Interdisciplinary symposium on modern density functional theory

RIKEN

June 22 (June 19-23), 2017

Quantum phase transition and quantum self organization in nuclear to mesoscopic many-body systems

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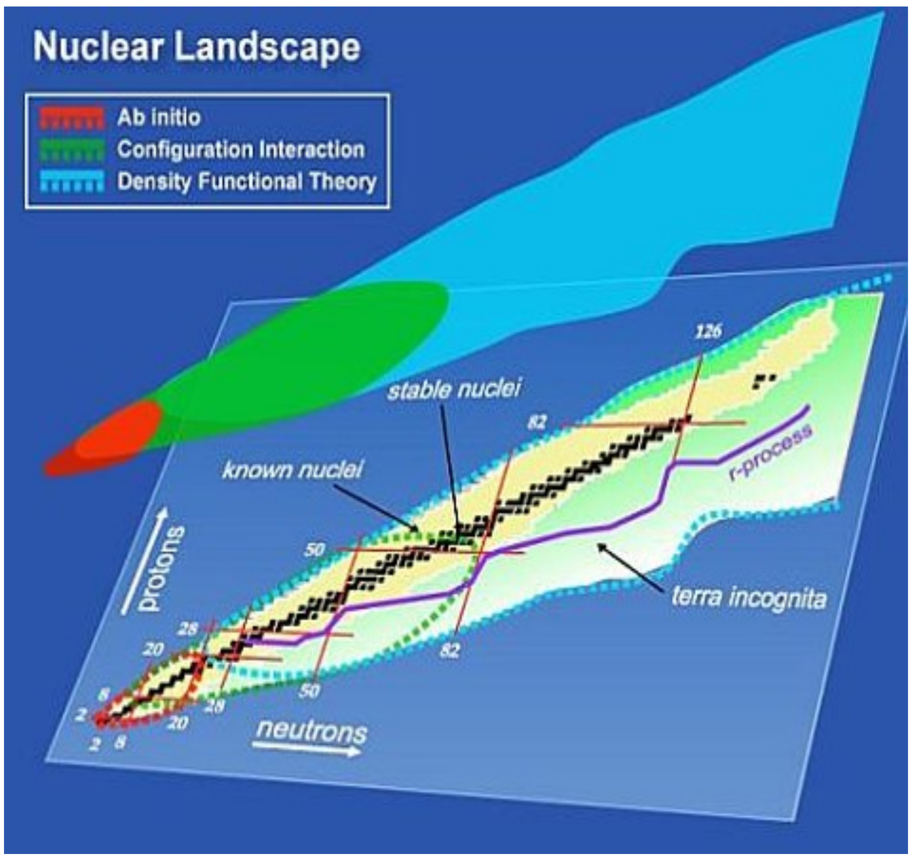
This work has been supported by MEXT and JICFuS as a priority issue (Elucidation of the fundamental laws and evolution of the universe) to be tackled by using Post 'K' Computer

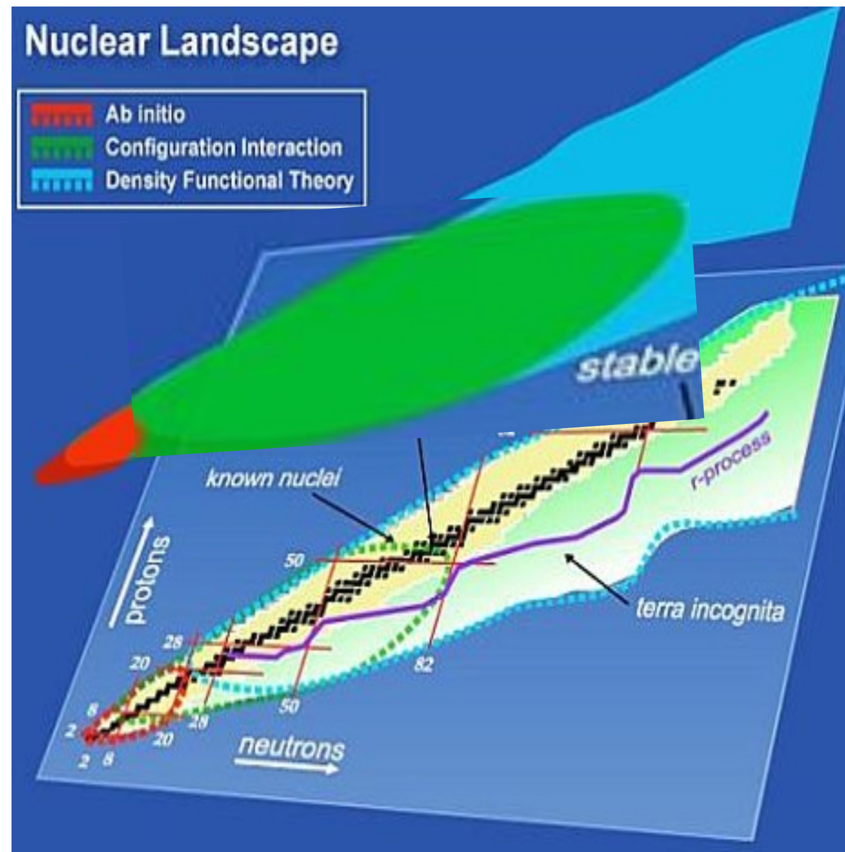
RIKEN NiSHiNA CENTER 東京大学 THE UNIVERSITY OF TOKYO KU LEUVEN MICHIGAN STATE UNIVERSITY Founded 1855

What can be done and what will come out with the (large-scale) shell-model studies at present and near future ?

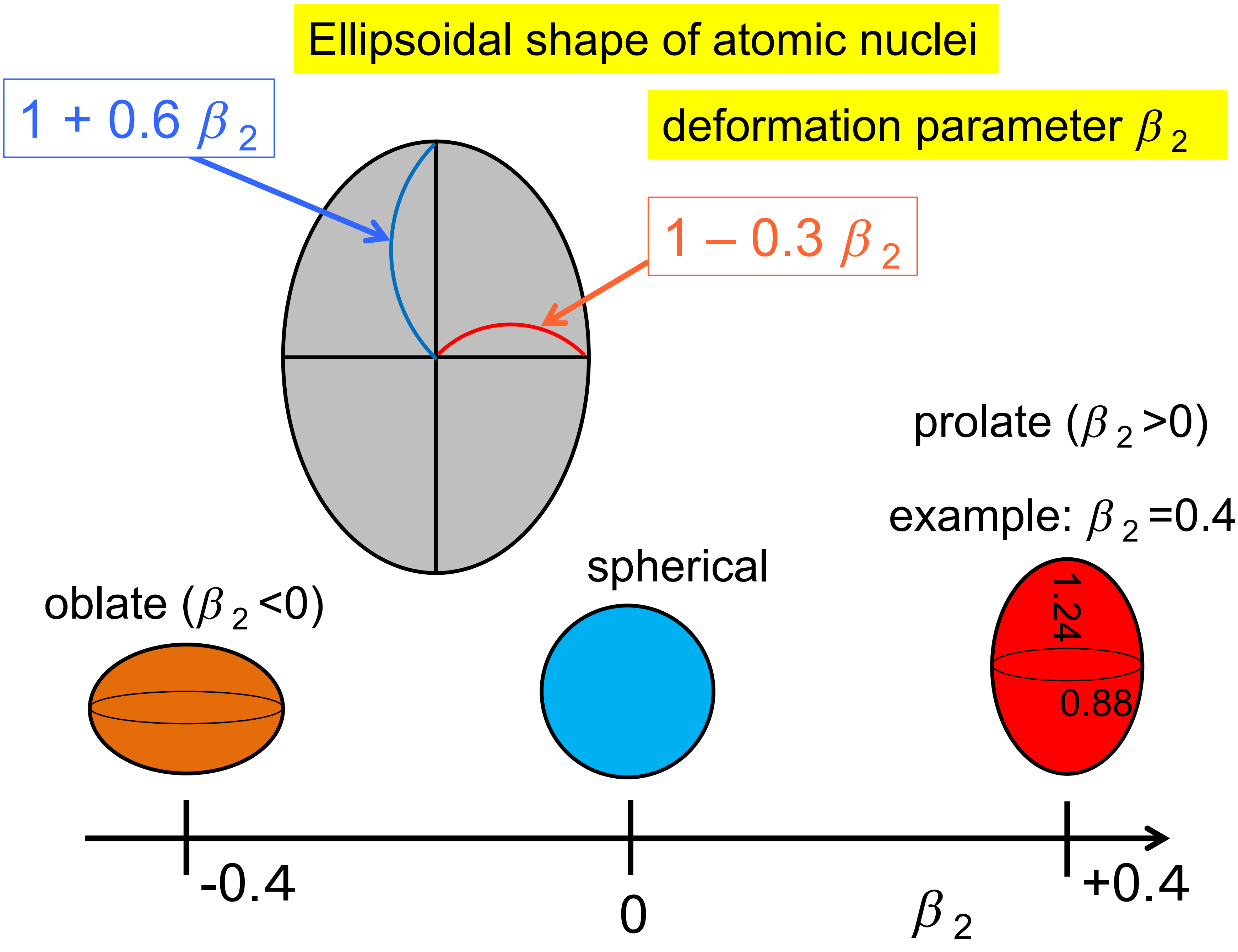
Could this challenge be feasible in a cooperative way with DFT ?

From UNEDF





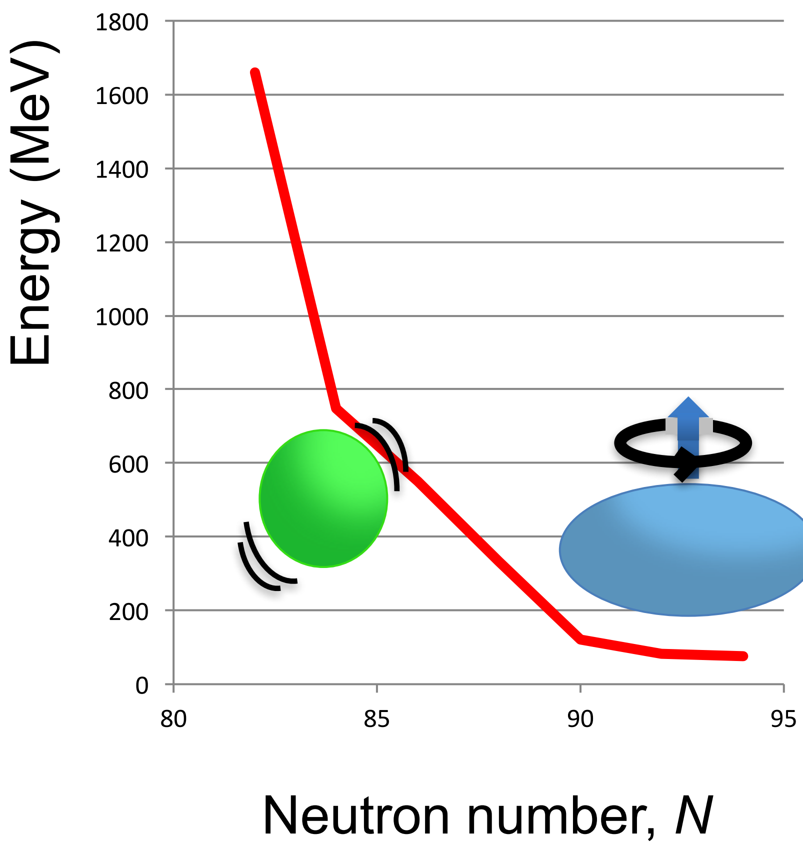
Nuclear shapes


Ellipsoidal shape of atomic nuclei
1 + 0.6 β 2
deformation parameter β 2
1 – 0.3 β 2
prolate (β 2 >0)
example: β 2 =0.4
spherical
oblate (β 2 <0)
1.24
0.88
-0.4
0
β 2
+0.4

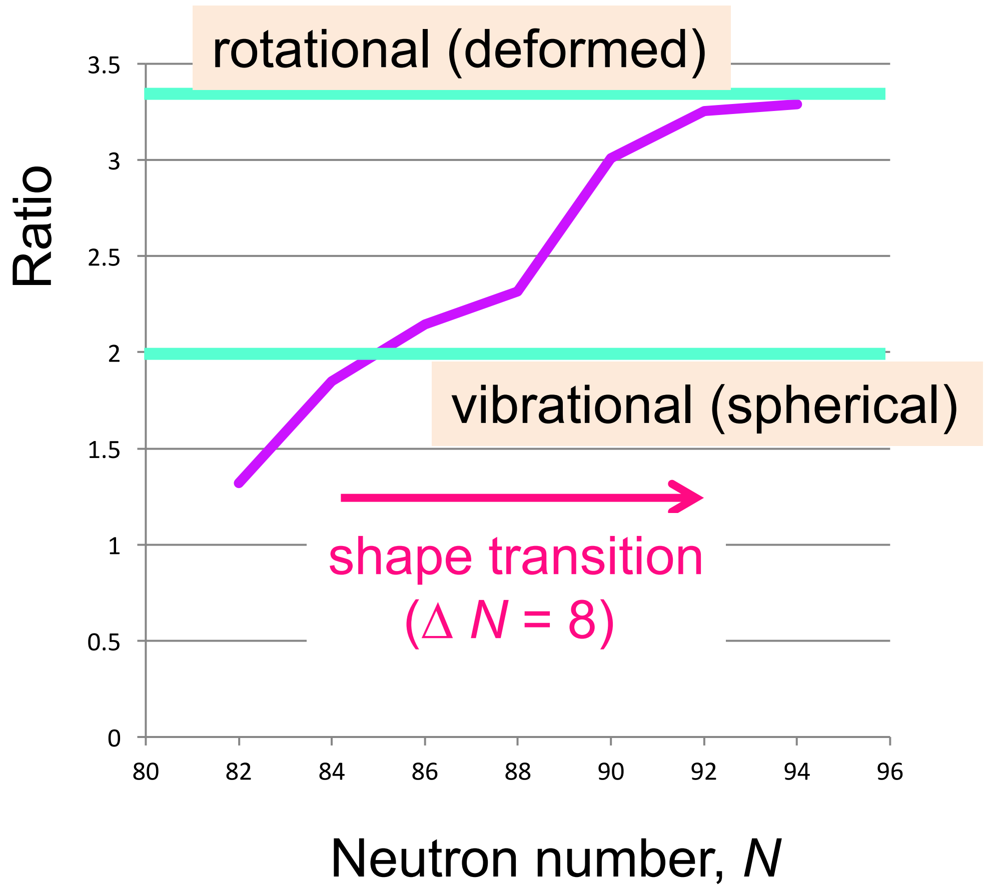
Nuclear shape evolution

2^+ and 4^+ level properties of $_{62}$Sm isotopes

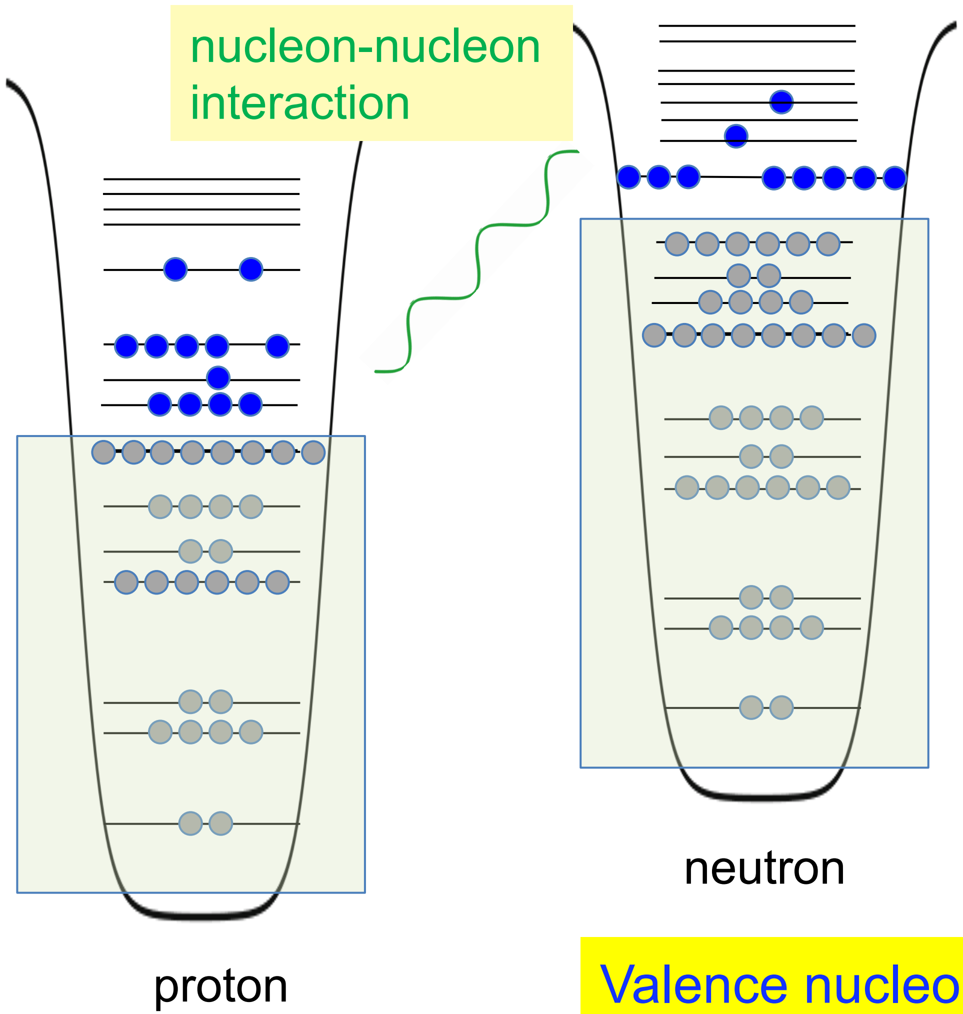
Ex (2^+) :
excitation energy of first 2^+ state



