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Octupole correlations in heavy and superheavy nuclei

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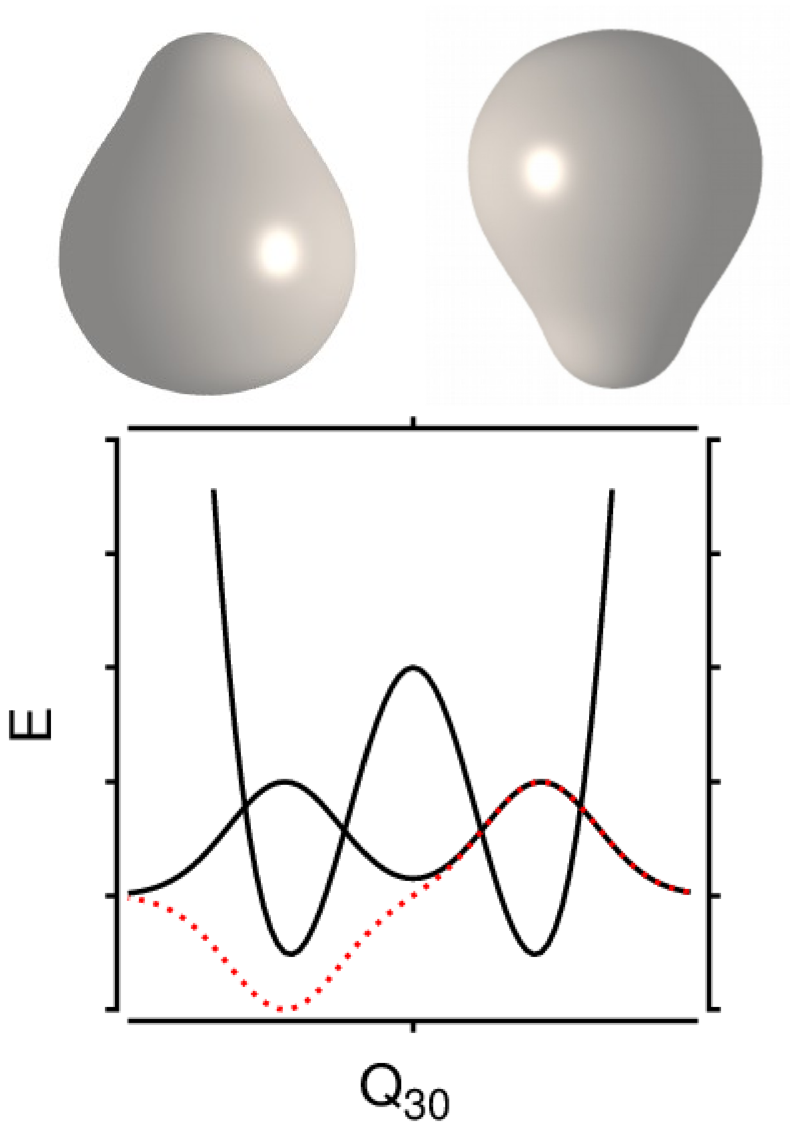
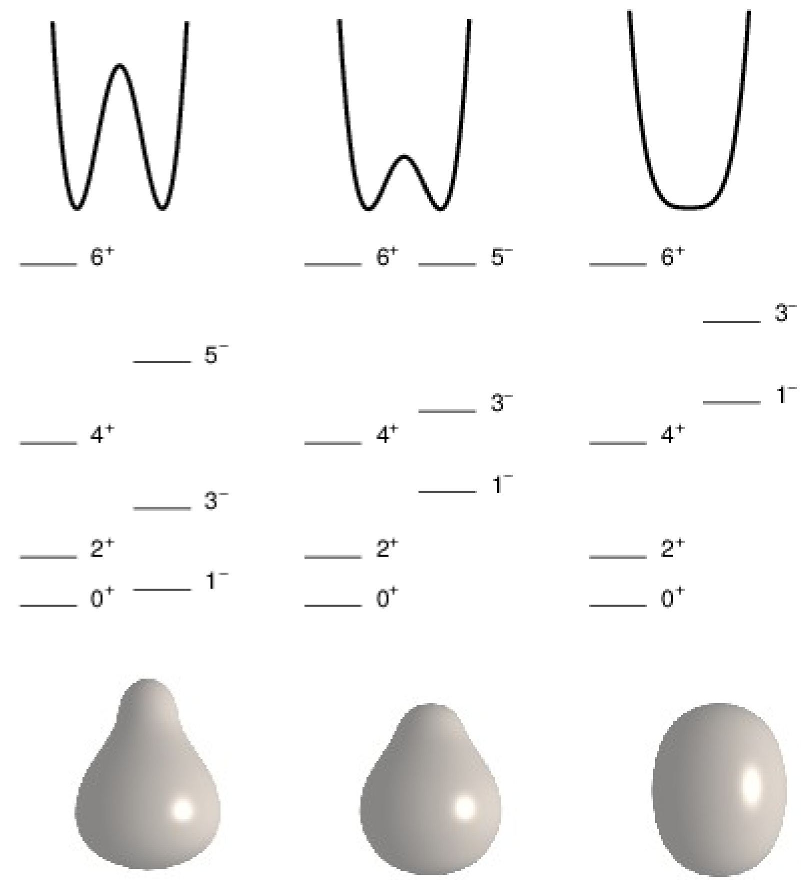
Octupoles 1.0



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



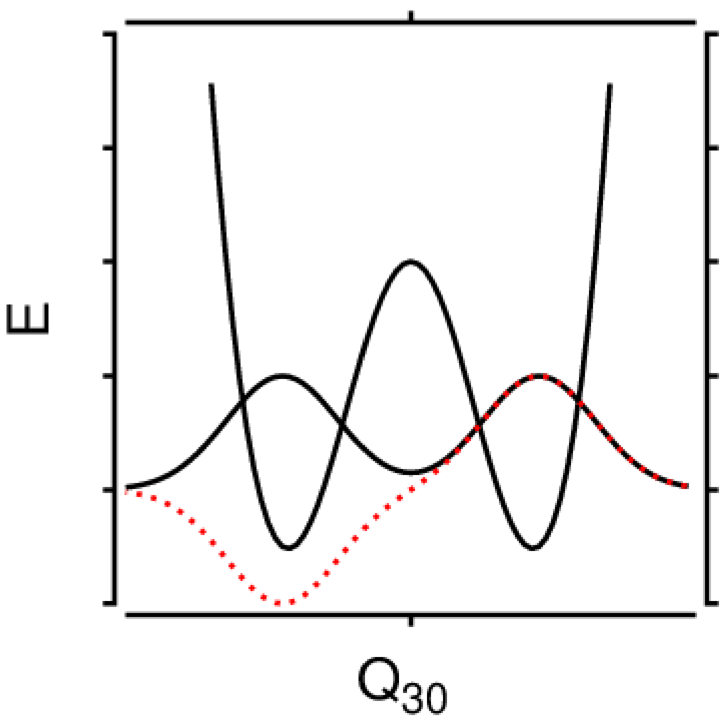
- Parity doublets
- Strong E3 transition strengths

Back in the 80's

Vivid debate about the existence of permanent octupole deformation in atomic nuclei.

- Shell Corrections method with different (HO, WS, FW, etc) single particle potentials (Leander, Nazarewicz, Moller, Ciowk, Chasman, etc)
- Self consistent HF, HF+BCS or HFB with Skyrme or Gogny forces (Heenen, Bonche, Flocard, Egido, Robledo, etc)
- Algebraic: p and f bosons (Iachello, Engel, Otsuka, Han, etc)

Predicted octupole deformed minima in the light Ra and Ba isotopes with depths in the range between a few hundred keV to 1.5 MeV



But the depth of the potential is not the only ingredient: collective wave functions also depend on the collective inertias

Different alternatives for the collective inertias used in different approximations: CSE, GCM, etc finally led to the conclusion that some nuclei around 224Ra (and 146Ba) can be considered as permanent octupole deformed

Strong E3 were obtained and the behavior of the E1 was more or less understood

First calculations with the Gogny force

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STABLE OCTUPOLE DEFORMATION IN SOME ACTINIDE NUCLEI ☆

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The possibility of permanent octupole deformation in the ground state of ^{222}Ra, ^{222}Rn and ^{224}Ra nuclei is studied using the constrained HF+BCS method and the Gogny density dependent interaction The calculation shows energy minima for non-zero values of octupole moment for all three nuclei studied, the minimum for ^{222}Rn being shallower than for the others This result is in agreement with the observed position of $I^{\pi}=1^-$ states. The dipole moments for these nuclei are also calculated

Nuclear Physics **A524** (1991) 65–87
North-Holland

PARITY-PROJECTED CALCULATIONS ON OCTUPOLE DEFORMED NUCLEI*

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Received 6 July 1990

Abstract: A microscopic parity-projected calculation, using as intrinsic states the ones obtained in the mean field approach with the Gogny interaction and constraining the octupole moment is carried out for several nuclei in the barium and radium isotope chains. Projected mean values and transition matrix elements are obtained for both, parities as well as for the 0^+-1^- splittings. These quantities are compared to previous results obtained in collective calculations. The differences are discussed and conclusions about the importance of the correlations associated to the projection are extracted.

Nuclear Physics **A494** (1989) 85–101
North-Holland, Amsterdam

MICROSCOPIC STUDY OF THE OCTUPOLE DEGREE OF FREEDOM IN THE RADIUM AND THORIUM ISOTOPES WITH GOGNY FORCES*

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Received 15 August 1988
(Revised 19 October 1988)

Abstract. The octupole degree of freedom of the nuclei $^{218-230}$Ra and $^{222-230}$Th is investigated in a microscopic way. Our analysis is based on the constrained Hartree–Fock plus BCS theory as well as on the adiabatic time-dependent Hartree–Fock in the cranking approximation (and generator coordinate method plus mean field). In the numerical applications we use the Gogny forces. From the mean field calculations we show octupole barrier heights, dipole moments as well as the values of β_2, β_4, β_5, β_6 and β_7 along the constrained path. From the symmetry conserving calculations we display the 0^+-1^- splitting, wave functions as well as the E1 and E3 transition probabilities. The overall agreement with the available experimental data is very good.

PHYSICAL REVIEW C VOLUME 46, NUMBER 1 JULY 1992

Characterization of octupole correlations in the Lipkin model

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The Lipkin model is used to study the transition to a parity-breaking system with the aim of understanding the features of negative parity low-lying levels associated with the octupole degree of freedom. The results of parity projection calculations for the energy splitting between the positive parity ground state and the lowest-lying negative parity state as well as the negative parity transition probability connecting them have been studied and compared to the exact results. A good agreement is observed for not-deformed and for well-deformed systems but at intermediate deformations the parity-projected results strongly differ from the exact ones. By analyzing the parity-projected energy curves, two characteristic configurations are observed in the problem: the mean-field and the tunneling configurations. By mixing these two configurations, a substantial improvement over the parity projection method is obtained for the two quantities studied in all the regions of deformation. It is suggested that this method could be used in realistic calculations to improve the understanding of the octupole dynamics in opposition to the most powerful but expensive generator coordinate method.

