# Nuclear deformations: origin and properties

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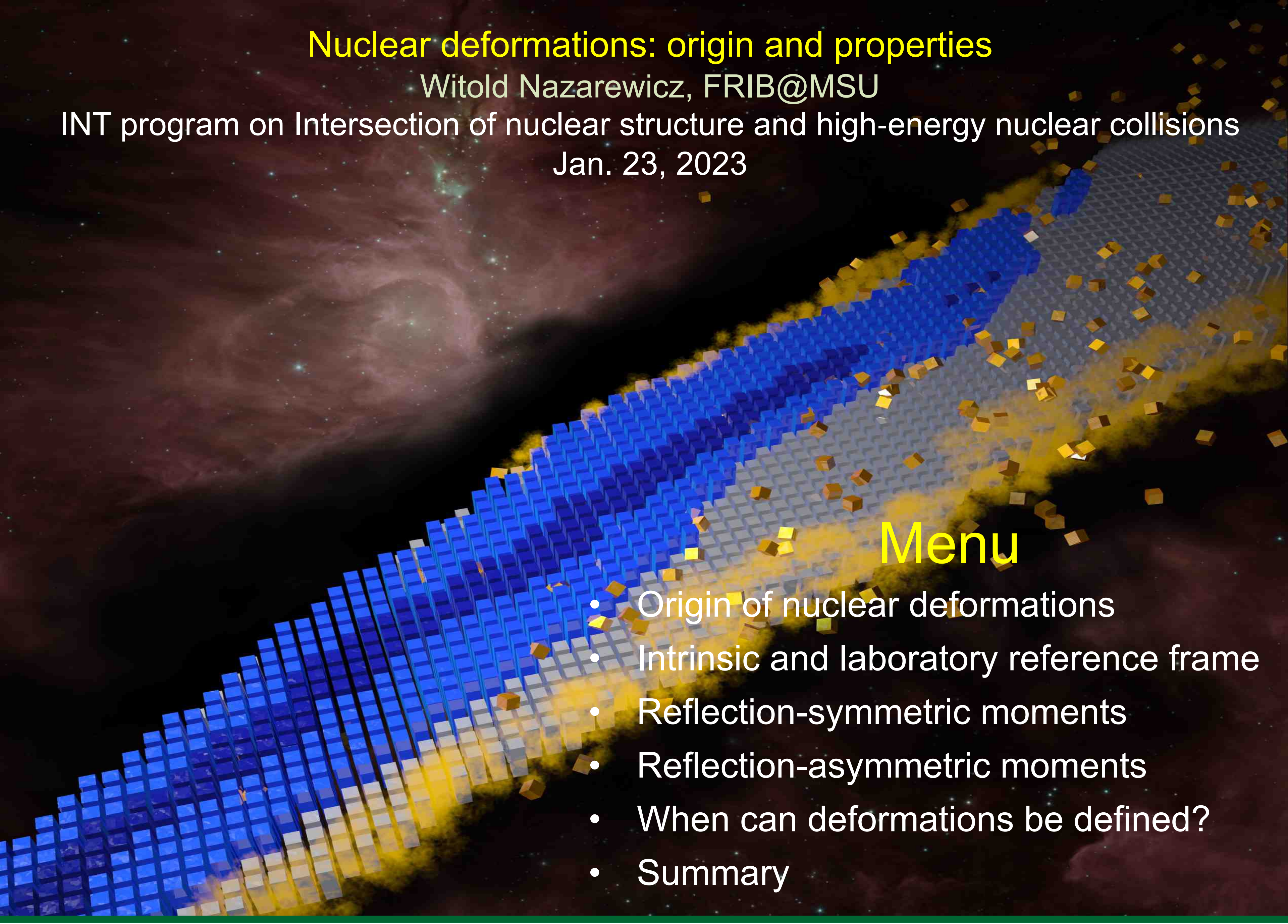
INT program on Intersection of nuclear structure and high-energy nuclear collisions

Jan. 23, 2023



## Menu

- Origin of nuclear deformations
- Intrinsic and laboratory reference frame
- Reflection-symmetric moments
- Reflection-asymmetric moments
- When can deformations be defined?
- Summary

# Nuclear shapes

The first evidence for a non-spherical nuclear shape came from the observation of a quadrupole component in the hyperfine structure of optical spectra. The analysis showed that the electric quadrupole moments of the nuclei concerned were more than an order of magnitude greater than the maximum value that could be attributed to a single proton and suggested a deformation of the nucleus as a whole.

- Schüler, H., and Schmidt, Th., Z. Physik 94, 457 (1935)
- Casimir, H. B. G., On the Interaction Between Atomic Nuclei and Electrons, Prize Essay, Taylor' s Tweede Genootschap, Haarlem (1936)

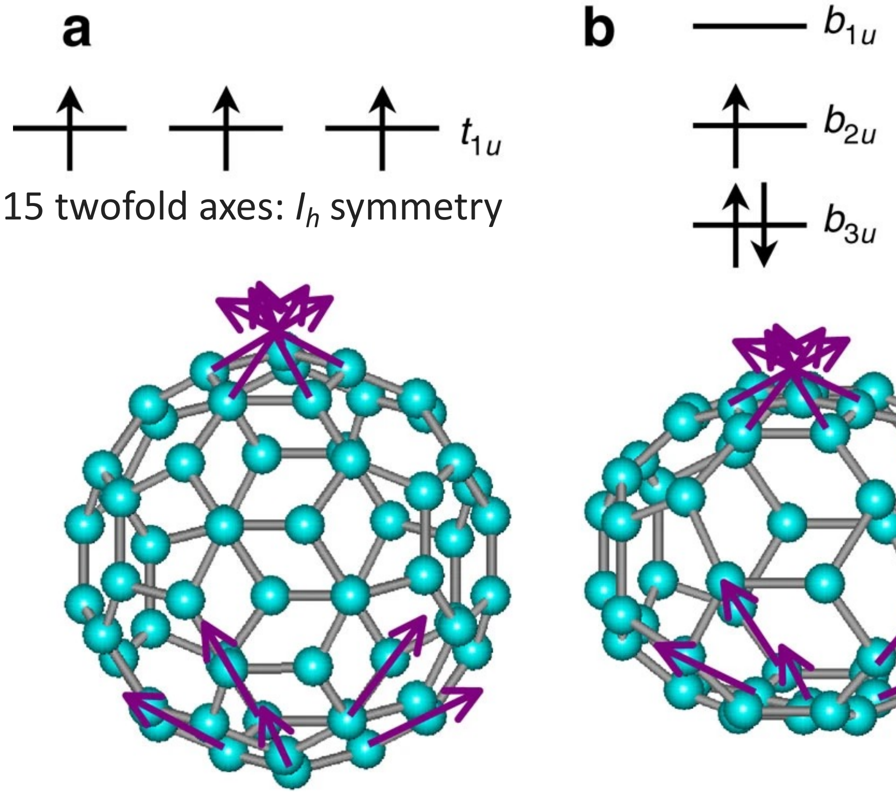
The question of whether nuclei can rotate became an issue already in the very early days of nuclear spectroscopy

- Thibaud, J., Comptes rendus 191, 656 ( 1930)
- Teller, E., and Wheeler, J. A., Phys. Rev. 53, 778 (1938)
- Bohr, N., Nature 137, 344 ( 1936)
- Bohr, N., and Kalckar, F., Mat. Fys. Medd. Dan. Vid. Selsk. 14, no, 10 (1937)

# Jahn-Teller effect

The Jahn–Teller theorem (1937) states that any nonlinear molecule with a spatially degenerate electronic ground state will undergo a geometrical distortion that removes that degeneracy, because the distortion lowers the overall energy of the species.

symmetry:
degeneracies



broken symmetry:
degeneracies lifted

fullerene
ion

Nature Comm. 3, 912 (2012)

# Nuclear deformations and spontaneous symmetry breaking

## Molecular physics: Jahn-Teller effect 1937

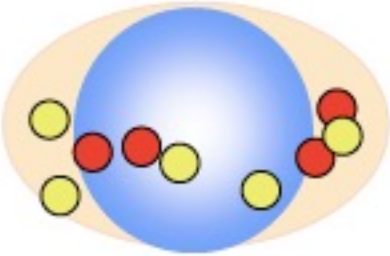
Any configuration of atoms or ions (except for a linear chain) can develop a stable symmetry-breaking deformation provided the coupling between degenerate electronic excitations and collective molecular vibrations is strong.

## Nuclear physics: Bohr-Mottelson 1952-53

Any nuclear configuration can develop a stable symmetry-breaking deformation provided the coupling between degenerate single-nucleonic excitations and collective nuclear modes is strong.

### The unified model. Particle vibration coupling

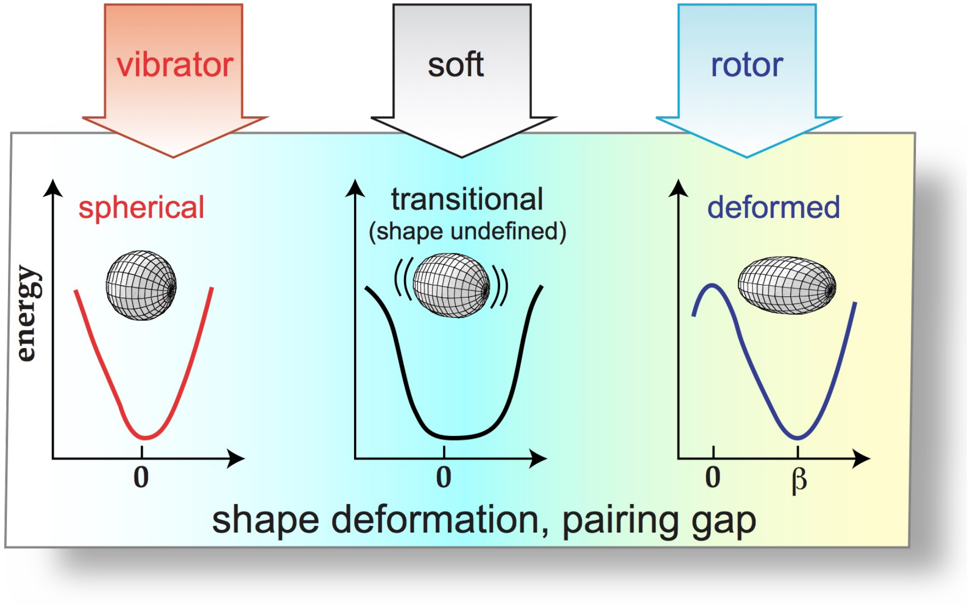
$$V_{\text{int}} = -\kappa(r)\sum_{\lambda\mu}\alpha_{\lambda\mu}Y_{\lambda\mu}(\Omega)$$

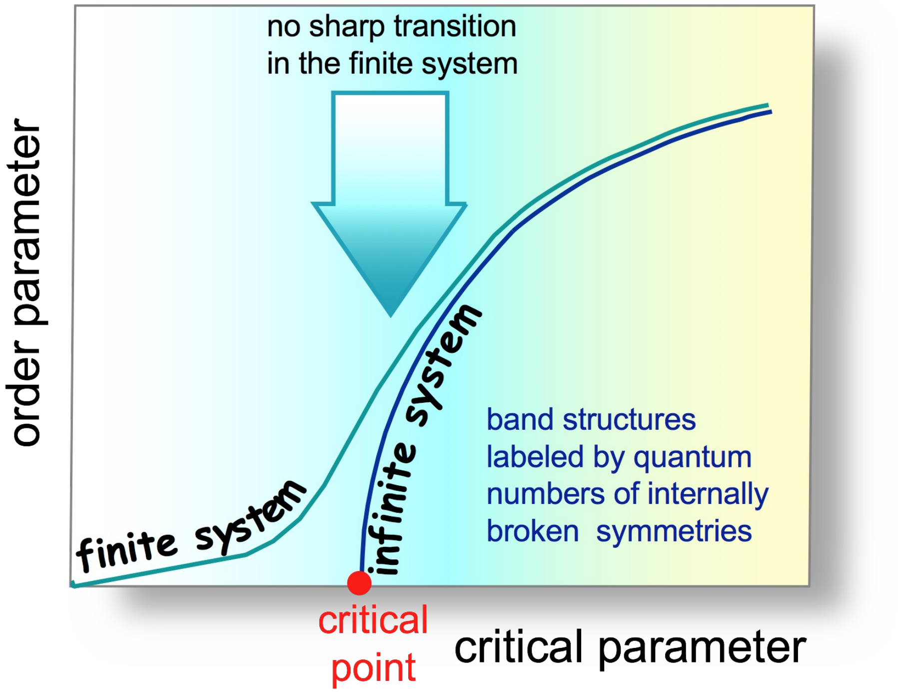


see also Nucl. Phys. A 420, 173 (1984) and Nucl. Phys. A 574, 27 (1994)

Nuclear deformations are governed by shell effects!

