

Reflections on the atomic nucleus  
Liverpool, UK

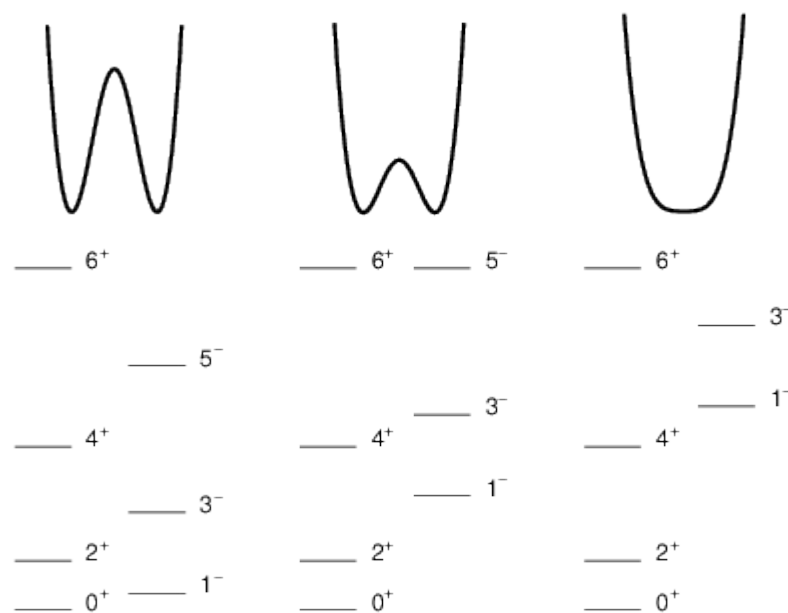
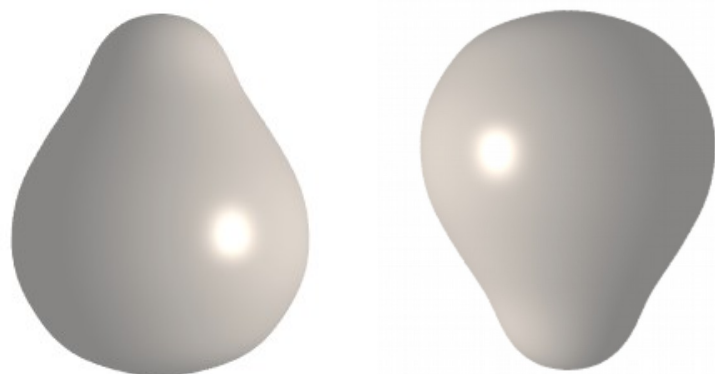


# Octupole correlations beyond the mean field

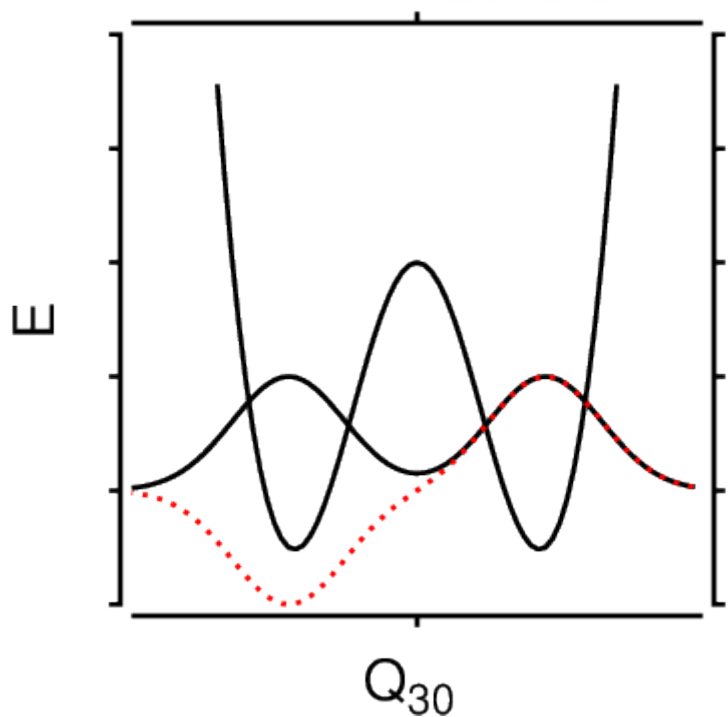
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- Parity doublets
- Strong E3 transition strengths

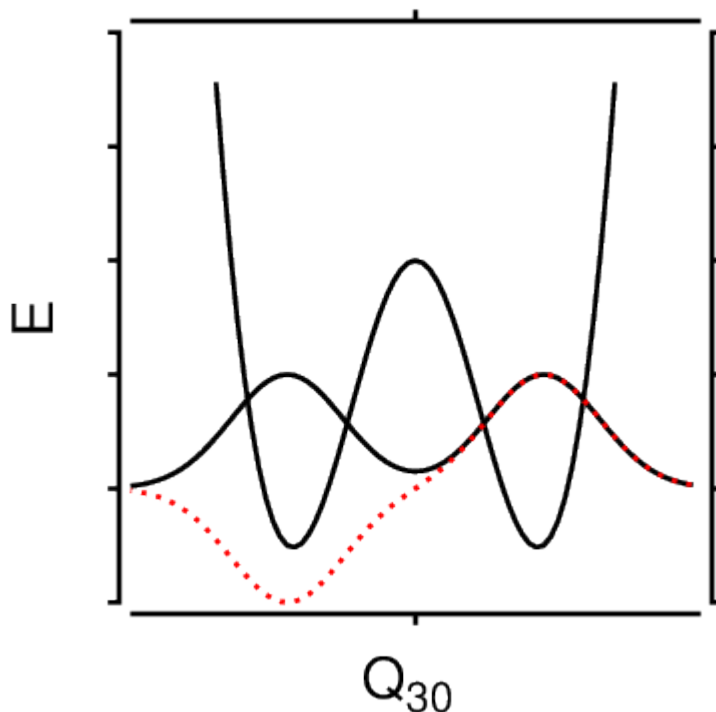


$$Q_{30} = z \left( z^2 - \frac{3}{2} r_{\perp}^2 \right)$$

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, Ciovek, 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  $^{224}\text{Ra}$  (and  $^{146}\text{Ba}$ ) 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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PHYSICS LETTERS B

26 March 1987

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

## STABLE OCTUPOLE DEFORMATION IN SOME ACTINIDE NUCLEI \*

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The possibility of permanent octupole deformation in the ground state of  $^{222}\text{Ra}$ ,  $^{222}\text{Rn}$  and  $^{224}\text{Ra}$  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  $^{222}\text{Rn}$  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 **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  $^{218-230}\text{Ra}$  and  $^{222-230}\text{Th}$  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  $\beta_2$ ,  $\beta_4$ ,  $\beta_5$ ,  $\beta_6$  and  $\beta_7$  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.

