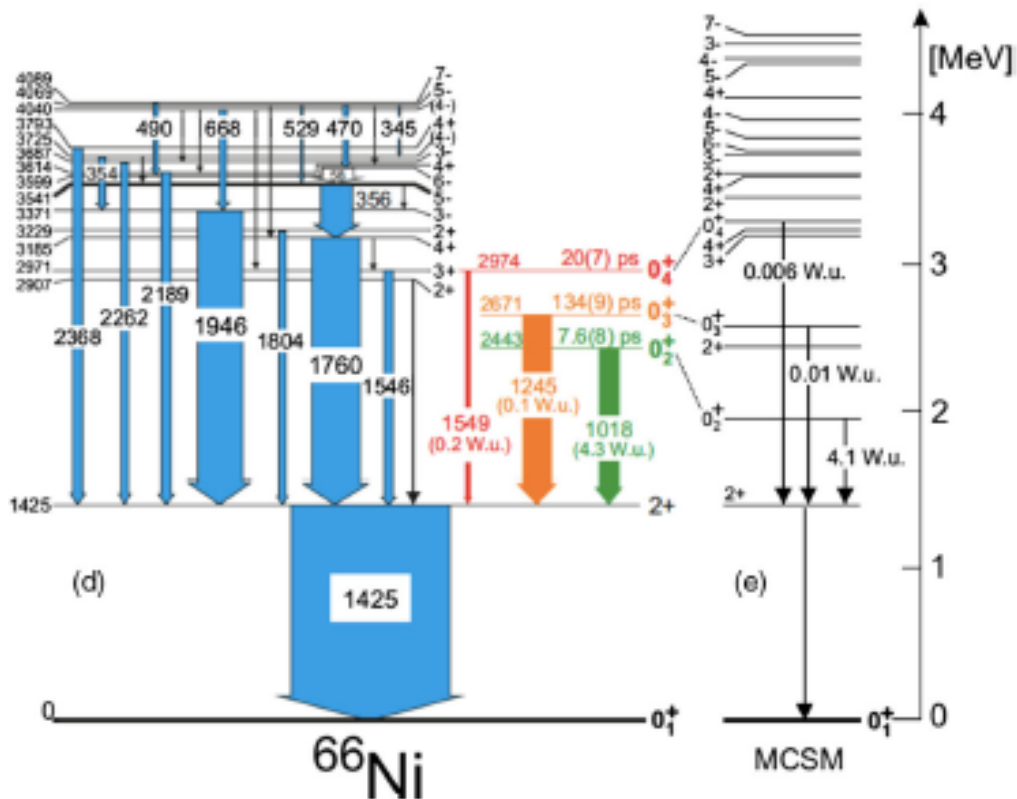
## Multifaceted Quadruplet of Low-Lying Spin-Zero States in $^{66}\text{Ni}$ : Emergence of Shape Isomerism in Light Nuclei

S. Leoni,<sup>1,2,\*</sup> B. Fornal,<sup>3</sup> N. Mărginean,<sup>4</sup> M. Sferrazza,<sup>5</sup> Y. Tsunoda,<sup>6</sup> T. Otsuka,<sup>6,7,8,9</sup> G. Bocchi,<sup>1,2</sup> F. C. L. Crespi,<sup>1,2</sup>  
A. Bracco,<sup>1,2</sup> S. Aydin,<sup>10</sup> M. Boromiza,<sup>4,11</sup> D. Bucurescu,<sup>4</sup> N. Cieplicka-Oryńczak,<sup>2,3</sup> C. Costache,<sup>4</sup> S. Călinescu,<sup>4</sup>  
N. Florea,<sup>4</sup> D. G. Ghiță,<sup>4</sup> T. Glodariu,<sup>4</sup> A. Ionescu,<sup>4,11</sup> Ł. W. Iskra,<sup>3</sup> M. Krzysiek,<sup>3</sup> R. Mărginean,<sup>4</sup> C. Mihai,<sup>4</sup> R. E. Mihai,<sup>4</sup>  
A. Mitu,<sup>4</sup> A. Negreț,<sup>4</sup> C. R. Niță,<sup>4</sup> A. Olăcel,<sup>4</sup> A. Oprea,<sup>4</sup> S. Pascu,<sup>4</sup> P. Petkov,<sup>4</sup> C. Petrone,<sup>4</sup> G. Porzio,<sup>1,2</sup> A. Șerban,<sup>4,11</sup>  
C. Sotty,<sup>4</sup> L. Stan,<sup>4</sup> I. Știru,<sup>4</sup> L. Stroe,<sup>4</sup> R. Șuvăilă,<sup>4</sup> S. Toma,<sup>4</sup> A. Turturică,<sup>4</sup> S. Ujeniuc,<sup>4</sup> and C. A. Ur<sup>1,2</sup>

<sup>1</sup>Dipartimento di Fisica, Università degli Studi di Milano, I-20133 Milano, Italy

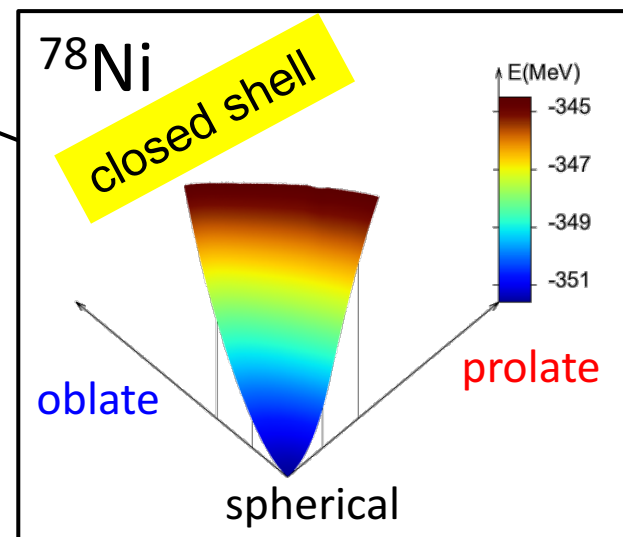
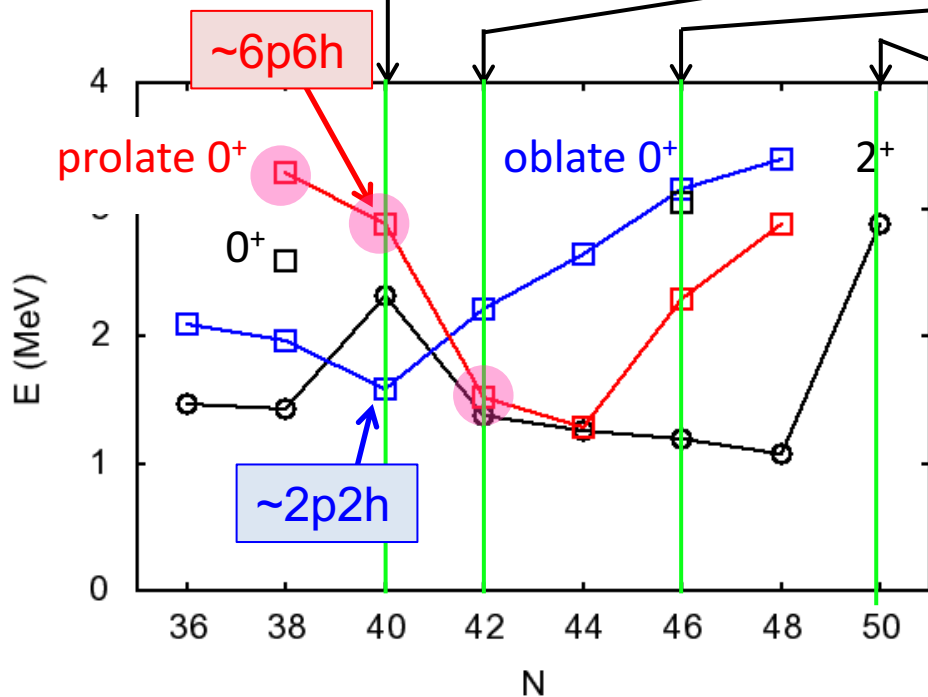
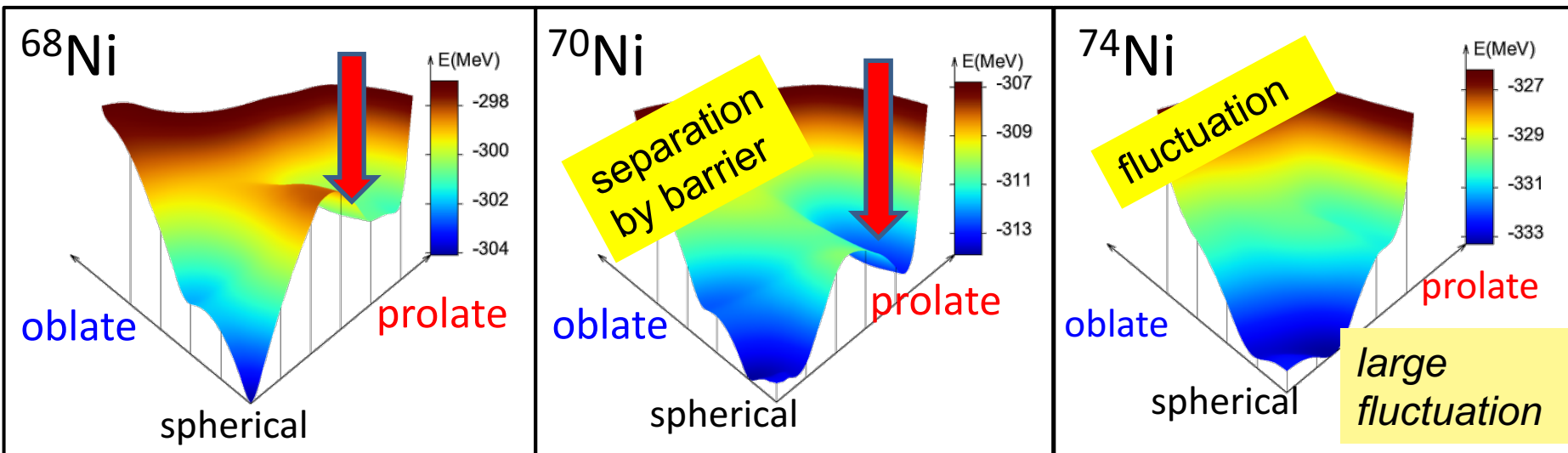
<sup>2</sup>INFN sezione di Milano via Celoria 16, 20133, Milano, Italy

<sup>3</sup>Institute of Nuclear Physics, PAN, 31-342 Kraków, Poland





# Shape or structure evolution of Ni isotopes



# *Outline*

I Introduction

II Presently used numerical methodology of many-body problems

III First application of MCSM to shape coexistence: Ni isotopes

IV An example from Quantum Phase Transition in Zr isotopes

V Basic mechanism

VI Shape coexistence and/or critical phenomena in Hg/Pb isotopes

VII Remarks

# An example : shapes of Zr isotopes by Monte Carlo Shell Model

- Effective interaction:

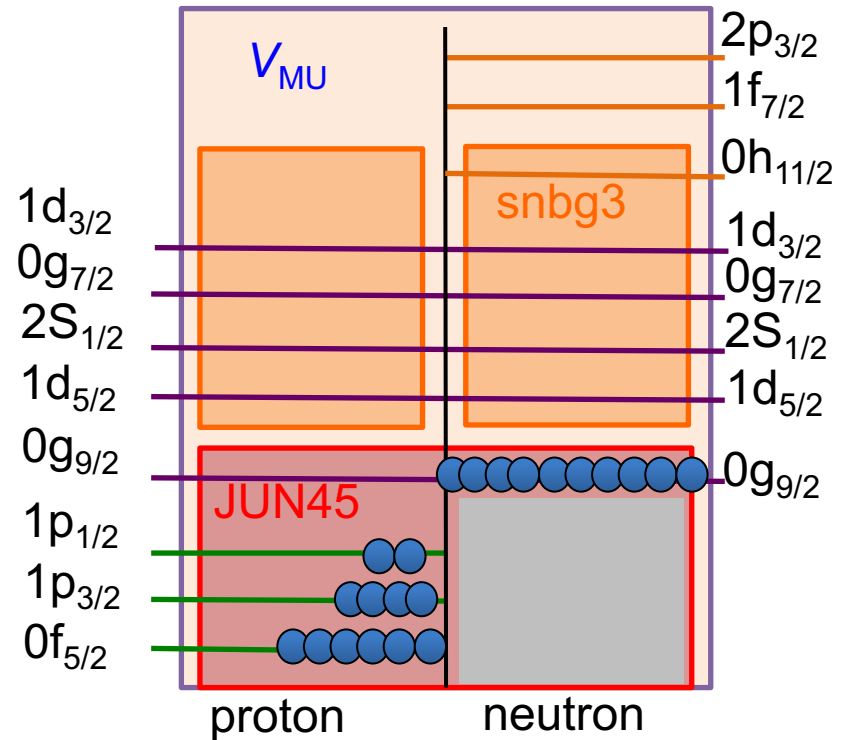
$$\text{JUN45} + \text{snbg3} + V_{\text{MU}}$$

*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  $3.7 \times 10^{23}$  **dimension** matrix.



$^{56}\text{Ni}$

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

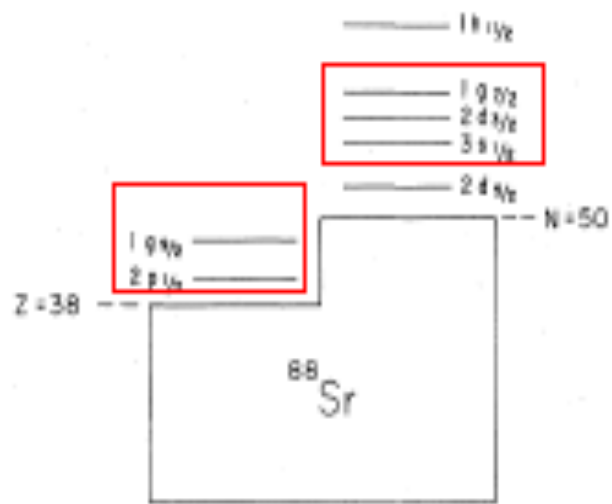


FIG. 3. Single-particle levels appropriate to a description of nuclei in the Zr-Mo region. An  $^{88}\text{Sr}$  core is assumed.

PHYSICAL REVIEW C 79, 064310 (2009)

## Shell model description of zirconium isotopes

K. Sieja,<sup>1,2</sup> F. Nowacki,<sup>3</sup> K. Langanke,<sup>2,4</sup> and G. Martínez-Pinedo<sup>1</sup>

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  $\pi(r3 - g)$ ,  $\nu(r4 - h)$ .

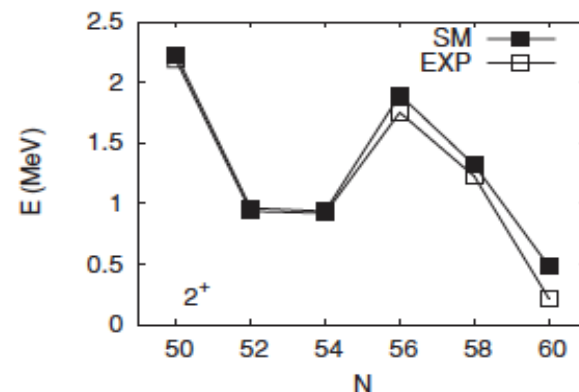
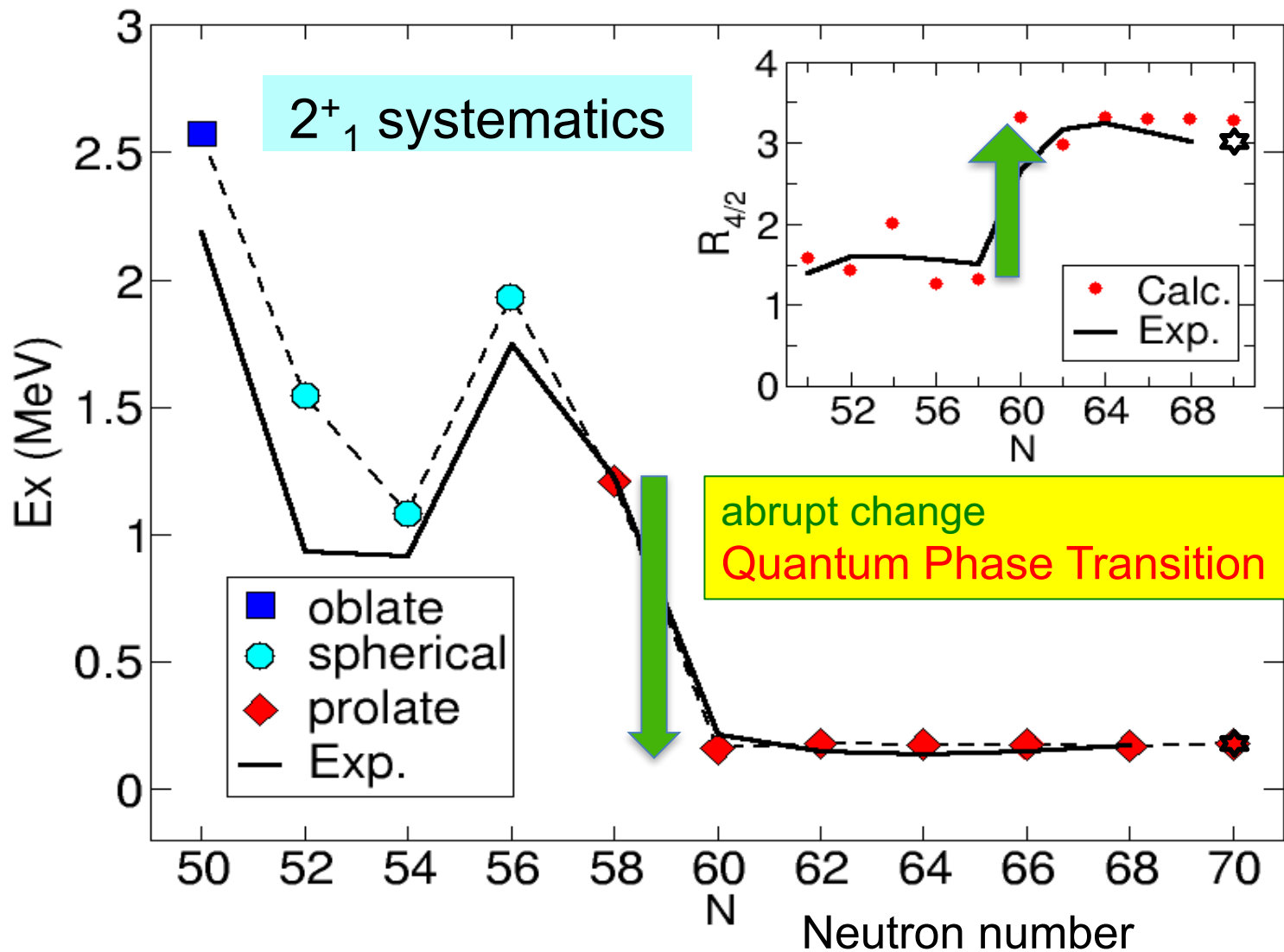


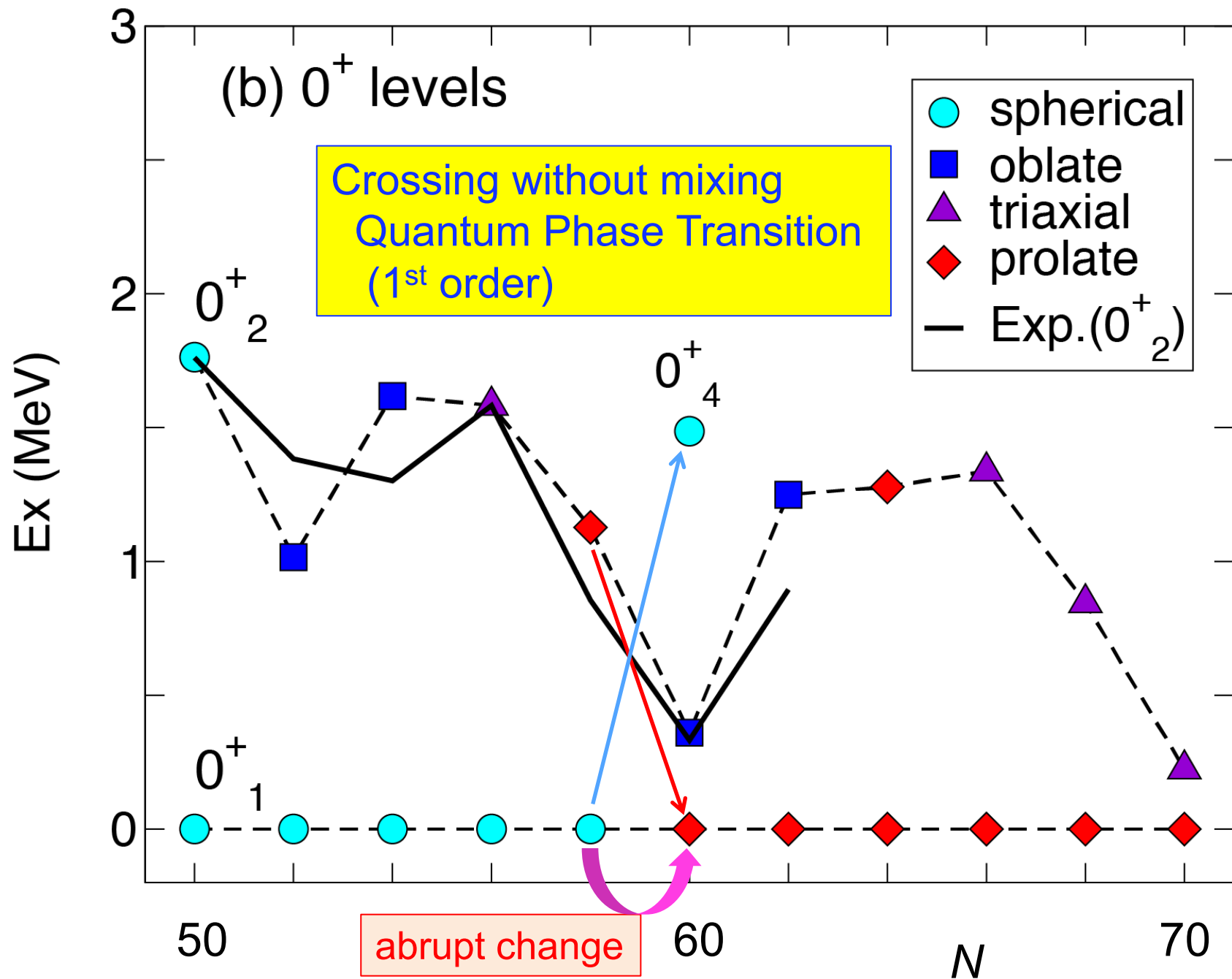
FIG. 12. Systematics of the experimental and theoretical first excited  $2^+$  states along the zirconium chain.