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

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

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

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

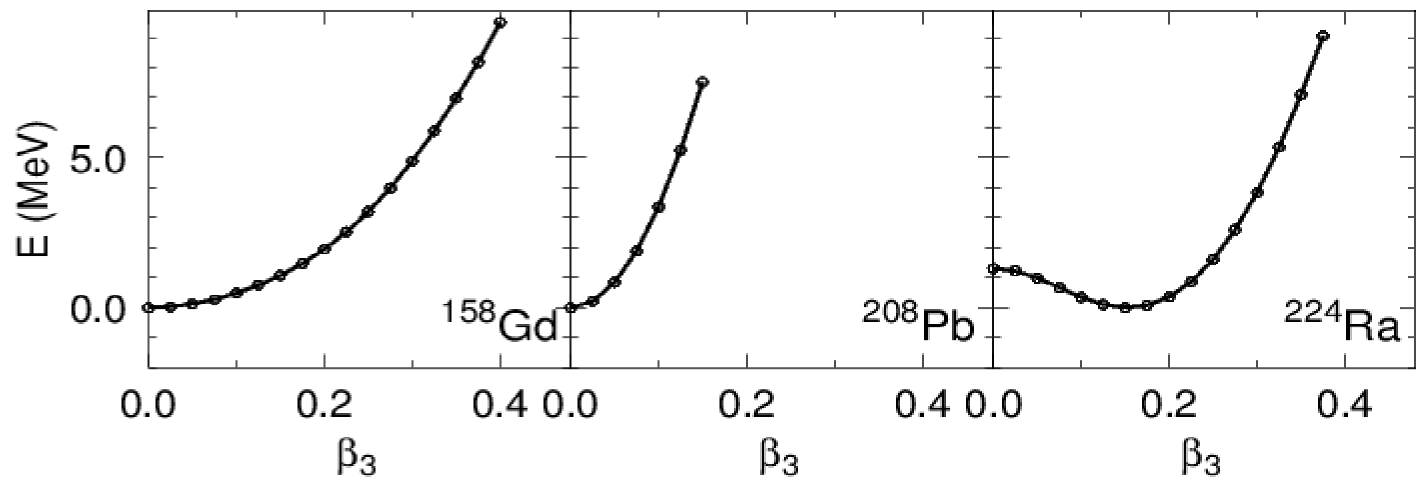
$$V_{DD}(1,2) = t_3 \delta(\vec{r}_1 - \vec{r}_2)(1 + x_0 P_\sigma)\rho^\alpha(\vec{R})$$

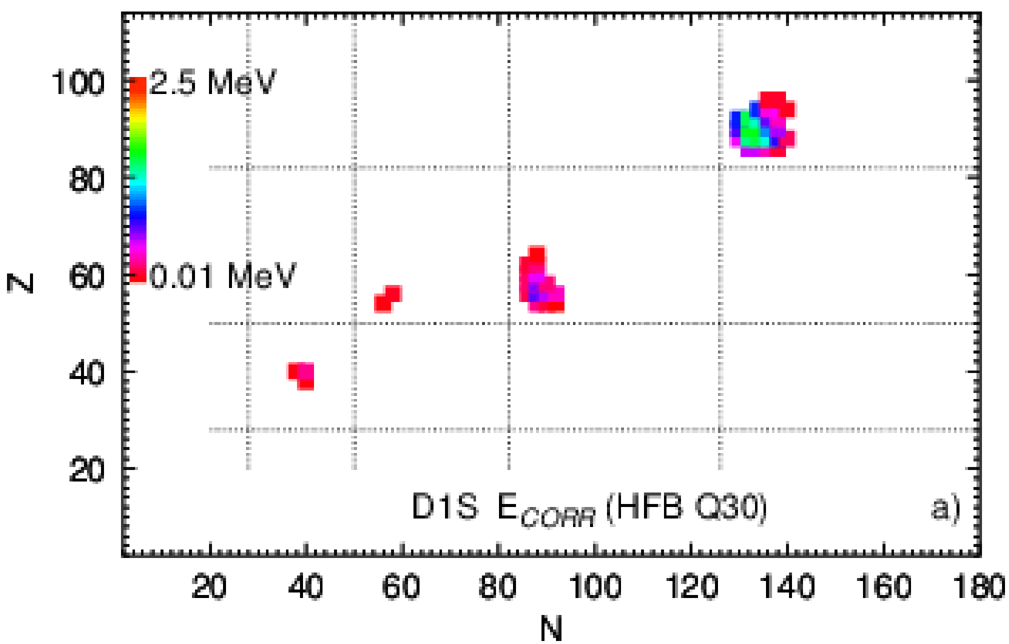
Parameters fixed by imposing some nuclear matter properties and a few values from finite nuclei (binding energies, s.p.e. splittings and some radii information).

- **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 beyond mean field effects

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

Mean field: Octupole constrained calculations



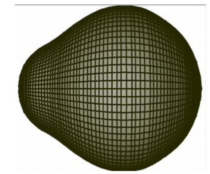
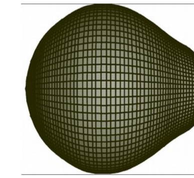


- Axially symmetric HFB with constraint in Q_{30}
- Around 900 nuclei (8<Z<110) analyzed
- Finite range Gogny (D1S, D1M, etc)

- Z and N values must have orbits of opposite parity and Δl=3 around the Fermi level for permanent octupole deformation
- Zr, Ba and Ra regions show octupole def
- Mean field correlations energies ≈ 1.5 MeV
- Many nuclei are soft against octupole deformation (eg Gd)
- Qualitative and almost quantitative independence with Gogny parametrization

L.M.Robledo and G.F. Bertsch, PRC84, 054302 (2011)

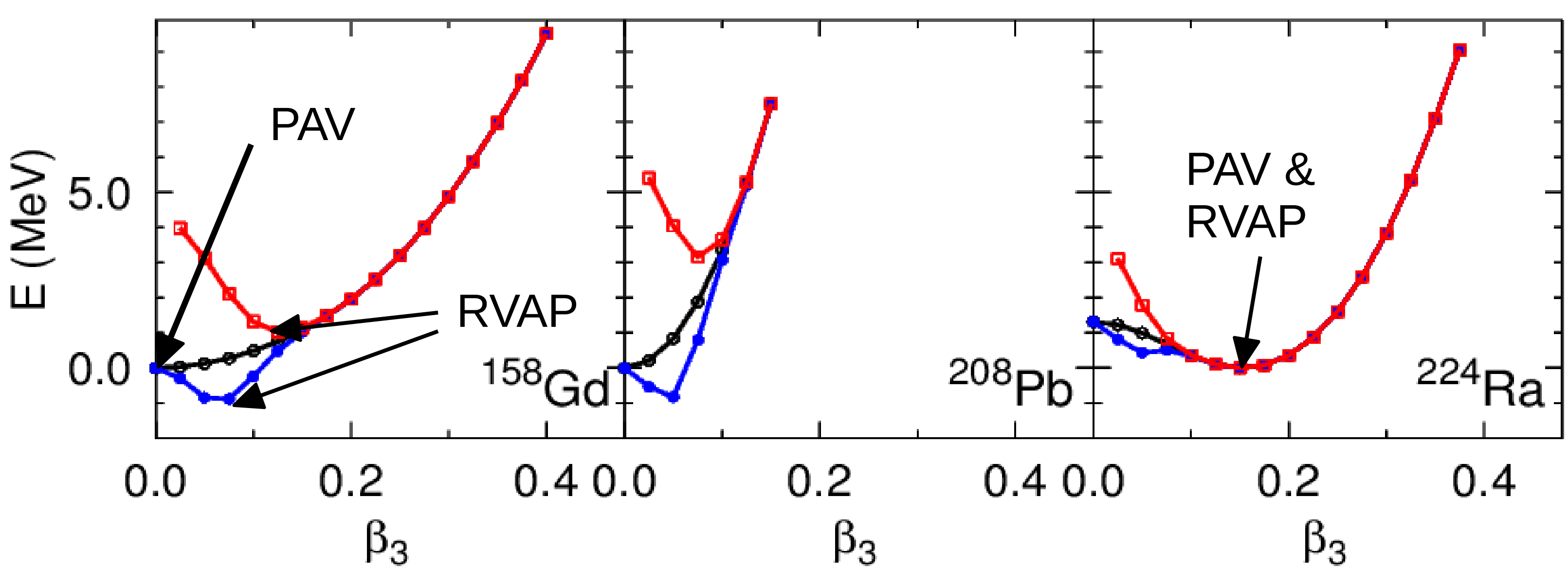
First step beyond the mean field: Parity projection

Parity symmetry is broken when $\beta_3 \neq 0$ $|\varphi(\beta_3)\rangle$  $\hat{\Pi}|\varphi(\beta_3)\rangle$ 

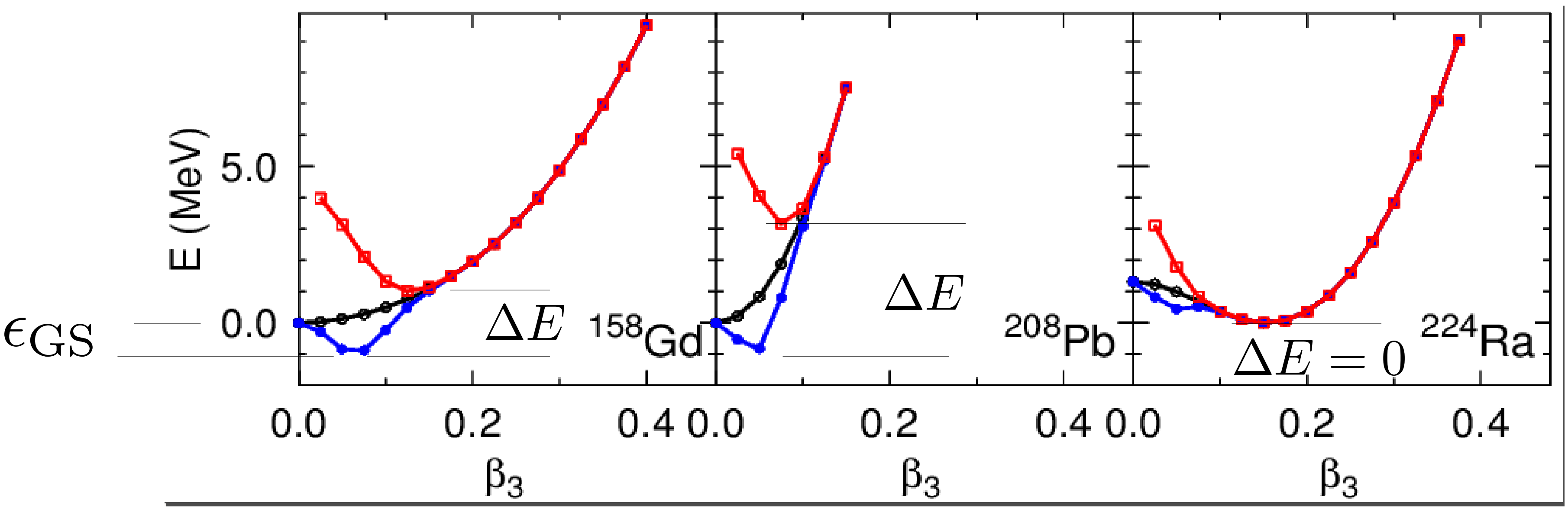
But a linear combination of the two shapes restores parity symmetry

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

1. Projection after variation (PAV): the intrinsic states are those minimizing the HFB energy
2. Projection before variation (VAP): the intrinsic states are chosen as to minimize the projected energy E_π One intrinsic state for each parity
3. Restricted VAP: VAP but the intrinsic states are restricted to $|\varphi(\beta_3)\rangle$



First step beyond the mean field: Parity projection



Excitation energy of K=0$^-$ band $\Delta E = E_+(\beta_3(+)) - E_-(\beta_3(-))$

Ground state correlation energy ϵ_{GS} : non zero for reflection symmetric mean field gs.