## 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.

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## Characterization of octupole correlations in the Lipkin model

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(Received 28 January 1992)

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

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

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

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

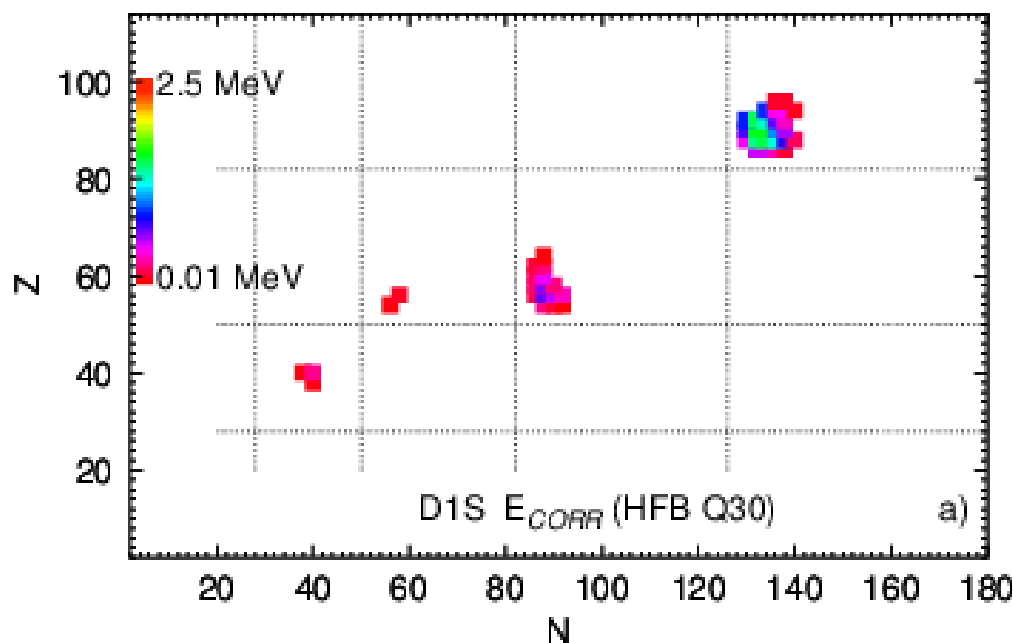
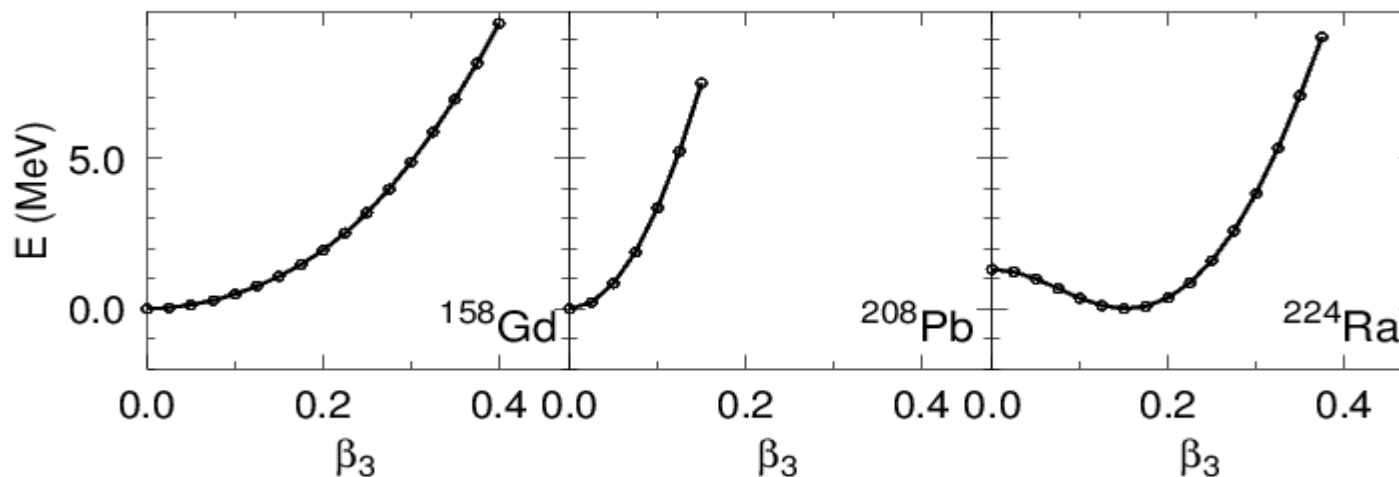
$$V_{DD}(1, 2) = t_3 \delta(\vec{r}_1 - \vec{r}_2) (1 + x_0 P_\sigma) \rho^\alpha(\vec{R})$$

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

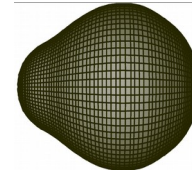


- Axially symmetric HFB with constraint in  $Q_{30}$
- Second order gradient solver
- Finite range Gogny (D1S, D1M, etc)
- Z and N values must have orbits of opposite parity and  $\Delta l=3$  around the Fermi level for permanent octupole deformation
- **Zr, Ba and Ra regions** show octupole def
- Mean field correlations energies  $\approx 1.5$  MeV
- **Many nuclei are soft** against octupole deformation (eg Gd)
- Results qualitatively and almost quantitatively independent of Gogny parametrization

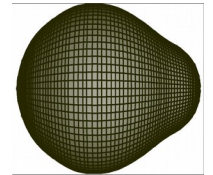
# First step beyond the mean field: Parity projection

