First Tsukuba-CSS-Riken workhop on microscopic theories of nuclear structure and dynamics

Octupole correlations in a full-symmetry restoring framework

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The shape of many nuclei is deformed in the intrinsic frame (a mean field artifact)

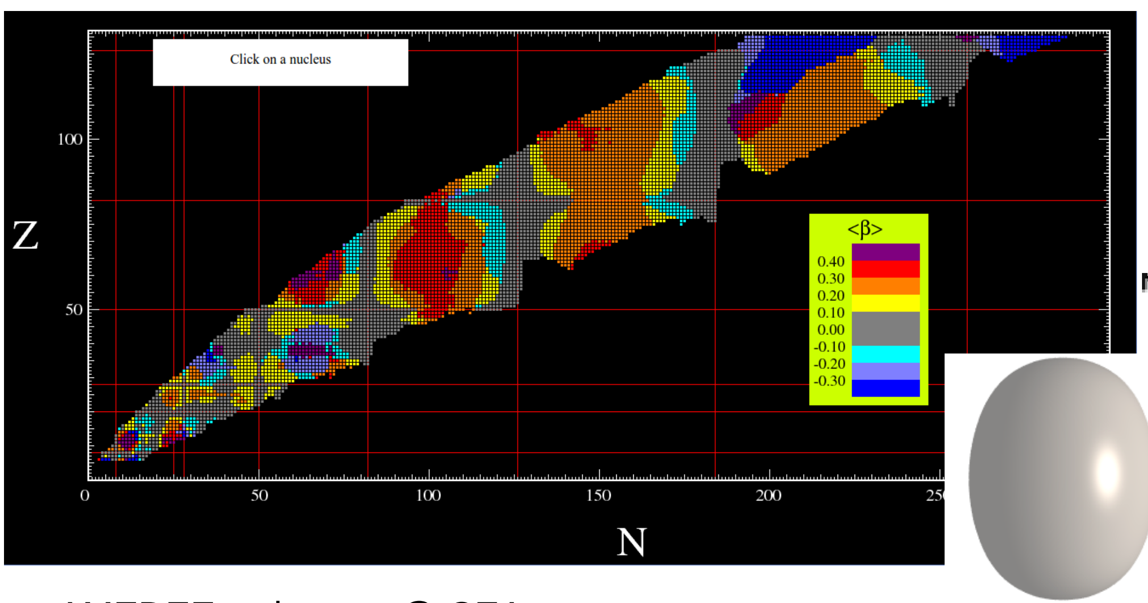
The restoration of broken symmetries (transformation to the LAB frame) generates a "band" for each intrinsic state. Band members have quantum numbers of the symmetry

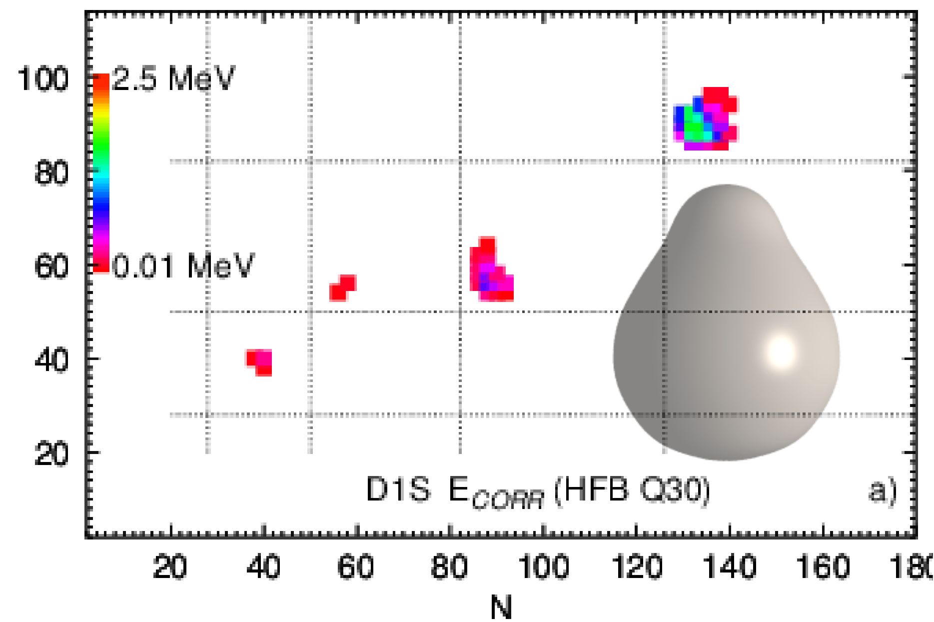
Deformation described in terms of multipole moments $R(\theta,\phi) = R_0(1+\sum_{LM}\alpha_{LM}Y_{LM})$

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

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

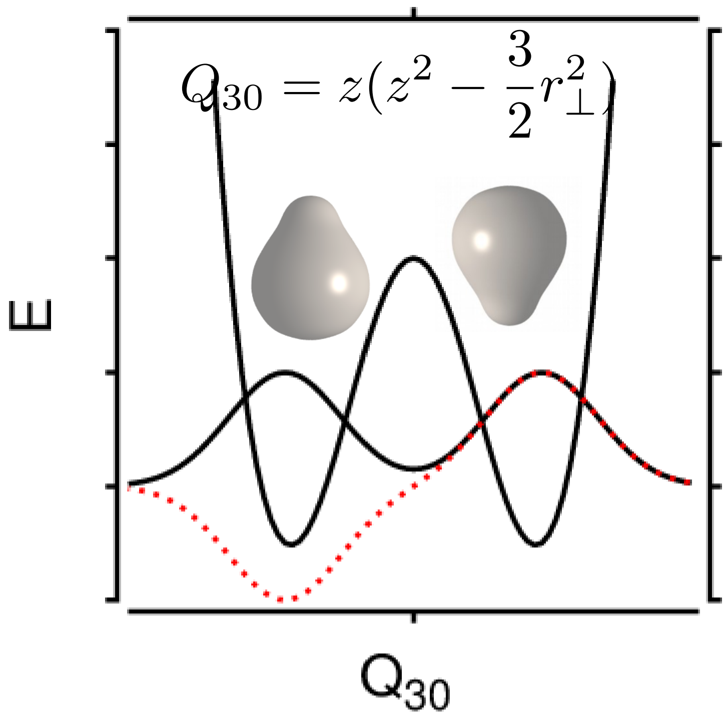
$$Q_{30} = z(z^2 - \frac{3}{2}r_\perp^2)$$

