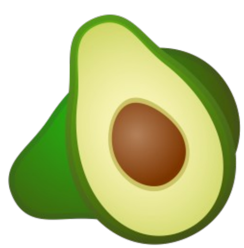
Nuclear deformation from a theoretical perspective

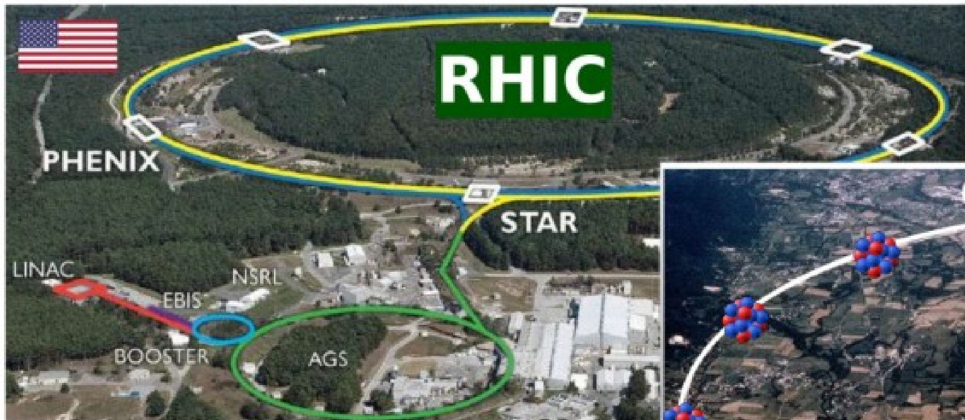


Luis M. Robledo

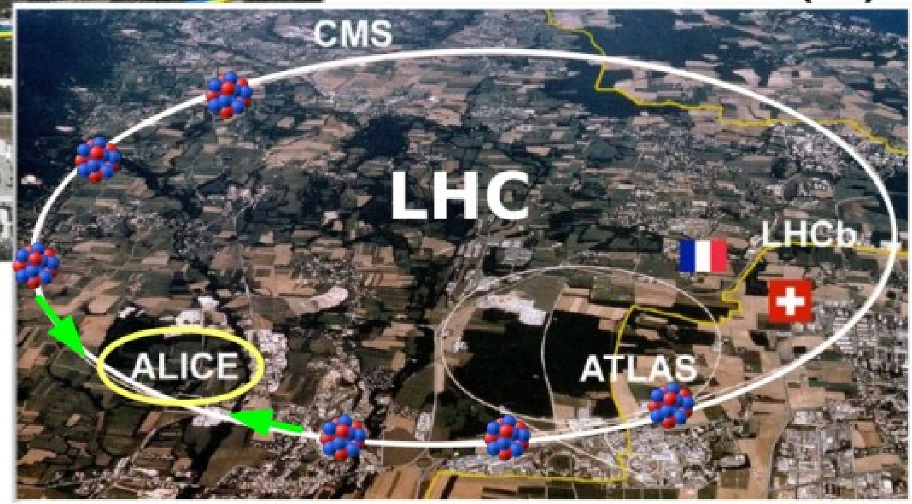
Universidad Autónoma de Madrid
Spain

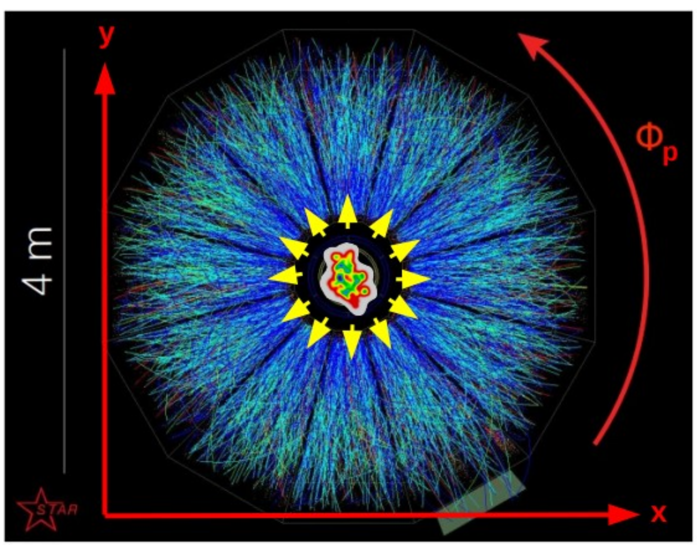
INT Workshop: Intersection of nuclear structure and high energy nuclear collisions, Feb 6th 2023

Long Island (NY)



Geneva (CH)





Low-momentum particles follow the hydrodynamic expansion.

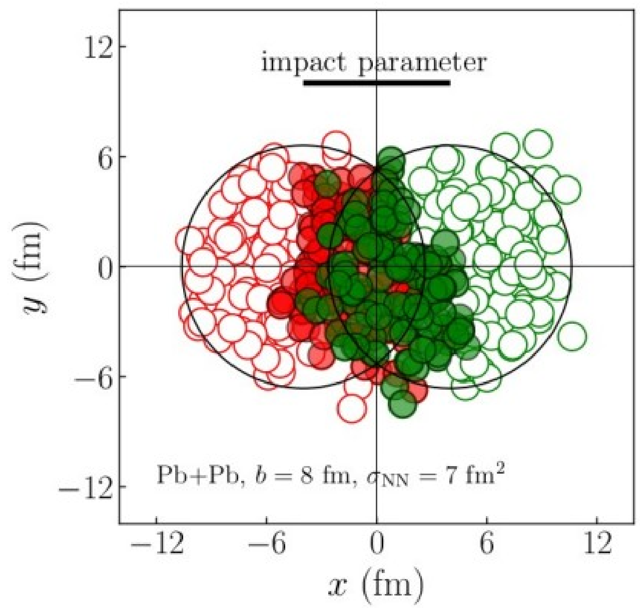
$$\frac{d^2N}{dp_T d\phi} = \frac{dN}{2\pi dp_T}\left(1 + 2\sum_{n=1}^{\infty} v_n \cos n(\phi - \Phi_n)\right)$$

EXPLOSIVENESS OF THE EXPANSION

ANISOTROPY OF AZIMUTHAL DISTRIBUTION

Heavy ion collisions at high energy produce a huge amount of particles characterized by hydrodynamic quantities like flux distributions, etc

Pictures taken from Giuliano’s talk …

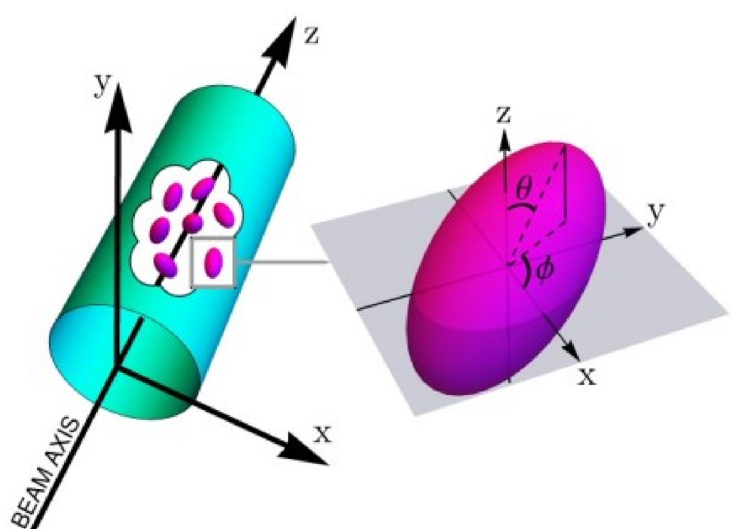


Density follows the nuclear mean field potential. Woods-Saxon parametrization

$$V(\vec{r}) = -\frac{V_0}{1 + \exp[(\vec{r} - \vec{R})/a]}$$

For spherical Pb only one parameter is required to characterize the density

Deformed systems



The bag of nucleons is now deformed and with a random orientation.

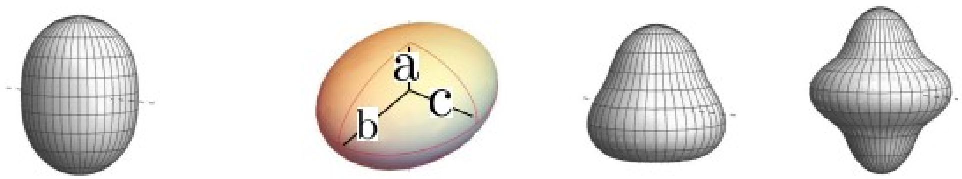
The collision selects one such orientation.

Pictures taken from Giuliano's talk …

Motivation

Generalize the Woods-Saxon profile to include intrinsic deformations:

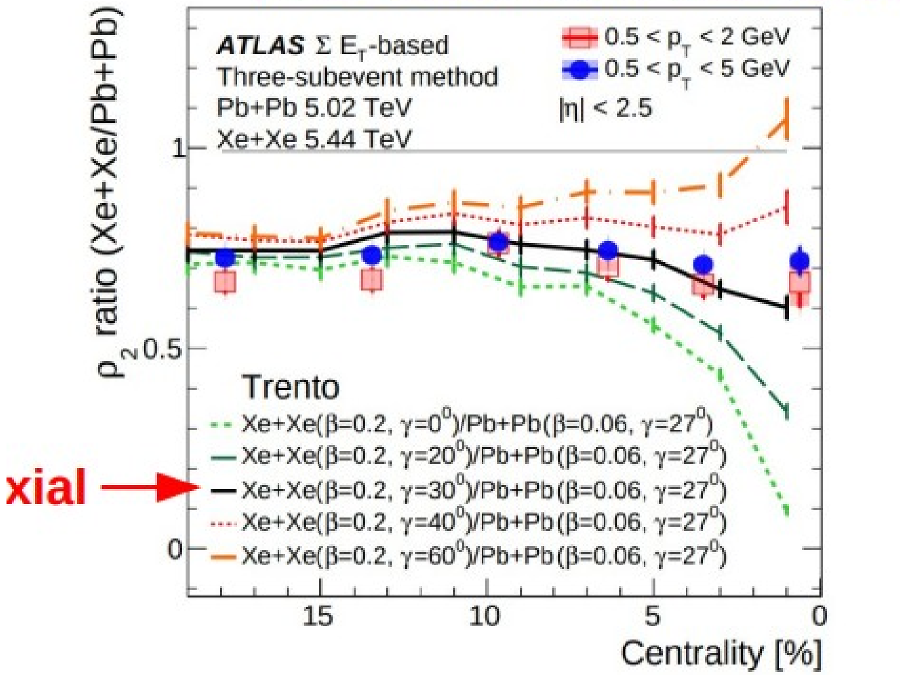
$$\rho(r,\Theta,\Phi) \propto \frac{1}{1+\exp\left(\left[r-R(\Theta,\Phi)\right]/a\right)} \;,\; R(\Theta,\Phi) = R_0\left[1+\underline{\beta_2}\left(\cos\underline{\gamma} Y_{20}(\Theta)+\sin\underline{\gamma} Y_{22}(\Theta,\Phi)\right)+\underline{\beta_3} Y_{30}(\Theta)+\underline{\beta_4} Y_{40}(\Theta)\right]$$



With this generalization is possible to reproduce with high accuracy experimental data not only for spherical 208Pb (LHC) but also for deformed and 129Xe (LHC) and 197Au, 238U, 96Ru and 96Zr (RHIC).