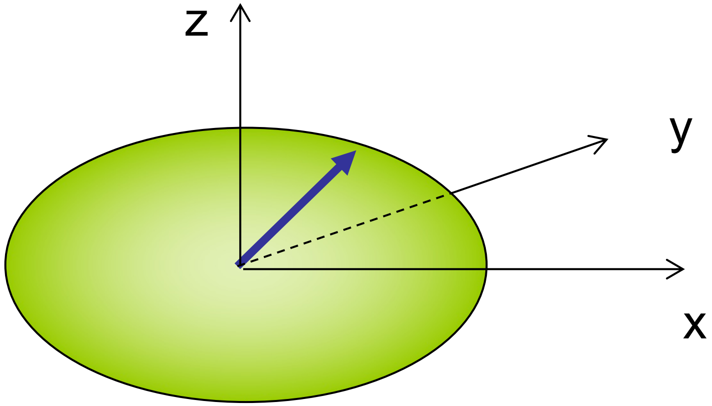
# Symmetry breaking (phase transition)





- Many nuclei are transitional systems.
- Quantum fluctuations are important.
- Characterization of individual phases is the first step towards understanding the phase diagram.

# How to describe nuclear shapes?



isoscalar deformations!

$$R(\theta,\varphi) = c(\alpha) R_0 \left[ 1 + \sum_{\lambda=1} \sum_{\mu=-\lambda}^{\lambda} \alpha^{*}_{\lambda\mu} Y_{\lambda\mu}(\theta,\varphi) \right]$$

volume conservation

radius of the sphere
with the same volume

deformation parameters
For axial shapes μ=0

$$\beta_\lambda \equiv \alpha_{\lambda\mu}$$

Another way: $Q_{\lambda 0} = \sqrt{\frac{16\pi}{2\lambda+1}} \langle r^\lambda Y_{\lambda 0} \rangle = \frac{3}{\sqrt{(2\lambda+1)\,\pi}} Z R_0^\lambda \tilde{\beta}_\lambda$

$$\tilde{\beta}_\lambda \neq \beta_\lambda$$

a) λ=1 (dipole); μ=-1,0,1

$$\int_V \vec{r}\, d^3 r = 0$$

center of mass conservation

3 conditions, they fix $\alpha_{1\mu}$

b) λ=2 (quadrupole); μ=-2,-1,0,1,2

$$\alpha_{2\,1} = \alpha_{2-1} = 0, \quad \alpha_{2\,2} = \alpha_{2-\,2}$$

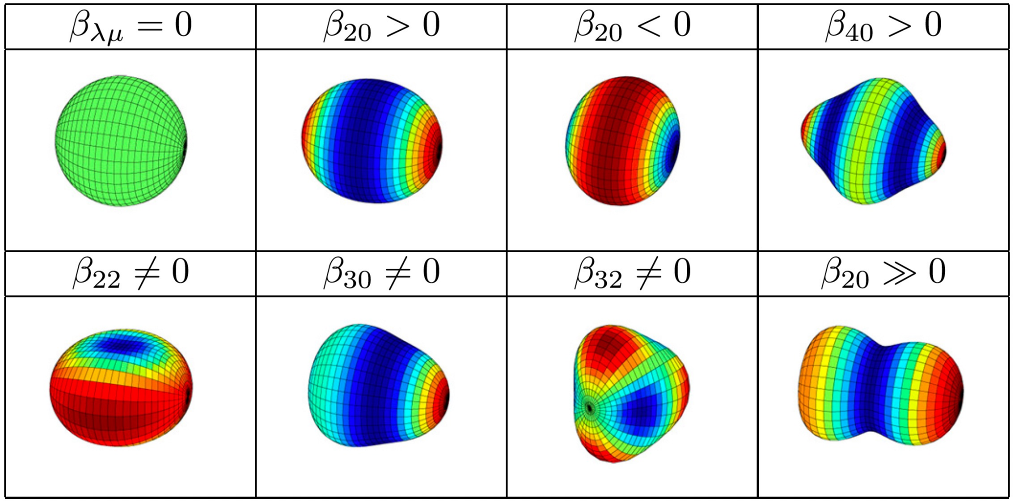
3 conditions, they fix three Euler angles

Only two deformation parameters left (Hill- Wheeler coordinates):

$$\alpha_{20} = \beta \cos\gamma, \quad \alpha_{22} = \frac{1}{\sqrt{2}} \beta \sin\gamma$$

c) λ=3 (octupole)
d) λ=4 (hexadecapole)
e) λ=5 (dotriacontapole)
f) λ=6 (hexacontatetrapole)

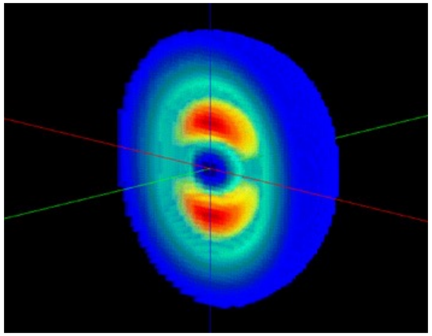
Phys. Scr. 89 (2014) 054028



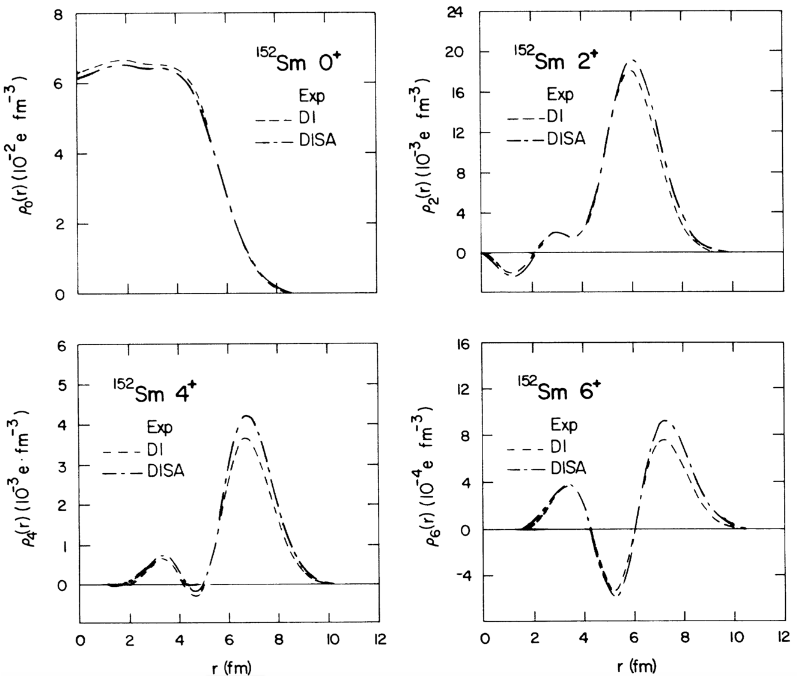
# Experimental techniques to probe nuclear shapes
## see K. Wimmer's presentation

Many powerful methods exist

- Coulomb excitation
- Strongly interacting probes
- Electron scattering
- Lifetime measurements
- Muonic atoms
- Hyperfine techniques (quadrupole moments, charge radii)
- Collective modes (e.g., giant resonances, rotational bands)
- …



The intrinsic shape of the deuteron from Jlab
Adv.Nucl.Phys.26, 293 (2001)



Shape of a charge distribution in $^{152}$Sm
Phys. Rev. C 39, 1645 (1989)

# Nuclear charge densities

Phys. Rev. C 103, 054310 (2021)

$$\rho_c(\boldsymbol{r}) = \frac{1}{(2\pi)^3}\int d^3q e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} F_c(\boldsymbol{q})$$

nuclear charge density

nuclear charge form factor

$$F_c(\boldsymbol{q}) = \sum_{t\in\{p,n\}} \Big[ G_{E,t}(\boldsymbol{q}) \left(1 - \tfrac{1}{2}\boldsymbol{q}^2\mathcal{D}\right) F_t(\boldsymbol{q}) - \mathcal{D}\left[2\mu_t G_{M,t}(\boldsymbol{q}) - G_{E,t}(\boldsymbol{q})\right] F_{\ell s,t}(\boldsymbol{q}) \Big].$$

$$\mathcal{D} = \frac{\hbar^2}{(2mc)^2}$$

$G_E$ and $G_M$ are the intrinsic proton and neutron electromagnetic form factors

$$F_t(\boldsymbol{q}) = \int d^3r\, e^{i\boldsymbol{q}\cdot\boldsymbol{r}} \rho_t(\boldsymbol{r}),$$

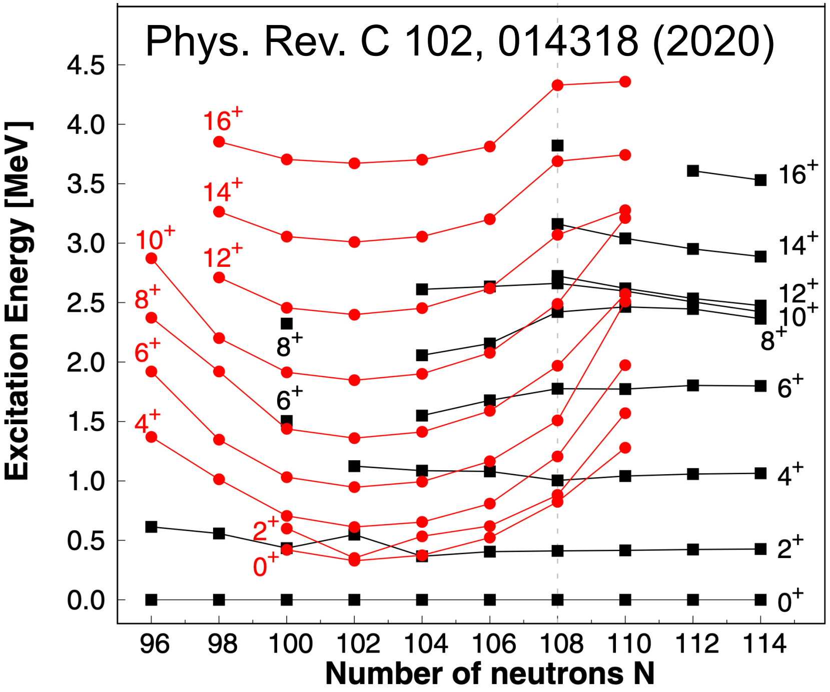
$$F_{\ell s,t}(\boldsymbol{q}) = \int d^3r\, e^{i\boldsymbol{q}\cdot\boldsymbol{r}} \boldsymbol{\nabla}\cdot\boldsymbol{J}_t(\boldsymbol{r})$$