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



shell structure and nucleon-nucleon interaction



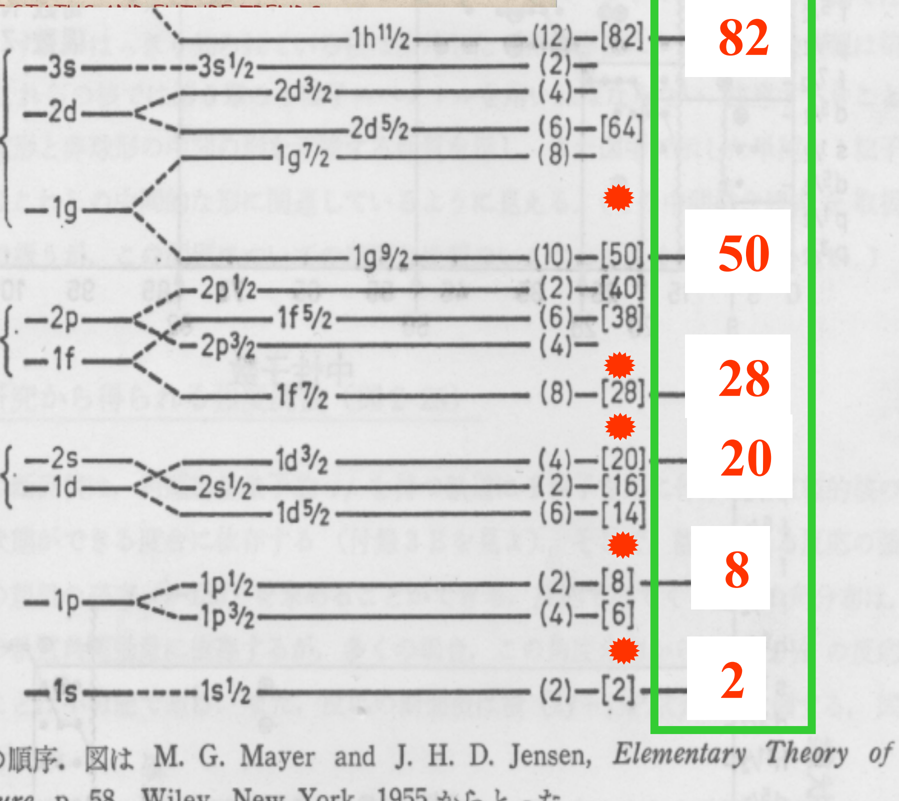
Protons and neutrons are orbiting in the mean potential like a vase
→ single-particle energies

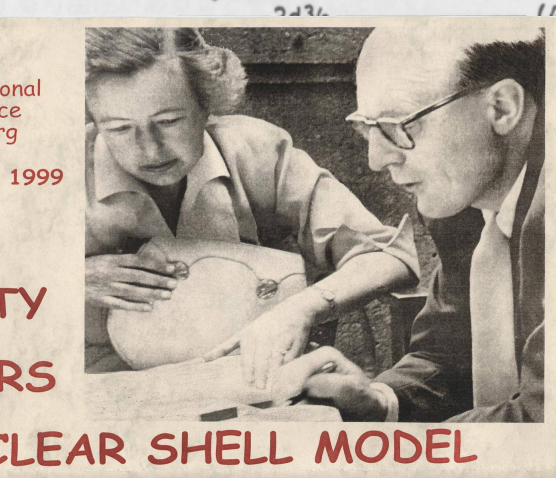
Lower orbits form the inert core
(shaded parts in the figure)

Upper orbits are only partially occupied
(valence orbits and nucleons).

Valence nucleons are the major source of nuclear dynamics at low excitation energy, because the inert core is *dead*.

Actual shell structure





Magic numbers by Mayer and Jensen (1949)

126

82

50

28

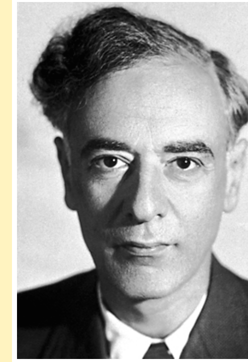
20

8

2

Atomic nucleus is a quantum Fermi liquid (of Landau) :

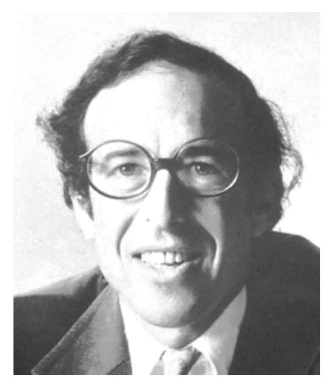
The nucleus is composed of almost free nucleons interacting weakly via residual forces in a (solid) (mean) potential



Surface deformation produced by additional deformed mean field

→ *Nilsson model*

Aage Bohr



Ben Mottelson

Sven Nilsson

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),

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

quadrupole deformed field

spherical field

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

constant within a region

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

$$\left.\begin{array}{ll} A=68 & 1.28 \\ A=100 & 1.12 \\ A=186 & 0.91 \end{array}\right\} (\mathbf{l}\cdot\mathbf{s})$$

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.

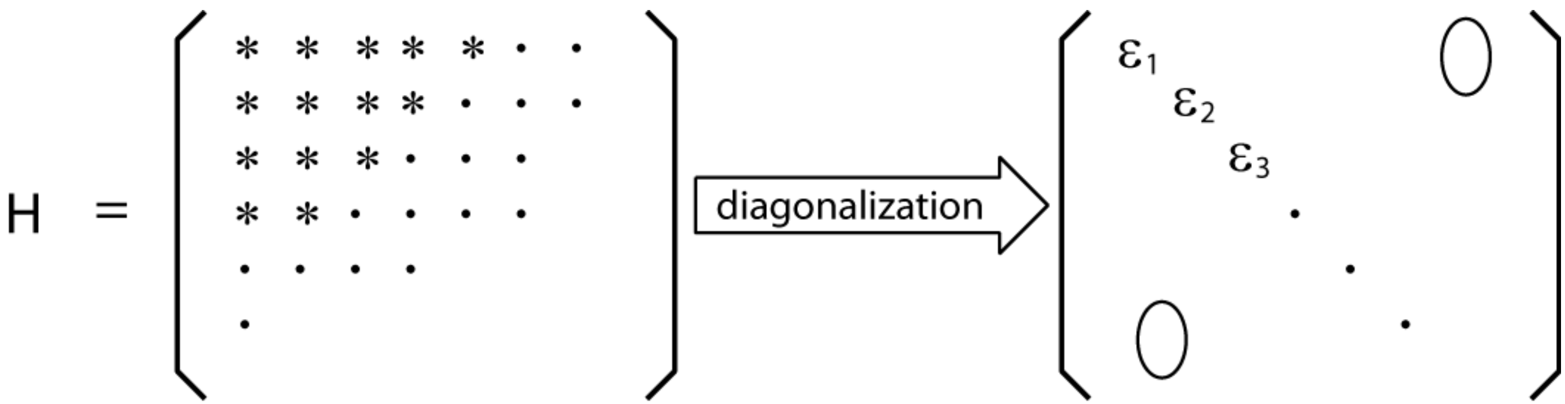
What else ?

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

Numerical methodology of many-body problems

Two types of shell-model calculations

dim. <~ 10^{10}



Conventional Shell Model

all Slater determinants

Direct diagonalization

For even bigger problem,

~100 dim.

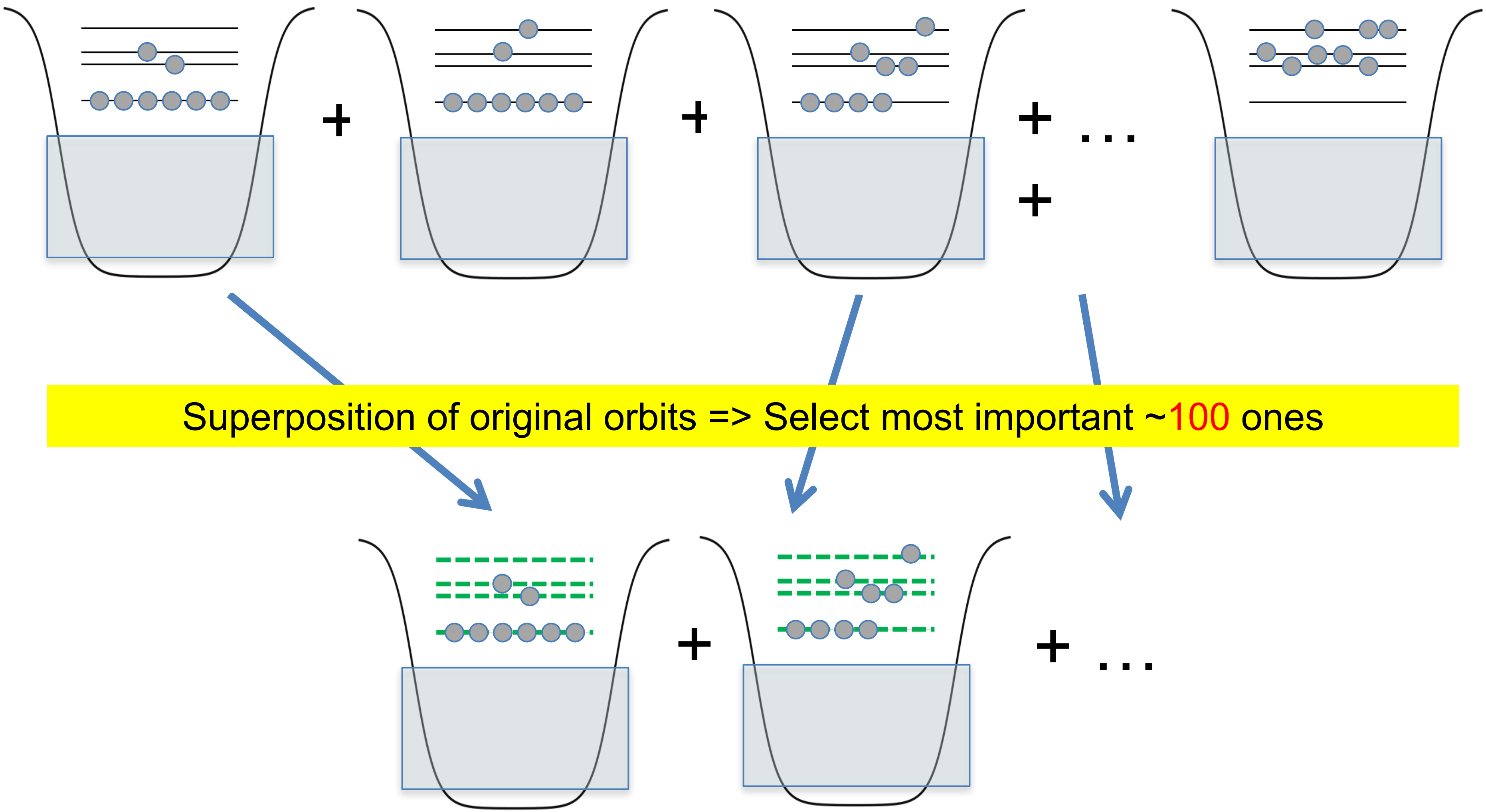
Monte Carlo Shell Model

bases important for a specific eigenstate

Selected

important basis vectors

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



Advanced Monte Carlo Shell Model

N_B : number of basis vectors (dimension)

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

amplitude

Projection op.

N_p : number of (active) particles

N_{sp} : number of single-particle states

$$\left|\phi(D^{(n)})\right\rangle = \prod_{\alpha=1}^{N_p} \underbrace{\left(\sum_{i=1}^{N_{sp}} a_i^{\dagger} D_{i\alpha}^{(n)} \right)}_{\text{Deformed single-particle state}} \left|-\right\rangle$$

n-th basis vector
(Slater determinant)

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

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

Step 1 : quantum Monte Carlo type method

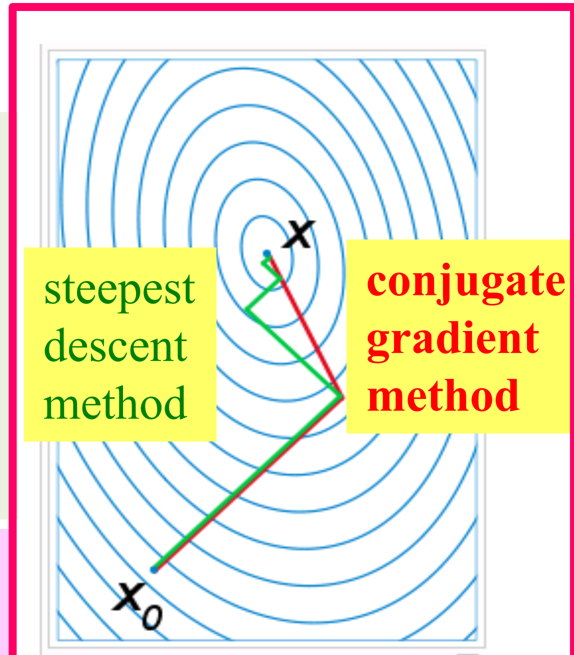
→ candidates of n-th basis vector (σ : set of random numbers)

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

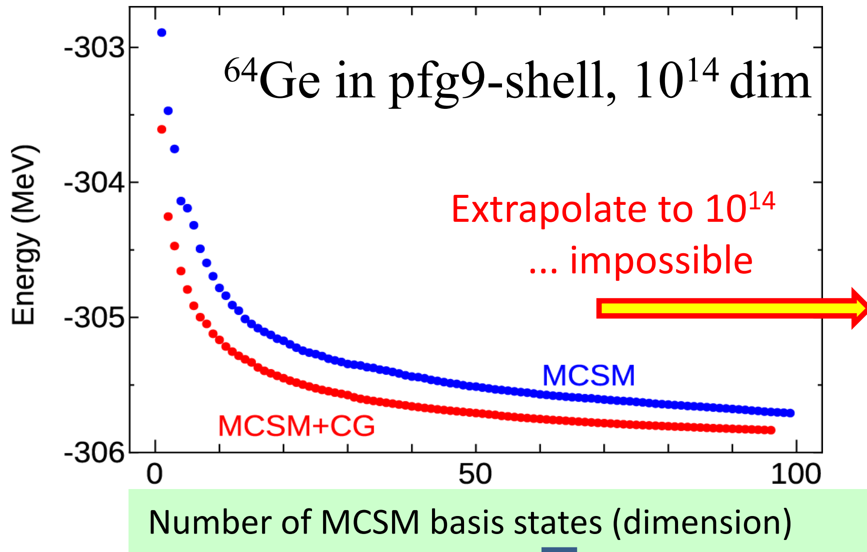
" σ" can be represented by matrix D

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

Step 2 : polish *D* by means of the conjugate gradient method "variationally".