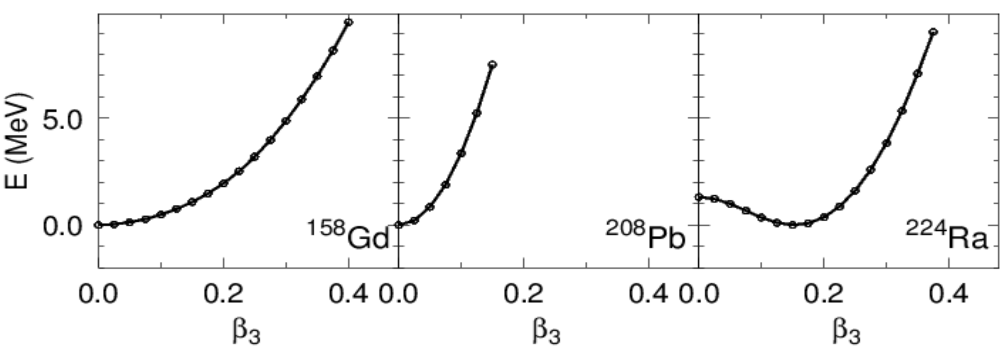




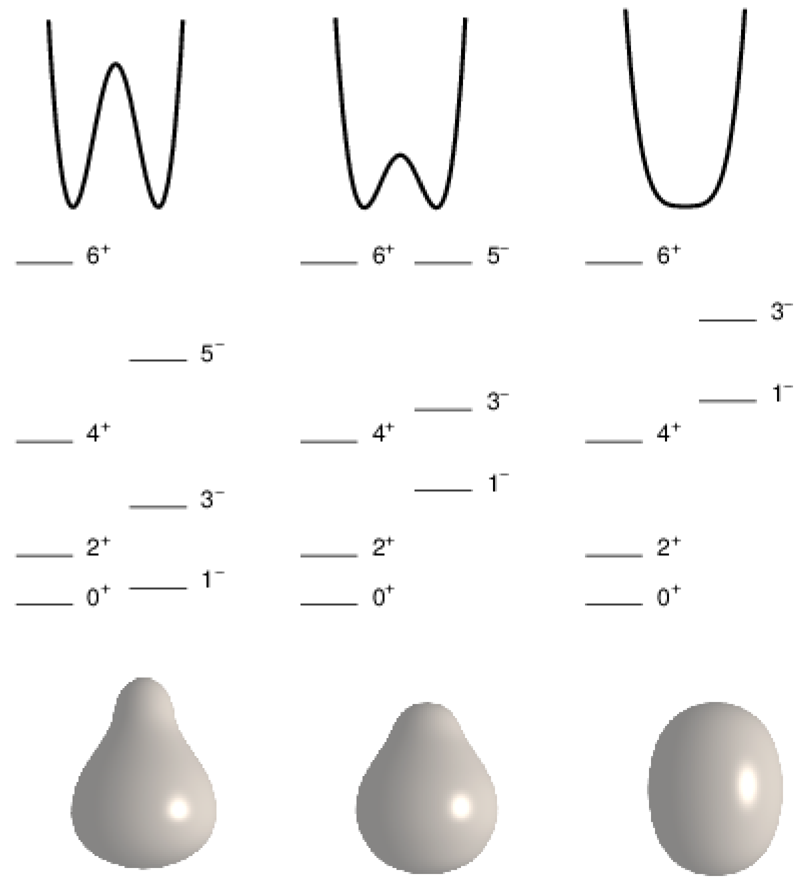
AMEDEE web page @ CEA

Octupoles 1.0 (Octupole deformation)





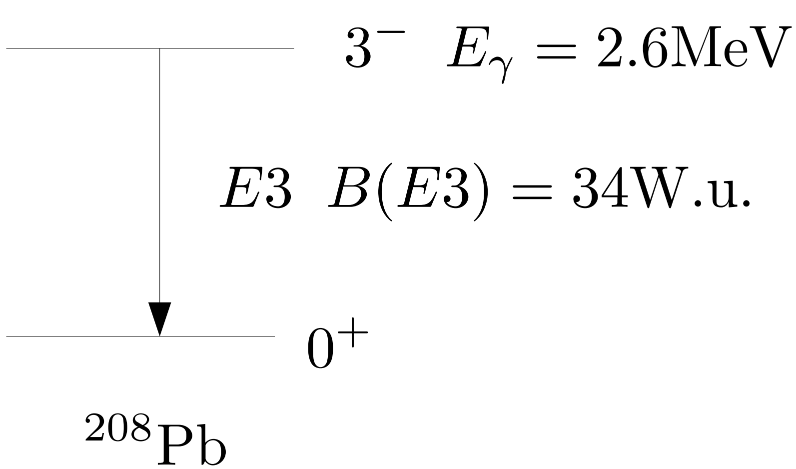
Three typical results obtained with Gogny D1S



- Octupole deformation shows up as minima of $E_{HFB}(Q_{30})$
- $E(Q_{30})=E(-Q_{30})$ (Parity invariance)
- In the LAB frame: parity doublets in the limit when there is no tunneling through the barrier
- Strong E3 transition strengths

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 π=(-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



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

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

- 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:

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

Can be avoided if the nucleus is strongly deformed (Rotational model) and quadrupole-octupole mixing neglegible

- Configuration mixing

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

Gogny force

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

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

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

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

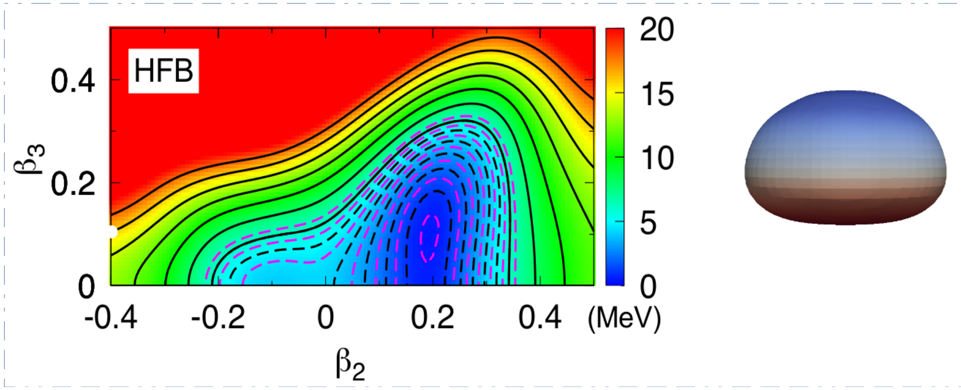
$$V_{DD}(1,2) = t_3\delta(\vec{r}_1 - \vec{r}_2)(1 + x_0 P_\sigma)\rho^\alpha(\vec{R})$$

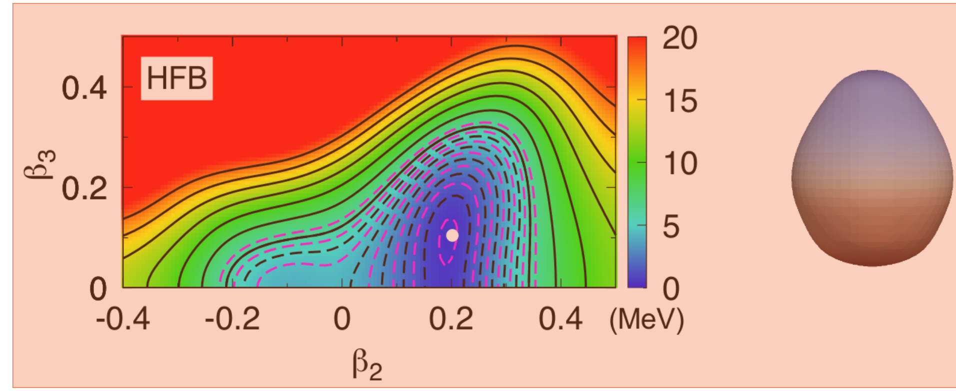
Parameters fixed by fitting some general nuclear matter properties and a few values from finite nuclei (binding energies, s.p.e. splittings and some radii information).

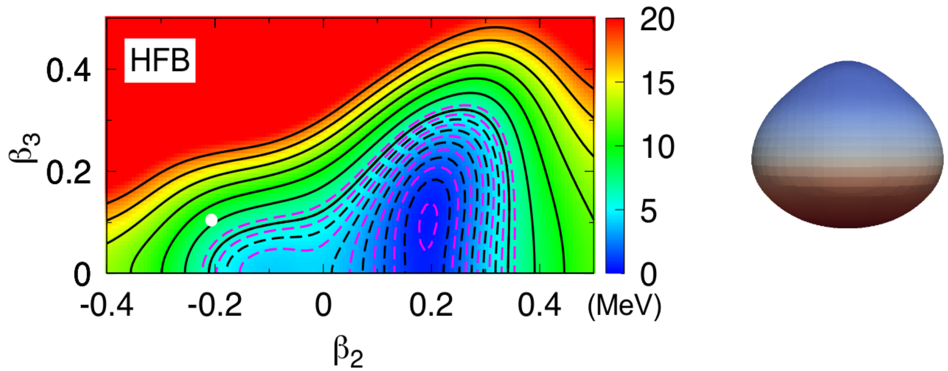
- **D1S:** surface energy fine tuned to reproduce fission barriers
- **D1N:** Realistic neutron matter equation of state reproduced
- **D1M**: Realistic neutron matter + Binding energies of essentially all nuclei with approximate beyond mean field effects

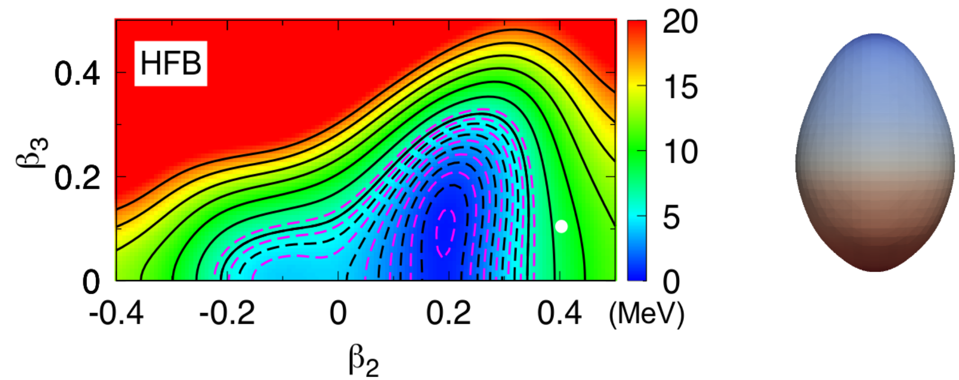
Pairing and time-odd fields are taken from the interaction itself