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

$|\varphi(\beta_3)\rangle$



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

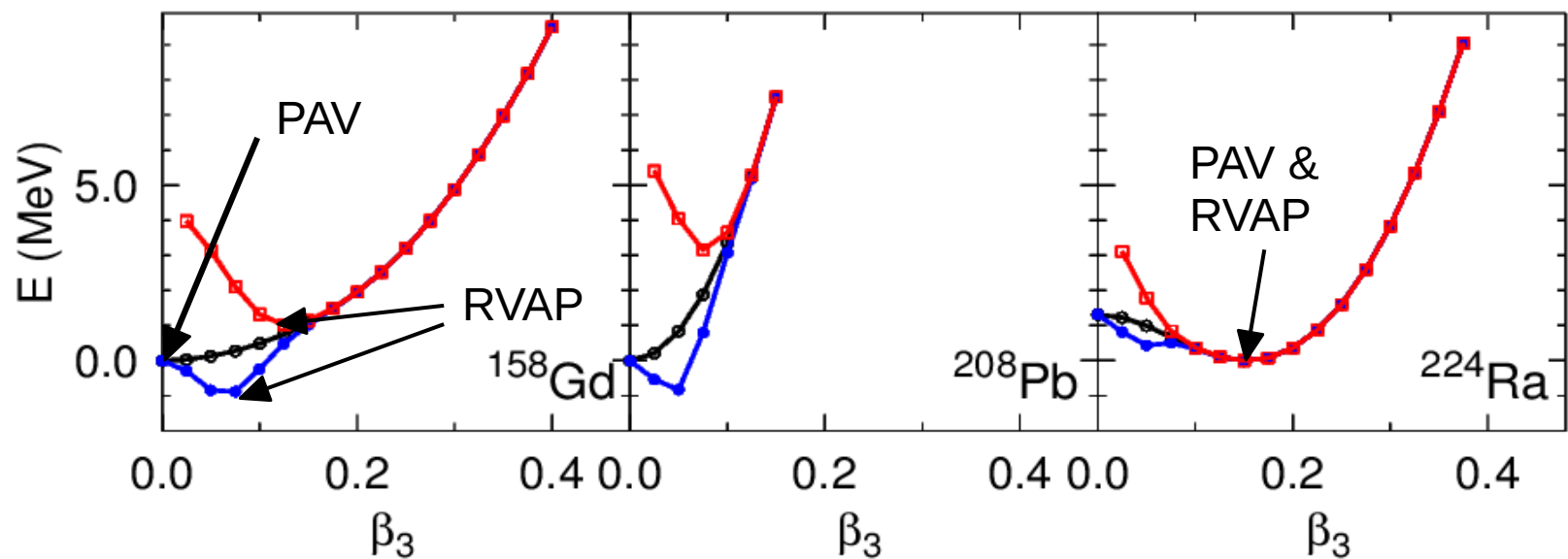


But a linear combination of the two shapes restores parity symmetry

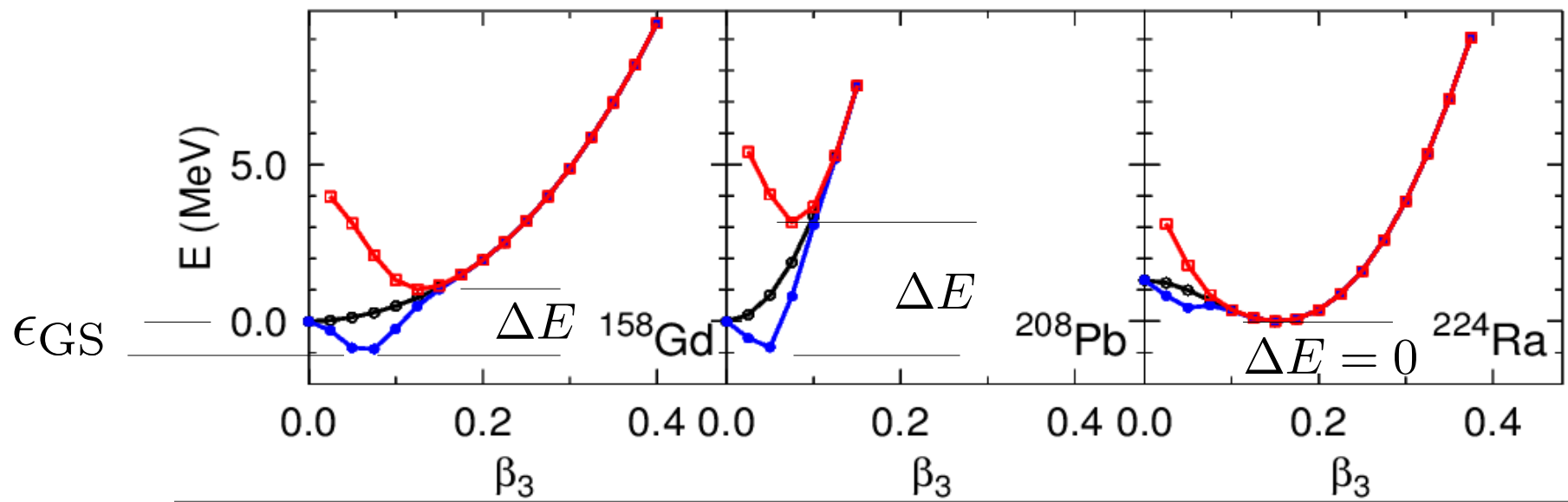
$$|\Psi_\pi\rangle = \mathcal{N}_\pi(1 + \pi\hat{\Pi})|\varphi(\beta_3)\rangle$$

$$E_\pi = \langle\Psi_\pi|\hat{H}|\Psi_\pi\rangle$$

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  $E_\pi$ . 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  $\epsilon_{GS}$  : non zero for reflection symmetric mean field gs.

Transition strengths  $E1$  and  $E3$  computed with the rotational formula

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

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  $Q_{30} \rightarrow -Q_{30}$

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

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

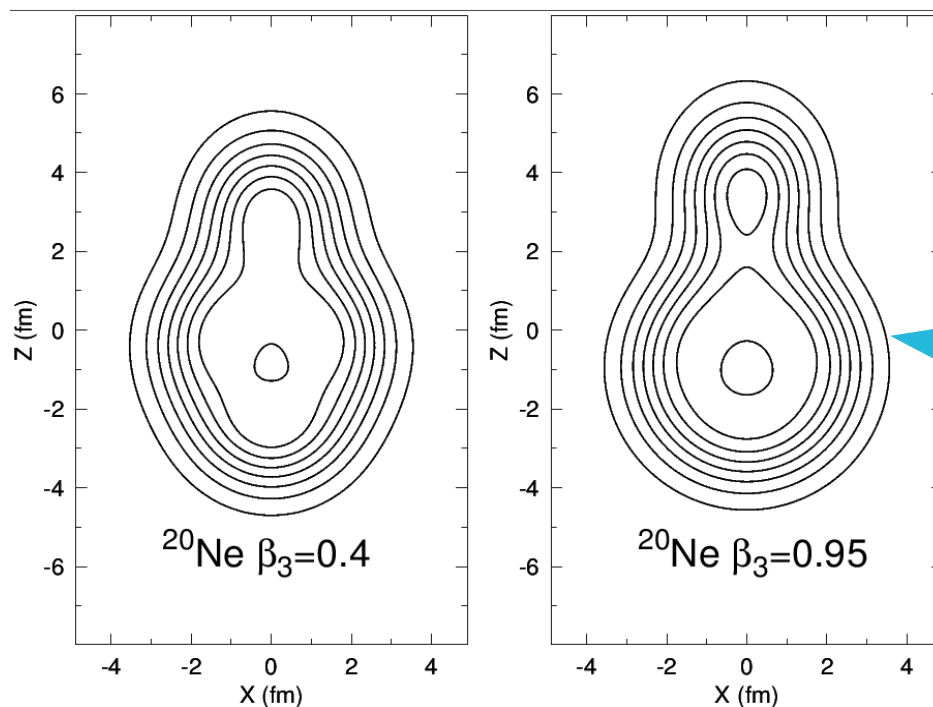
Transition strengths with the rotational approximation

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

# Assorted GCM results

Nucleus	E <sub>1</sub> (MeV)			W(E3)		
	Exp	GCM	RPA	Theory	Sph-Def	Exp
<sup>20</sup> Ne	5.6	6.7		12	Def	13
<sup>208</sup> Pb	2.6	4.0	3.46	53	Sph	34
<sup>158</sup> Gd	1.26	1.7		11.6	Def	12
<sup>226</sup> Ra	0.32	0.16		43	Def	54

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



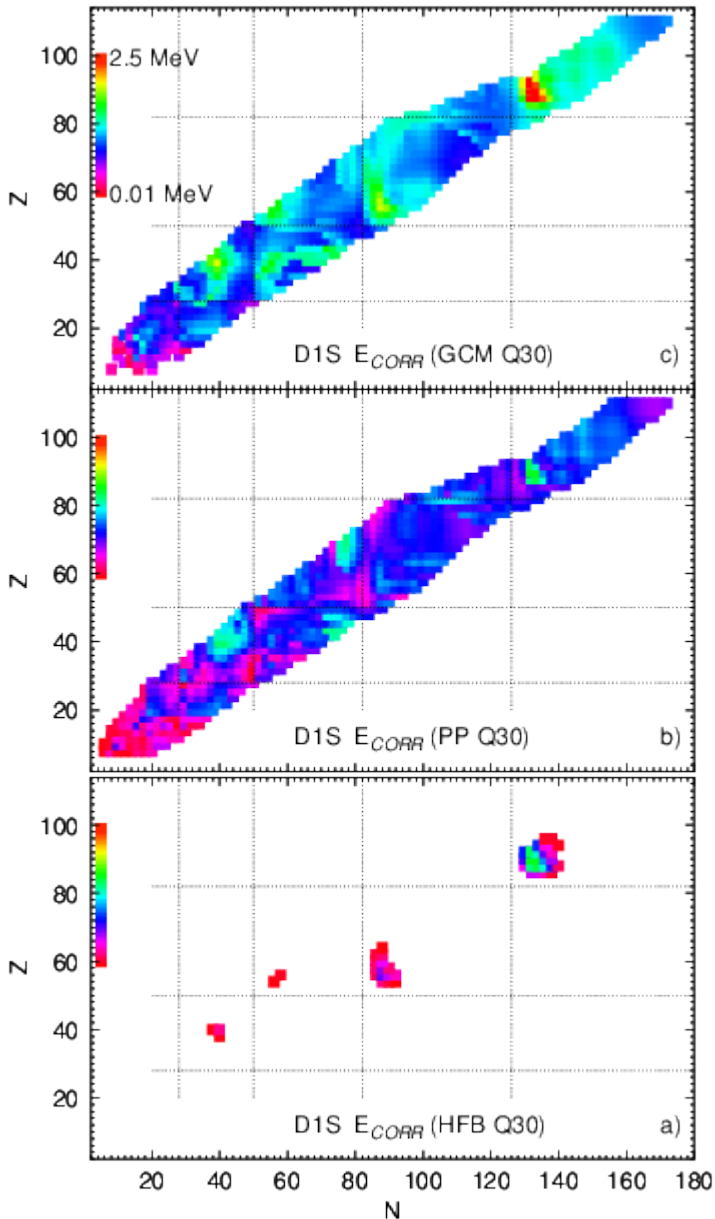
## Alpha clustering in light nuclei

- $\beta_3 = 0.4$  Positive parity intrinsic state
- $\beta_3 = 0.95$  Negative parity intrinsic state

