Overview of Dynamic and static octupole correlations in atomic nuclei

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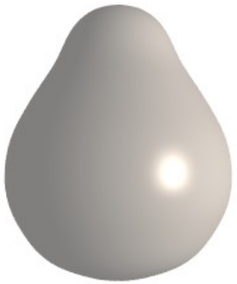
Octupole deformation is a relevant concept in nuclear structure of atomic nuclei

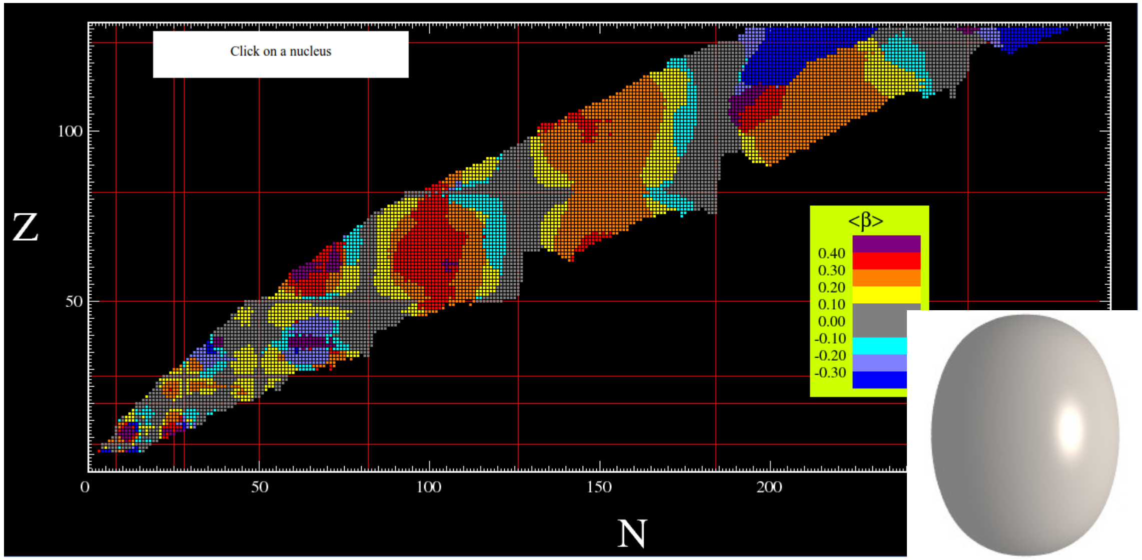
- *Next multipole moment after quadrupole (L=3)*
- *Breaks reflection symmetry (parity). Pear shape*
- *Parity doublets and alternating parity rotational bands*
- *Strong E3 electromagnetic transitions (E1 also but caution applies)*
- *Octupole ''magic'' numbers: 34, 56, 88, 134 and 196*

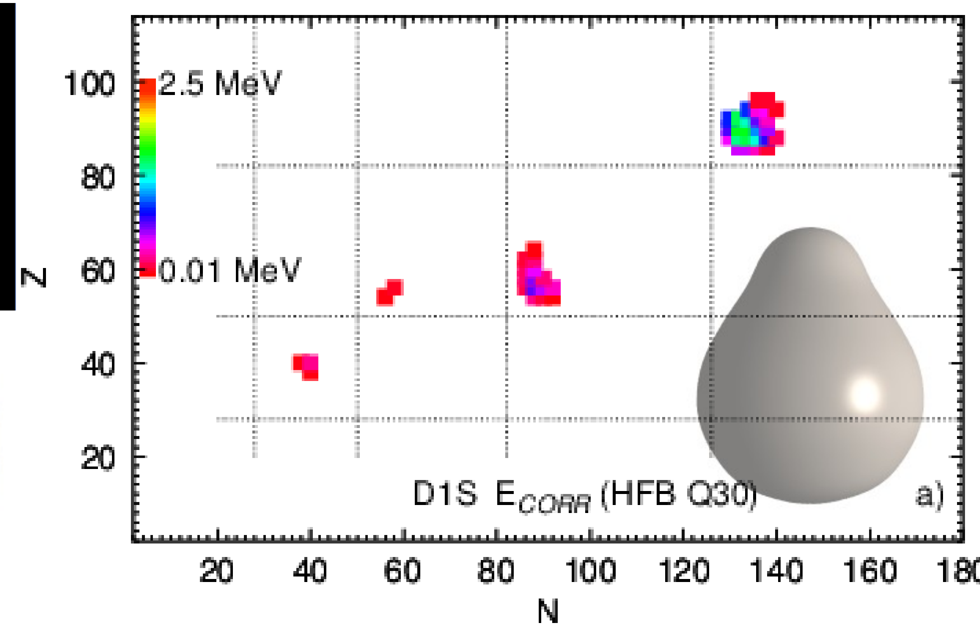


and also in other fields of research

- *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*

Octupoles 0.0





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

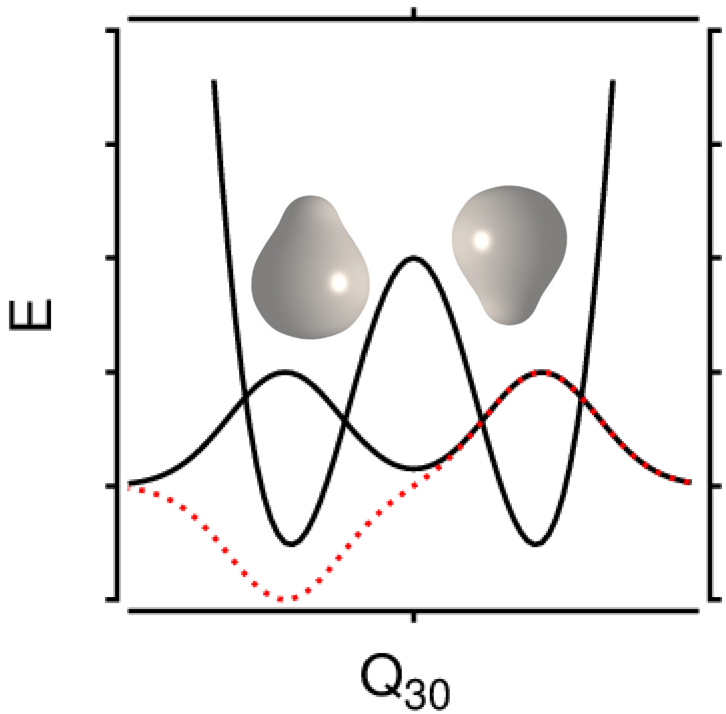
Deformation	L	Symmetry	Bands	Transitions
Quadrupole	2	Rotational	Rotational (J)	E2
Octupole	3	Parity	Parity doublets (π)	E1,E3

Order parameters

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

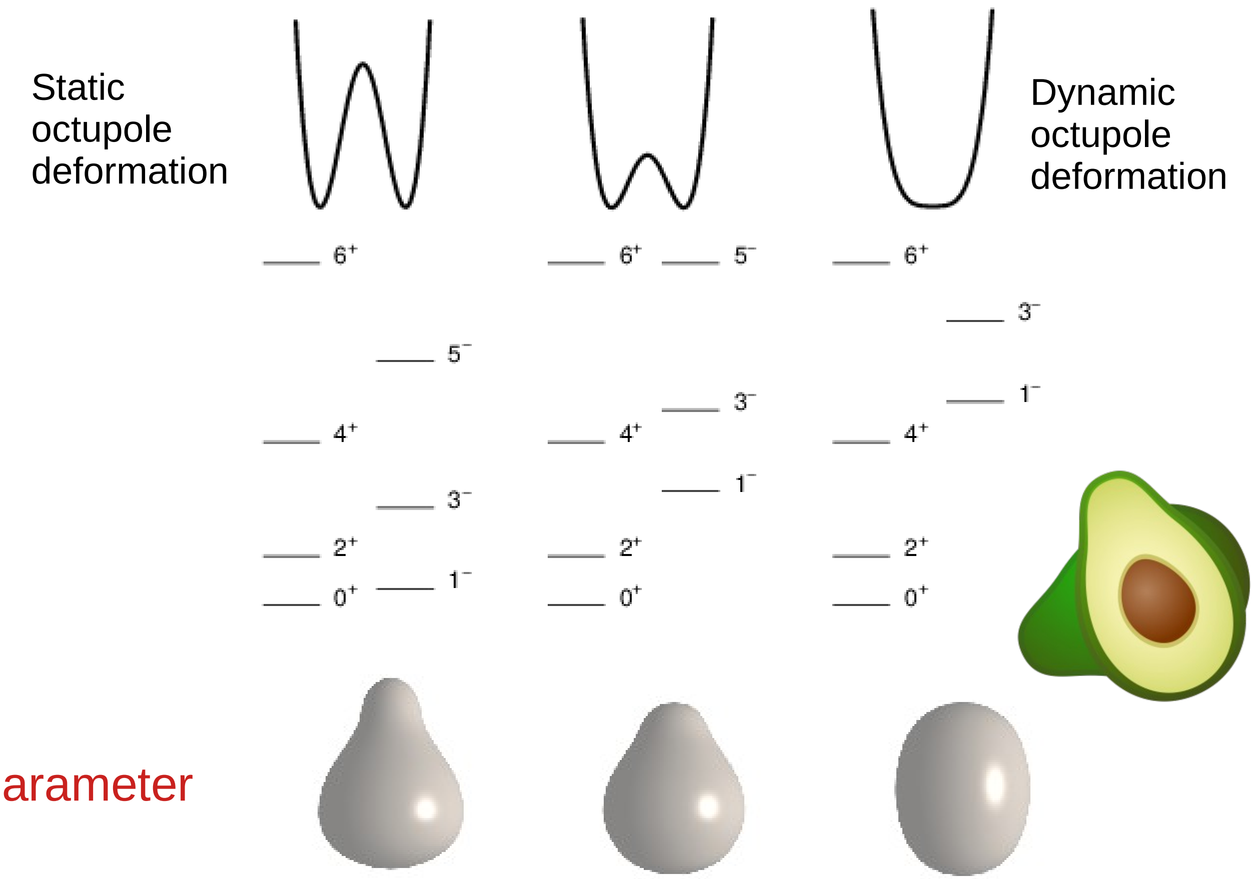
$$Q_{30} = z(z^2 - \frac{3}{2}r_\perp^2)$$

Octupoles 1.0 (Octupole deformation)



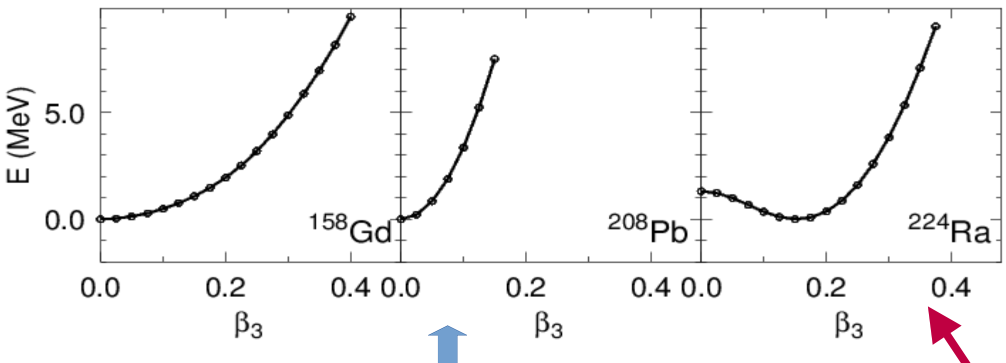
$$Q_{30} = z(z^2 - \frac{3}{2} r_\perp^2)$$

