On shape coexistence in zirconium region

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Theoretical Nuclear Physics in Padova:
a meeting in honor of Prof. Andrea Vitturi
20-21 May 2019

Few remarks about Andrea

- He was one of my first collaborators from abroad during my PhD in Seville.
- Only 3 publications in common:
  - J.E. García-Ramos, C.E. Alonso, J.M. Arias, P. Van Isacker y A. Vitturi, "Intrinsic structure of two-phonon states in the interacting boson model", Nuclear Physics A **637**, 529-546 (1998).
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   - Interacting Boson Model calculations
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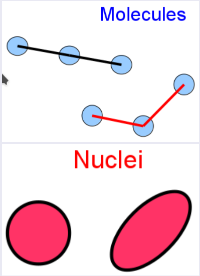
What Shape Coexistence (SC) is?

It appears in quantum systems where eigenstates with very different density distribution coexist.
Therefore, the existence of a geometric interpretation is implicit.



Quadrupole shape invariants

$$q_{2,i} = \sqrt{5}\langle 0_i^+ | [\hat{Q} \times \hat{Q}]^{(0)} | 0_i^+ \rangle,$$

$$q_{3,i} = -\sqrt{\frac{35}{2}} \langle 0_i^+ [\hat{Q} \times \hat{Q} \times \hat{Q}]^{(0)} | 0_i^+ \rangle,$$

$$q_2 = q^2, q_3 = q^3 \cos 3\ \delta.$$

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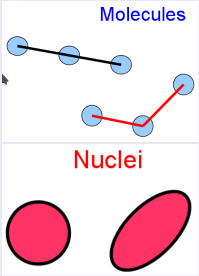

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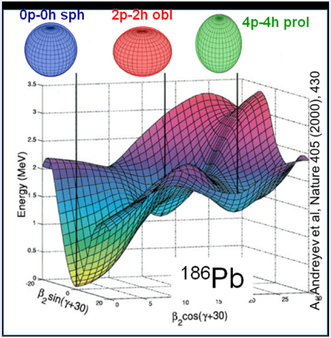
Mean field: example of triple coexistence



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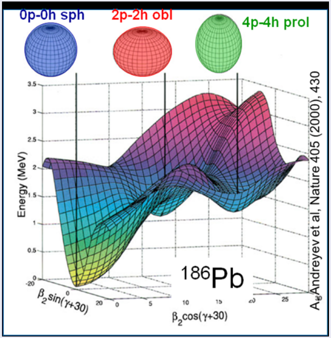
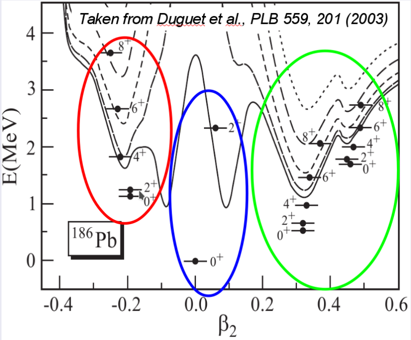


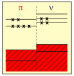
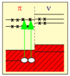


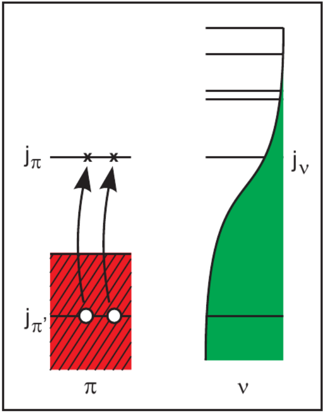
The angular momentum projected mean field plus the Generator Coordinate Method generates different bands with very different deformation.

Shell model. Where to be used

- For nuclei near to closed shells, either for neutrons or for protons, it can be energetically favorable to have excitations of 2p-2h, 4p-4h ... crossing the energy gap.
- The np-nh excitations have a lower excitation energy than expected due to the correlation energy: pairing and deformed correlations.
- Restricted to light and medium-heavy nuclei, at present.