$^{16}\text{O} + ^4\text{He}$

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

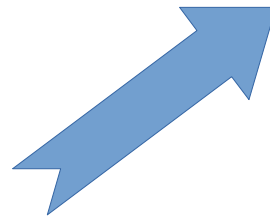
# Beyond mean field: Correlation energies



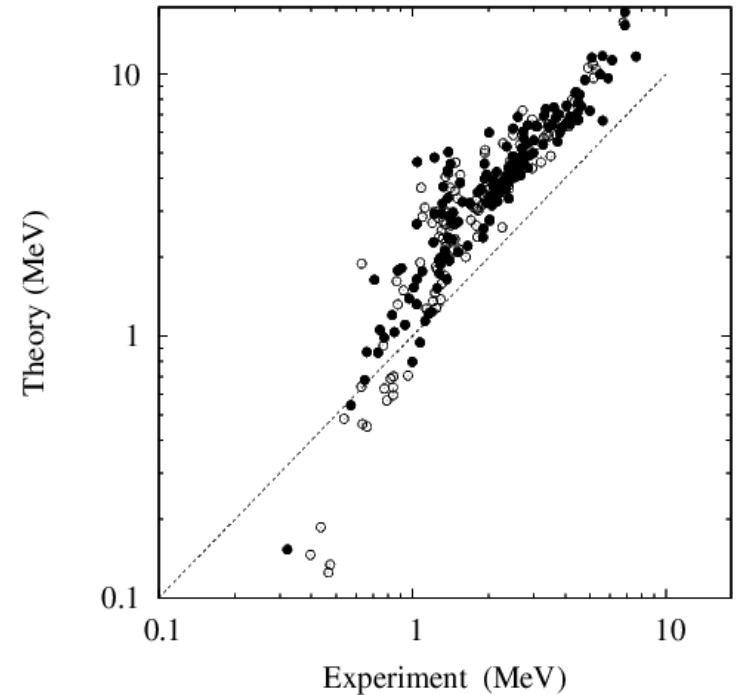
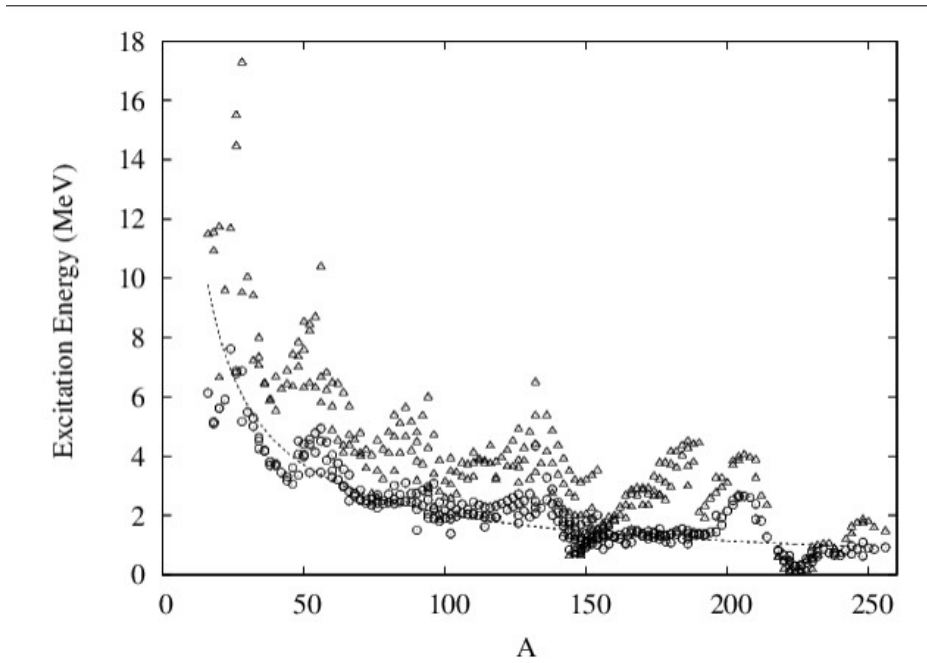
## GS correlation energies $\epsilon_{GS}$

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

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

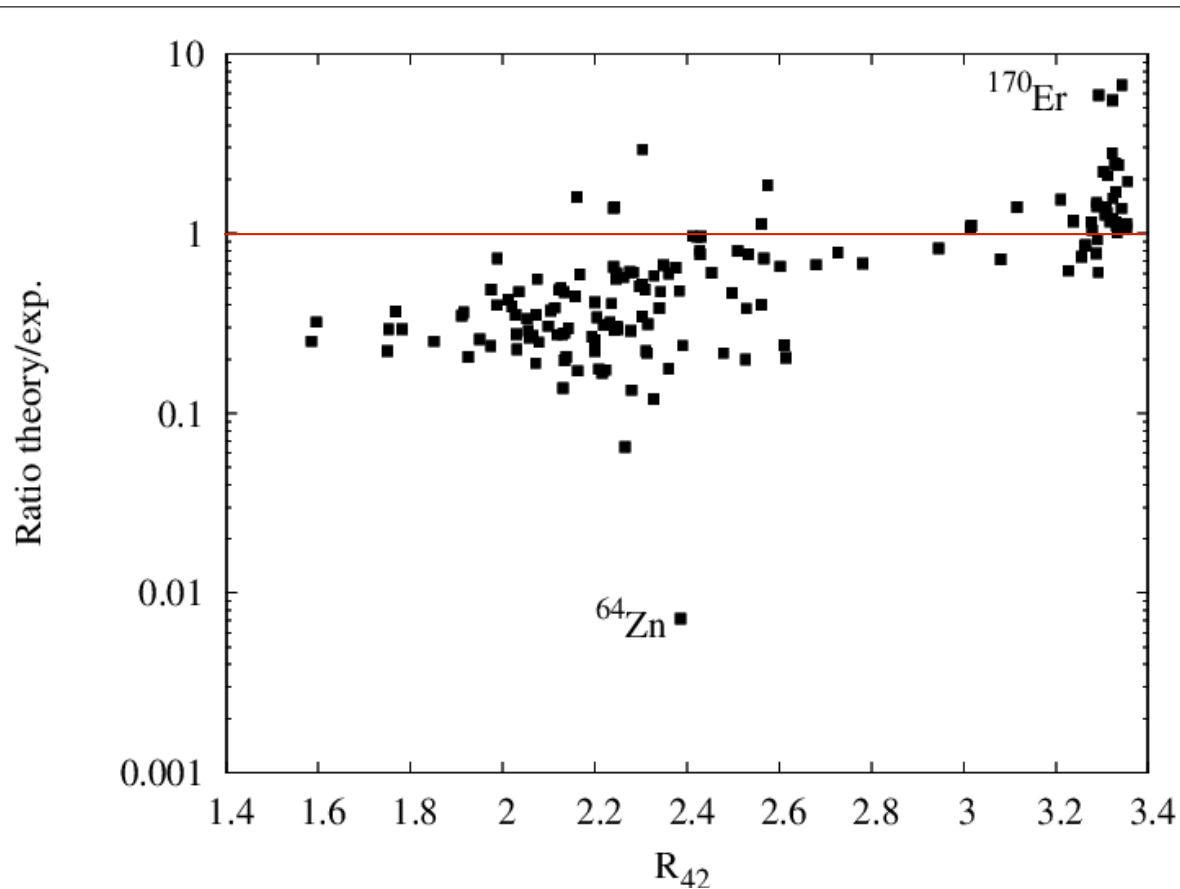


# Excitation energies



- The excitation energies of the  $K=0^-$  are plotted vs A (GCM)
- and compared to experimental data (including  $K \neq 0$  excitations in def nuclei)
- **Theory is systematically too high** ( $\sim$  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 ?
- › What happens with  $^{64}\text{Zn}$  ?