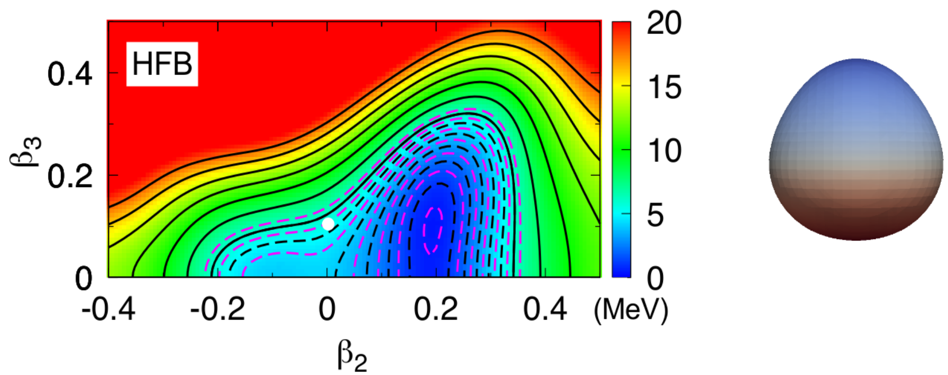
Intrinsic HFB configurations











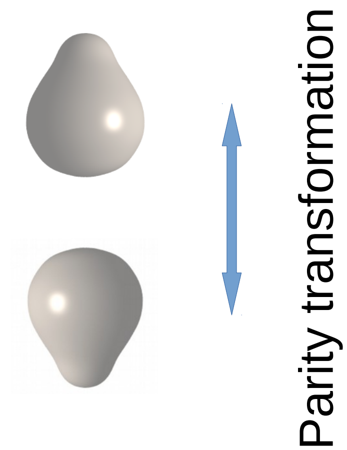
- Configurations at and around the HFB minimum
- Axially symmetric HFB with constraints in $Q_{20}\, Q_{30}$
- Efficient second order gradient solver
- Finite range Gogny (D1S, D1M, etc)

The example corresponds to 144Ba with rather strong quadrupole-octupole mixing

Symmetry restoration

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

To restore the symmetry, apply the symmetry operator to the intrinsic wave function $\hat{\Pi}|\varphi(\beta_3)\rangle$



And take the appropriate linear combination of the two shapes to restore the symmetry

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

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 made of two elements: identity and parity

Symmetry restoration: Continuous symmetries

Particle number and angular momentum restoration involve continuous symmetries

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

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)

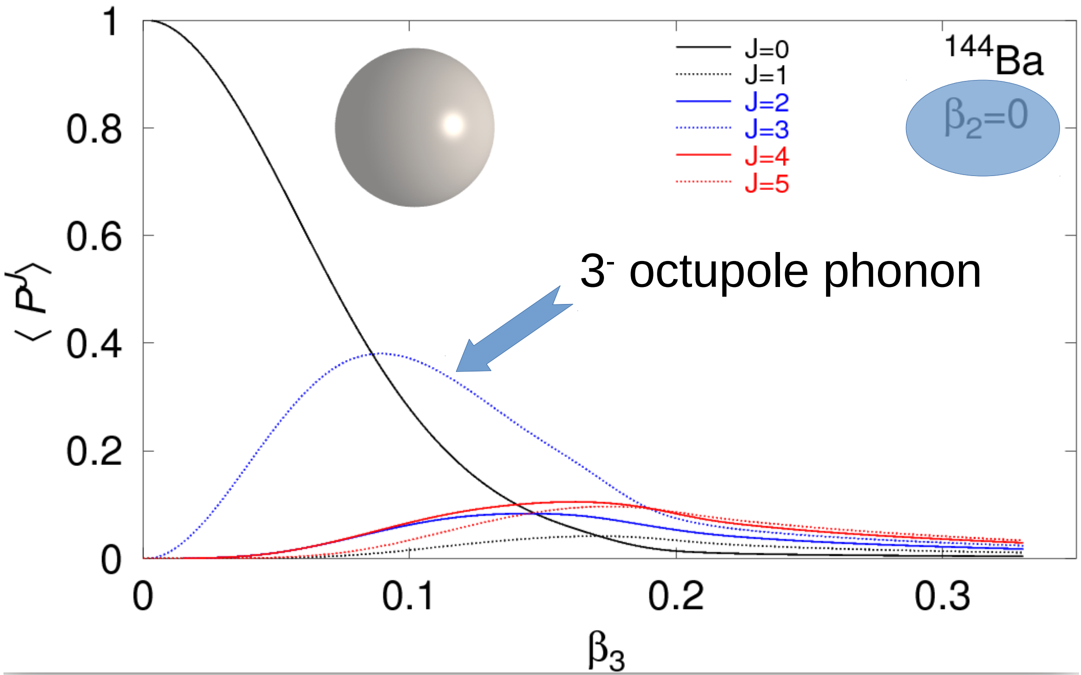
$$P^J|\Phi\rangle = \sum_K g_K \int d\Omega \mathcal{D}^{*J}_{KM}(\Omega)\hat{R}(\Omega)|\Phi\rangle$$

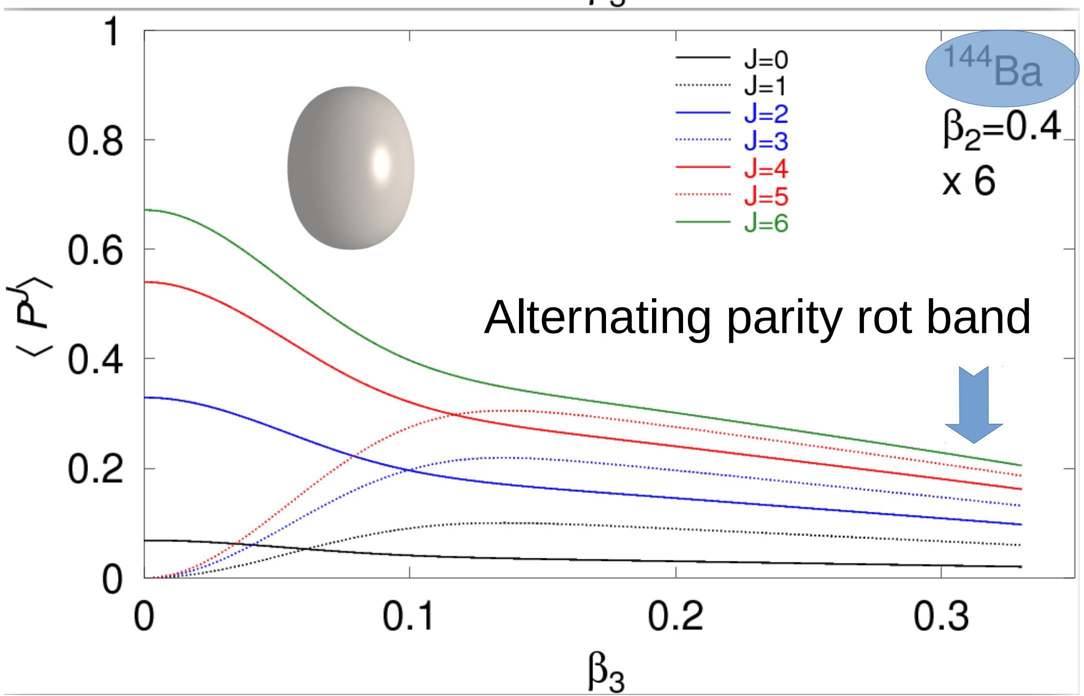
We assume axial symmetry and good signature in the intrinsic wave function.