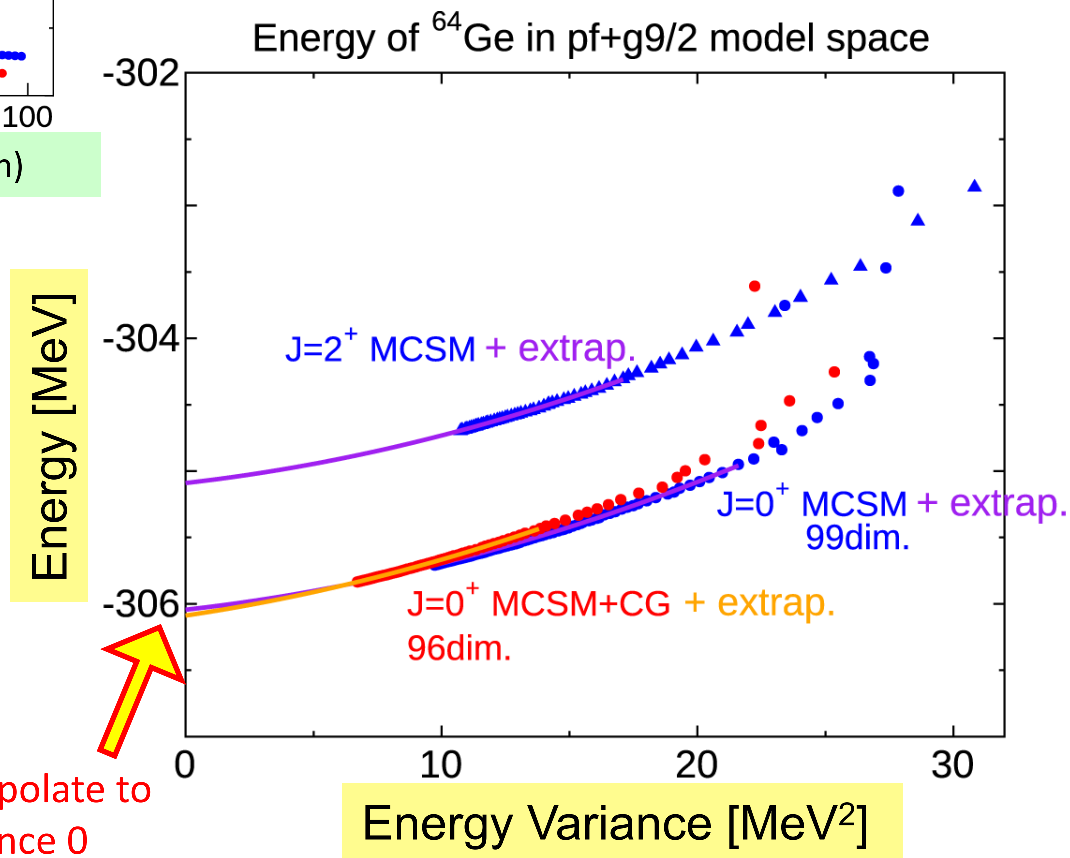
Step 3 : Energy variance extrapolation

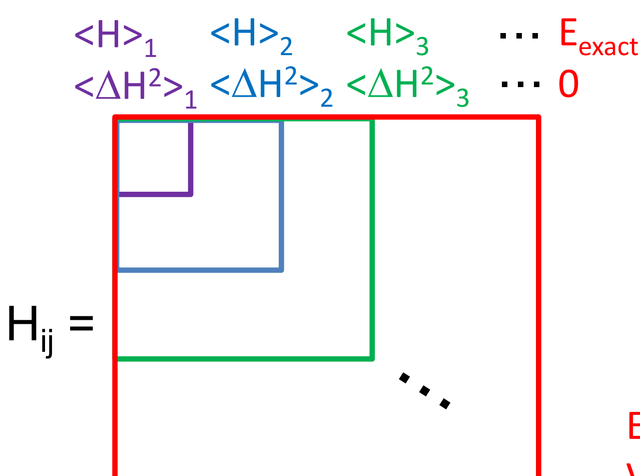


Energy variance : $\langle \Delta H^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2$

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

Extrapolate towards $\langle \Delta H^2 \rangle \to 0$





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

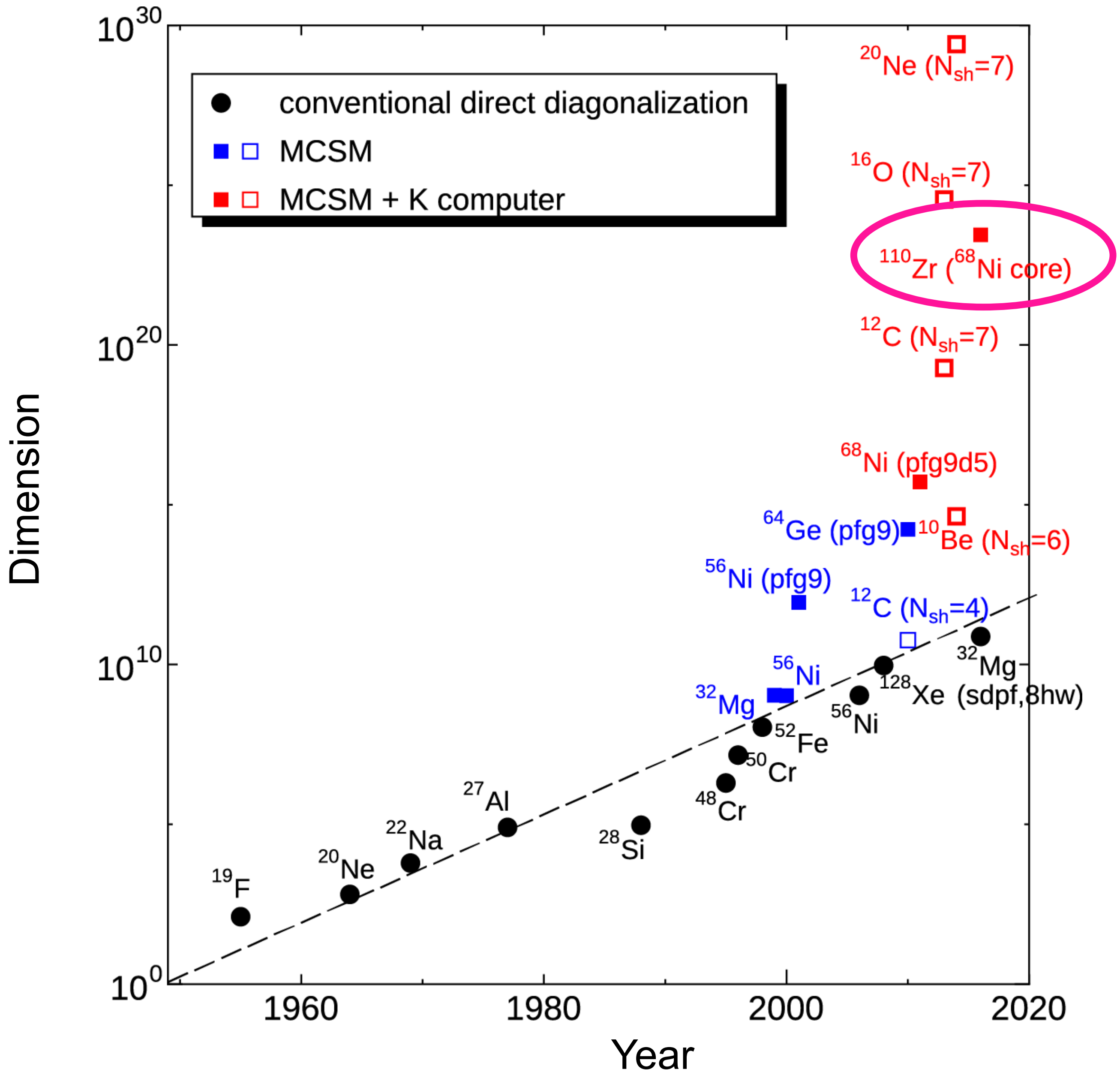
$\Rightarrow$ *Projection of basis vectors*

Rotation with three Euler angles

with about 50,000 mesh points

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

Development of shell-model calculation



~ Avogadro number

MCSM wave function on Potential Energy Surface (*T-plot*)

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

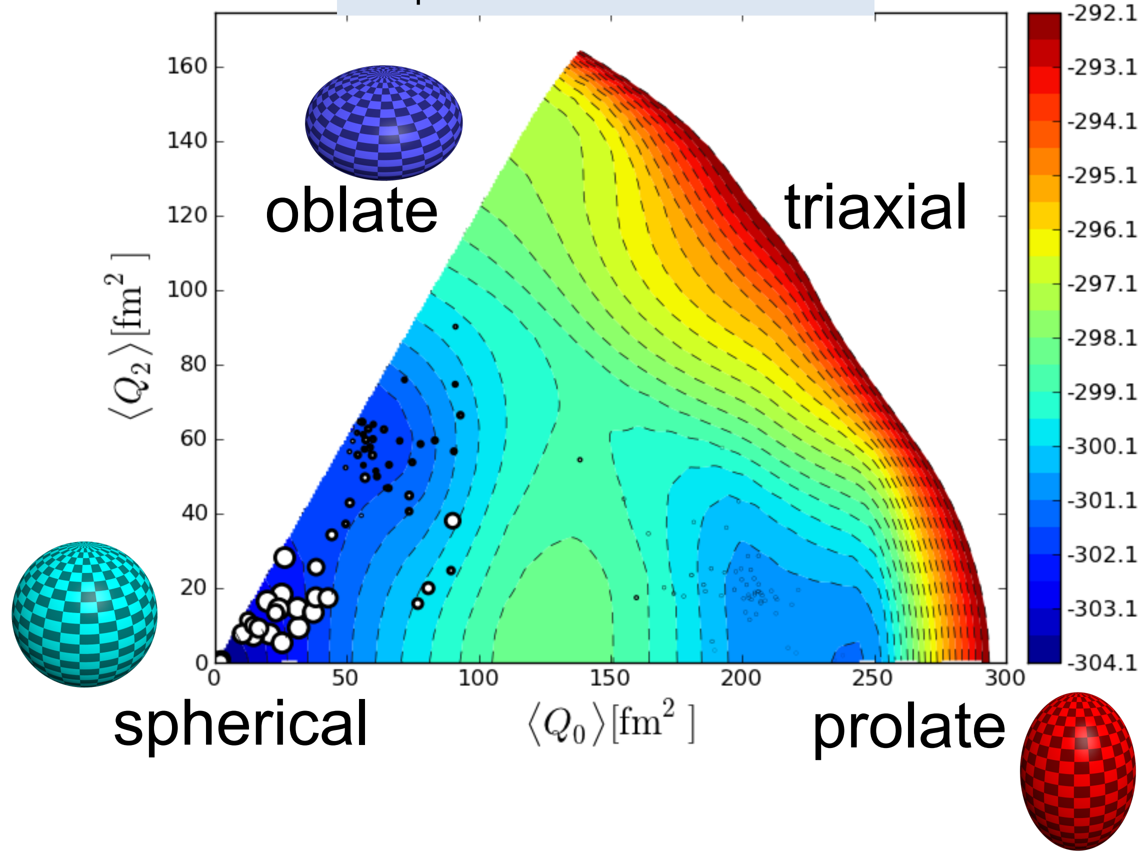
amplitude

projection on J^π

Slater determinant
→ intrinsic deformation

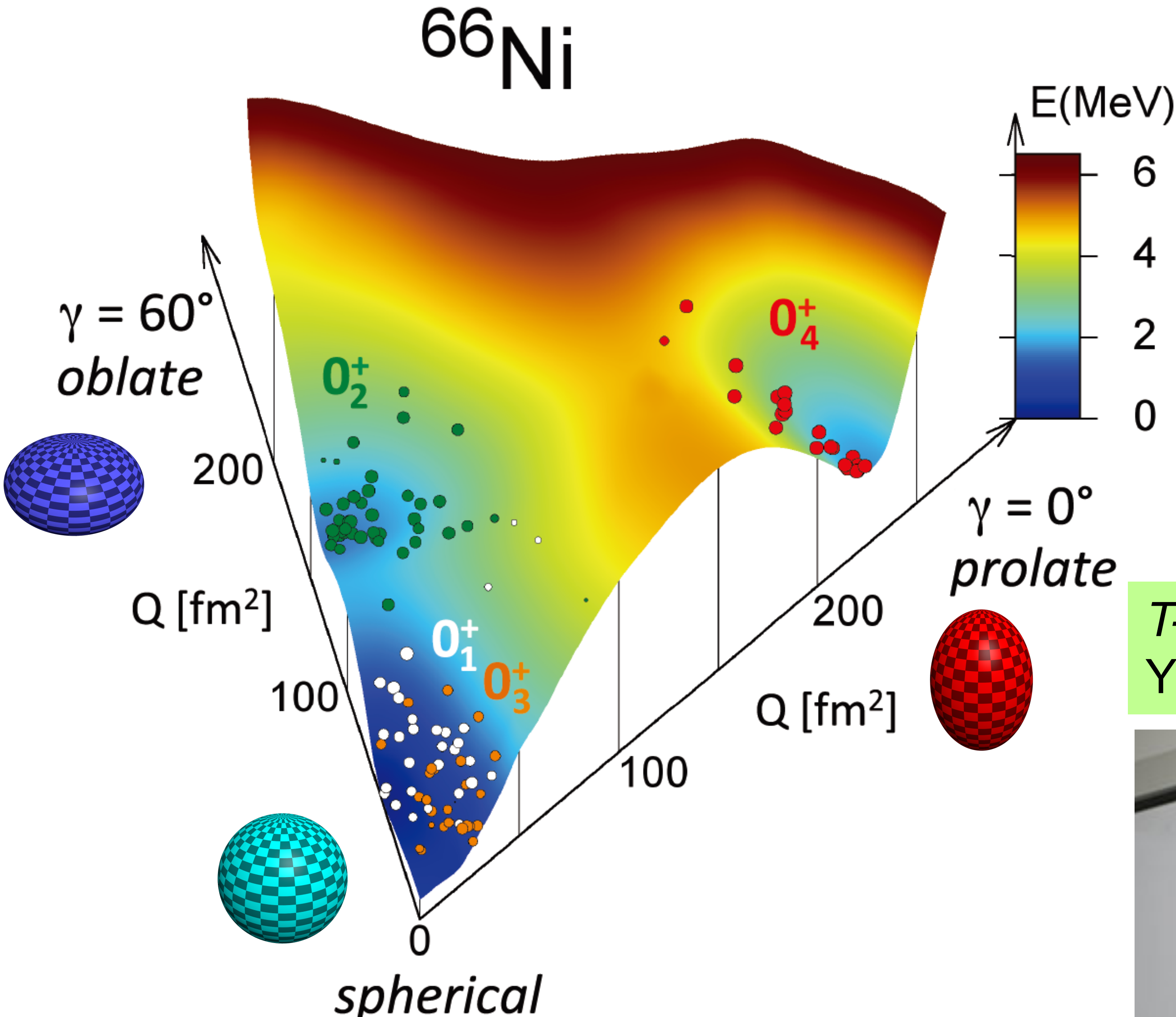
- PES is calculated by CHF
- Location of circle : quadrupole deformation of unprojected MCSM basis vectors
- Area of circle : overlap probability between each projected basis and eigen wave function

0^+_1 state of ^{68}Ni



3-dimensional T-plot

~ Alpine villages

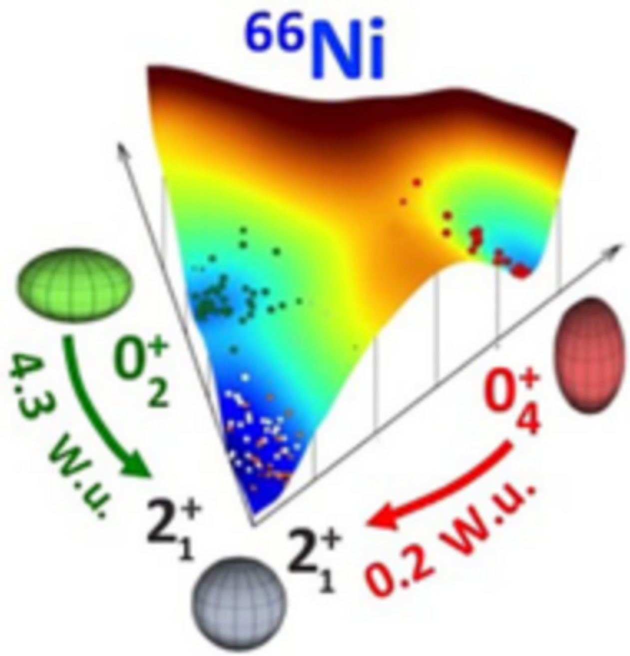


T-plot invented by Yusuke Tsunoda

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

S. Leoni *et al.*

Phys. Rev. Lett. **118**, 162502 (2017) – Published 20 April 2017



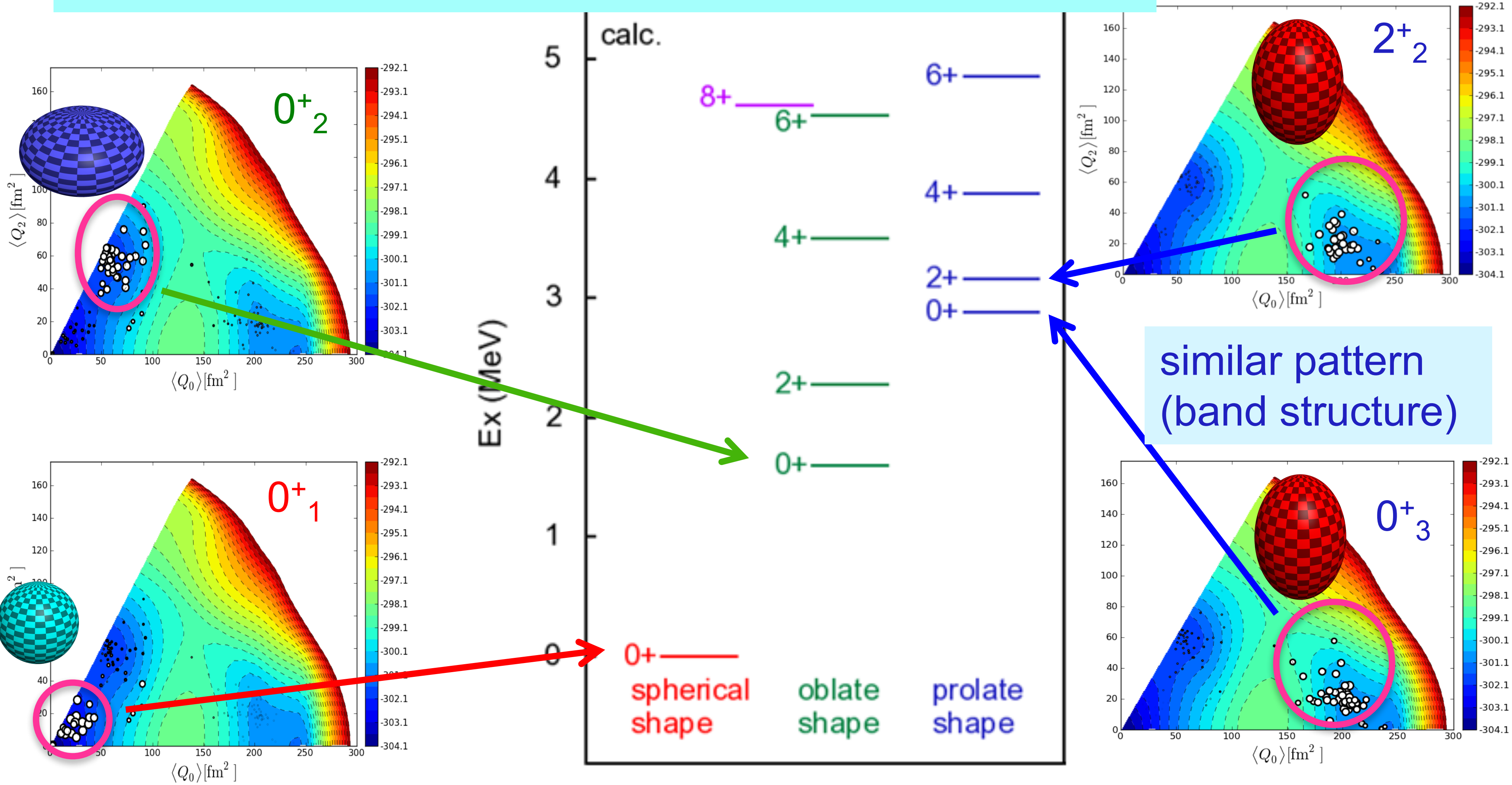
General properties of T-plot :

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}Ni



Quantum Phase Transition

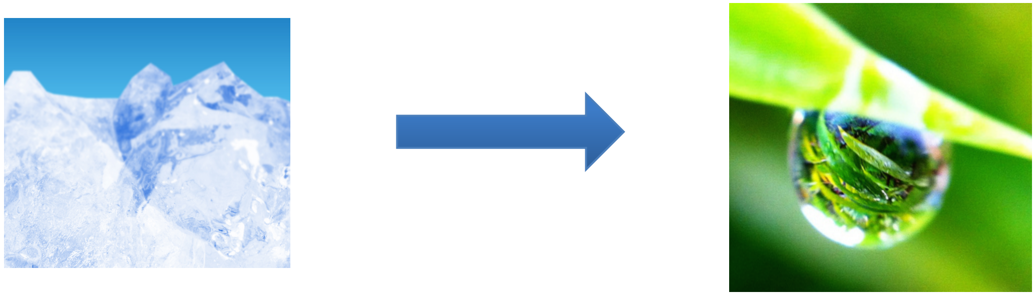
Can the shape transition be a "Phase Transition" ?