Transition strengths E1 and E3 computed with the rotational formula

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

Valid for well deformed nuclei. For spherical ones multiply by 2L+1 (see below)

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

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

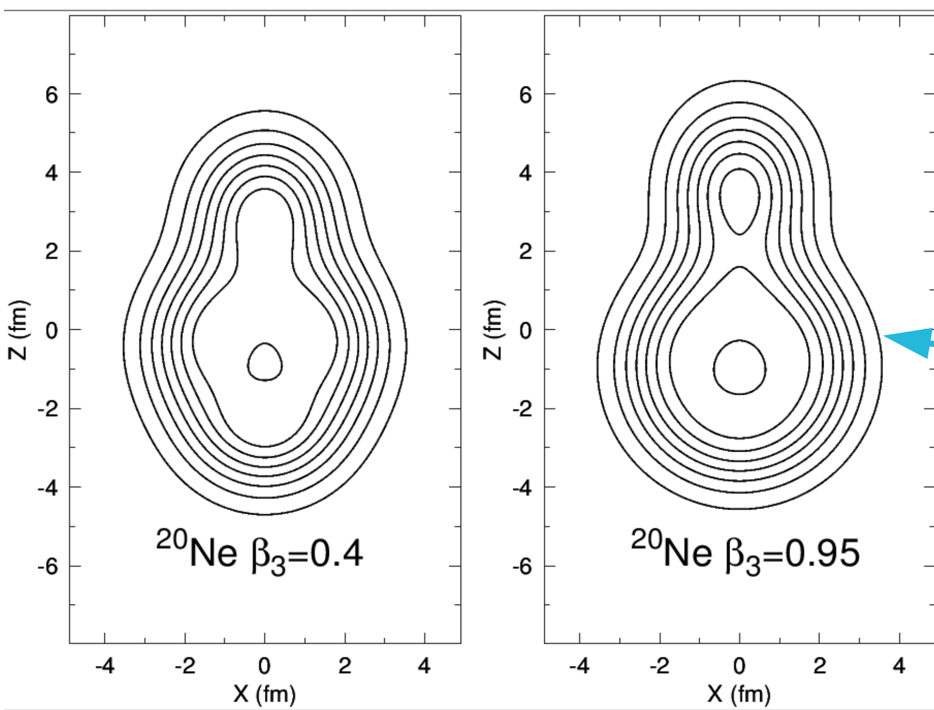
Transition strengths with the rotational approximation

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

Assorted GCM results

Nucleus	E_- (MeV)			W(E3)		
	Exp	GCM	RPA	Theory	Sph-Def	Exp
^{20}Ne	5.6	6.7		12	Def	13
^{208}Pb	2.6	4.0	3.46	53	Sph	34
^{158}Gd	1.26	1.7		11.6	Def	12
^{226}Ra	0.32	0.16		43	Def	54

W(E3) Sph =W(E3) Def x7



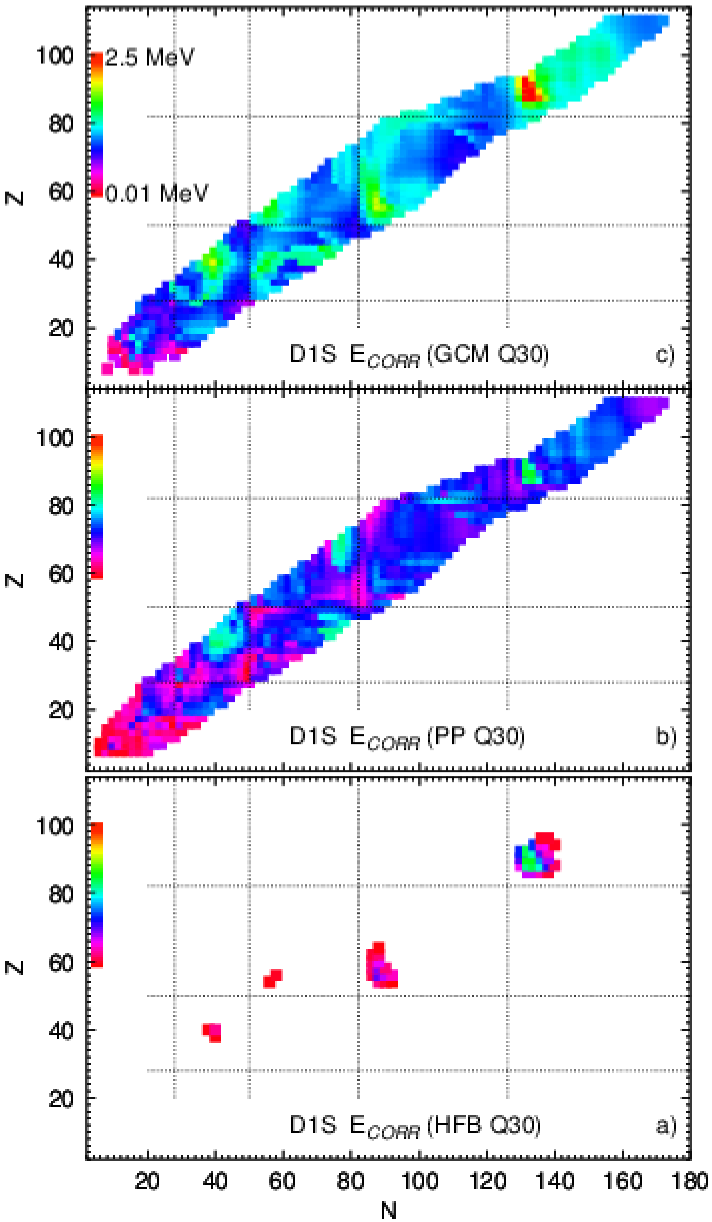
^{16}O+^{4}He

Alpha clustering in light nuclei

- β_3= 0.4 Positive parity intrinsic state
- β_3=0.95 Negative parity intrinsic state

Connected with asymmetric fission physics and cluster emission in heavy nuclei (^{223}Ra → ^{209}Pb+ ^{14}C)

Beyond mean field: Correlation energies



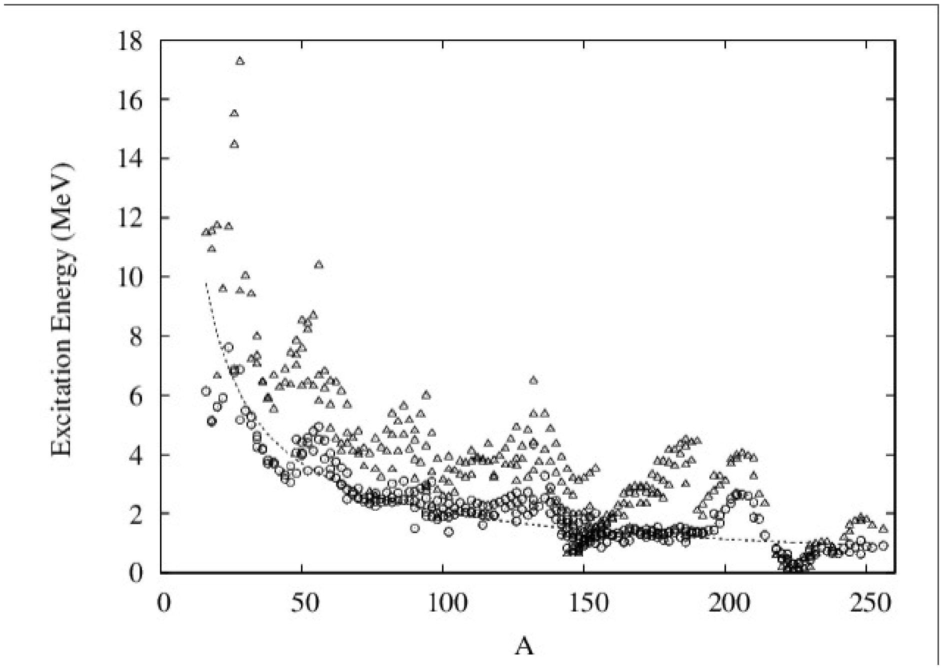
GS correlation energies ϵ_{GS}

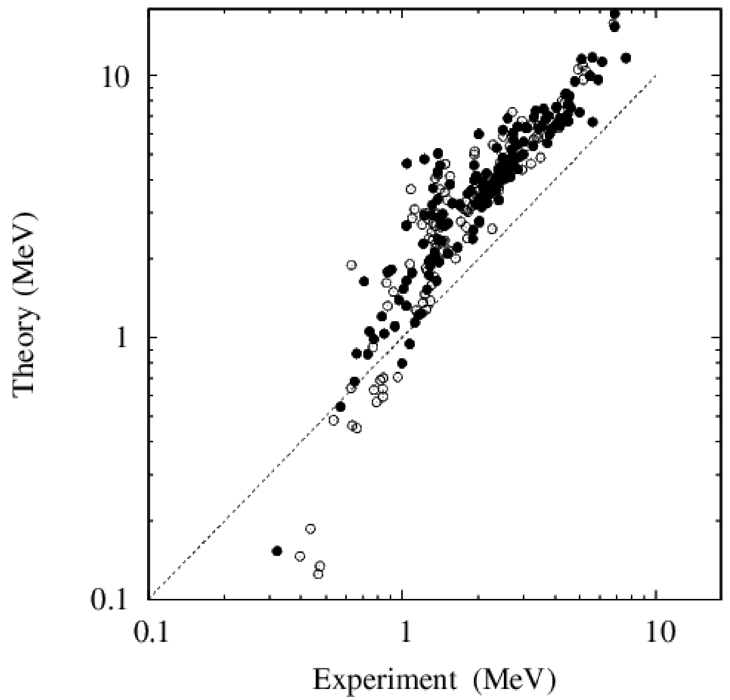
- HFB: Present in just a few nuclei and around 1 MeV
- Parity projection: Present in all nuclei (except octupole deformed) ≈ 0.8 MeV
- GCM; Present in all nuclei ≈ 1.0 MeV

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.