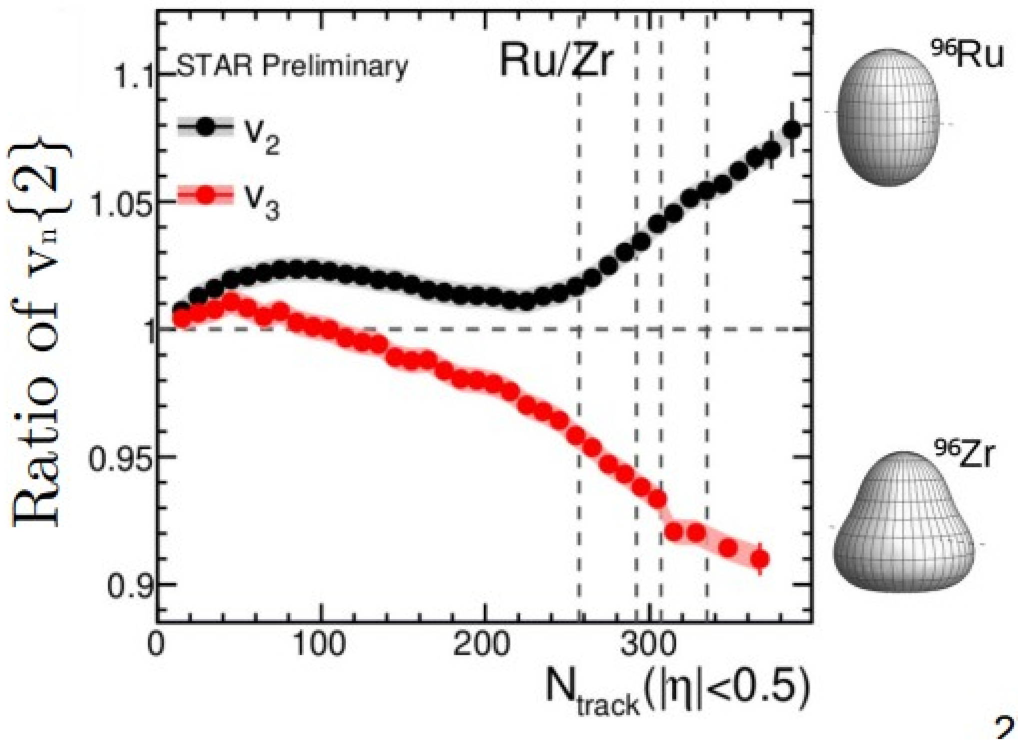
Nuclear intrinsic deformations involve not only axial quadrupole deformation, but also triaxial deformation (129Xe), hexadecapole (238U) and octupole (96Zr)

[ATLAS collaboration, arXiv:2205.00039]



Pictures taken from Giuliano's talk …

Motivation



2021 data on isobar collisions depart from the expected relationships for isobars

$$\frac{O_{X+X}}{O_{Y+Y}} = 1$$

Deviations seem to imply that 96Ru is more strongly quadrupole deformed than 96Zr

96Zr is octupole deformed while 96Ru is not

Conclusion: Low energy nuclear structure data can be extracted from heavy-ion collisions

Caveat: Intrinsic shapes and the deformation parameters characterizing them are not physical observables

Pictures taken from Giuliano's talk …

In the first week of the program Witek gave a nice introduction to intrinsic deformations from a physics oriented point of view. Here, I will describe the problem from a different perspective

Quick reminder:

- A physical system posses a given symmetry if its Hamiltonian commutes with all the operators of the underlying symmetry group
  - Parity $$[\hat{H}, \hat{\Pi}] = 0$$
  - Rotational invariance $$[\hat{H}, \hat{R}(\Omega)] = 0$$

  If the symmetry group is continuous the Hamiltonian also commute with the generators of the symmetry (elements of the group's algebra).

- The consequence is the quantum numbers of the eigenstates of H (physical states !) **can** contain the quantum numbers of the generators or the group elements
  - Reflection symmetry: Parity good quantum number
  - Rotational invariance: J (SU(2) Casimir) and M are good quantum numbers

Caveats:

- Only valid for **stationary** states eigenstates of H
- If the eigenstate is **degenerate** there can be other choices (electric dipole moment hidrogen atom and hibridation in atoms)

Deformation and intrinsic frame

- The **mean field** concept is a fruitful one in nuclear physics as it allows to explain naturally **magic numbers**
- The underlying **mean field grasps** most of the dynamic **correlations** present in the nucleus
- The mean field can be obtained by means of the **Hartree-Fock or HFB** variational **approximations** to the full many body problem
- As an **approximation** to the full problem, the **mean field** does not necessarily preserve the symmetries of the full Hamiltonian. In this case we say the mean field approximation **spontaneously breaks** the symmetries of the Hamiltonian
- Same mechanism as **unrestricted Hartree Fock** in atoms and molecules
- By **breaking symmetries** in the approximate solution many **correlations** are **incorporated into the simple mean field picture** (that incorporates the symmetrization principle in an straightforward way)
- The mean field symmetry breaking solutions live in the **intrinsic frame** and are denoted as **intrinsic wave functions**
- As already pointed out by Wigner, **linear combinations** of rotated **deformed** intrinsic wave functions can **restore** the angular momentum **quantum numbers** of the state

Intrinsic and Laboratory frame connection

The eigenstates of the Hamiltonian have the quantum numbers of the symmetries, and therefore, to improve the symmetry breaking mean field approximate solution one has to **restore the broken symmetries** (i.e. go from the intrinsic to the Lab frame).

Symmetry restoration is a well defined **procedure** rooted on **group theory** grounds

$$|\Psi^J_M(\pi, N)\rangle = \sum_K g_K P^J_{MK} P^N P^\Pi |\phi\rangle$$

The projectors are **linear combinations** with the appropriate weights, tailored to the quantum numbers to be restored, of the **symmetry group elements** (see below)

Physical observables have to be computed with the **symmetry restored wave functions** as well as transition probabilities

$$\langle \Psi^J_M(\pi, N)|\hat{O}|\Psi^J_M(\pi, N)\rangle \quad \langle \Psi^J_M(\pi, N)|\hat{O}|\Psi^{J'}_{M'}(\pi', N')\rangle$$

Please note that in the **successful shell model approach**, where the problem is solved from the beginning in the Lab frame, and the exact solutions within the given configuration space are obtained, there is no need to define an intrinsic frame

From the intrinsic to the Lab frame

In **Bohr and Mottelson's rotational model** the passage from the intrinsic to the Lab frame was based on the introduction of "orientation wave functions" (Wigner functions) times intrinsic deformed ones.

The calculation of **physical quantities** was always carried out in the **Lab frame**, but within the realm of the model those quantities could be expressed in terms of the corresponding **quantities in the intrinsic frame**. For instance

$$\langle I_1 K_1 || \hat{Q}_\lambda || I_2 K_2 \rangle = \sum_\mu Q^{int}_{\lambda\mu} (-)^{I_1 - K_1} \sqrt{(2I_1+1)(2I_2+1)} \begin{pmatrix} I_1 & \lambda & I_2 \\ -K_1 & \mu & K_2 \end{pmatrix}$$

Where $Q^{int}_{\lambda\mu}$ are the intrinsic deformation parameters. For K=0 bands and quadrupole transitions one obtains

$$B(E2, I+2) = Q_0^2 \frac{5}{16\pi} \frac{3}{2} \frac{(I+1)(I+2)}{(2I+3)(2I+5)} \qquad Q_0 = \sqrt{\frac{16\pi}{5}} \frac{3}{4\pi} A R_0^2 \beta$$

In **BM's rotational model** physical quantities can be obtained from intrinsic ones

The **BM model** can be **justified** microscopically (i.e. with projections) in the **strong deformation limit**, i.e. the intrinsic wave function is **well deformed**

The passage from the **LAB to the intrinsic** frame requires a **careful evaluation** of the assumptions made in the **strong deformation limit**

Some reflections

- It would be very interesting to analyze the changes in the **spatial matter distribution** after symmetry restoration and configuration mixing

- Not a common chore in standard nuclear structure calculations

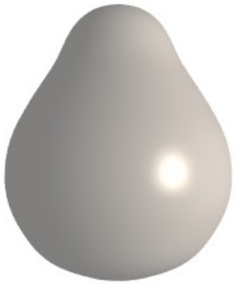
- Computationally intensive

- **Analyze the role of LAB density in the Glauber Montecarlo Model used to study the flux anisotropies**

- Perhaps it could be the clue to solve the 96Zr puzzle

  - HI analysis point to an octupole deformed nucleus
  - Nuclear structure also point to strong octupole correlations
  - Calculations point to dynamic instead of static octupole correlations

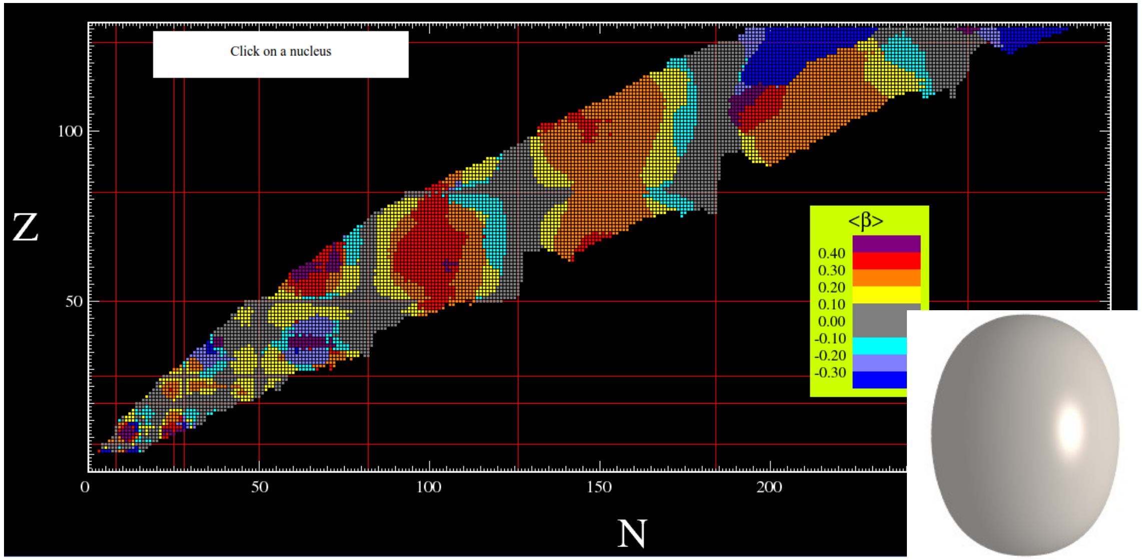
Octupole deformation is a relevant concept in nuclear structure of atomic nuclei