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

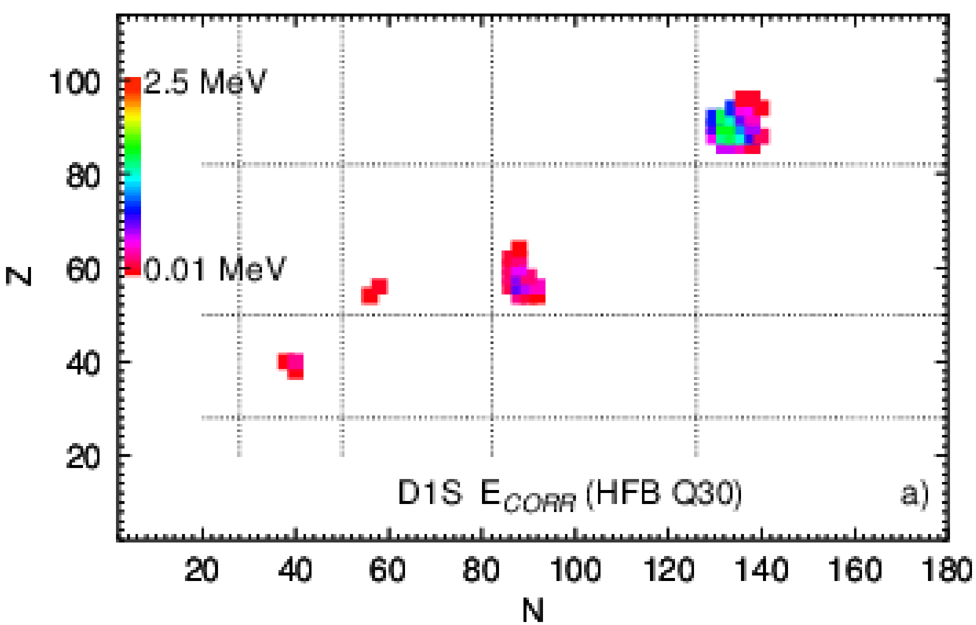


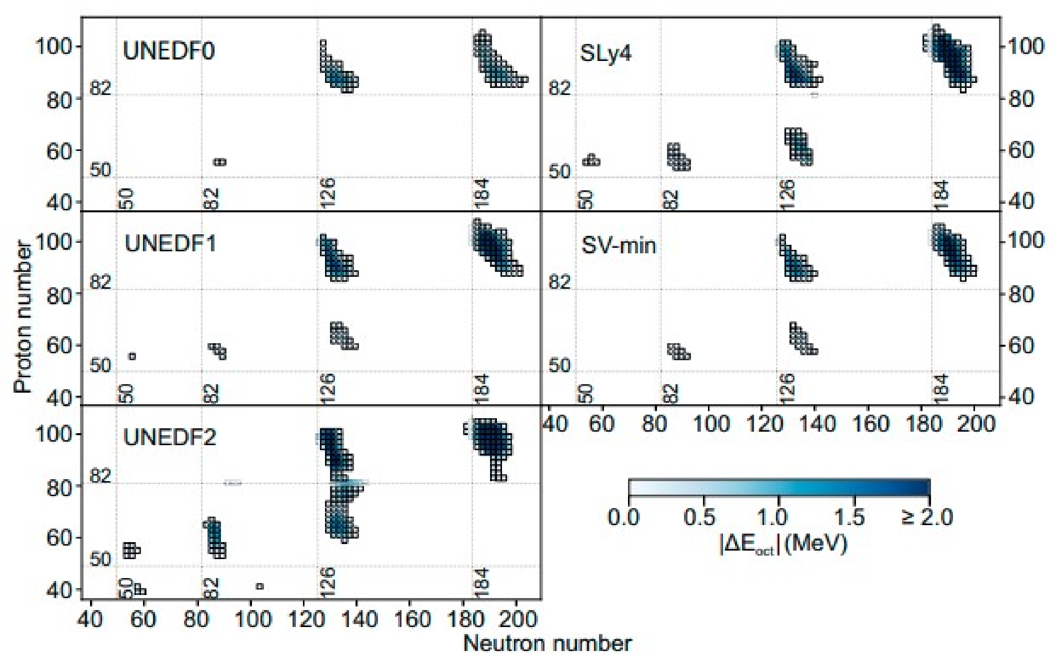
Gogny D1S HFB results

Octupole magic numbers

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

Static octupole correlations

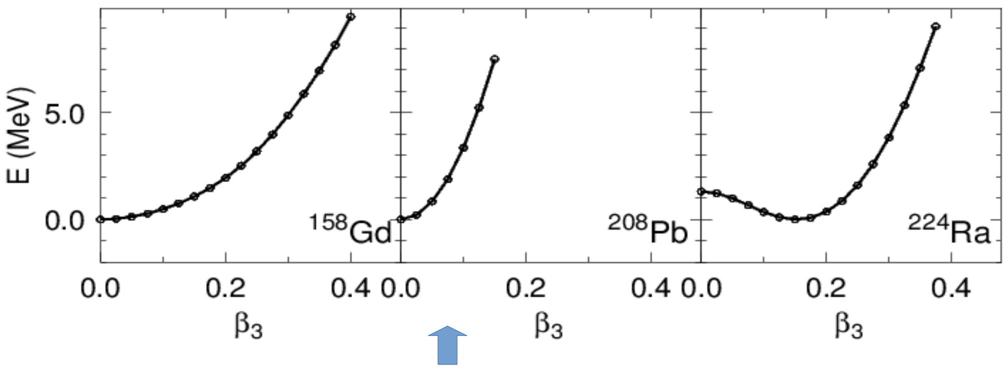




LM Robledo and GF Bertsch, Phys. Rev. C **84**, 054302

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

Permanent octupole deformation



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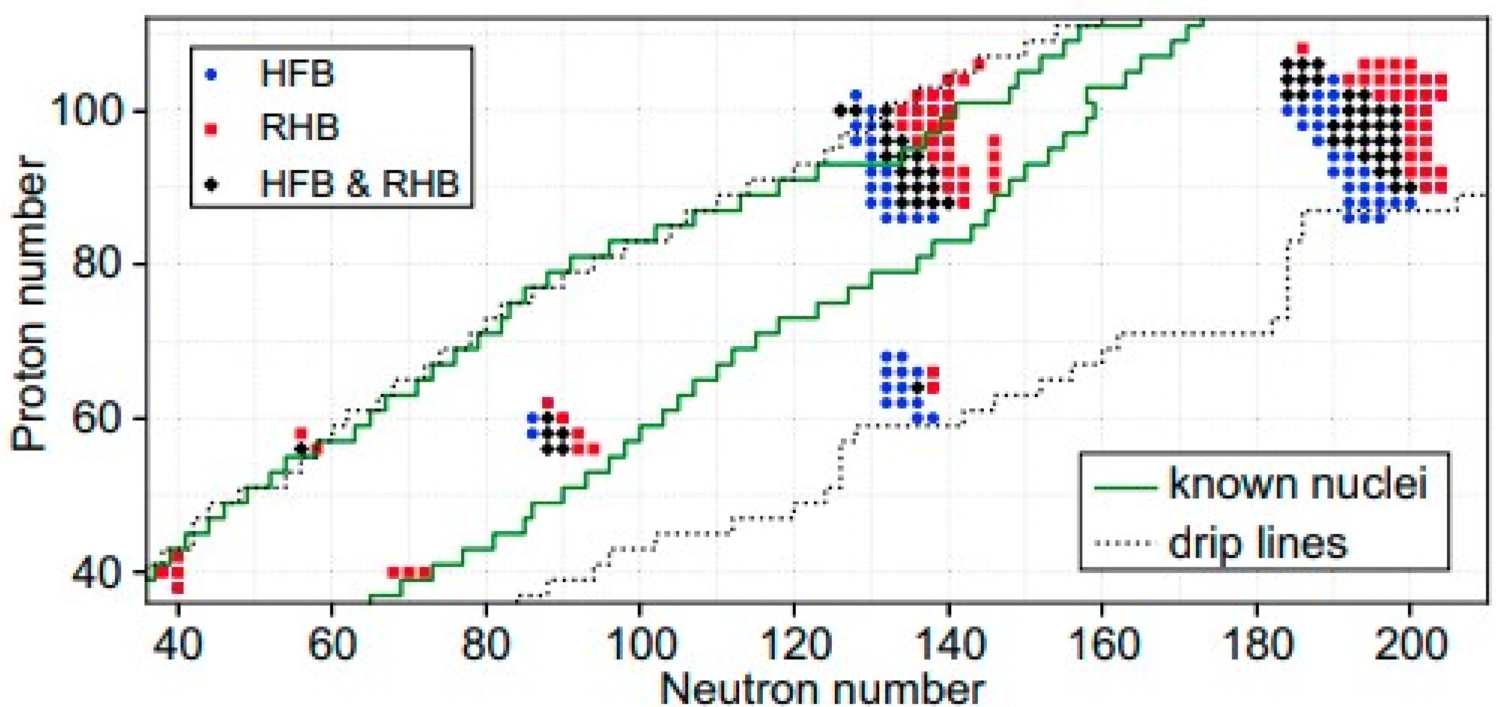
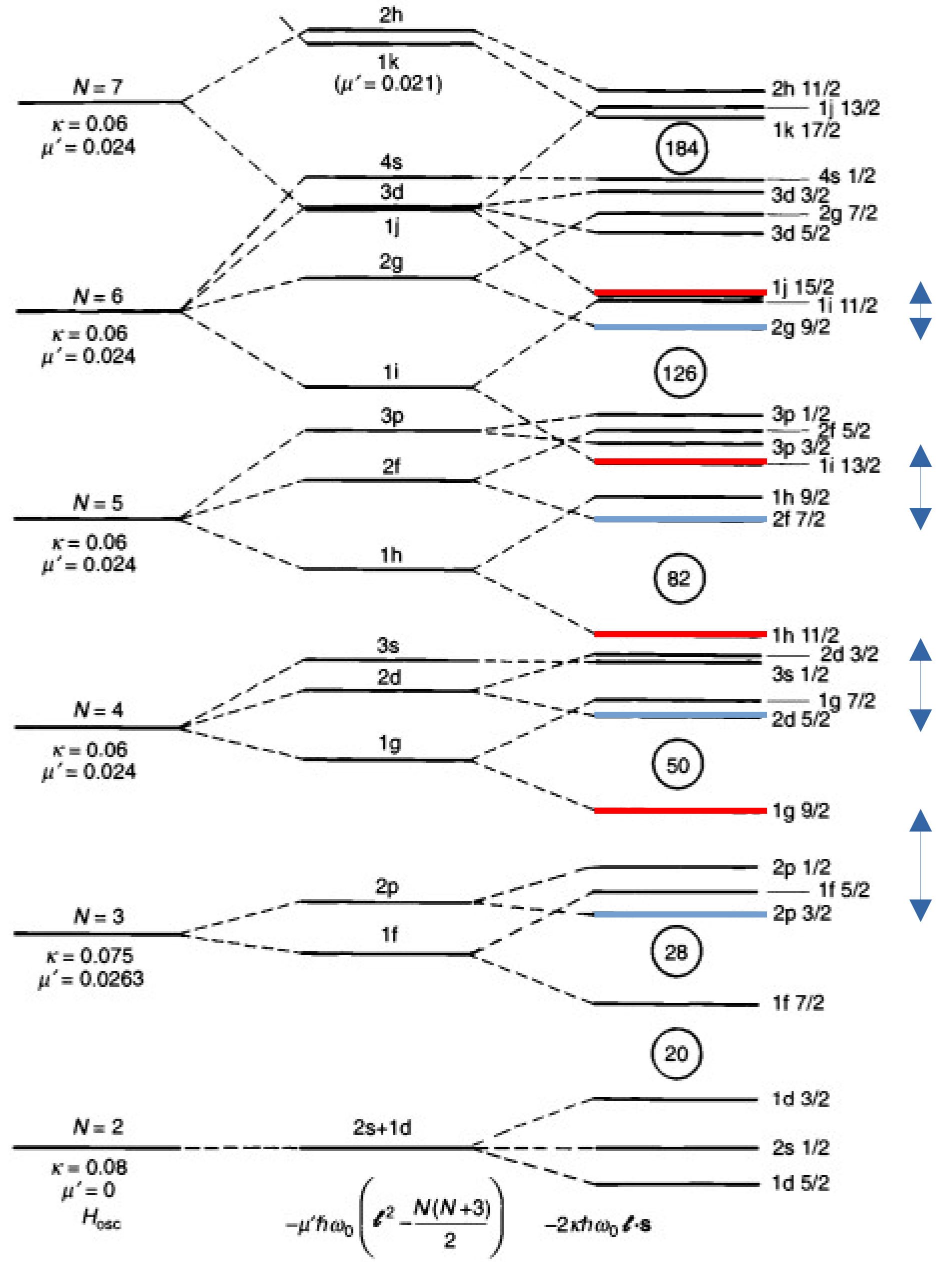


Y. Cao et al Phys Rev C 102, 024311 (2020)

HFB means non-relativistic with Skyrme interactions



N = 7
κ = 0.06
μ′ = 0.024
2h
1k
(μ′ = 0.021)
2h 11/2
1j 13/2
1k 17/2
184
4s
3d
1j
4s 1/2
3d 3/2
2g 7/2
3d 5/2
N = 6
κ = 0.06
μ′ = 0.024
2g
1j 15/2
1i 11/2
2g 9/2
1i
126
3p
2f
3p 1/2
2f 5/2
3p 3/2
1i 13/2
N = 5
κ = 0.06
μ′ = 0.024
1h 9/2
2f 7/2
1h
82
3s
2d
1h 11/2
2d 3/2
3s 1/2
1g 7/2
2d 5/2
N = 4
κ = 0.06
μ′ = 0.024
1g
50
1g 9/2
2p
2p 1/2
1f 5/2
2p 3/2
N = 3
κ = 0.075
μ′ = 0.0263
1f
28
1f 7/2
20
1d 3/2
N = 2
κ = 0.08
μ′ = 0
2s+1d
2s 1/2
1d 5/2
H_{osc}
$-\mu'\hbar\omega_0\left(\ell^2 - \frac{N(N+3)}{2}\right)$
$-2\kappa\hbar\omega_0\,\ell\cdot s$

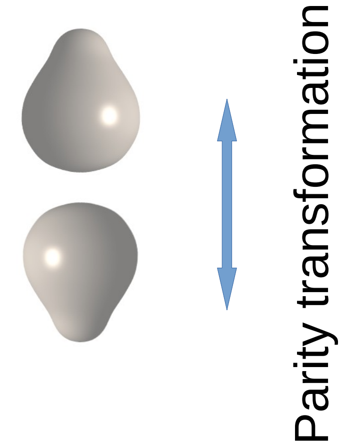
Symmetry restoration and dynamic octupole correlations

Parity symmetry is broken when $\beta_3 \neq 0$

$$|\varphi(\beta_3)\rangle$$

The application of the symmetry operator to the intrinsic wave function changes the orientation

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



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

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

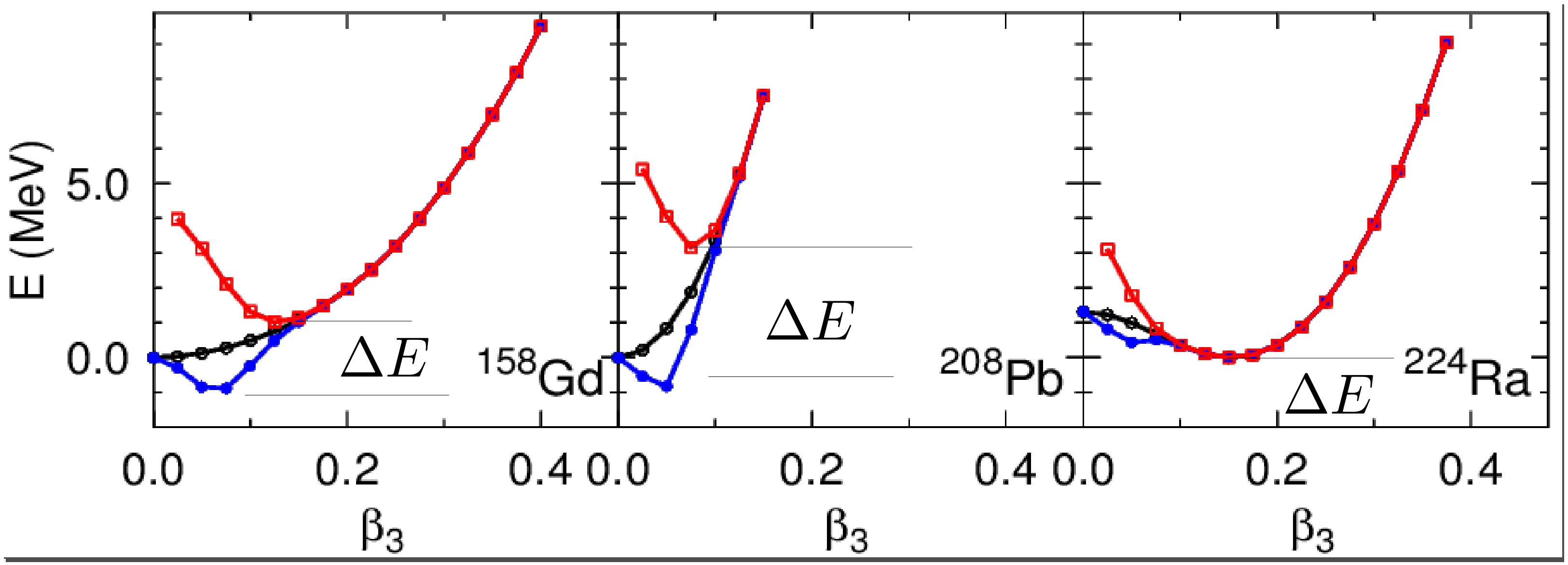
The procedure works because of the **special properties** (group theory) of the symmetry operator $\hat{\Pi}^2 = 1$

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**

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

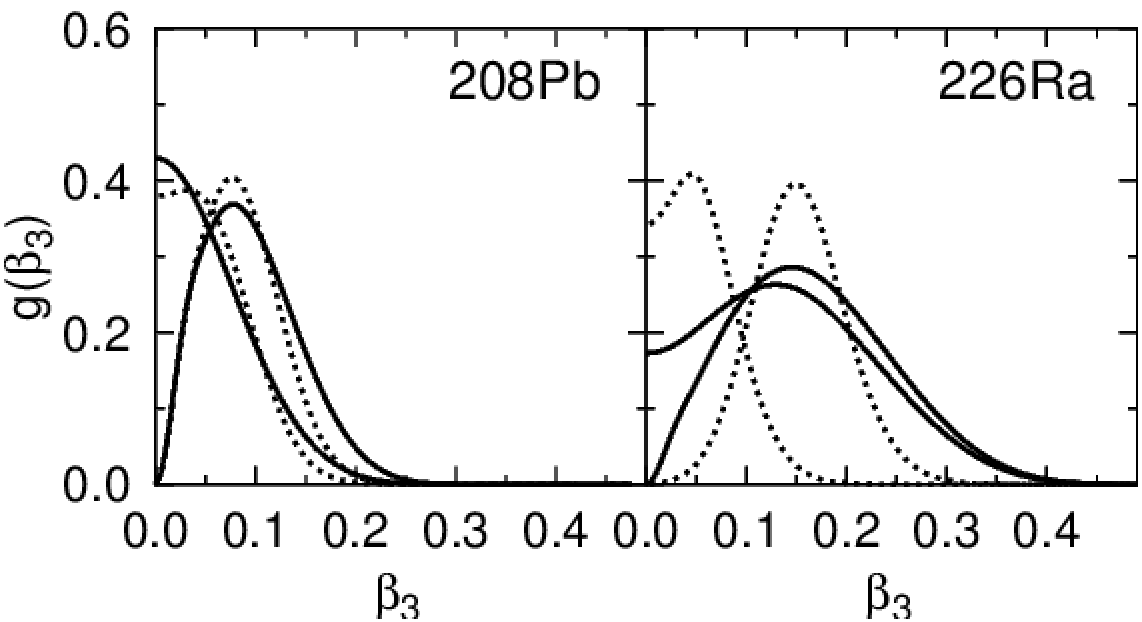
Collective wave functions $g_\sigma(\beta_3) = \int d\beta'_3\, \mathcal{N}^{1/2}(\beta_3, \beta'_3)\, f_\sigma(\beta'_3)$