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

Natural parity selection rule

AM 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 deformation limit of the octupole, both positive and negative parity amplitudes exactly follow the same pattern (alternating parity rotational bands)

Configuration mixing

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 intrinsic states are determined by solving the HFB equation

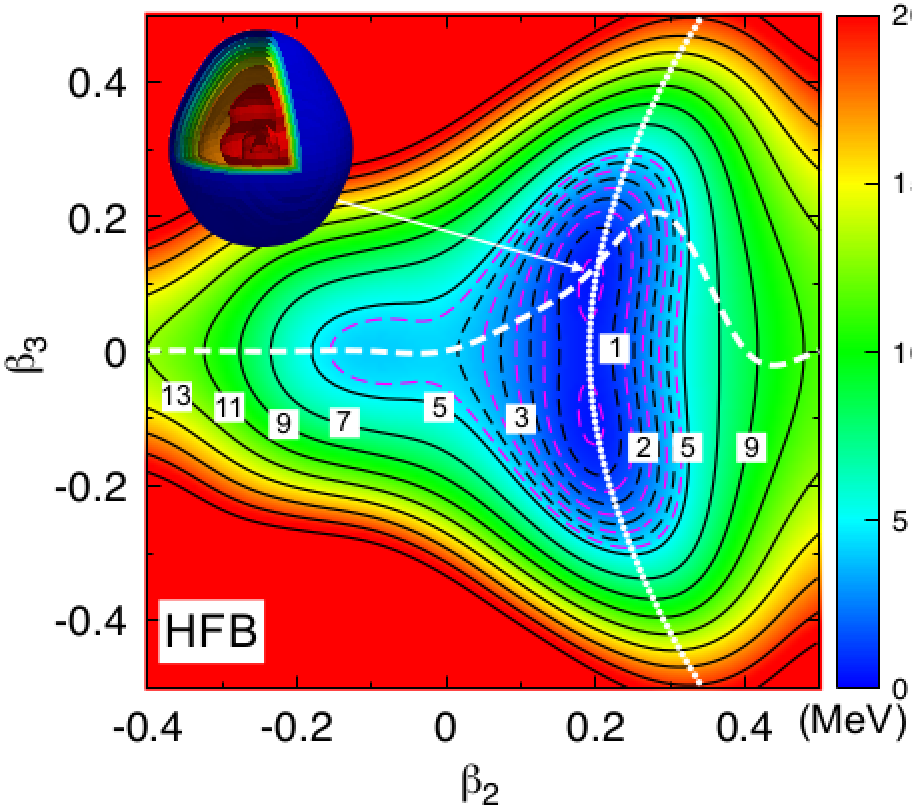
The f amplitudes are obtained by solving the Schrodinger equation in the reduced configuration space (Hill-Wheeler equations for each J, π)

The final wf has good quantum numbers J, N , etc. 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

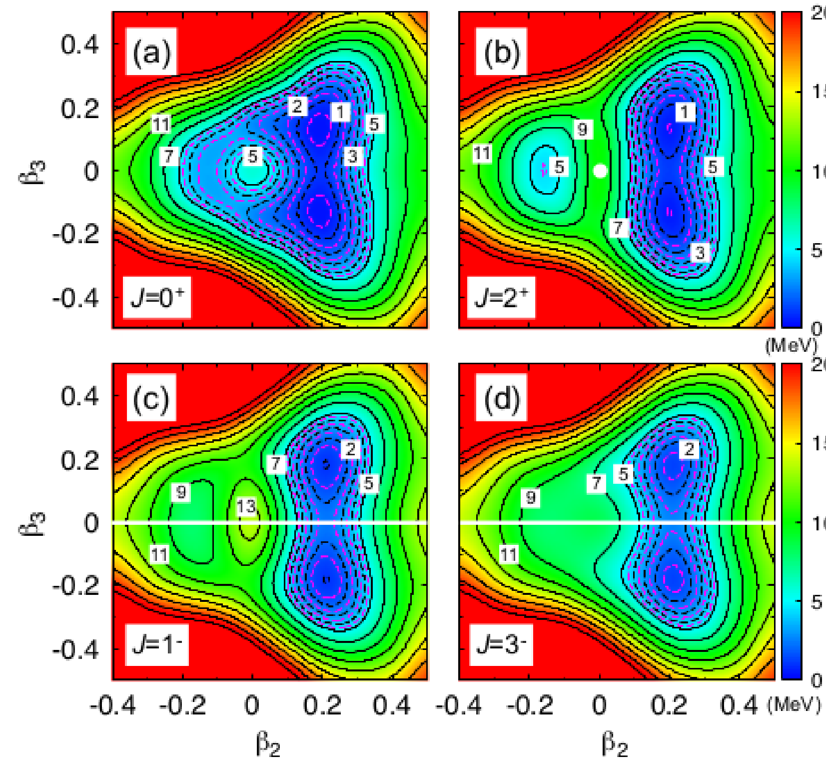
$$\langle \Psi_{\sigma_1}^{J_1\pi_1} | \hat{O} | \Psi_{\sigma_2}^{J_2\pi_2} \rangle \longrightarrow \langle \Phi(Q_2,Q_3) | P^{J_1} P^{\pi_1} \hat{O} P^{J_2} P^{\pi_2} | \Phi(Q_2',Q_3') \rangle$$

In the present approach, assumptions like the "rotational formula" often used to compute transition strengths are not required !

The "rotational formula" B(EL) α β_L^2 fails in weakly deformed nuclei and in computing transitions among different intrinsic states