# Quantum Phase Transition in the Shape of Zr isotopes

Tomoaki Togashi,<sup>1</sup> Yusuke Tsunoda,<sup>1</sup> Takaharu Otsuka,<sup>1,2,3,4</sup> and Noritaka Shimizu<sup>1</sup>



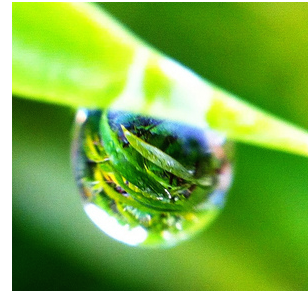


## Can this be a “Phase Transition” ?

### *Phase Transition* :

A **macroscopic** system can change qualitatively from a stable state (e.g. ice for H<sub>2</sub>O) to another stable state (e.g., water for H<sub>2</sub>O) as a function of a certain parameter (e.g., temperature).

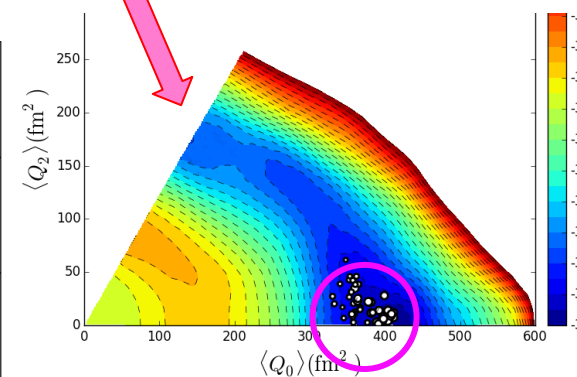
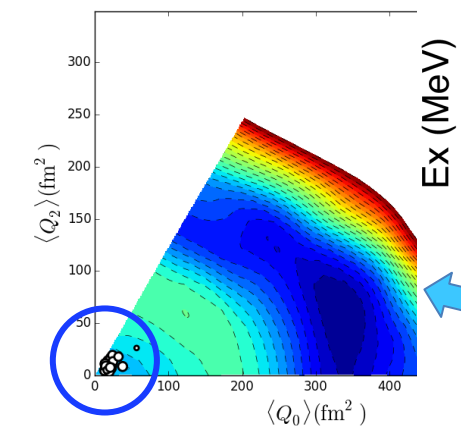
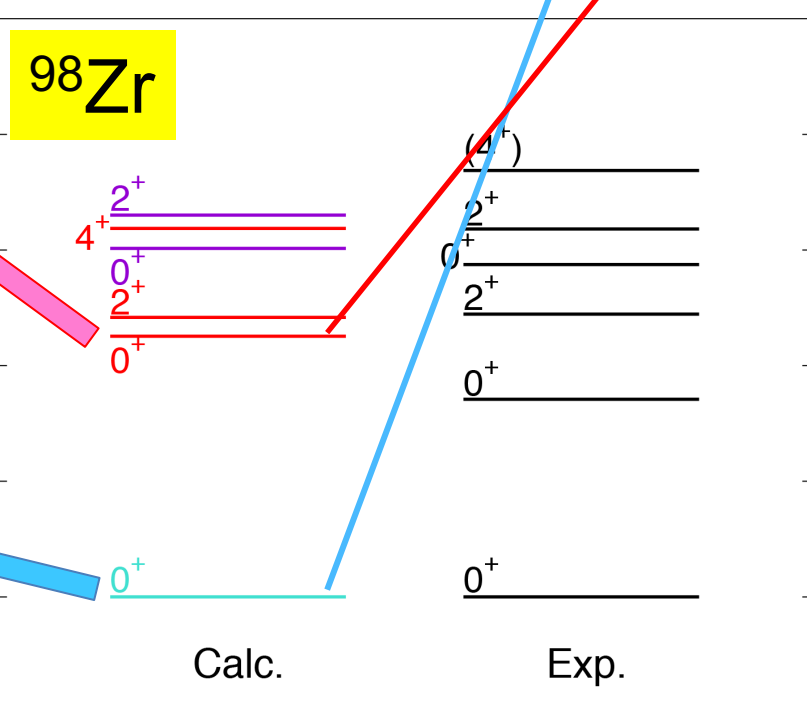
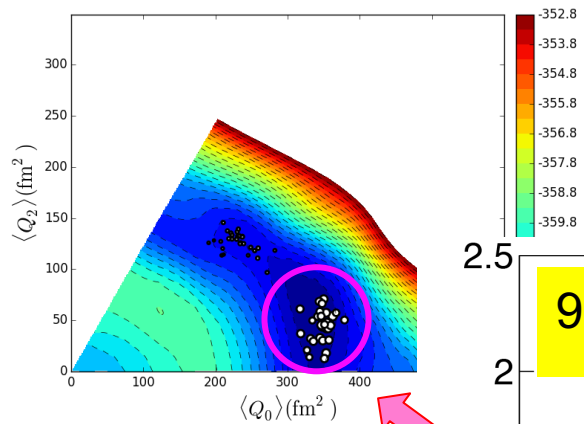
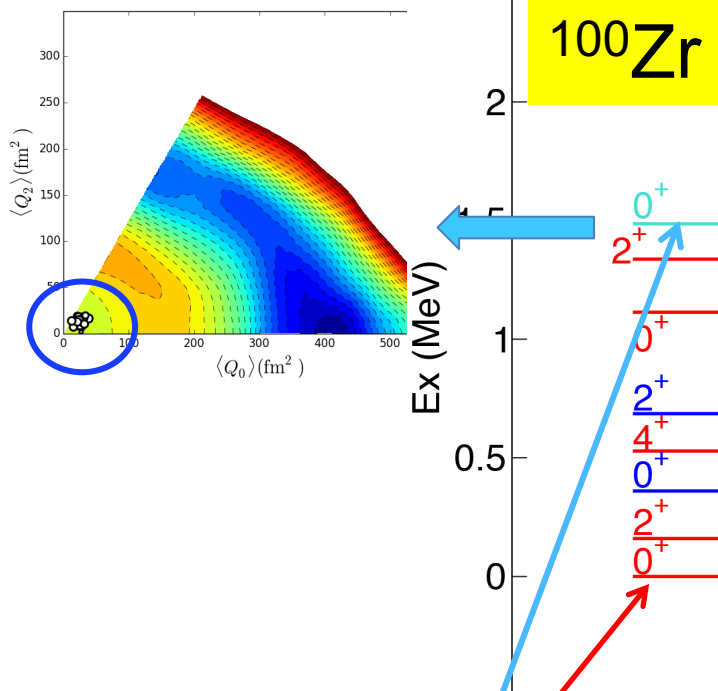
The phase transition implies this kind of phenomena of macroscopic systems consisting of **almost infinite number of molecules**.

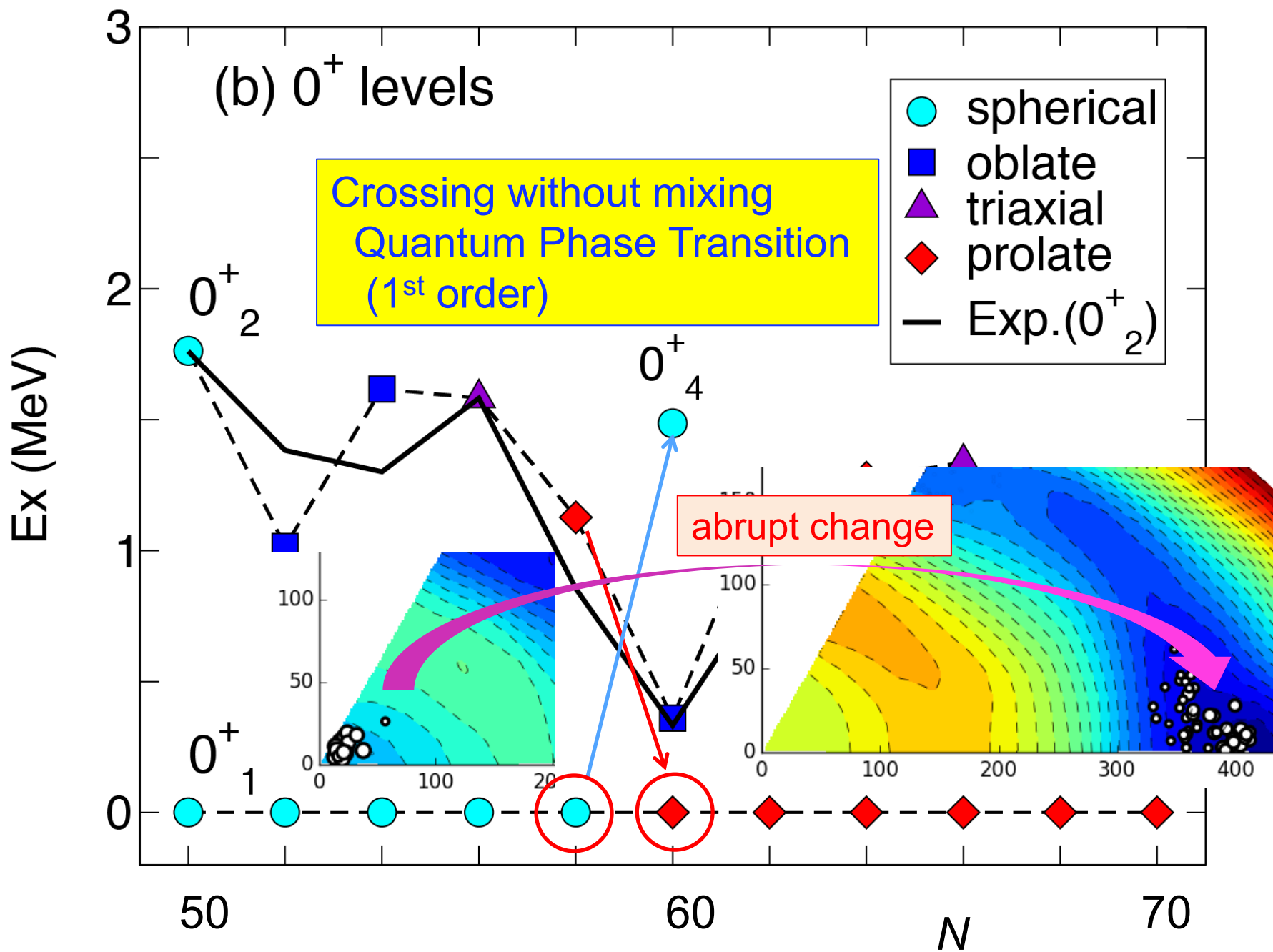


### *Quantum Phase Transition (QPT)*

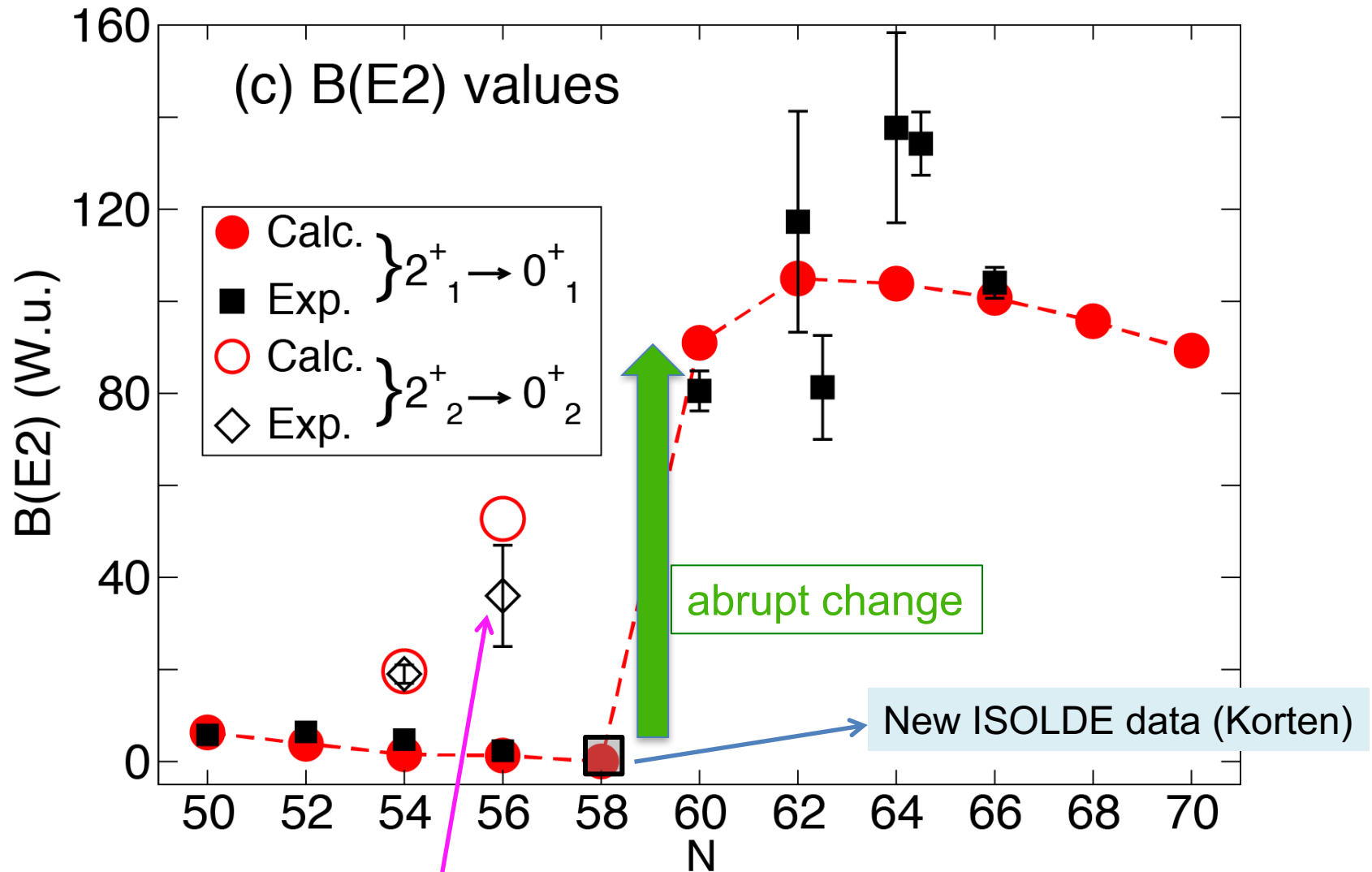
The concept of the phase transition cannot be applied to microscopic systems as it is. The QPT has been introduced as *an abrupt change (of order parameter) in the ground state of a many-body system by varying a physical (i.e., control) parameter at zero temperature. (cf., Wikipedia)*

Quantum Phase Transition  
(1<sup>st</sup> order)  
due to crossing  
without mixing





# B(E2; 2<sup>+</sup> -> 0<sup>+</sup>) systematics

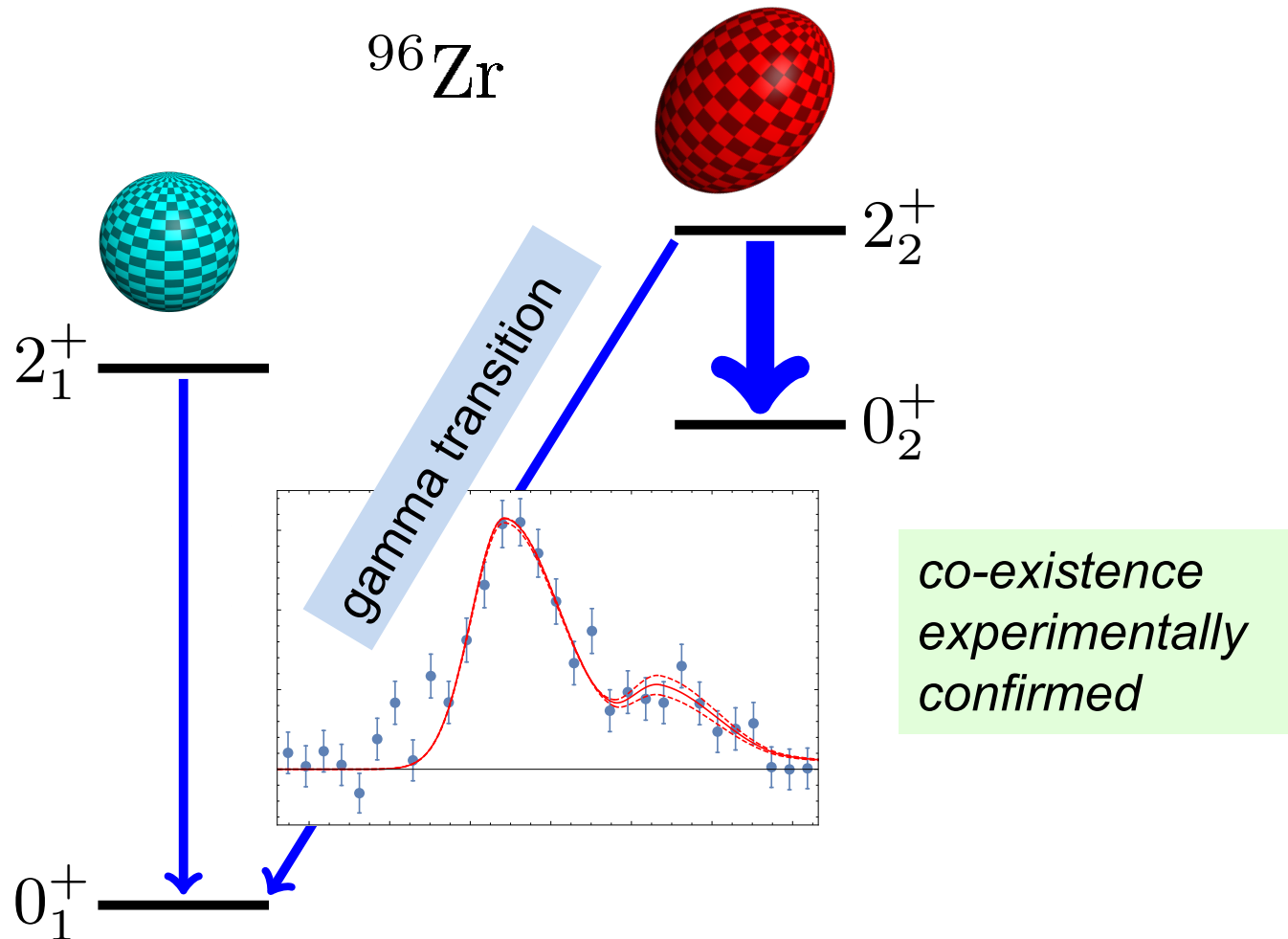


New data from Darmstadt, Kremer *et al.* PRL 117, 172503 (2016)