"Sum" of configurations

$\phi(J,M) = a(J,M)$  $+\ b(J,M)$ 



In heavy nuclei the huge model space imposes some kind of truncation: symmetry dictated truncation.

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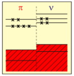
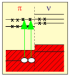
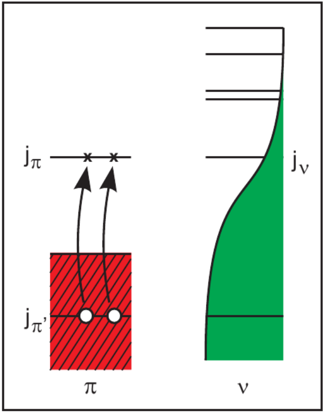
$\phi(J,M) = a(J,M)$ 

$+\ b(J,M)$ 



In heavy nuclei the huge model space imposes some kind of truncation: symmetry dictated truncation.

A symmetry guided approximation: the IBM

Nucleons couple preferably in pairs with angular momentum either equal to 0 (S) or equal to 2 (D). Those pairs are then described by means of bosons: s and d.

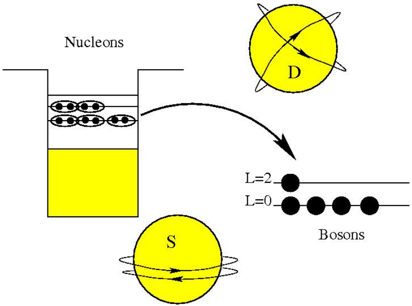
$$s^\dagger, d_m^\dagger (m = 0, \pm 1, \pm 2)$$
$$s, d_m (m = 0, \pm 1, \pm 2)$$

with

$$[\gamma_{lm}, \gamma^\dagger_{l'm'}] = \delta_{ll'}\delta_{mm'},$$
$$[\gamma^\dagger_{lm}, \gamma^\dagger_{l'm'}] = 0, [\gamma_{lm}, \gamma_{l'm'}] = 0$$

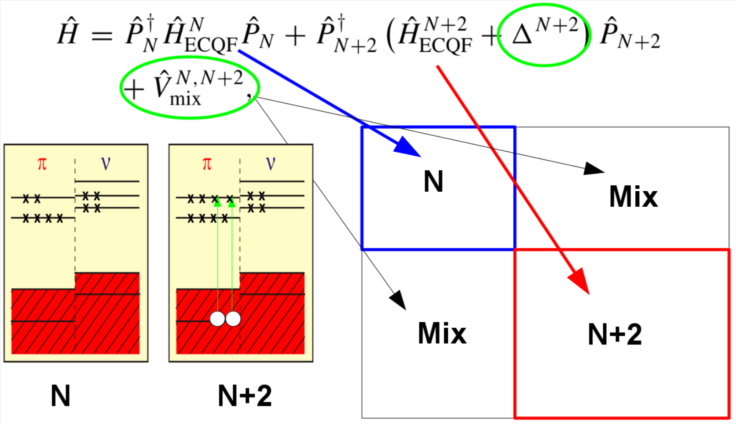
Simplified Hamiltonian

$$\hat{H}_{ECQF} = \varepsilon \hat{n}_d + \kappa \hat{Q} \cdot \hat{Q} + \kappa' \hat{L} \cdot \hat{L}$$



Model based on a u(6) spectrum generator algebra. It is especially suited for medium and heavy-mass nuclei.
The number of bosons, N, corresponds the number of nucleons pairs, regardeless its proton, neutron, particle or hole nature.