Intrinsic energy

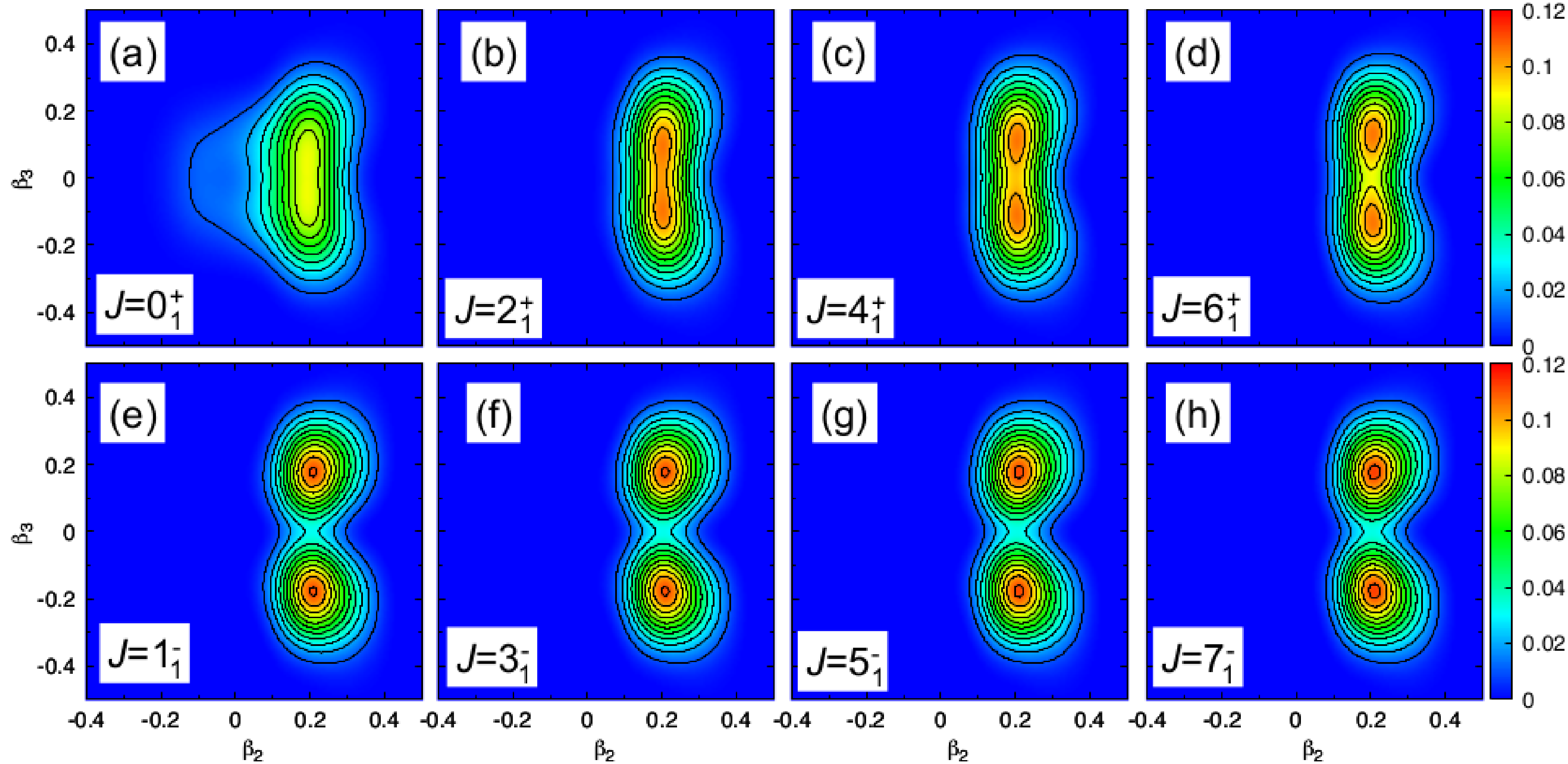


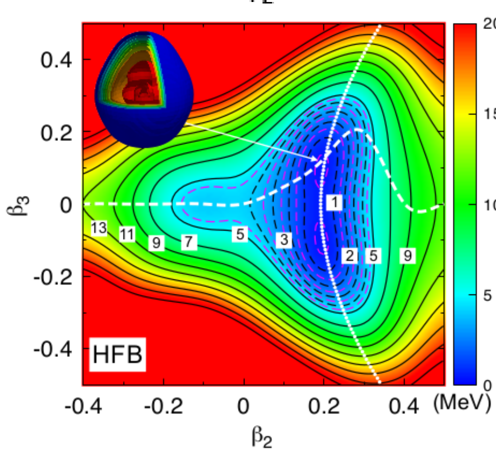
Projected LAB energies

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

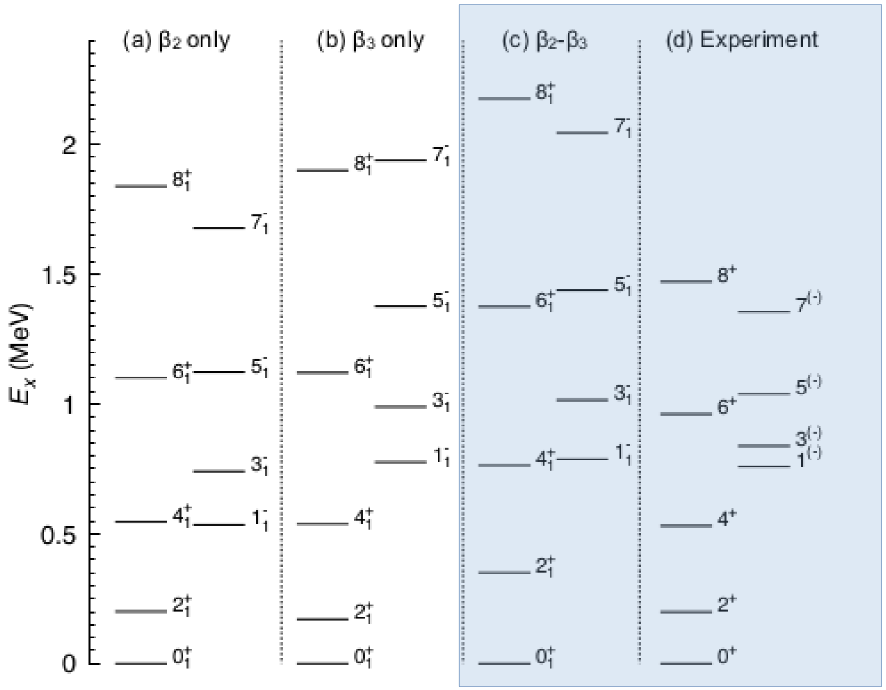




Collective amplitudes:

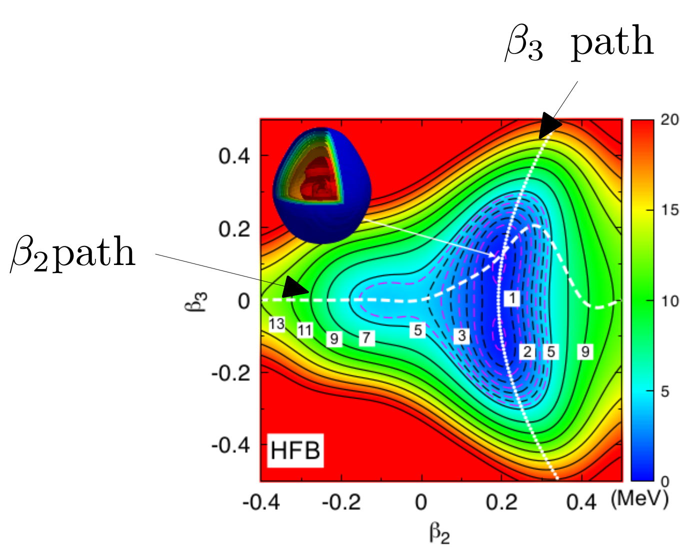
- Follow the topology of the energy surface
- Symmetry restrictions (wf zero if π=-1 and β_3=0)
- Fairly constant as a function of J (collective rotational band)
- Positive parity amplitudes evolve to match negative parity ones (stabilization of octupole deformation at high spins)

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

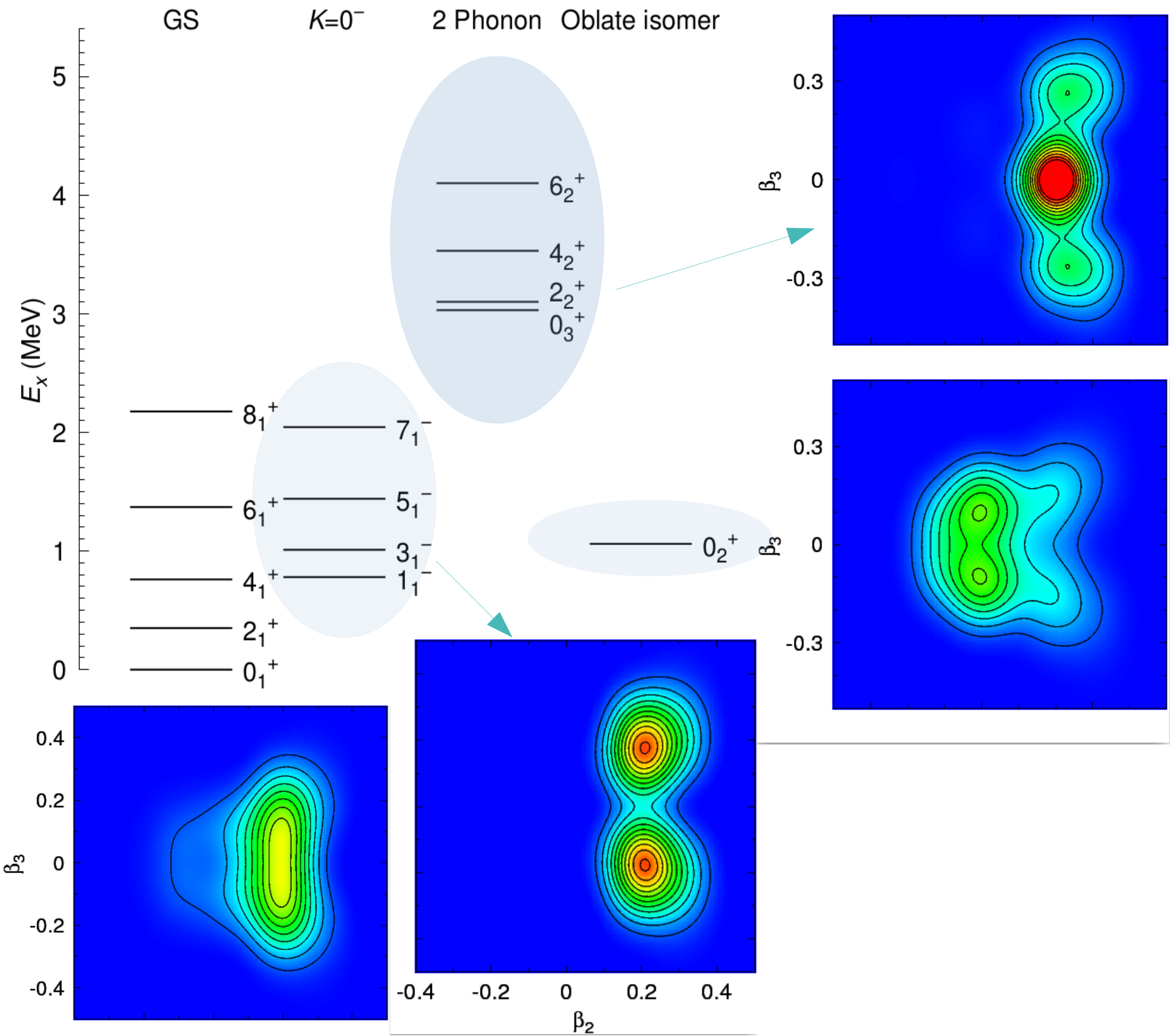
TABLE I. Absolute values of the transition matrix elements $|\langle J_i^\pi||E\lambda||J_f^\pi\rangle|$ (in $eb^{\lambda/2}$) for several transitions of interest.