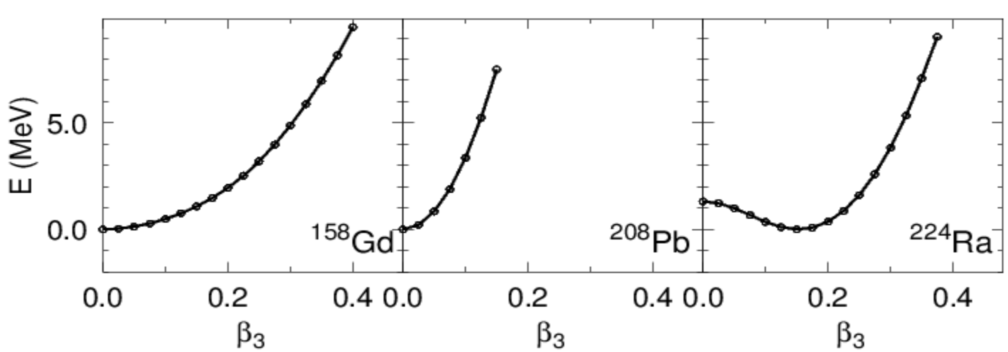
Under some conditions in the norm the complicated HW equation reduces to a **collective Schrodinger-like equation** where Q_{30} is the coordinate

Second step beyond mean field: configuration mixing

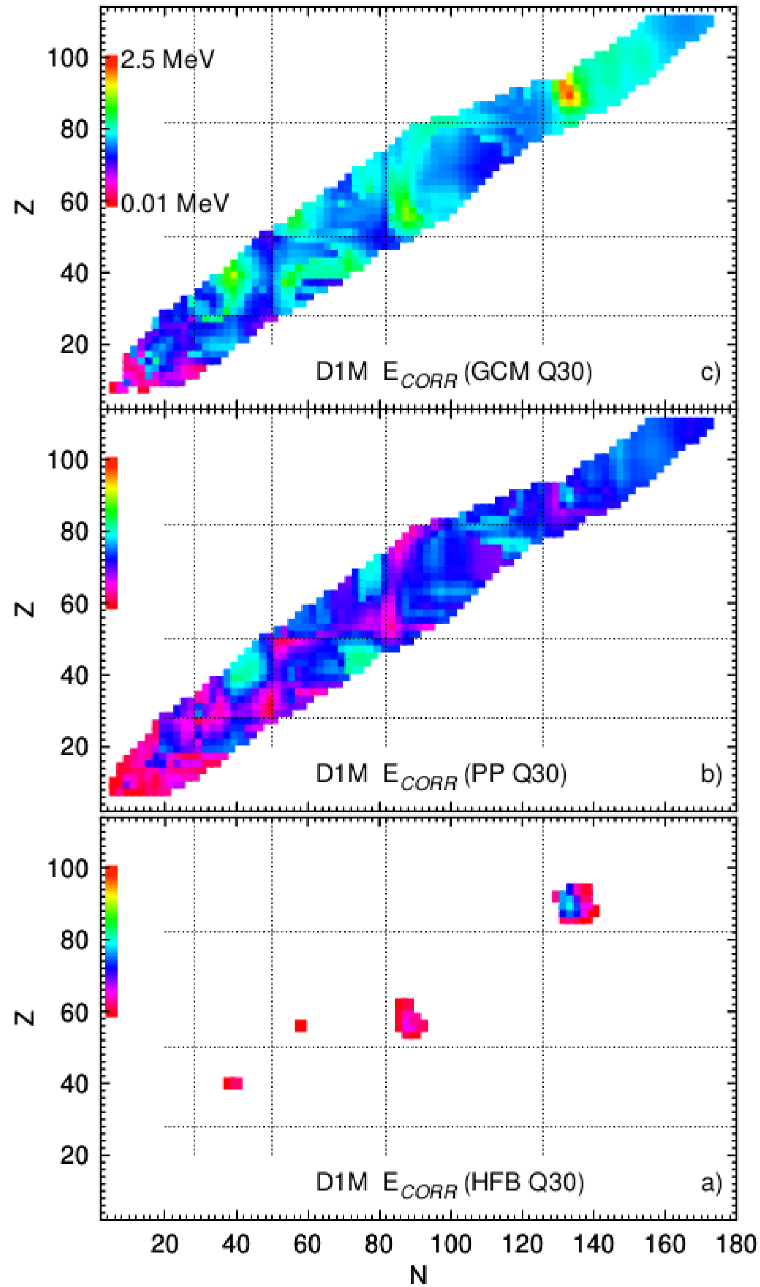
Collective wave functions

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





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

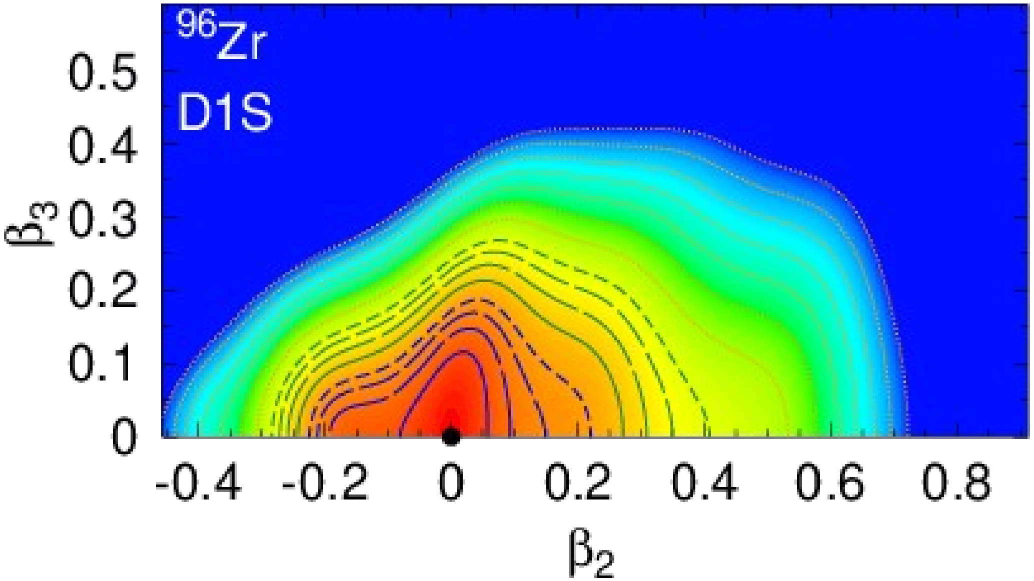
- Computationally intensive

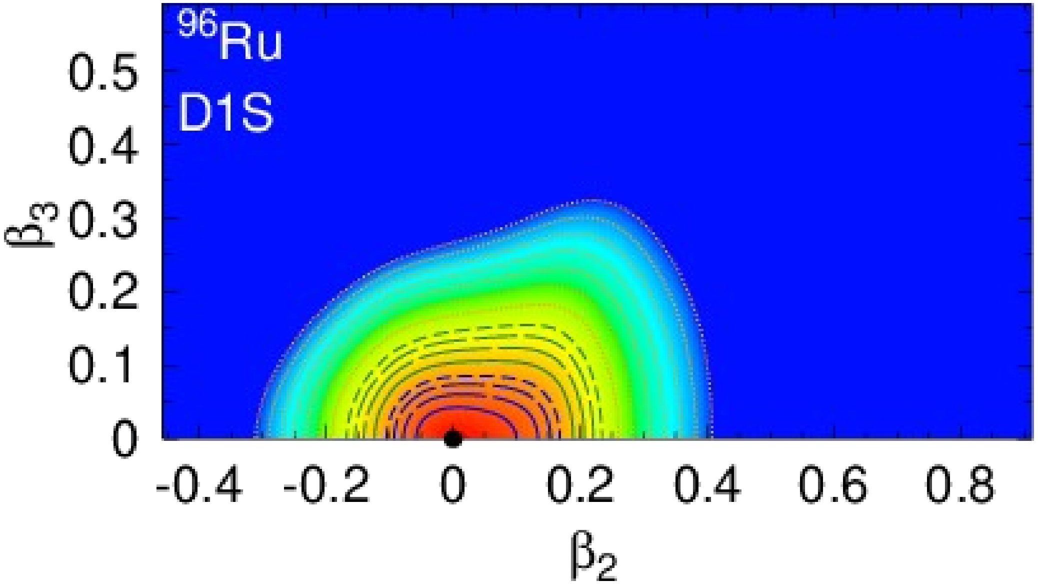
- **Analyze the role of LAB density in the Glauber Montecarlo Model used to study the flux anisotropies**

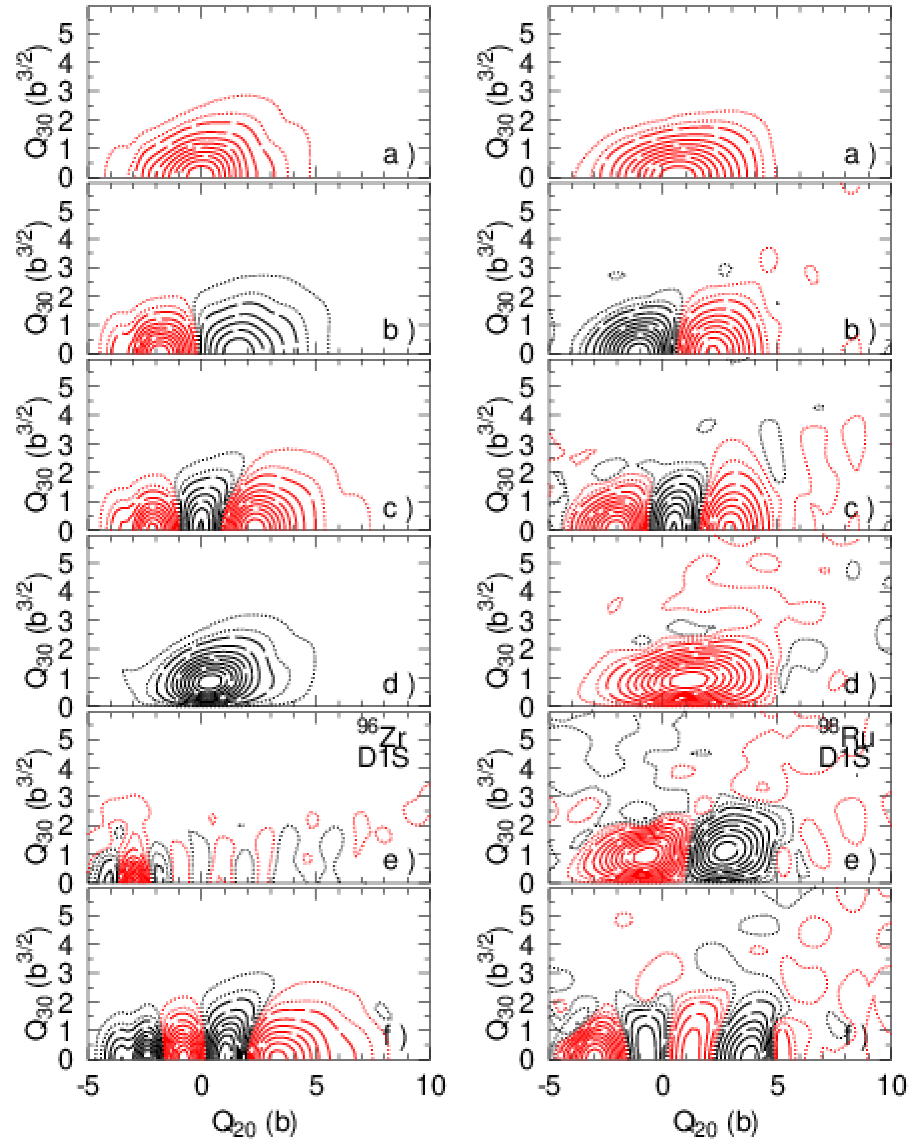
- Perhaps it could be the clue to solve the 96Zr puzzle

    - 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)

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)

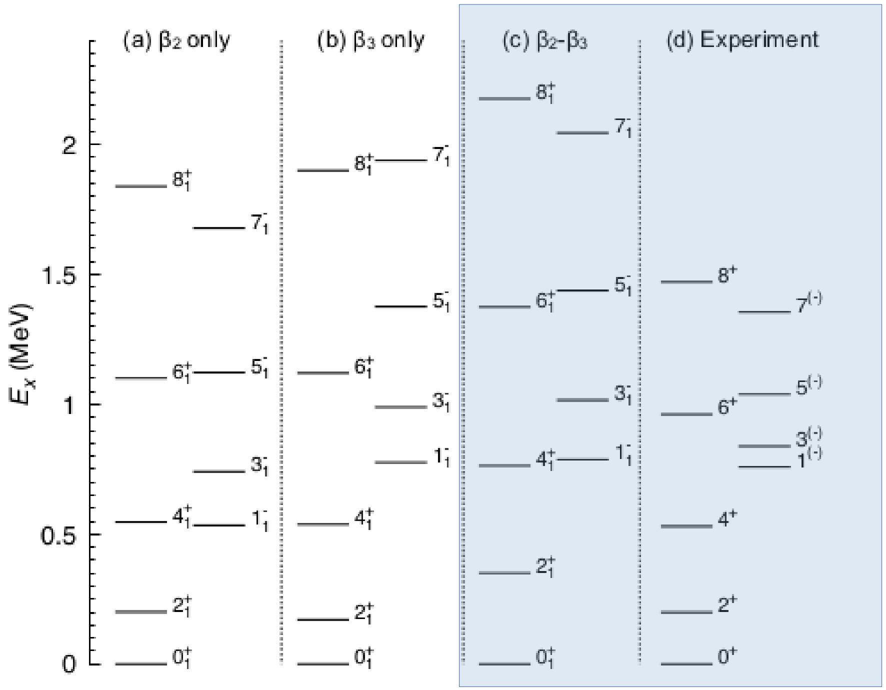
  - Angular momentum projection P^J
  - Particle Number projection P^N
  - Parity projection P^π

- Configuration mixing

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

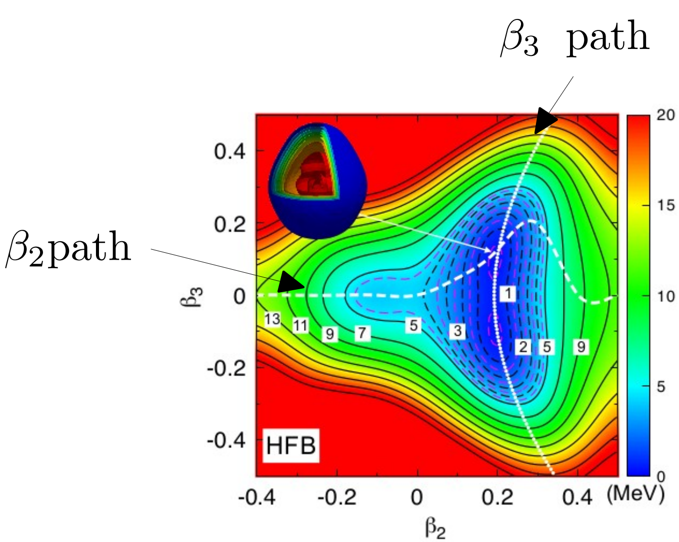
144Ba

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 !