# Transition strengths

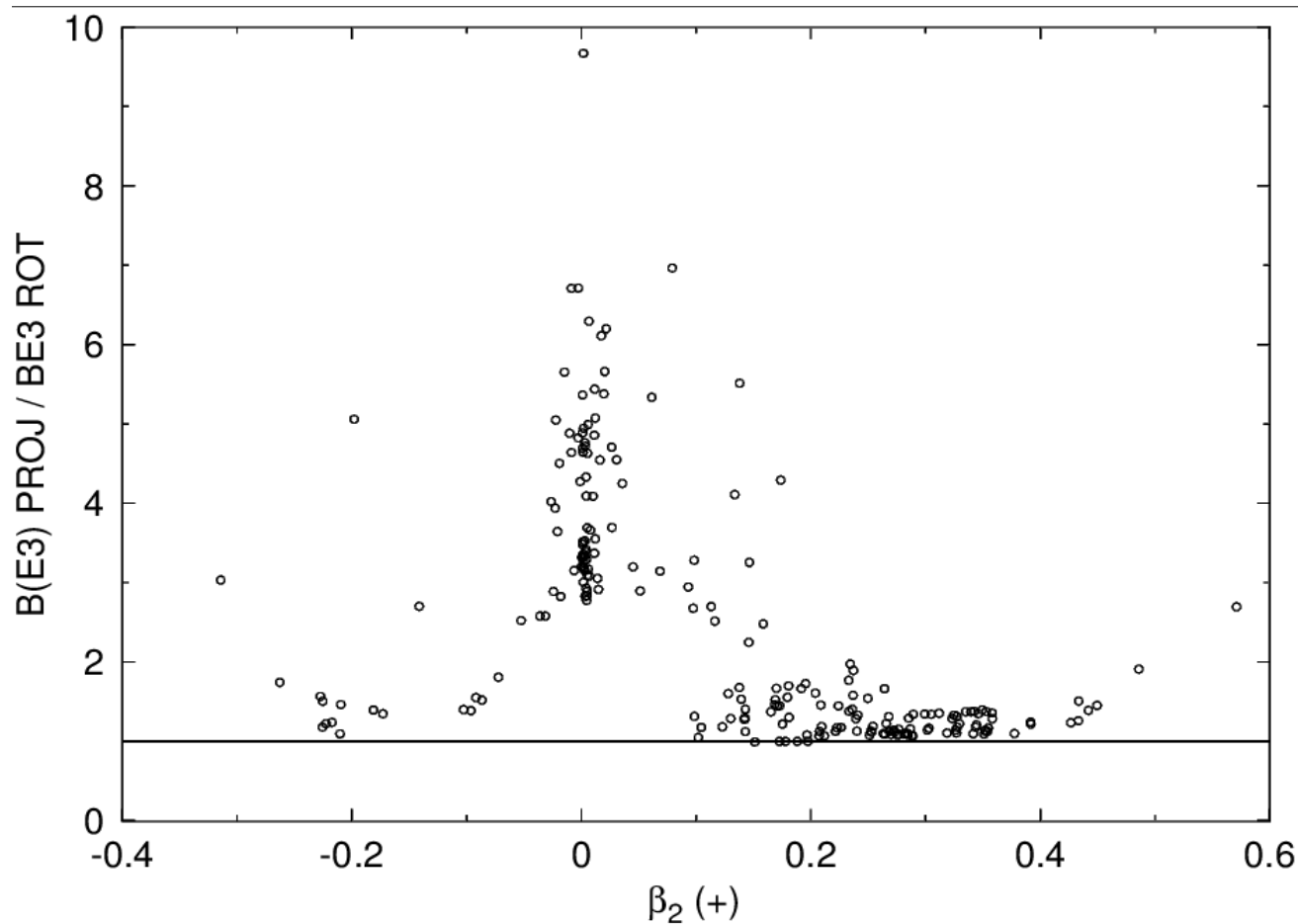
- The **rotational formula** used to relate intrinsic deformation parameters and transition strengths can be justified in the **strong deformation limit**
- **Not valid for spherical or near spherical nuclei**
- The proper treatment involves angular momentum projected wave functions
- Contrary the rotational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

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

- **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  $\beta_2$  values less than 0.1 (**0.2**) in heavy (**light**) nuclei
  - Simple formula to relate  $B(E2)$  and  $\beta_2$



# Projected B(E3) transition strengths



$$|\Psi^{3^-}\rangle = \mathcal{N}P^{J=3}|\varphi(\beta_3(-))\rangle$$
$$|\Psi^{0^+}\rangle = \mathcal{N}P^{J=0}|\varphi(\beta_3(+))\rangle$$

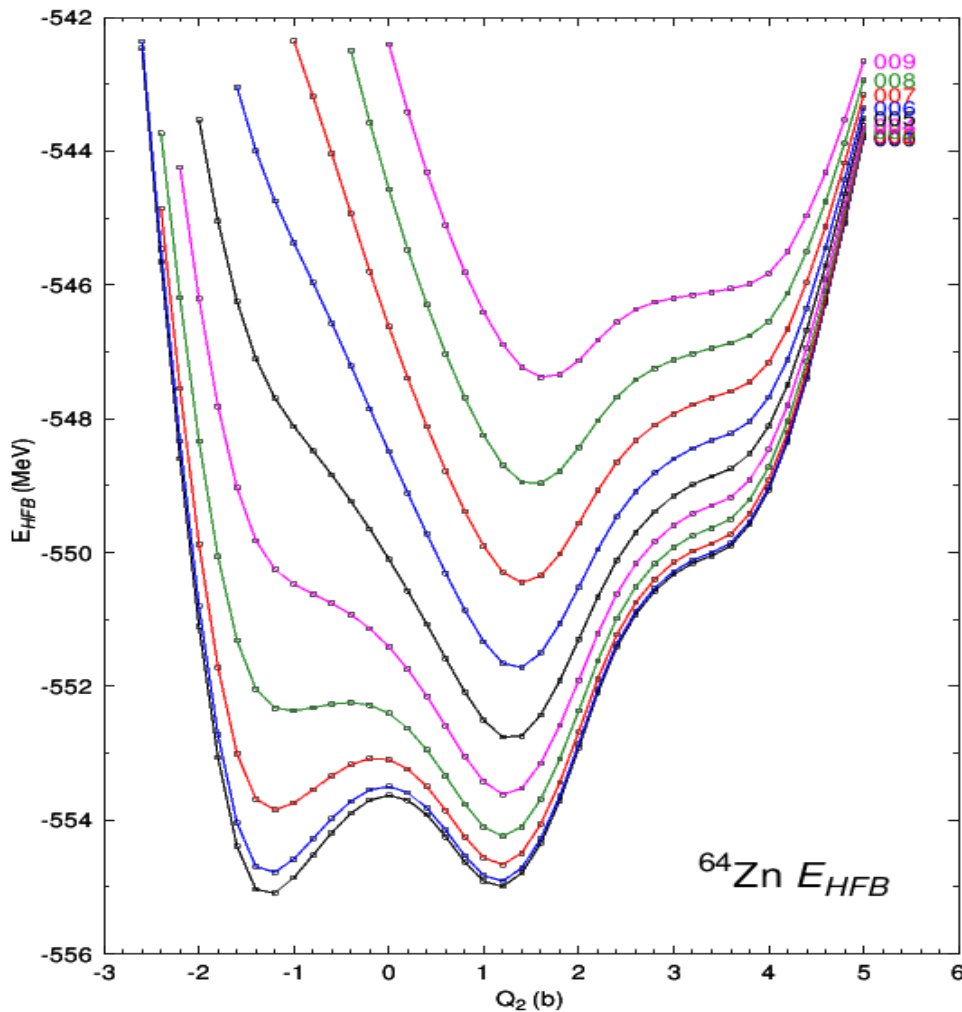
- Only RVAP intrinsic wf
- A factor  $\sim 7$  is seen !
- $\beta_2 (+)$  quadrupole deformation of the gs