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

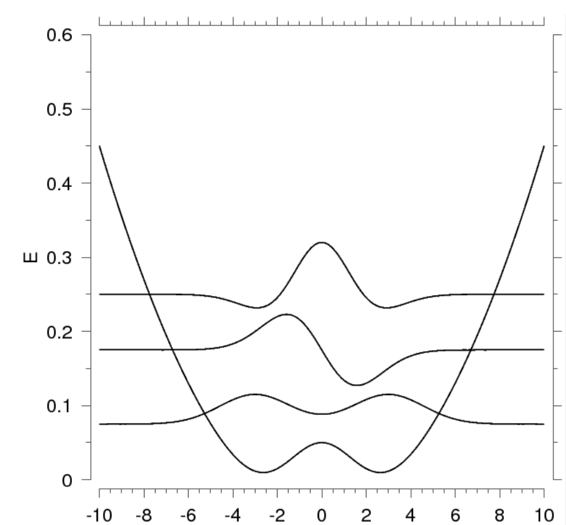
(*) PRC62, 054319; PLB746, 341

144Ba double octupole phonon

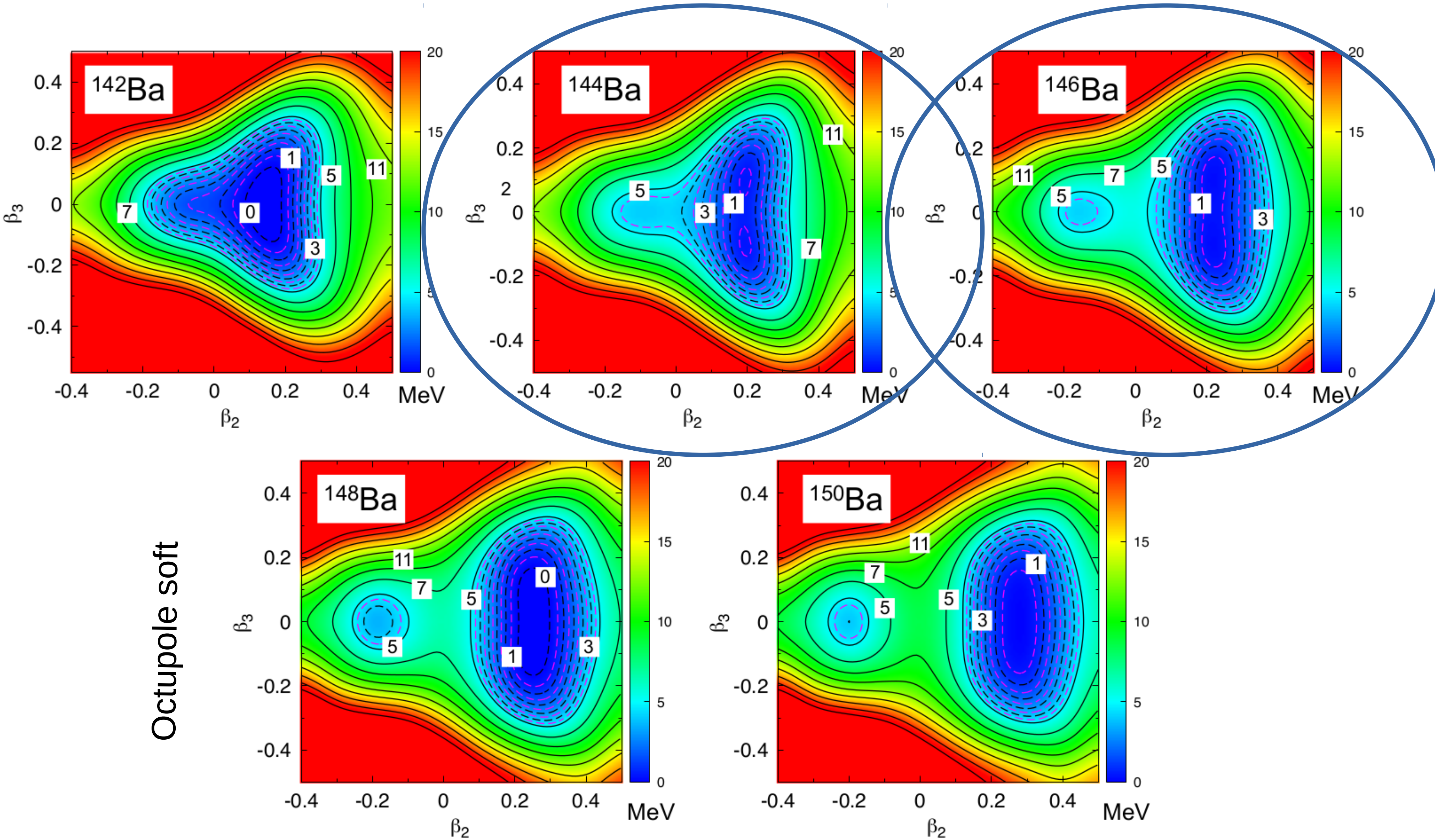


Additional collective states observed

- Oblate isomer
- Two octupole phonon multiplet



Other Ba isotopes

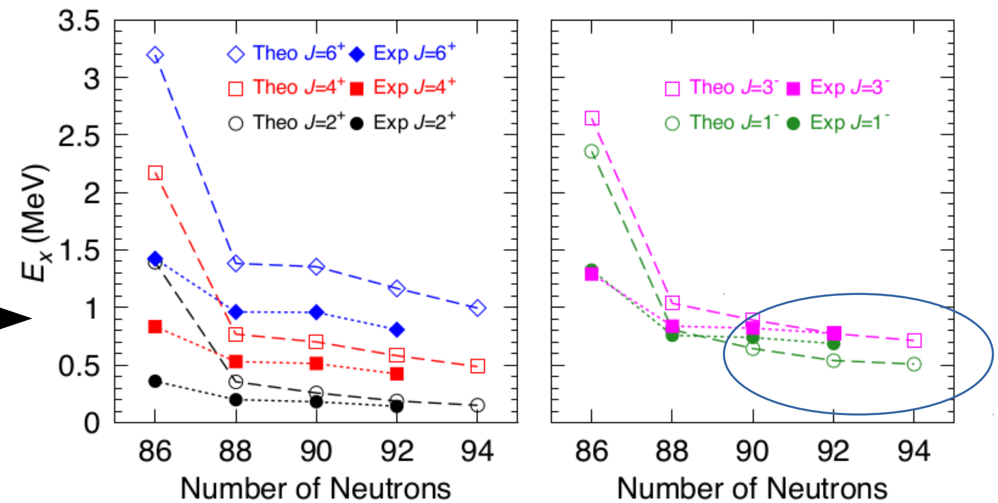


Gogny D1S
HFB potential energy surfaces

Other Ba isotopes

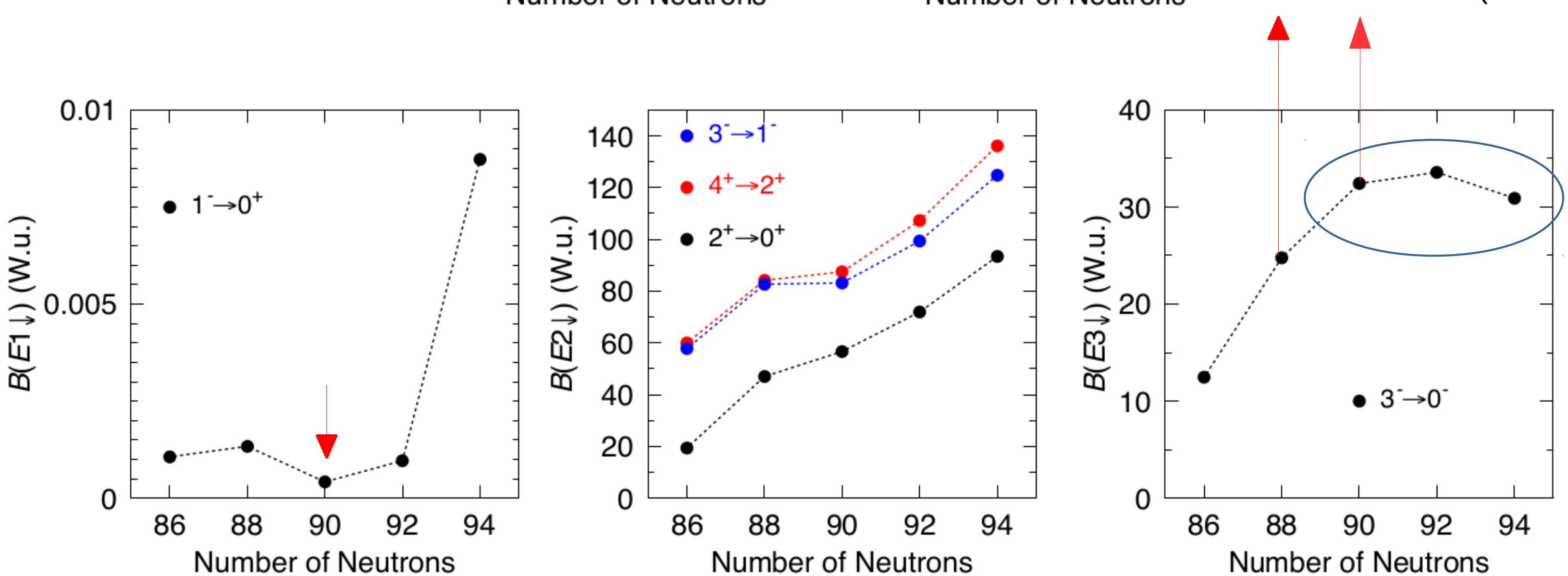
Gogny D1S
GCM results

Too small moments of inertia

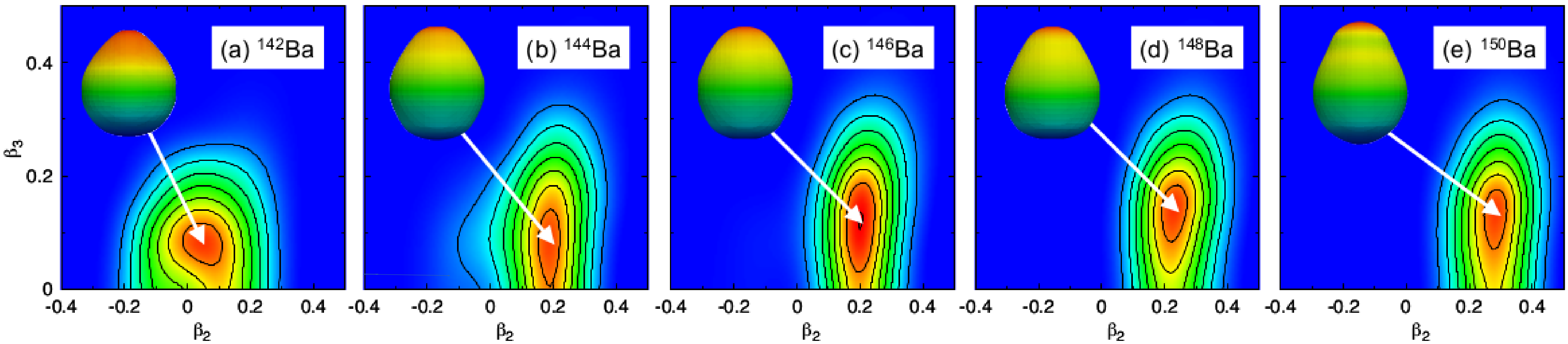


Enhanced octupolarity

Bucher et al (~48 Wu)



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

Conclusions

- Our computational framework reproduces quite nicely many of the experimental features of octupole deformed nuclei in the Ba region
- 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 excitations (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

- Tomás Rodríguez (UAM)