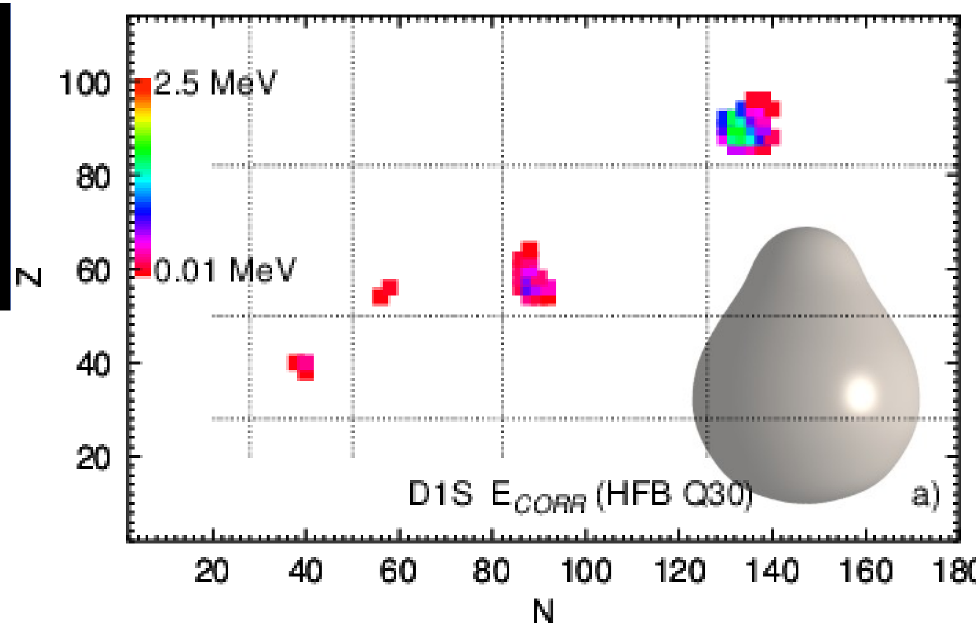


- *Next multipole moment after quadrupole (L=3)*
- *Breaks reflection symmetry (parity). Pear shape*
- *Parity doublets and alternating parity rotational bands*
- *Strong E3 electromagnetic transitions (E1 also but caution applies)*
- *Octupole ‘’magic” numbers: 34, 56, 88, 134 and 196*

and also in other fields of research

- *Devise experiments looking for beyond the standard model of particle physics (electric dipole moment of elementary particles)*
- *Interpretation of heavy-ion collision results regarding the flow distribution in the transverse plane after quark-gluon plasma creation*





AMEDEE web page @ CEA

The shape of many nuclei is deformed in the intrinsic (body fixed) frame (a mean field artifact). Wave function factorizes: deformed x orientation

Deformation described in terms of multipole moments $R(\theta,\phi) = R_0(1+\sum_{LM}\alpha_{LM}Y_{LM})$

The restoration of broken symmetries via orientation fluctuations (transformation to the LAB frame) generates a “band” for each intrinsic state. Band members labeled by the quantum numbers of the restored symmetry

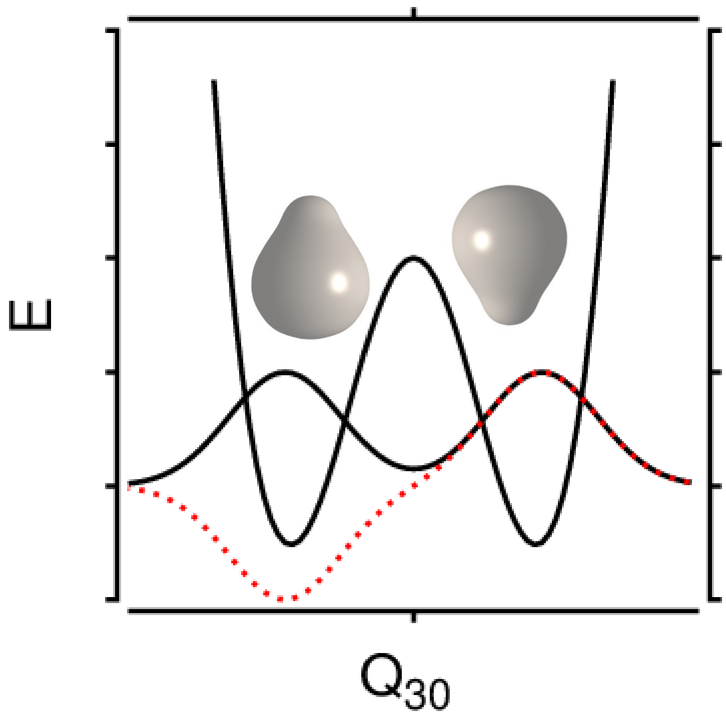
Deformation	L	Symmetry	Bands	Transitions
Quadrupole	2	Rotational	Rotational (J)	E2
Octupole	3	Parity	Parity doublets (π)	E1,E3

Order parameters

$$Q_{20} = z^2 - \frac{1}{2}r_\perp^2$$

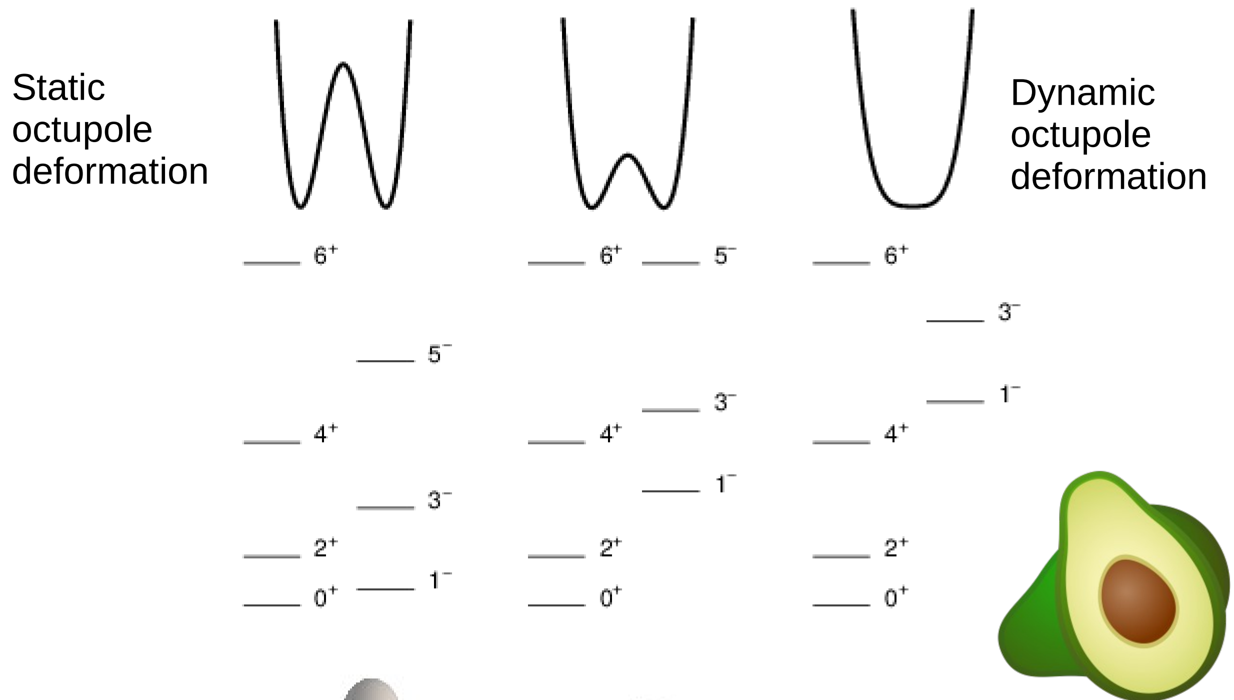
$$Q_{30} = z(z^2 - \frac{3}{2}r_\perp^2)$$

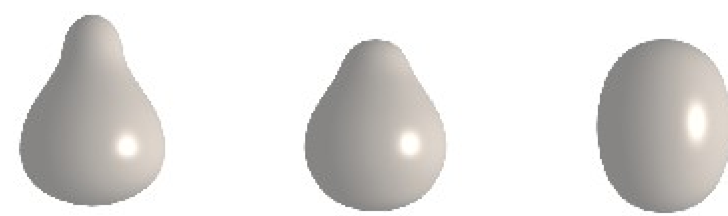
Octupoles 1.0 (Octupole deformation)



$$Q_{30} = z(z^2 - \frac{3}{2}r_\perp^2)$$

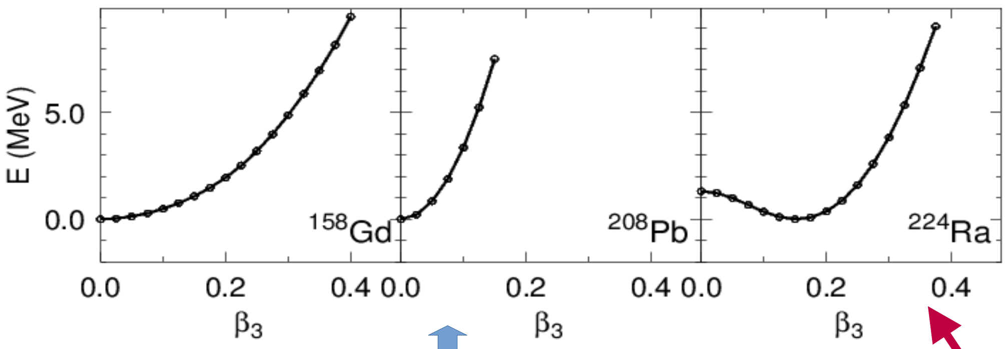
Order parameter





- Octupole deformation shows up as minima of $E_{HFB}(Q_{30})$ (2MeV depth at most)
- The largest the depth of the octupole well the largest the def at the minimum
- $E(Q_{30})=E(-Q_{30})$ (Interaction invariant under parity)
- In the LAB frame: parity doublets in the limit when there is no tunneling through the barrier
- Alternating parity rotational bands (def. nuclei)
- Strong E3 transition strengths