Excitation energies



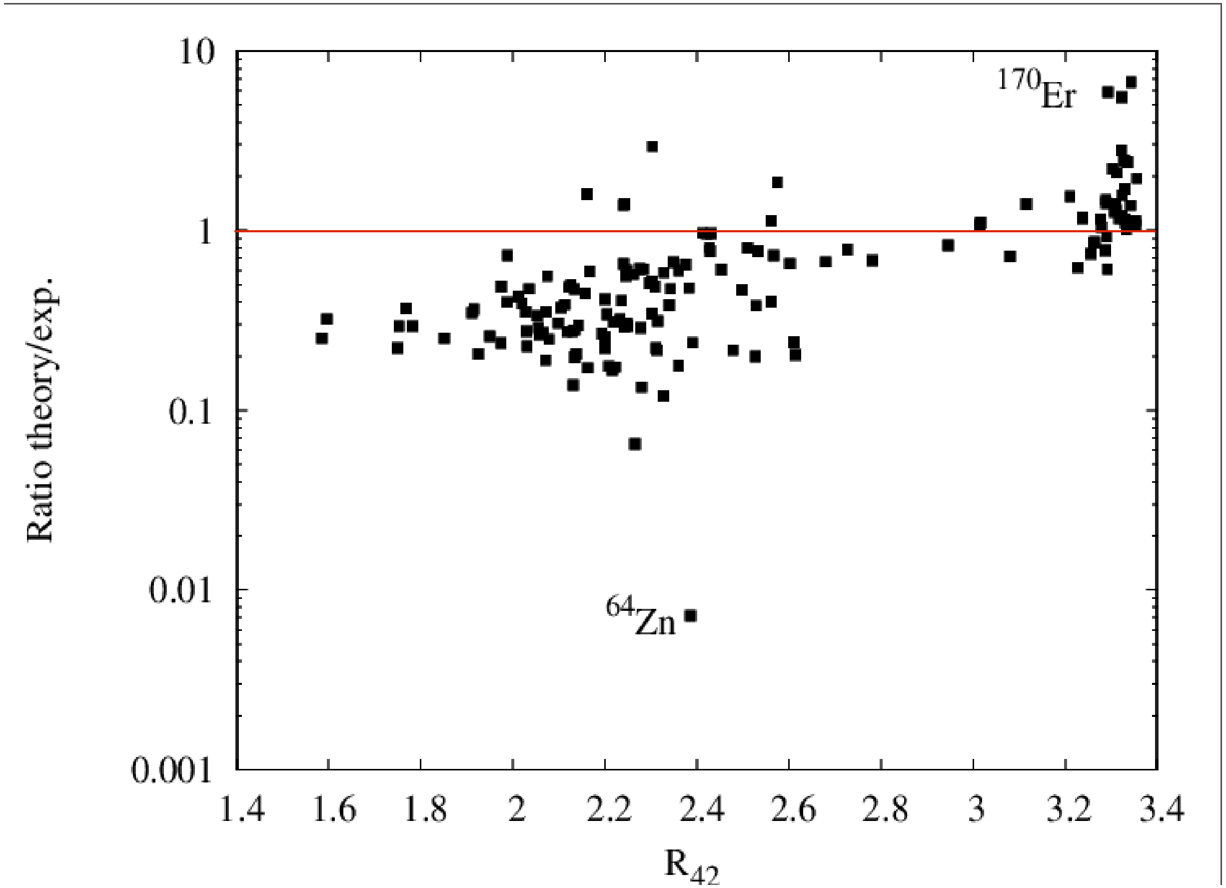


- The excitation energies of the $K=0^-$ are plotted vs A (GCM)
- and compared to experimental data (including K≠0 excitations in def nuclei)

- Theory is systematically too high (~ factor 1.5) (irrespective of interaction)
- Also for 2+ (quadrupole) excitations with GCM approaches

- Other degrees of freedom ?
  - Pairing, quadrupole-octupole coupling
  - Time odd, momentum like collective variables

Electromagnetic strengths



- B(E3) strength vs R_{42}
- Log scale
- Good for $R_{42} \sim 3.3$
- Underestimation for $R_{42} < 2.8$

- B(E1) is not smooth as a function of N and Z (strongly dependent upon single particle occupancies)
- Is the rotational formula valid ? Ans: Only for strongly deformed systems
- What is happening with ^{64}Zn ?

Transition strengths

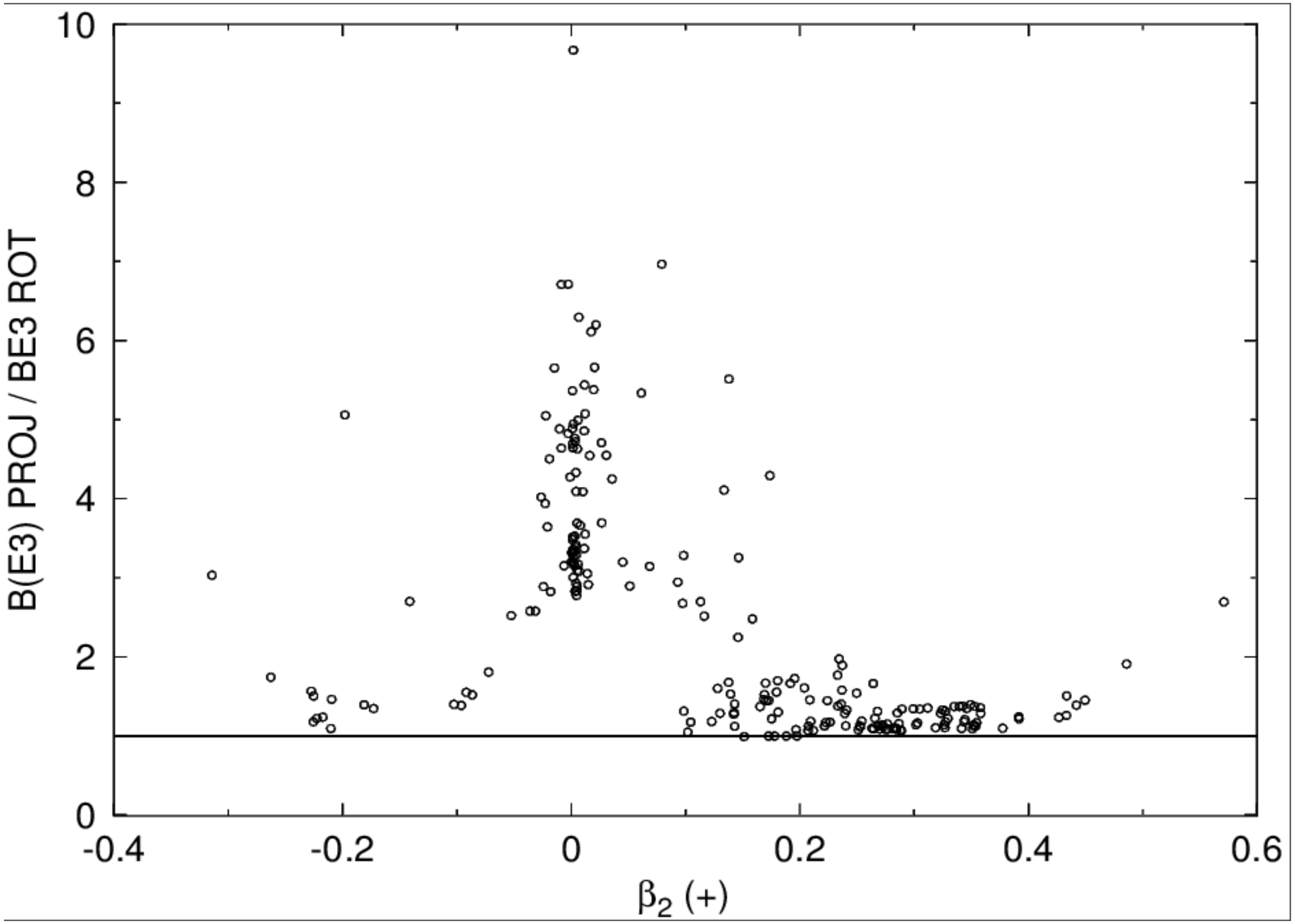
- The rotational formula used to relate intrinsic deformation parameters and transition strengths can be justified in the strong deformation limit
- Not valid for spherical or near spherical nuclei
- The proper treatment involves angular momentum projected wave functions
- Contrary the rotational formula, the projected B(EL,L→0) is not zero in the spherical limit

$$|\Psi^J\rangle = \mathcal{N}_J P^J |\varphi\rangle \to \text{p-h excitations}$$

- For B(E3) strength the spherical limit equals a factor 7=(2L+1) times the rotational formula value but using the parity projected wave functions instead
- The rotational formula for B(E2) is not valid for β_2 values less than 0.1 (0.2) in heavy (light) nuclei
  - Simple formula to relate B(E2) and β_2

LMR, G.F. Bertsch, PRC86, 054306 (2012)

Projected B(E3) transition strengths



$$|\Psi^{3^-}\rangle = \mathcal{N} P^{J=3} |\varphi(\beta_3(-))\rangle$$

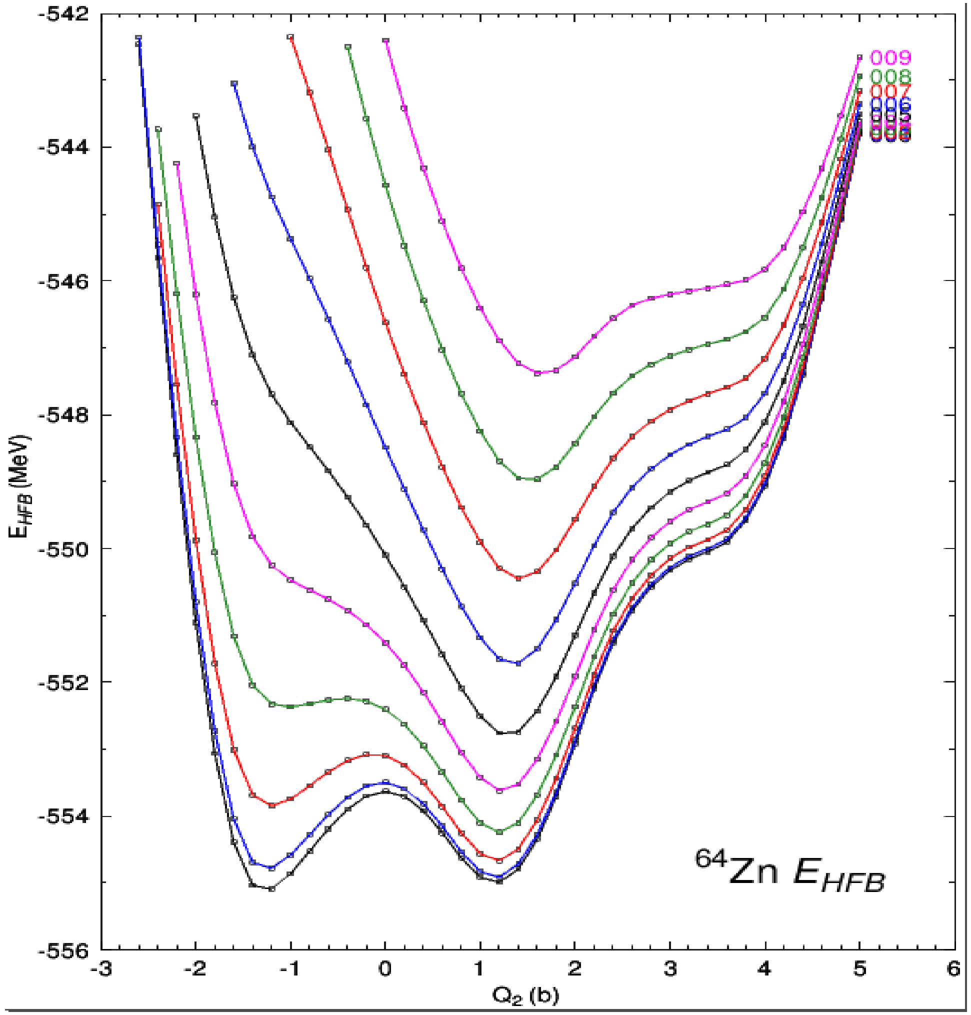
$$|\Psi^{0^+}\rangle = \mathcal{N} P^{J=0} |\varphi(\beta_3(+))\rangle$$