Backup slides

Octupoles 1.0 (Vibrational states)

- The nucleus can vibrate around its equilibrium position $R(\theta,\phi) = R_0(1 + \sum_{LM} \alpha_{LM} Y_{LM})$
- Vibration characterized by the new dynamical variables α_{LM}
- Harmonic oscillator like quantum states (phonons) carrying angular momentum L and parity $\pi=(-1)^L$

$$B^{\dagger}_{LM}$$

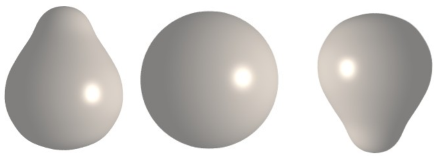
- The oscillator frequency and characteristic length depend upon two parameters: spring constant and inertia. The latter is not easy to determine in mean field theories.
- Energies and transition strength depend on those two parameters.
- Octupole vibration corresponds to L=3 and the corresponding phonon carries 3 units of angular momentum

3^- $E_\gamma = 2.6\mathrm{MeV}$

$E3$ $B(E3) = 34\mathrm{W.u.}$

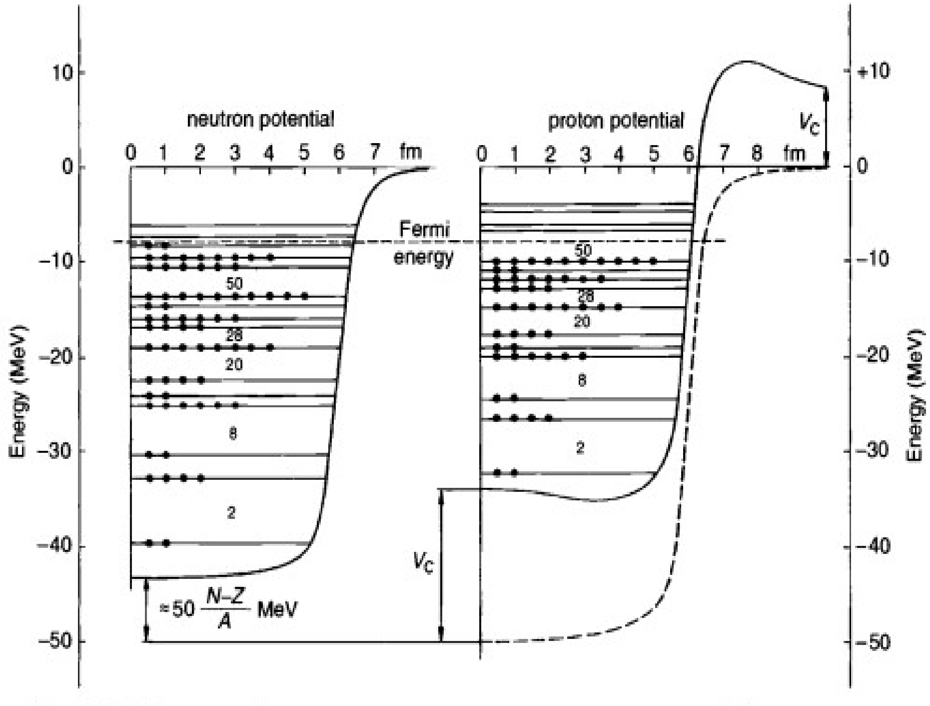
0^+

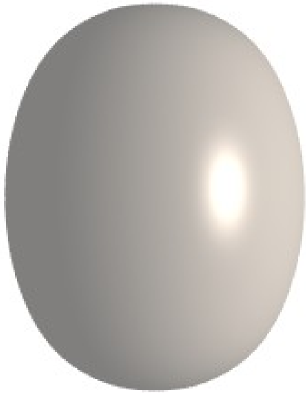
$^{208}\mathrm{Pb}$



- Well defined only in weakly deformed nuclei ?
- Quadrupole-Octupole coupling
- Two octupole phonons and 0^+_2

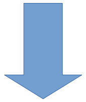
The two pillars of our present understanding of nuclear structure





Single particle model

Collective model



Mean field approximation and spontaneous symmetry breaking

Symmetry restoration to recover quantum numbers

In the strong symmetry breaking regime observables can be computed in simple yet approximate way

Microscopic description: the force

The Gogny force is a popular choice but others (Skyrme, relativistic, etc) are possible

$$V(\vec{r}_1 - \vec{r}_2) = V_C(1,2) + V_{LS}(1,2) + V_{Coul}(1,2) + V_{DD}$$

$$V_C(\vec{r}_1 - \vec{r}_2) = \sum_i (W_i - H_i P_\tau + B_i P_\sigma - M_i P_\sigma P_\tau) \exp\left((\vec{r}_1 - \vec{r}_2)^2/\mu_i^2\right)$$

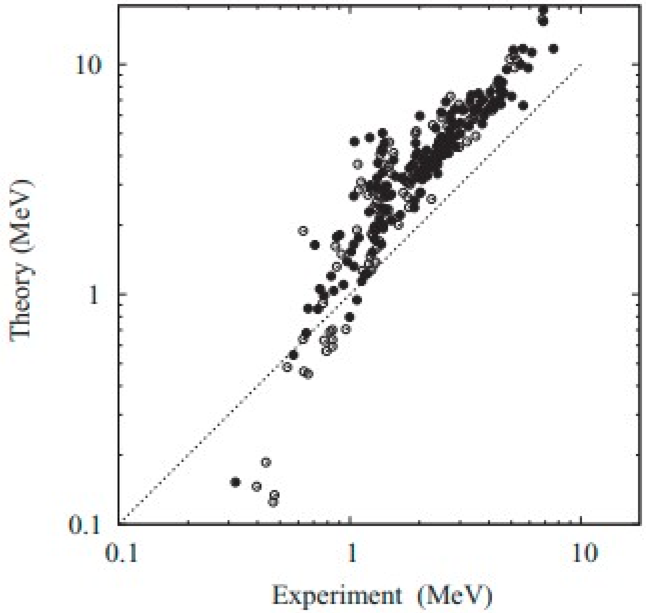
$$V_{LS}(1,2) = W_{LS}(\nabla_{12}\delta(\vec{r}_1 - \vec{r}_2)\nabla_{12})(\vec{\sigma}_1 + \vec{\sigma}_2) \qquad V_C(1,2) = \frac{e^2}{4\pi\epsilon_0 r}$$

$$V_{DD}(1,2) = t_3\delta(\vec{r}_1 - \vec{r}_2)(1 + x_0 P_\sigma)\rho^\alpha(\vec{R})$$

Parameters fixed by fitting some general nuclear matter properties and a few values from finite nuclei (binding energies, s.p.e. splittings and some radii information).

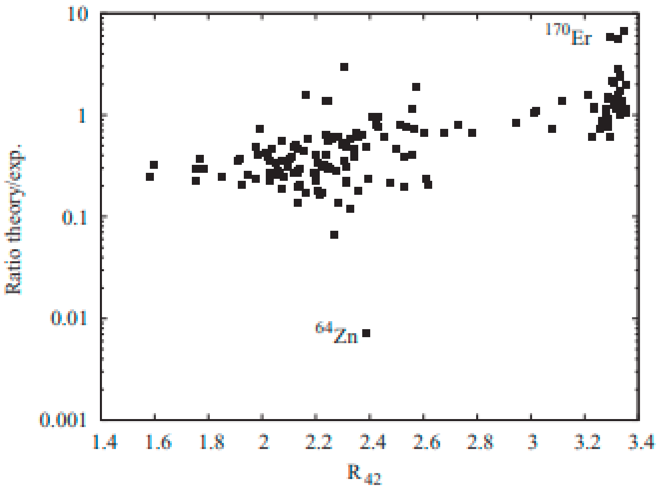
- **D1S:** surface energy fine tuned to reproduce fission barriers
- **D1N:** Realistic neutron matter equation of state reproduced
- **D1M**: Realistic neutron matter + Binding energies of essentially all nuclei with approximate beyond mean field effects

Pairing and time-odd fields are taken from the interaction itself



Systematically too high excitation energies: other degrees of freedom are important, specially in octupole soft systems

B(E1)s not considered in this analysis because they are less collective (see below)

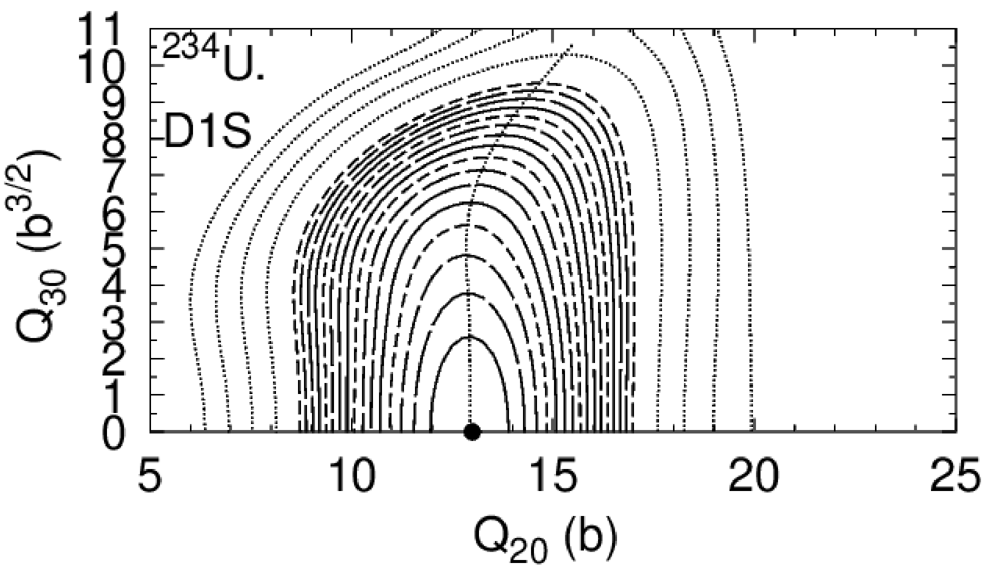


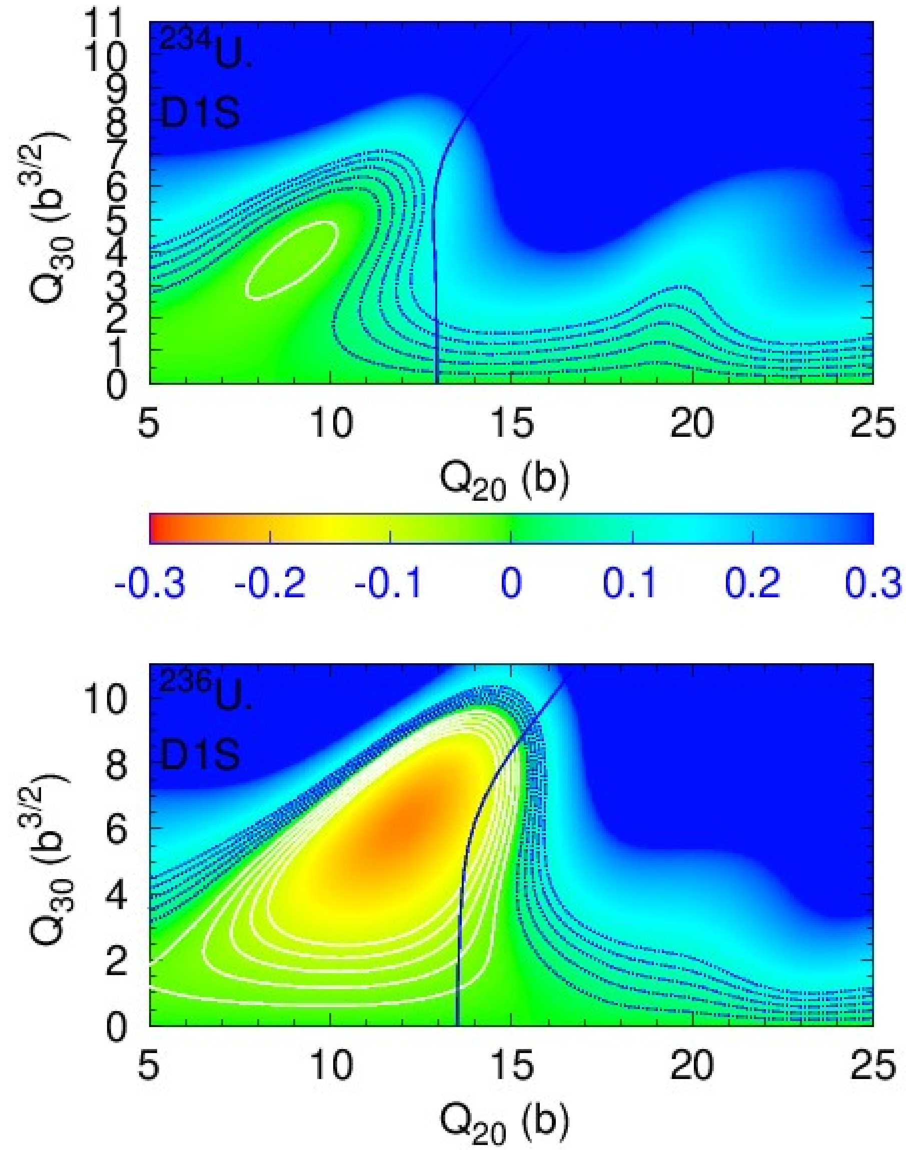
B(E3)s show a systematic deviation for not so well quadrupole deformed systems.

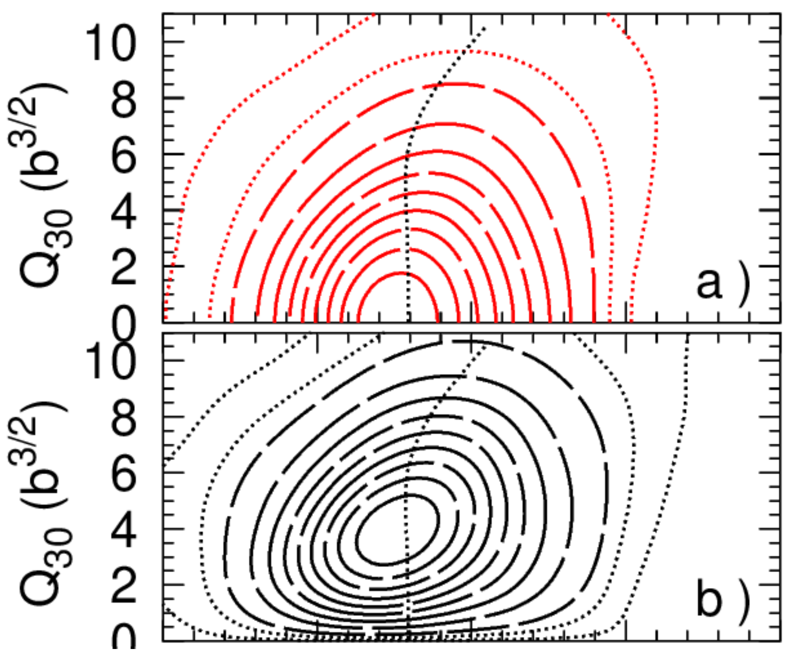
The **rotational formula is not valid,** as expected

$$B(E3, 3^- \to 0^+) = \frac{e^2}{4\pi} \langle \Psi_{\sigma_2} | \hat{Q}_3 \frac{1+t_z}{2} | \Psi_{\sigma_1} \rangle^2$$