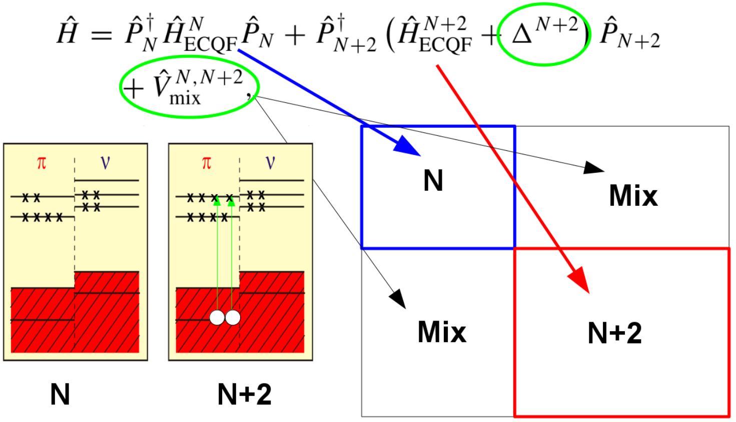
How IBM with configuration mixing works



A different Hamiltonian, $\hat{H}_{ECQF}^{N}$ and $\hat{H}_{ECQF}^{N+2}$, acts on the regular [N] and intruder [N+2] sectors, separately.

The offset Δ^{N+2} and the mixing interaction $\hat{V}_{mix}^{N,N+2}$ should be provided.

How IBM with configuration mixing works



A different Hamiltonian, $\hat{H}^N_{ECQF}$ and $\hat{H}^{N+2}_{ECQF}$, acts on the regular [N] and intruder [N+2] sectors, separately.

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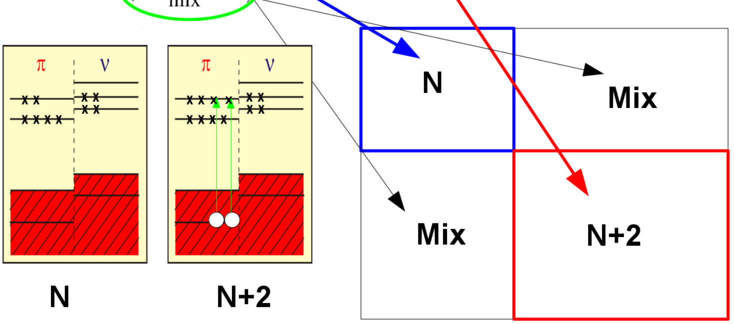
How IBM with configuration mixing works

$$\hat{H} = \hat{P}_N^\dagger \hat{H}_{\mathrm{ECQF}}^N \hat{P}_N + \hat{P}_{N+2}^\dagger \left(\hat{H}_{\mathrm{ECQF}}^{N+2} + \Delta^{N+2}\right) \hat{P}_{N+2} + \hat{V}_{\mathrm{mix}}^{N,N+2},$$



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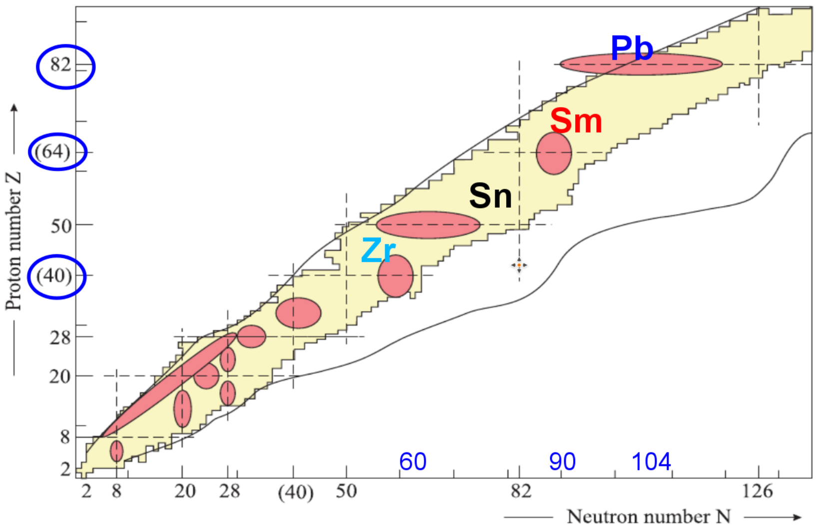
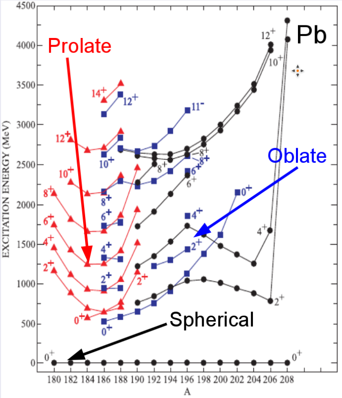
Regions of interest



Shape coexistence

Pb isotopes



Three families of states are present.