Phase Transition :

A macroscopic system can change qualitatively from a stable state (*e.g.* ice for H_2O) to another stable state (*e.g.*, water for H_2O) 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,

where thermodynamics can be applied.



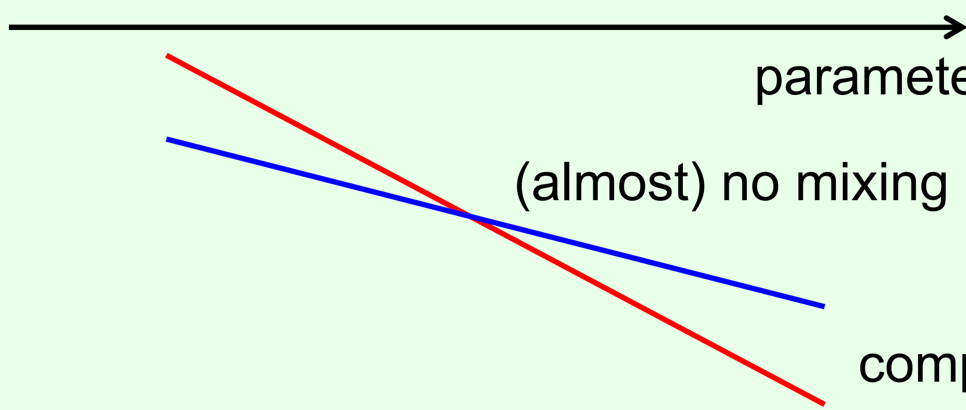
Quantum Phase Transition (QPT)

The concept of the phase transition cannot be applied to microscopic systems as it is. In the QPT, the ground state of a quantum (microscopic) system undergoes abrupt and qualitative change (of order parameter) as a (control) parameter changes.

The shape transition occurs rather gradually.

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 ?

possible scenario



Note that sizable mixing occurs usually in finite quantum systems.

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. (cf., Wikipedia)

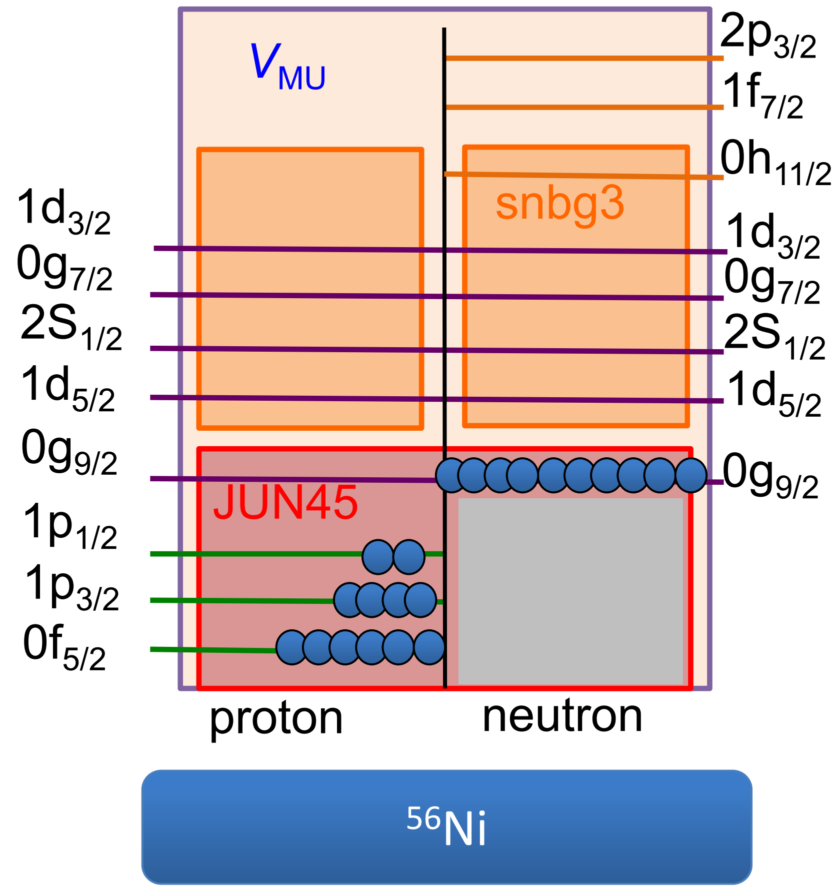
An example : shapes of Zr isotopes by Monte Carlo Shell Model

- Effective interaction:
  JUN45 + snbg3 + V_{MU}

  known effective interactions

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

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



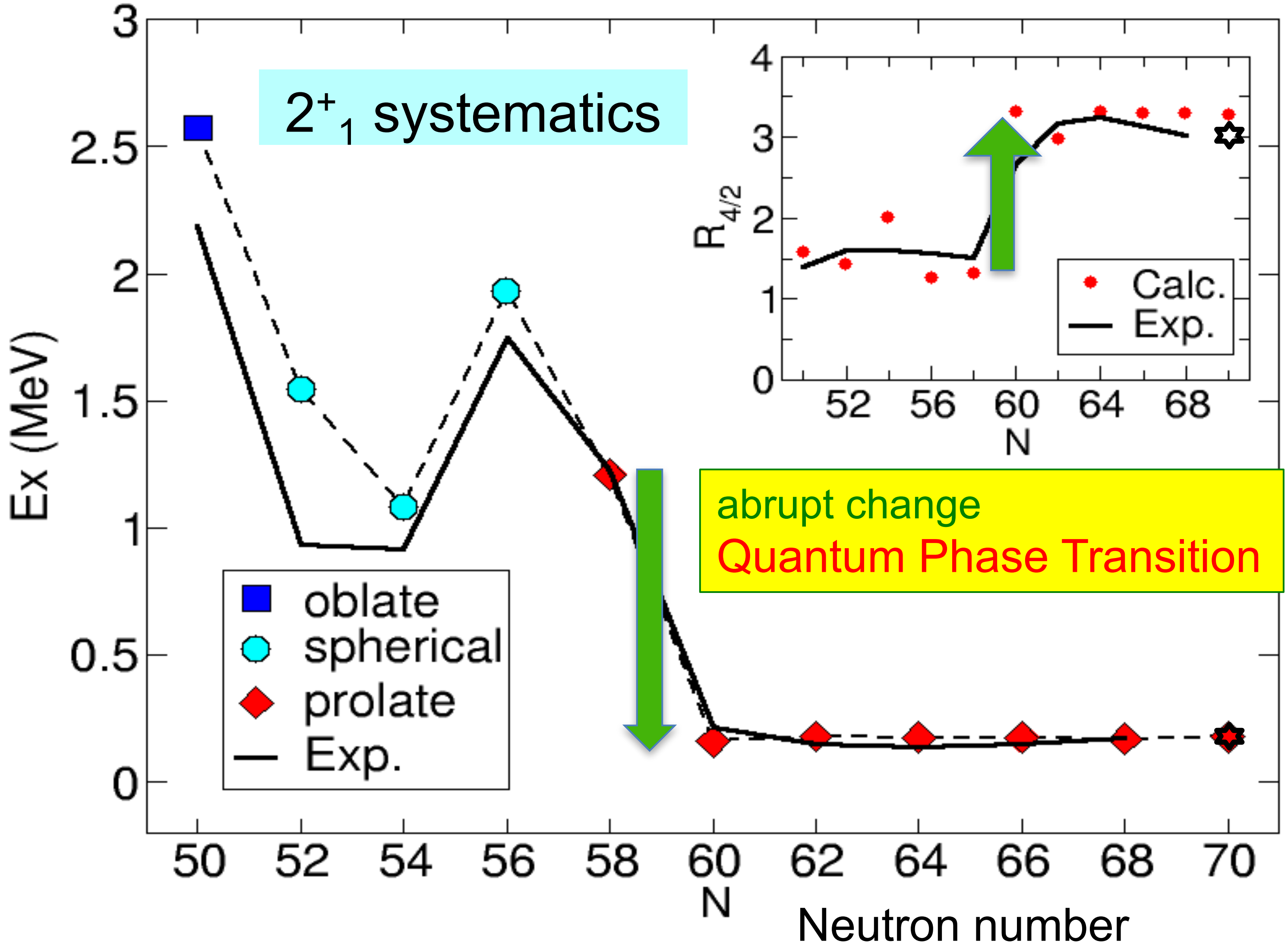
We performed Monte Carlo Shell Model (MCSM) calculations, where the largest case corresponds to the diagonalization of 3.7×10^{23} dimension matrix.

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

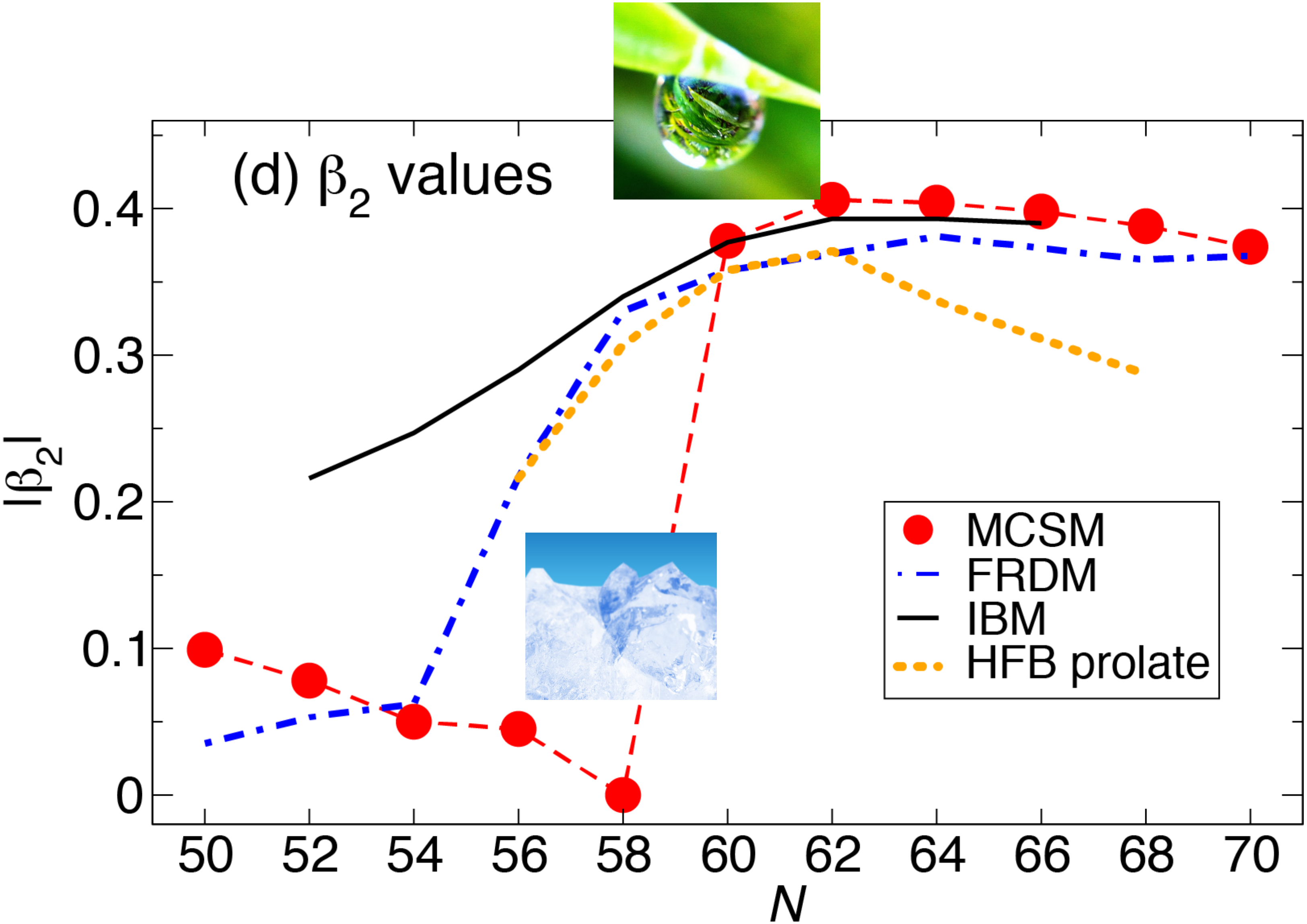
PRL 117, 172502 (2016) PHYSICAL REVIEW LETTERS week ending 21 OCTOBER 2016

Quantum Phase Transition in the Shape of Zr isotopes

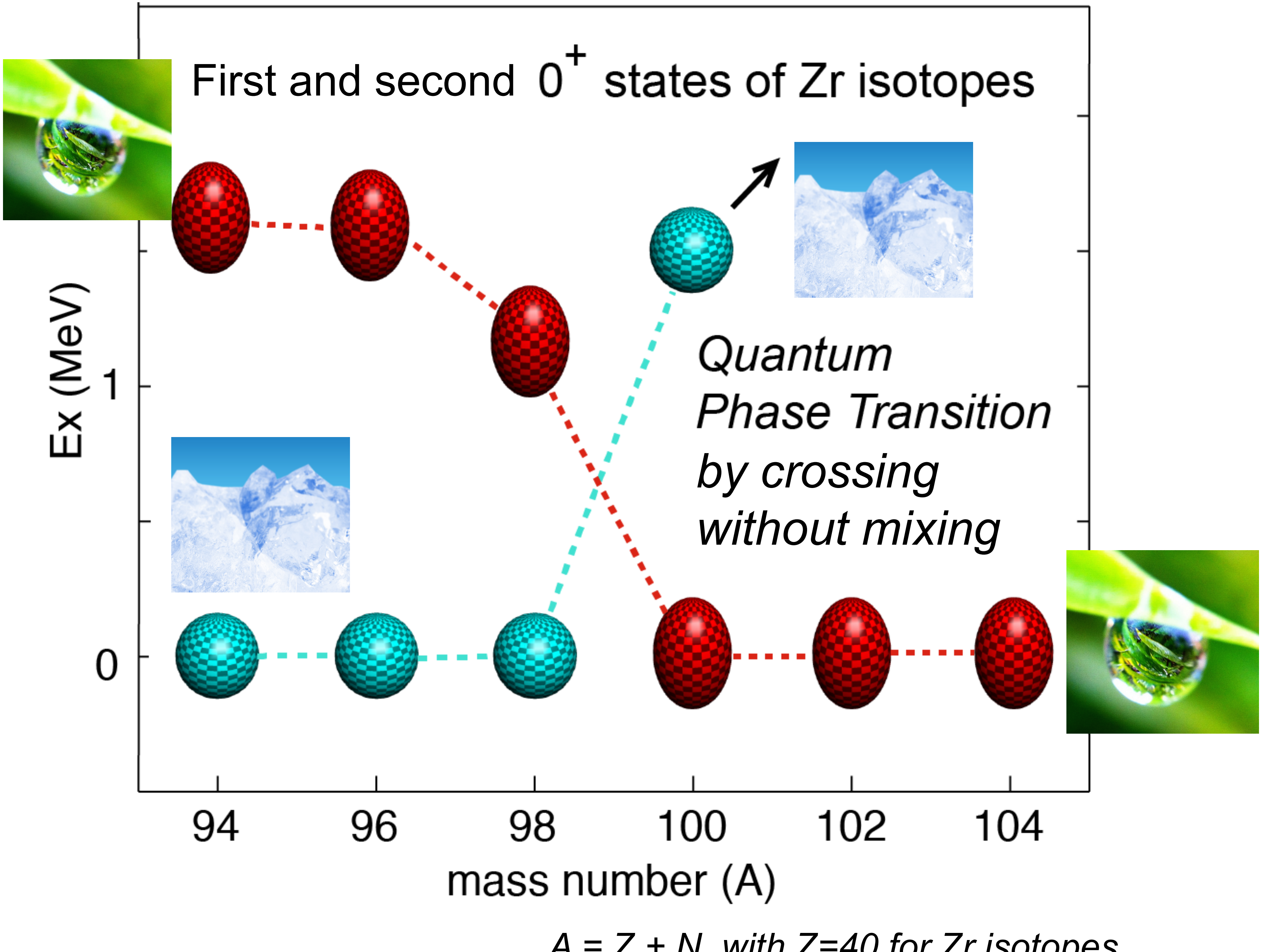
Tomoaki Togashi,[1] Yusuke Tsunoda,[1] Takaharu Otsuka,[1,2,3,4] and Noritaka Shimizu[1]