B(E1) strength of ^{234}U



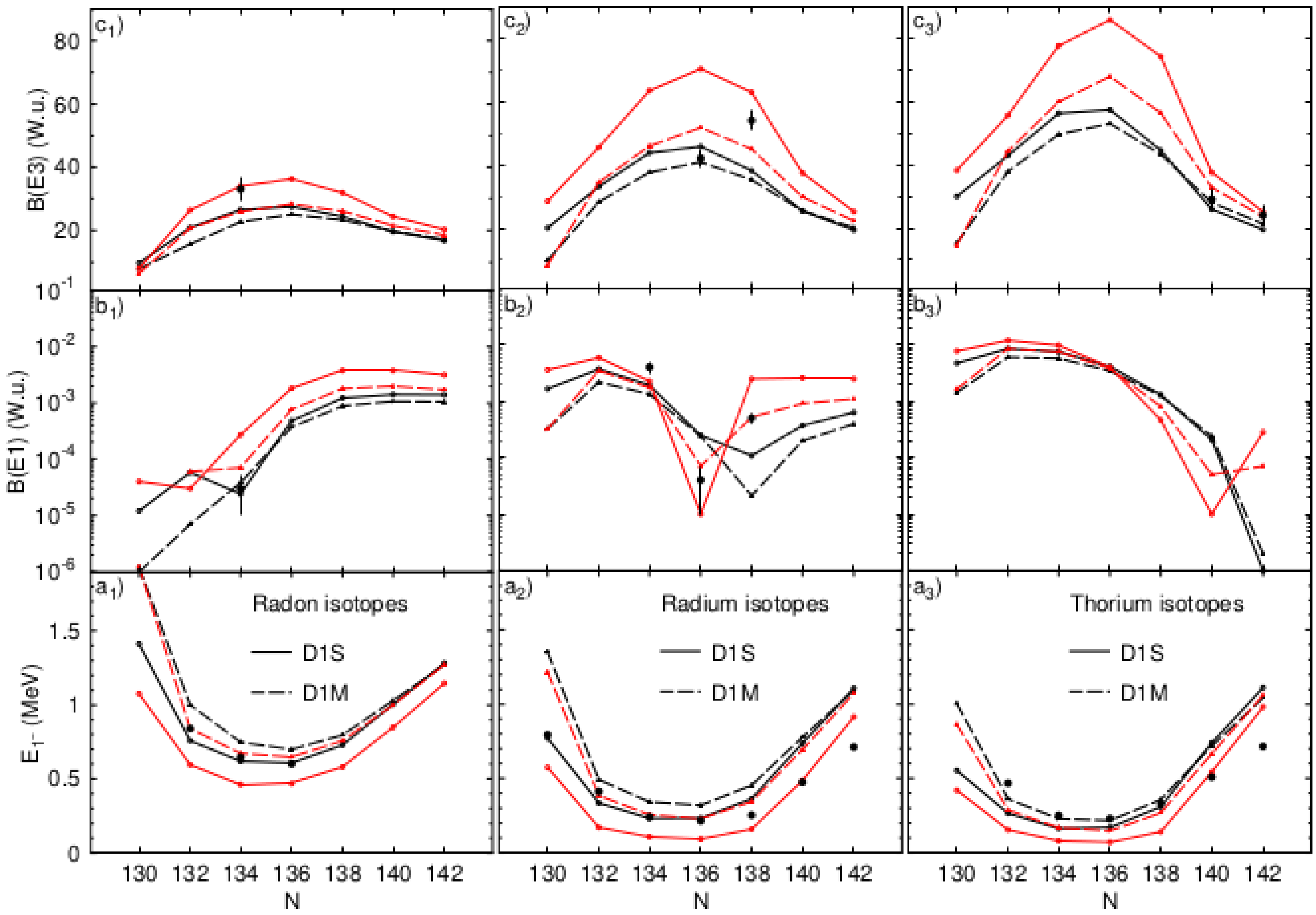




In collaboration with UWS' Dave O' Donnell

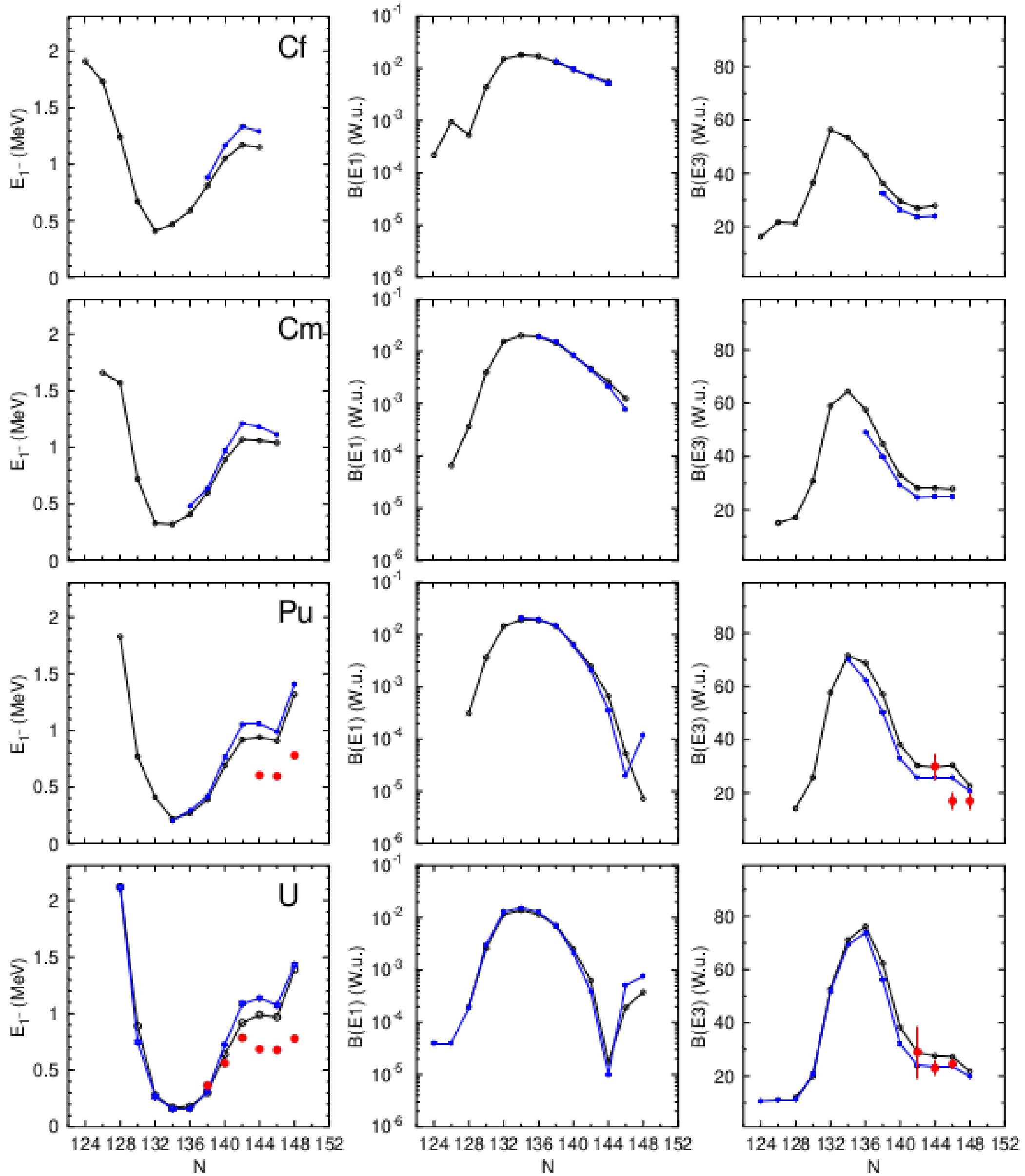
Improvements: Quadrupole – Octupole coupling

LMR and P Butler, Phys. Rev. C 88, 051302(R)

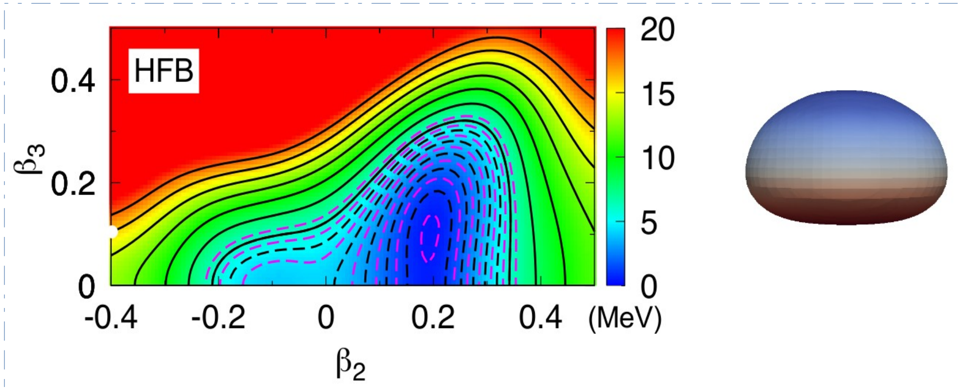


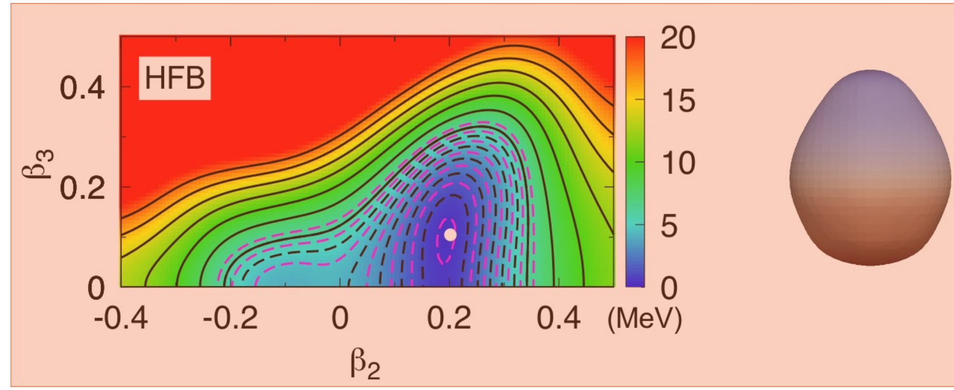
Improvements: Quadrupole – Octupole coupling

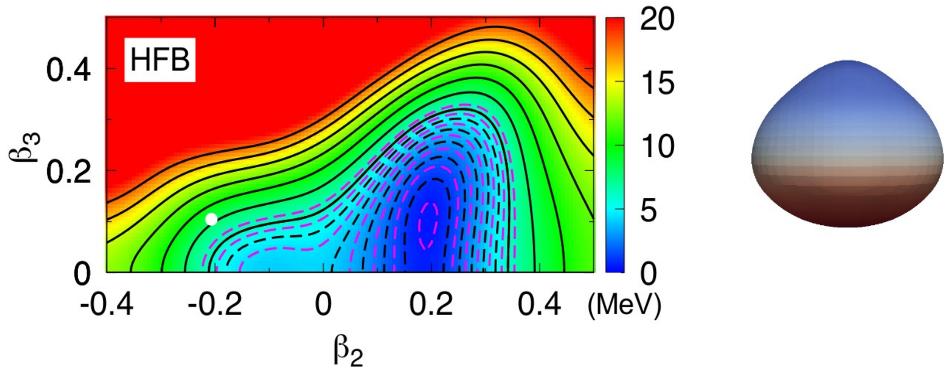
R.R.Rodriguez-Guzman et al, JPG in press

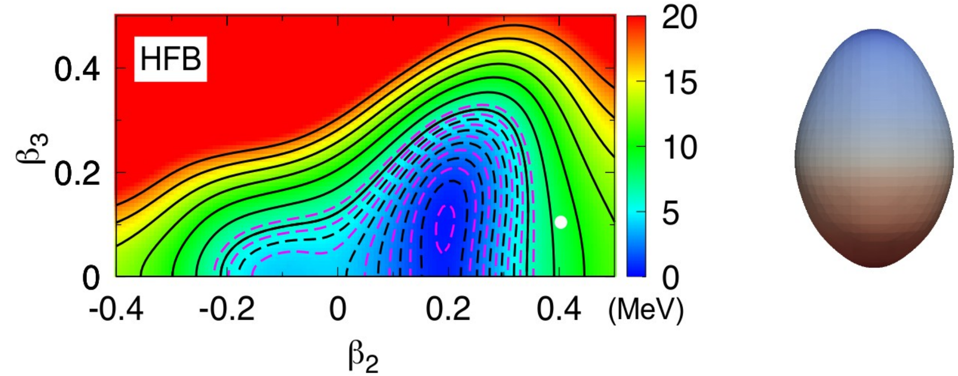


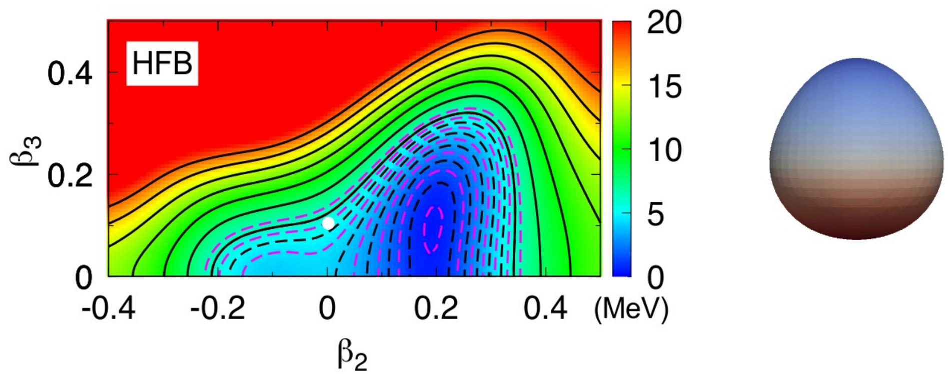
Microscopic description: Intrinsic HFB configurations











- Configurations at and around the HFB minimum
- Axially symmetric HFB with constraints on Q_{20} Q_{30}
- Efficient second order gradient solver
- Finite range Gogny (D1S, D1M, etc)

The example corresponds to ^{144}**Ba** with moderate **quadrupole-octupole mixing**

Symmetry restoration: Continuous symmetries

Particle number and angular momentum restoration involve continuous symmetries

$$e^{i\varphi\hat{N}} \qquad\qquad \hat{R}(\alpha,\beta,\gamma)=\exp(-i\alpha J_z)\exp(-i\beta J_y)\exp(-i\gamma J_z)$$

And "linear combinations of rotated intrinsic states" become integrals

$$P^N|\Phi\rangle=\int_0^{2\pi}d\varphi\, e^{-i\varphi N}e^{i\varphi\hat{N}}|\Phi\rangle$$

Linear combination weight rotated intrinsic state

This "simple" structure is due to the Abelian character of the underlying group U(1)

In the angular momentum case the symmetry group is SU(2) (not Abelian)

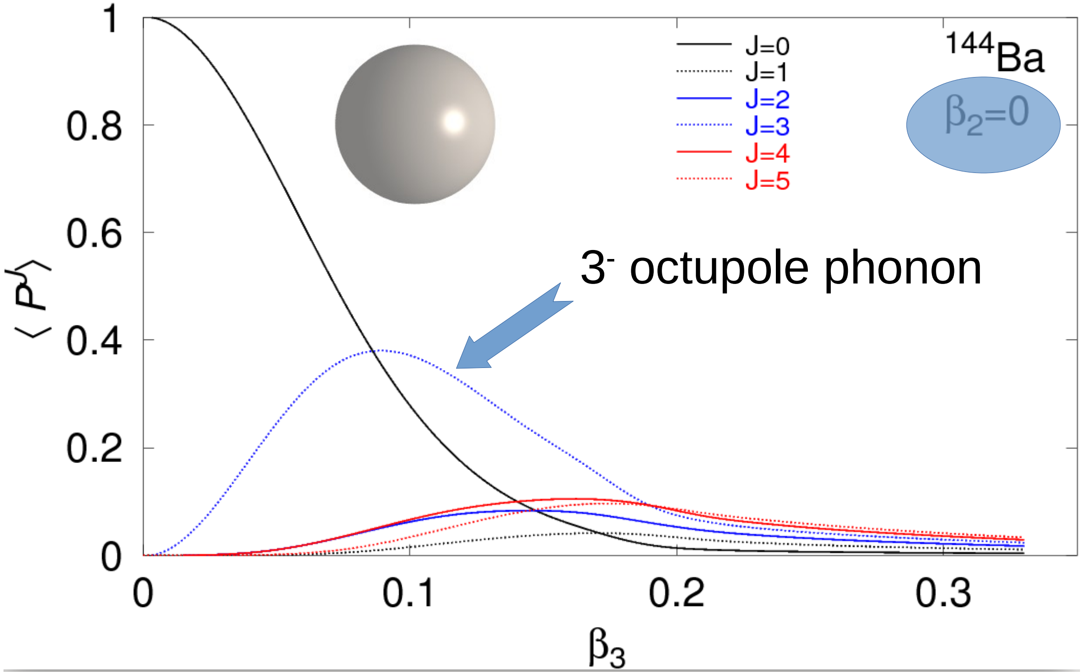
$$P^J|\Phi\rangle=\sum_K g_K\int d\Omega\mathcal{D}^{*J}_{KM}(\Omega)\hat{R}(\Omega)|\Phi\rangle$$