Shape coexistence

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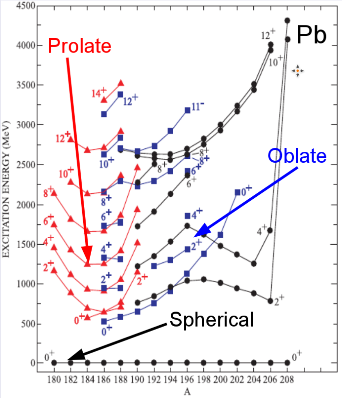

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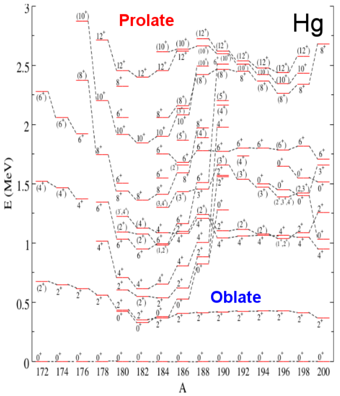
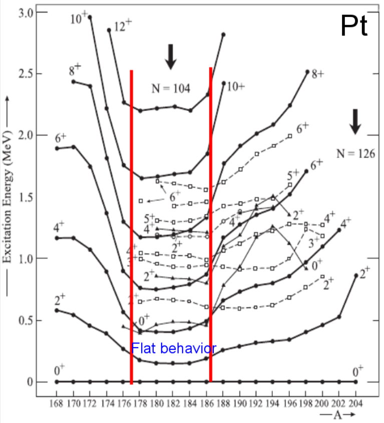
Hg isotopes



The presence of two families of states is self-evident.

Lead region

Pt isotopes



In this case only a *suspicious* flat area appears at midshell.

Lead region

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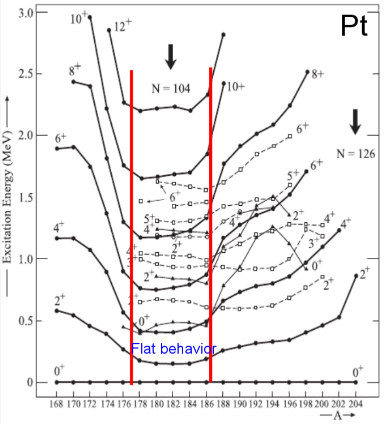

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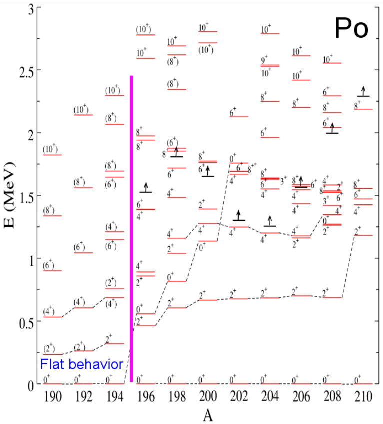
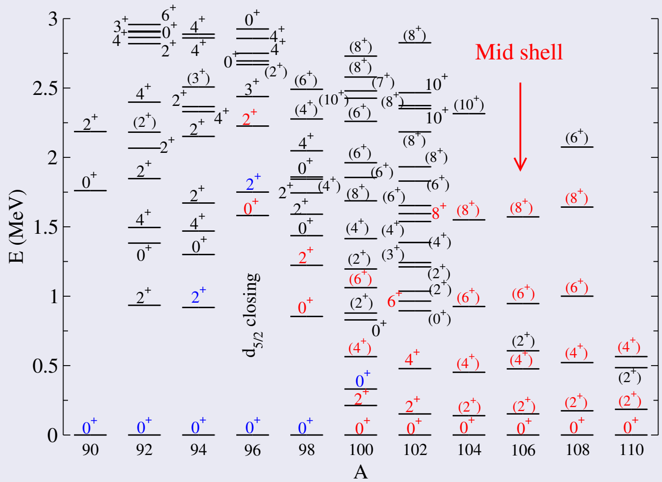
Po isotopes