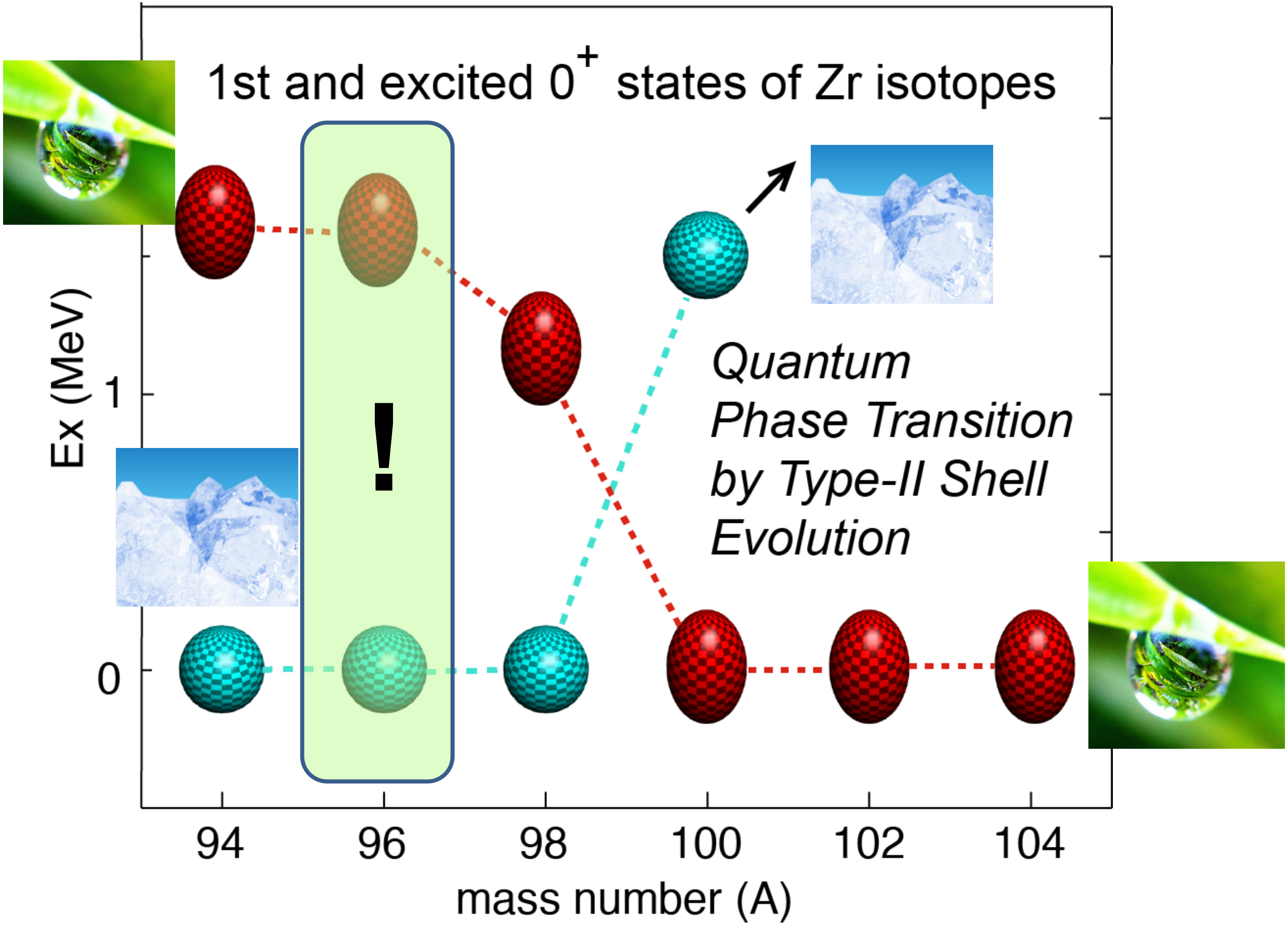


Deformation parameter β_2 varies as the neutron number N



Neutron number


First and second 0^+ states of Zr isotopes
Ex (MeV)
1
0
Quantum
Phase Transition
by crossing
without mixing
94
96
98
100
102
104
mass number (A)
A = Z + N with Z=40 for Zr isotopes

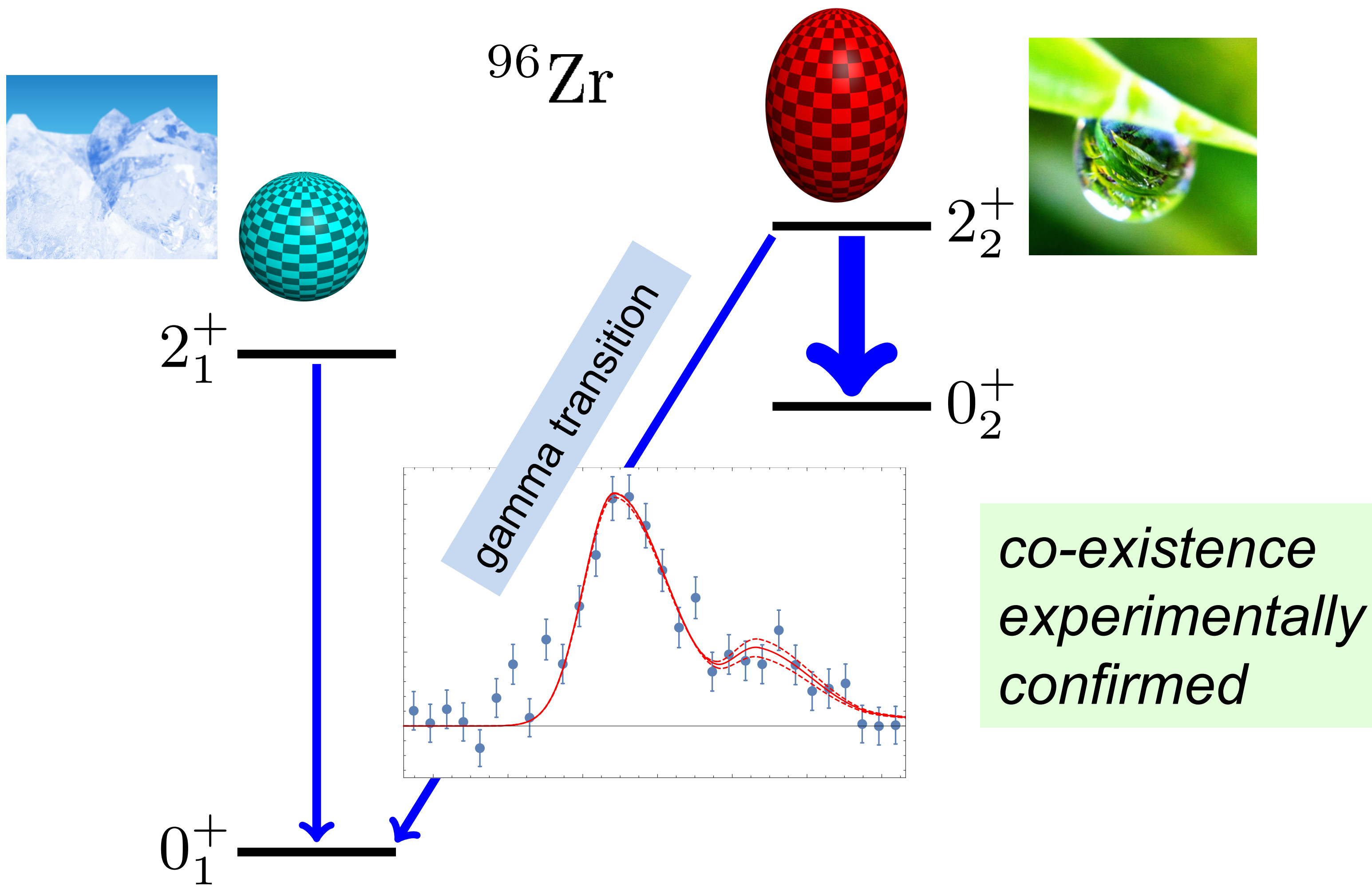


A = Z + N with Z=40 for Zr isotopes

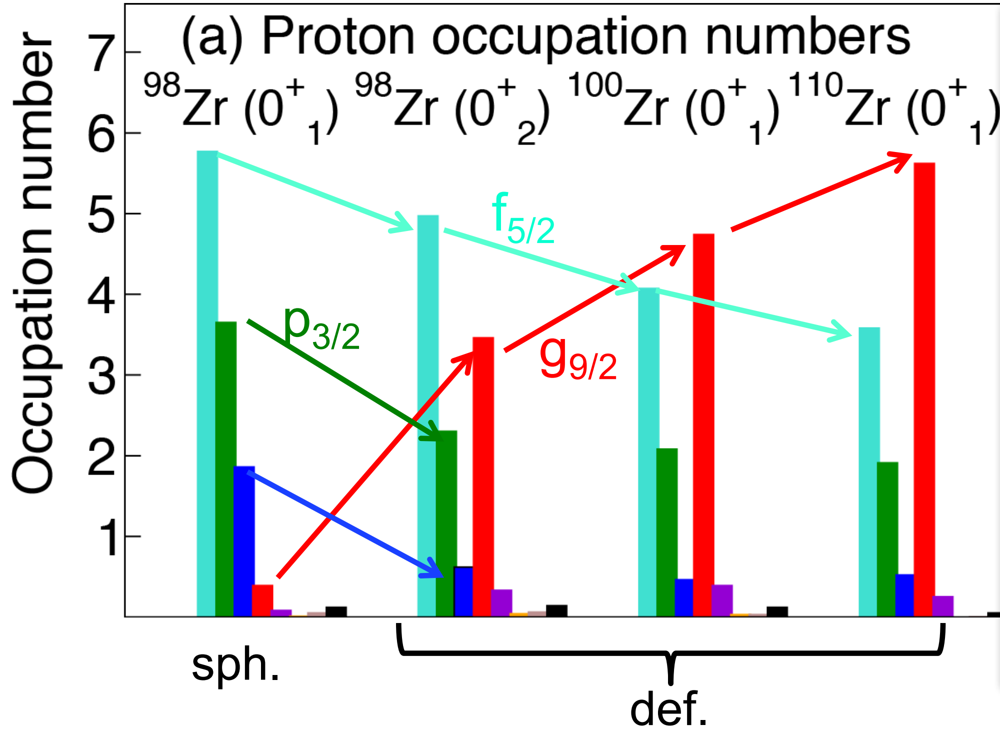
PRL 117, 172503 (2016) PHYSICAL REVIEW LETTERS week ending 21 OCTOBER 2016

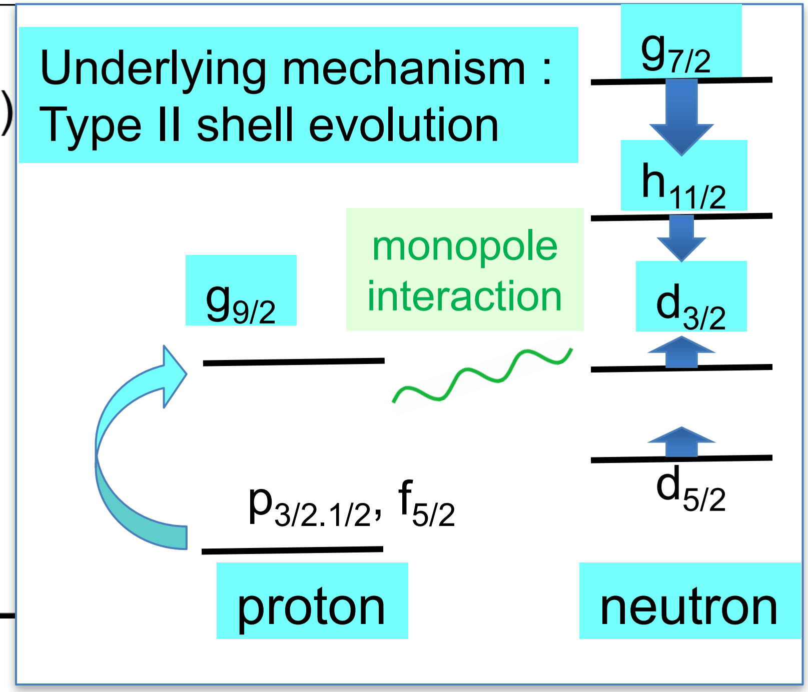
First Measurement of Collectivity of Coexisting Shapes Based on Type II Shell Evolution: The Case of ^{96}Zr

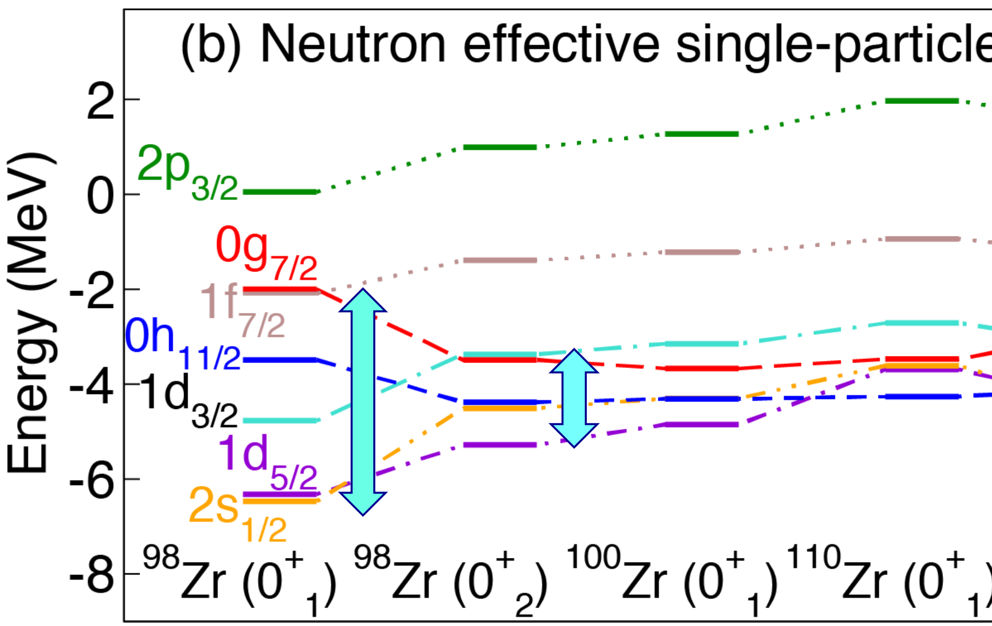
C. Kremer,[1] S. Aslanidou,[1] S. Bassauer,[1] M. Hilcker,[1] A. Krugmann,[1] P. von Neumann-Cosel,[1] T. Otsuka,[2,3,4,5] N. Pietralla,[1] V. Yu. Ponomarev,[1] N. Shimizu,[3] M. Singer,[1] G. Steinhilber,[1] T. Togashi,[3] Y. Tsunoda,[3] V. Werner,[1] and M. Zweidinger[1]



Basic mechanism







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 ➔ crossing w/o mixing

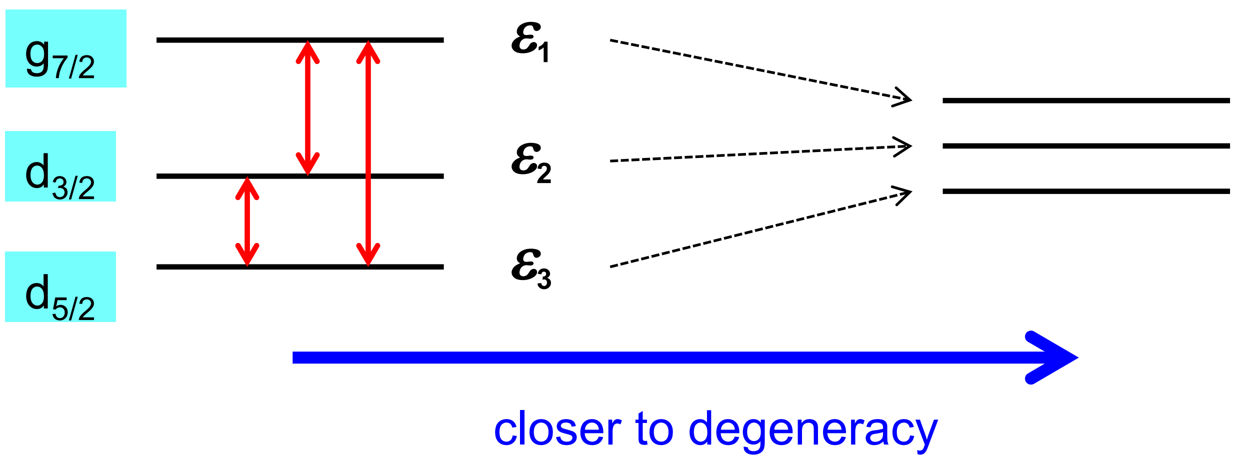
Reminder I : Jahn –Teller effect for nuclear deformation

(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 ε_1, ε_2, ε_3, etc.



larger deformation for the same deformed field

Reminder II ： Monopole interaction

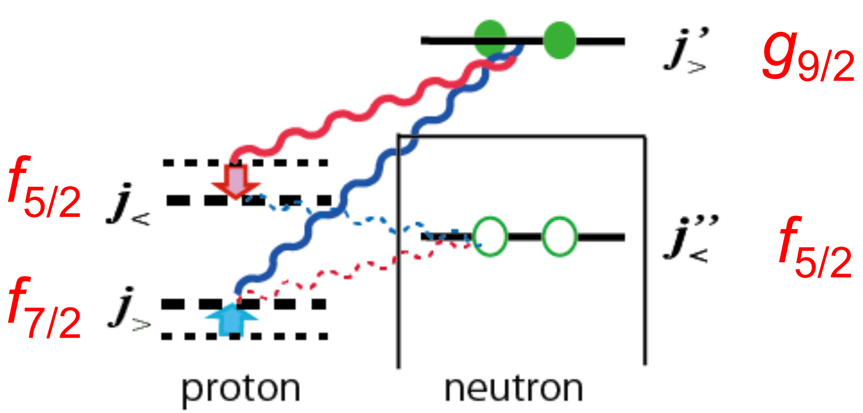
Any effective nucleon-nucleon interaction can be decomposed in terms of the spin-tensor decomposition, independently as to how it was derived. The monopole interaction is one of such components.