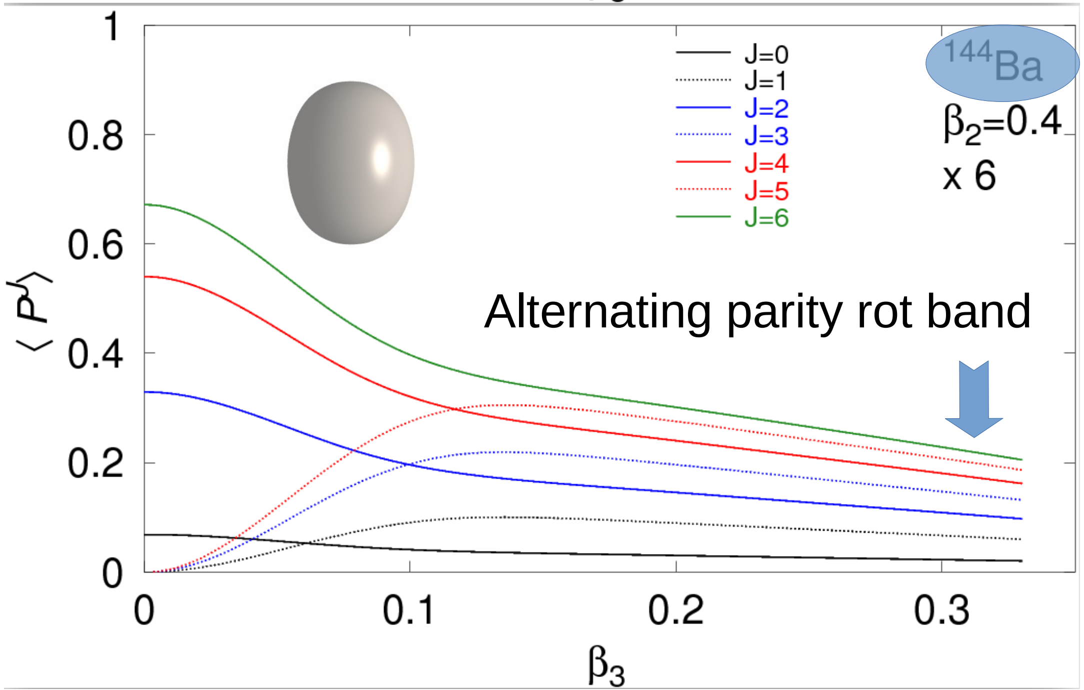
We assume axial symmetry and good signature in the intrinsic wave function.

$$\mathcal{S}=\mathcal{P}\mathcal{R}_y(\pi)\rightarrow \pi=(-1)^J$$

Natural parity selection rule

Angular momentum contents of the intrinsic states





- $|\langle P^J \rangle|^2$ is the probability of finding angular momentum J in the intrinsic state
- The **3^- configuration is dominant** for **negative parity states and spherical nuclei**
- **For deformed nuclei, the ordering of the negative parity states is similar to the one of positive parity states**
- In the **strong octupole deformation** limit, both positive and negative parity amplitudes exactly follow an interwinding pattern (alternating parity rotational bands)
- The model contains the right physics to describe both vibrations and rotations at the same time.

The last step is configuration mixing

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

This is a Projection After Variation (PAV) procedure because the <u>intrinsic states are determined by solving the HFB equation and then projected</u>

The f amplitudes of the GCM are obtained by solving the Schrodinger equation in the reduced configuration space (Hill-Wheeler equations for each J, π)

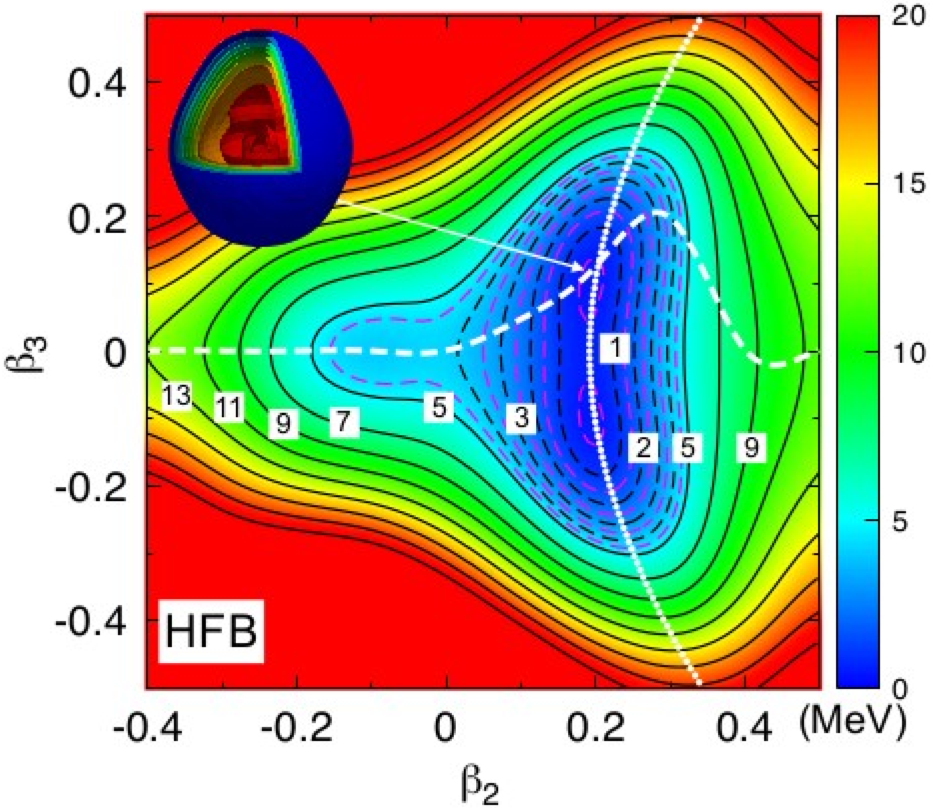
The final wf has good quantum numbers J, N, and π. This is very important as electromagnetic transition strengths and their associated selection rules strongly depend on them. To compute transition strengths we need the overlaps of the EM transition operators

$$\langle \Psi_{\sigma_1}^{J_1\pi_1} | \hat{O} | \Psi_{\sigma_2}^{J_2\pi_2} \rangle \longrightarrow \langle \Phi(Q_2,Q_3) | P^{J_1} P^{\pi_1} \hat{O} P^{J_2} P^{\pi_2} | \Phi(Q_2', Q_3') \rangle$$

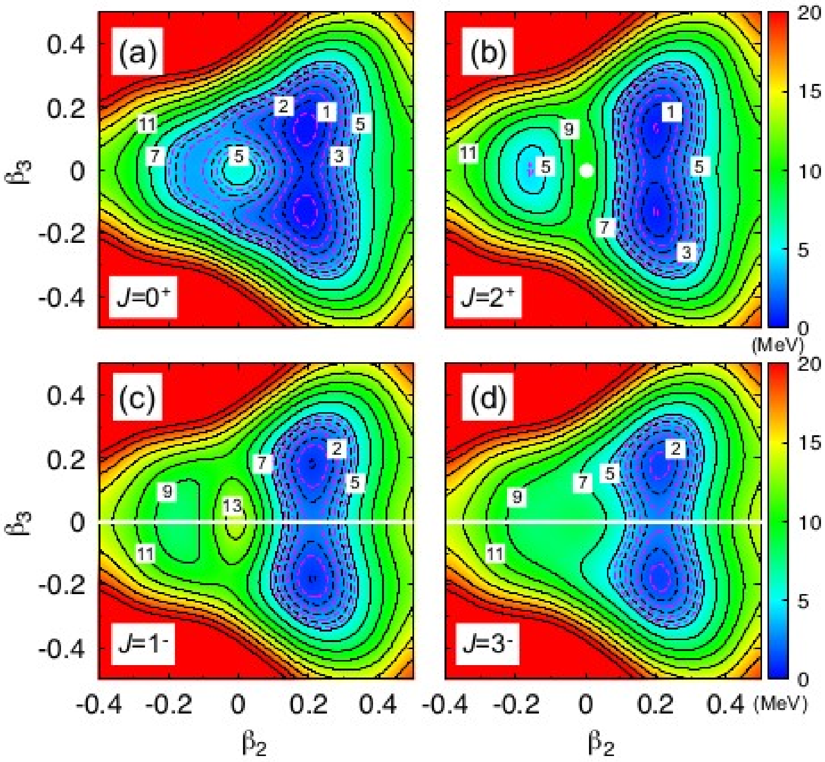
In the present approach, the assumption of the “rotational formula” often used to compute transition strengths is not required !

The “rotational formula” B(EL) α $\beta_L^{\,2}$ fails in weakly deformed nuclei and in computing transitions among different bands

144Ba: Mean field and projection



Intrinsic energy

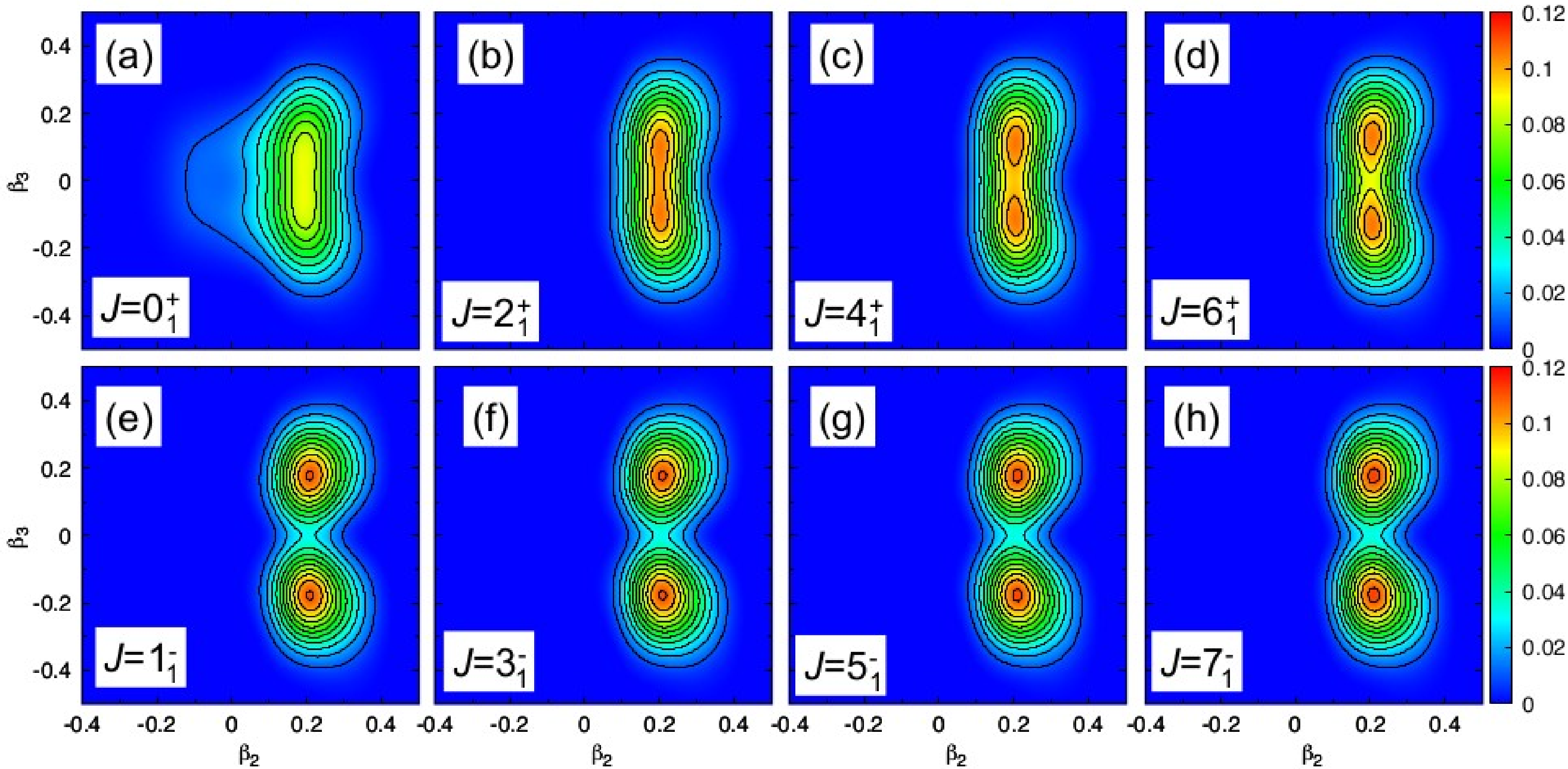


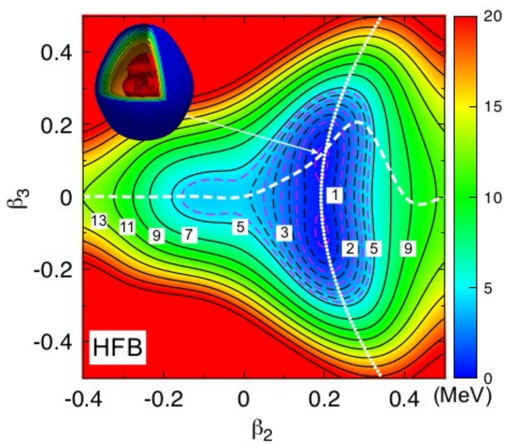
Projected LAB energies

Gogny D1S calculation (one day in a 600 node computer farm)

R.N. Bernard, L.M. Robledo and T.R. Rodriguez
Octupole correlations in the nucleus 144Ba described with symmetry conserving configuration mixing calculations
Phys. Rev. C 93, 061302 (R) (2016)