- **Much better agreement with experiment:** in  $^{208}\text{Pb}$  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
- AMP is not used to determine the intrinsic states



# Quadrupole-octupole coupling

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



GCM with Gogny D1S

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

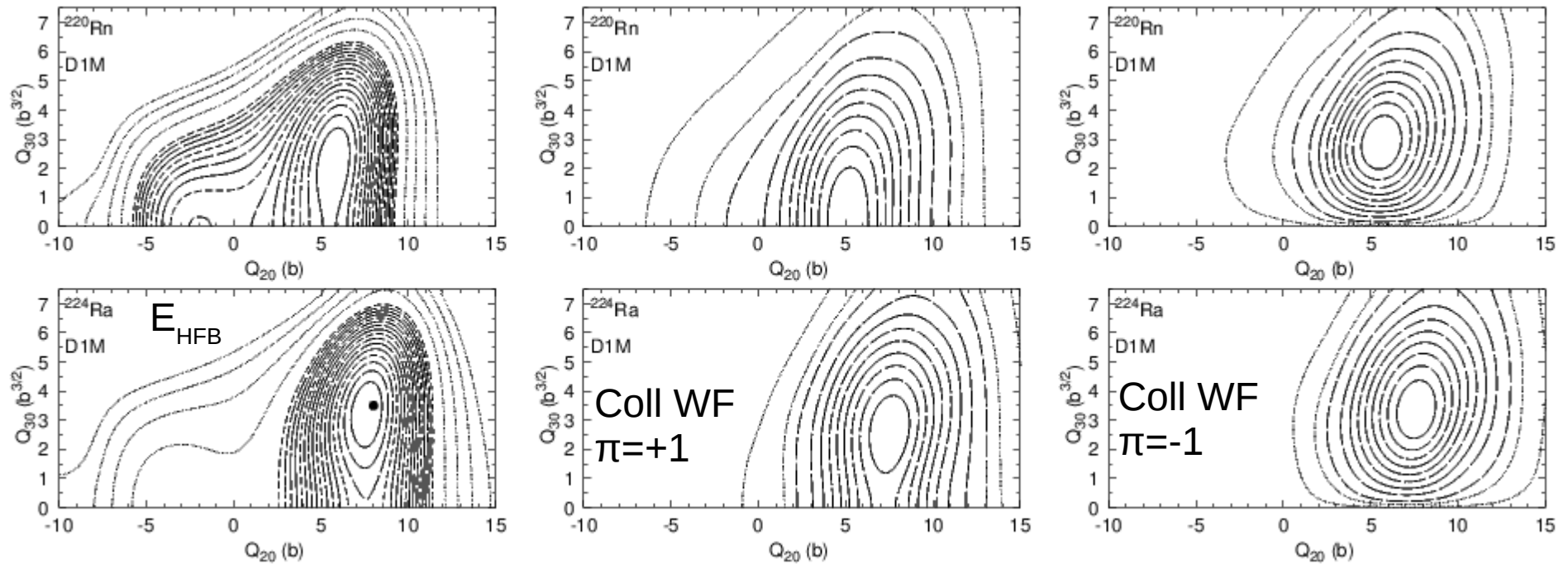
Also relevant in other nuclei (see below)

Two-phonon octupole states and  $0_2^+$  ?

Computationally intensive



# Quadrupole-octupole coupling

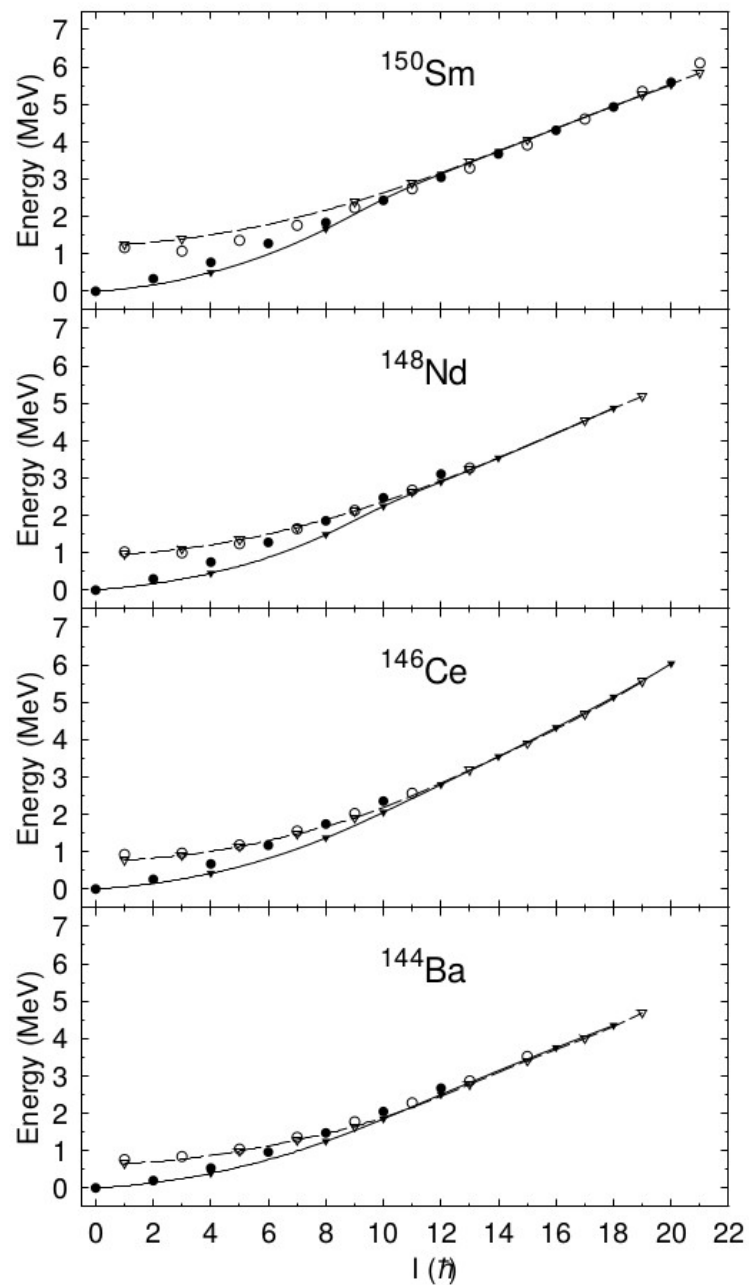
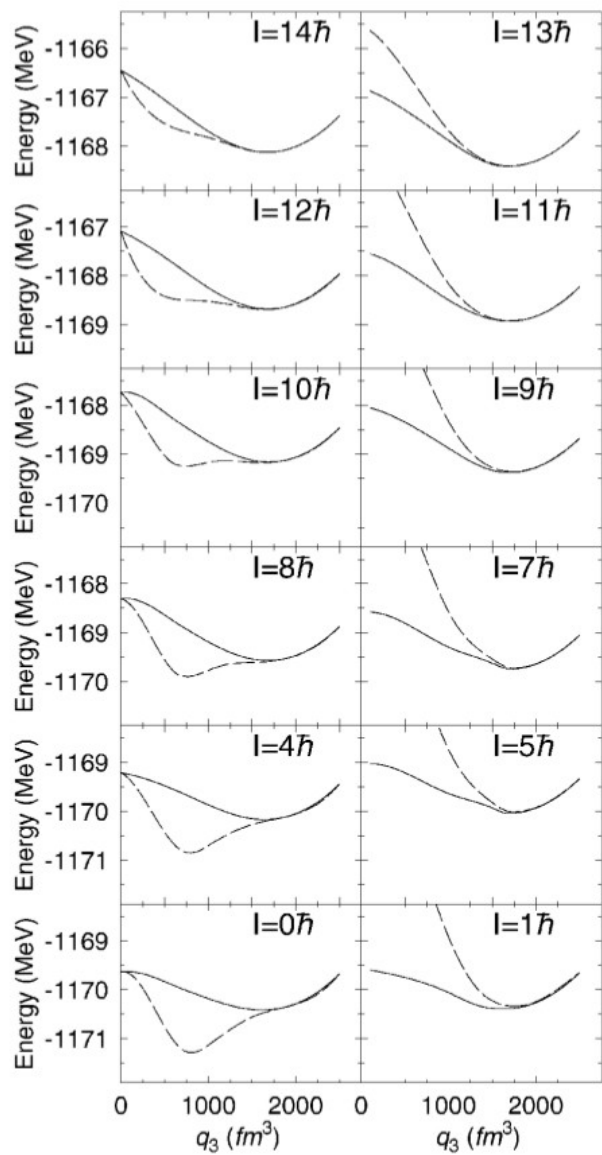