- Only RVAP intrinsic wf
- A factor ~7 is seen !
- β_2 (+) quadrupole deformation of the gs

- Much better agreement with experiment: in ^{208}Pb the experimental B(E3) is 34 Wu The parity projected value is 7.5 Wu and the angular momentum one is 24 Wu
- When both regimes are intermixed: full use of AMP is required
- Caveat: AMP is not used (yet) to determine the intrinsic states

Quadrupole-octupole coupling

- Important in shape coexistent nuclei like ^{64}Zn



GCM with Gogny D1S

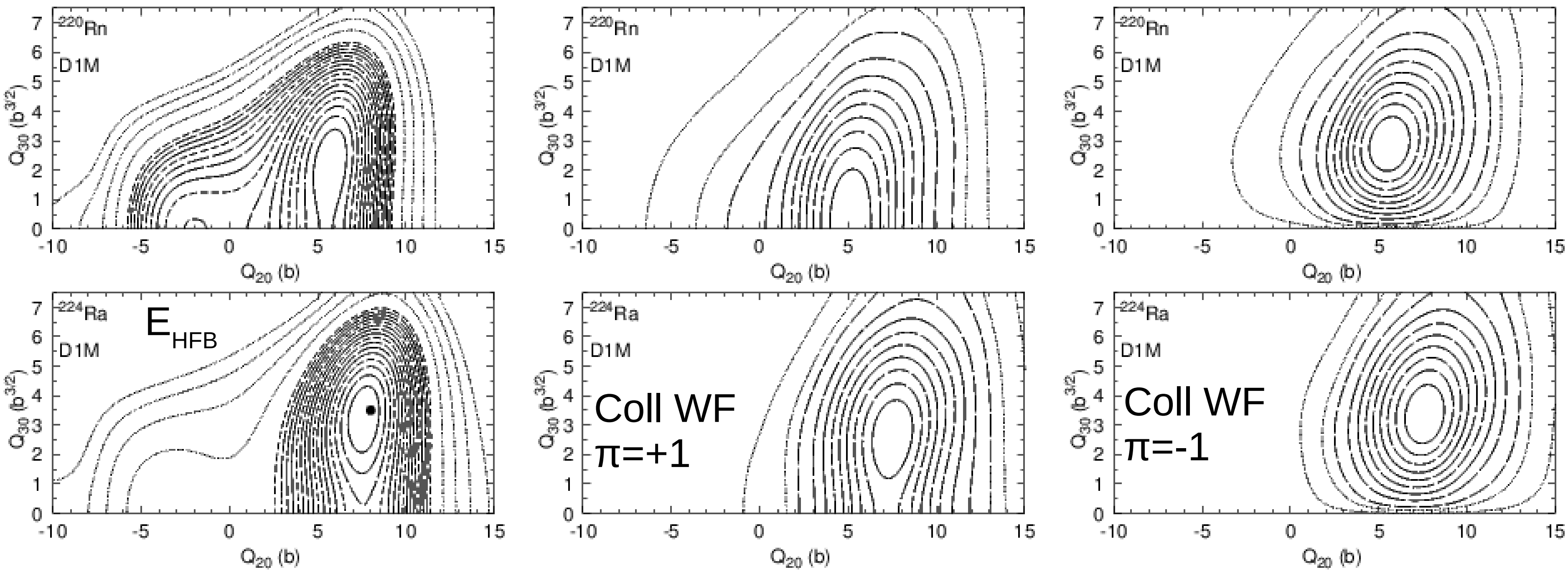
	Q_2-Q_3	Q_3
E_- (MeV)	4.2	7.20
E_{corr} (MeV)	1.63	0.72
W(E3)	6.80	Wild

Also relevant in other nuclei (see below)

Two-phonon octupole states and 0_2^+ ?

Computationally intensive

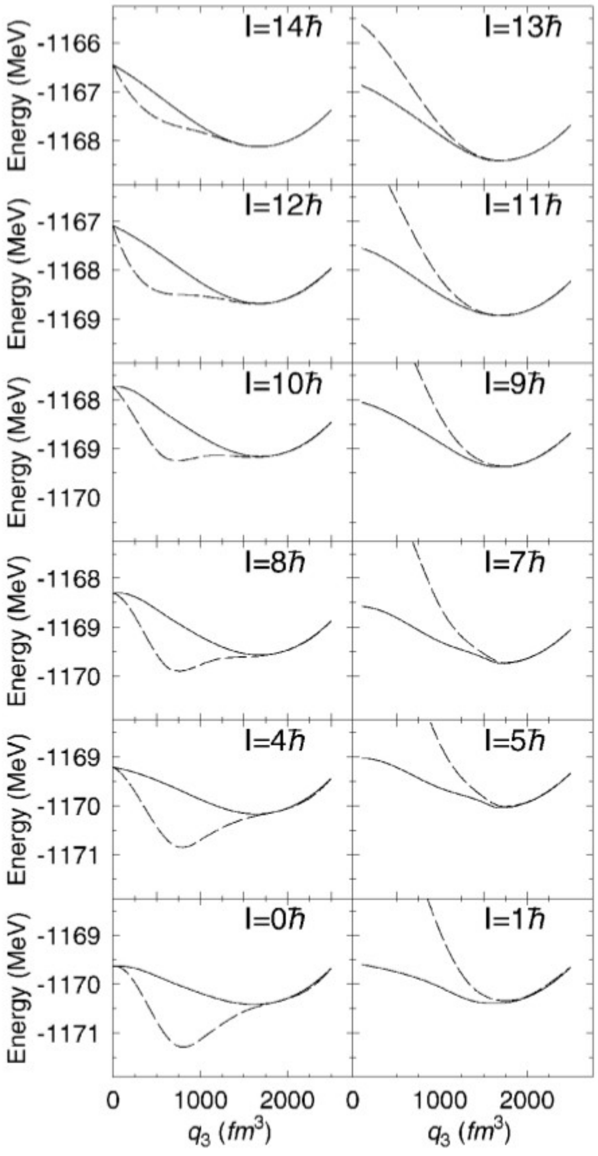
Quadrupole-octupole coupling



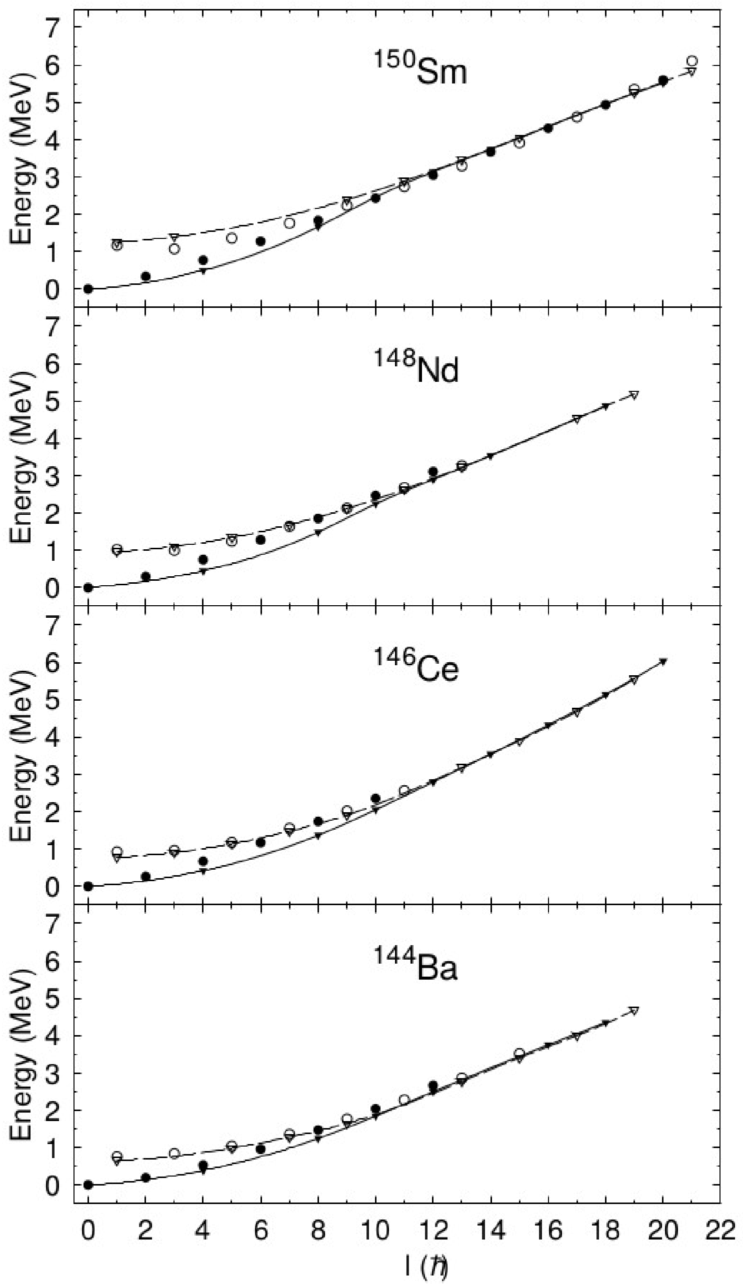
220 Rn	Q_2-Q_3	Exp
E_- (MeV)	0.618	0.645
W(E1)	2.4 10^{-5}	< 1.5 10^{-3}
W(E3)	26.50	33±4
E_2^+ (MeV)	1.35	0.94
W(E2)	48.5	48±3

224 Ra	Q_2-Q_3	Exp
E_- (MeV)	0.234	0.216
W(E1)	2.4 10^{-4}	< 5 10^{-5}
W(E3)	45.7	42±3
E_2^+ (MeV)	1.75	0.97
W(E2)	92.8	98±3

Good agreement with recent experimental data (LMR and P.A. Butler, PRC 88 051302 (R))