Schematically, K=0 piece of $V = \Sigma_K \; f_K \; (U^{(K)} U^{(K)})$

$U^{(K)}$: rank K one-body op. ; K=2 -> quadrupole interaction

$v(j, j') \, n^p_j \, n^n_{j'}$ between a proton in the orbit *j* and a neutron in the orbit *j'*

Ex. Monopole effect from tensor force

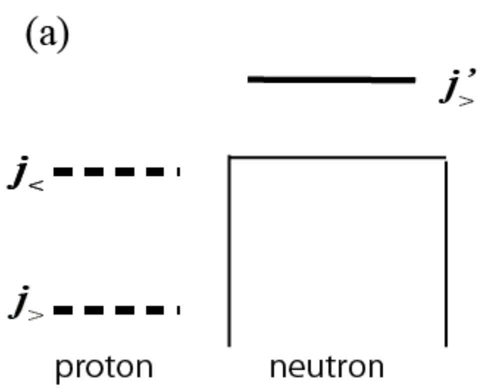


1. Proportional to occupation number (linear effect)
2. Single-particle energies are changed effectively
3. Also for holes with the opposite sign
4. We need to know the forces

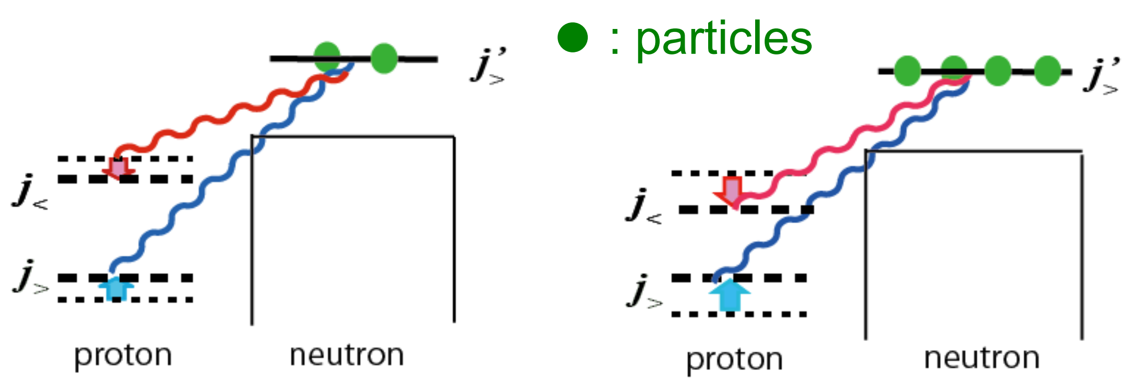
Shell Evolution - Type I and Type II -

Monopole effects on the shell structure - tensor force as an example -

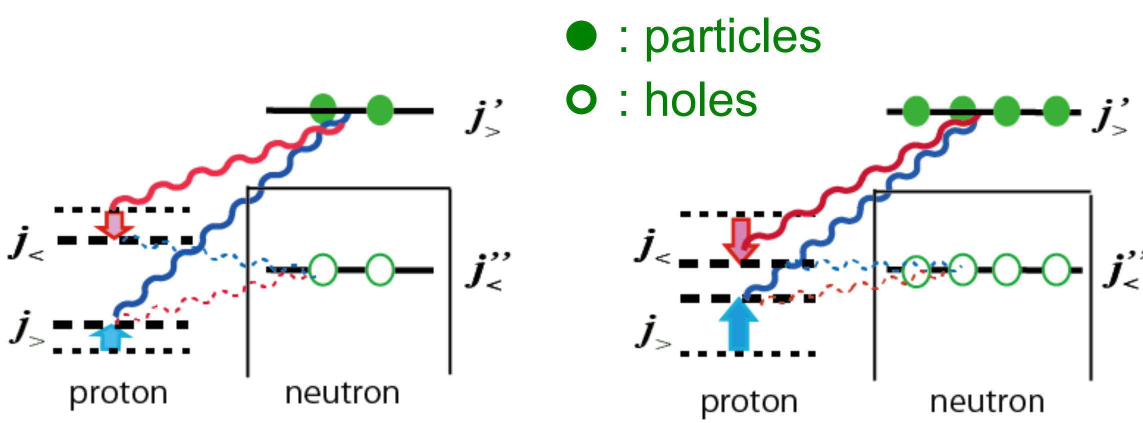
single-particle levels on top of closed shells



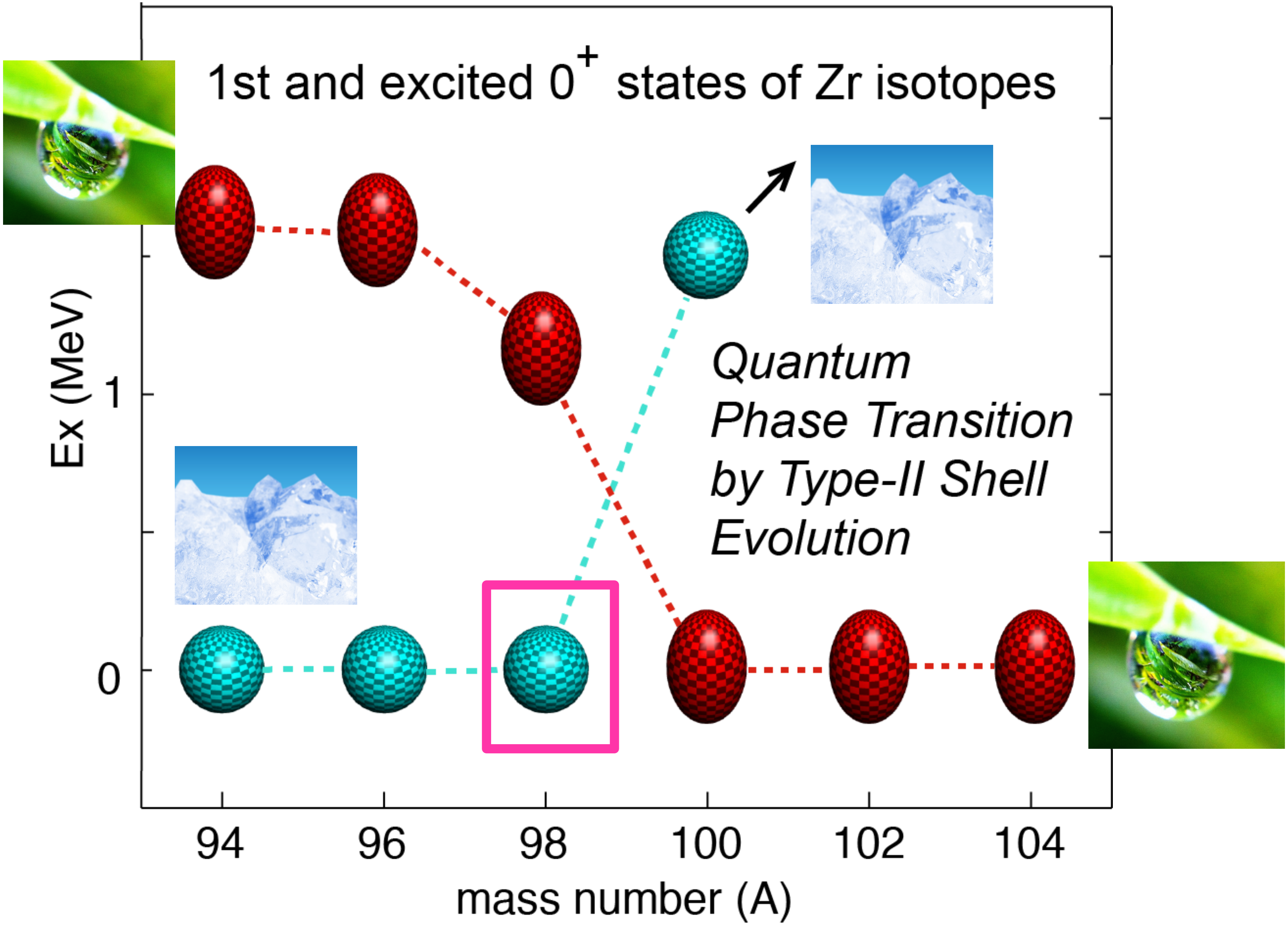
Type I Shell Evolution : different isotopes



Type II Shell Evolution : within the same nucleus



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

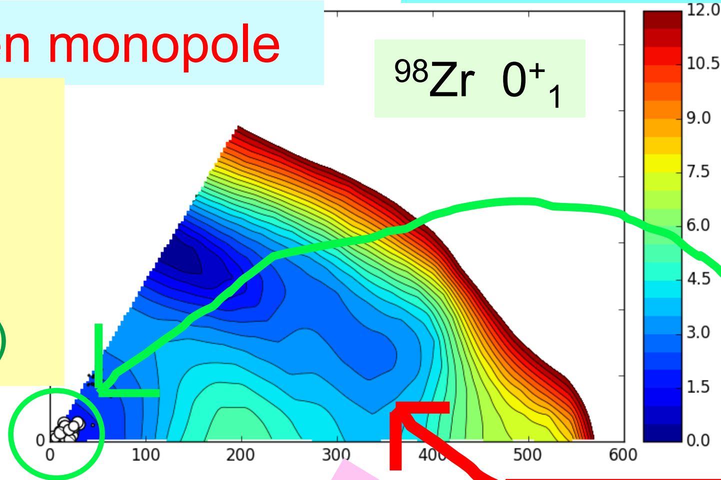

1st and excited 0^+ states of Zr isotopes
Ex (MeV)
1
0
Quantum Phase Transition by Type-II Shell Evolution
94
96
98
100
102
104
mass number (A)

Anatomy of this effect : example by ^{98}Zr spherical 0^+_1 and deformed 0^+_2

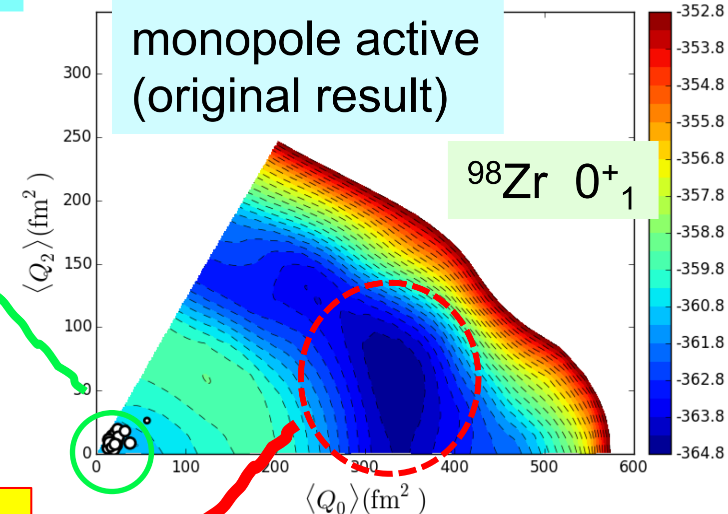
PES with T-plot

Frozen monopole

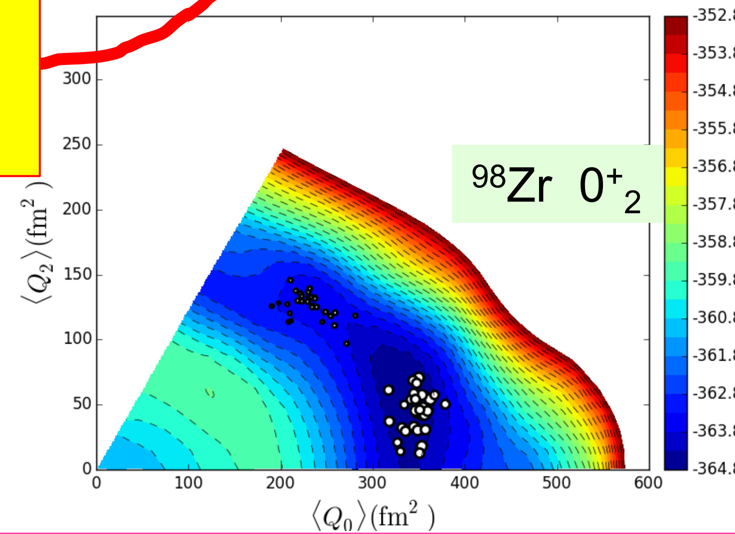
spherical ground state do not change (overlap~0.98)



monopole active (original result)