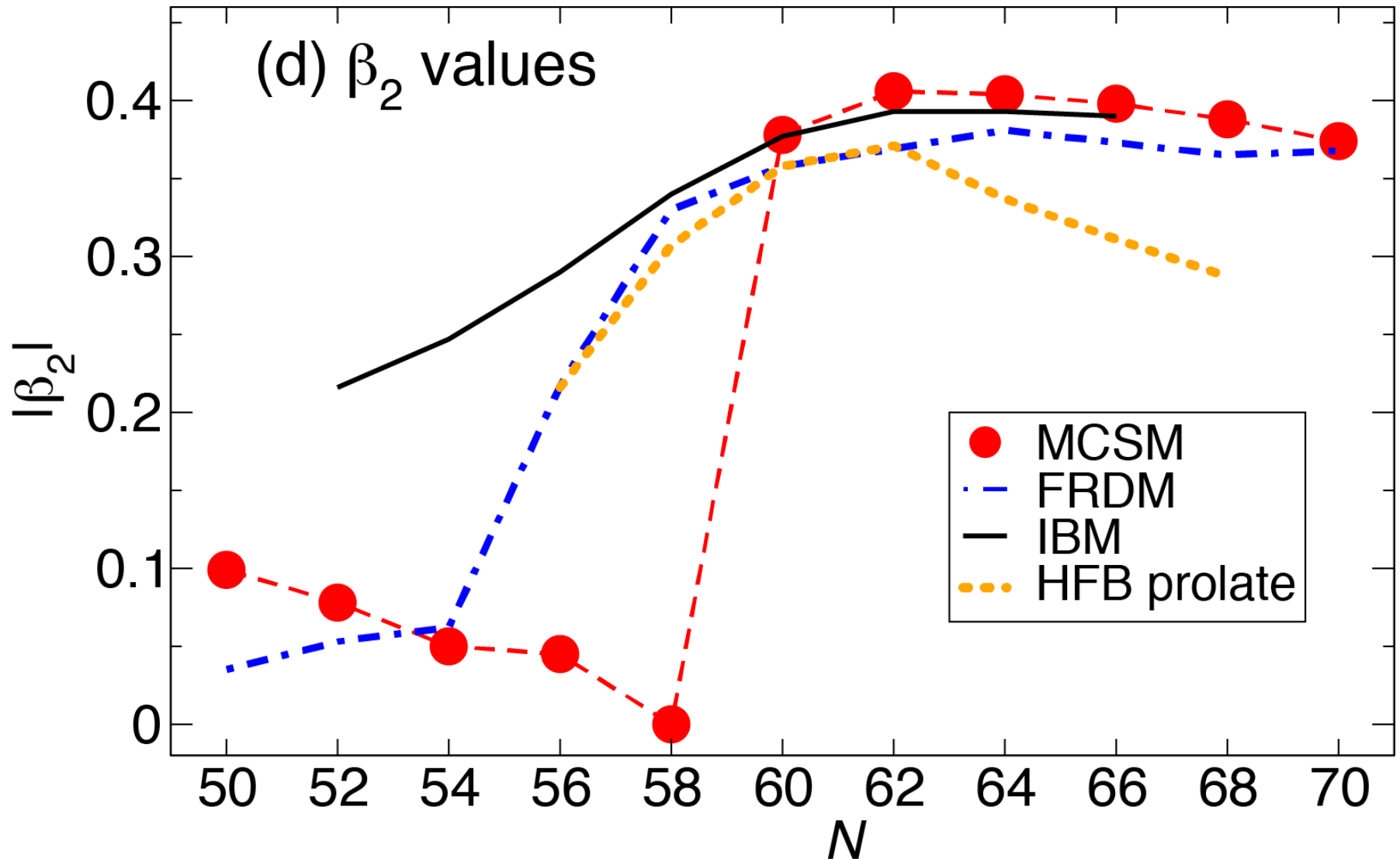


# First Measurement of Collectivity of Coexisting Shapes Based on Type II Shell Evolution: The Case of $^{96}\text{Zr}$

C. Kremer,<sup>1</sup> S. Aslanidou,<sup>1</sup> S. Bassauer,<sup>1</sup> M. Hilcker,<sup>1</sup> A. Krugmann,<sup>1</sup> P. von Neumann-Cosel,<sup>1</sup>  
T. Otsuka,<sup>2,3,4,5</sup> N. Pietralla,<sup>1</sup> V. Yu. Ponomarev,<sup>1</sup> N. Shimizu,<sup>3</sup> M. Singer,<sup>1</sup> G. Steinhilber,<sup>1</sup>  
T. Togashi,<sup>3</sup> Y. Tsunoda,<sup>3</sup> V. Werner,<sup>1</sup> and M. Zweidinger<sup>1</sup>







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. Rodriuez-Guzman et al. Phys. Lett. B 691, 202 (2010).

# *Outline*

I Introduction

II Presently used numerical methodology of many-body problems

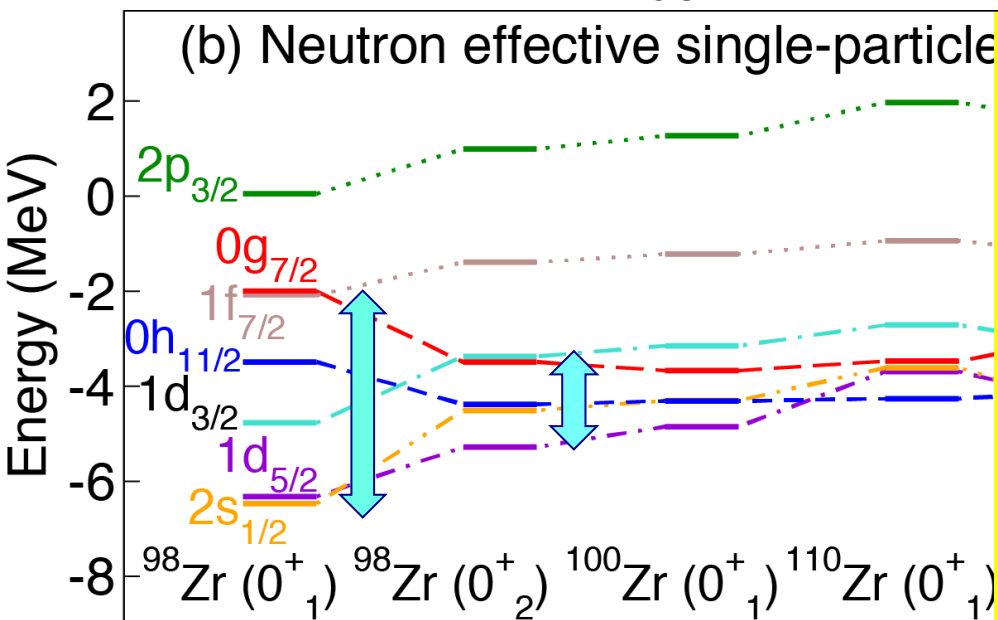
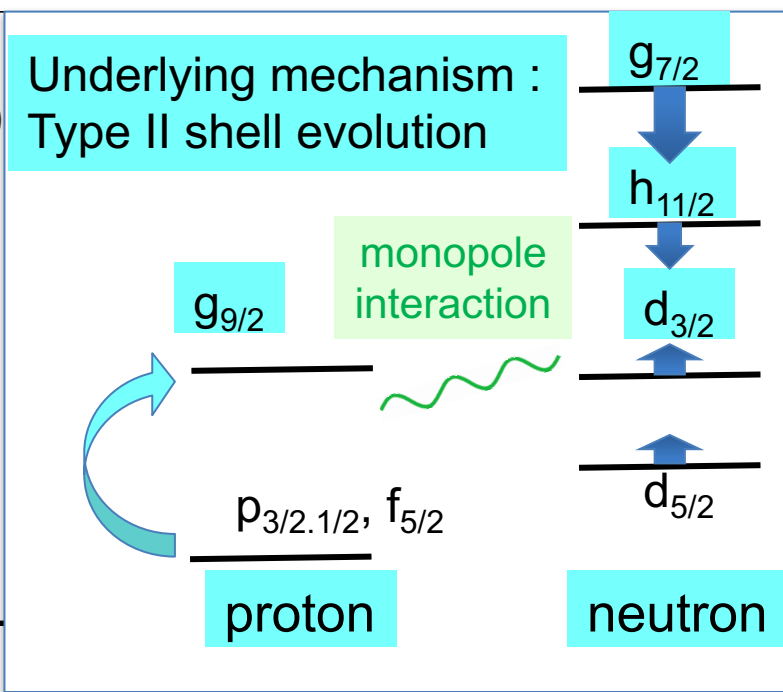
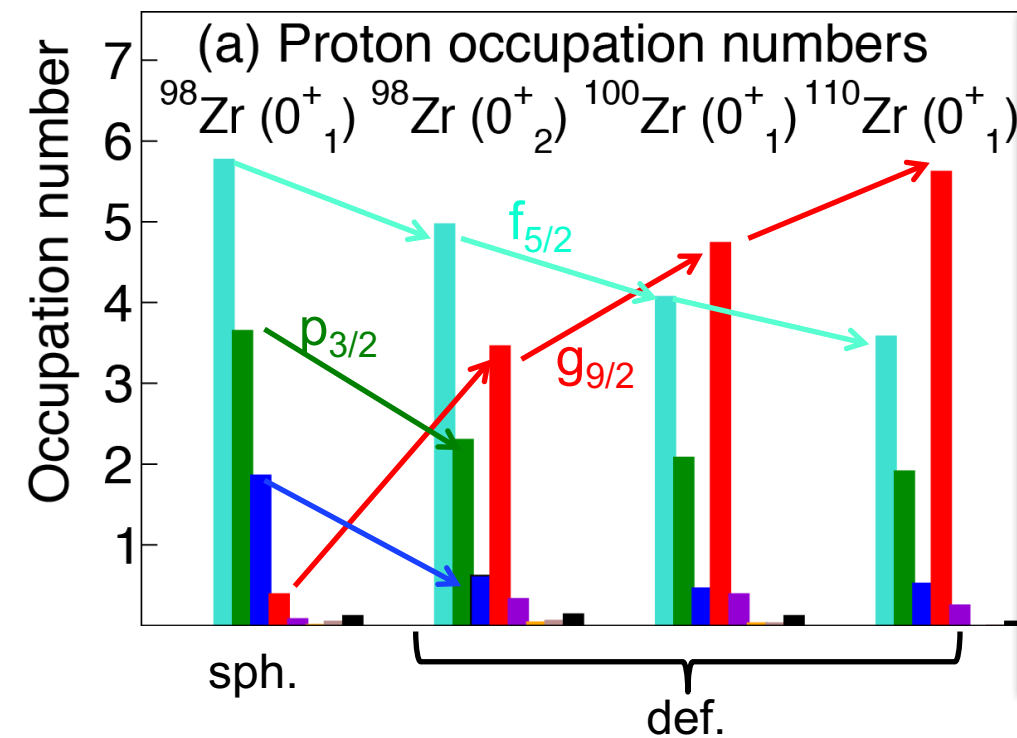
III First application of MCSM to shape coexistence: Ni isotopes

IV An example from Quantum Phase Transition in Zr isotopes

V **Basic mechanism**

VI Shape coexistence and/or critical phenomena in Hg/Pb isotopes

VII Remarks



Relevant neutron single-particle levels get **closer** as a combined effect of nuclear forces (tensor and central) and particular configurations. The **resistance power against deformation is then reduced**. Large difference in ESPEs and configurations  $\rightarrow$  crossing w/o mixing

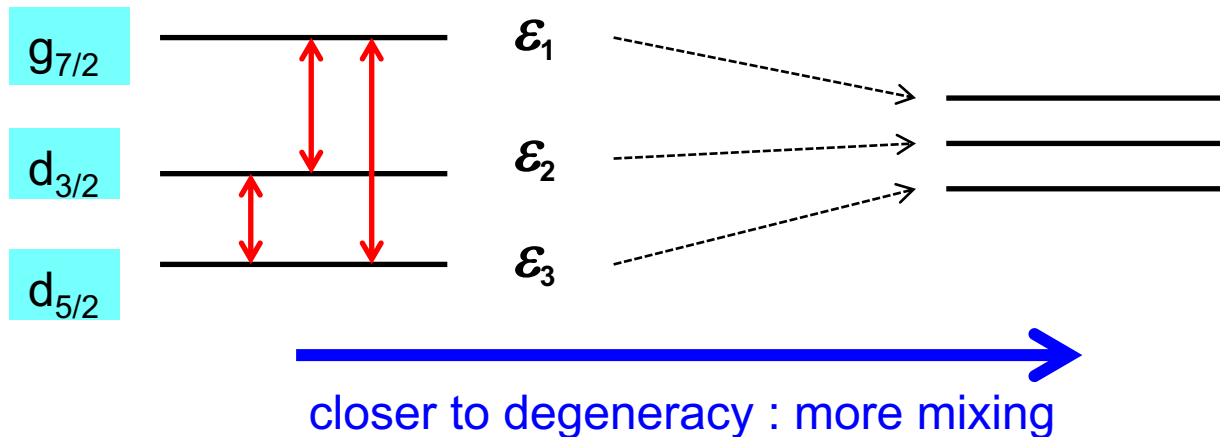
## Reminder I : Jahn –Teller effect for nuclear deformation

(Self-consistent) quadrupole deformed field  $\propto Y_{2,0}(\theta, \phi)$  mixes the orbits below

$$\Psi (J_z=1/2) = c_1 |g_{7/2}; j_z=1/2\rangle + c_2 |d_{3/2}; j_z=1/2\rangle + c_3 |d_{5/2}; j_z=1/2\rangle$$

stronger mixing = larger quadrupole deformation

Mixing depends not only on the strength of the  $Y_{2,0}(\theta, \phi)$  field, but also the spherical single-particle energies  $\epsilon_1, \epsilon_2, \epsilon_3$ , etc.



large (or maybe realistic) splitting is certainly an enemy of deformation

## Reminder II : Monopole interaction

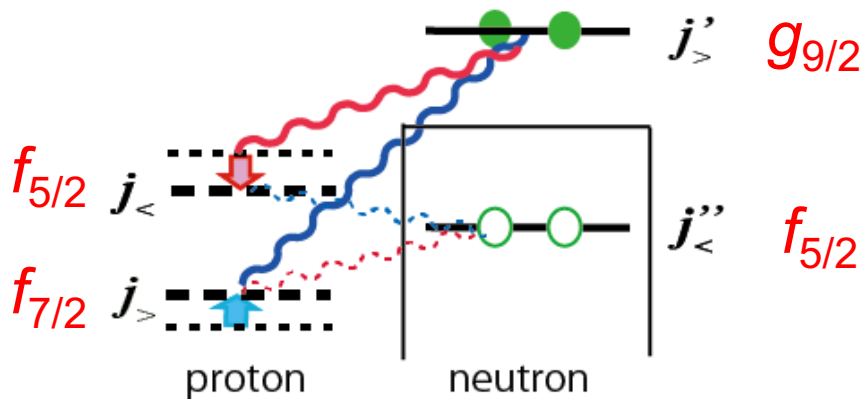
A part of the nucleon-nucleon interaction.

Between a proton in the orbit  $j$  and a neutron in the orbit  $j'$ , it is written as

$$v(j, j') n_j^p n_j^n$$

$v(j, j')$ : monopole matrix element,  $n_j^p$  &  $n_j^n$  : number operators

Ex. Monopole effect from tensor force



1. Proportional to occupation number (**linear scaling**)  
Its effect can be magnified.
2. **Single-particle energies are changed effectively**  
Ex:  $\Delta\varepsilon_j^p = v(j, j') \Delta n_j^n$
3. Also for holes with the opposite sign
4.  $v(j, j')$  **not uniform**  
central and tensor forces

# Variation of monopole matrix element from a central force : A=70

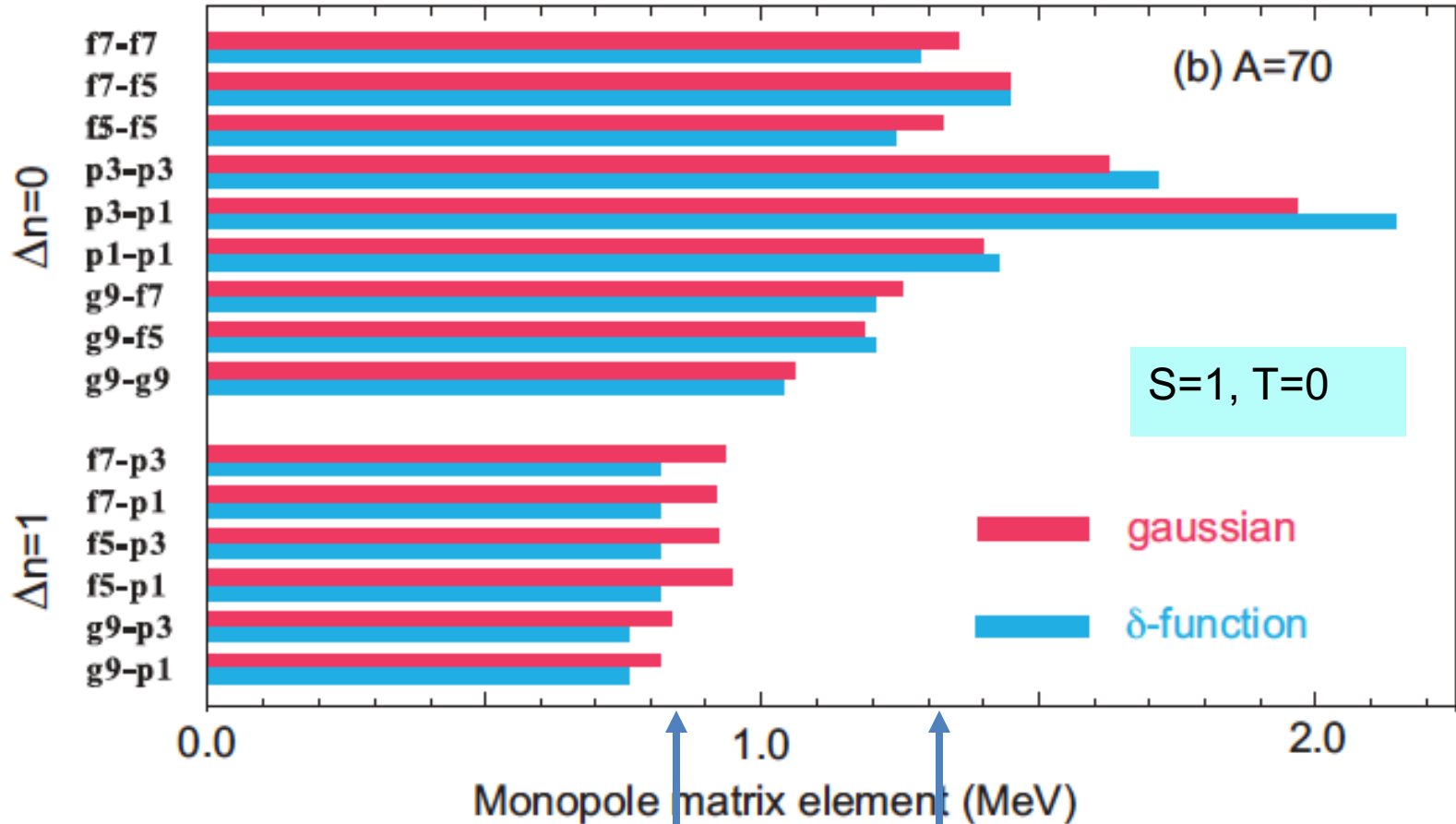


Figure 26 Monopole matrix elements of central gaussian and delta interactions for ( $S = 1, T = 0$ ) channel. The orbit labeling is abbreviated like g9 for  $1g_{9/2}$ , etc. The orbits are from valence shell for (a)  $A = 100$  and (b)  $A = 70$ .