144Ba: GCM collective amplitudes

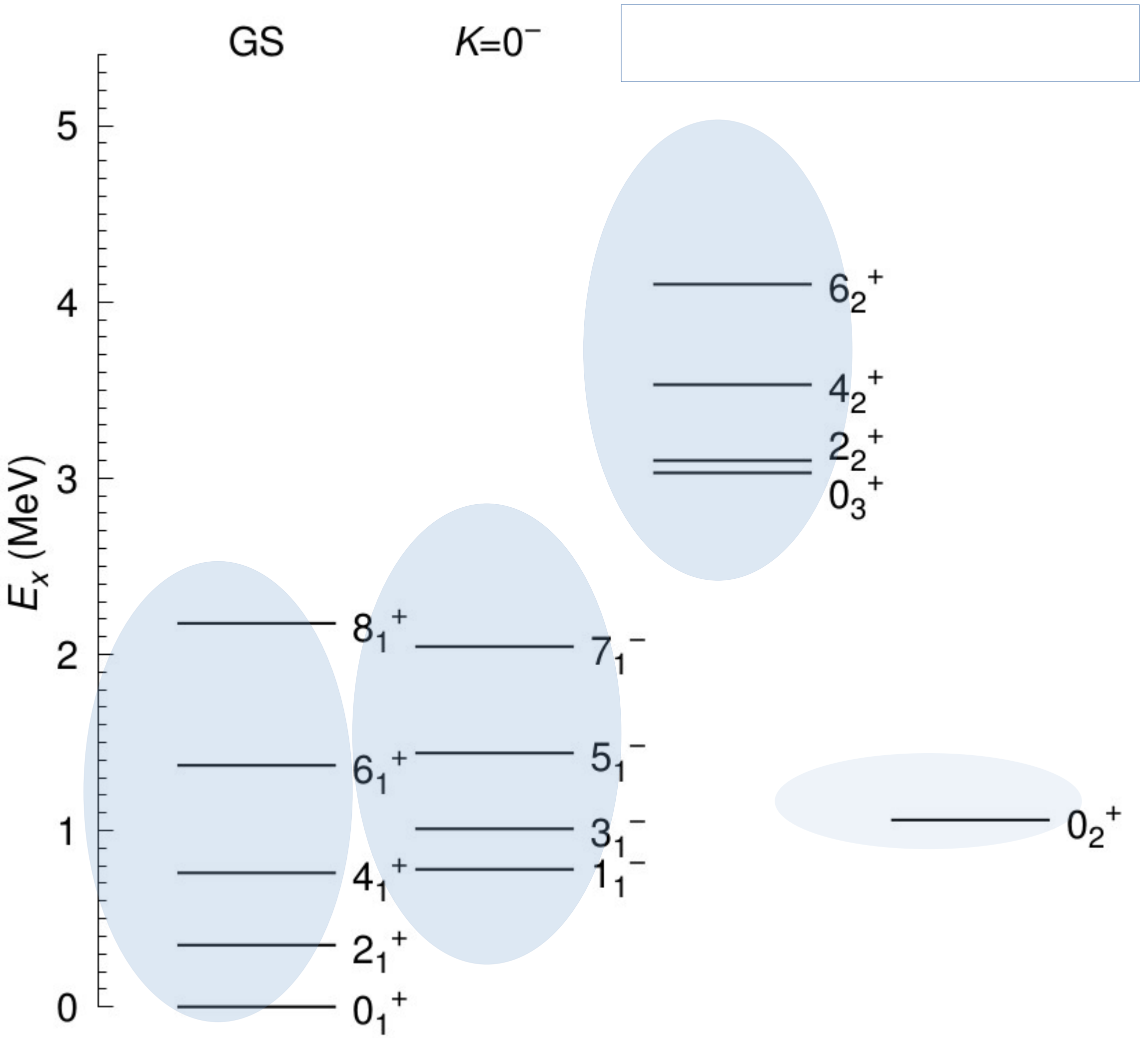




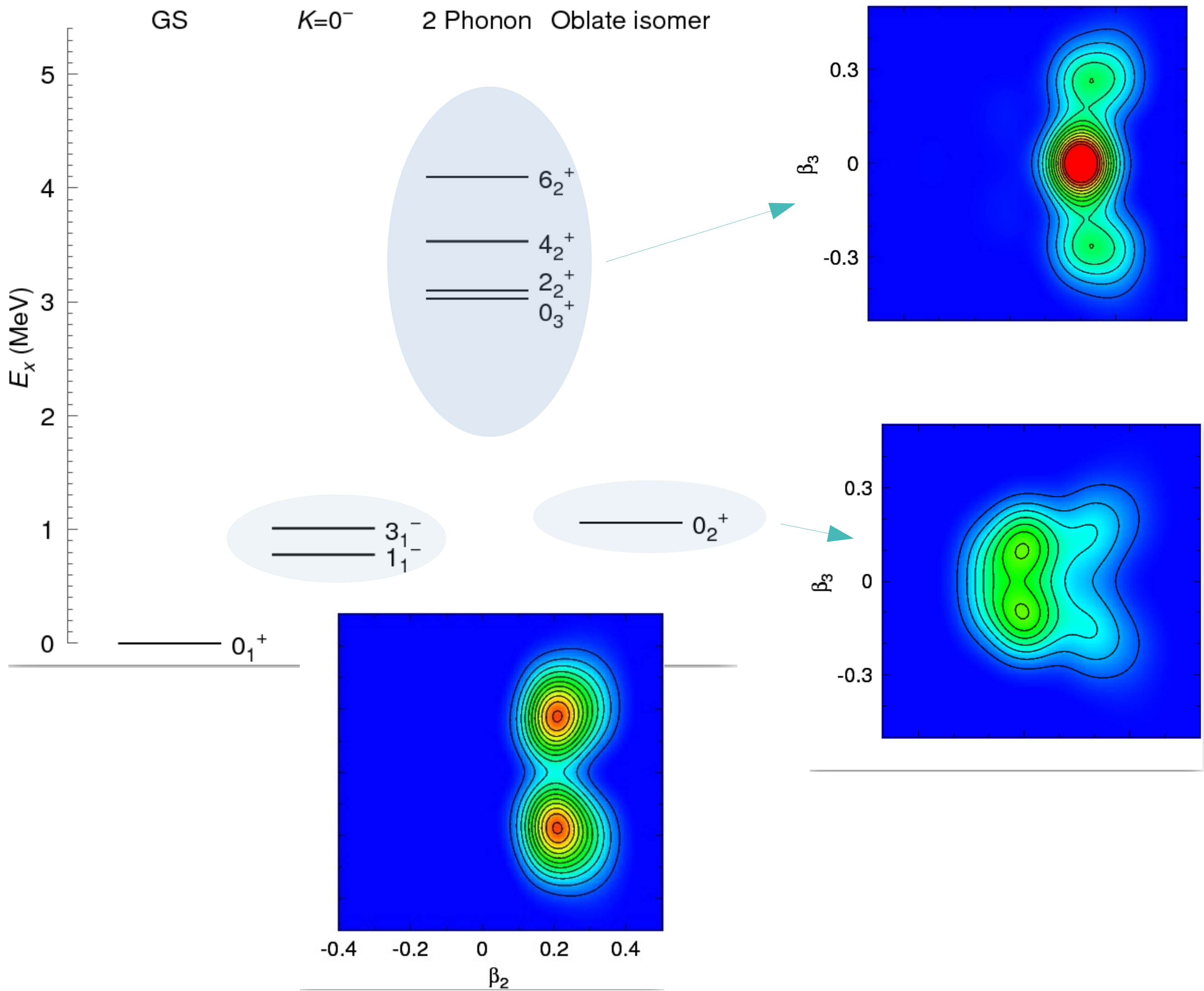
Collective amplitudes:

- Follow the topology of the energy surface
- Symmetry restrictions (wf zero if π=-1 and β_3=0)
- Fairly constant as a function of J (collective rotational band)
- Positive parity amplitudes evolve to match negative parity ones (stabilization of octupole deformation at high spins)