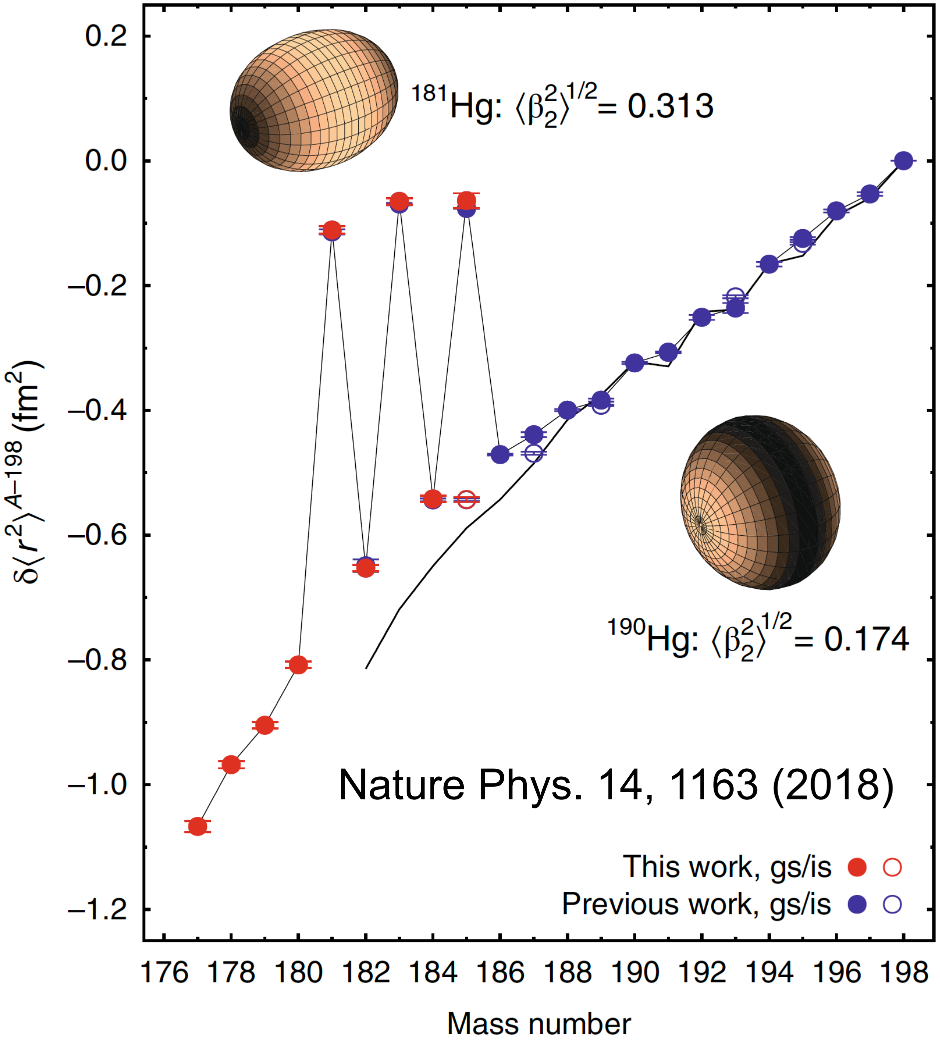
spin-orbit current

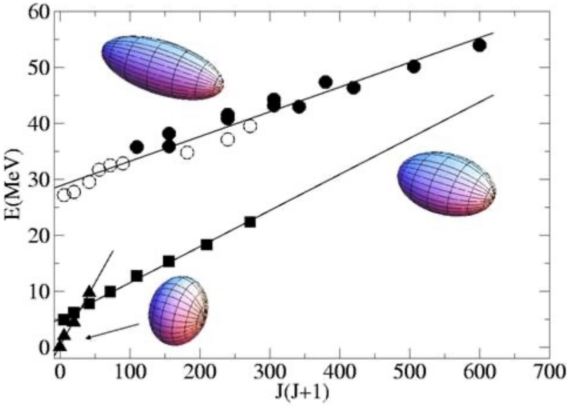
General expression. Valid for spherical and deformed nuclei

# Shape-staggering effect in mercury nuclei

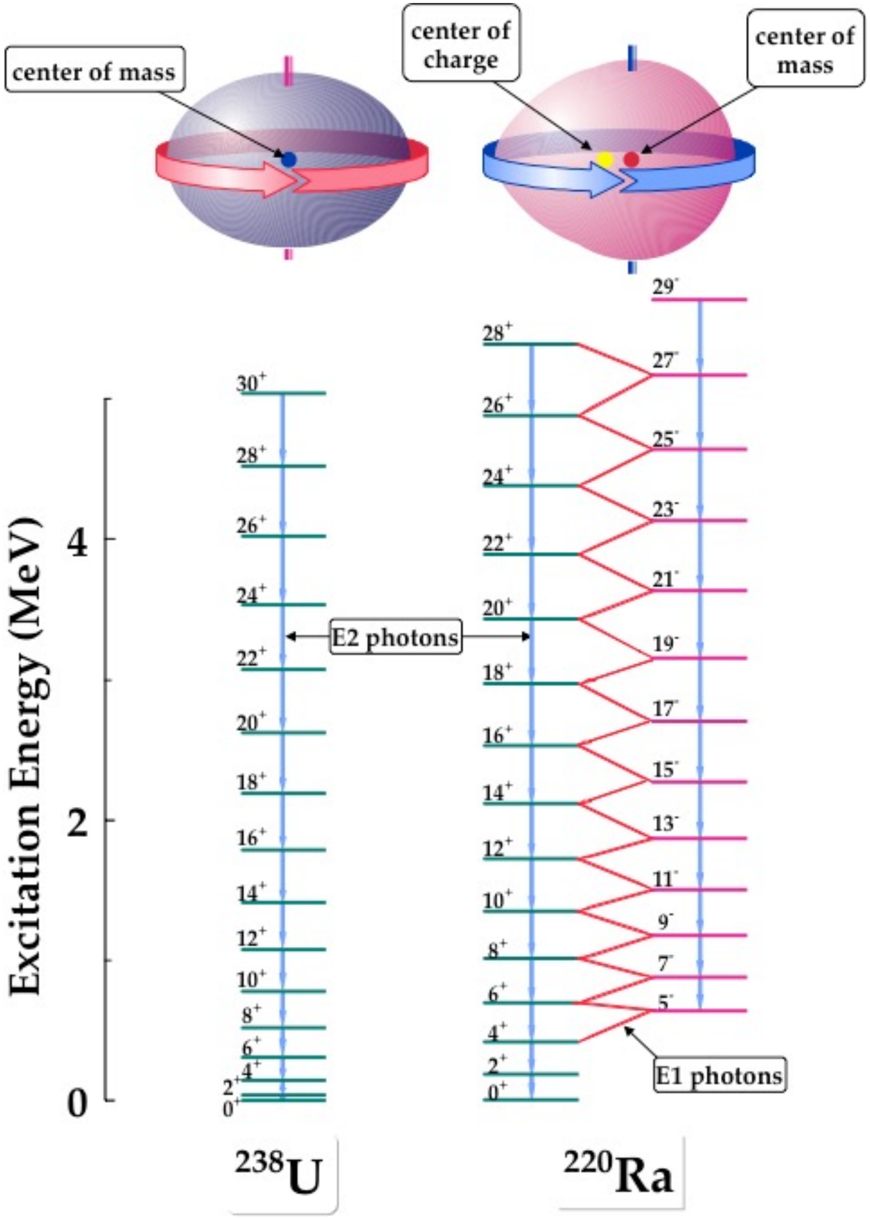
## Coexistence of oblate and prolate configurations

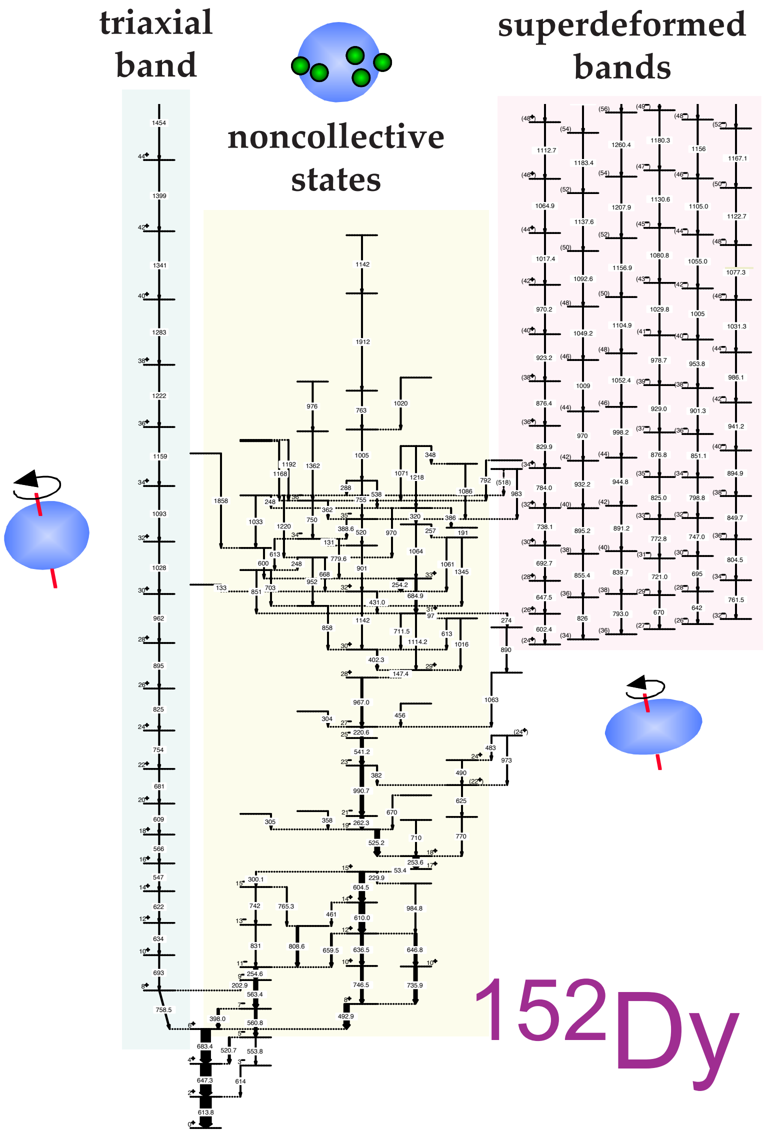

Phys. Rev. C 102, 014318 (2020)


Nature Phys. 14, 1163 (2018)



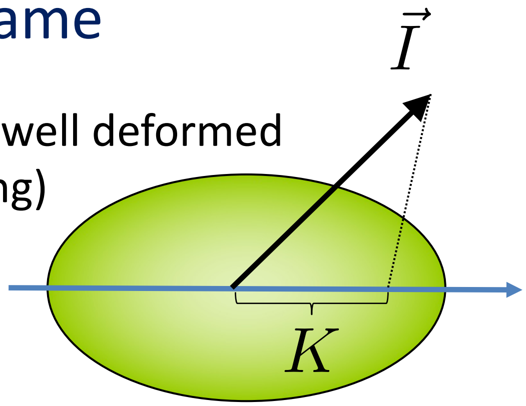
$$\langle r^2\rangle = \langle r^2\rangle_{\rm sph}\left(1+\frac{5}{4\pi}\langle\beta_2^2\rangle\right)$$


center of mass
center of charge
center of mass
Excitation Energy (MeV)
0
2
4
0+
2+
4+
6+
8+
10+
12+
14+
16+
18+
20+
22+
24+
26+
28+
30+
E2 photons
E1 photons
5-
7-
9-
11-
13-
15-
17-
19-
21-
23-
25-
27-
29-
238U
220Ra


triaxial band
noncollective states
superdeformed bands
152Dy

# Laboratory frame and intrinsic frame

Shape is axial, well deformed
(strong coupling)



$$Q = \frac{2K^2\text{-}I(I+1)}{(I+1)(2I+3)}\, Q_0$$

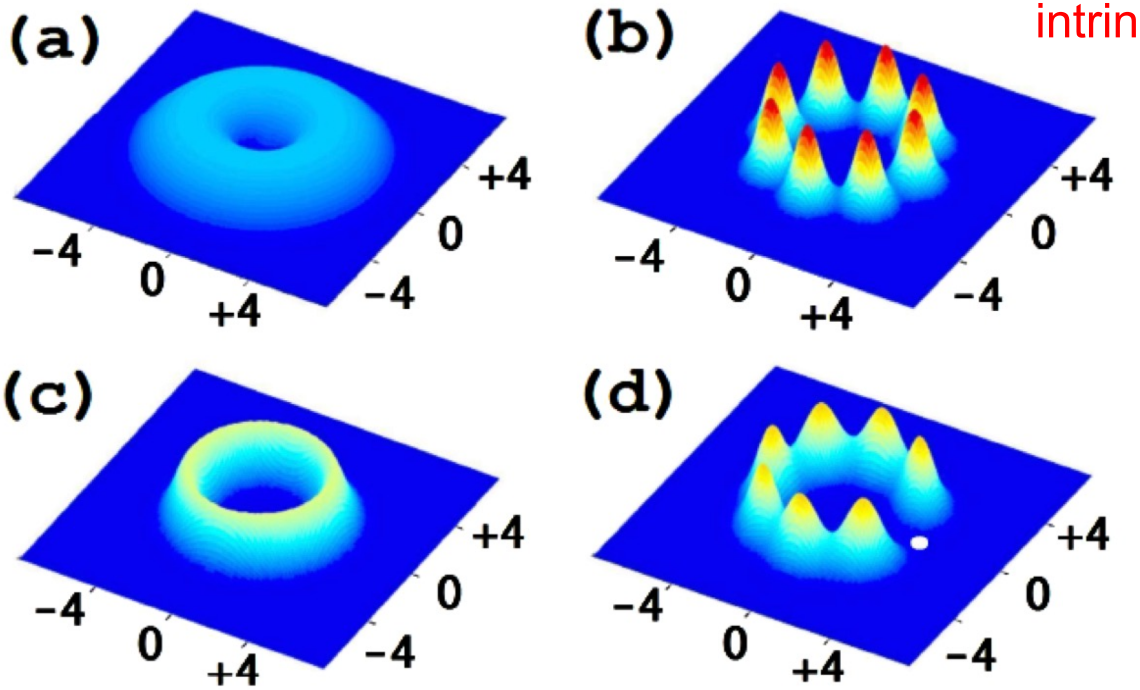
**MEASURED**

**RELATIVE MOTION**

**INTRINSIC**

**$Q=0$ for $I=K=0$, independently of $Q_0$!**

- How to define the intrinsic system?
- How to extract intrinsic deformations in the lab-system models?