mean values ~0.8 MeV      ~1.3 MeV

difference ~ 0.5 MeV

variations ~0.1 MeV      ~0.3 MeV

Variation of monopole matrix element from tensor force :  $A=70$

variations 0.5 ~ 1 MeV

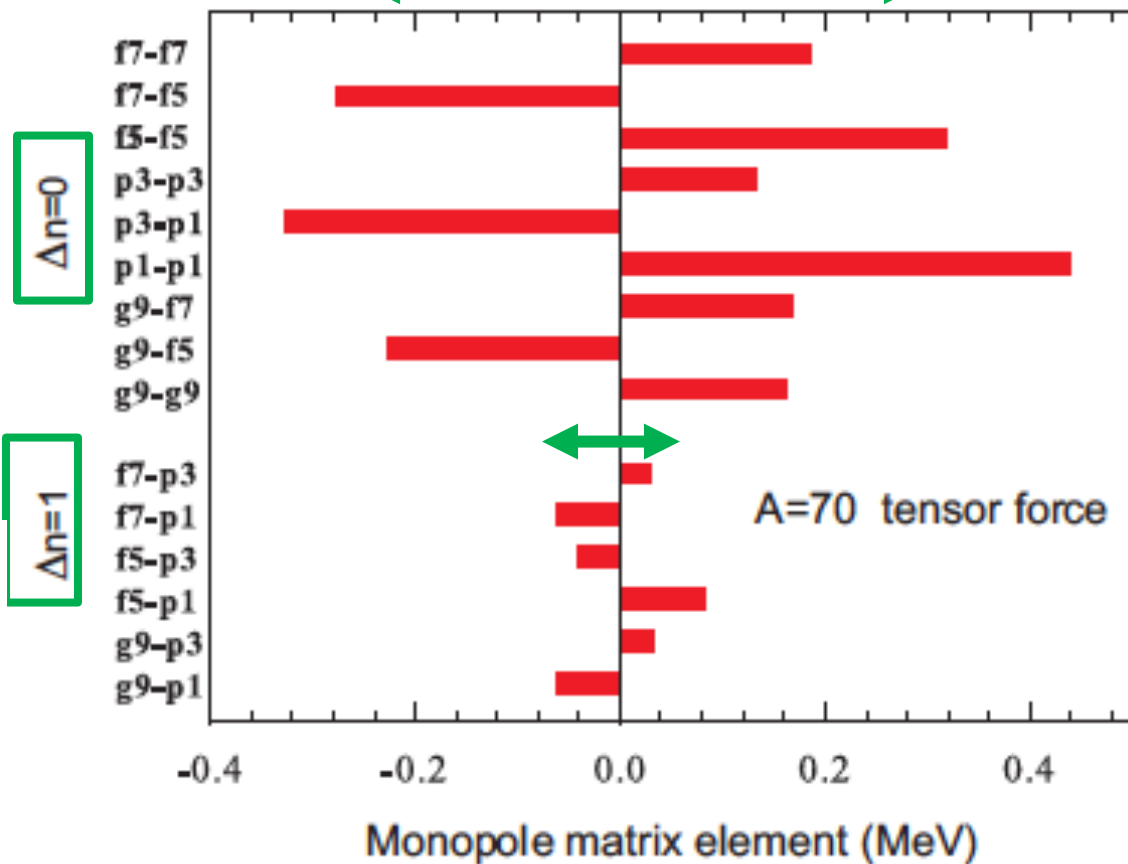
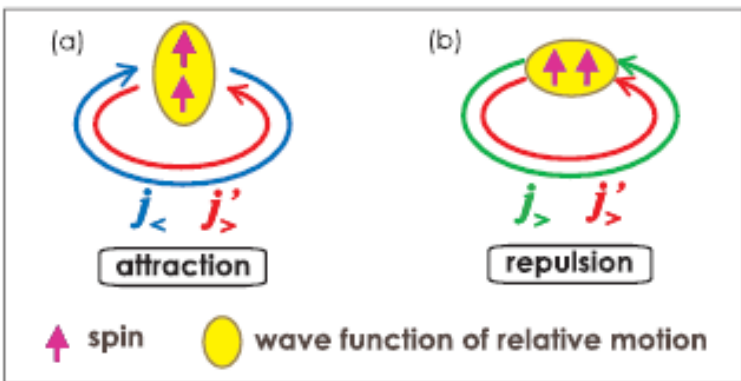
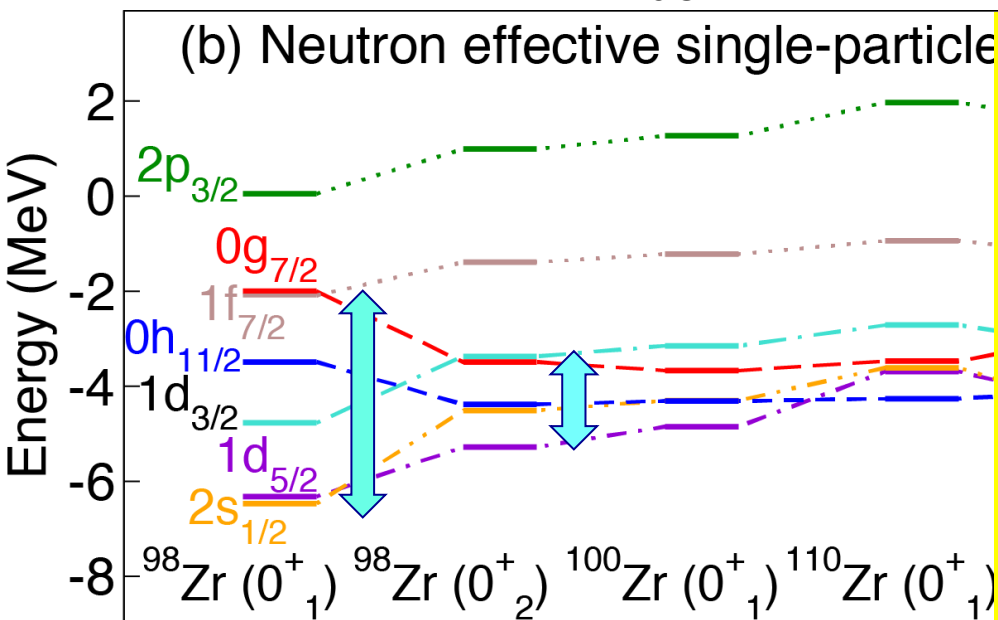
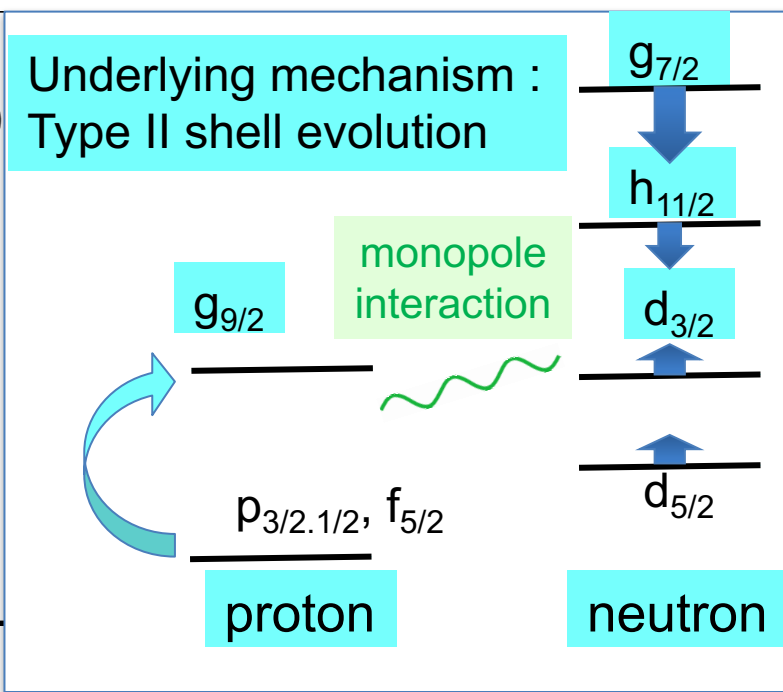
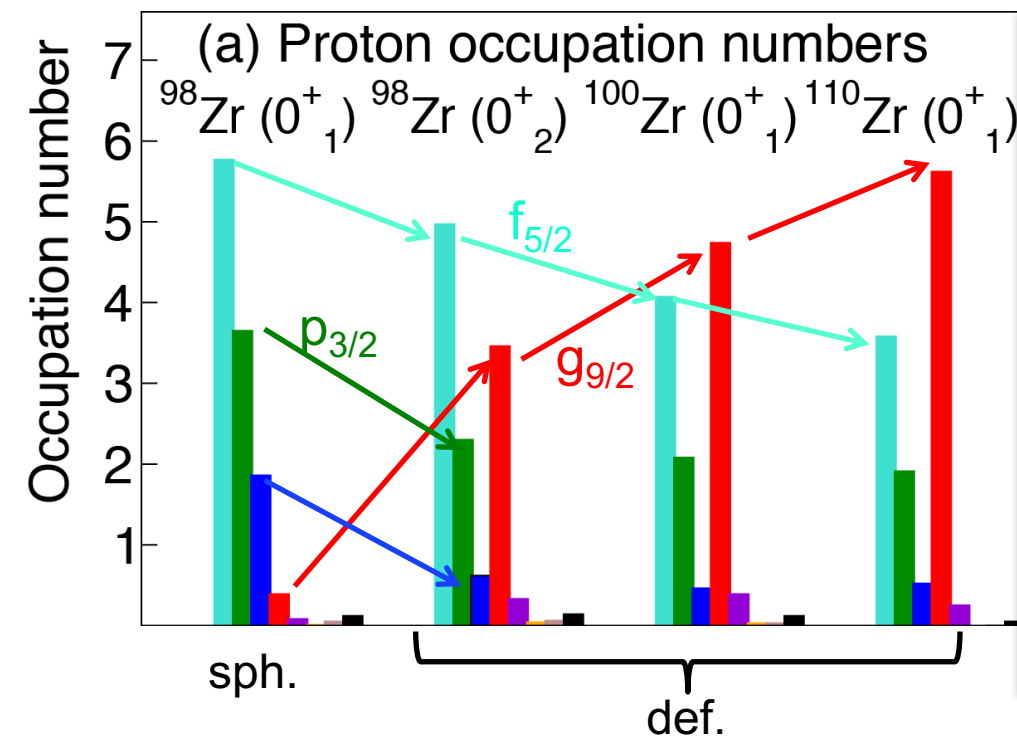


Figure 34 Monopole matrix elements of the tensor force in the  $T=0$  channel. The orbit labeling is abbreviated like f7 for  $1f_{7/2}$ , etc. The orbits are from valence shell for  $A = 70$ .



Relevant neutron single-particle levels get **closer** as a combined effect of nuclear forces (tensor and central) and particular configurations. The **resistance power against deformation is then reduced**. Large difference in ESPEs and configurations  $\rightarrow$  crossing w/o mixing

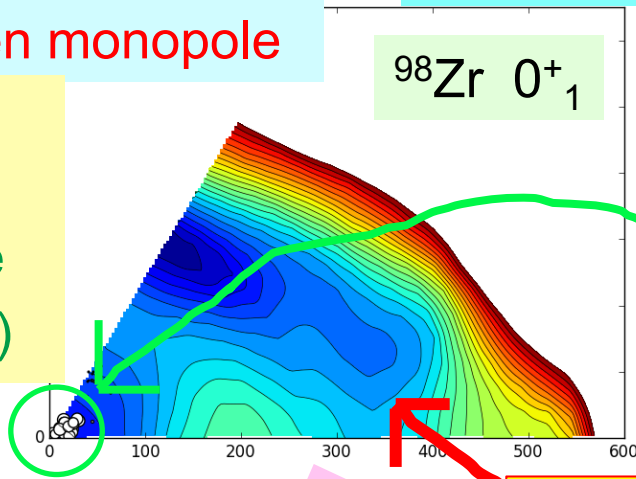


# Anatomy of this effect : $^{98}\text{Zr}$ spherical $0^+_1$ and deformed $0^+_2$

## PES with T-plot

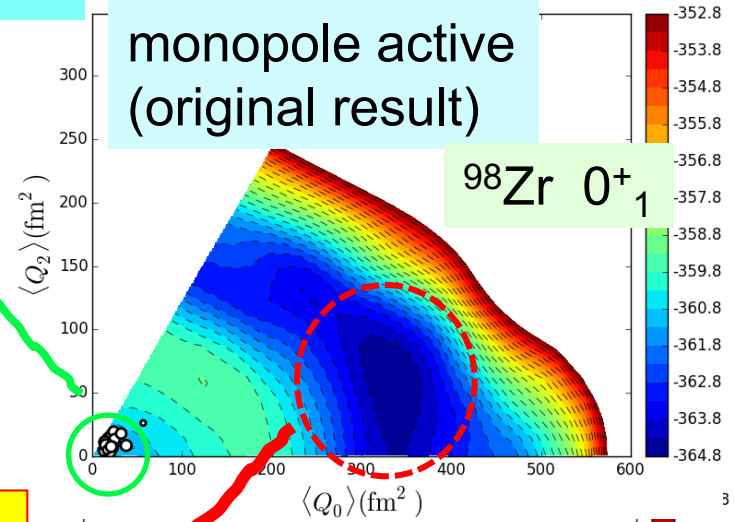
Frozen monopole

spherical ground state do not change (overlap  $\sim 0.98$ )



$^{98}\text{Zr}$   $0^+_1$

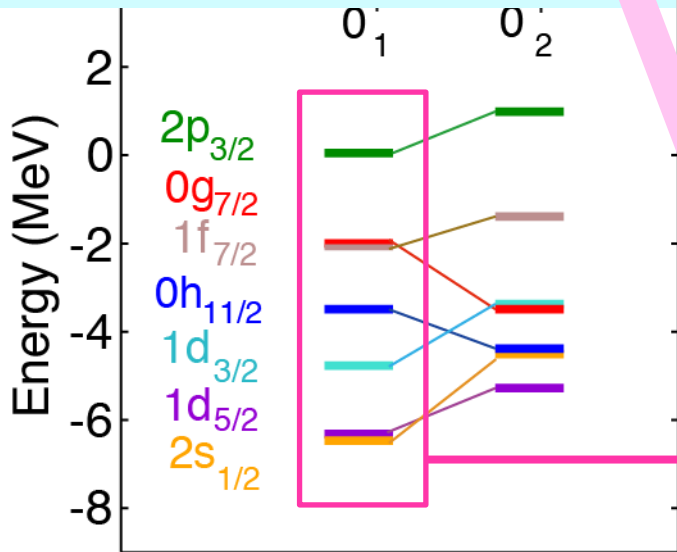
monopole active (original result)



$^{98}\text{Zr}$   $0^+_1$

Effective SPE

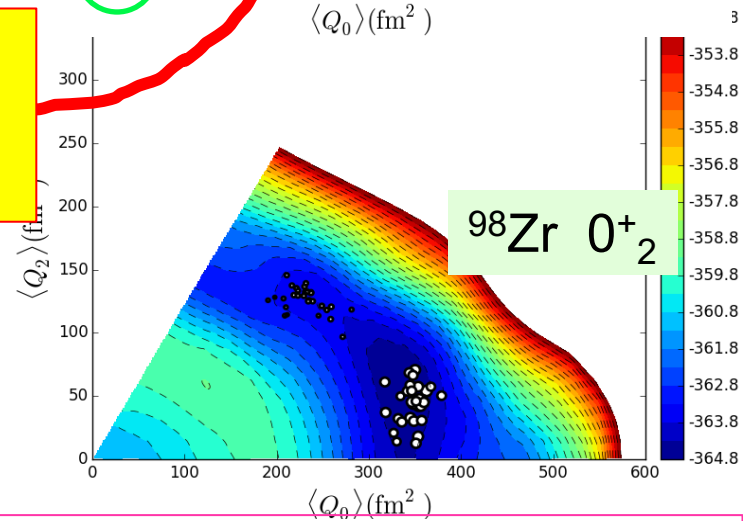
- configuration dependent -



prolate minimum is gone

Use them as constant SPEs independent of configurations, putting monopole int. aside

→ Frozen monopole treatment



$^{98}\text{Zr}$   $0^+_2$

Type II shell evolution is a simplest and visible case of

## *Quantum Self Organization*

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

resistance power ← pairing force

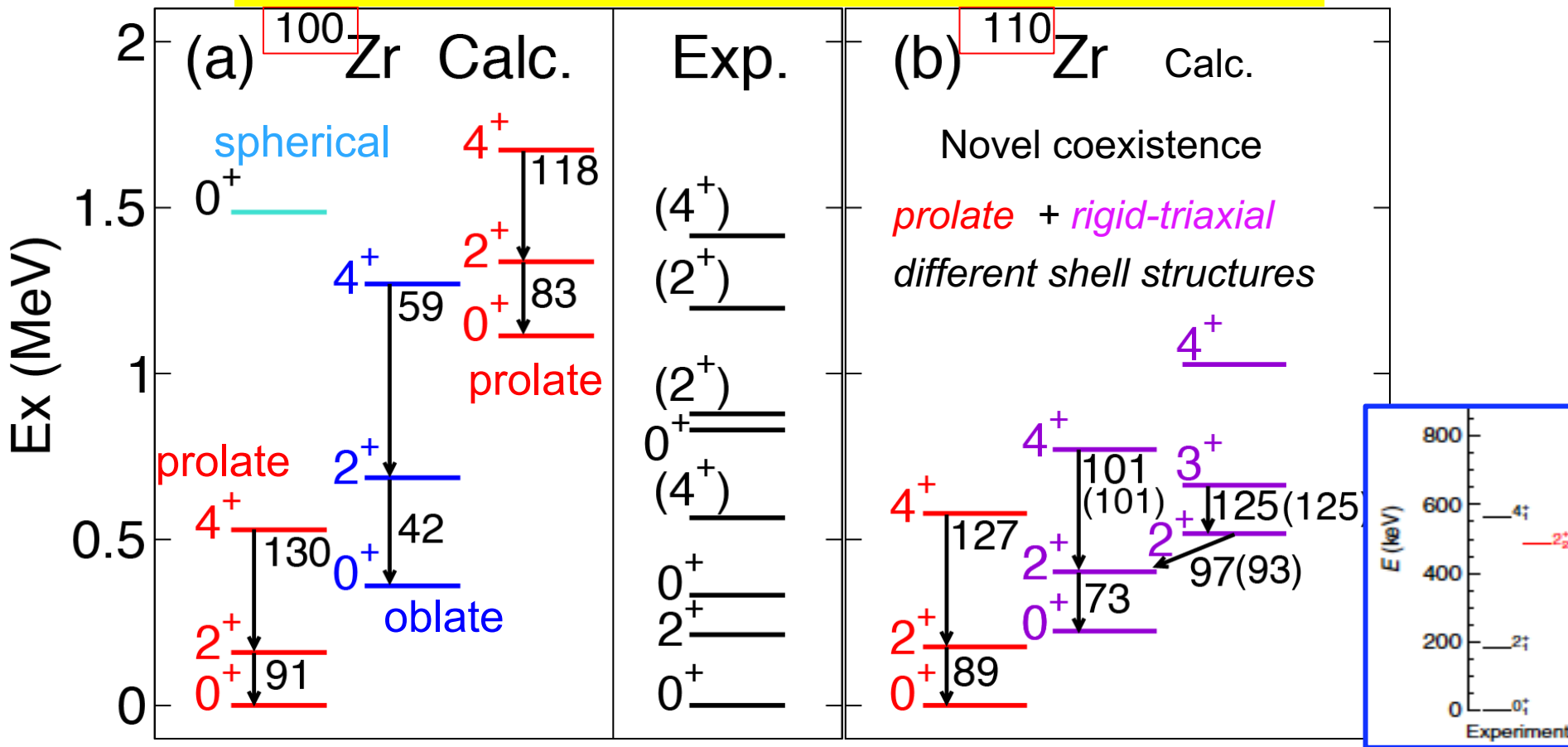
↑ single-particle energies

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

→ an enhancement of Jahn-Teller effect.

Single-particle levels and the number of particles  
determines  
the shapes

# Prolate – rigid-triaxial shape coexistence



( ) : Rigid-triaxial rotor with  $\gamma=28$  degrees normalized at  $2^+_2 \rightarrow 0^+_2$

week ending  
20 JANUARY 2017

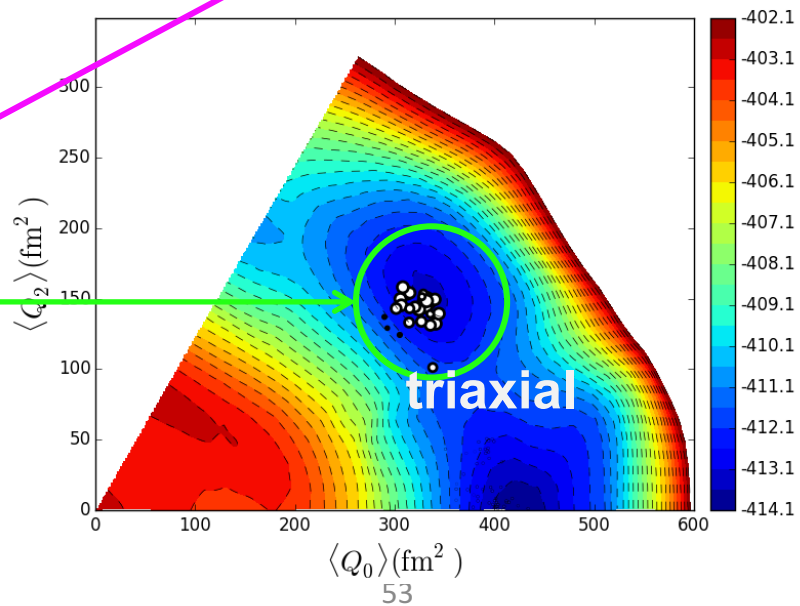
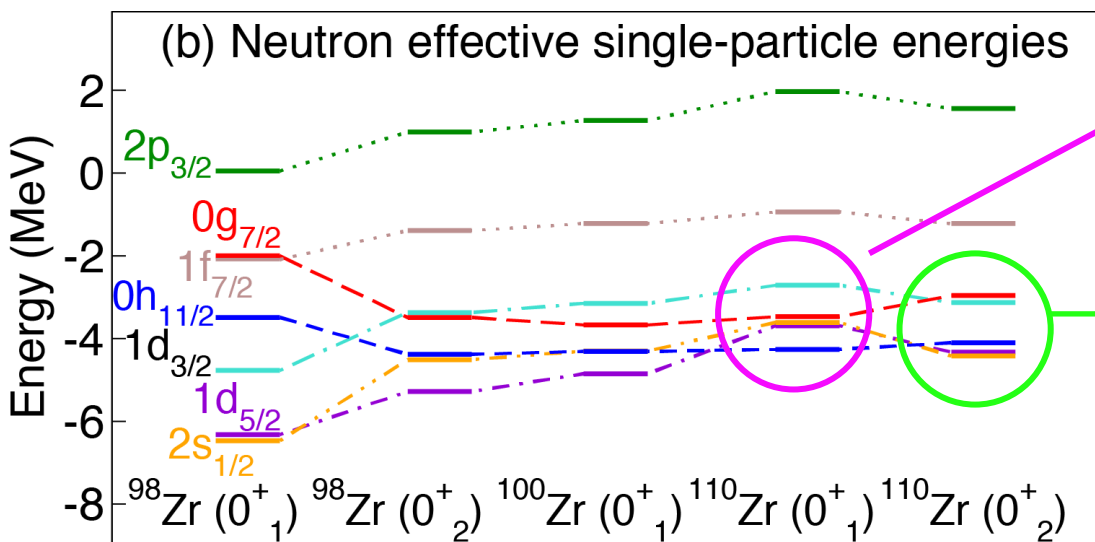
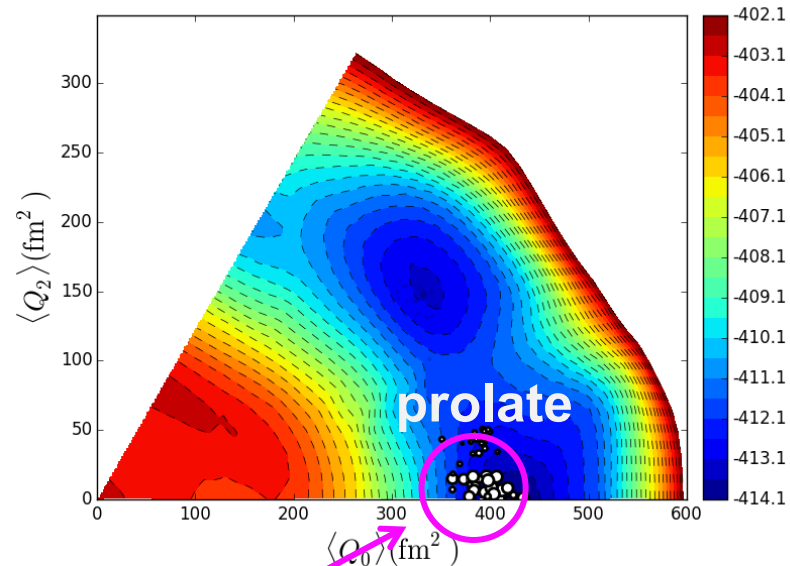
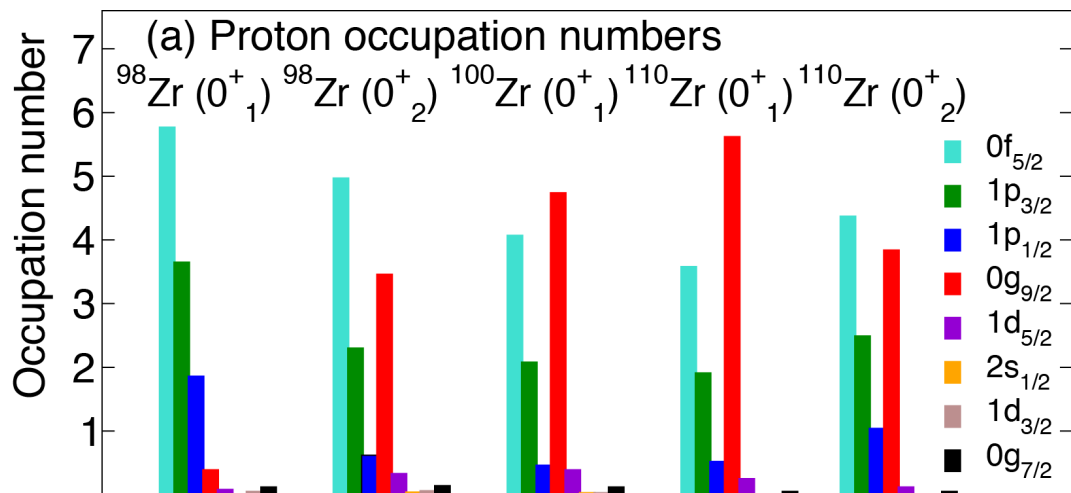
PHYSICAL REVIEW LETTERS