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

Title

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

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

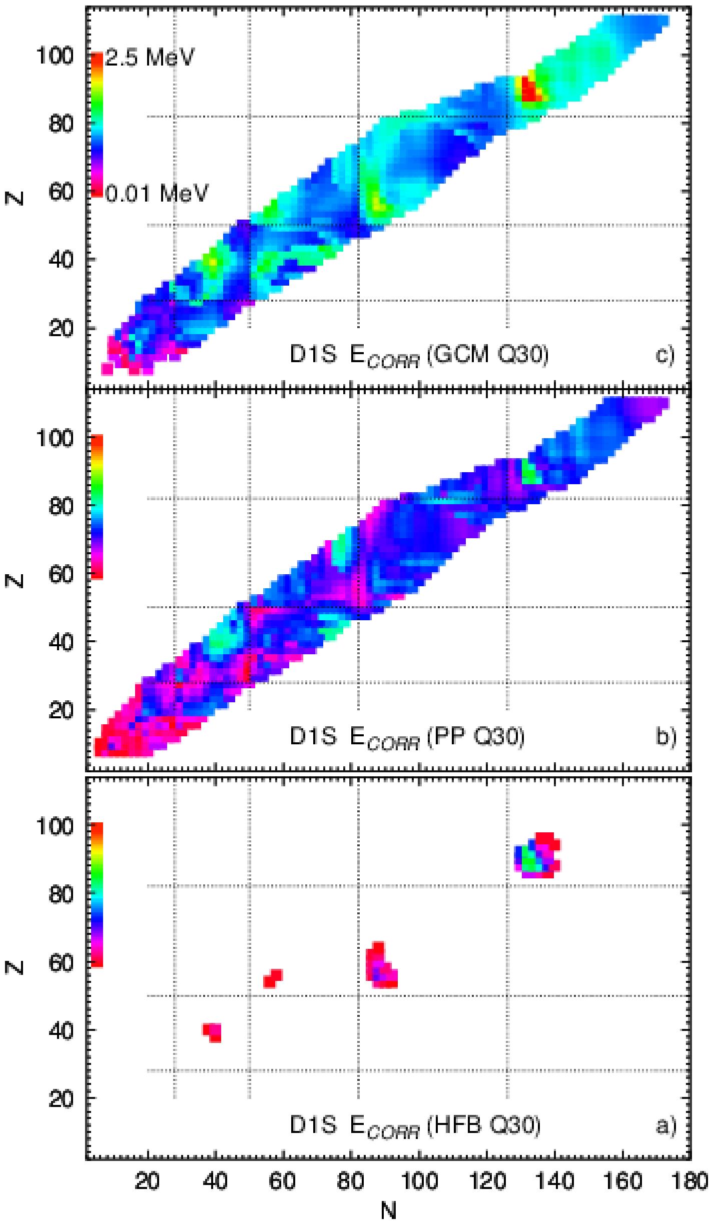
Collective wave functions

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

Transition strengths with the rotational approximation

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

Beyond mean field: Correlation energies

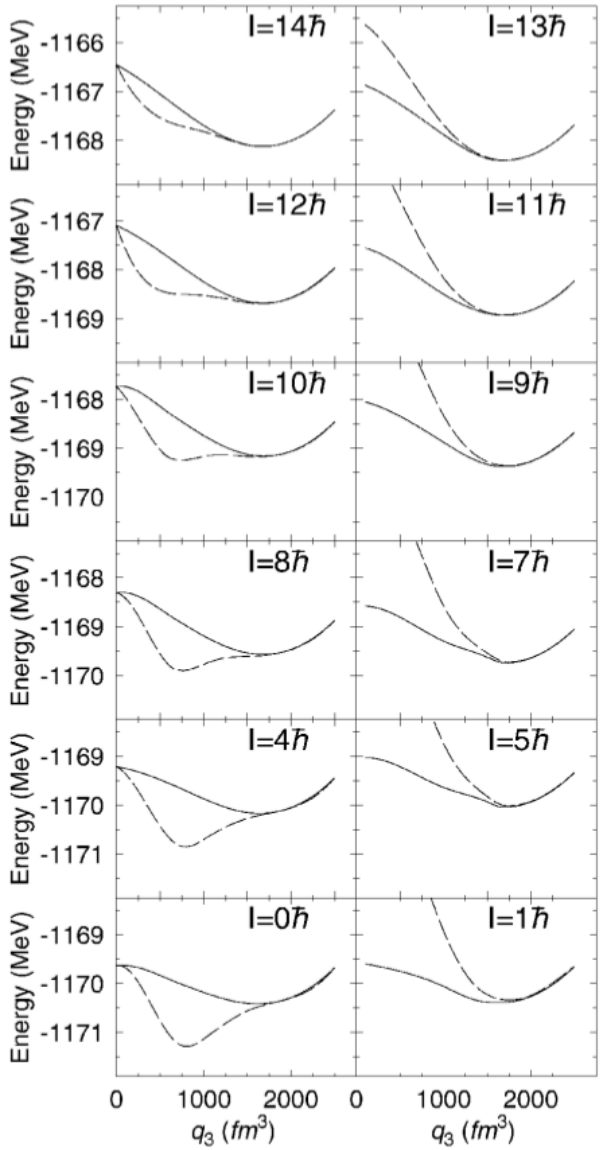


GS correlation energies $\epsilon_{\rm GS}$

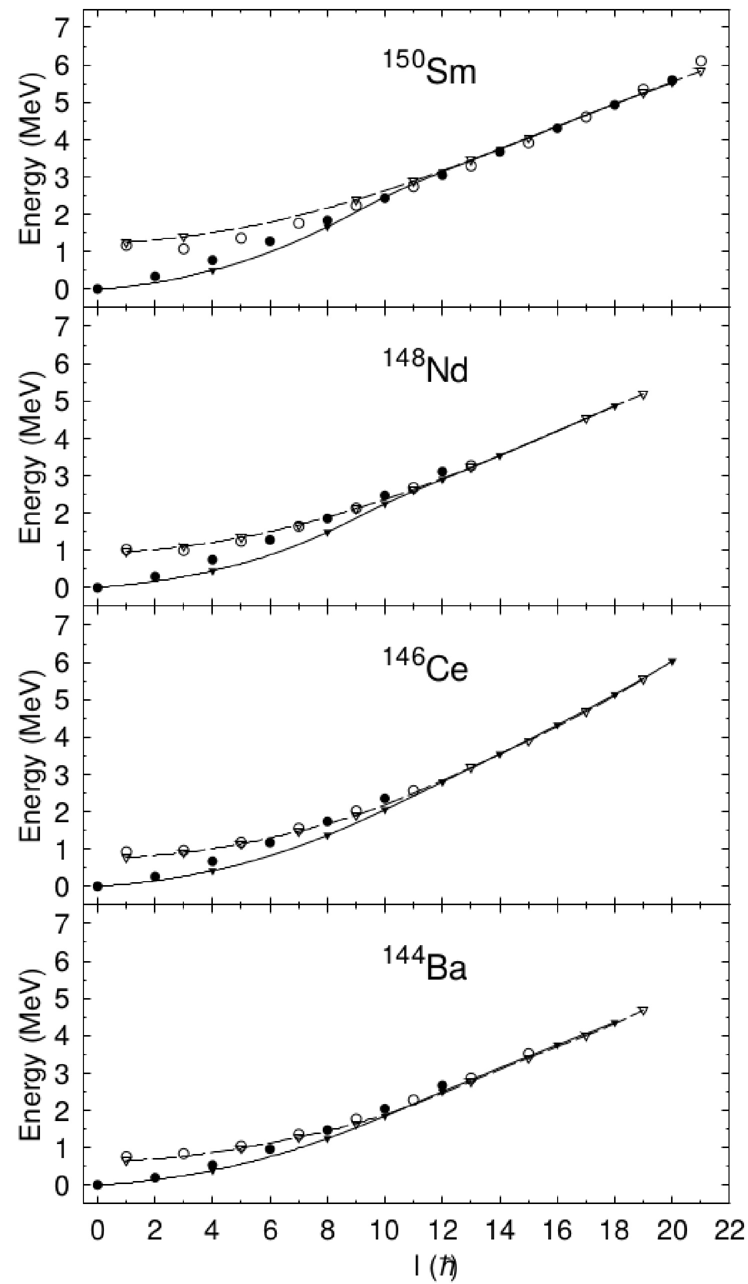
- HFB: Present in just a few nuclei and around 1 MeV