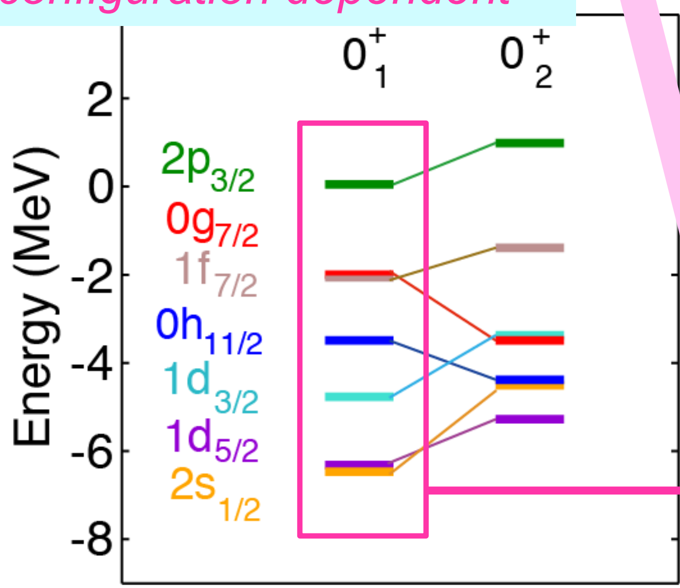


prolate minimum is *gone*



Effective SPE

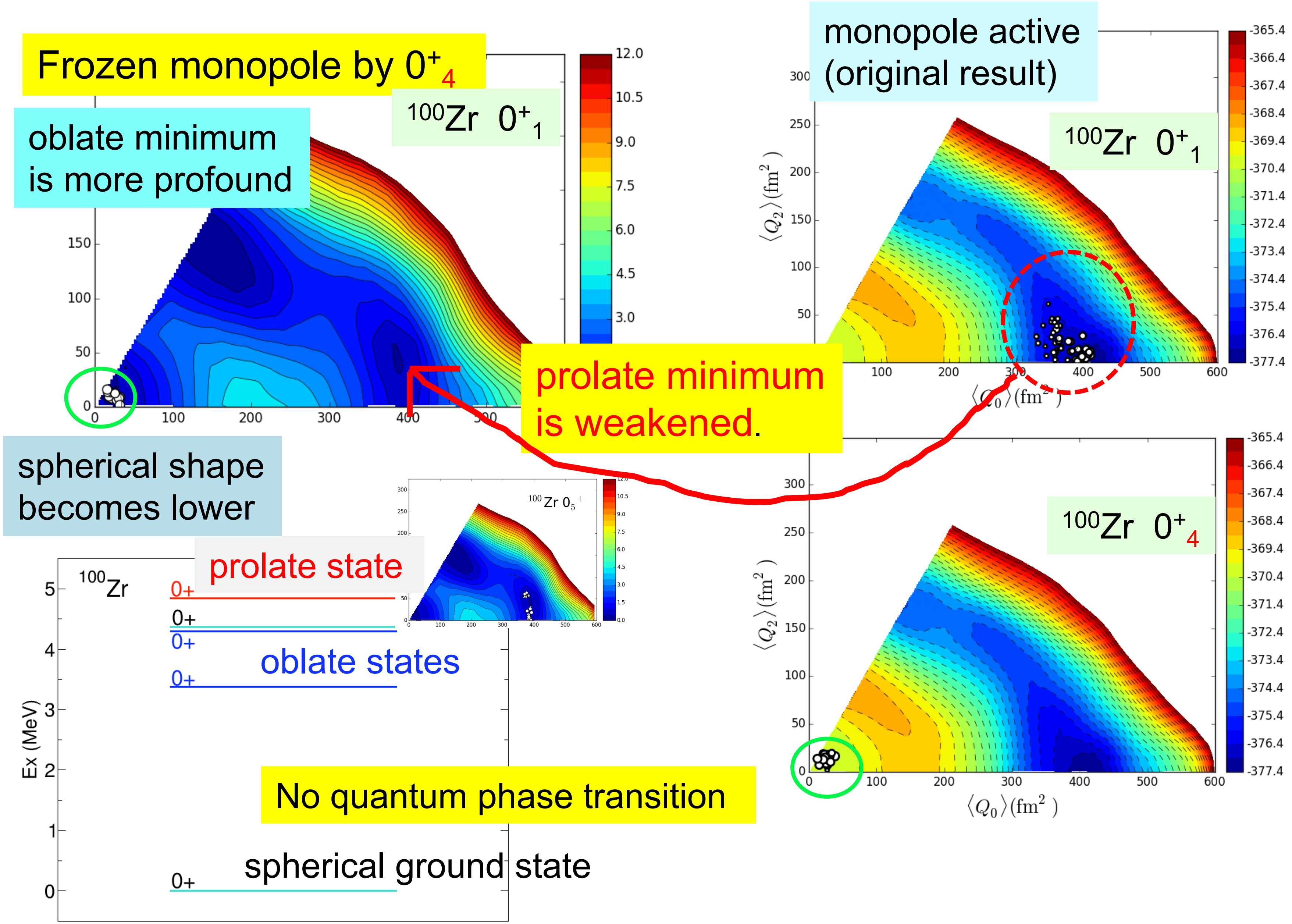
- *configuration dependent* -

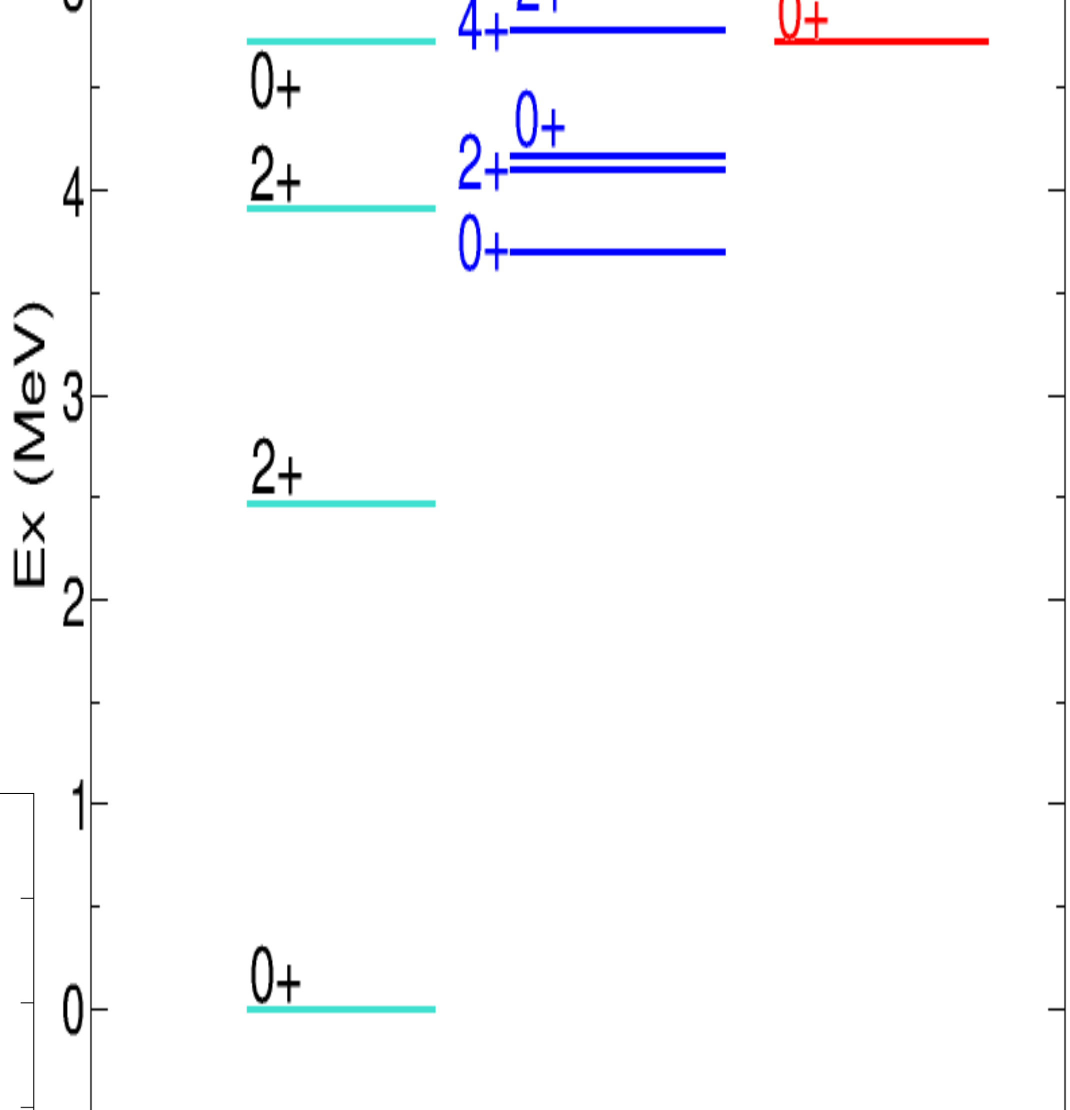


Use them as constant SPEs *independent of configurations, putting monopole int. aside*

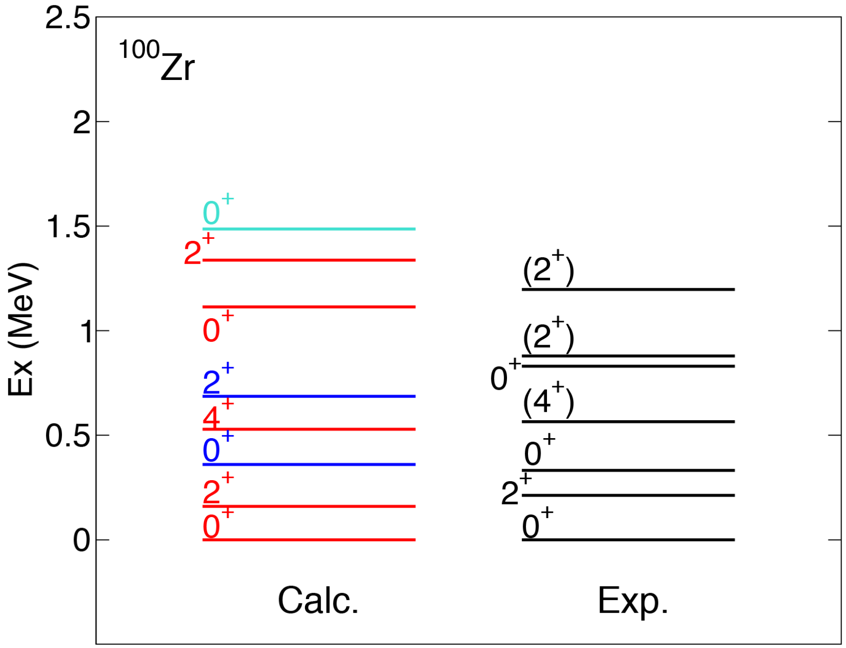
➔ Frozen monopole treatment

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



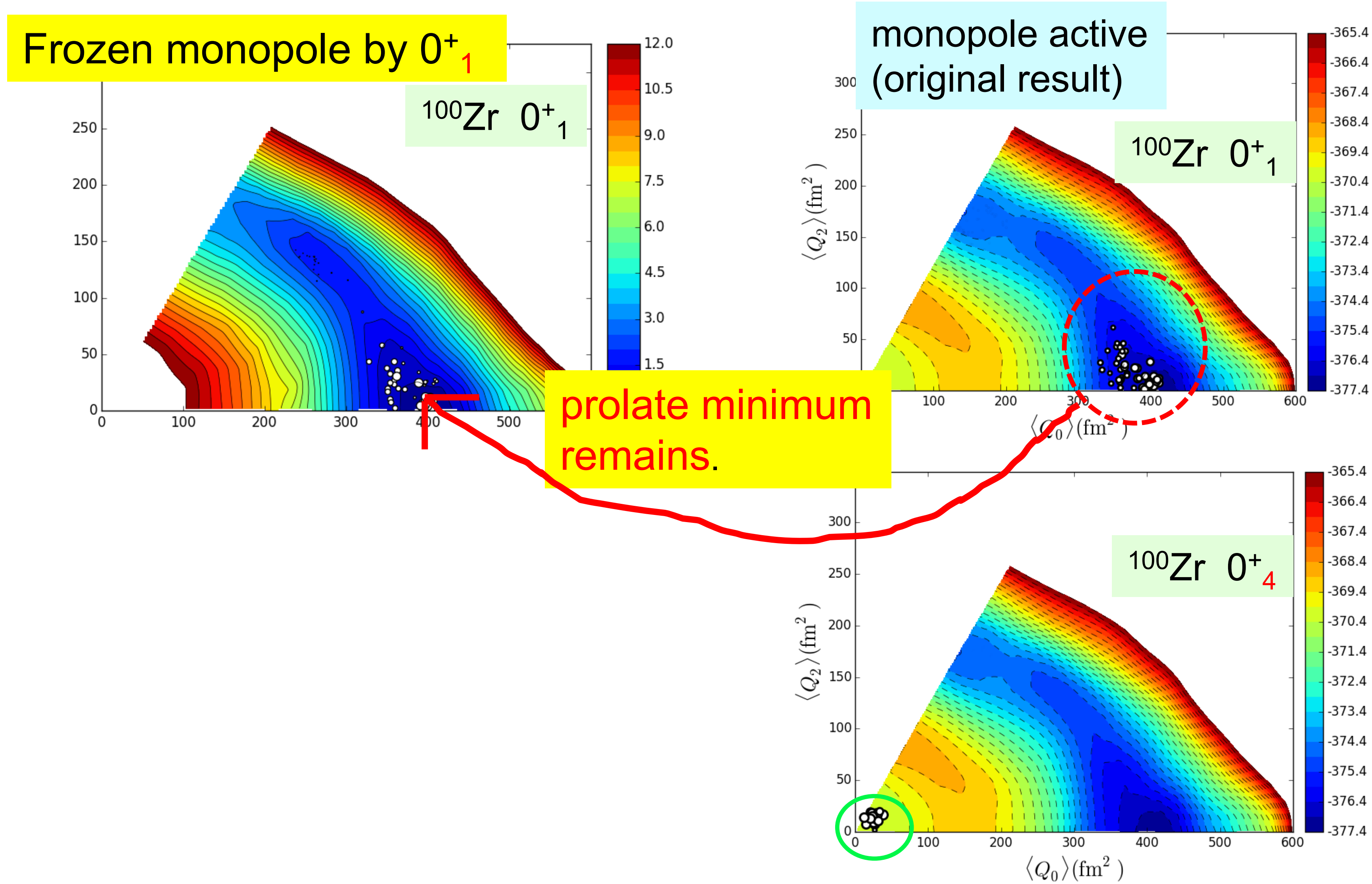


Ex (MeV)
0
1
2
3
4
0+
2+
2+
0+
4+
0+
2+
0+
0+



^{100}Zr
Ex (MeV)
2.5
2
1.5
1
0.5
0
0^+
2^+
0^+
2^+
4^+
0^+
2^+
0^+
(2^+)
(2^+)
0^+
(4^+)
0^+
2^+
0^+
Calc.
Exp.

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



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.

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

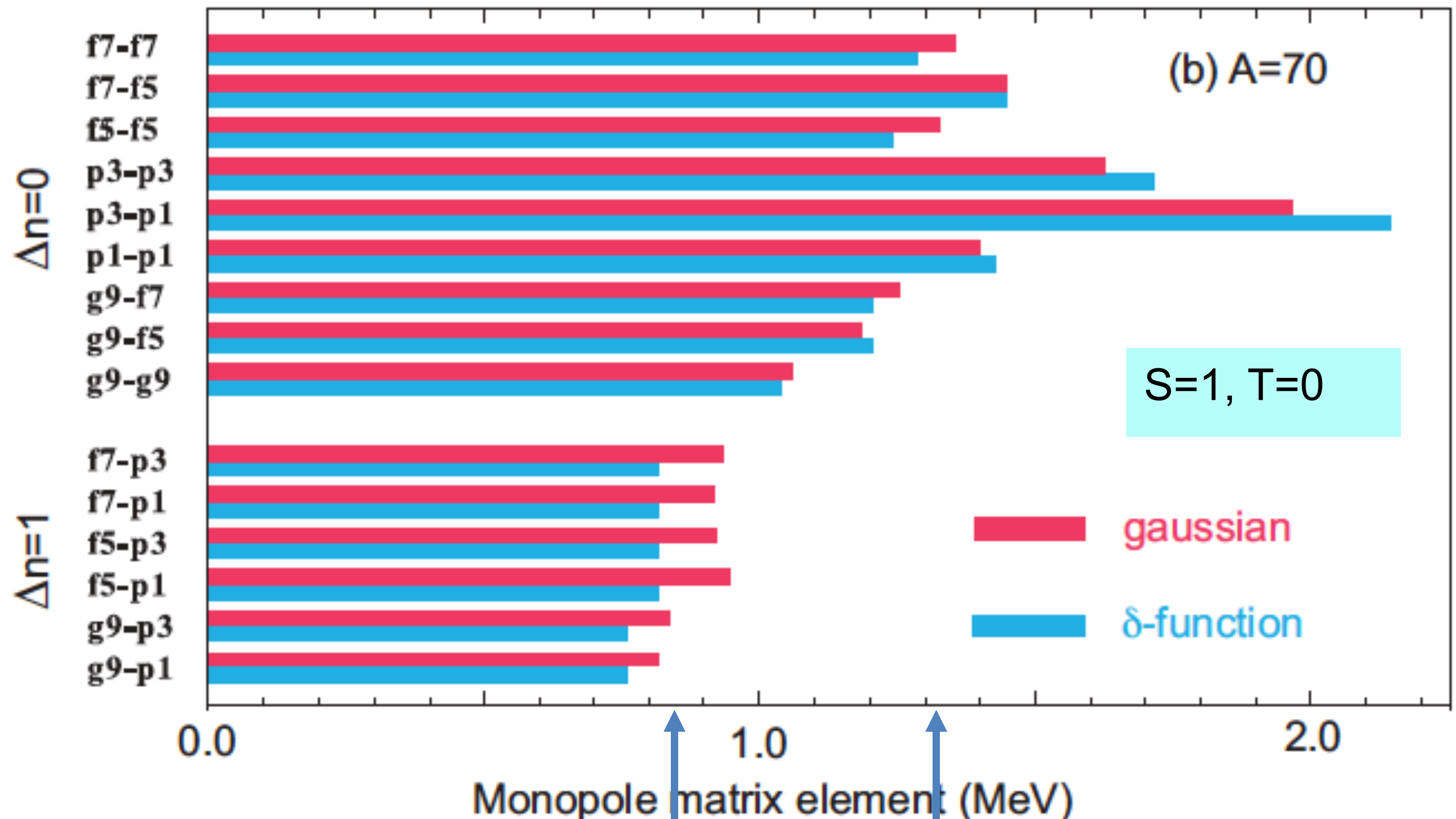


Figure 26 Monopole matrix elements of central gaussian and delta interactions for $(S = 1, T = 0)$ channel. The orbit labeling is abbreviated like g9 for $1g_{9/2}$, *etc.* The orbits are from valence shell for (a) $A = 100$ and (b) $A = 70$.