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**Are There Signatures of Harmonic Oscillator Shells Far from Stability?  
 First Spectroscopy of  $^{110}\text{Zr}$**

N. Paul,<sup>1,2,\*</sup> A. Corsi,<sup>1</sup> A. Obertelli,<sup>1,2</sup> P. Doornenbal,<sup>2</sup> G. Authelet,<sup>1</sup> H. Baba,<sup>2</sup> B. Bally,<sup>3</sup> M. Bender,<sup>4</sup> D. Calvet,<sup>1</sup>

# different shell structures ~ like “different nuclei”



Sr & Kr isotopes within the scope but not yet done well

PHYSICAL REVIEW C 95, 054319 (2017)

**Abrupt shape transition at neutron number  $N = 60$ :  $B(E2)$  values in  $^{94,96,98}\text{Sr}$  from fast  $\gamma$ - $\gamma$  timing**

J.-M. Régis,<sup>1,\*</sup> J. Jolie,<sup>1</sup> N. Saed-Samii,<sup>1</sup> N. Warr,<sup>1</sup> M. Pfeiffer,<sup>1</sup> A. Blanc,<sup>2</sup> M. Jentschel,<sup>2</sup> U. Köster,<sup>2</sup> P. Mutti,<sup>2</sup> T. Soldner,<sup>2</sup>

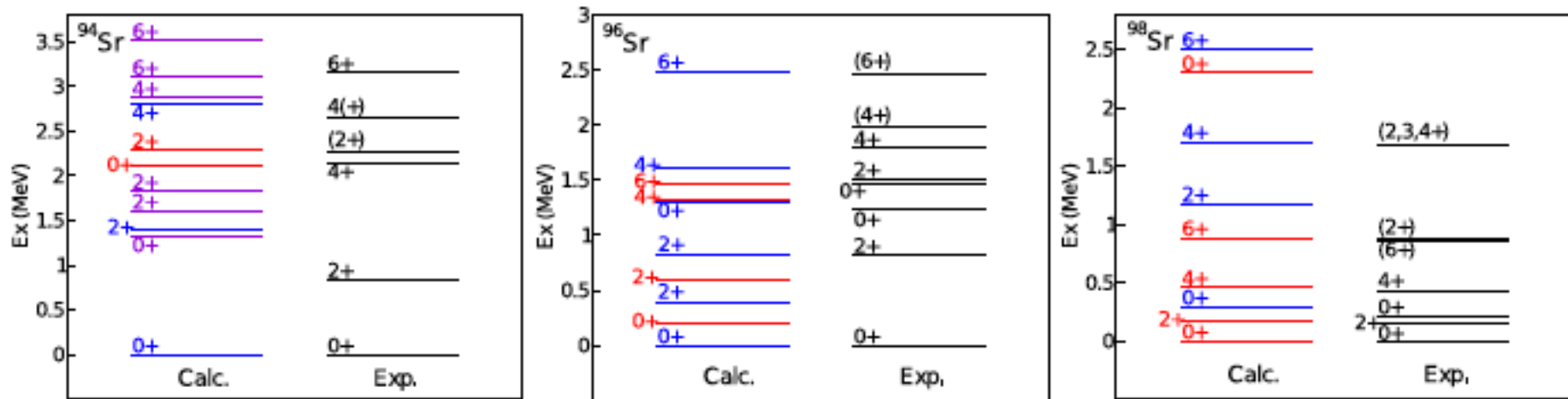


FIG. 7. Comparison between level schemes from MCSM calculations and experimental values for the lowest two excited  $I^\pi = 0^+, 2^+, 4^+, 6^+$  states in  $^{94,96,98}\text{Sr}$ . Oblate (prolate) deformed states are given in blue (red) and triaxial ones in purple. The experimental data are taken from Refs. [21,26].

# *Outline*

I Introduction

II Presently used numerical methodology of many-body problems

III First application of MCSM to shape coexistence: Ni isotopes

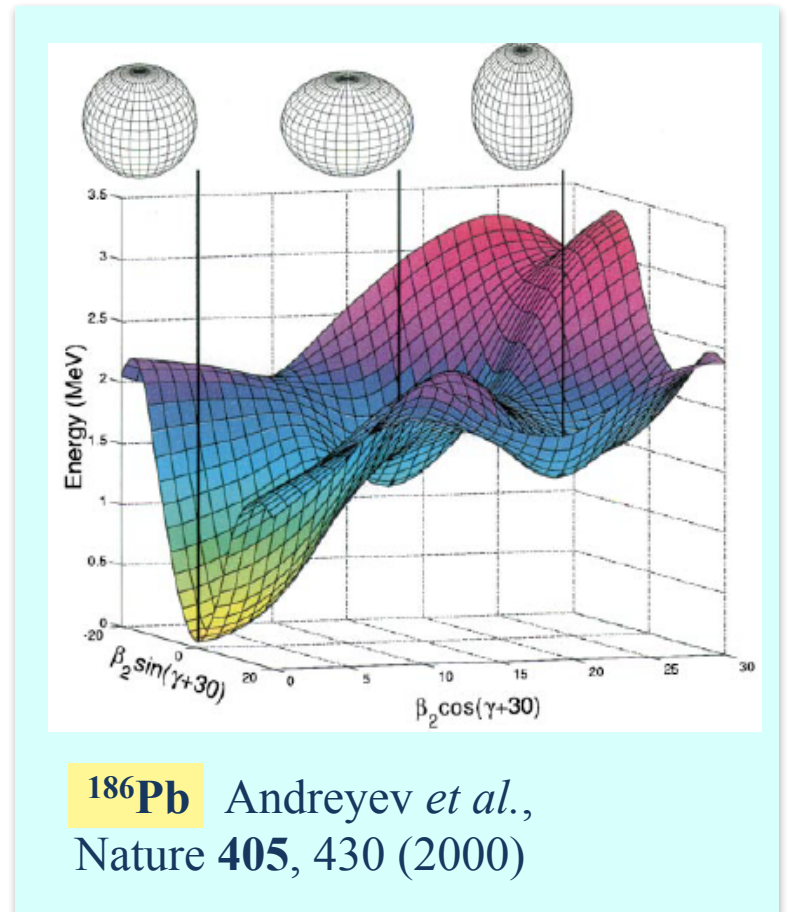
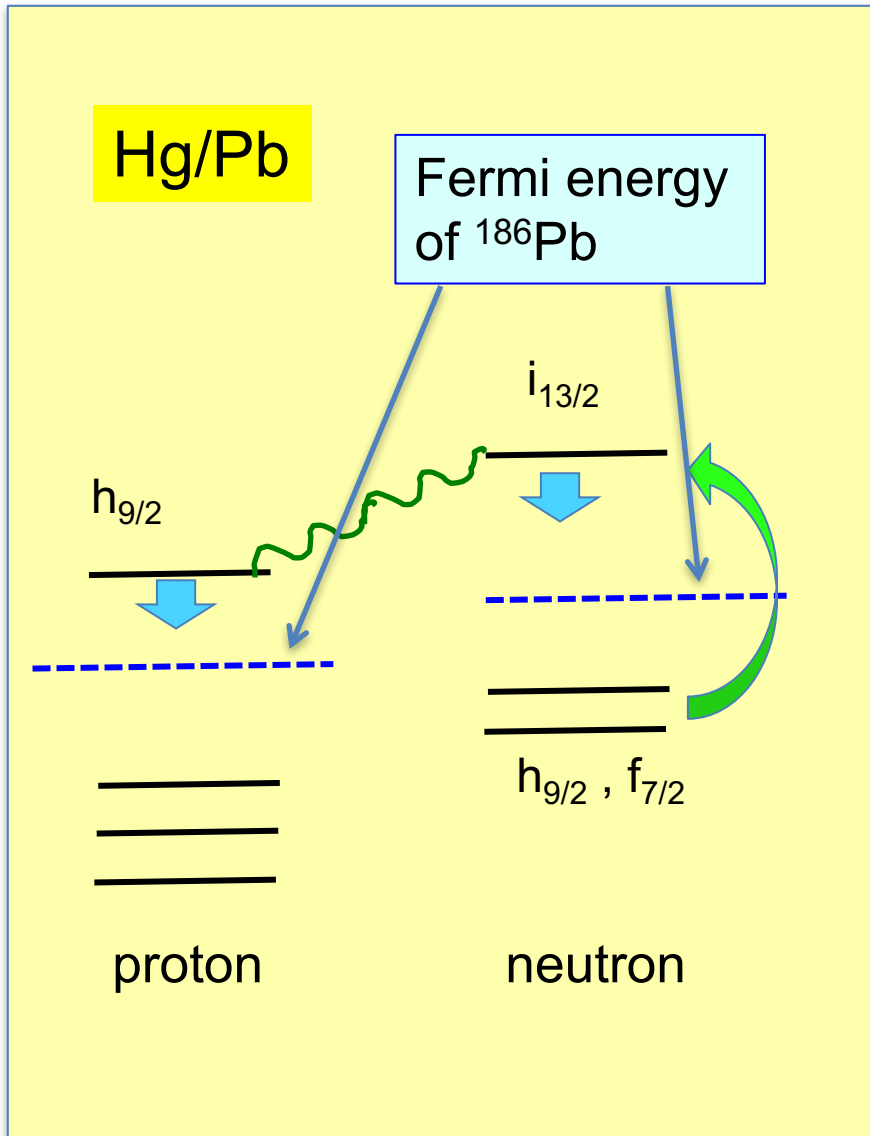
IV An example from Quantum Phase Transition in Zr isotopes

V Basic mechanism

VI Shape coexistence and/or critical phenomena in Hg/Pb isotopes

VII Remarks

# Moving to heavier nuclei





## MCSM calculation setup

<u>-0.68</u>	$2p_{1/2}$			$2d_{3/2}$
<u>-0.17</u>	$2p_{3/2}$			$1g_{7/2}$
<u>-0.98</u>	$1f_{5/2}$	<u>-1.40</u>	<u>-1.45</u>	$3s_{1/2}$
<u>-2.19</u>	$0i_{13/2}$		<u>-1.90</u>	$2d_{5/2}$
<u>-2.90</u>	$1f_{7/2}$		<u>-2.37</u>	$0j_{15/2}$
<u>-3.80</u>	$0h_{9/2}$	<u>-3.16</u>	<u>-2.51</u>	$0i_{11/2}$
		<u>-3.94</u>		$1g_{9/2}$

$^{208}\text{Pb}$

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				$2p_{1/2}$
<u>-8.01</u>	$2s_{1/2}$	<u>-7.37</u>		$1f_{5/2}$
<u>-8.36</u>	$1d_{3/2}$	<u>-7.94</u>		$2p_{3/2}$
<u>-9.36</u>	$0h_{11/2}$	<u>-9.00</u>	<u>-8.27</u>	$0i_{13/2}$
<u>-9.70</u>	$1d_{5/2}$	<u>-9.71</u>		$1f_{7/2}$
<u>-11.49</u>	$0g_{7/2}$	<u>-10.78</u>		$0h_{9/2}$

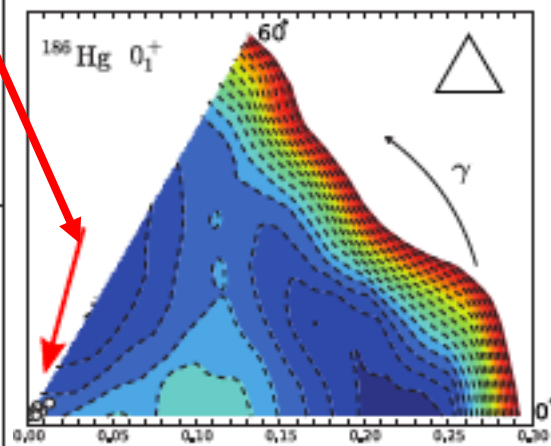
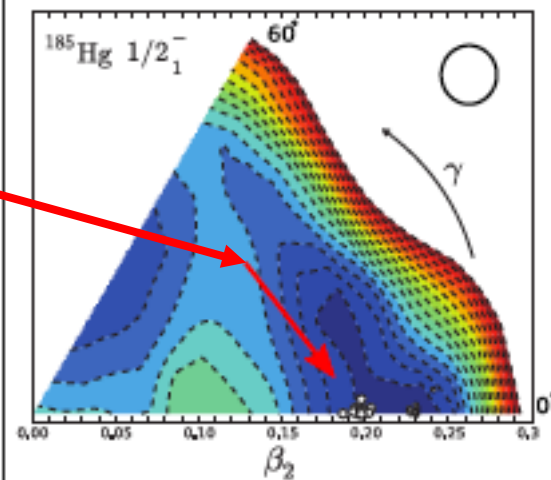
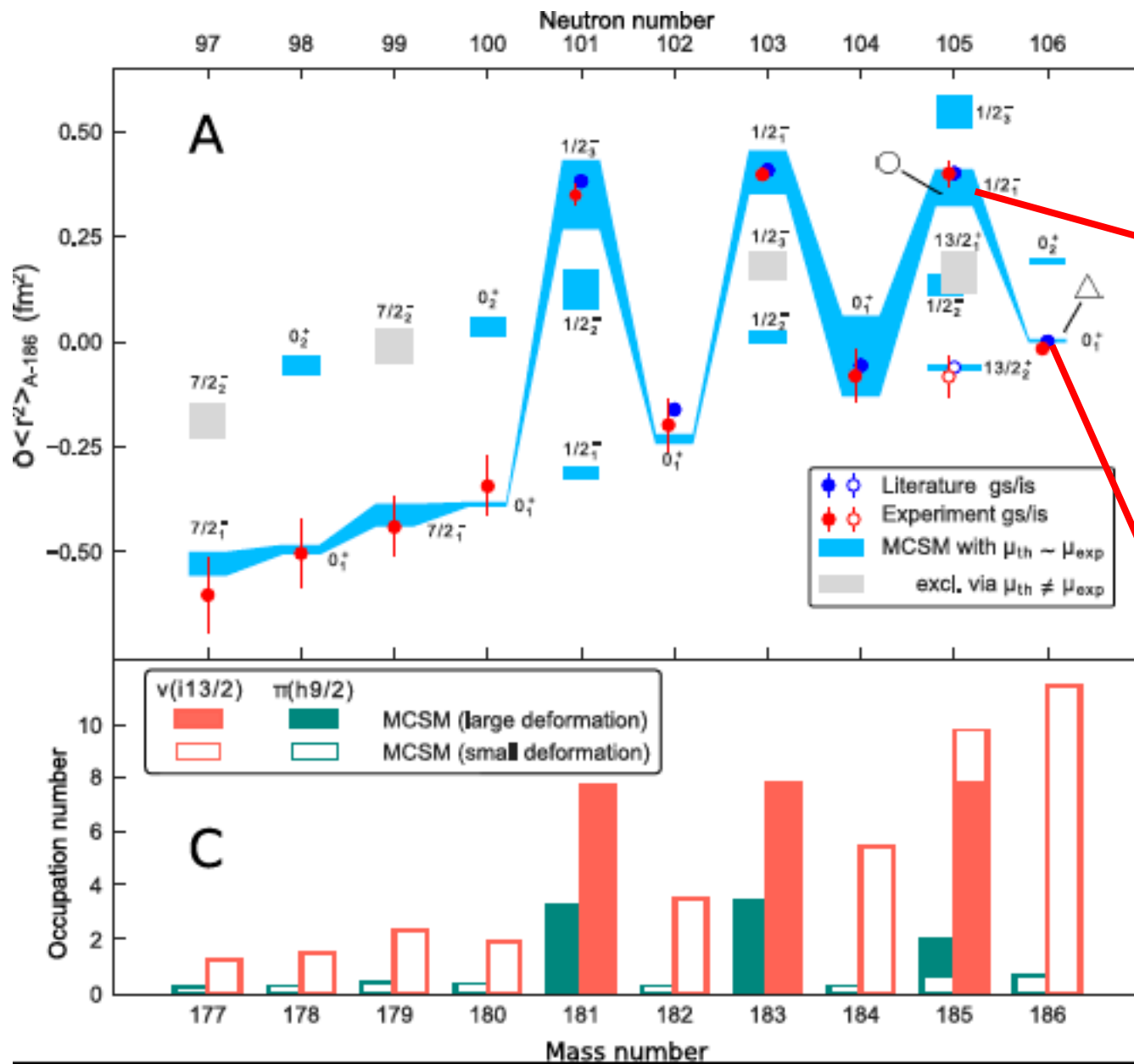
All these orbits are included in the MCSM calculation.

30 protons activated  
 15 ( $^{177}\text{Hg}$ ) – 24 ( $^{188}\text{Hg}$ )  
 neutrons activated

max dimension in conventional diagonalization  $\sim 2 \times 10^{42}$   
 (feasible in 60 years)

p-p, n-n effective interactions are taken from  
 B.A. Brown, PRL 85, 5300 (2000)

p-n effective interaction is taken from  
 T. Otsuka, PRL 104, 012501 (2010) (VMU: central + tensor)  
 + 2body LS from M3Y

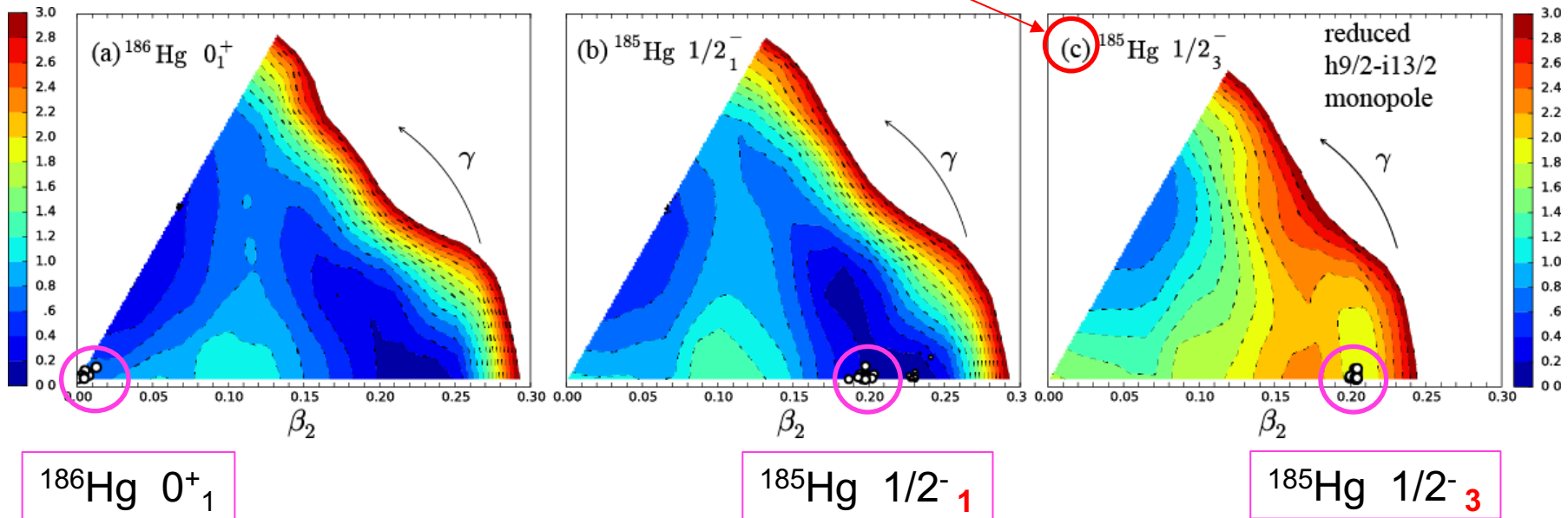


Energy (MeV)

Single-particle structure is self-organized in prolate states:

proton  $h_{9/2}$  – neutron  $i_{13/2}$  monopole interaction is particularly strong due to the central + tensor force.