- Parity projection: Present in all nuclei (except octupole deformed) ≈ 0.8 MeV
- GCM; Present in all nuclei ≈ 1.0 MeV

Almost all even-even nuclei have dynamic octupole correlation and their intrinsic ground state is octupole deformed

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

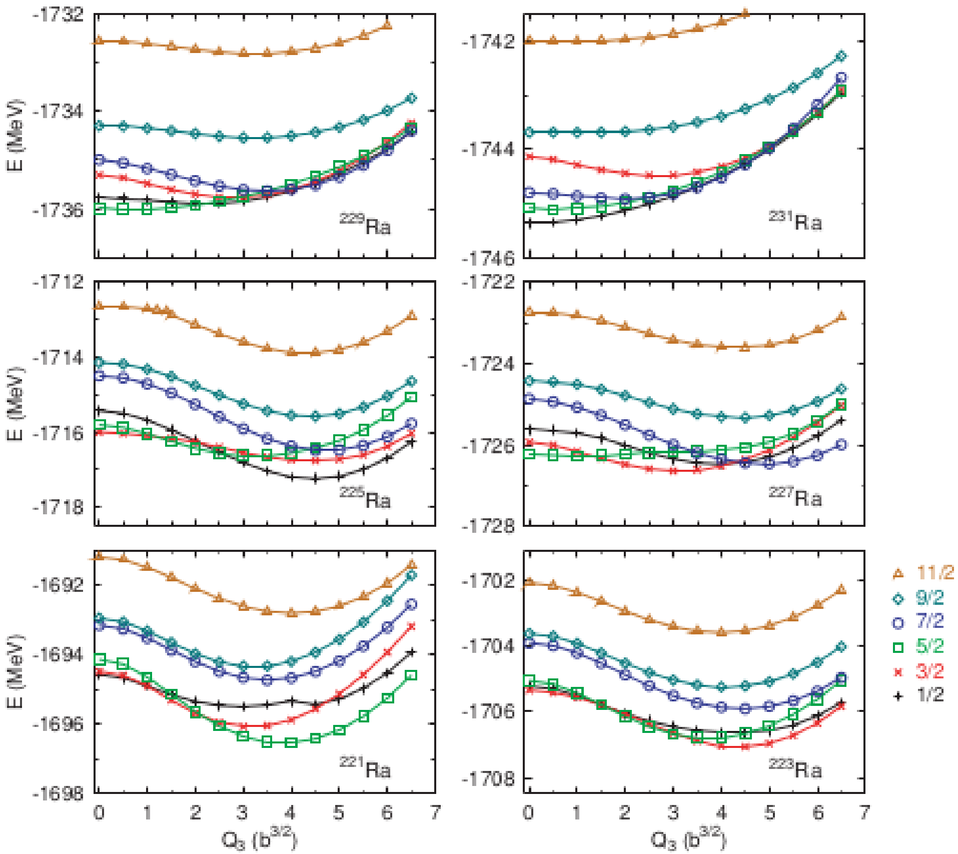


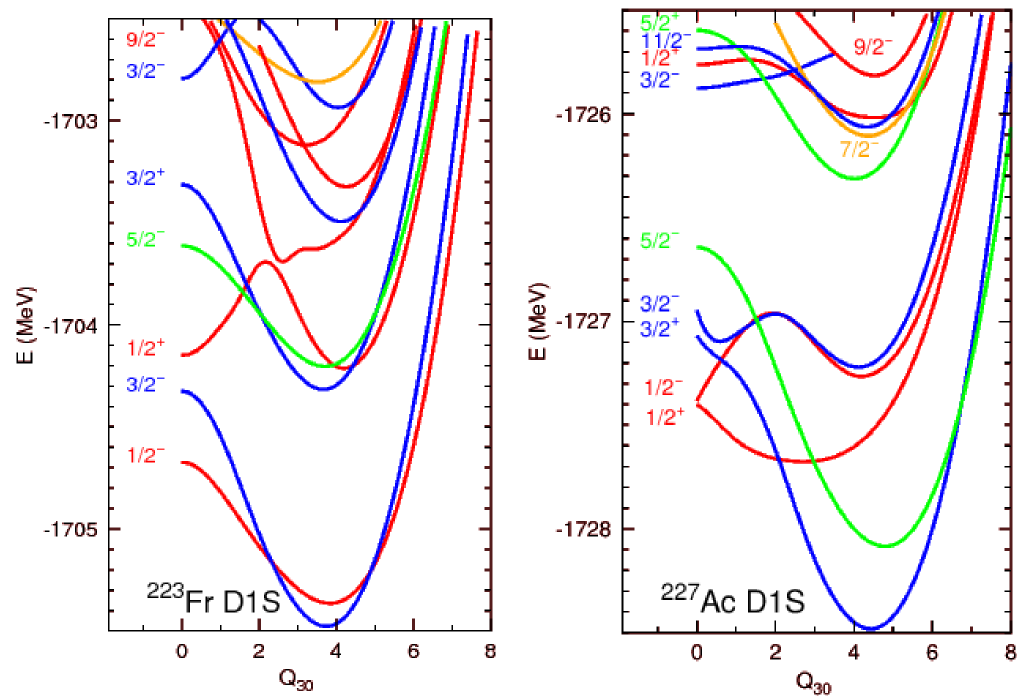
E. Garrote et al PRL 75, 2466



Odd-A and octupole deformation

Unpaired nucleon expected to polarize the even-even core





- Gogny D1S
- Uniform filling approximation
- Octupolarity changes level ordering

- Full blocking (time odd fields)
- Parity projection
- Octupole GCM

S. Perez, LMR PRC 78, 014304

Work in progress