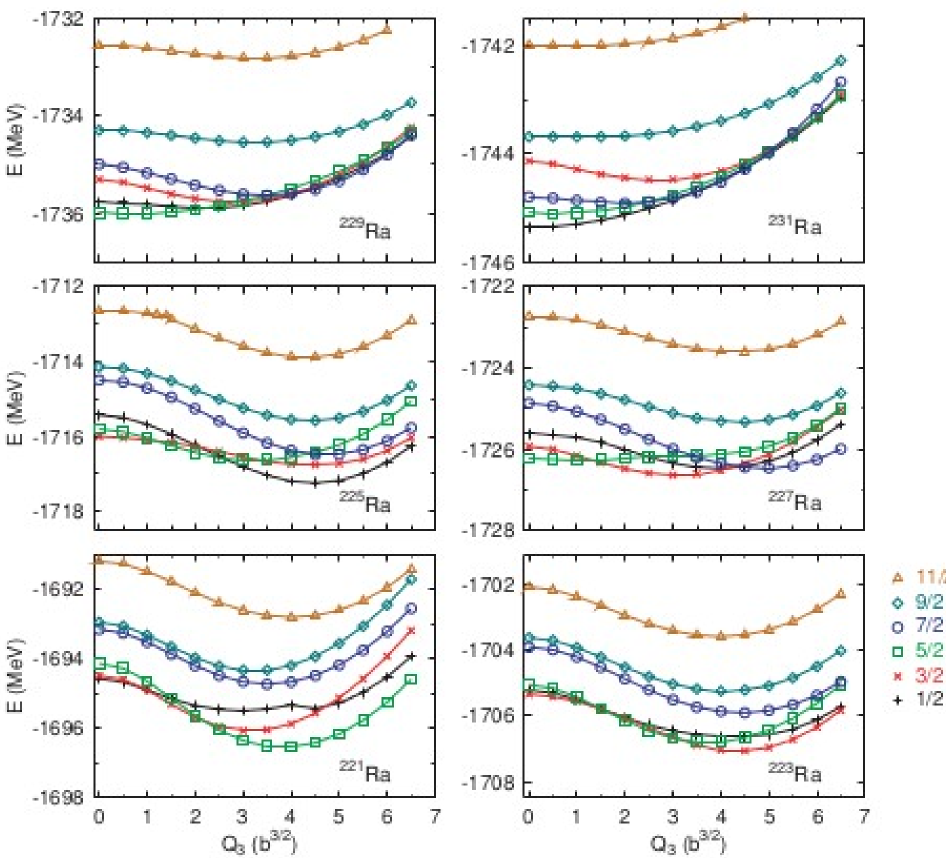


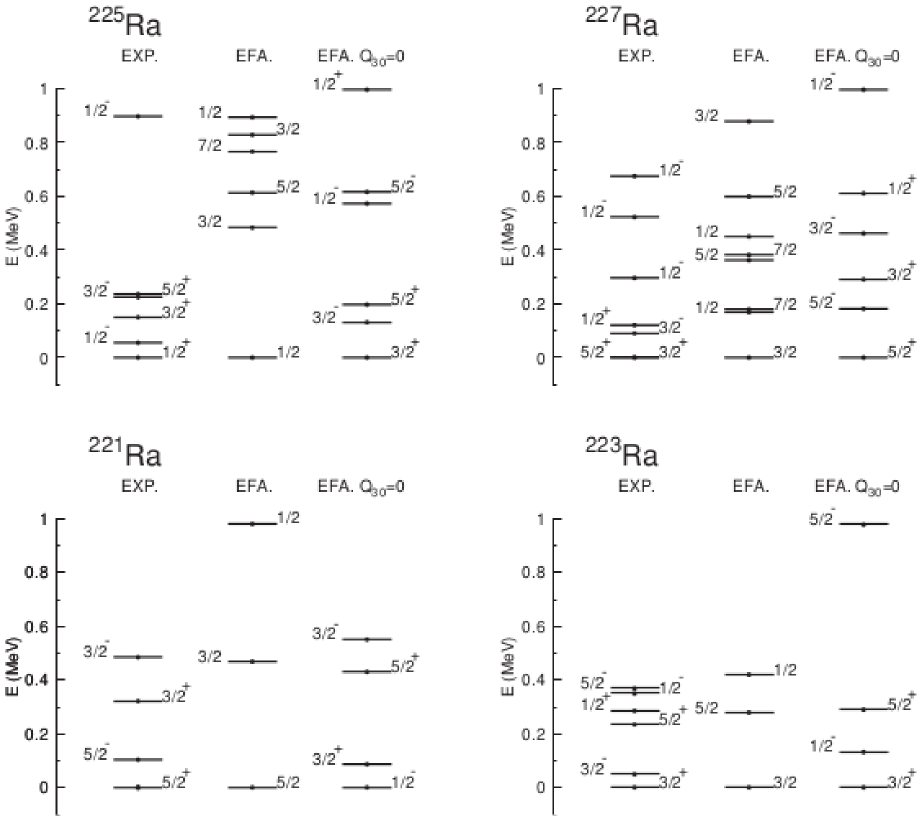
E. Garrote et al PRL 75, 2466



Odd-A and octupole deformation

Unpaired nucleon expected to polarize the even-even core





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

No time odd fields
“States” are not orthogonal

S. Perez, LMR PRC 78, 014304

Full blocking with the Hartree- Fock- Bogoliubov

Fully paired even systems: ρ has doubly degenerated eigenvalues

$$|\Phi\rangle = \prod_k (u_k + v_k a^\dagger_k a^\dagger_{\bar{k}})|-\rangle \quad \mathbb{R} = \begin{pmatrix} \langle\Phi|\beta^\dagger_\mu \beta_\nu|\Phi\rangle & \langle\Phi|\beta^\dagger_\mu \beta^\dagger_\nu|\Phi\rangle \\ \langle\Phi|\beta_\mu \beta_\nu|\Phi\rangle & \langle\Phi|\beta_\mu \beta^\dagger_\nu|\Phi\rangle \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{I} \end{pmatrix}$$

Odd (number parity) systems (1qp excitation):

$$|\Phi_\mu\rangle = \beta^\dagger_\mu|\Phi_0\rangle = a^\dagger_\mu \prod_{k\neq\mu} (u_k + v_k a^\dagger_k a^\dagger_{\bar{k}})|-\rangle \qquad \mathbb{R}_\mu = \begin{pmatrix} I_\mu & 0 \\ 0 & \mathbb{I} - I_\mu \end{pmatrix}$$

Vacuum of $\beta_1, \ldots, \beta_{\mu-1}, \beta^\dagger_\mu, \beta_{\mu+1}, \ldots$

Two quasiparticle excitations

$$|\Phi_{\mu\nu}\rangle = \beta^\dagger_\mu \beta^\dagger_\nu|\Phi_0\rangle = a^\dagger_\mu a^\dagger_\nu \prod_{k\neq\mu\nu} (u_k + v_k a^\dagger_k a^\dagger_{\bar{k}})|-\rangle$$

$$\mathbb{R}_{\mu\nu} = \begin{pmatrix} I_\mu + \mathbb{I}_\nu & 0 \\ 0 & \mathbb{I} - \mathbb{I}_\mu - \mathbb{I}_\nu \end{pmatrix}$$

Full blocking with Hartree- Fock- Bogoliubov

The HFB equation and the gradient expression for blocked odd-A states, 2qp excitations, etc are the same but replacing the generalized density matrix by the corresponding one

$$\mathbb{R}_\mu = \begin{pmatrix} \mathbb{I}_\mu & 0 \\ 0 & \mathbb{I} - \mathbb{I}_\mu \end{pmatrix} \qquad \mathbb{R}_{\mu\nu} = \begin{pmatrix} \mathbb{I}_\mu + \mathbb{I}_\nu & 0 \\ 0 & \mathbb{I} - \mathbb{I}_\mu - \mathbb{I}_\nu \end{pmatrix}$$

They can be written as $\mathbb{R}_\mu = \mathbb{S}_\mu \mathbb{R} \mathbb{S}_\mu^\dagger$ $\qquad \mathbb{R}_{\mu\nu} = \mathbb{S}_\mu \mathbb{S}_\mu \mathbb{R} \mathbb{S}_\mu^\dagger \mathbb{S}_\nu^\dagger$

$$\mathbb{S}_\mu = \begin{pmatrix} \mathbb{I} - \mathbb{I}_\mu & \mathbb{I}_\mu \\ \mathbb{I}_\mu & \mathbb{I} - \mathbb{I}_\mu \end{pmatrix}$$

The “swapping” matrix can be re-absorbed in the Bogoliubov amplitude matrix

$$W_\mu = W \mathbb{S}_\mu$$

explaining in a natural way the “swap U and V columns in the Bogoliubov amplitudes” recipe used in solving the HFB equation for 1qp, 2qp, etc systems. It allows to extend the gradient method to the 1qp, 2qp, etc cases (advantageous for handling many constraints)

The solution of the HFB equation follows the strategy

- Solve HFB (even number parity, time reversal invariant) for the target N and Z values
- Choose the quasiparticles to block (usually the 10 with the lowest qp energy)
- Swap the appropriate U and V columns in the Bogoliubov amplitudes and start the iterative solution of the HFB equation computing all time-odd fields

Problem

- Orthogonality is not preserved by the iterative process
  - Initial quasiparticles are orthogonal even if they have the same quantum numbers
  - However, orthogonality is lost in the iterative process and usually, no matter the initial quasiparticle is, the final solution is the same and corresponds to the lowest energy
- This is the most prominent advantage of preserving axial symmetry: K is a good quantum number and quasiparticles with different K values are orthogonal by construction. The orthogonality problem only matters within quasiparticles with the same K

The orthogonality constraint

The orthogonality issue

- In odd mass systems, or two- four- etc quasiparticle states it is common to consider several excited states. Most of them are orthogonal to the others because of symmetry considerations like the K quantum number or parity.

- When the symmetries are not preserved or the quantum numbers are the same the states are not necessarily orthogonal and the solution of the HFB equation based on the minimization of the energy usually ends up in the lowest energy solution.

  - For instance, in even-even nuclei is very difficult to reach 2qp $K=0^+$ solutions if orthogonality is not addressed in the proper way (always converge to the ground state)

  - It is very difficult to obtain solutions different from the ground state with triaxial, codes

- Another typical situation is when two different solutions of the HFB equations have a non-zero overlap meaning, according to the rules of QM, that they are not true excited states and a re-orthogonalization is required (modifying excitation energies and other properties)

The orthogonality constraint

To minimize the energy of $|\Phi\rangle$ imposing orthogonality to $|\Phi_i\rangle$

use Lagrange multipliers $-\sum_i \lambda_i \langle \Phi_i | \Phi \rangle$

Gradient

$$-\sum_i \lambda_i \langle \Phi_i | \alpha_\mu^+ \alpha_\nu^+ | \Phi \rangle$$

with

$$\langle \Phi_i | \alpha_\mu^+ \alpha_\nu^+ | \Phi \rangle = \langle \Phi_i | \Phi \rangle (A^{-1} B)_{\mu\nu}$$

$$\langle \Phi_i | \Phi \rangle = (\det A)^{1/2} \qquad A_i = U_{0i}^\dagger U + V_{0i}^\dagger V$$

The gradient is the product of a singular matrix A^{-1} times a tiny number det A