intrinsic state

angular-momentum projected state

conditional probability distribution (CPD)

See PRL 97, 090401 (2006) on bosonic molecules in rotating traps and discussion in J. Phys. G 48, 123001 (2021)

CPD

$$P(\boldsymbol{r},\boldsymbol{r}_0)=\langle\Psi_I|\sum_{i\neq j}\delta(\boldsymbol{r}_i-\boldsymbol{r})\delta(\boldsymbol{r}_j-\boldsymbol{r}_{\mathbf{0}})[\Psi_I\rangle$$

proportional to the conditional probability of finding a nucleon at ***r*** under the condition that a second nucleon is located at $\boldsymbol{r}_0$

$$\hat{H} = \hat{H}_0 + \frac{1}{2}\kappa_0 \hat{Q}_0 \hat{Q}_0 + \frac{1}{2}\kappa_1 \hat{Q}_1 \hat{Q}_1$$

$$\hat{Q}_0 = \hat{Q}_n + \hat{Q}_p, \qquad \hat{Q}_1 = \hat{Q}_n - \hat{Q}_p$$

isoscalar isovector

The quadrupole-quadrupole (octupole-octupole) neutron-proton interaction is responsible for the development of the quadrupole (octupole) deformation

| | |
|---|---|
| Quadrupole case: | Phys. Rev. Lett. 60, 2254 (1988) |
| Octupole case: | Phys. Rev. C 103, 034303 (2021) |

$$Q_\lambda = Q_\lambda^{\rm bare} + Q_\lambda^{\rm pol}$$

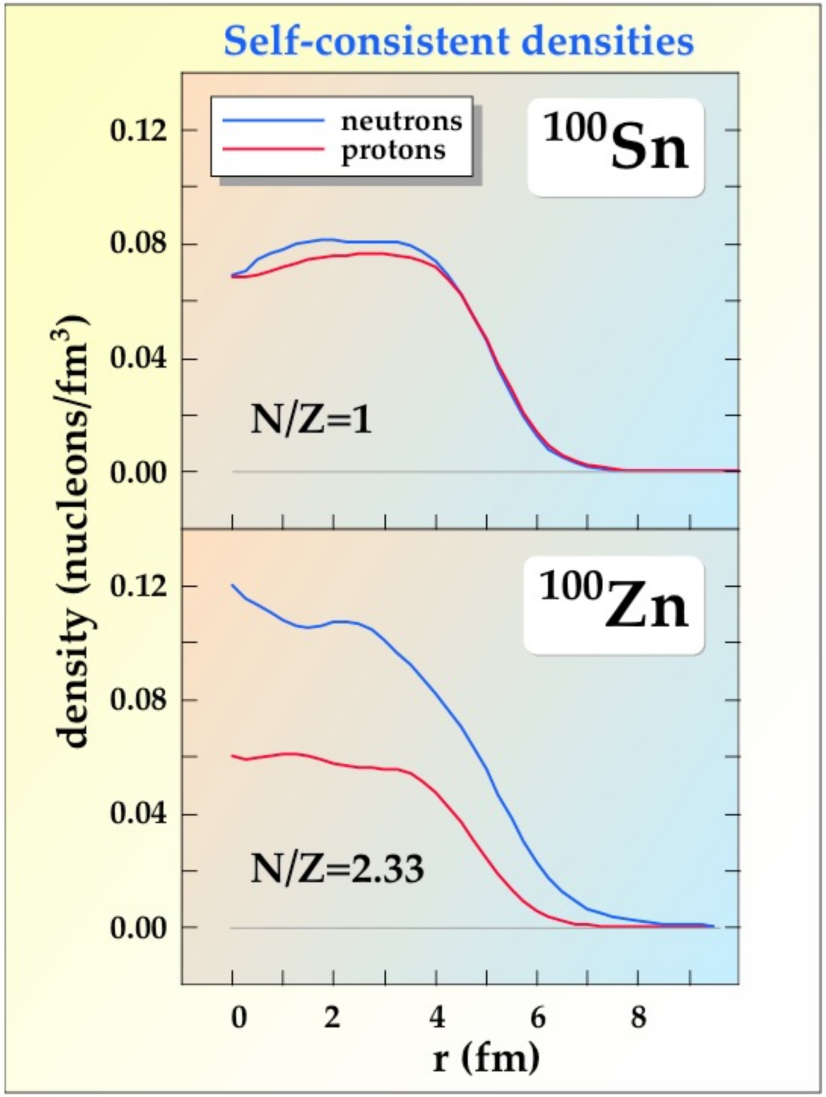
Nuclear polarization effects entering through the self-consistency of the nuclear mean field are very large!

$$Q_\lambda^{\rm pol} \approx Q_\lambda^{\rm bare} \quad \text{for } \lambda = 2$$ (coupling to the GQR)

… a big problem for ab-initio theory in spherical Hilbert space

# Nuclear Density Functional Theory

## *Degrees of freedom: local nucleonic densities*



- two fermi liquids
- self-bound
- superfluid

- mean-field ⇒ one-body densities
- zero-range ⇒ local densities
- finite-range ⇒ gradient terms
- particle-hole and pairing channels
- the *energy density functional* does not have to be related to a force
- a broken-symmetry generalized product state is a powerful concept
- deformations can be extracted from DFT densities

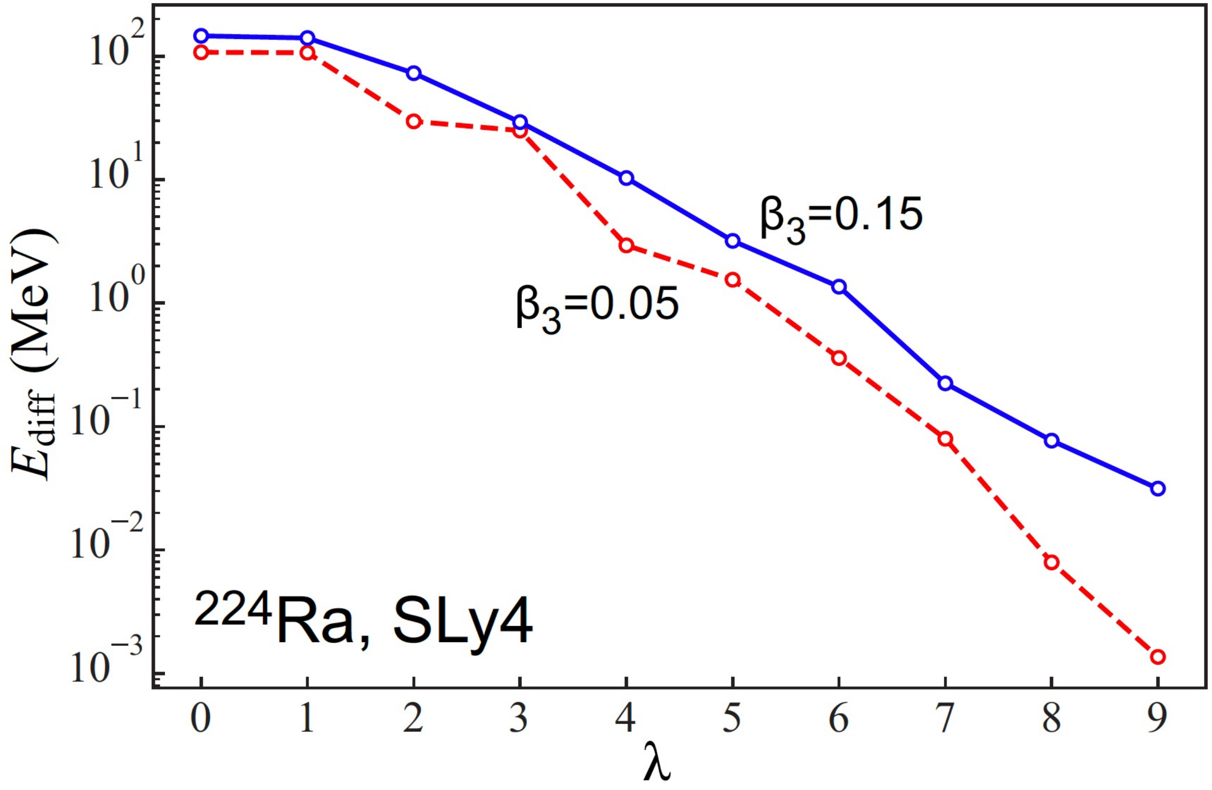
$$\rho(\vec{r}) = \sum_J \rho_{[\lambda]}(r) Y_{J,M=0}(\Omega)$$

functions $\rho_{[\lambda]}$ determine deformations

$$E = E_{[0]} + E_{[1]} + E_{[2]} + E_{[3]} + \ldots$$

$$E_{[\lambda]} = \frac{1}{2}\mathrm{Tr}(\Gamma_{[\lambda]}\rho_{[\lambda]}) + \frac{1}{2}\mathrm{Tr}(\tilde{\Gamma}_{[\lambda]}\tilde{\rho}_{[\lambda]})$$

Phys. Rev. C 103, 034303 (2021)



$$E_{\mathrm{diff}}(\lambda) = \sum_{\lambda'=0}^{\lambda} E_{[\lambda']} - E$$

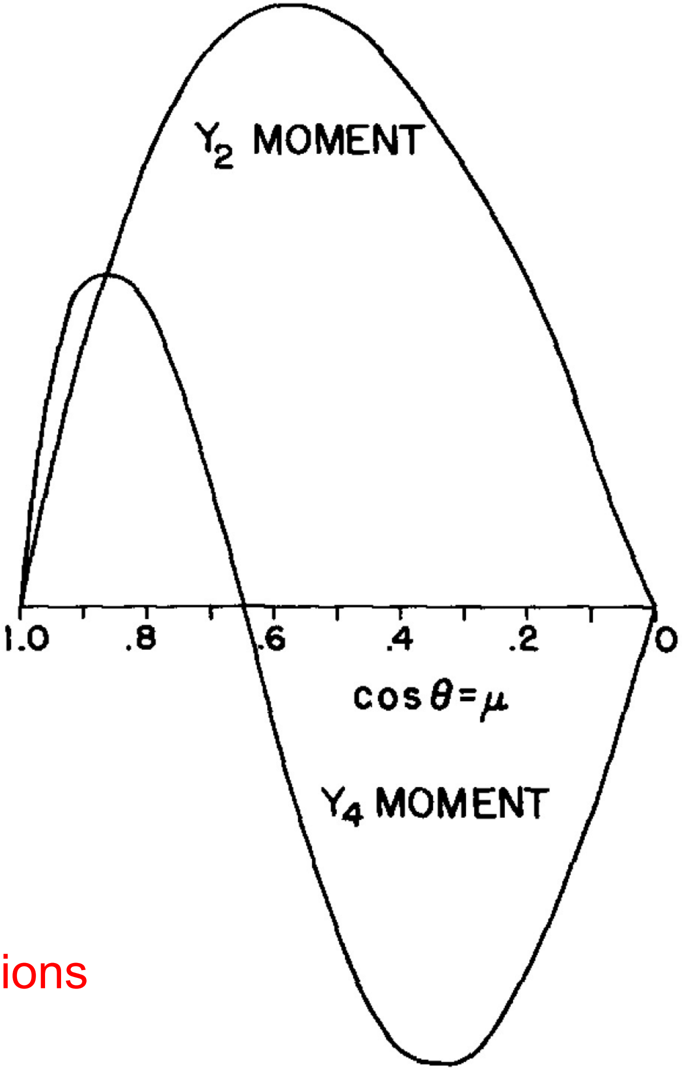
# Trend of deformations with shell filling