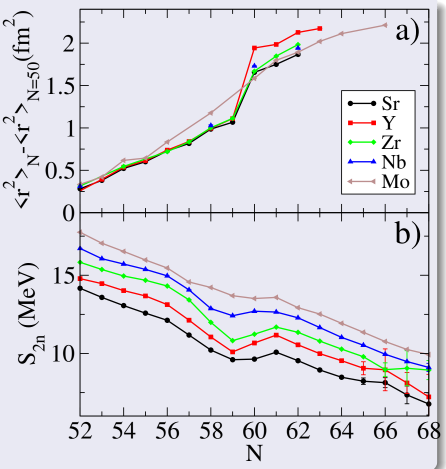
Here we hardly reach the midshell and no clear conclusions can be obtained.

Energy systematics for even-even Zr nuclei



Blue labels for spherical states while red labels for deformed ones.

Radii and two-neutron separation energies



- Radii show a shudden increase at $N = 60$ for Sr, Y and Zr, being almost smoothed out for Mo.
- S_{2n} present a similar trend to the observed one in rare-earth region, although, once more, the *discontinuity* is smoothed out for Mo.

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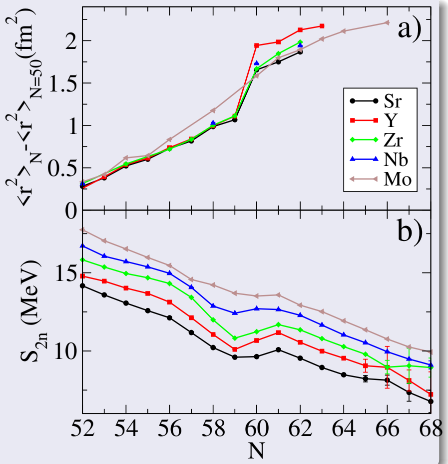

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The fitting procedure

Energies

Error (keV)	States
$\sigma = 1$	2_1^+
$\sigma = 10$	$4_1^+, 0_2^+, 2_2^+, 4_2^+$
$\sigma = 100$	$2_3^+, 2_4^+, 3_1^+, 4_3^+, 4_4^+$

χ^2 test

The χ^2 function is defined in the standard way as

$$\chi^2 = \frac{1}{N_{data} - N_{par}} \sum_{i=1}^{N_{data}} \frac{(X_i(data) - X_i(IBM))^2}{\sigma_i^2},$$

We minimize the χ^2 function for each isotope separately using the package MINUIT which allows to minimize any multi-variable function.

The fitting procedure

The operators

$$\hat{H}^{i}_{\mathrm{ecqf}} = \varepsilon_i \hat{n}_d + \kappa'_i \hat{L} \cdot \hat{L} + \kappa_i \hat{Q}(\chi_i) \cdot \hat{Q}(\chi_i).$$

$$\hat{Q}_\mu(\chi_i) = [s^\dagger \times \tilde{d} + d^\dagger \times s]^{(2)}_\mu + \chi_i [d^\dagger \times \tilde{d}]^{(2)}_\mu, \;\; \hat{T}(E2)_i = e_i \hat{Q}_i$$