If we weaken it to an averaged magnitude of monopole interactions between other orbits, we get ( c )



**Note : oblate region is not affected so much**

## Remarks

*Naïve Fermi liquid picture (a la Landau) is revised, as atomic nuclei are not necessarily like simple solid vases containing almost free nucleons.*

Nuclear forces are rich enough to optimize single-particle energies for each eigenstate (especially in the cases of collective-mode states), as referred to as **quantum self-organization**.

The **quantum self-organization** produces sizable effects with

- (i) **two quantum fluids** (protons and neutrons),
- (ii) **two major forces** : e.g., quadrupole interaction to **drive collective mode**  
monopole interaction to **control resistance**

Thus, non-specific forces, e.g. monopole interaction, work coherently so that single-particle states are not always enemies but can be friends of collective modes.

Interesting topics may include

- **prolate shape is more favored** (reason for prolate > oblate ?)
- **Majorana force in IBM** may be explained for the first time
- more important for heavier nuclei → stability of **superheavy** elements
- time dependent version ... intriguing project

## Remarks - *continued*

Type II shell evolution is a simpler case of the quantum self-organization, involving closed-shell structure ( $\sim$ shape coexistence).

Quantum phase transition, shape coexistence, shape transition (e.g., Sm), superdeformation, fission, ... seem to be relevant.

*heavier nuclei : more particles and more orbits => more important*

From known examples,

Ni (+Co ..) shape coexistence with lowest  $E_x \sim 1$  MeV

Zr (+Sr ..) quantum phase transition at  $N=60$

Hg (+Pb ..) even-even isotopes : shape coexistence

even-odd : alternation between spherical/weak oblate and

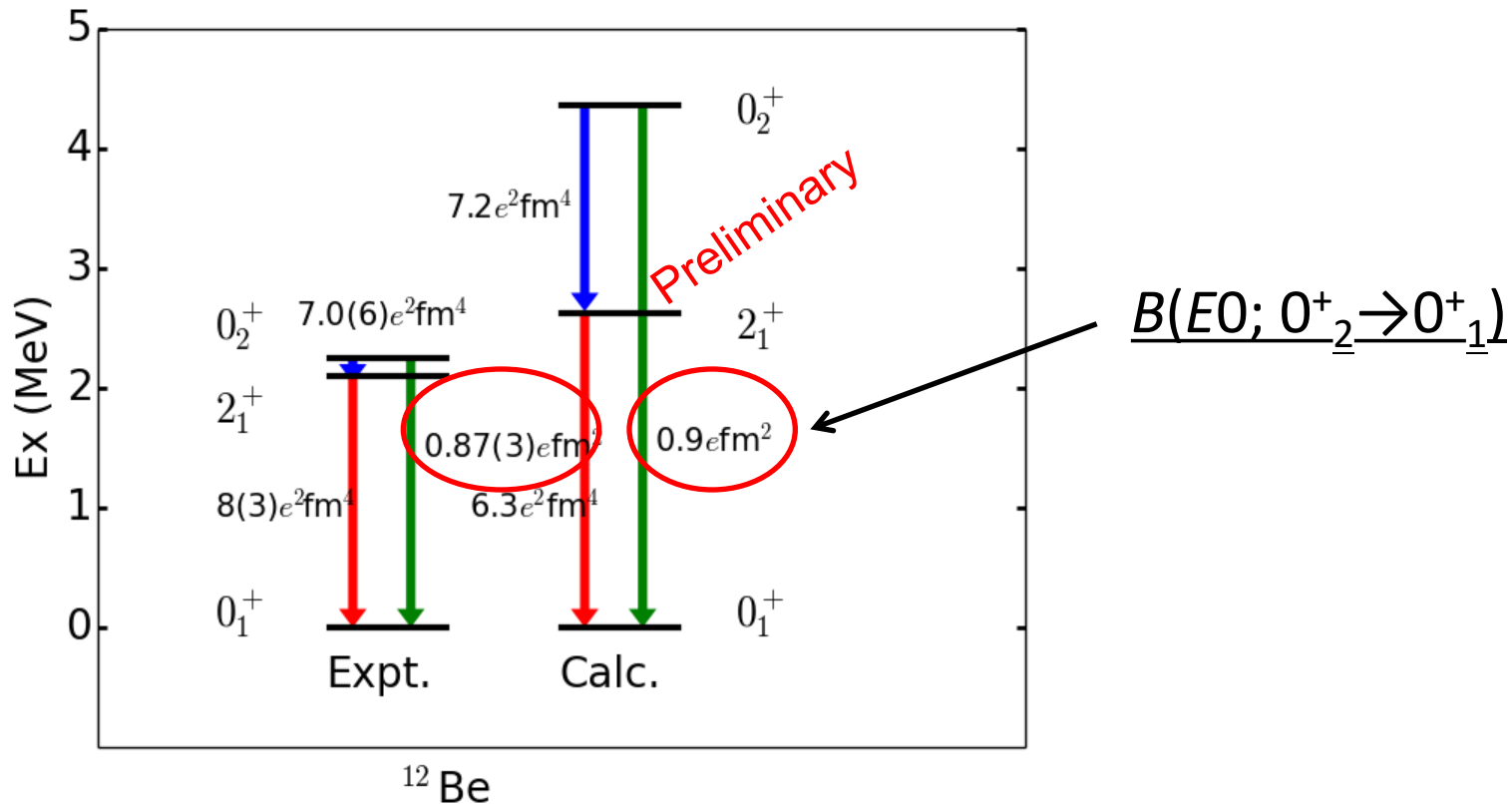
prolate  $\rightarrow$  degeneracy of phases (critical phenomenon)

even or odd of neutron number controls

# E2 & E0 Transition strength of $^{12}\text{Be}$

Current status

E0 is difficult for the shell model. But could ab initio shell model solve this ?



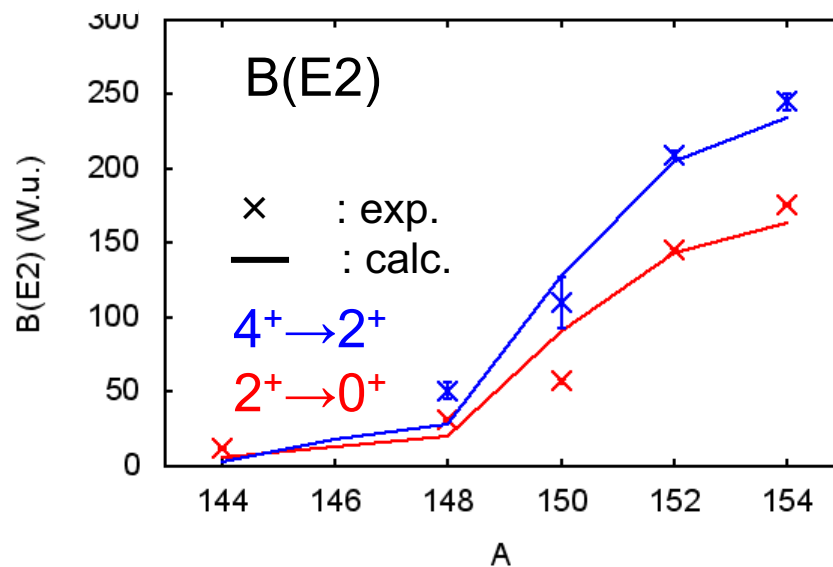
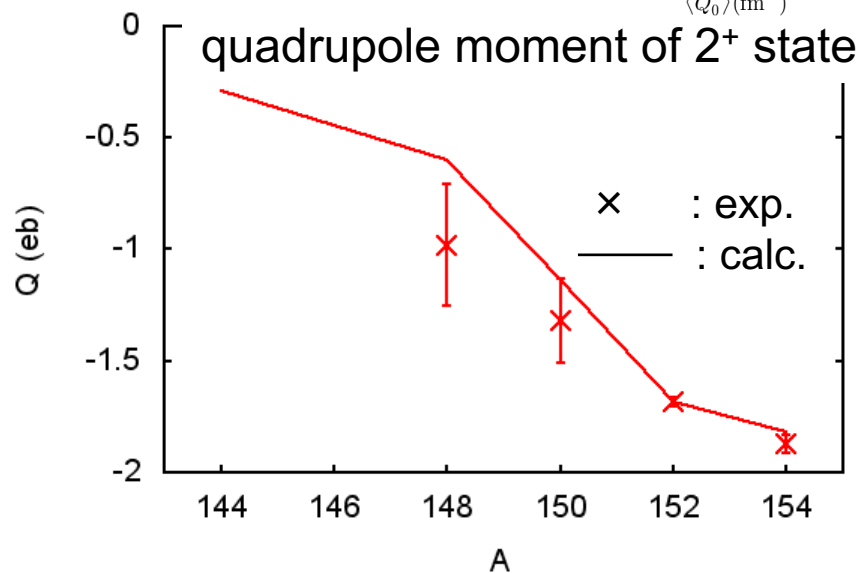
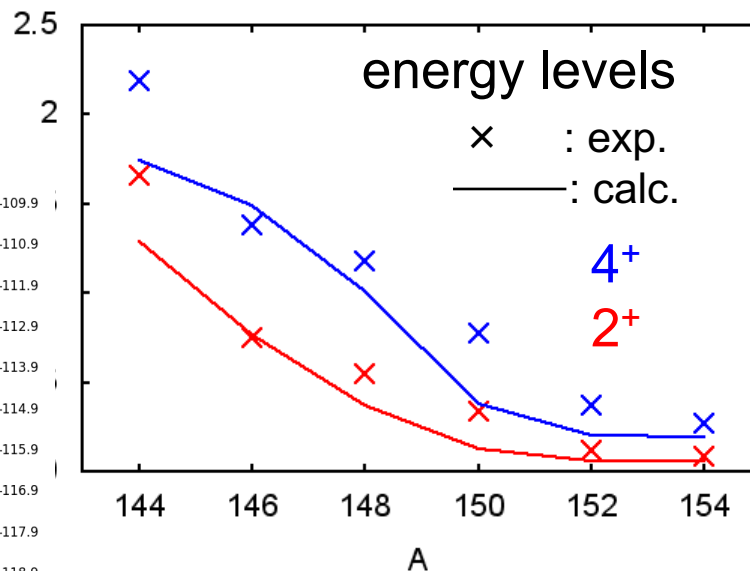
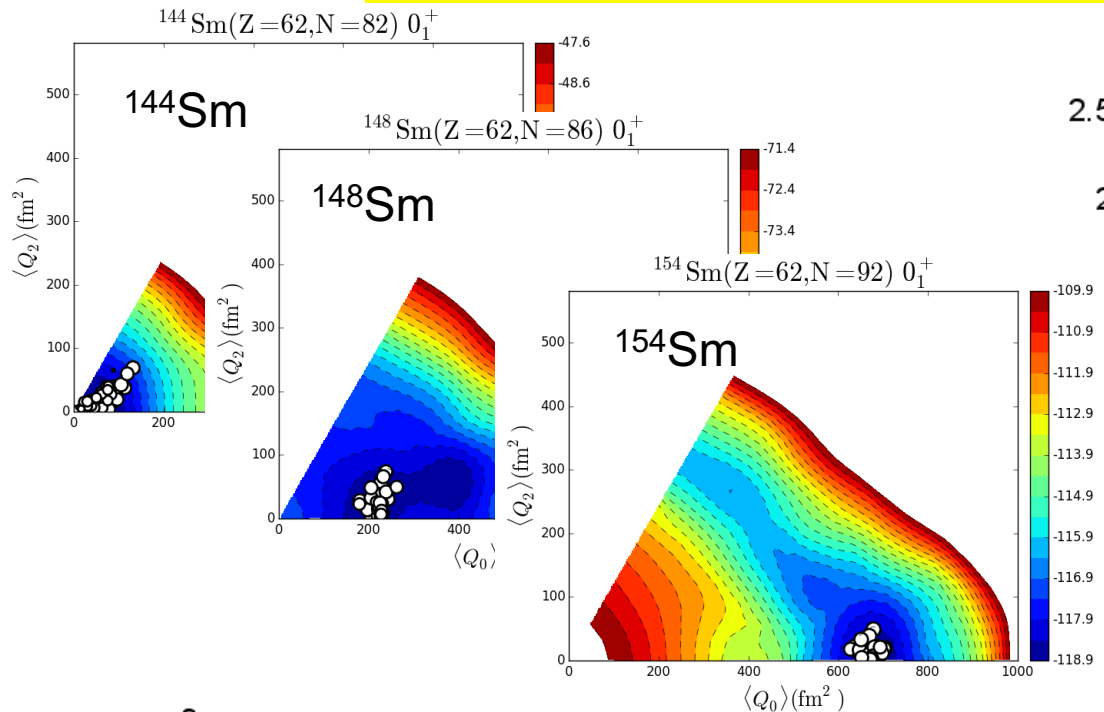
Expt.:

S. Shimoura, et al., Phys. Lett. B 654 87 (2007)

N. Imai, et al., Phys. Lett. B 673 179 (2009)

*Thank you*

# Shape evolution in Sm isotopes (very preliminary)

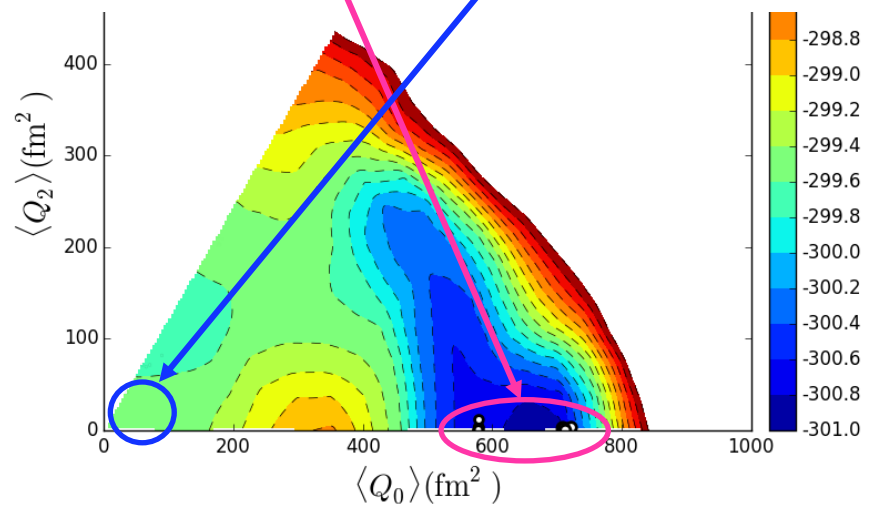
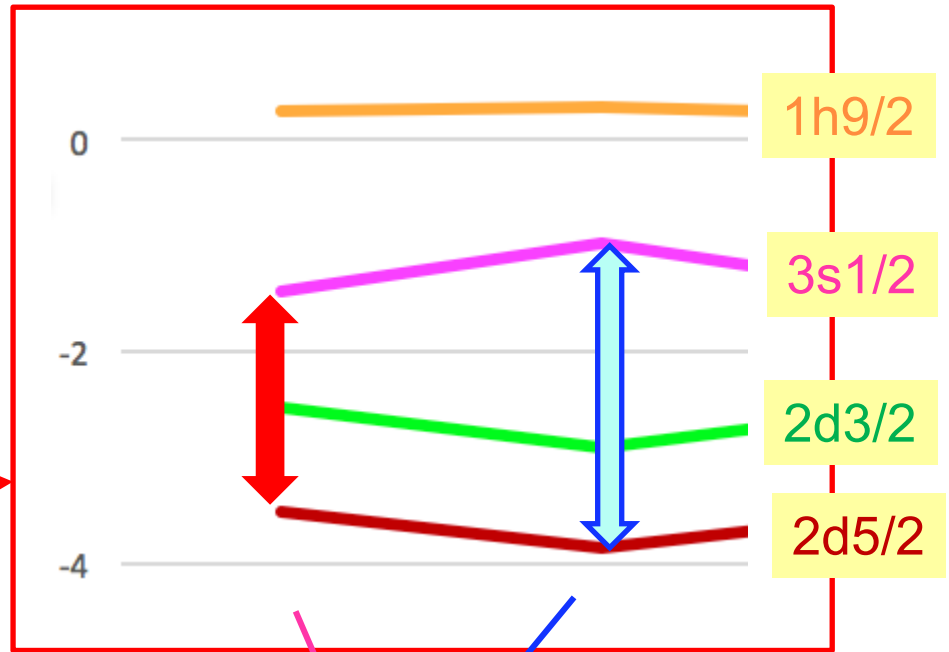
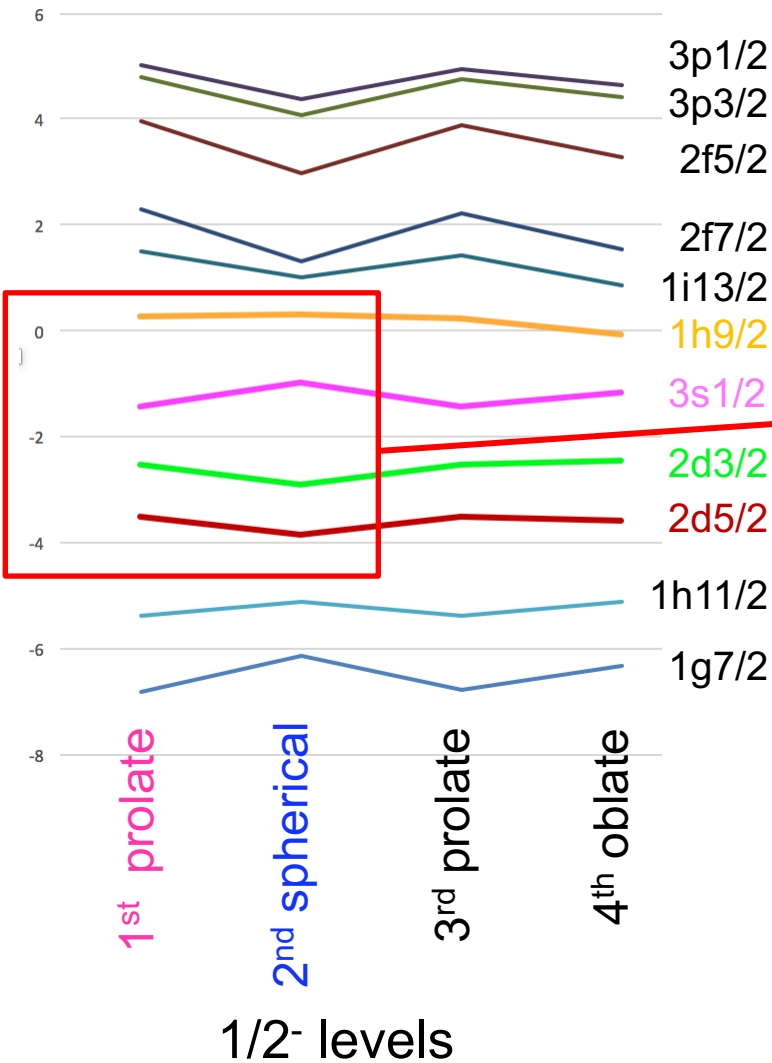




# Shape coexistence in Hg/Pb region

*Very Preliminary*

$^{181}\text{Hg}$  proton ESPE (MeV)



11 proton orbits, 13 neutron orbits  
nn, pp Brown (PRL85, 5300), pn VMU

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

resistance power ← pairing force

↑  
single-particle energies

Analogy to electric current,

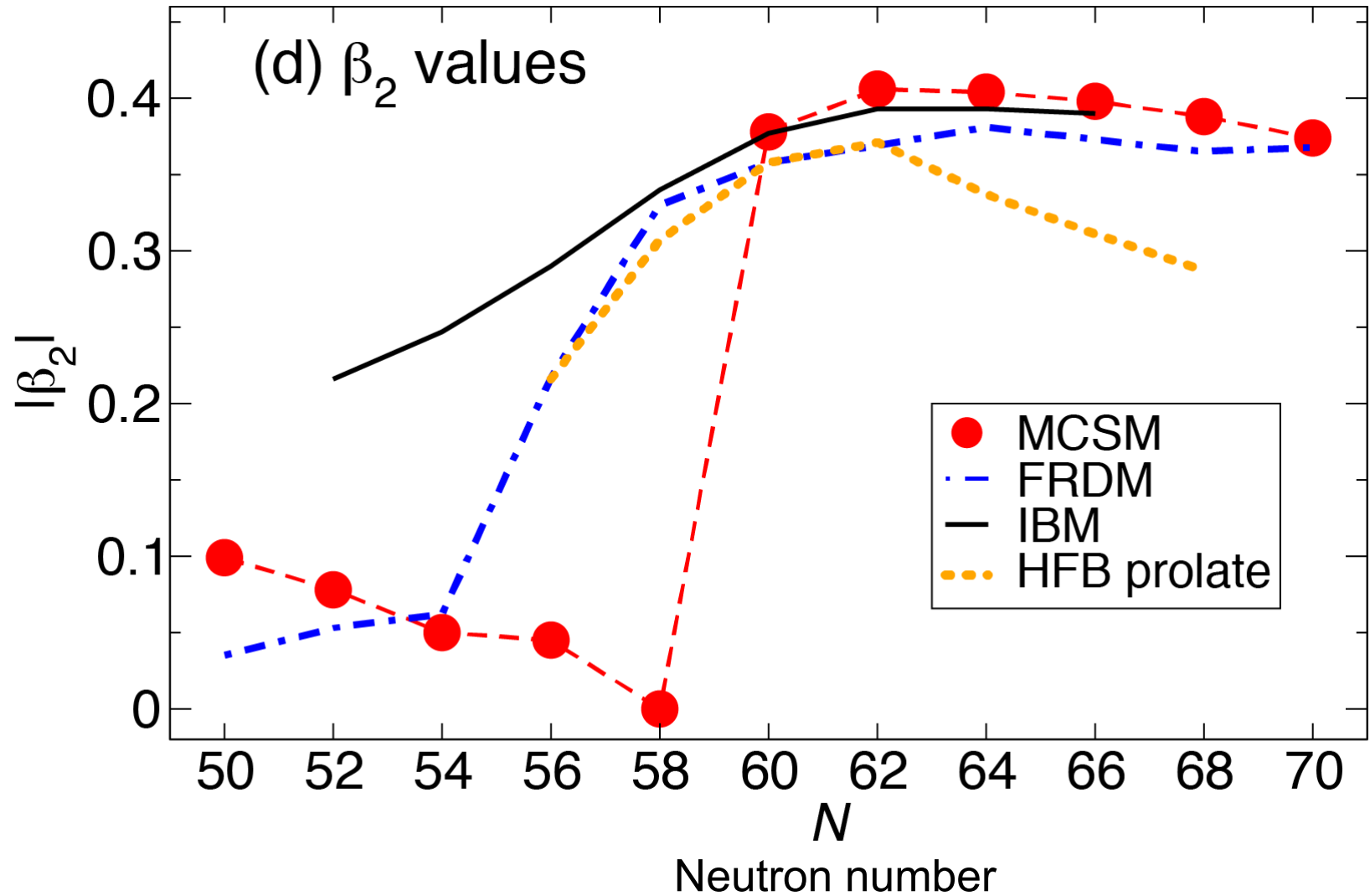
$$\text{current} = \frac{\text{voltage}}{\text{resistance}}$$

Additional remark:

The atomic nucleus can optimize its single-particle properties for actual mode/shape (or any final form of the structure), by choosing favorable configurations.