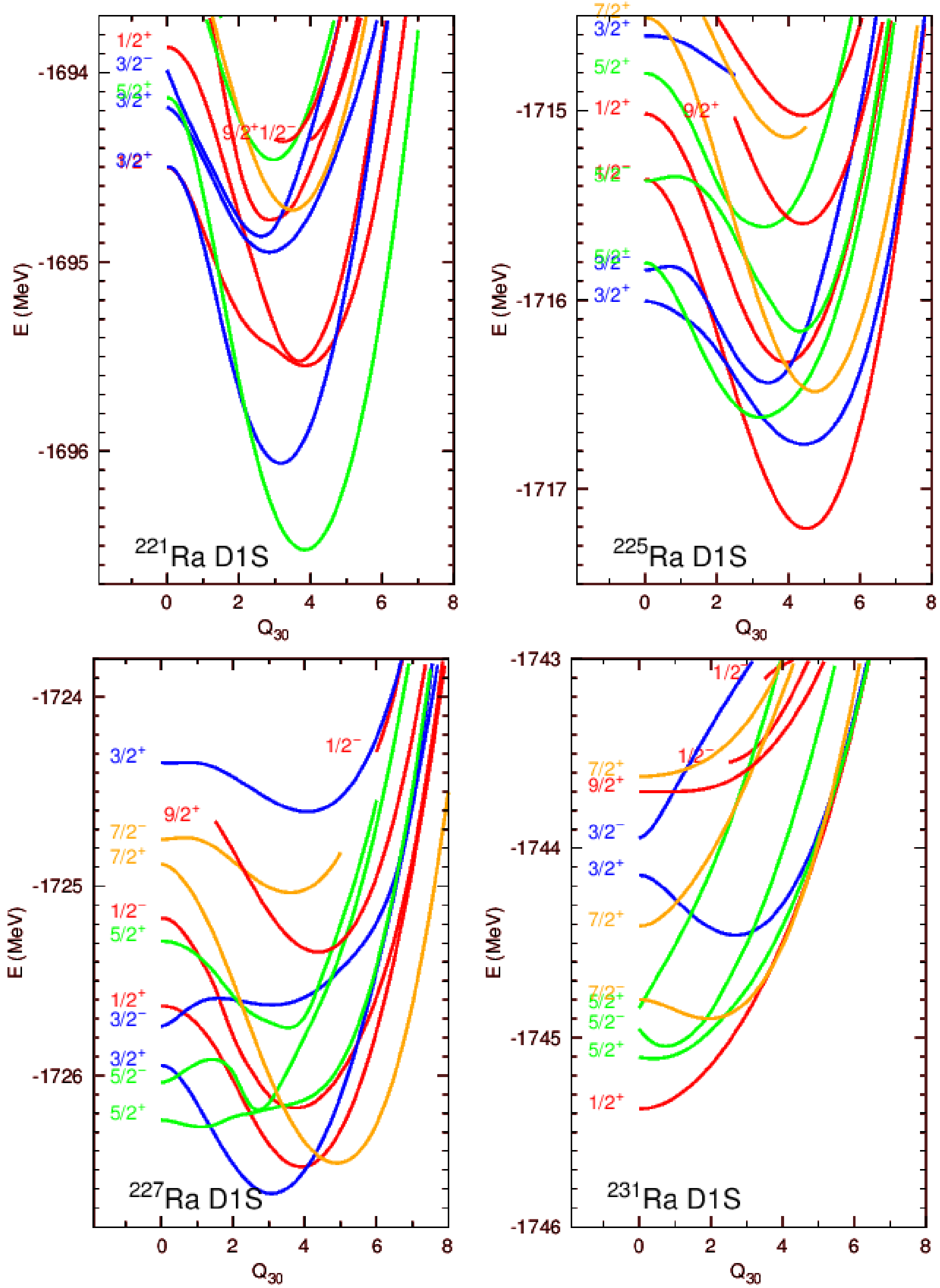
To handle this situation the SVD of A is very handy $A = C \sigma D^T$

C, D are orthogonal matrices and σ is diagonal.

$$A^{-1} = D \sigma^{-1} C^T \qquad \det A = \prod_\mu \sigma_\mu$$

$$\det(A)^{1/2} \times A^{-1} = D \tilde{\sigma} C^T \qquad \tilde{\sigma} = \prod_{k \neq \mu} \sigma_k$$

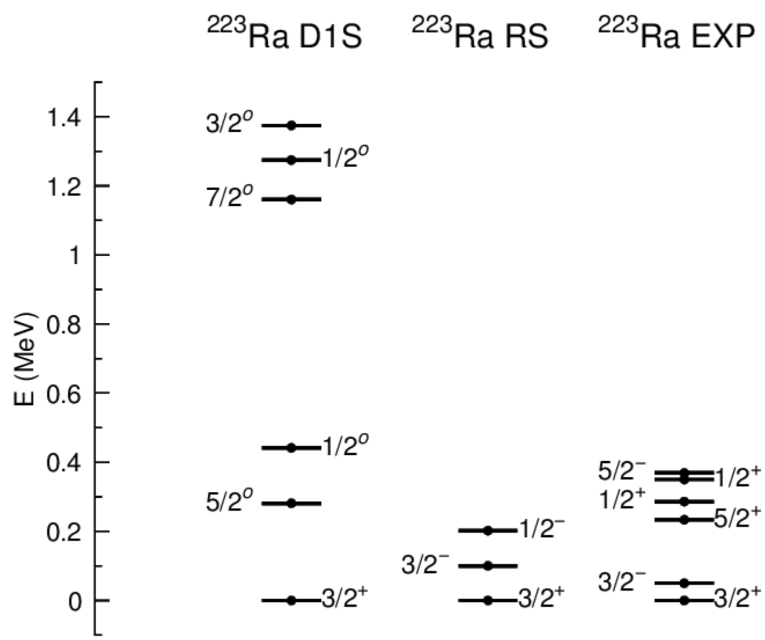
Odd-A and octupole deformation (full blocking)



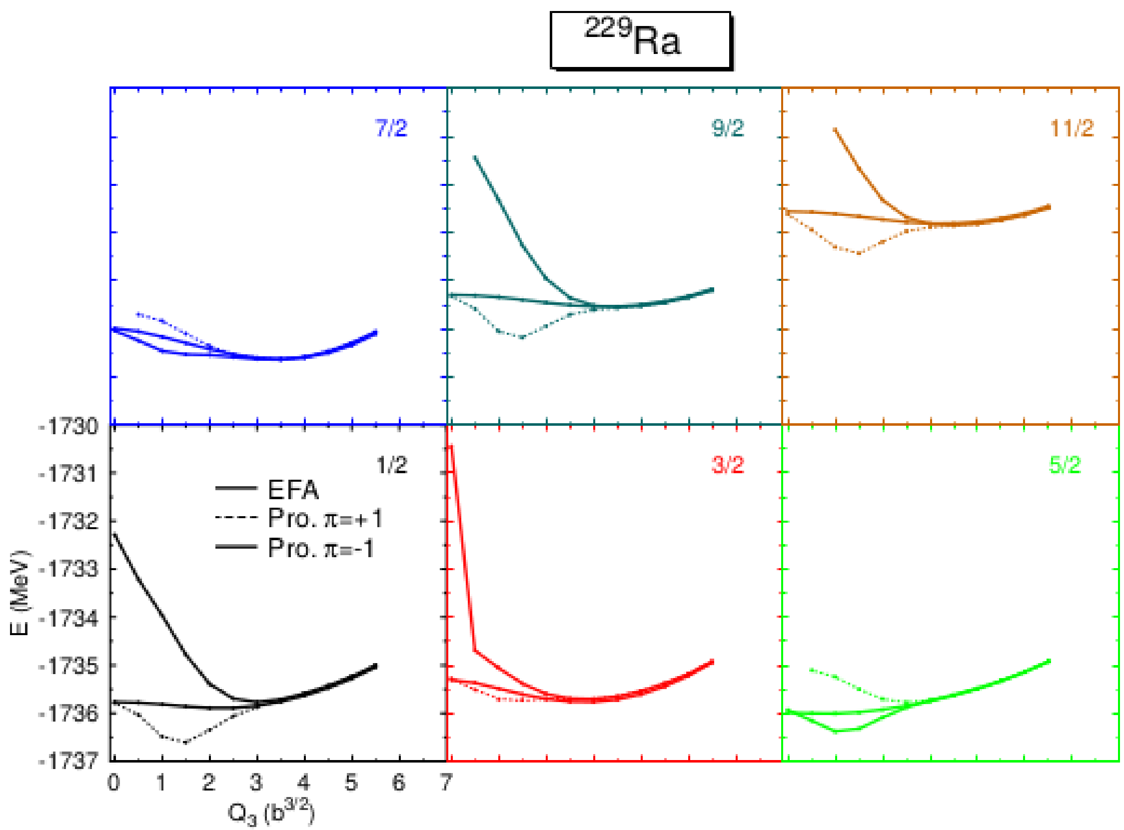
Different levels react differently to octupole deformation

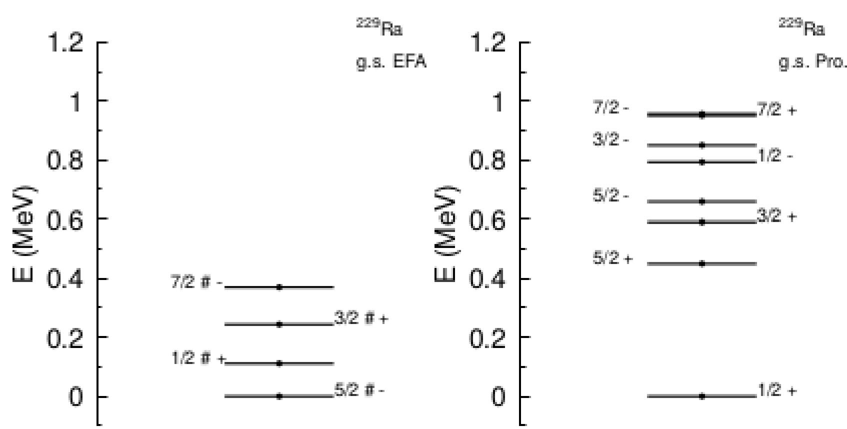
Minimum not always at the same octupole deformation

Deformation parameters and correlation energies very similar to that of e-e neighbors



Very preliminary results on parity projection
(time-odd fields not considered in the hamiltonian overlap)





Very significant change in excitation energies and ordering of levels !

2QP excitations and octupole deformation

^{236}Pu ground state is reflection symmetric in our calculations but there are several 2qp excitations with a quite large octupole deformation

Polarization effects (no weak coupling for those states)

K	E_{exc}	β_2	β_3	
2+	1.1	0.26	0.045	prot
3+	1.15	0.26	0.044	prot
6-	1.50	0.26	0.078	prot
1-	1.67	0.25	0.075	prot
4-	1.81	0.27	0.101	prot
2-	1.82	0.26	0.103	prot