220 Rn	$Q_2$ - $Q_3$	Exp
$E_-$ (MeV)	0.618	0.645
$W(E1)$	$2.4 \cdot 10^{-5}$	$< 1.5 \cdot 10^{-3}$
$W(E3)$	26.50	$33 \pm 4$
$E_2^+$ (MeV)	1.35	0.94
$W(E2)$	48.5	$48 \pm 3$

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

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

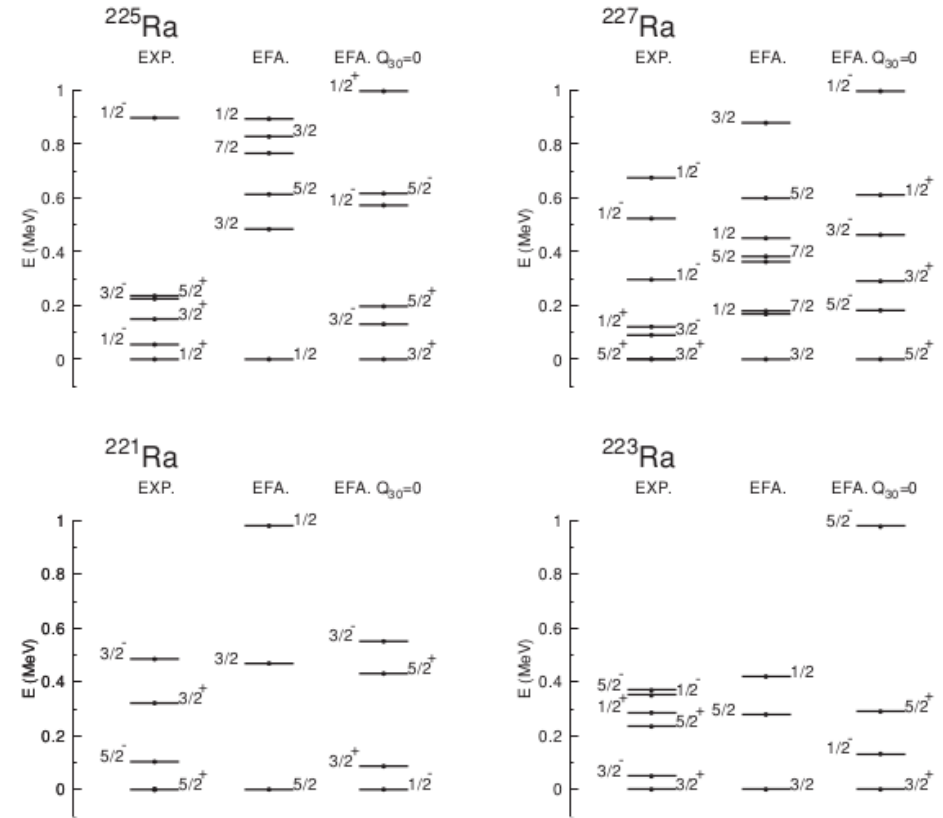
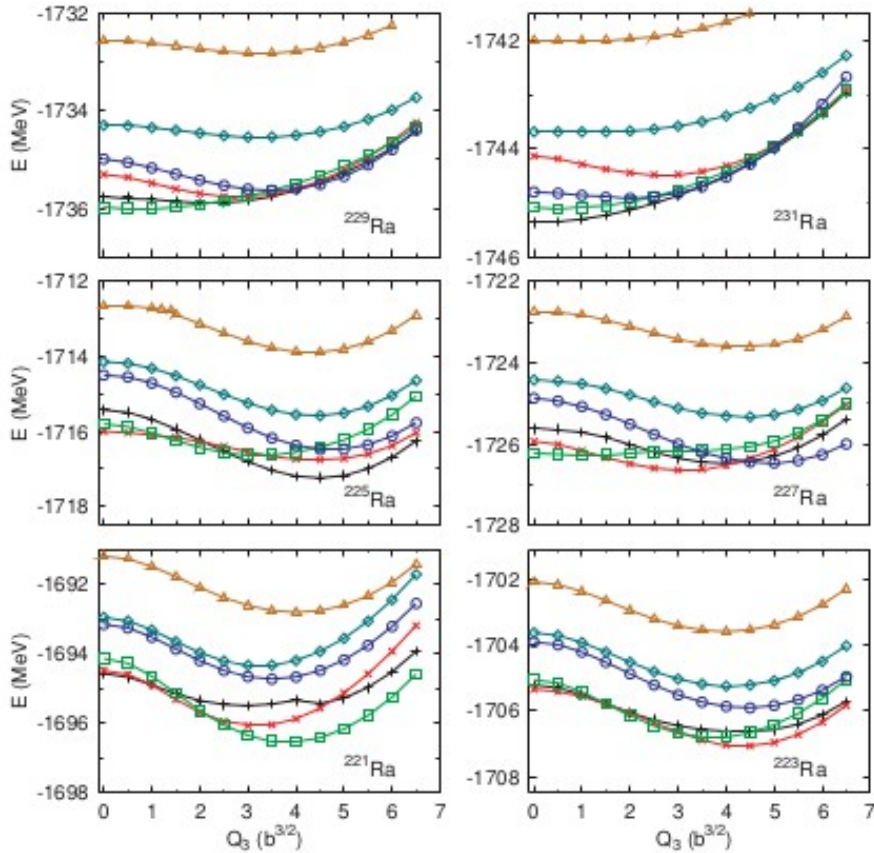
# Octupoles at high spin