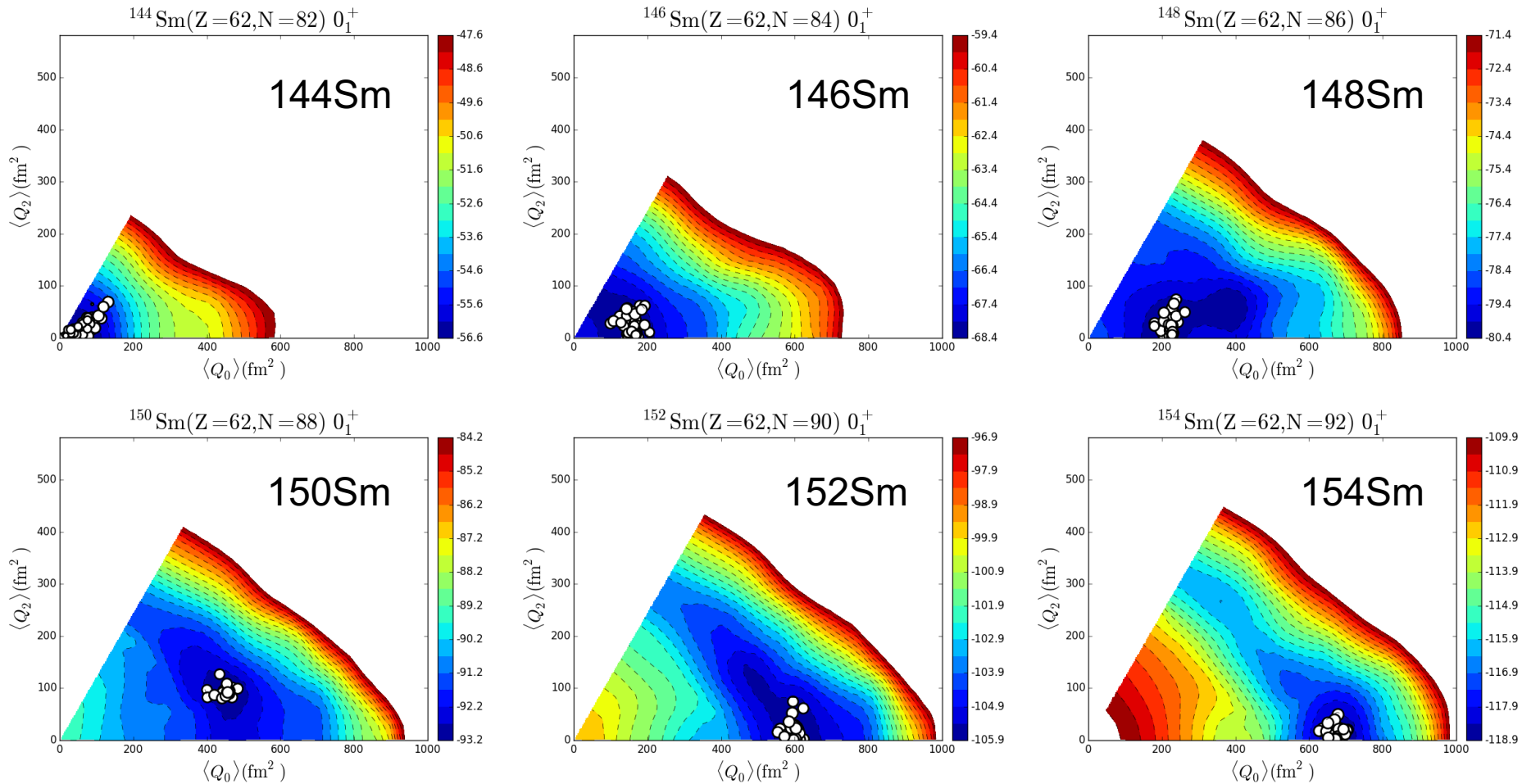
This aspect of the quantum self-organization may be (one of) the missing correlations Nakatsukasa-san mentioned this morning.

Deformation parameter  $\beta_2$  varies as the neutron number  $N$



# Sm同位体(Z=62)のT-plot

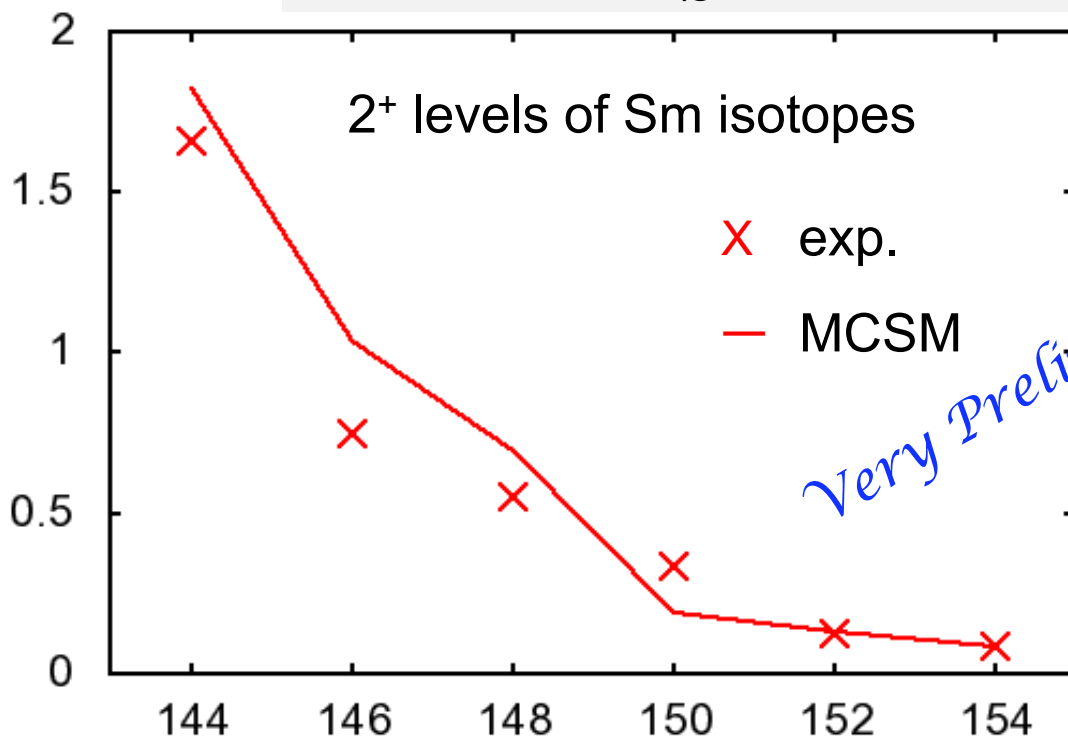
- $^{144}\text{Sm}$ から $^{154}\text{Sm}$ にかけて変形度が増加( $^{154}\text{Sm}$ で $\beta \sim 0.3$ )
- $^{150}\text{Sm}$ から配位が変わり、 $\pi 0h_{11/2}$ ,  $\nu 0g_{9/2}$ ,  $\nu 0i_{13/2}$ などに励起する



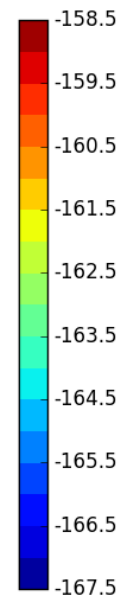
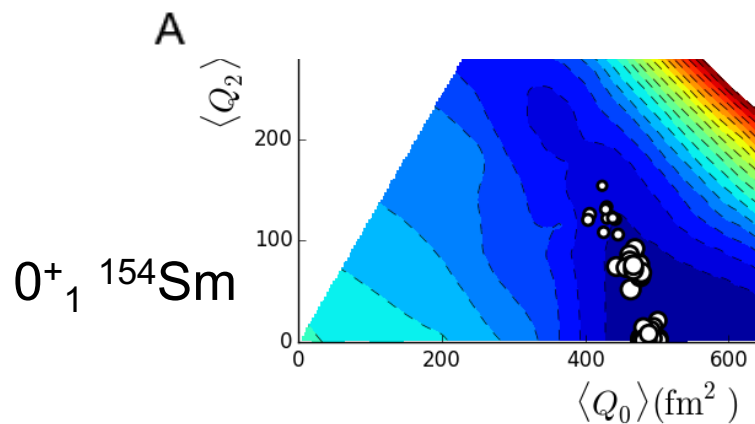
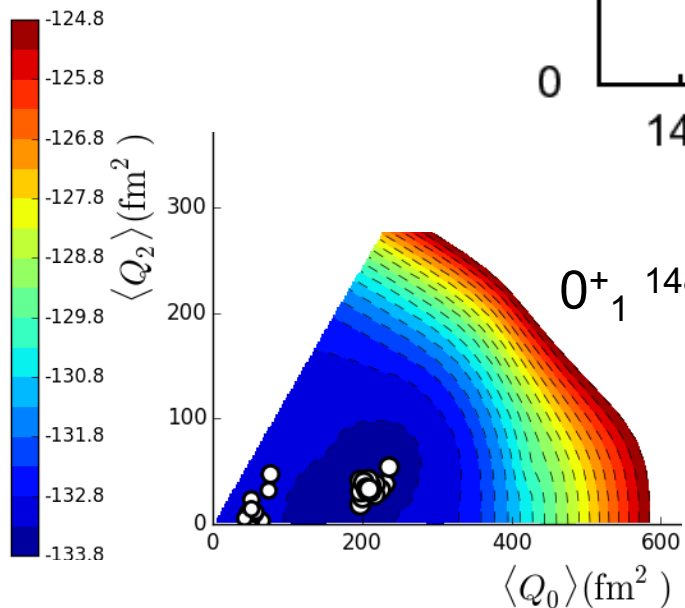
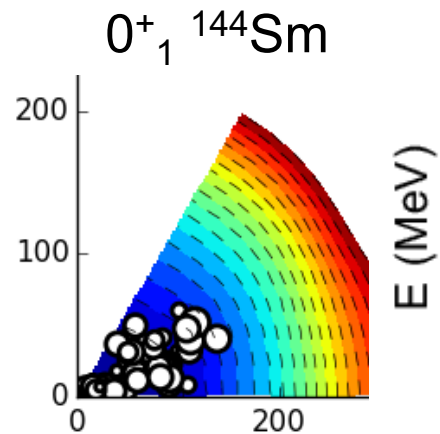
# Sm isotopes

proton 8 orbits  
neutron 10 orbits

Interaction VMU (gaussian central +  $\pi+\rho$  tensor)



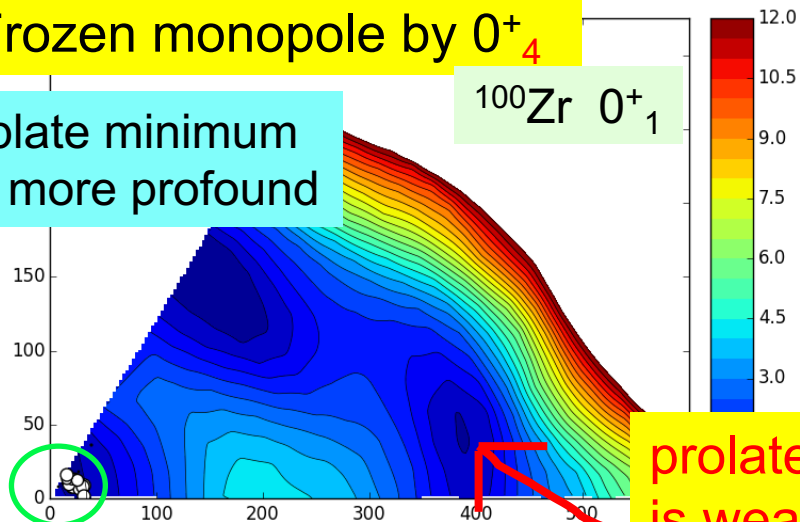
*Very Preliminary*



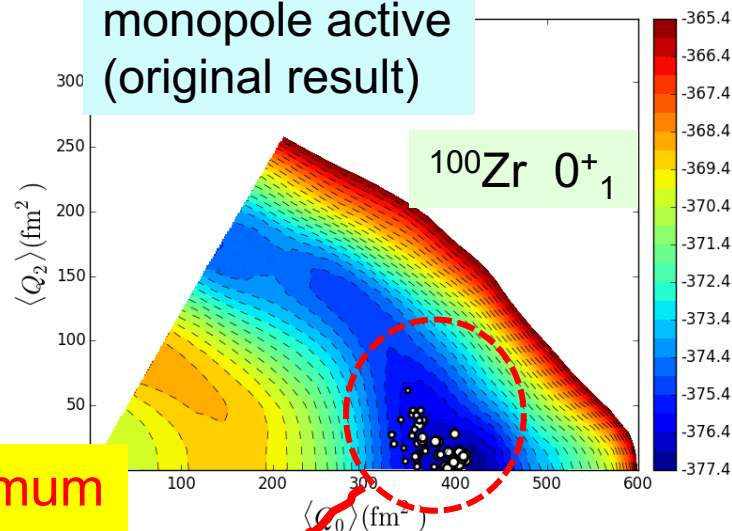
# $^{100}\text{Zr}$ prolate $0^+_1$ and spherical $0^+_4$ (T-plot)

Frozen monopole by  $0^+_4$

oblate minimum is more profound

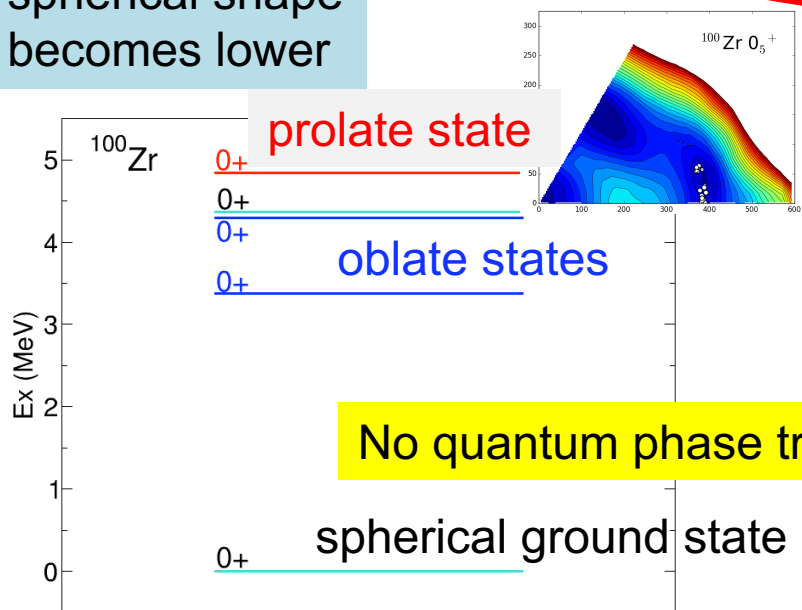


monopole active (original result)



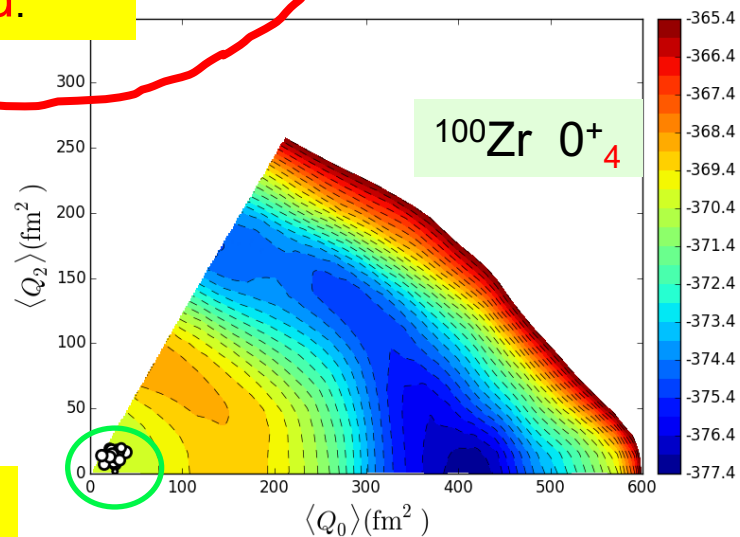
prolate minimum is weakened.