See A. Afanasjev's presentation

Phys. Lett. B 26, 130 (1968)

$$Q_{\lambda 0} \propto \int_0^{\mu} P_\lambda(x)dx$$

$\mu$ = partial filling of the valence shell

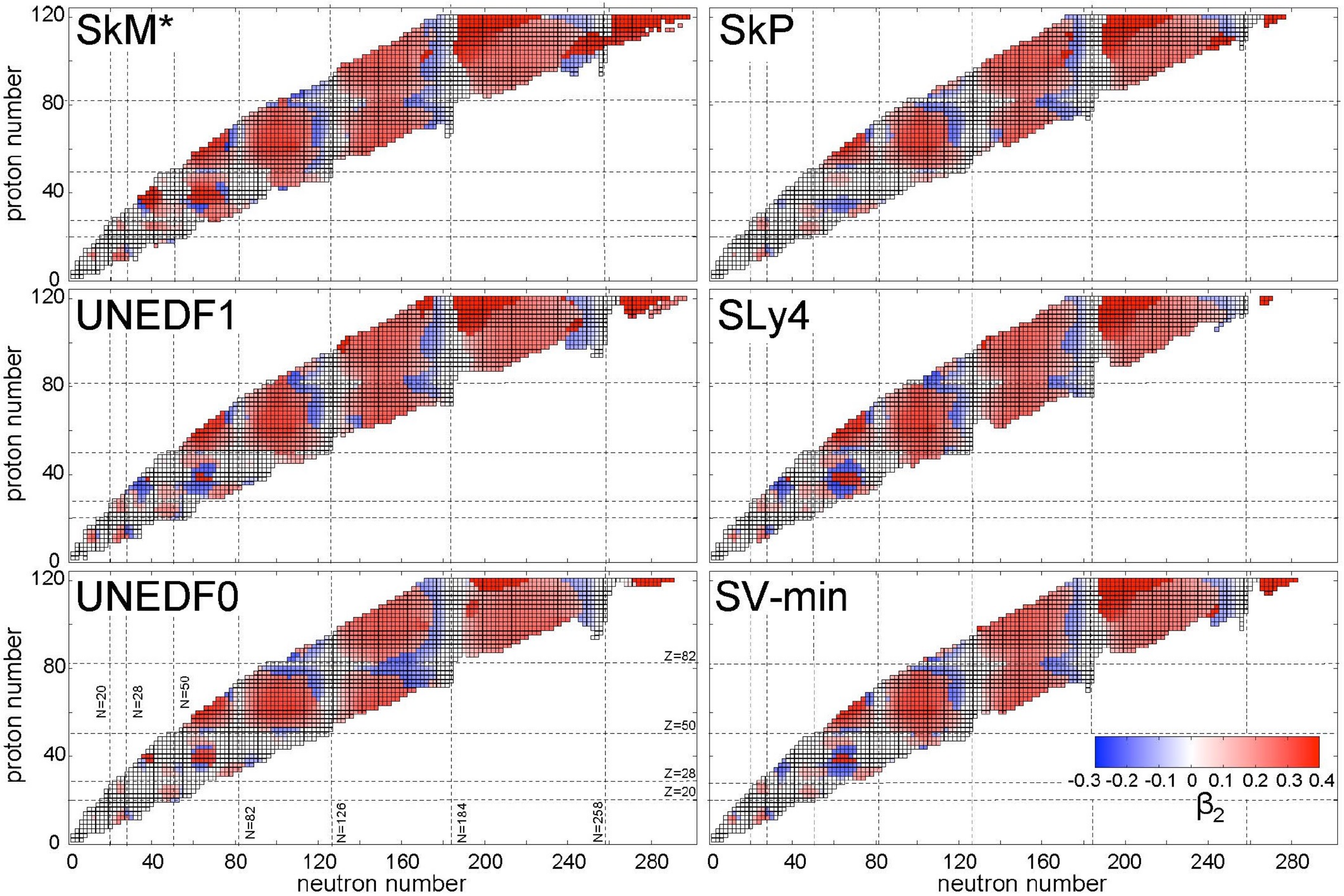


See also a paper:

Simple parameterization of nuclear deformations

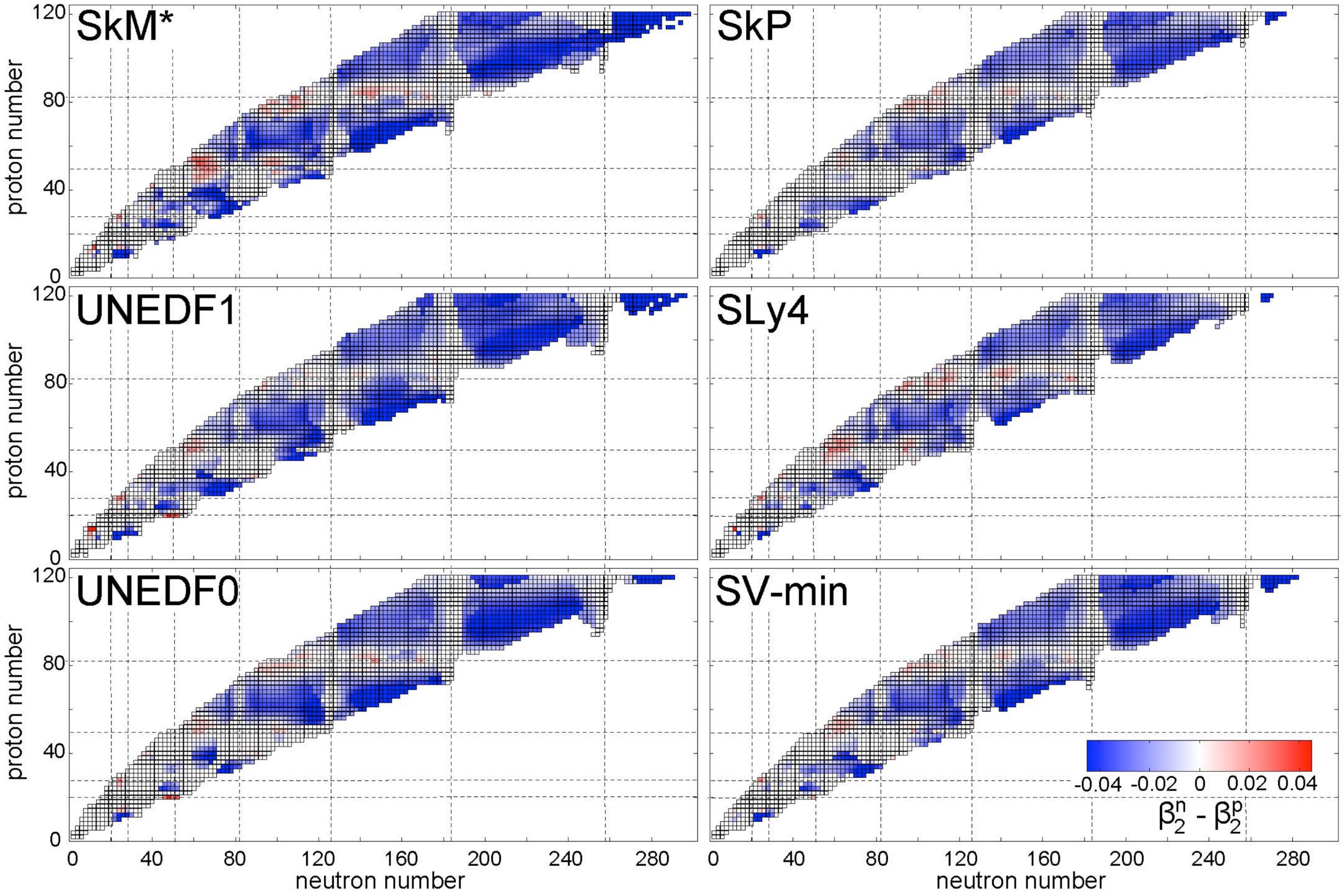
Phys. Lett. B 103, 1 (1981)

# Quadrupole deformations in nuclei



Nature 486, 509–512 (2012)

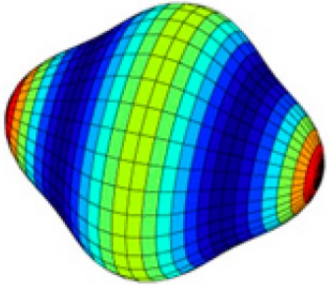
# Isovector quadrupole deformations in nuclei



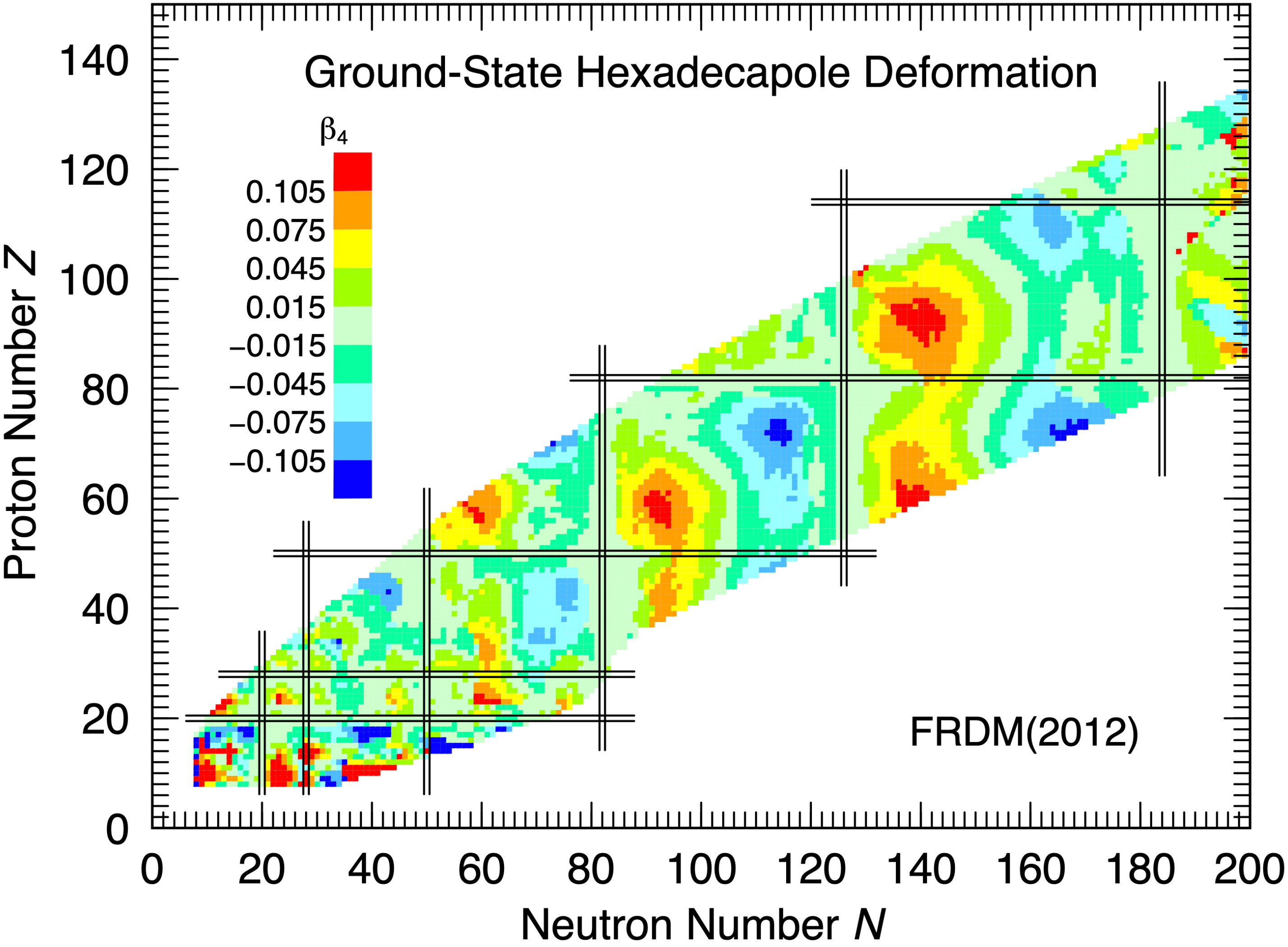
Nature 486, 509–512 (2012)