Permanent octupole deformation

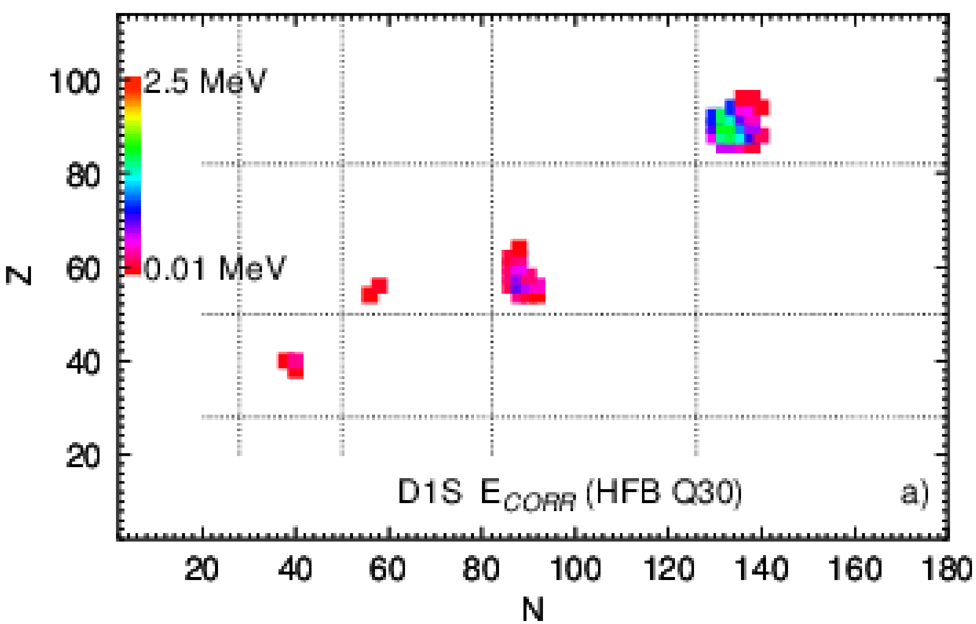


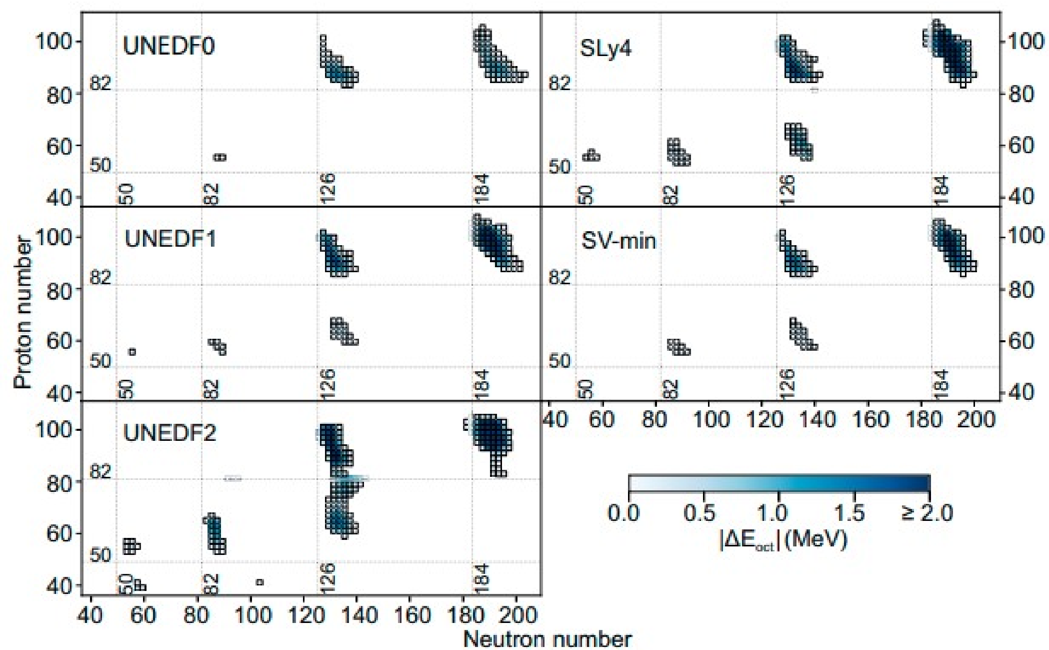
Gogny D1S HFB results

Octupole magic numbers

- 34 ($g_{9/2}$-$p_{3/2}$) 40 ?
- 56 ($h_{11/2}$-$d_{5/2}$)
- 88 ($i_{13/2}$-$f_{7/2}$) $\Delta j=\Delta l=3$
- 134 ($j_{15/2}$-$g_{9/2}$)
- 196 ($k_{17/2}$-$h_{11/2}$)