E. Garrote et al PRL 75, 2466

# Odd-A and octupole deformation

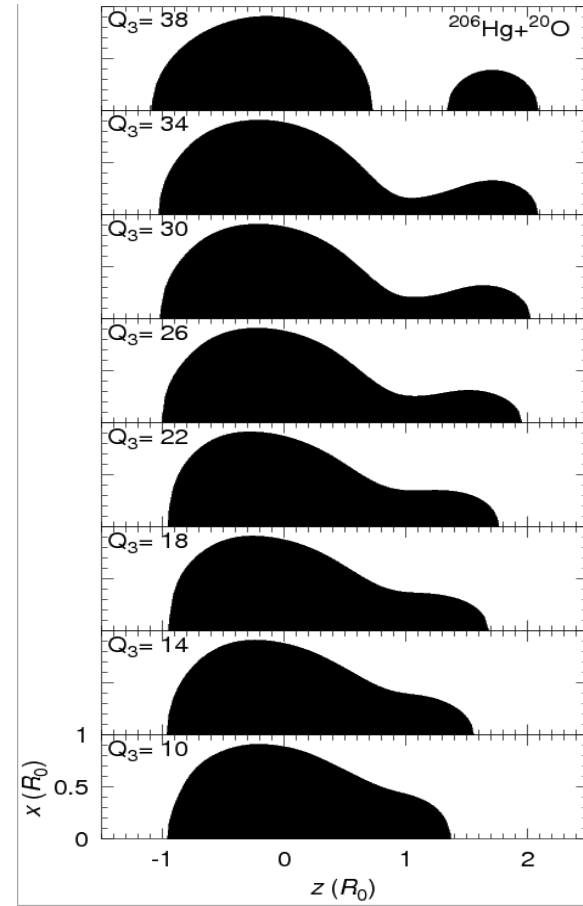
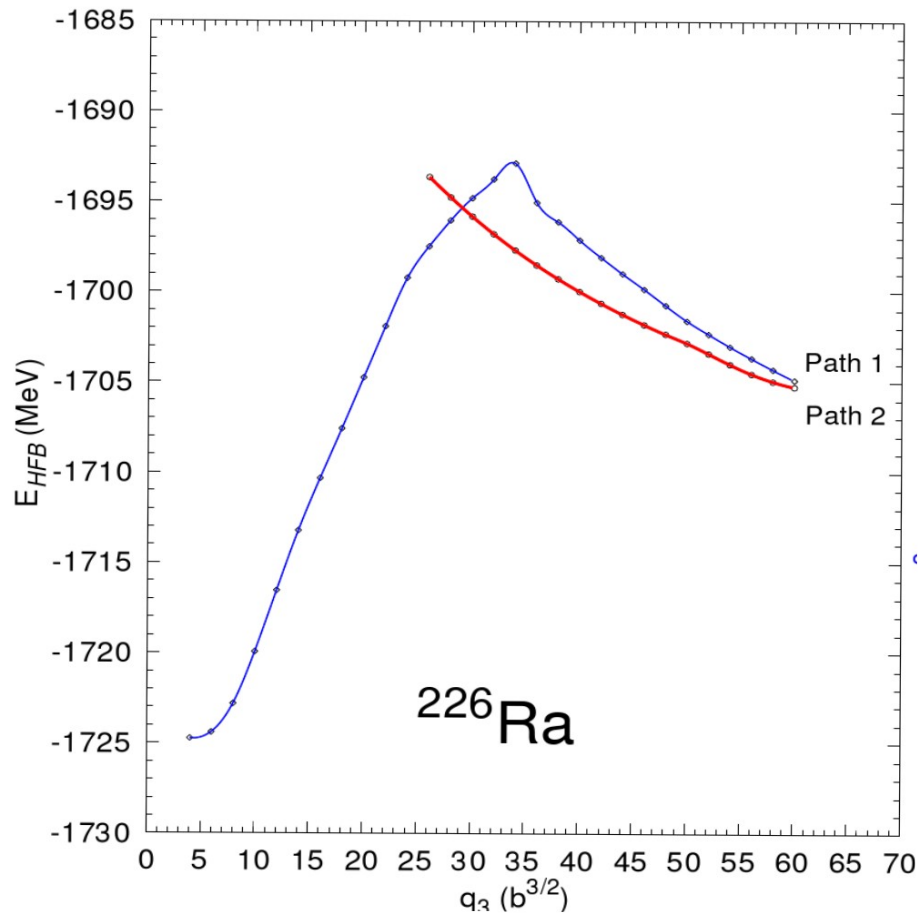
Unpaired nucleon expected to polarize the even-even core



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

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

# Octupoles and cluster emission

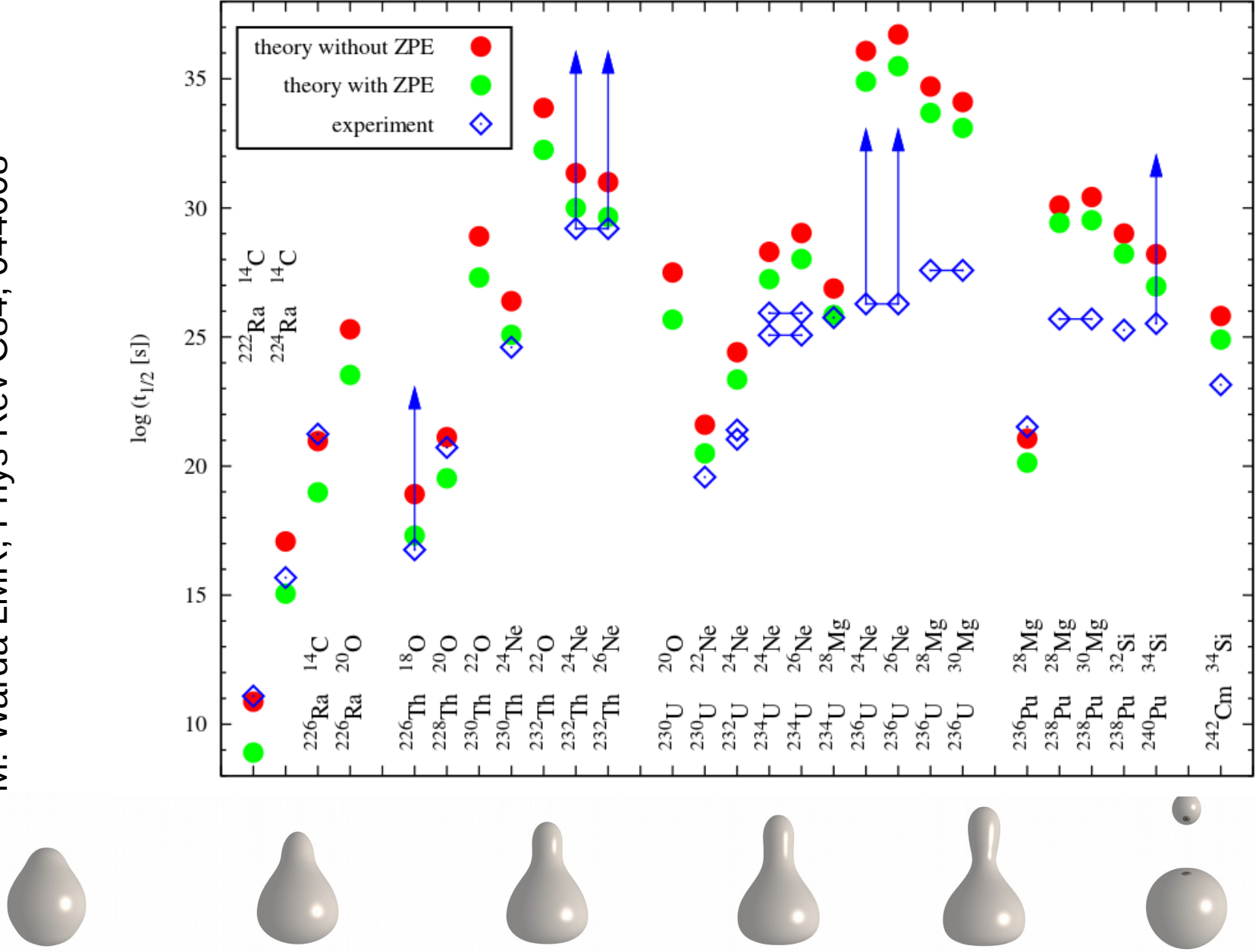


Emission of heavy clusters ( $^{14}\text{C}$ ,  $^{20}\text{Ne}$ ,  $^{20}\text{O}$ ,  $^{30}\text{Mg}$  ... ). Very asymmetric fission



# Octupoles and cluster emission

M. Warda LMR, Phys Rev C84, 044608



# Summary and conclusions

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- 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
- 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)