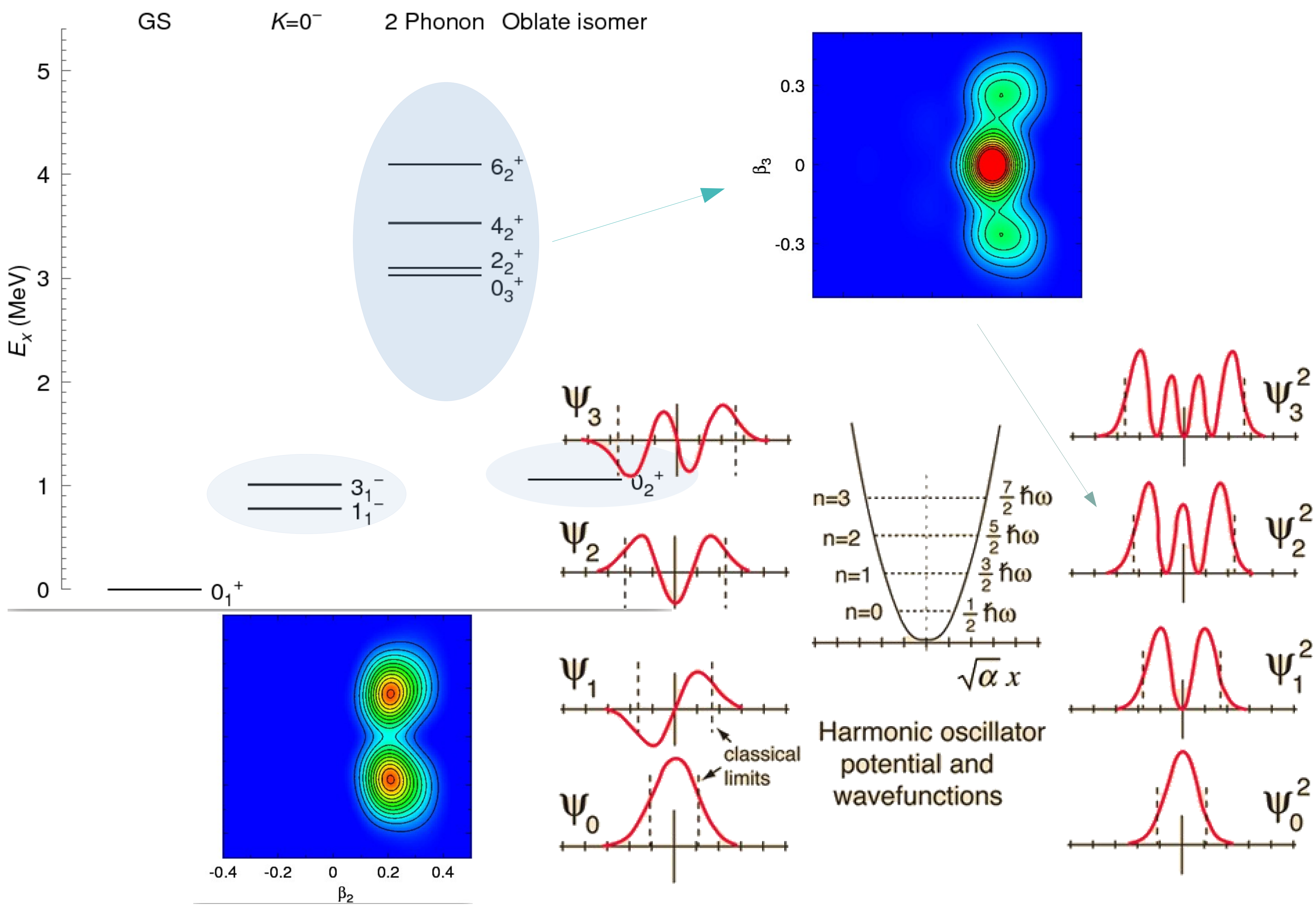
144Ba: double octupole phonon



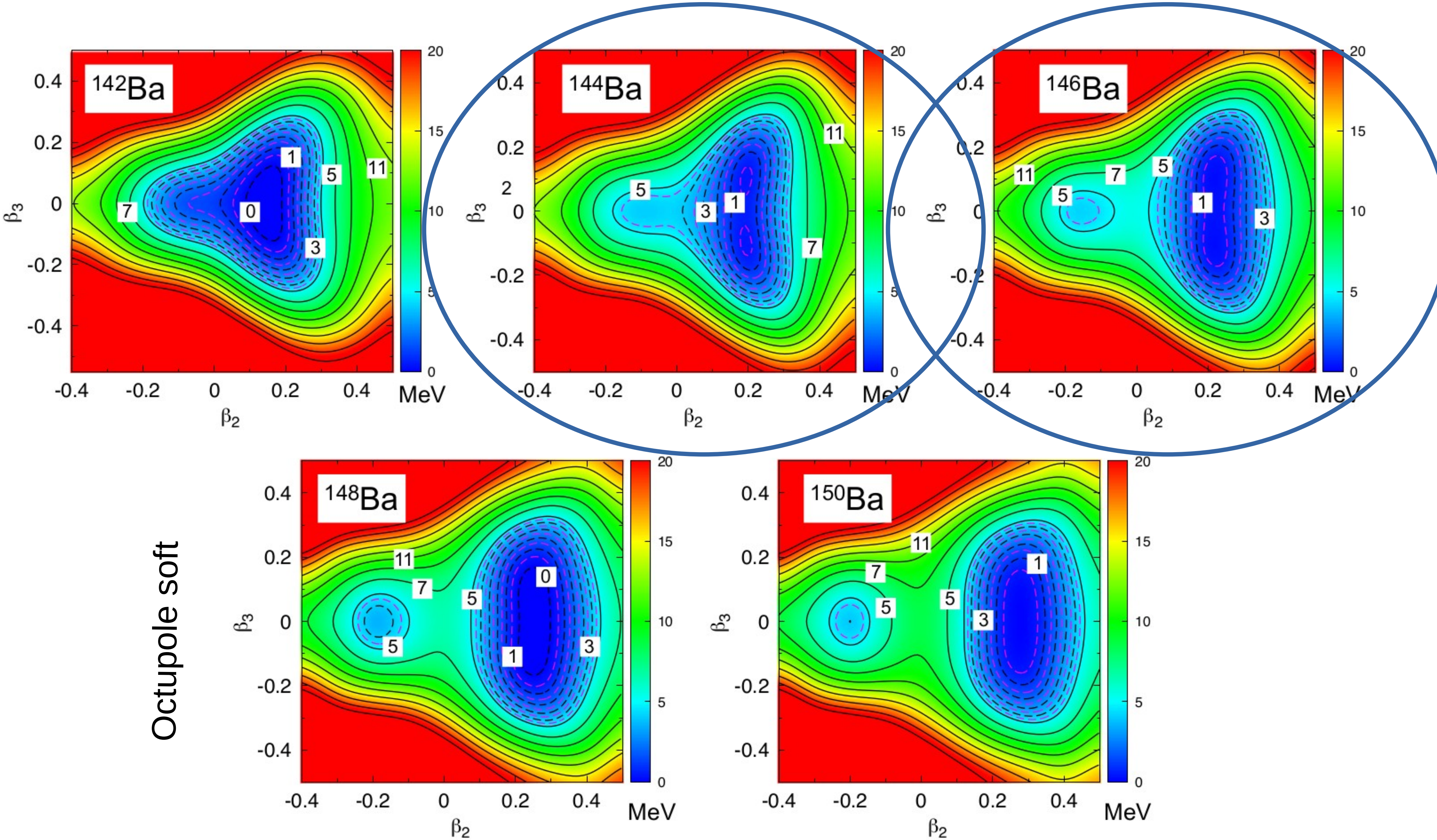
144Ba: double octupole phonon



144Ba: double octupole phonon

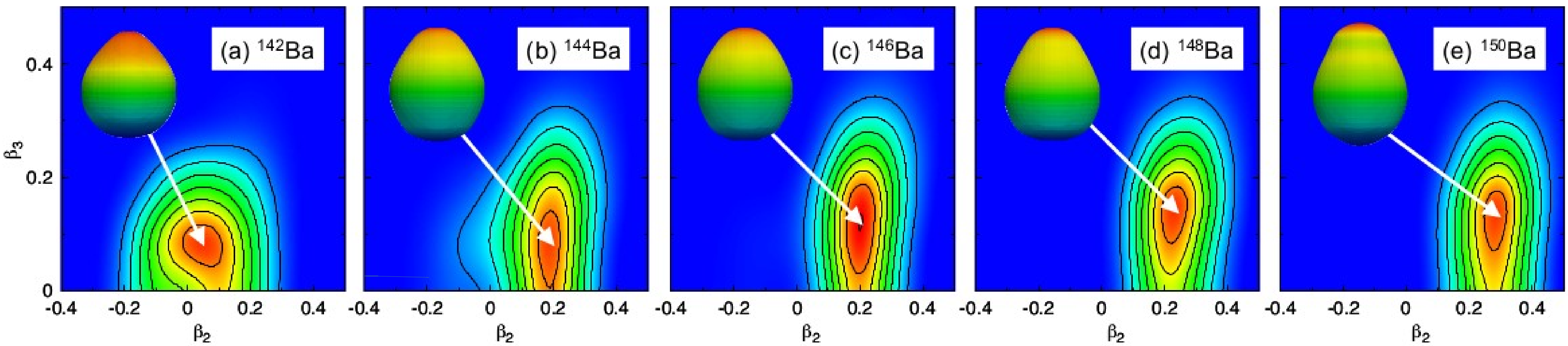


Other Ba isotopes



Gogny D1S
HFB potential energy surfaces

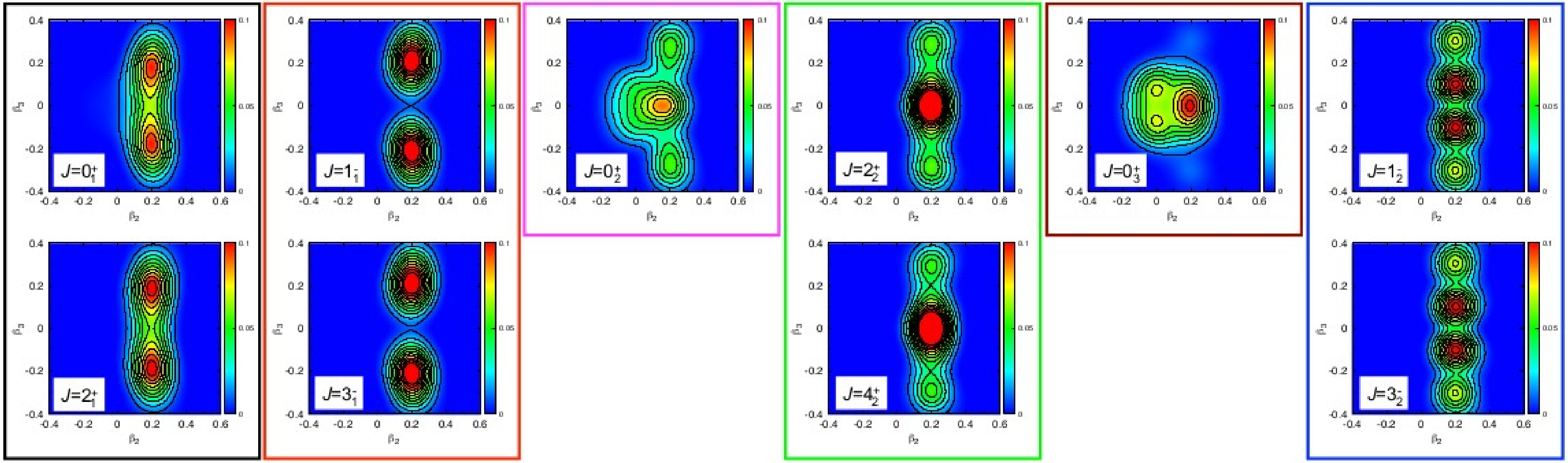
Other Ba isotopes

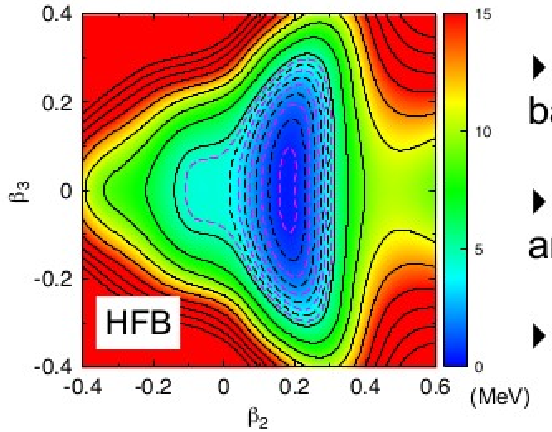


Gogny D1S
ground state collective wave functions

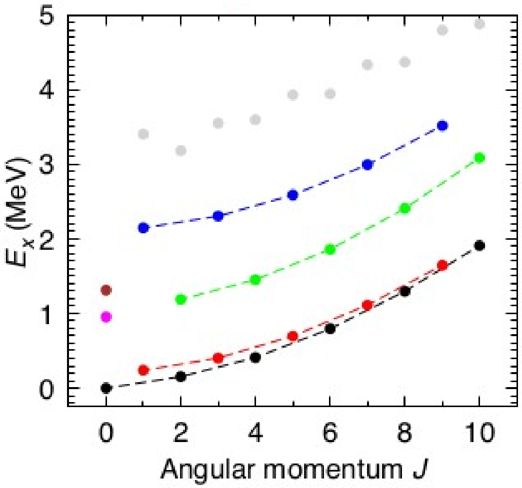
- Larger quadrupole-octupole mixing in $^{142\text{-}144}$Ba
- Coll w.f. peaked at Q_{30} different from zero ! Not so well correlated with E_{HFB} topology: consequence of dynamical quantum correlations

Responsible for enhanced B(E3) in N=90, 92, 94





- Quadrupole+octupole g.s. rotational bands
- Octupole vibrations as 2nd excited positive and negative parity bands.
- Shape mixing in 0^+_3

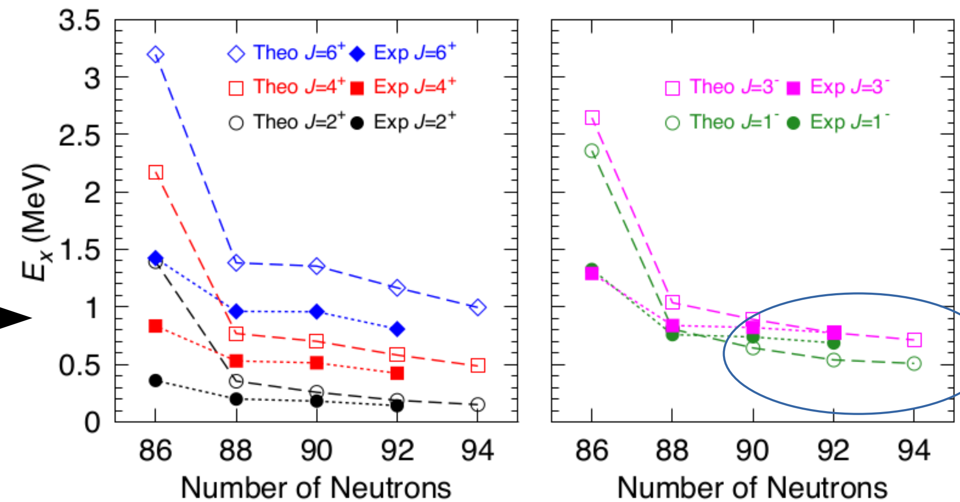


Working now in the actinide region: more nuclei to come

Other Ba isotopes

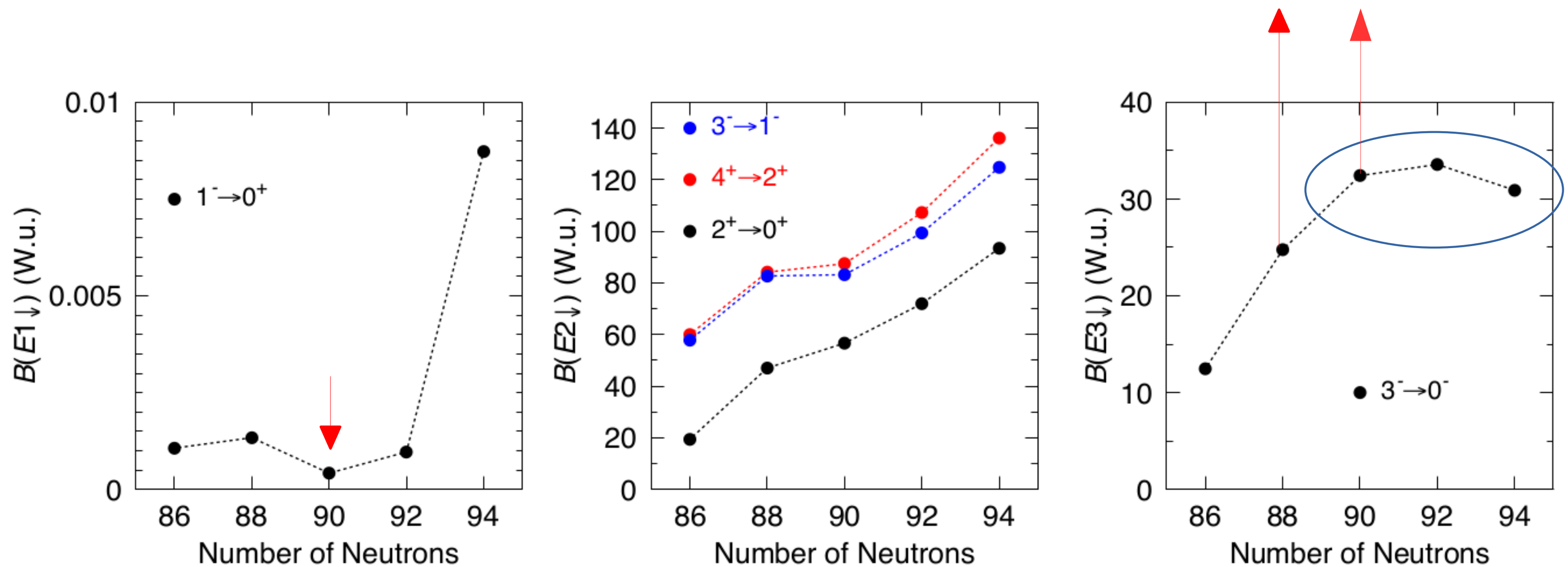
Gogny D1S
GCM results

Too small moments of inertia

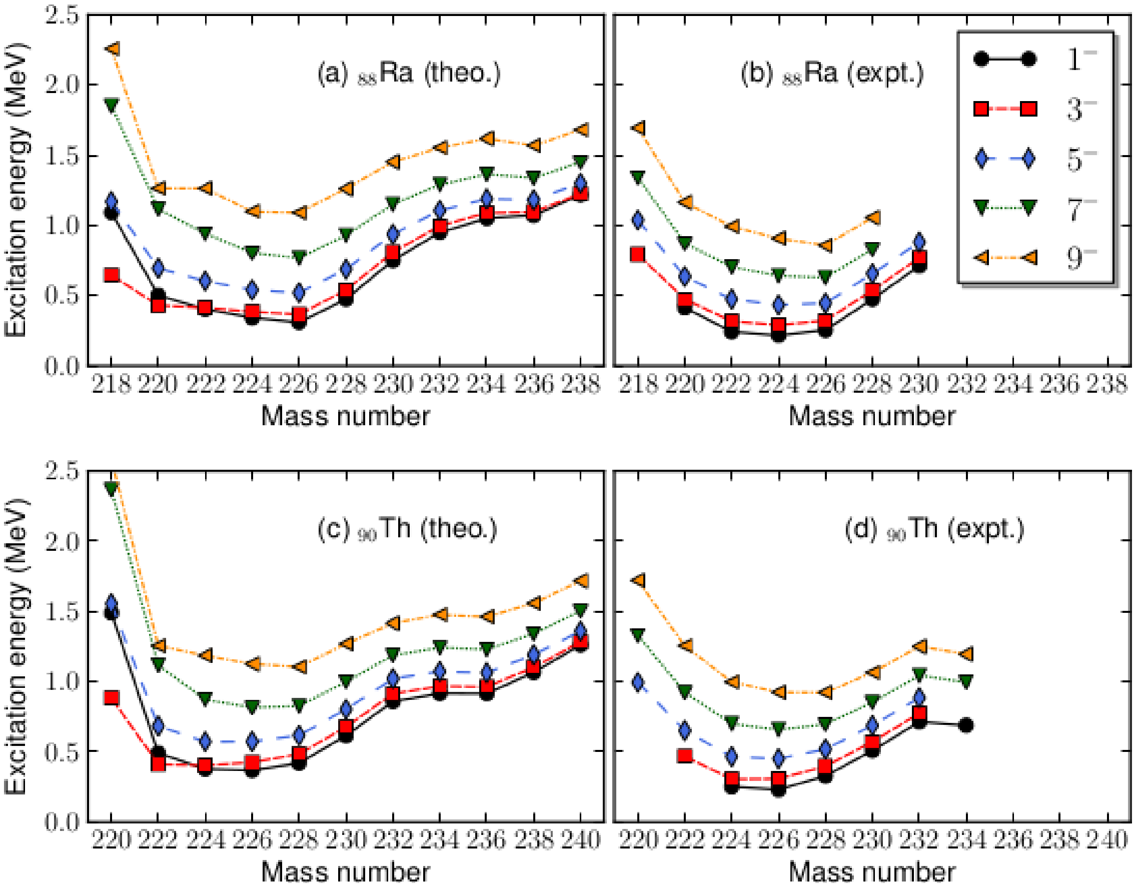


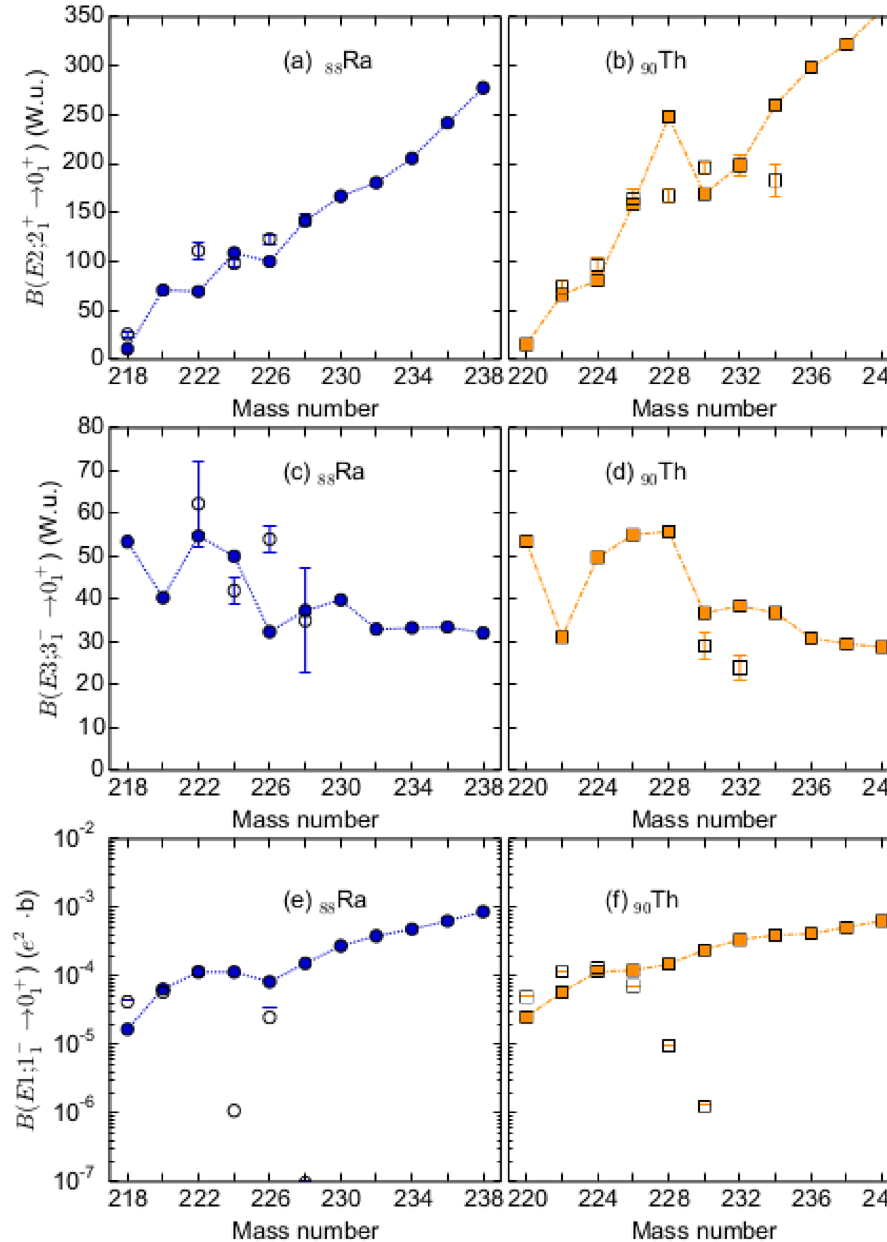
Enhanced octupolarity

Bucher et al (~48 Wu)



Other approaches





spdf IBM hamiltonian with microscopic input

K.Nomura et al. PRC

Conclusions

- Our computational framework reproduces quite nicely many of the experimental features of octupole deformed nuclei in the Ba (and other) regions
- Its microscopic foundation **avoids uncontrolled assumptions** of phenomenological models (vibrational or octupole deformed) as well as approximations (like the **rotational formula for transition strengths**)
- Its use of “global” EDFs like Gogny allows its use in other regions of the periodic table (work in progress!)
- Computationally demanding but still within the reach of modest computational facitilites
- It can be extended to consider the coupling with other relevant degrees of freedom like pairing or single particle excitation modes (work in progress!)

ToDo

- Release axial symmetry assumption
- Release time reversal invariance assumption (cranking)
- Extend to odd mass nuclei

Collaborators

This work is the result of a collaboration with

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  (UAM, tomas.rodriguez@uam.es)

- Remi Bernard
  (former postdoc@UAM, now at CEA)

Title