Static octupole correlations

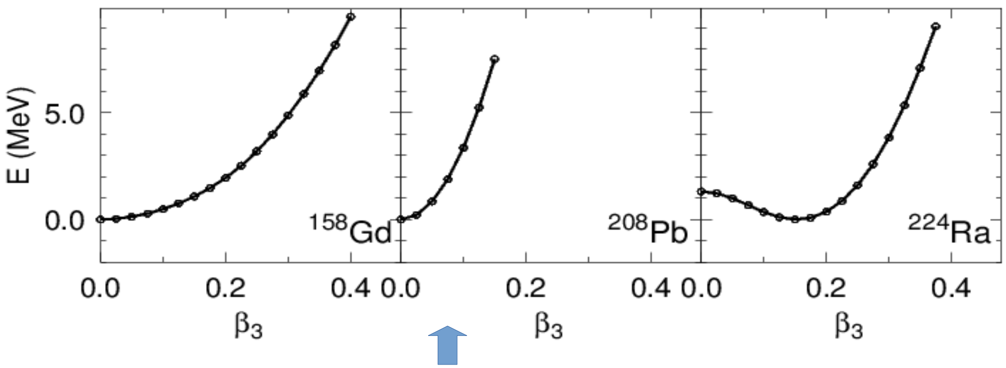




LM Robledo and GF Bertsch, Phys. Rev. C **84**, 054302

Y. Cao et al Phys Rev C**102**, 024311 (2020)

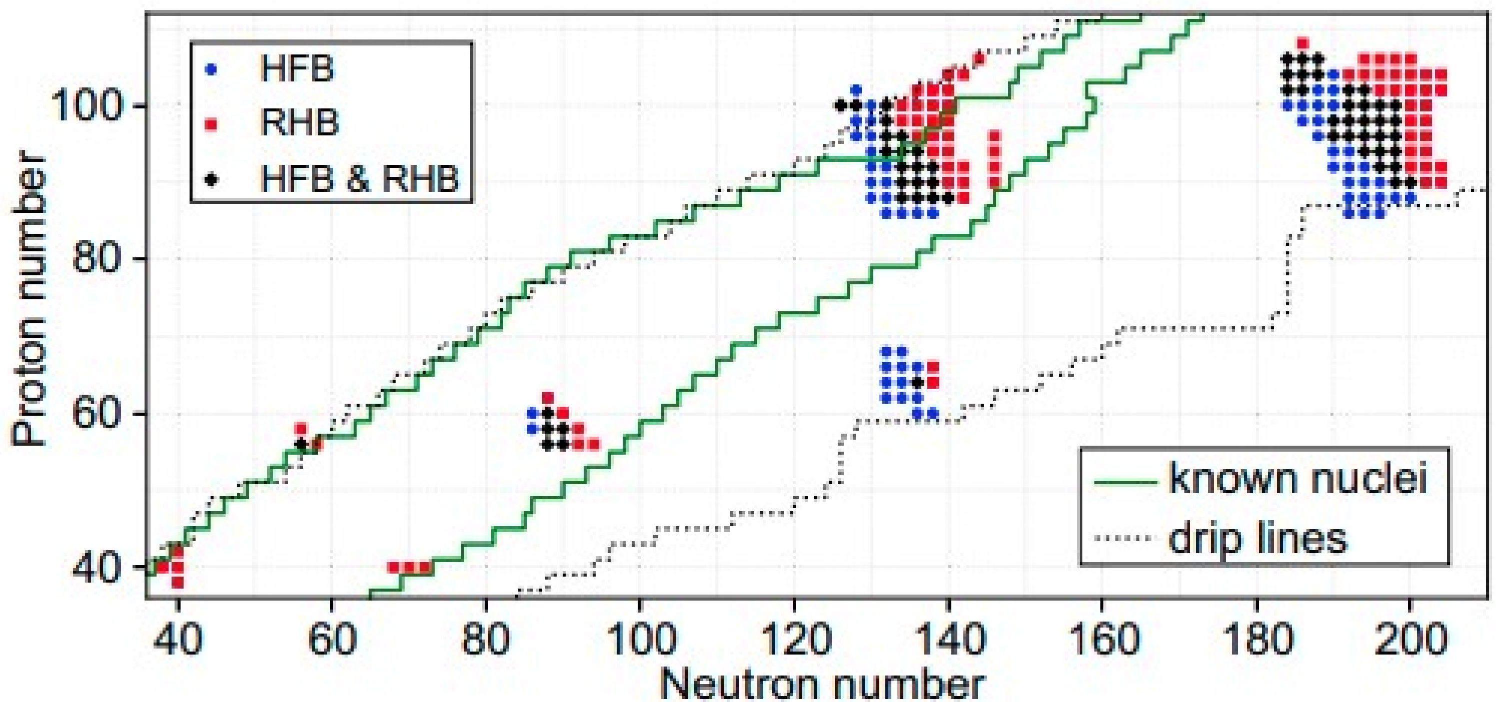
Permanent octupole deformation



Gogny D1S HFB results

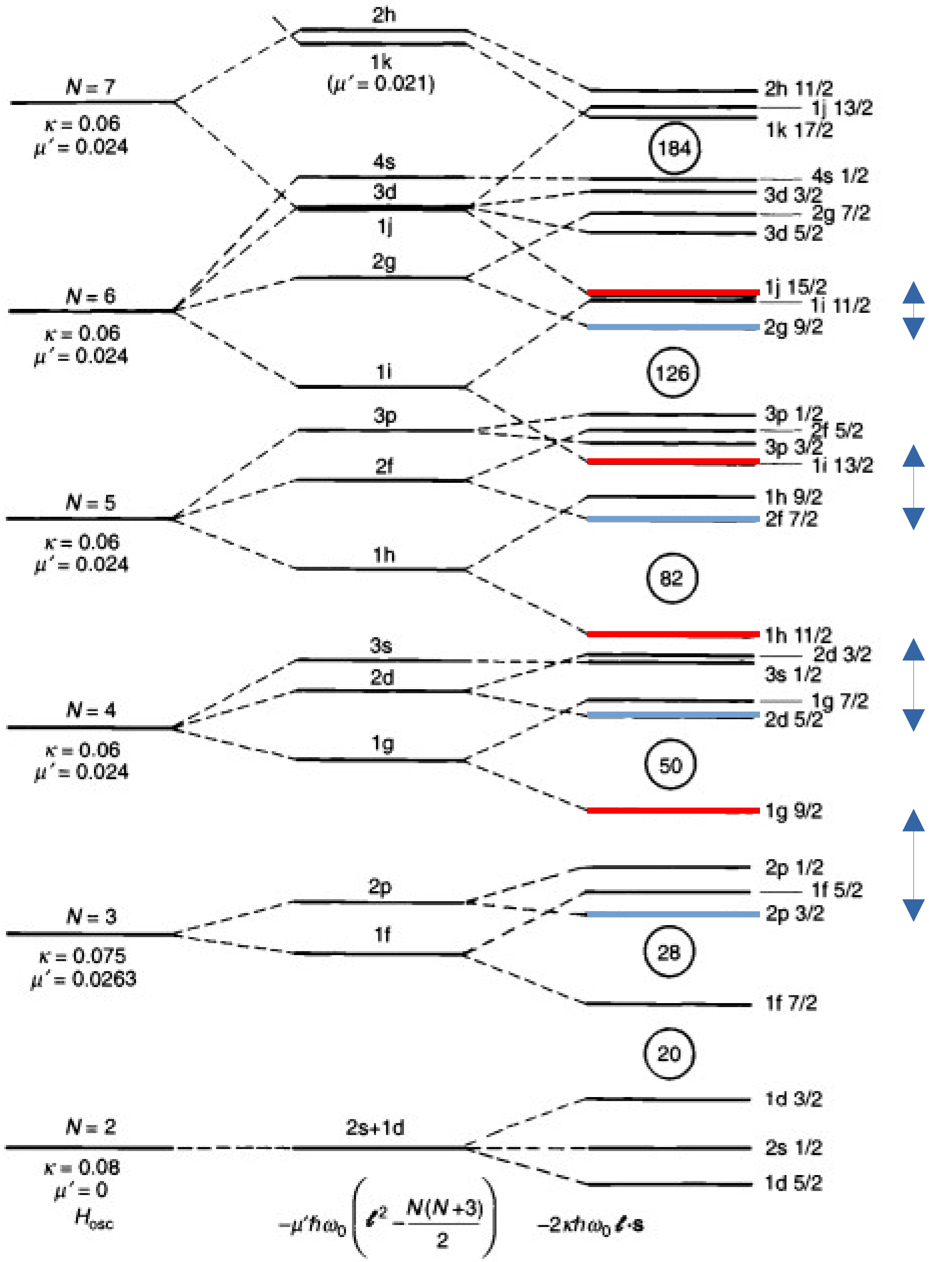
Octupole magic numbers

- 34 $(g_{9/2}$-$p_{3/2})$ 40 ?
- 56 $(h_{11/2}$-$d_{5/2})$
- 88 $(i_{13/2}$-$f_{7/2})$
- 134 $(j_{15/2}$-$g_{9/2})$
- 196 $(k_{17/2}$-$h_{11/2})$



Y. Cao et al Phys Rev C 102, 024311 (2020)

HFB means non-relativistic with Skyrme interactions

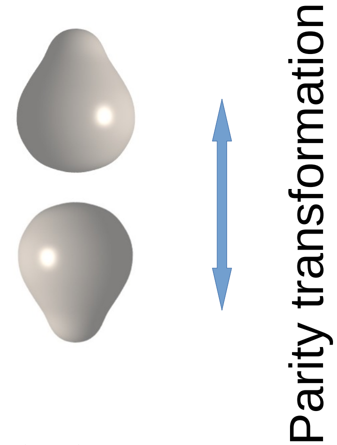


N = 7
κ = 0.06
μ' = 0.024
N = 6
κ = 0.06
μ' = 0.024
N = 5
κ = 0.06
μ' = 0.024
N = 4
κ = 0.06
μ' = 0.024
N = 3
κ = 0.075
μ' = 0.0263
N = 2
κ = 0.08
μ' = 0
H_osc
2h
1k
(μ' = 0.021)
4s
3d
1j
2g
1i
3p
2f
1h
3s
2d
1g
2p
1f
2s+1d
−μ'ħω₀ (ℓ² − N(N+3)/2)
−2κħω₀ ℓ·s
2h 11/2
1j 13/2
1k 17/2
184
4s 1/2
3d 3/2
2g 7/2
3d 5/2
1j 15/2
1i 11/2
2g 9/2
126
3p 1/2
2f 5/2
3p 3/2
1i 13/2
1h 9/2
2f 7/2
82
1h 11/2
2d 3/2
3s 1/2
1g 7/2
2d 5/2
50
1g 9/2
2p 1/2
1f 5/2
2p 3/2
28
1f 7/2
20
1d 3/2
2s 1/2
1d 5/2

Symmetry restoration and dynamic octupole correlations

Parity symmetry is broken when $\beta_3 \neq 0$ $\quad |\varphi(\beta_3)\rangle$

The application of the symmetry operator to the intrinsic wave function changes the orientation $\quad \hat{\Pi}|\varphi(\beta_3)\rangle$



Both states have the same intrinsic energy

$$\langle\varphi(\beta_3)|\hat{H}|\varphi(\beta_3)\rangle = \langle\varphi(\beta_3)|\hat{\Pi}\hat{H}\hat{\Pi}|\varphi(\beta_3)\rangle$$

Taking the appropriate linear combination of the two shapes the symmetry is restored

$$|\Psi_\pi\rangle = \mathcal{N}_\pi(1+\pi\hat{\Pi})|\varphi(\beta_3)\rangle \quad \pi = \pm 1 \quad \Rightarrow \quad \hat{\Pi}|\Psi_\pi\rangle = \pi|\Psi_\pi\rangle$$

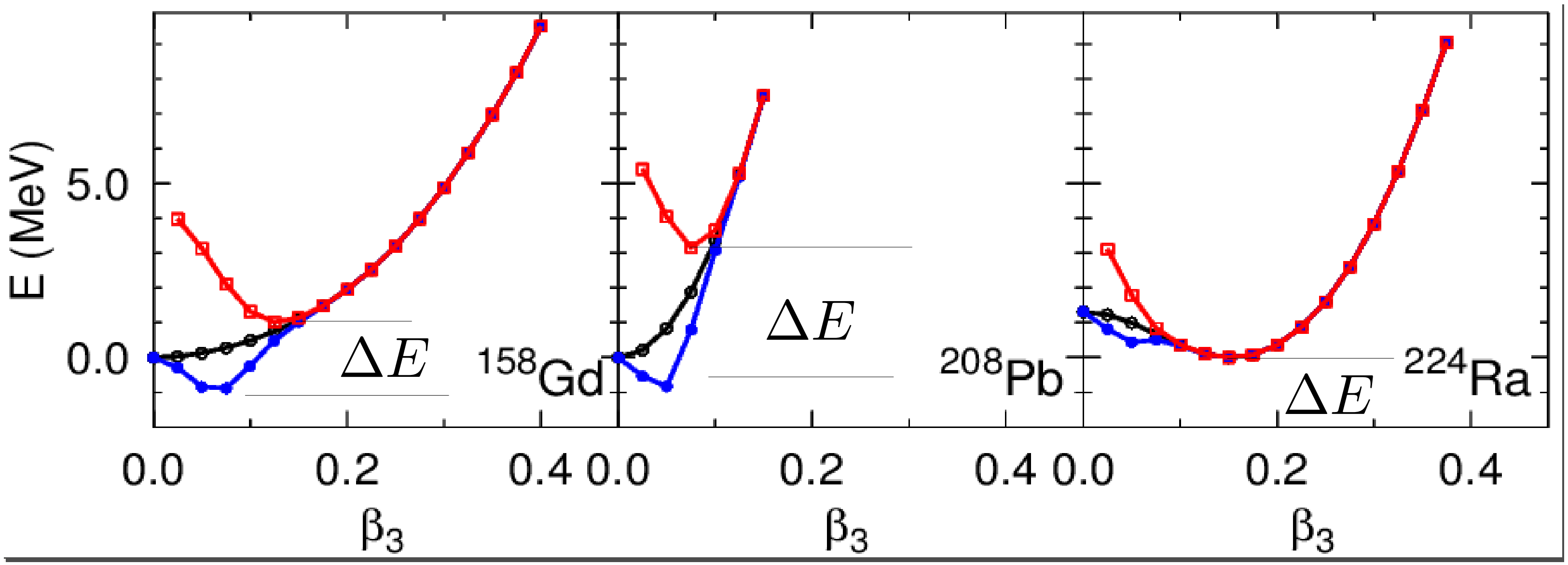
The procedure works because of the **special properties** (group theory) of the symmetry operator $\quad \hat{\Pi}^2 = 1$

Parity restoration is so simple because it is a discrete symmetry. The symmetry group is made of two elements: identity and parity and it is Abelian (1D irreps). Life gets a bit more involved for continuous symmetries …

First step beyond the mean field: Parity projection

Dynamic octupole correlation energies

Static correlations



Excitation energy of K=0$^-$ band

$$\Delta E = E_+(\beta_3(+)) - E_-(\beta_3(-))$$

Ground state correlation energy: non zero for reflection symmetric mean field ground states. Dynamic correlations imply non-zero intrinsic octupole moment even in 208Pb !