In this case, protons are very effective polarizing the nucleus

Other nuclei as well as 4qp excitations are worth exploring

The β_3 of ^{224}Ra is 0.15 for comparison

Odd-Odd systems and octupole deformation

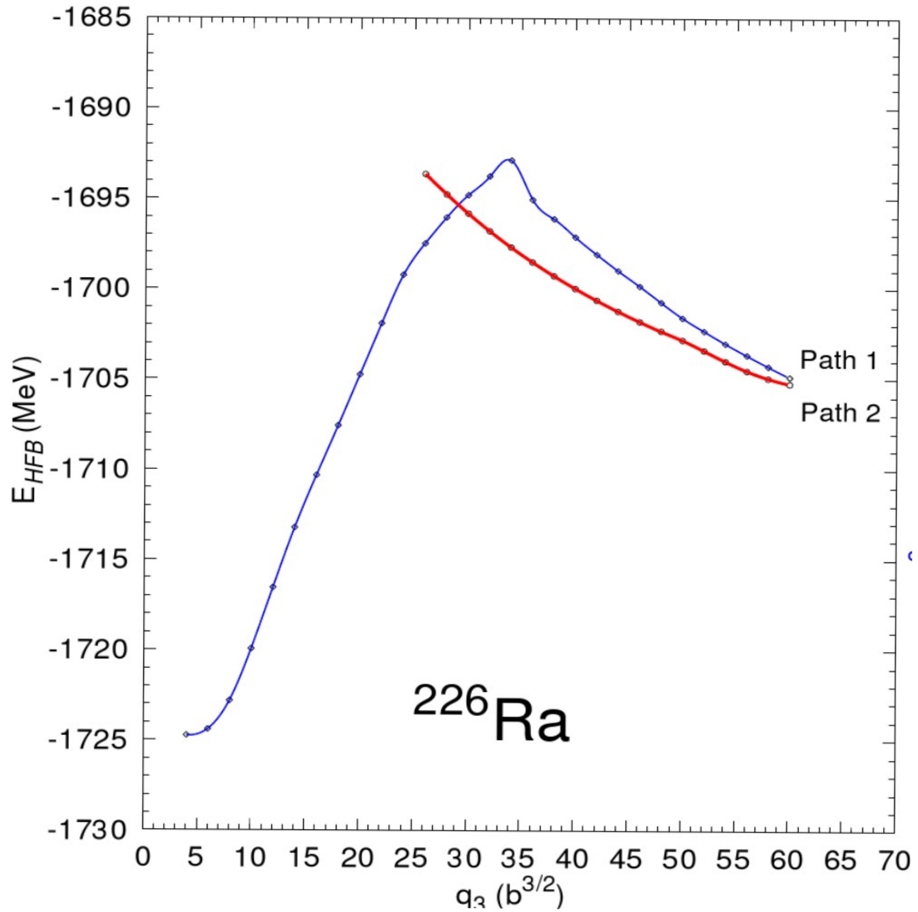
^{224}Fr and ^{226}Fr are good candidates for EDM experiments: Strong octupole correlations are expected (polarization effects)

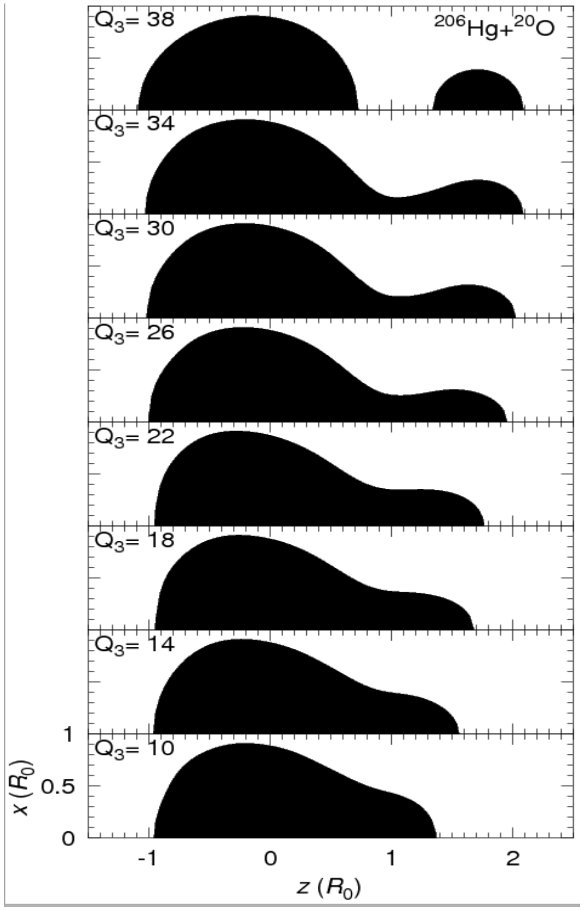
In our calculations the 1^- state (experimental gs) with the lowest energy has strong octupole deformation but similar to the one of e-e neighbors: No polarization effects

	β_2	β_3
^{222}Fr	0.16	0.141
^{224}Fr	0.18	0.136
^{226}Fr	0.19	0.070

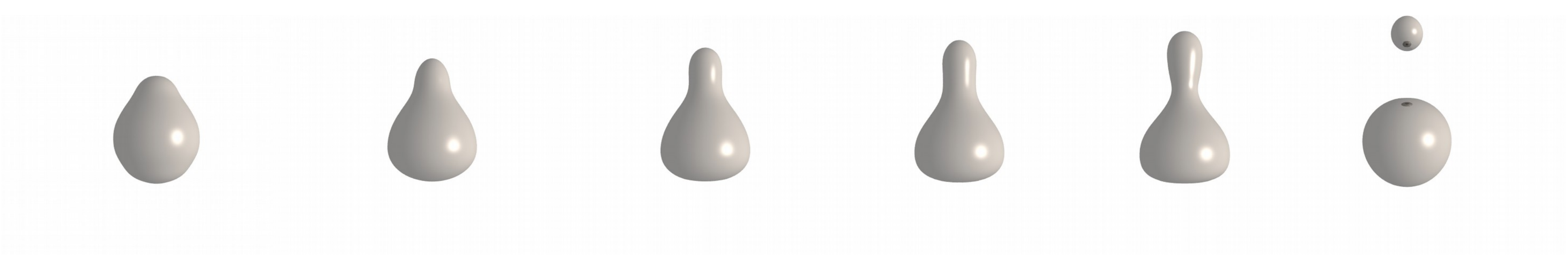
Calculation of Schiff moments will be considered soon

Octupoles and cluster emission



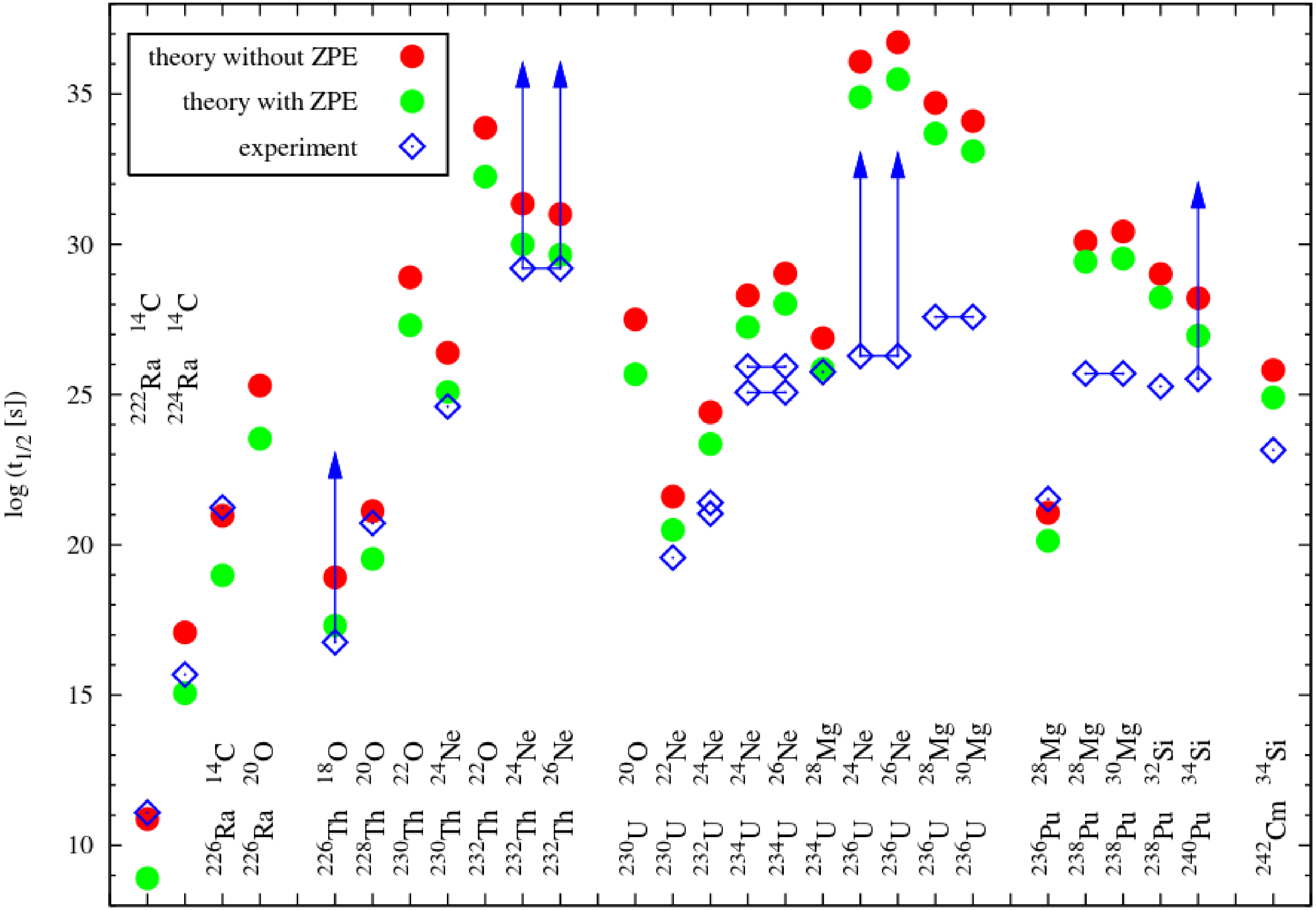


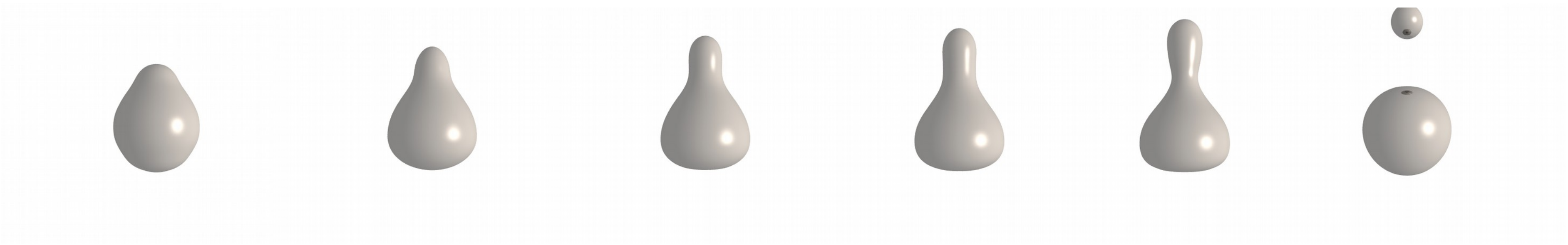
Emission of heavy clusters (^{14}C, ^{20}Ne, ^{20}O, ^{30}Mg …). Very asymmetric fission



Octupoles and cluster emission

M. Warda LMR, Phys Rev C84, 044608





Summary and conclusions

- Octupole correlations
  - Static: present in a few nuclei around Zr, Ba, Ra
  - Dynamic: present in all nuclei (Parity projection and configuration mixing)
- Gogny GCM (Q_3) is a reasonable theory
- B(E3) strengths require angular momentum projected wave functions
- Quadrupole-octupole coupling important
- Enhancement at high spin well described by Parity Projection
- Large impact in spectroscopy of odd-A nuclei
- Octupoles in 2qp excitations and odd-odd systems
- Microscopic basis of cluster emission

to do

- Systematic $Q_2 - Q_3$ calculations
- Consider other degrees of freedom (pairing, time odd momenta)
- Extend parity projection to odd-A nuclei (time odd fields)
- Extend GCM to odd-A nuclei (time odd fields)