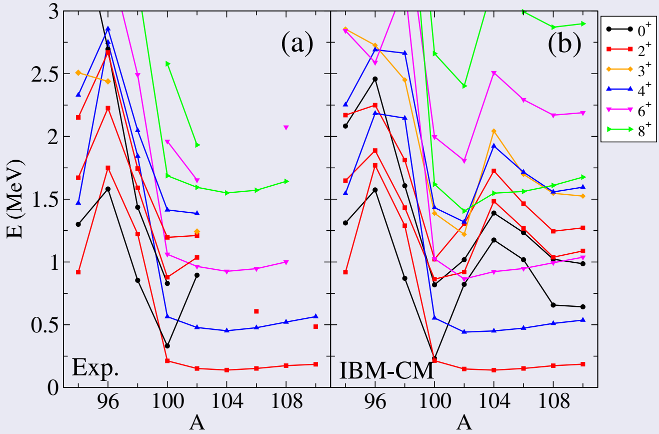
The parameters

Nucleus	ε_N	κ_N	χ_N	κ'_N	ε_{N+2}	κ_{N+2}	χ_{N+2}	κ'_{N+2}	ω	Δ	e_N	e_{N+2}
^{94}Zr	1201	-0.00	1.30	-39.93	0.1	-26.32	-2.35	21.97	150	3200	2.01	-1.36
^{96}Zr	1800	-34.41	1.82	25.12	333.2	-29.18	0.09	-4.50	15	2000	0.90	3.35
^{98}Zr	1044	-25.23	1.80	78.71	439.6	-14.32	0.67	26.48	15	814	1.55	3.11
^{100}Zr	1063	-23.26	2.53	0.00	438.3	-28.76	-0.95	0.00	15	820	0.46	2.26
^{102}Zr	1050	-23.58	2.46	0.00	337.9	-32.01	-0.68	0.00	15	820	0.46	2.32
^{104}Zr	1050	-23.58	2.46	0.00	616.5	-32.00	-1.35	0.00	15	820	0.46	2.32
^{106}Zr	1050	-23.58	2.46	0.00	580.5	-31.03	-0.93	0.00	15	820	0.46	1.79
^{108}Zr	1050	-23.58	2.46	0.00	540.2	-30.00	-0.90	0.00	15	820	0.46	1.81
^{110}Zr	1050	-23.58	2.46	0.00	498.9	-32.00	-0.90	0.00	15	820	0.46	1.81

All quantities have the dimension of energy (given in keV), except χ_N and χ_{N+2}, which are dimensionless and e_N and e_{N+2} which are given in $\sqrt{\mathrm{W.u.}}$

Comparing theory and experimental data

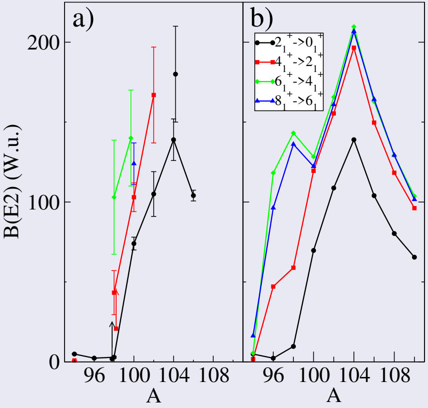
Energies



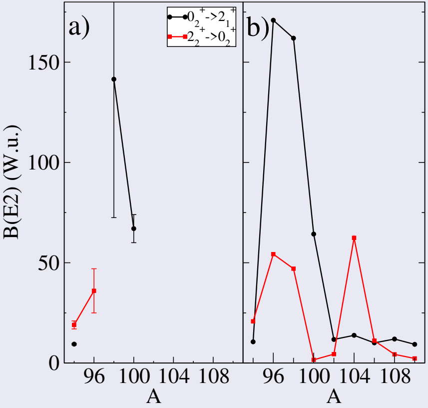
A very similar work has been recently published: N. Gavrielov, A. Leviatan and F. Iachello, to appear in PRC.