Static versus dynamic

Second step beyond mean field: configuration mixing

Flat energy surfaces imply **configuration mixing** can lower the ground state energy

Generator Coordinate Method (GCM) ansatz

$$|\Psi_\sigma\rangle = \int dQ_{30}\, f_\sigma(Q_{30})|\varphi(Q_{30})\rangle$$

The amplitude $f_\sigma(Q_{30})$ has good parity under the exchange $Q_{30} \to -Q_{30}$

Parity projection recovered with $f_\pm(Q_{30}) = \delta(Q_{30} - Q'_{30}) \pm \delta(Q_{30} + Q'_{30})$

Energies and amplitudes solution of the **Hill-Wheeler equation**

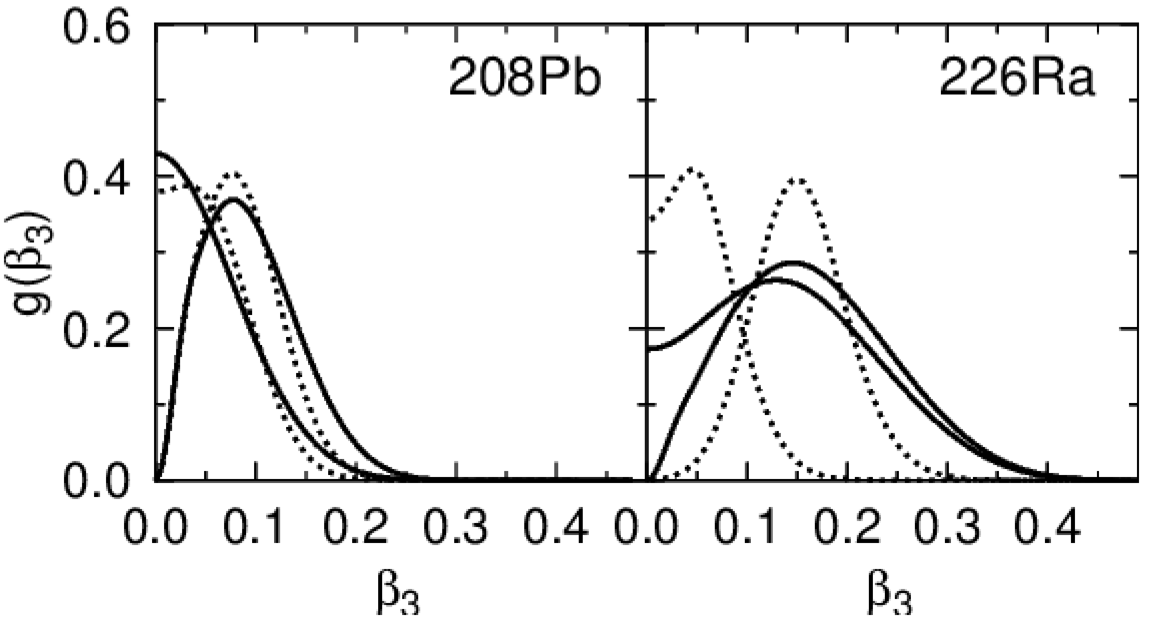
$$\int dQ'_{30} \mathcal{H}(Q_{30}, Q'_{30}) f_\sigma(Q'_{30}) = E_\sigma \int dQ'_{30} \mathcal{N}(Q_{30}, Q'_{30}) f_\sigma(Q'_{30})$$

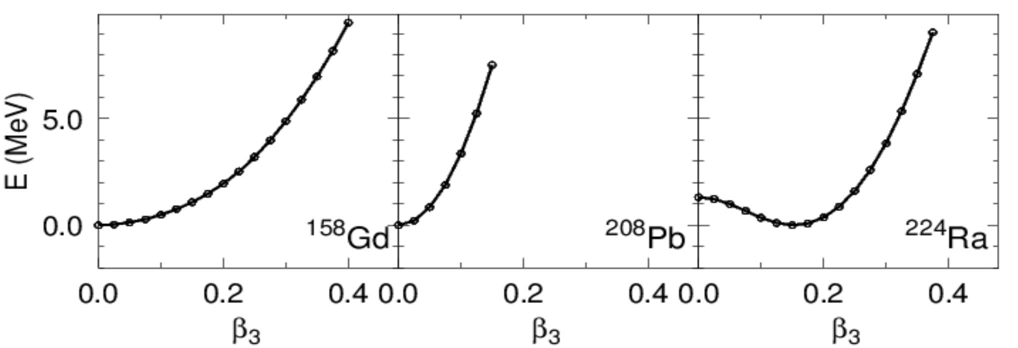
Collective wave functions $g_\sigma(\beta_3) = \int d\beta'_3\, \mathcal{N}^{1/2}(\beta_3, \beta'_3)\, f_\sigma(\beta'_3)$

Under some conditions in the norm the complicated HW equation reduces to a **collective Schrodinger-like equation** where Q_{30} is the coordinate

Second step beyond mean field: configuration mixing

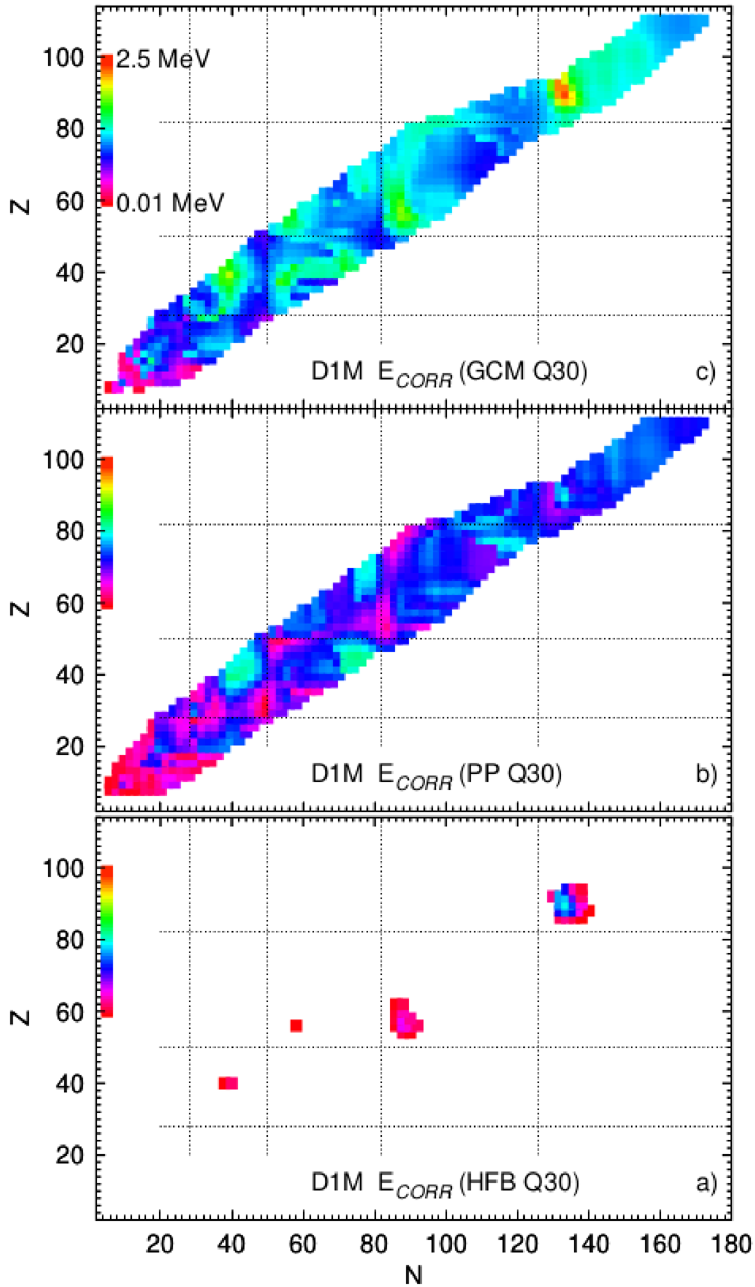
Collective wave functions $$g_\sigma(\beta_3) = \int d\beta_3' \, \mathcal{N}^{1/2}(\beta_3, \beta_3') \, f_\sigma(\beta_3')$$





Static and dynamic octupole correlations

J. Phys. G: Nucl. Part. Phys. 42 (2015) 055109



Static octupole correlations are only present in a very restricted set of nuclei

Dynamic octupole correlations associated to symmetry restoration (parity) are present everywhere (represent around 0.8 MeV)

Dynamic octupole correlations associated to fluctuations in the octupole degree of freedom are present everywhere (around 1 MeV extra)

- Beyond mean field effects are relevant for binding energies

Calculations were restricted to a limited set of around 800 even-even nuclei not too far from the stability line. Exploratory calculations in very neutron rich nuclei indicate the same trend.

Some reflections

- It would be very interesting to analyze the changes in the **spatial matter distribution** after symmetry restoration and configuration mixing

- Not a common chore in standard nuclear structure calculations

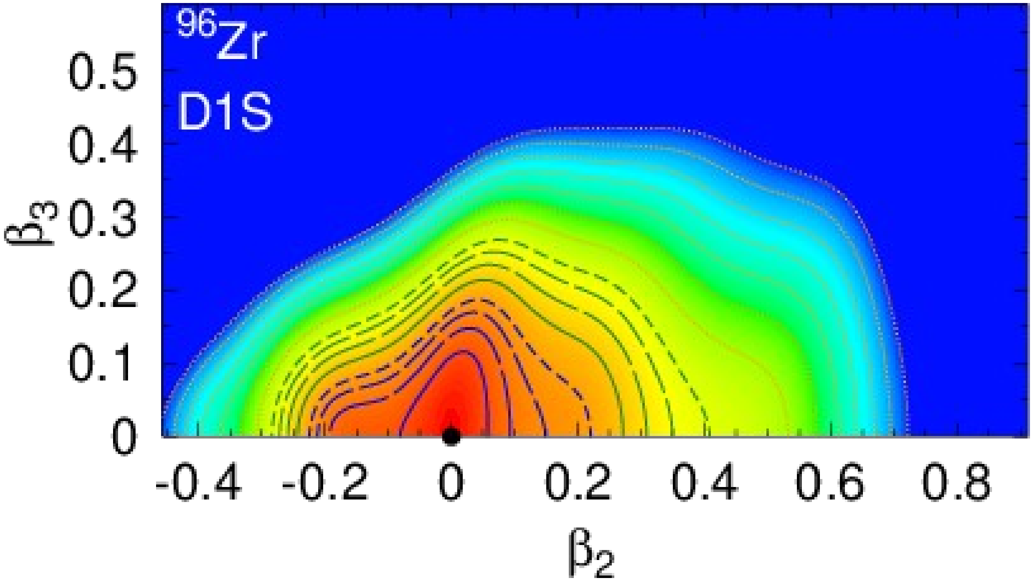
- Computationally intensive

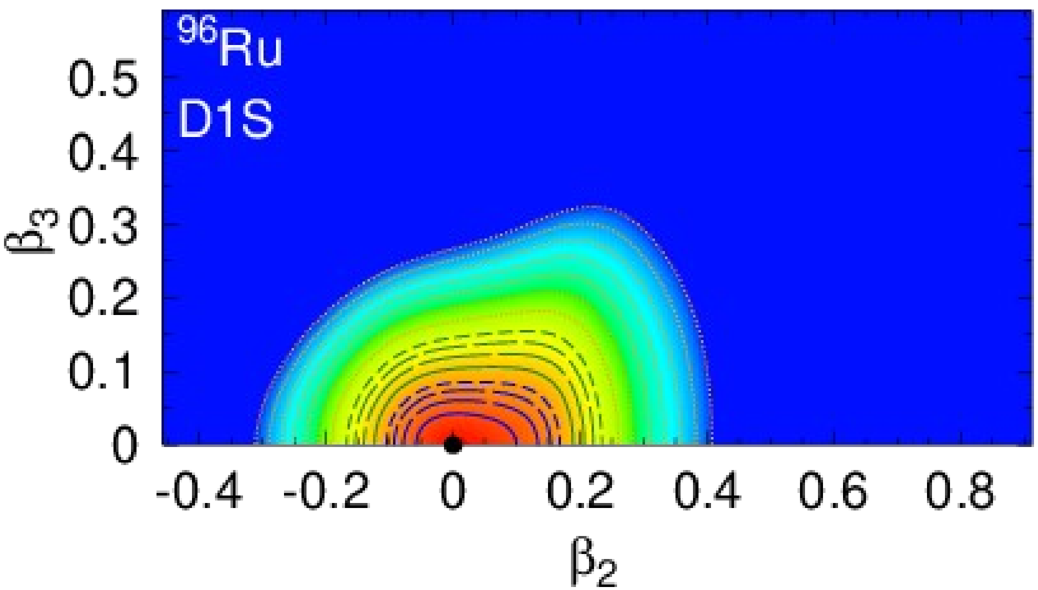
- **Analyze the role of LAB density in the Glauber Montecarlo Model used to study the flux anisotropies**