# Hexadecapole deformations in nuclei

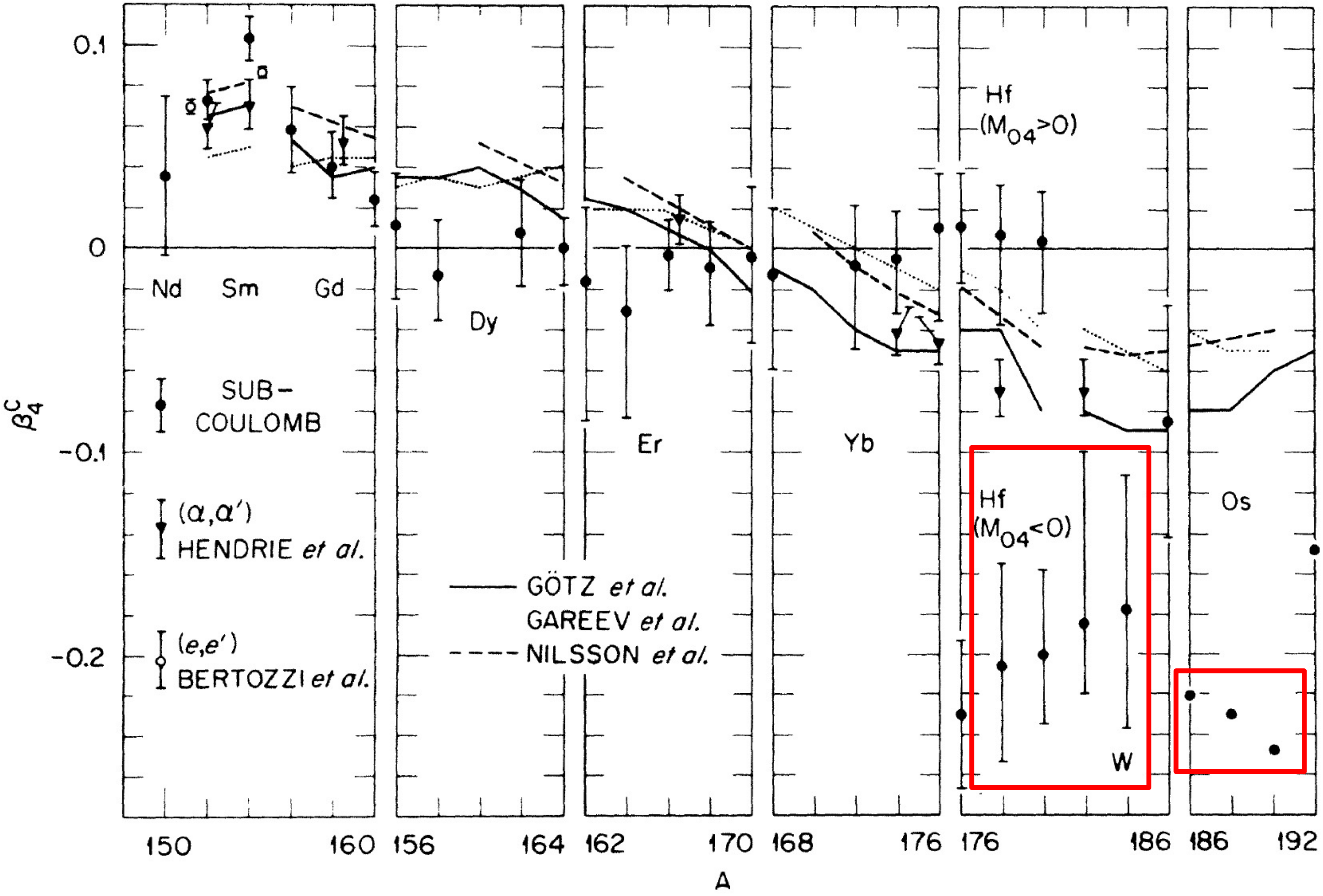
$\beta_4>0$



At. Data Nucl. Data Tables 109, 1 (2016)

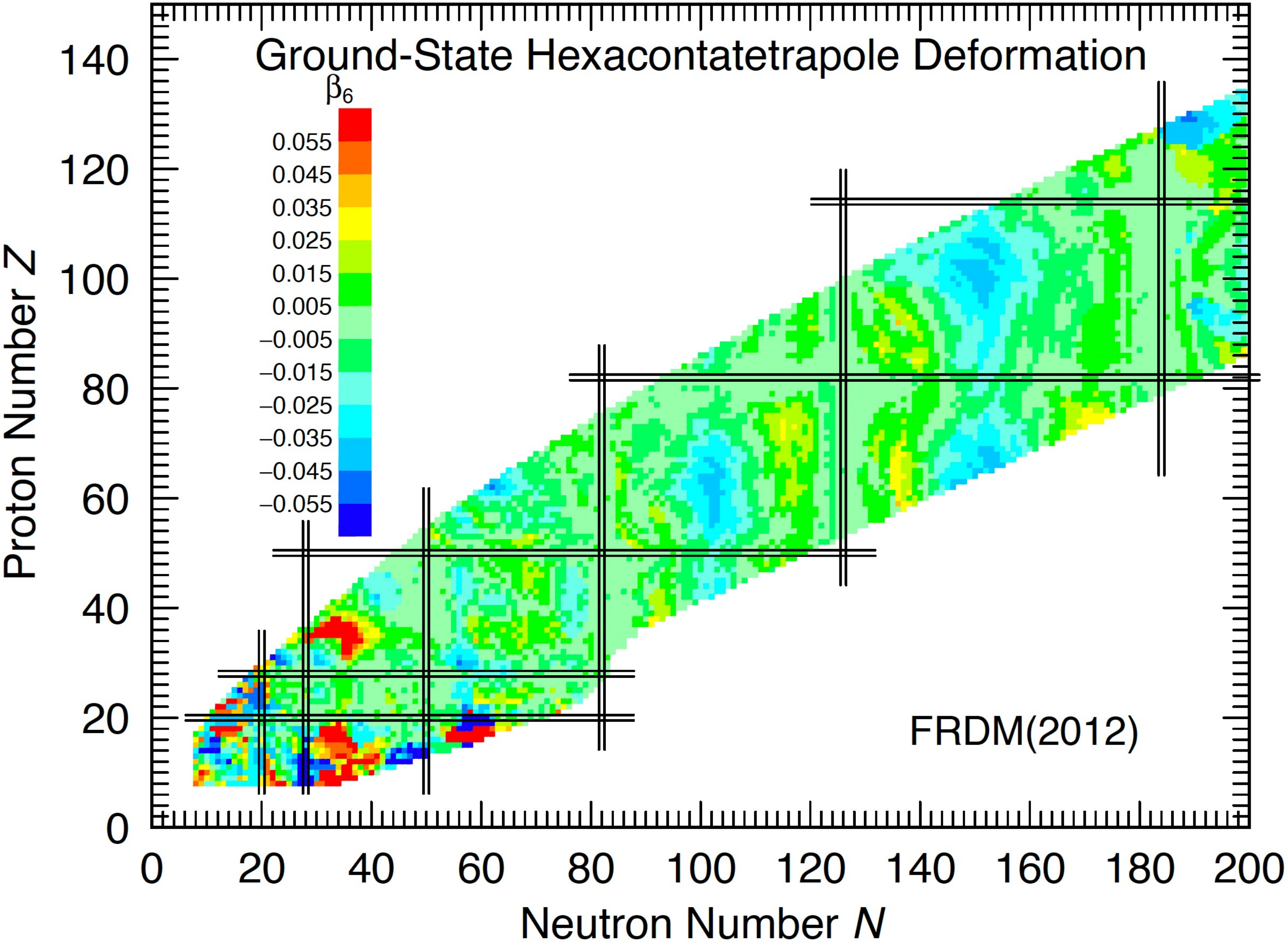


# Phys. Rev. C 16, 2208 (1977)

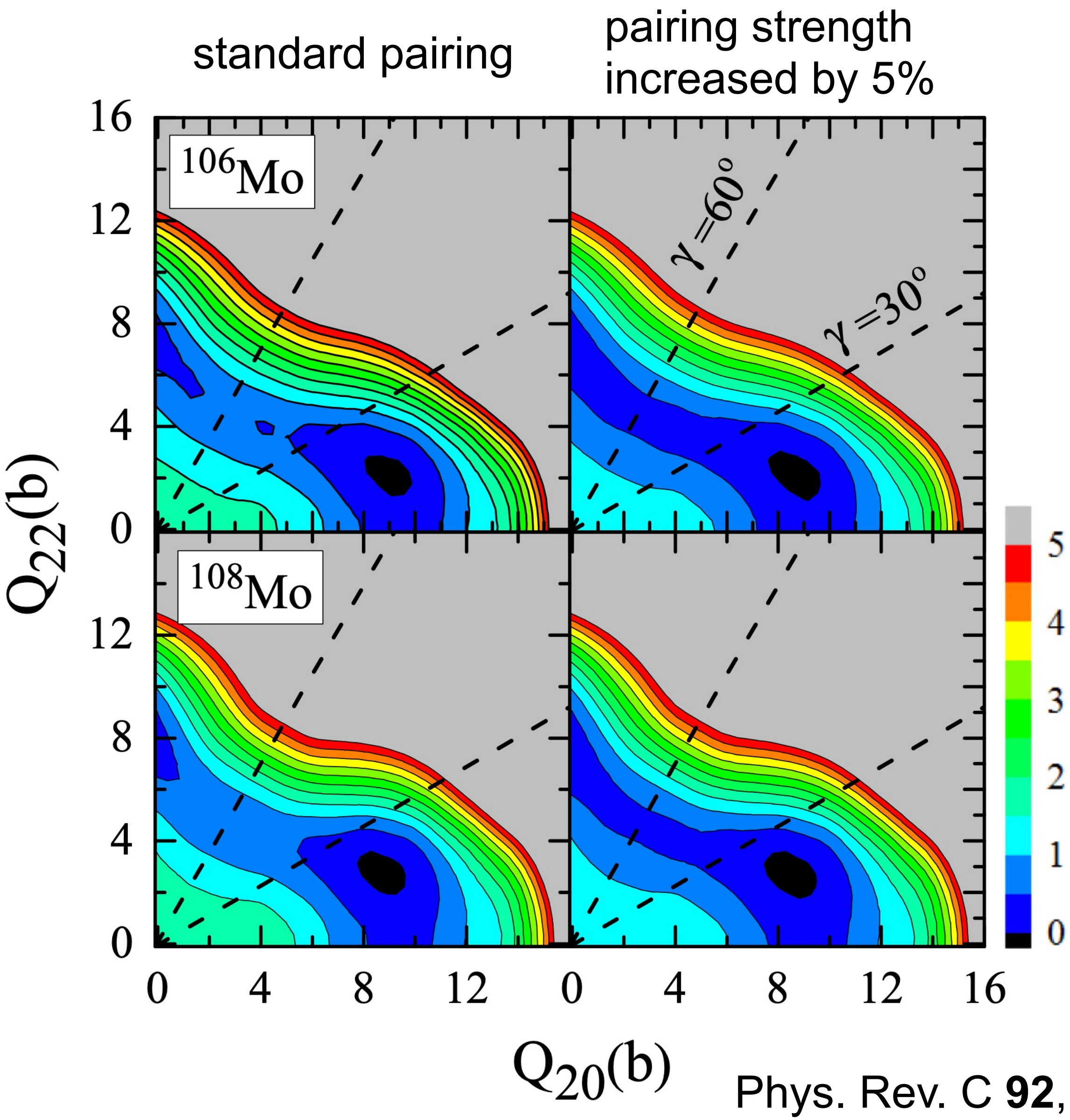


# Hexacontatetrapole deformations in nuclei

At. Data Nucl. Data Tables 109, 1 (2016)



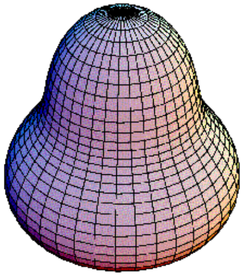
# Triaxial deformations in nuclei



- Triaxial shapes expected in transitional nuclei with small prolate-oblate energy difference
- Very soft minima: multireference theory needed

Phys. Rev. C **92**, 034307 (2015)