B(E2) transition rates

Intraband

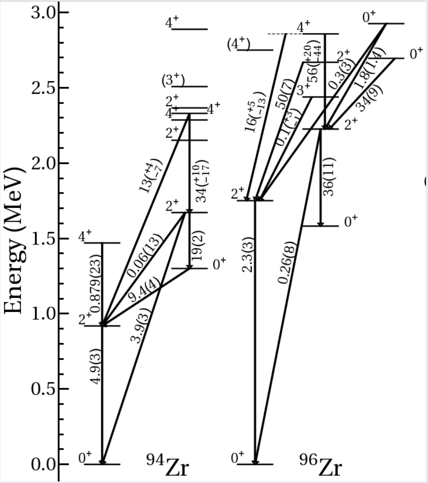


Interband

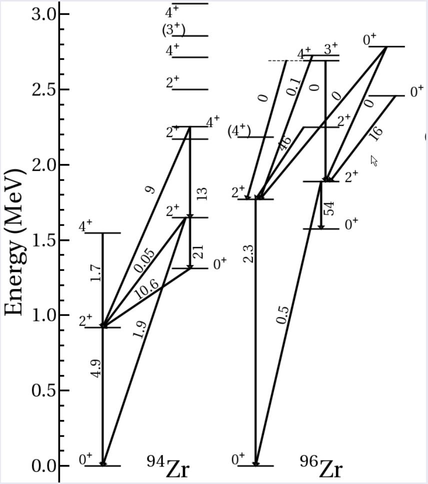


Comparing theory and experimental data

Experimental

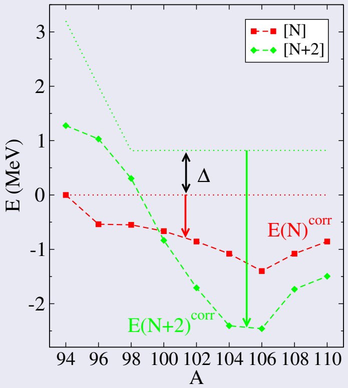


Theoretical



Unperturbed energies

Correlation energies

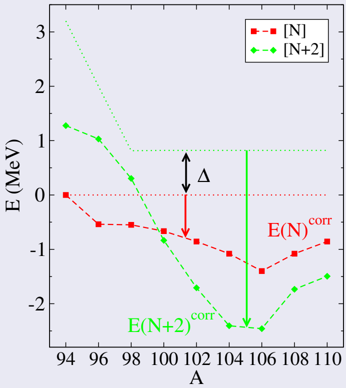


The intruder configuration becomes ground state for

$A = 100$ and onwards.

Unperturbed energies

Correlation energies



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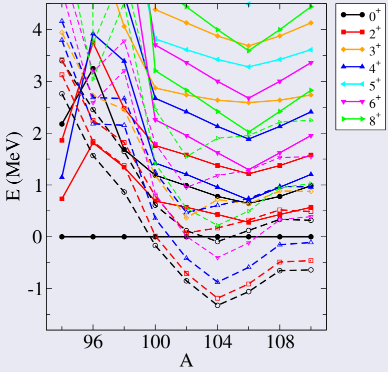
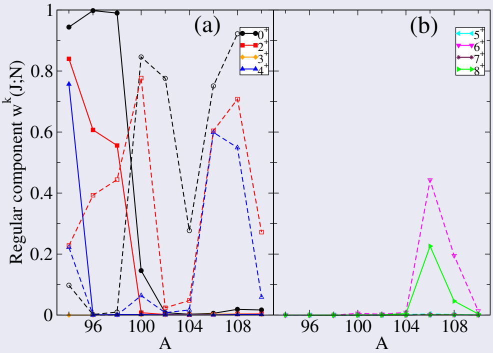
Unperturbed spectra



Intruder states present a *parabolic* behaviour while regular ones *flat*.