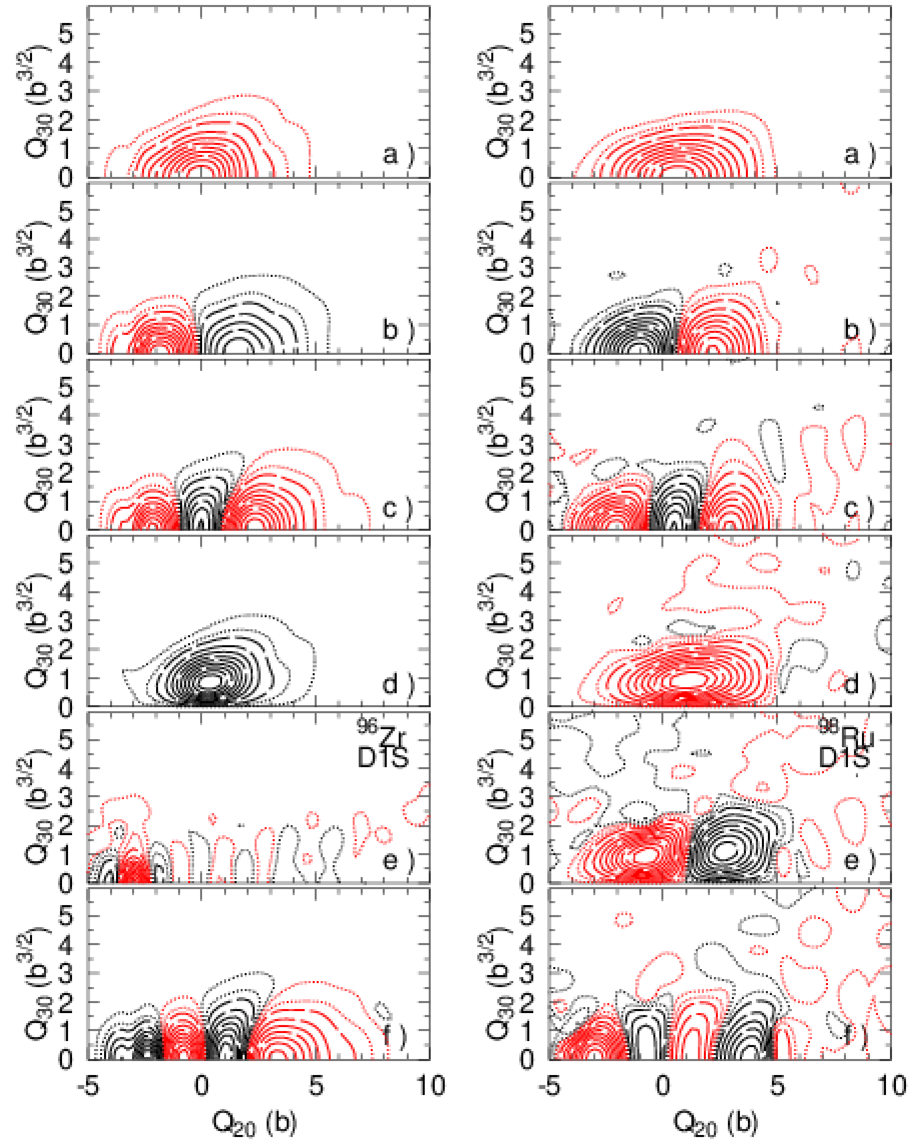
- Perhaps it could be the clue to solve the 96Zr puzzle

  - HI analysis point to an octupole deformed nucleus
  - Nuclear structure also point to strong octupole correlations
  - Calculations point to dynamic instead of static octupole correlations

Quadrupole-Octupole coupling: 96Zr and 96Ru

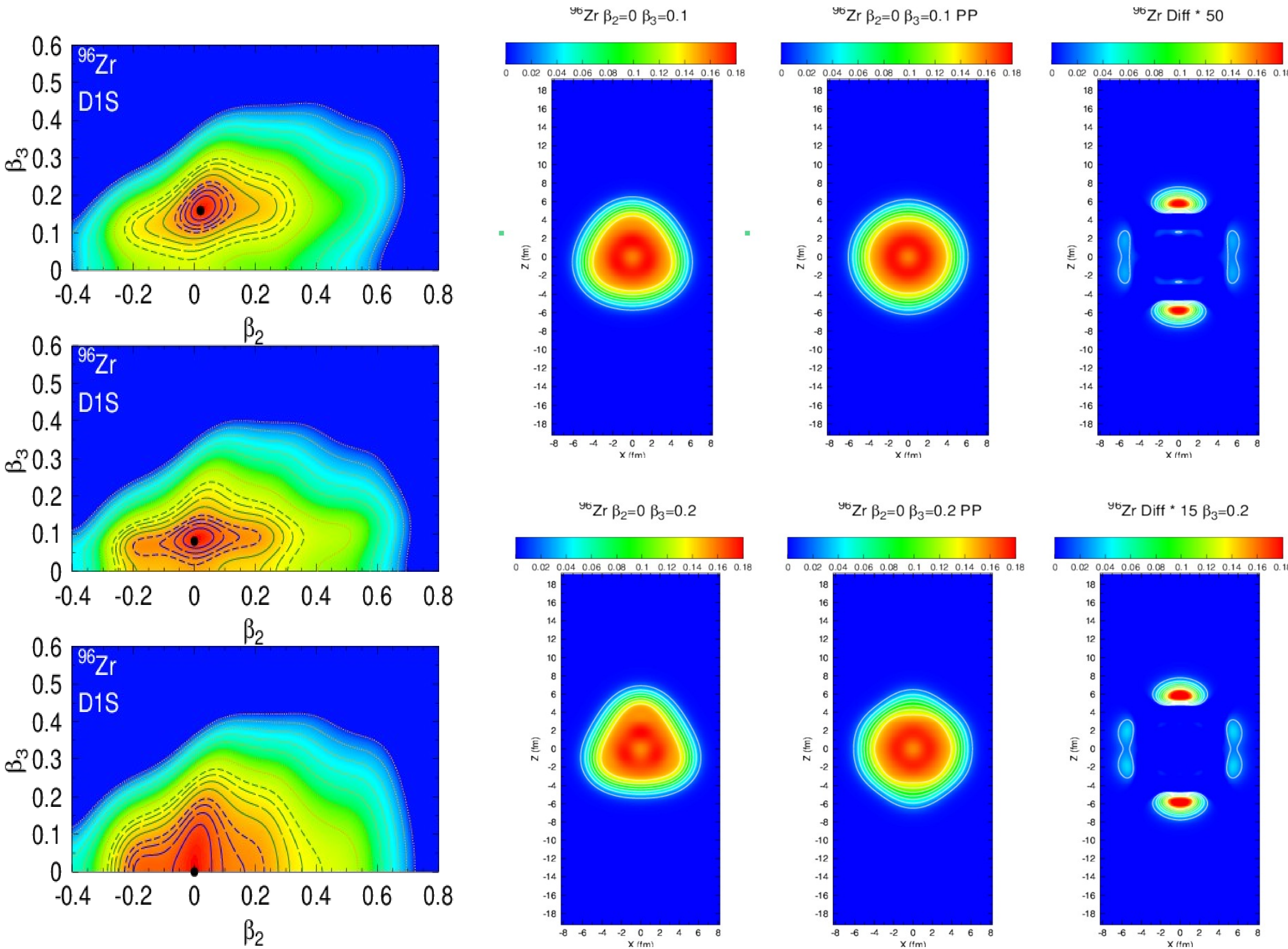






Zr puzzle: 96Zr, lowest 3- energy in the N=56 isotonic chain and largest B(E3)

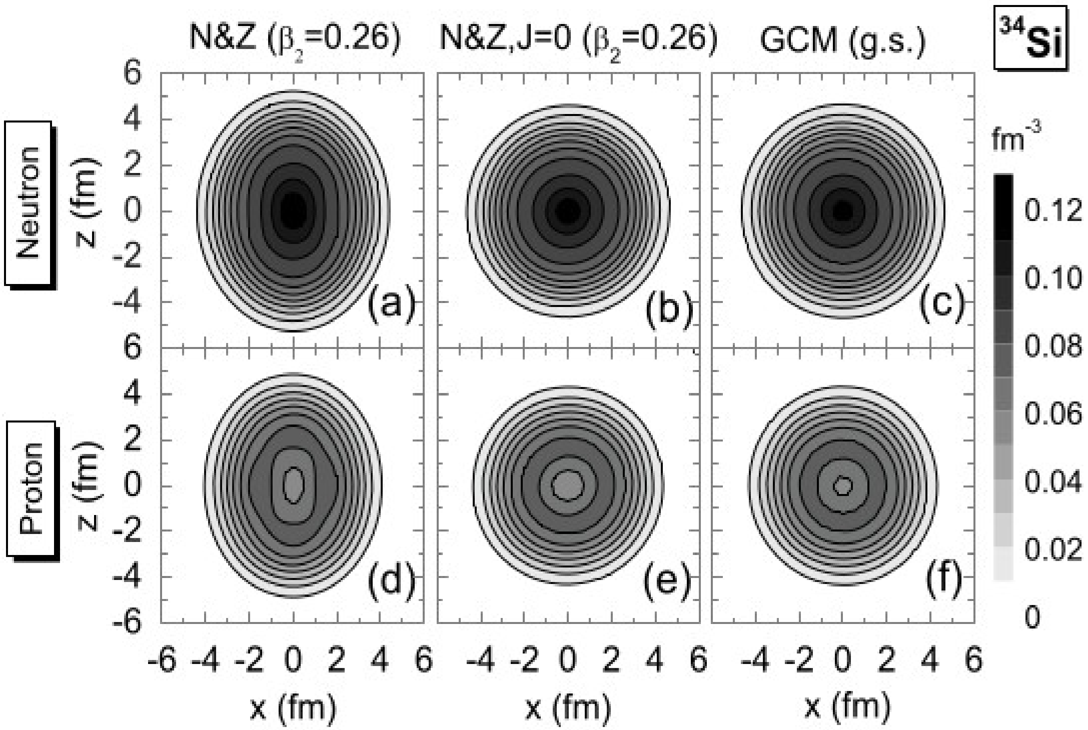
96Ru is spherical (but 098Zr deformed)