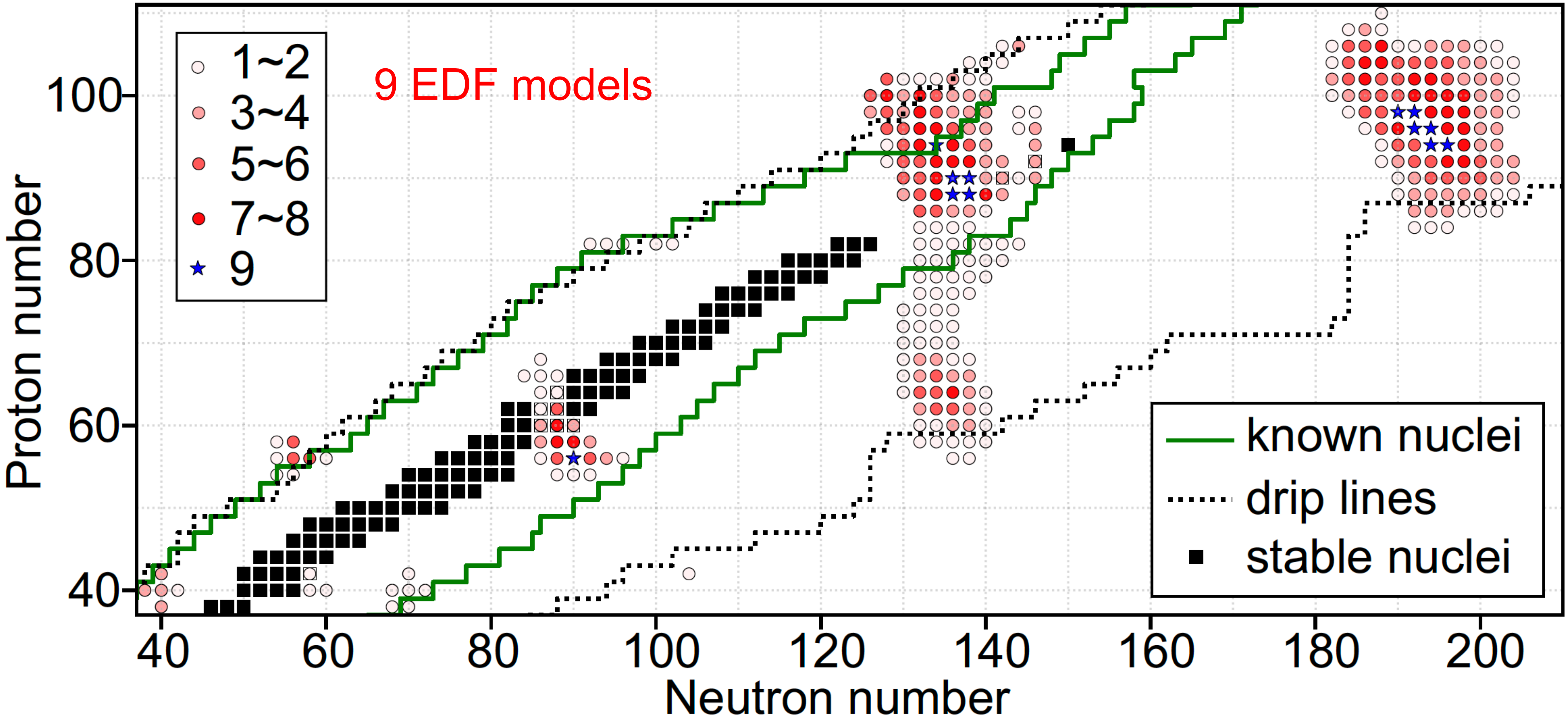
# Reflection-asymmetric nuclei



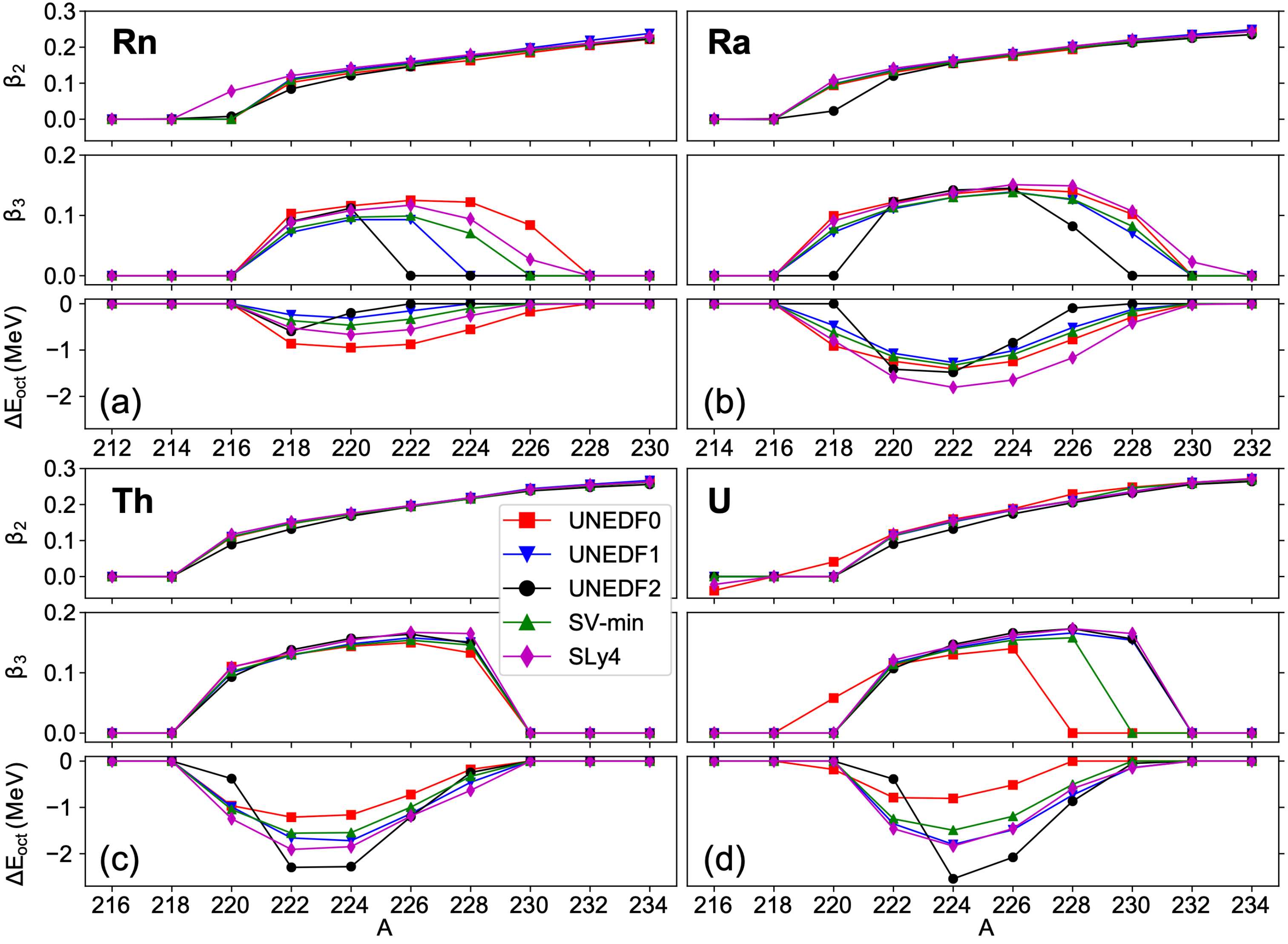
Landscape of pear-shaped even-even nuclei

Phys. Rev. C 102, 024311 (2020)

The regions of strong octupole collectivity are defined by the presence of close-lying proton and neutron shells with $\Delta l = \Delta j = 3$

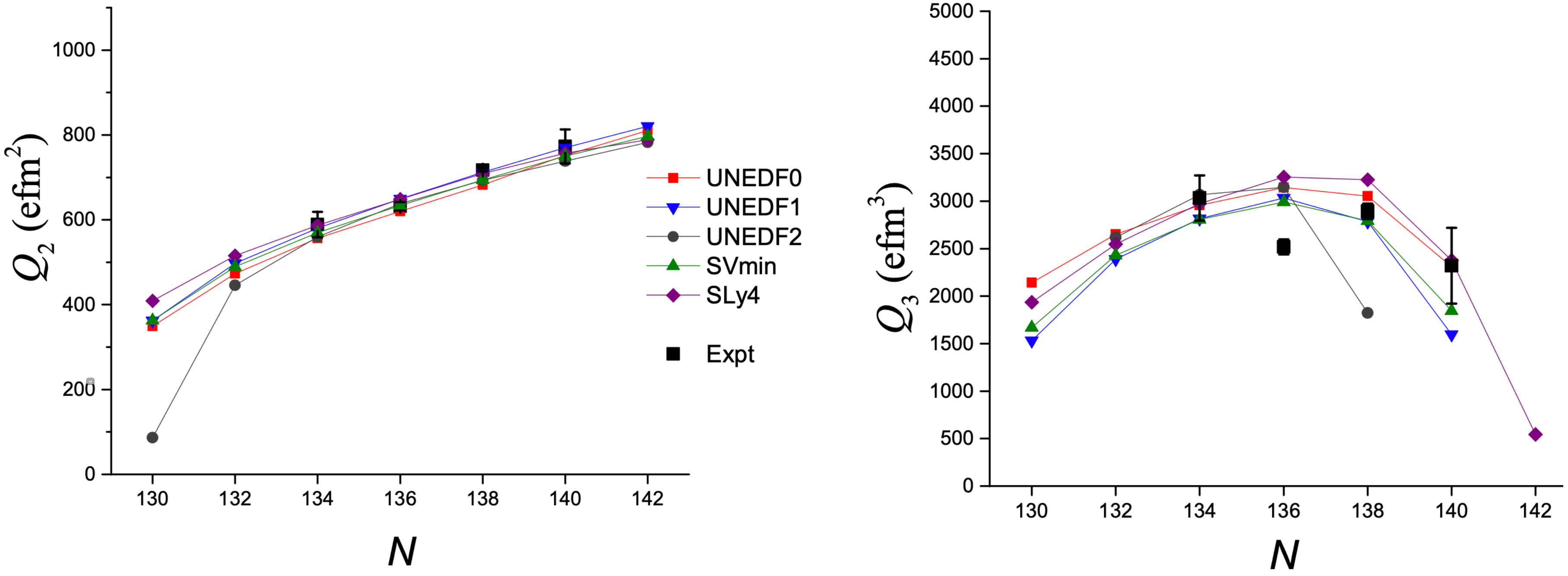


# Octupole deformations in nuclei



Phys. Rev. C 102, 024311 (2020)

# Theory vs experiment Ra (Z = 88) isotopes



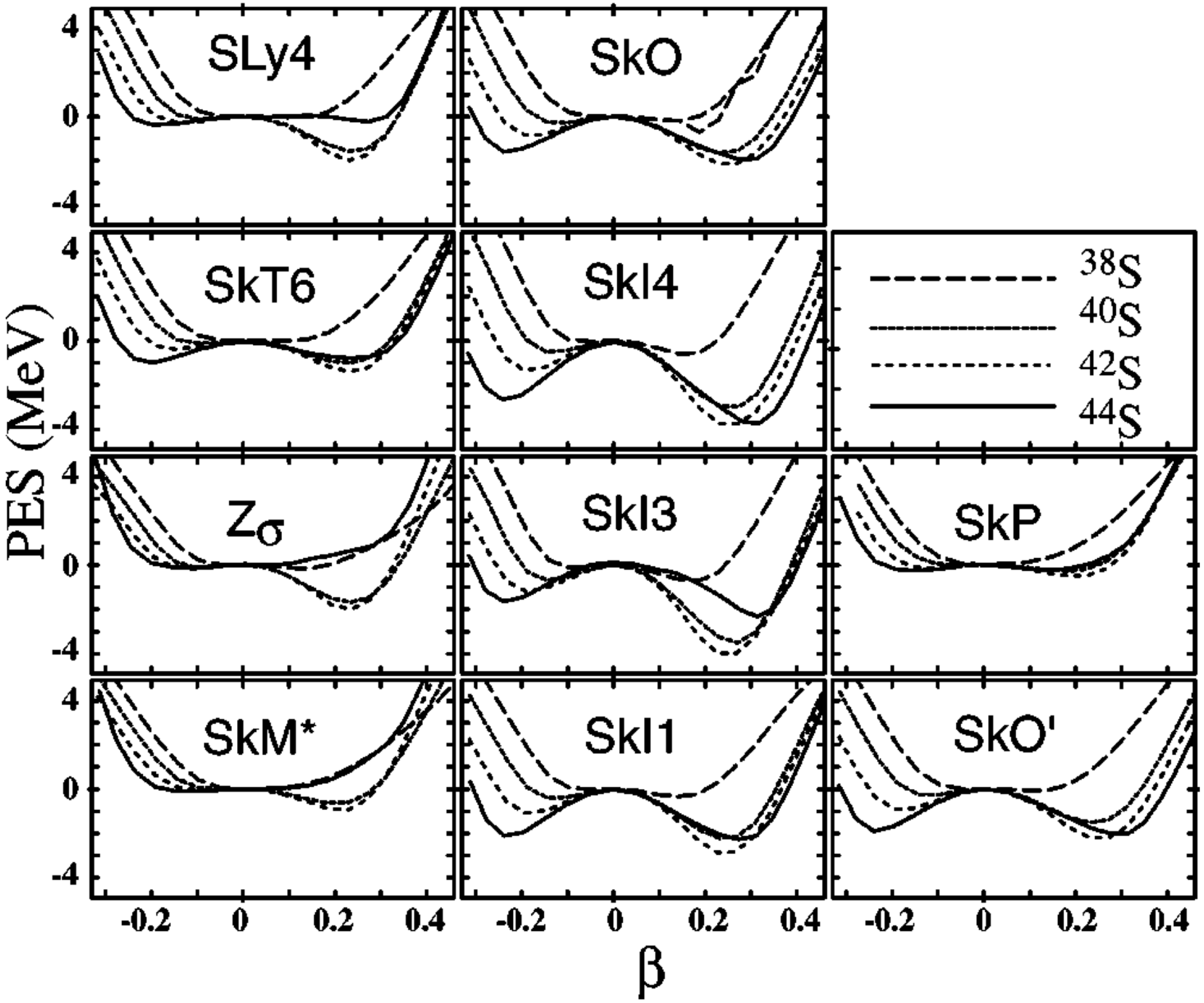
Experimental data from Proc. R. Soc. A 476: 20200202 (2020)