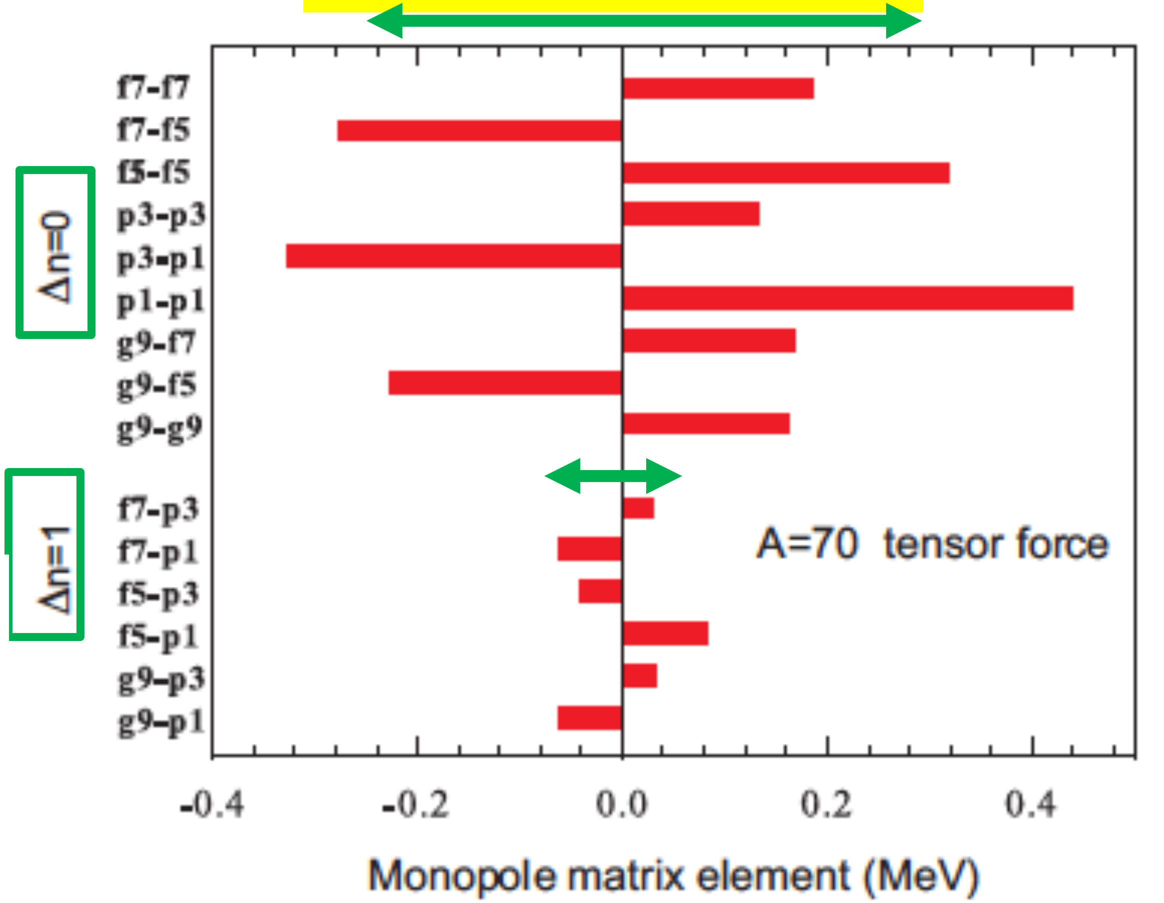
mean values ~0.8 MeV ~1.3 MeV

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



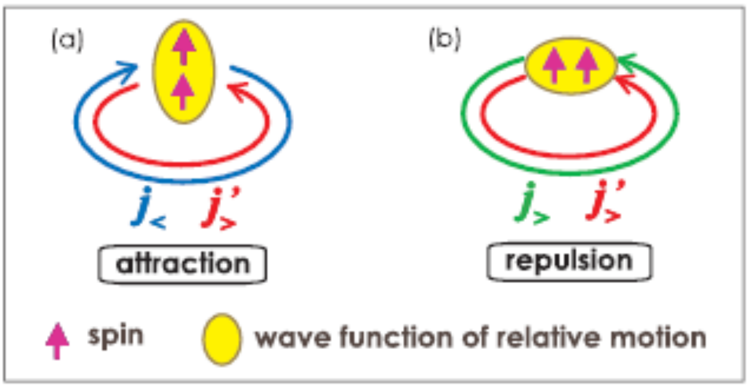
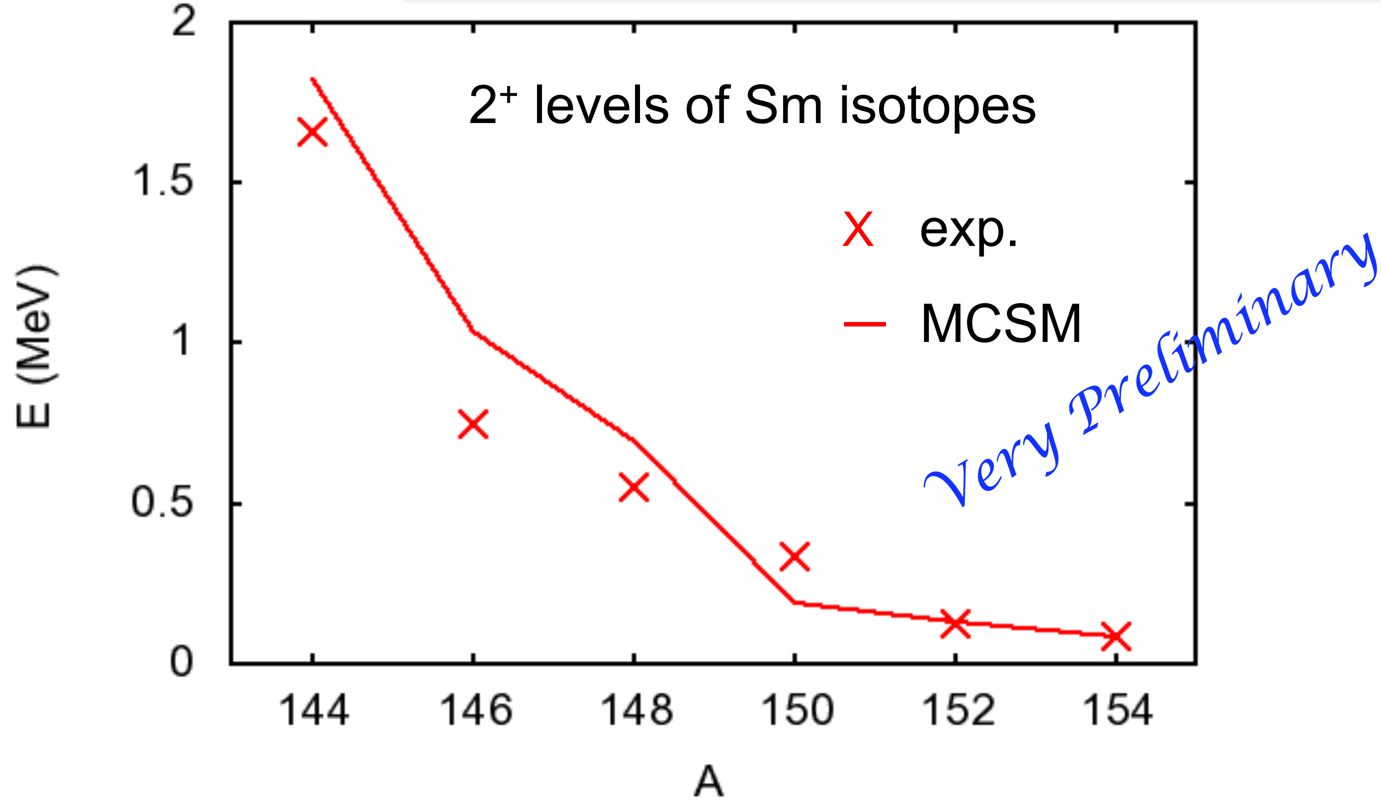


Figure 34 Monopole matrix elements of the tensor force in the T=0 channel. The orbit labeling is abbreviated like f7 for $1f_{7/2}$, *etc.* The orbits are from valence shell for $A = 70$.

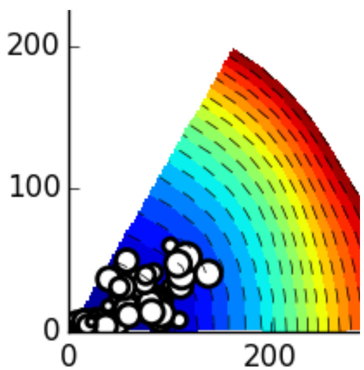
Sm isotopes

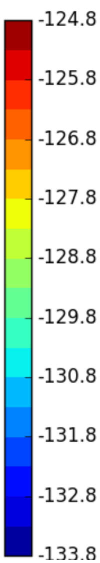
proton 8 orbits
neutron 10 orbits

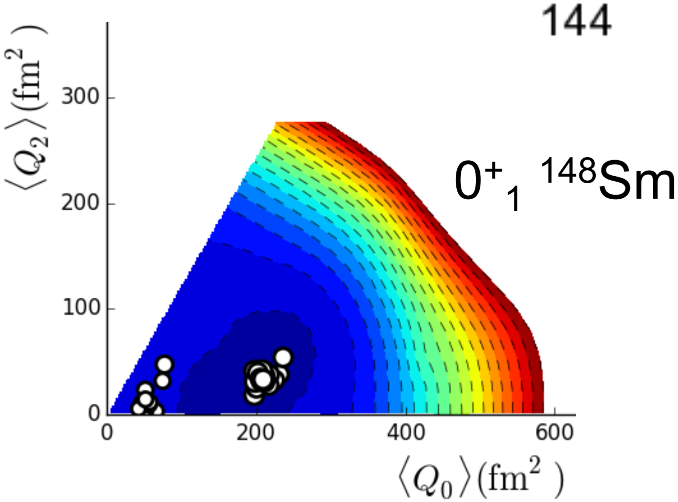
Interaction VMU (gaussian central + π+ρ tensor)



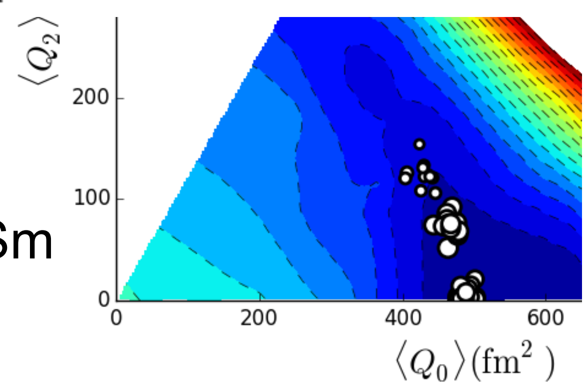
0^+_1 ^{144}Sm

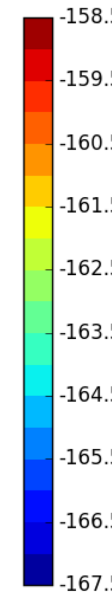






0^+_1 ^{154}Sm

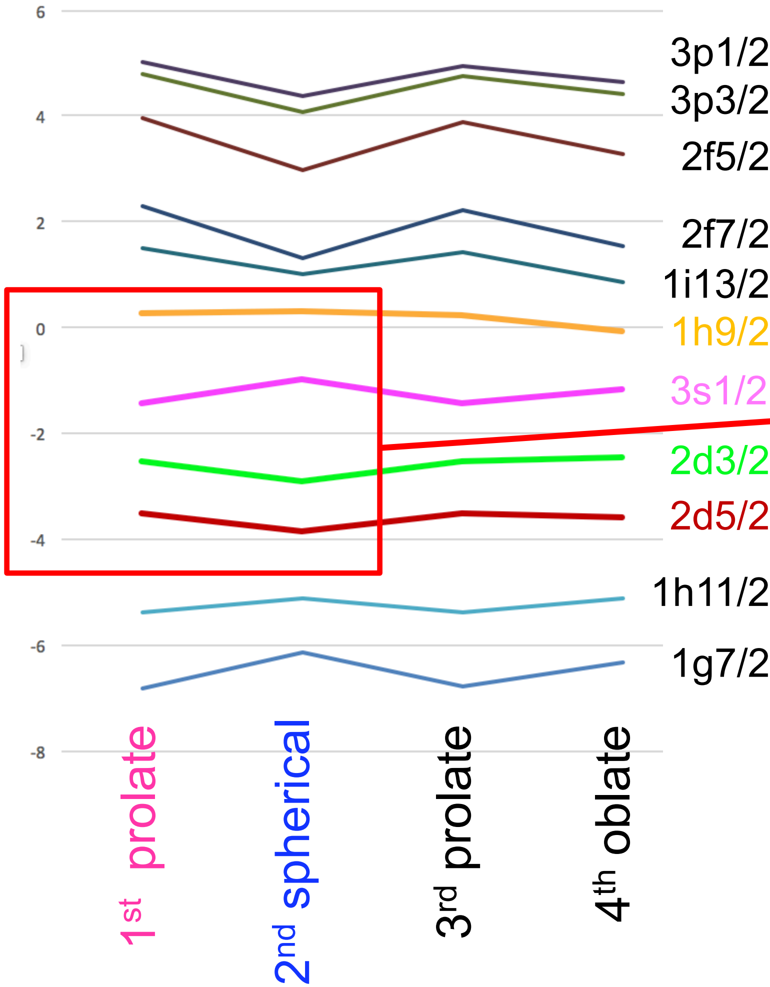


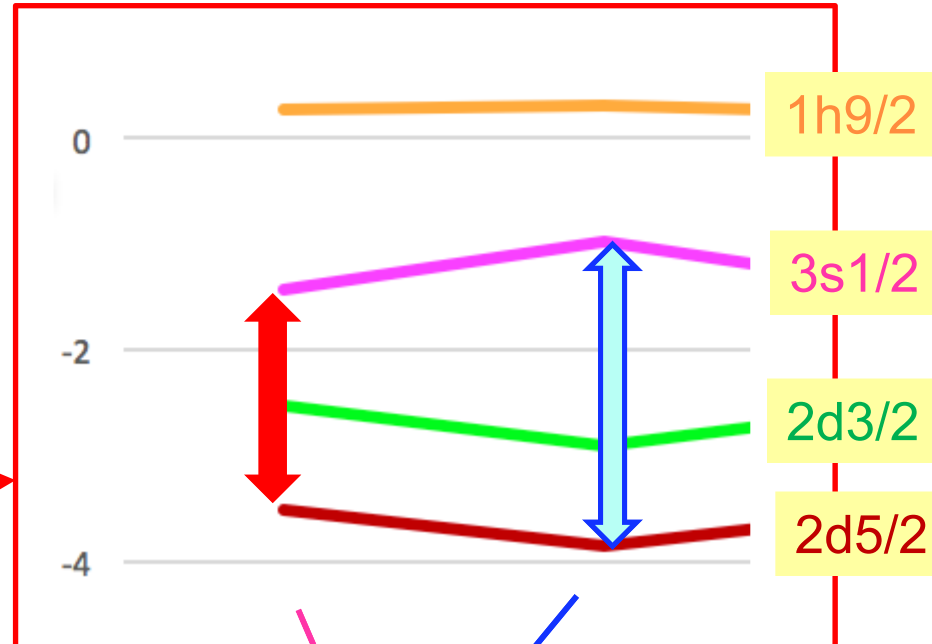


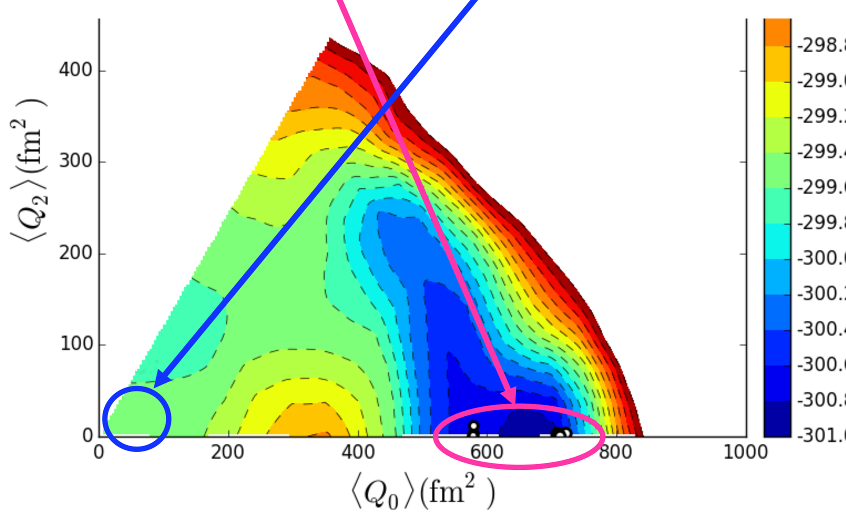
Shape coexistence in Hg/Pb region

Very Preliminary

^{181}Hg proton ESPE (MeV)







1/2$^-$ levels

11 proton orbits, 13 neutron orbits

nn, pp Brown (PRL85, 5300), pn VMU

Summary

- The Monte Carlo Shell Model calculations can handle cases corresponding to the diagonalization of 10^{23}-dimension Hamiltonian matrix or more.
- The Monte Carlo Shell Model can bridge from the shell-model (CI) calculation to mean-field (DFT) calculation because of deformed basis vectors.
- The atomic nuclei are not necessarily like simple rigid vases containing almost free nucleons. $\Longleftrightarrow$ *Naïve Fermi liquid picture (a la Landau)*
- Nuclear forces are rich enough to change single-particle energies for each eigenstate, leading to quantum self-organization. This effect becomes visible for
  (i) two quantum liquids (protons and neutrons),
  (ii) two major forces : *e.g.*, quadrupole interaction : to drive collective mode
  monopole interaction : to control resistance
- Relevance to shape coexistence and quantum phase transition, with actual cases in Ni, Sm, Hg/Pb, ……, island of stability, ...
- Prolate deformation is favored by this, whereas oblate shape is not much. Any relevance to the dominance of prolate shapes in nuclei ?
- What about mesoscopic systems ?

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

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.

Thank you