^{96}Zr
D1S
β_3
β_2
^{96}Zr β_2=0 β_3=0.1
^{96}Zr β_2=0 β_3=0.1 PP
^{96}Zr Diff * 50
^{96}Zr β_2=0 β_3=0.2
^{96}Zr β_2=0 β_3=0.2 PP
^{96}Zr Diff * 15 β_3=0.2
Z (fm)
X (fm)

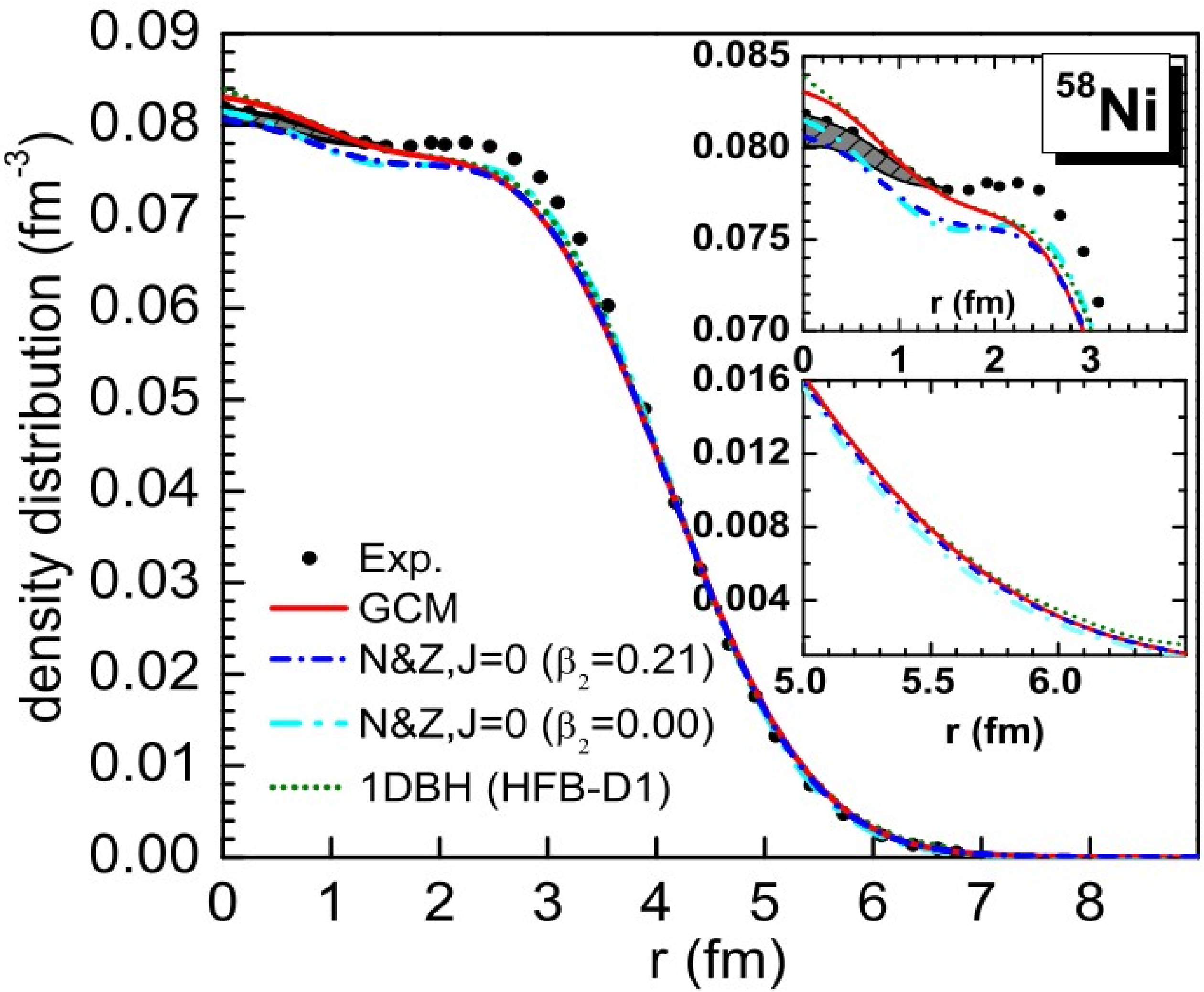
Angular momentum projection in 34Si

YAO, BARONI, BENDER, AND HEENEN



PHYSICAL REVIEW C **86**, 014310 (2012)

Symmetry restoration in 58Ni



J. M. YAO, M. BENDER, AND P.-H. HEENEN

PHYSICAL REVIEW C **91**, 024301 (2015)

State of the art microscopic description

Our goal is to describe octupole correlations in an unified framework to treat in the same footing vibrations, octupole deformed states and any intermediate situation

- The use of an "universal" interaction (EDF) is required for predictability
- Based on Hartree Fock Bogoliubov (HFB) intrinsic states. Must be flexible enough to accommodate many physical situations like quadrupole and octupole coupling

$$|\Phi(Q_2, Q_3)\rangle$$

- Symmetry restoration:

Can be avoided if the nucleus is strongly deformed (Rotational model)

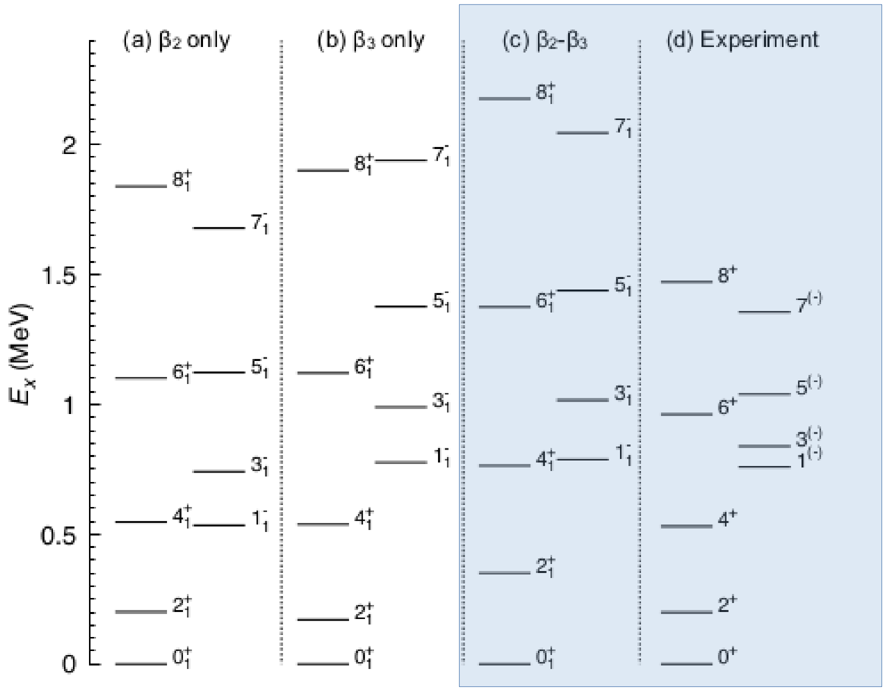
  - Angular momentum projection P^J
  - Particle Number projection P^N
  - Parity projection P^π

- Configuration mixing

$$|\Psi_\sigma\rangle = \int dQ_2 dQ_3 \, f_\sigma(Q_2, Q_3) P^J P^N P^\pi |\Phi(Q_2, Q_3)\rangle$$

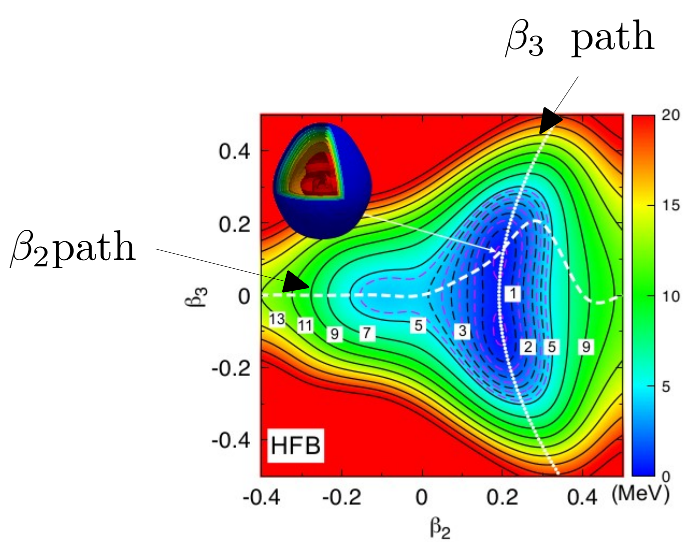
144Ba

Recent experimental data from *B. Bucher et al PRL 116, 112503 (2016)*



$J_i^\pi \to J_f^\pi$	$E\lambda$	GCM β_2	GCM β_3	GCM $\beta_2-\beta_3$	Exp
$0^+ \to 2^+$	E2	1.148	1.121	1.023	1.042^{+17}_{-22}
$2^+ \to 4^+$	E2	1.865	1.803	1.845	1.860^{+86}_{-81}
$4^+ \to 6^+$	E2	2.371	2.287	2.360	1.78^{+12}_{-10}
$6^+ \to 8^+$	E2	2.800	2.696	2.793	2.04^{+35}_{-23}
$0^+ \to 1^-$	E1	0.007	0.006	0.008	
$1^- \to 2^+$	E1	0.005	0.009	0.006	
$0^+ \to 3^-$	E3	0.450	0.477	0.460	0.65^{+17}_{-23}
$1^- \to 4^+$	E3	0.599	0.635	0.695	
$2^+ \to 5^-$	E3	0.708	0.745	0.810	< 1.2
$3^- \to 6^+$	E3	0.804	0.865	0.810	
$4^+ \to 7^-$	E3	0.887	0.945	1.031	< 1.6

TABLE I. Absolute values of the transition matrix elements $|\langle J_i^\pi||E\lambda||J_f^\pi\rangle|$ (in $eb^{\lambda/2}$) for several transitions of interest.



- Weakly deformed nucleus (both quadrupole and octupole) with strong Q_2-Q_3 coupling
- Good agreement for the 1^- excitation energy
- Wrong moments of inertia for rotational bands (understood: missing cranking-like states (*))
- Good transition strengths E2 and E3

(*) *PRC62, 054319; PLB746, 341*

Thank you for your attention !