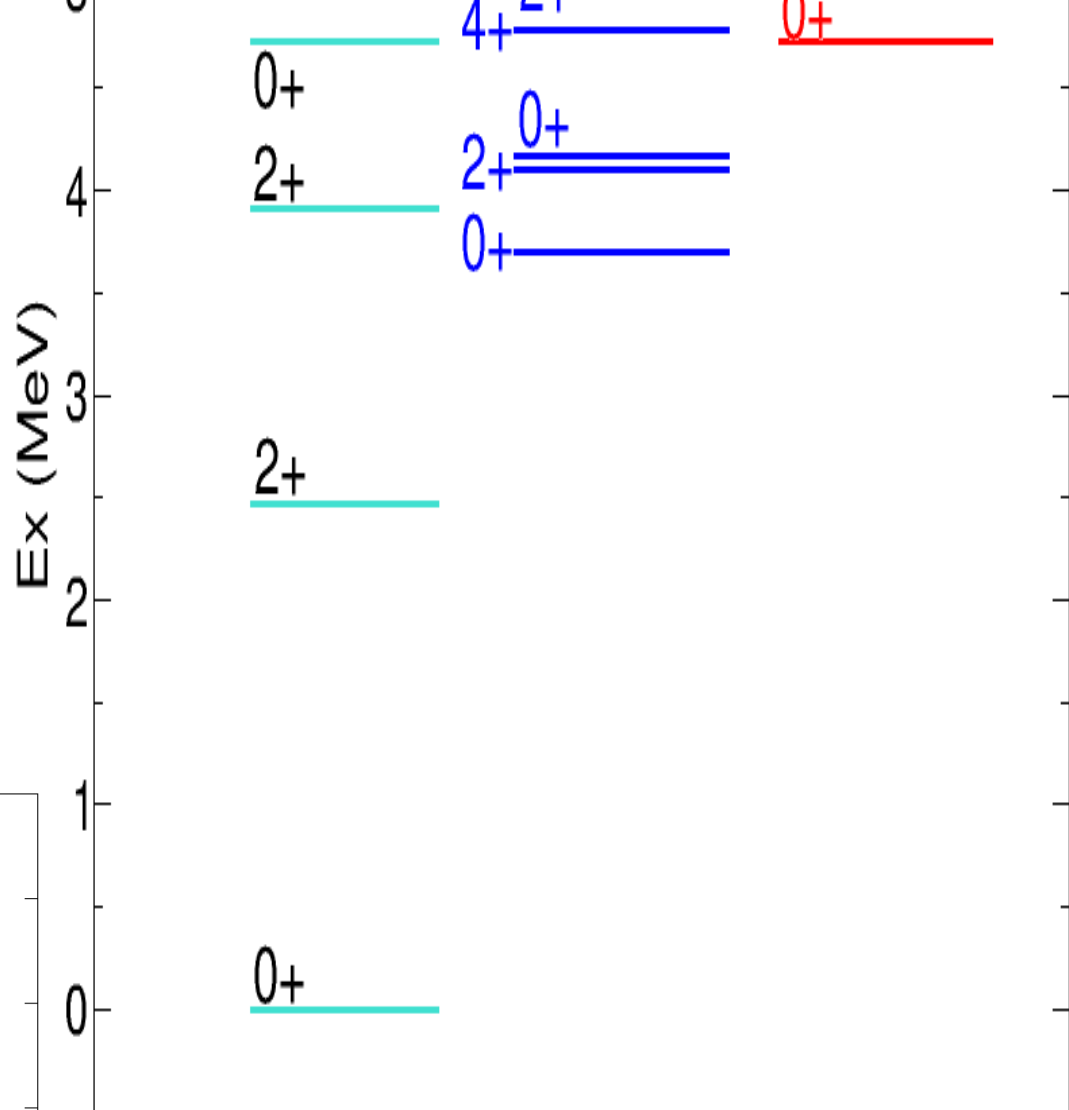
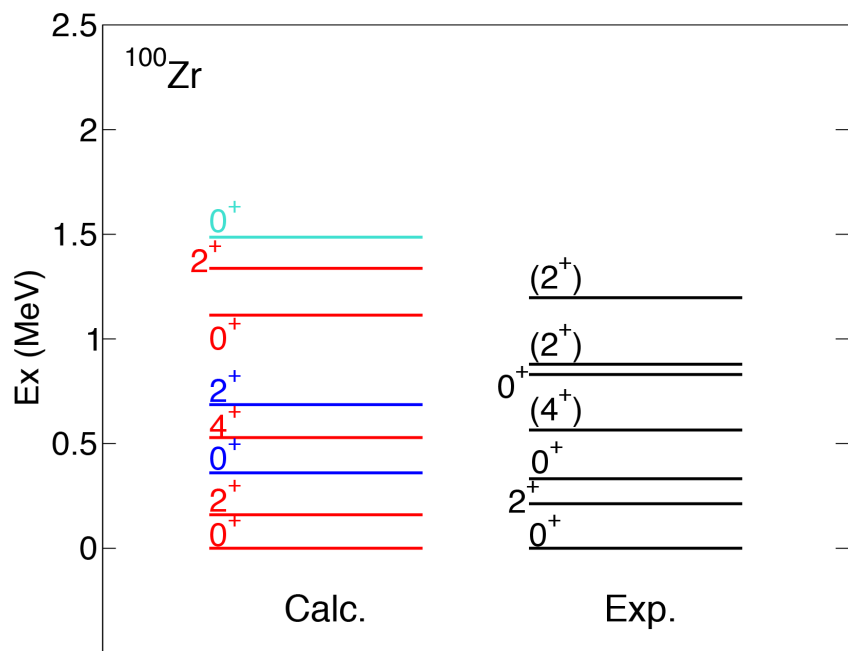
spherical shape becomes lower



No quantum phase transition

spherical ground state

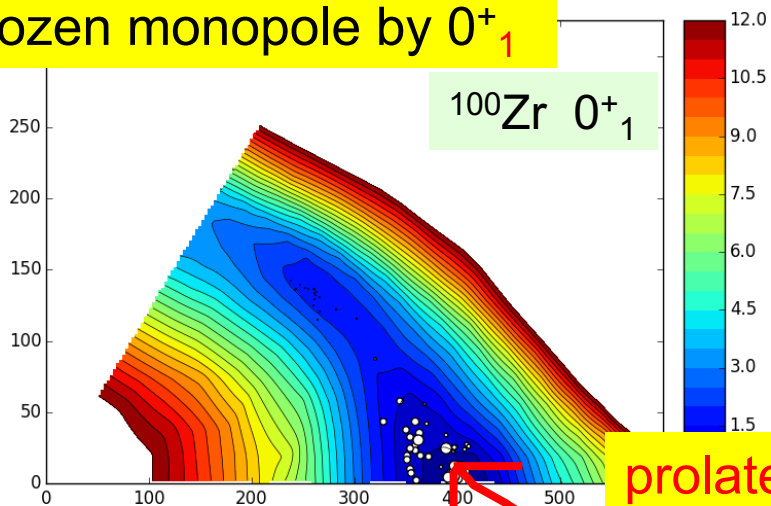






# $^{100}\text{Zr}$ prolate $0^+_1$ by frozen S.P.E. (T-plot)

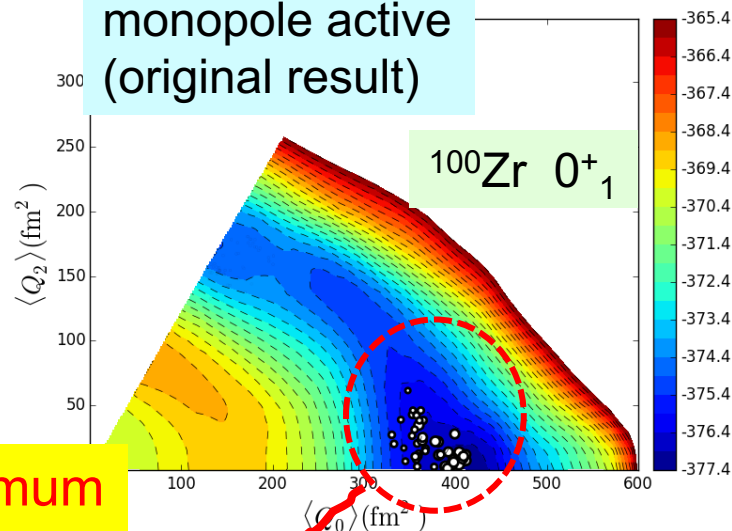
Frozen monopole by  $0^+_1$



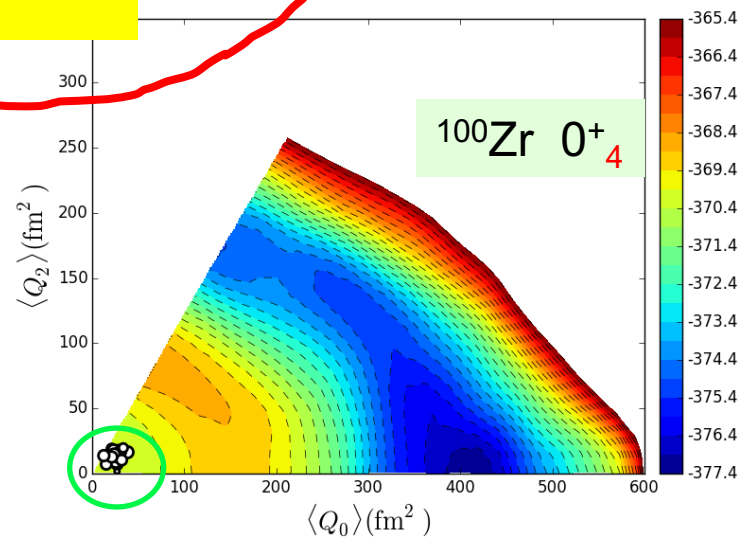
$^{100}\text{Zr}$   $0^+_1$

prolate minimum remains.

monopole active (original result)

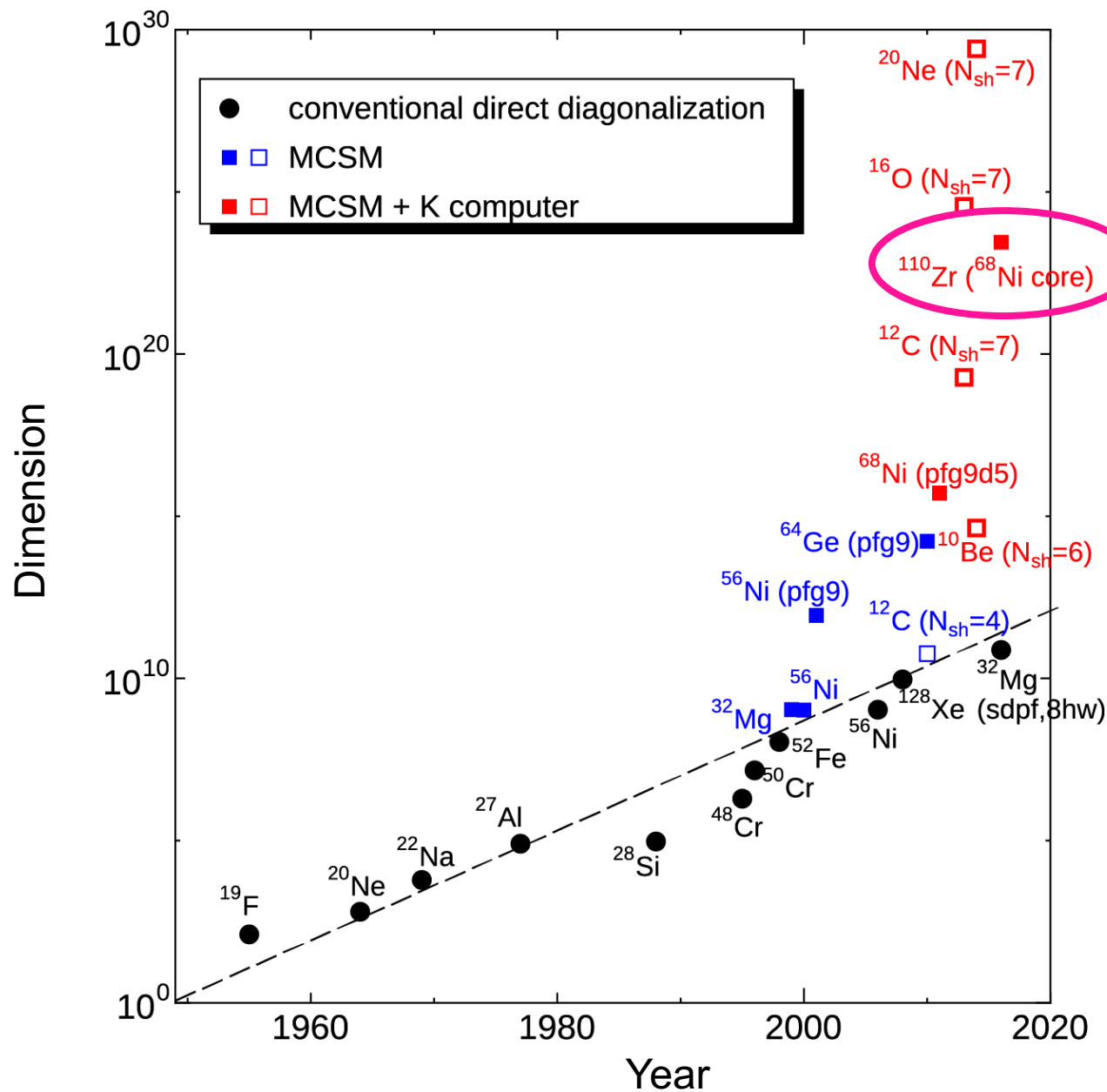


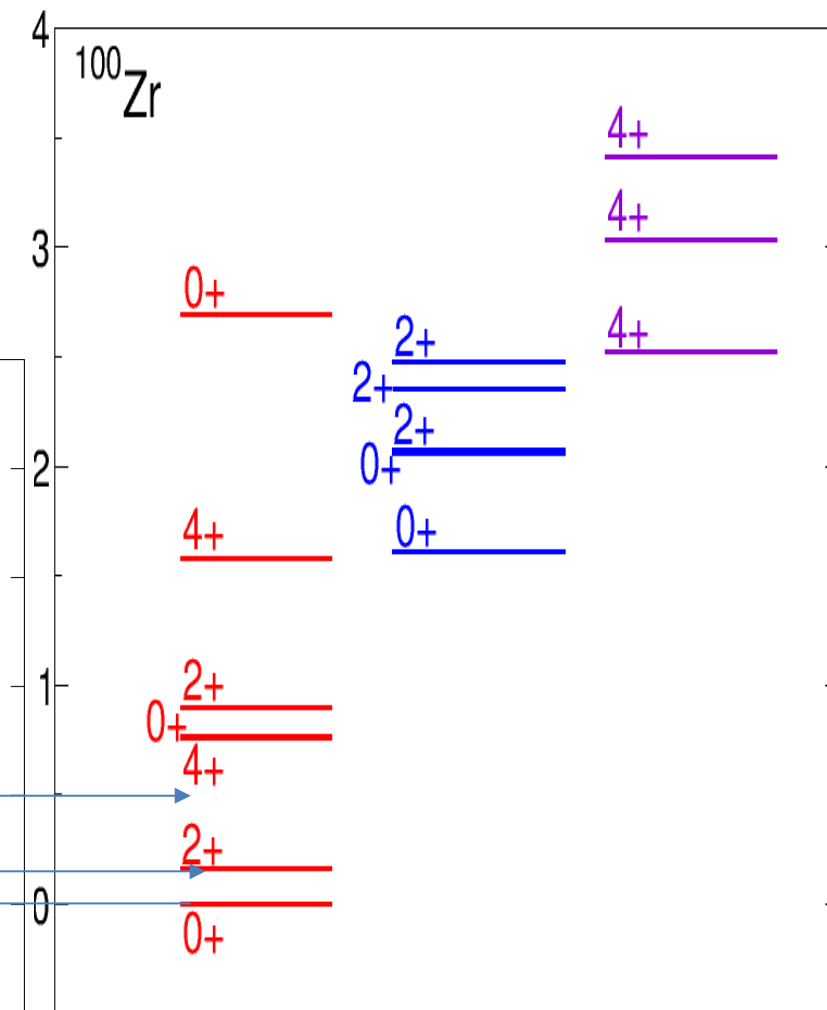
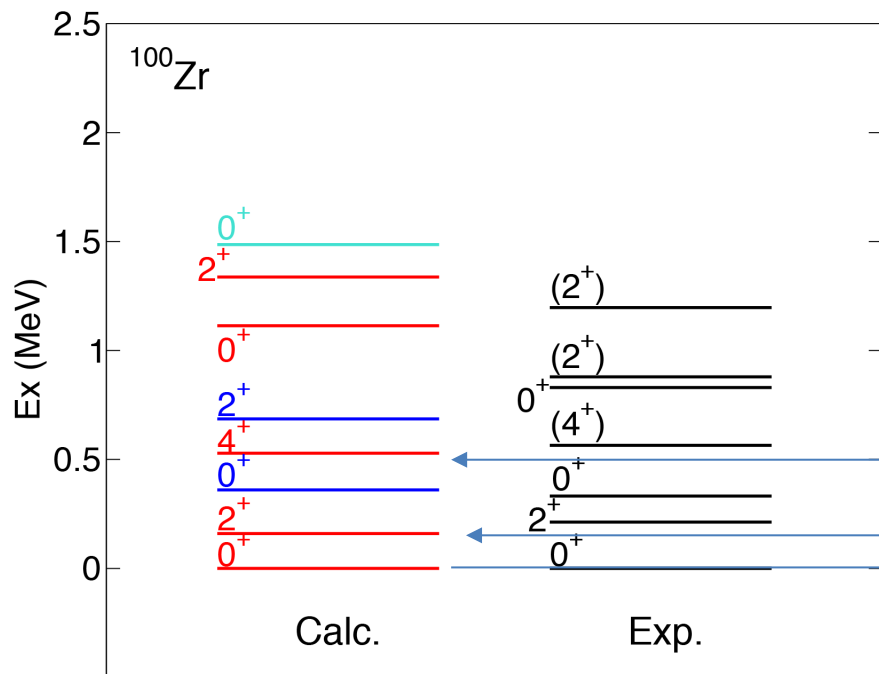
$^{100}\text{Zr}$   $0^+_1$



$^{100}\text{Zr}$   $0^+_4$

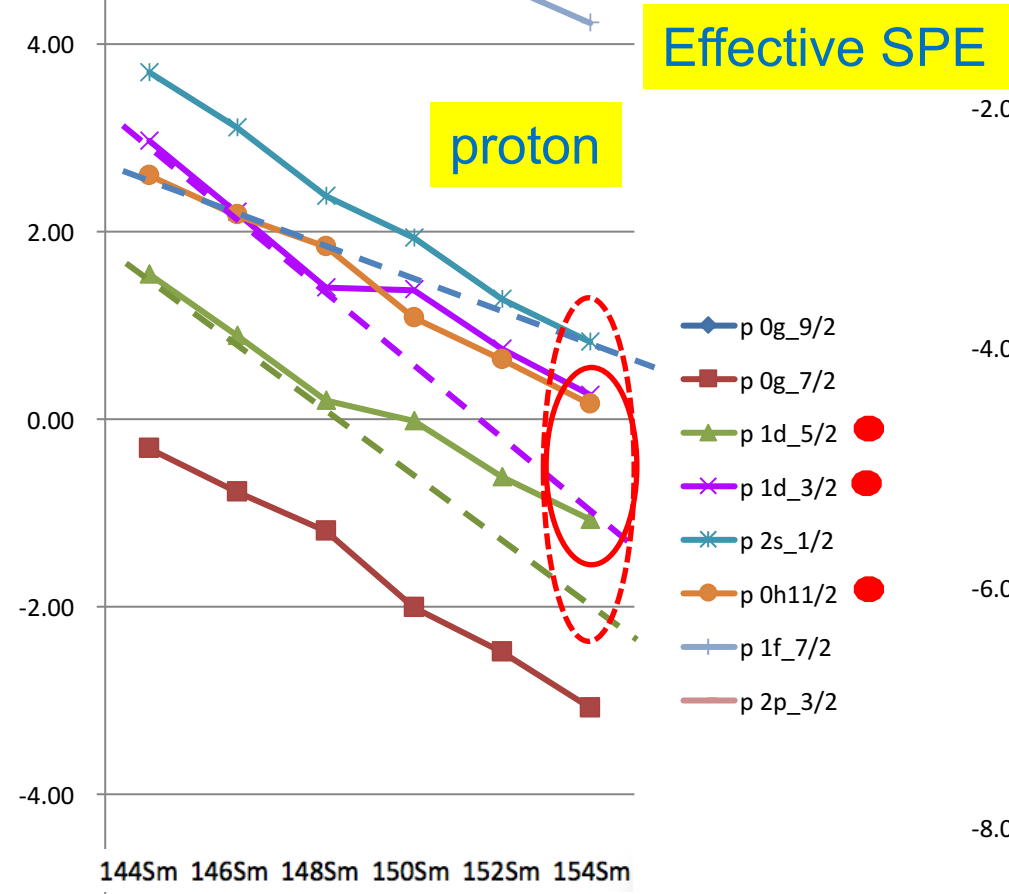
# Development of shell-model calculation



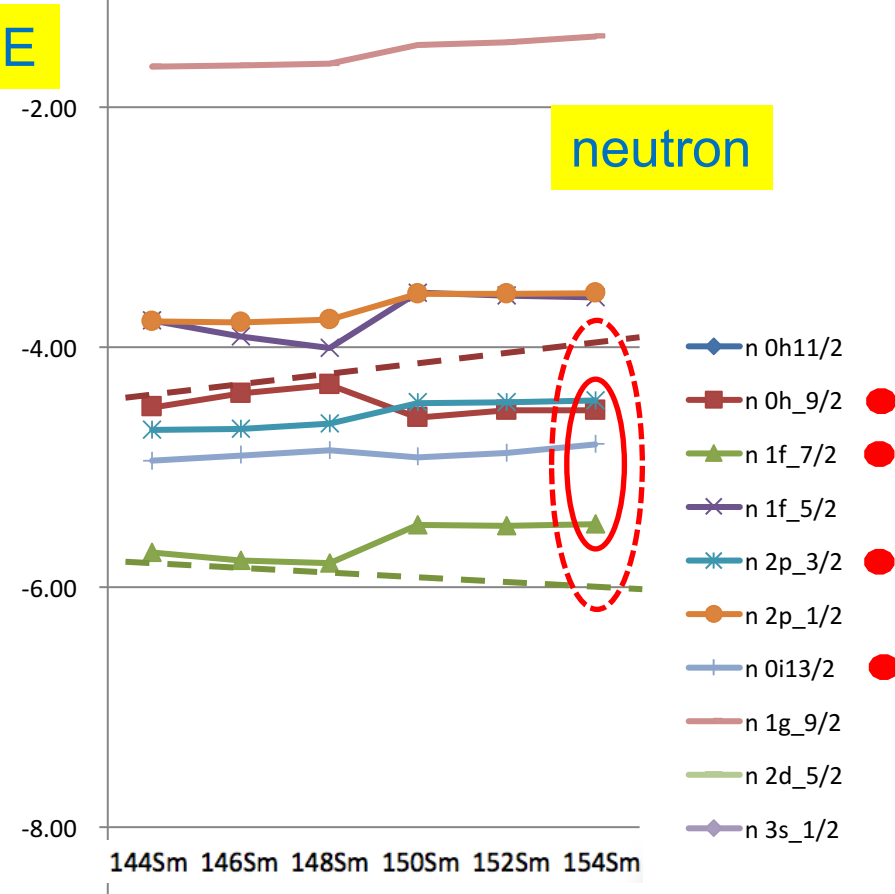


# Effective SPE

## proton



## neutron



Very Preliminary