Microscopic origin of reflection-asymmetric nuclear shapes
Rev. C 103, 034303 (2021)

- pear-shape deformations are driven by the odd-multipolarity isoscalar interactions
- isoscalar octupole polarizability large in atomic nuclei
- dotriacontapole (λ=5) couplings very important

# Generator Coordinate Method

This variational approach can be viewed as a “horizontal expansion”. The GCM wave function is a superposition of HFB states



# Generator Coordinate Method

## See B. Bally's and T. Rodríguez's presentation

This variational approach can be viewed as a "horizontal expansion". The GCM wave function is a superposition of HFB states (⇒ multireference method)

In molecules, where the Born-Oppenheimer adiabatic approximation works, we can write the many-body wave function as

$$\Psi(Q,x) = \sum_n \Phi_n(Q,x)\chi_n(Q)$$

where the coordinates $Q$ are slow compared to the fast coordinates $x$. In atomic nuclei, such a separation is imperfect: slow coordinates do not strictly exist. Still, we can assume the many body wave function in a form:

$$\Psi(x) = \int_{coll} dQ\, \Phi(Q,x) f(Q)$$

generator coordinates

HFB wave functions

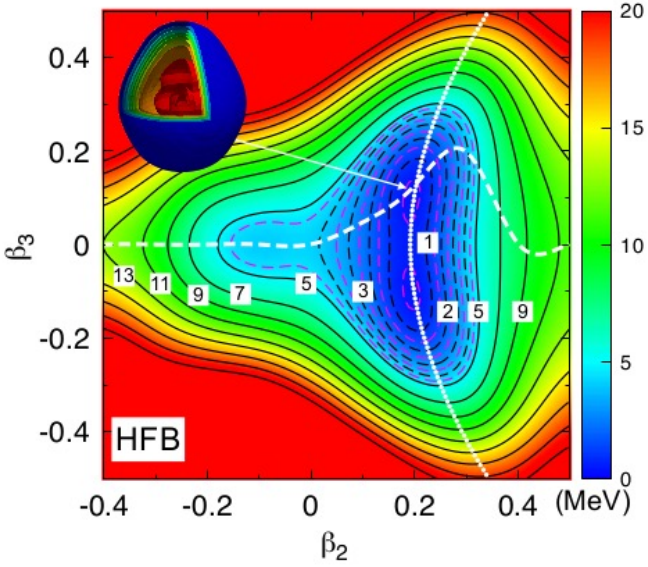
weight functions

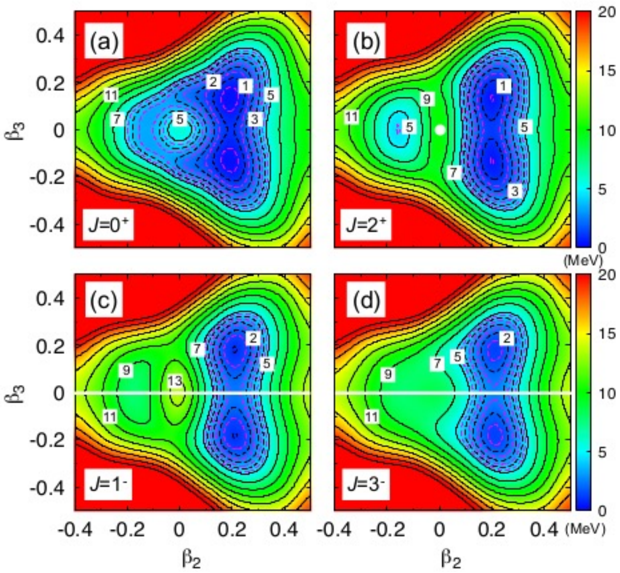
Note that the generator coordinates are integrated out. Their choice us up to us! Depending on the choice of the intrinsic (HFB) states and $Q$, the GCM wave function may contain the exact solution of the variational problem.

# Example of GCM calculations

$^{144}$Ba: Phys. Rev. C 93, 061302 (R) (2016)

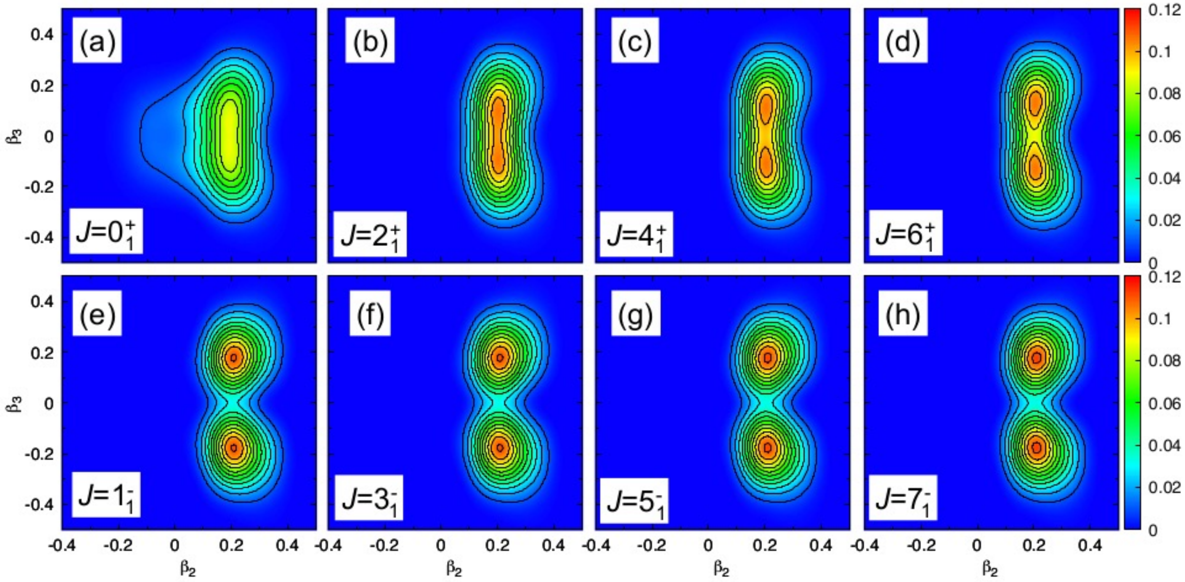
PES





projected PES

Collective wave functions

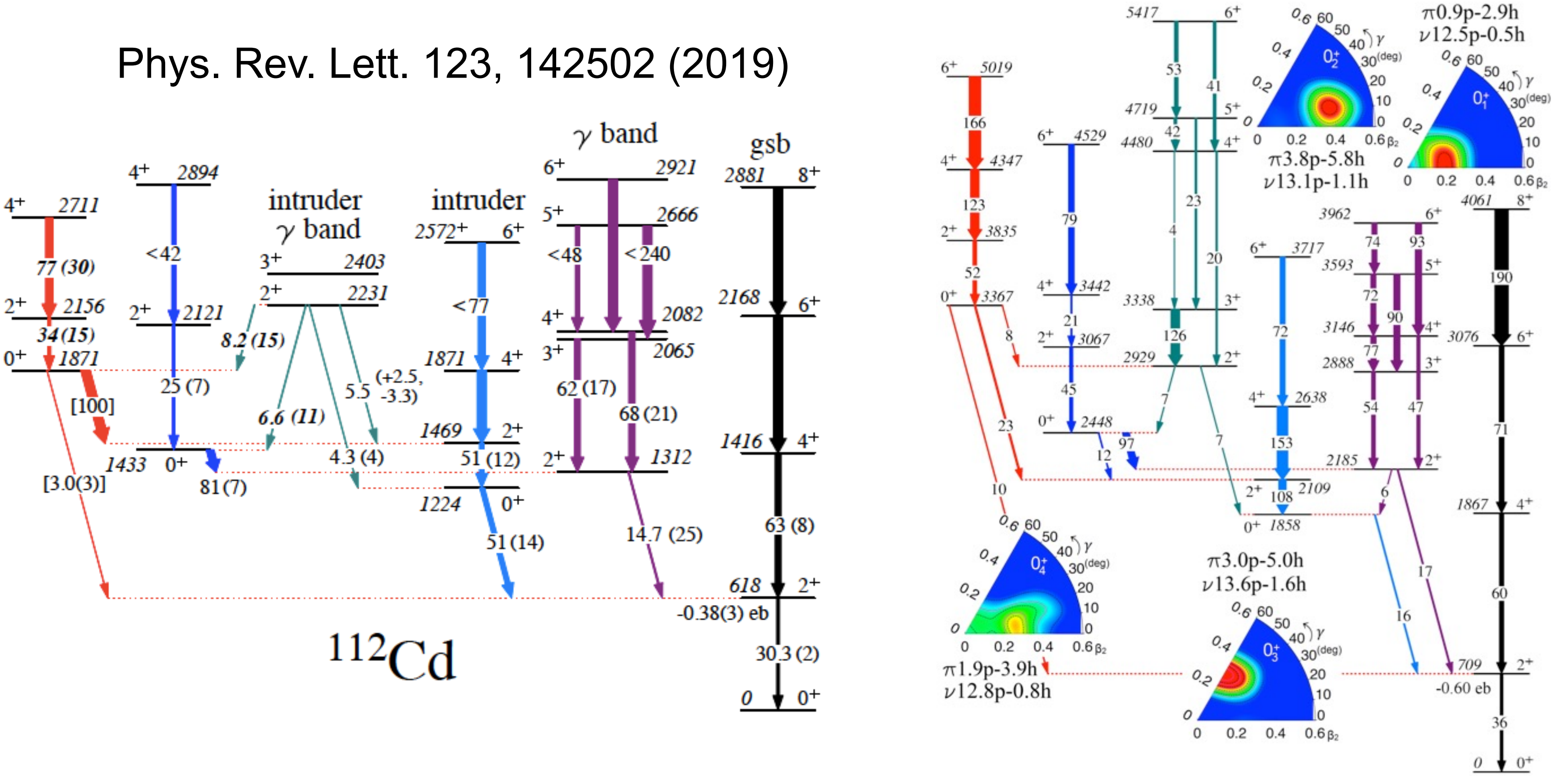


# GCM applications: Spectroscopy of complex nuclei

See T. Rodríguez’s presentation

Symmetry conserving configuration method with D1S energy density functional

Phys. Rev. Lett. 123, 142502 (2019)



- From schematic labels to a microscopic picture

# Summary

- Majority of nuclei are deformed due to the Jahn Teller effect
- Nuclear deformations are not fundamental degrees of freedom: they are nucleonic density features
- Nuclear deformations (appearance, magnitude) are governed by microscopic shell effects.
- The presence of intrinsic deformed shapes results in the occurrence of collective excitations in the laboratory system
- Deformations are configuration dependent!
- In many cases, nuclear deformation cannot be defined as intrinsic configurations having similar shape appear close in energy. In such cases, multireference analysis (such as GCM) is needed

# BACKUP