Wave function

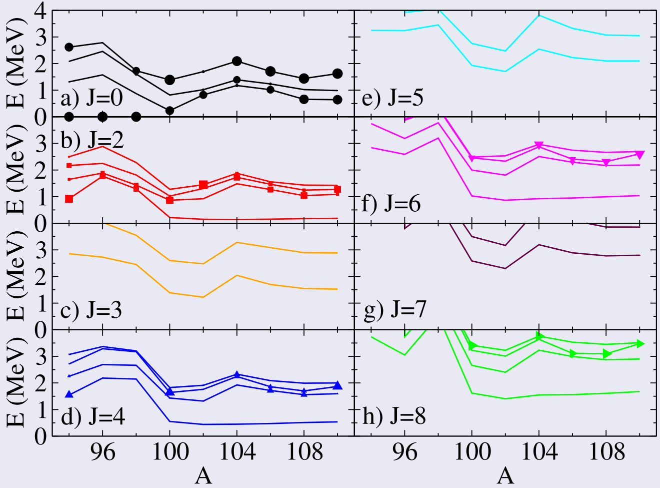
Regular component



$\Psi(k, JM) = \sum_i a_i^k(J;N)\psi((sd)_i^N; JM) + \sum_j b_j^k(J;N+2)\psi((sd)_j^{N+2}; JM)$ and
$w^k(J,N) \equiv \sum_i \mid a_i^k(J;N) \mid^2$.

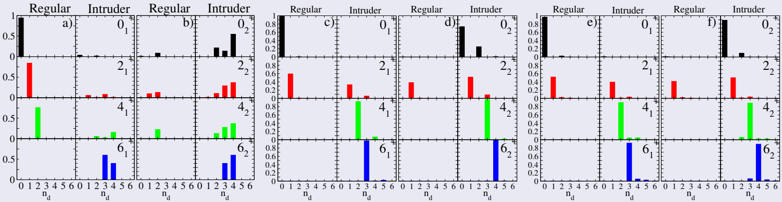
Wave function

Regular component and energy



Wave function: U(5) decomposition

^{94}Zr, ^{96}Zr and ^{98}Zr



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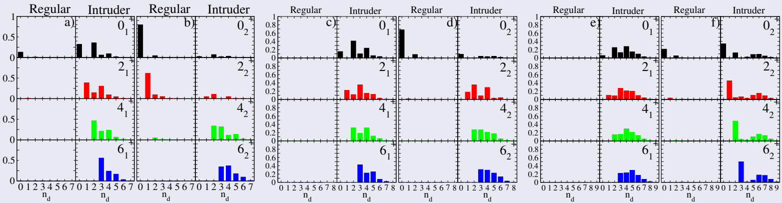

Radii

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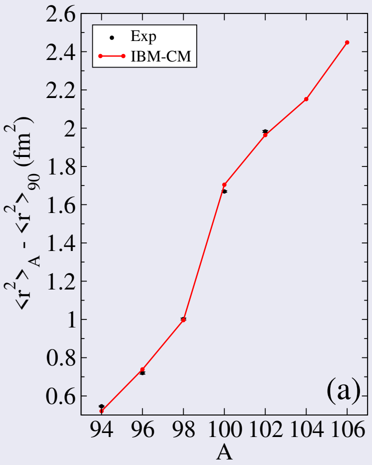
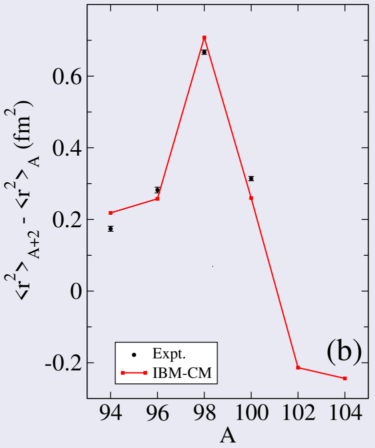
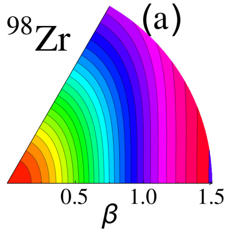


Isotopic shift

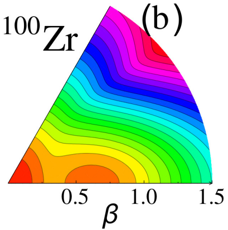


Mean-field energy surfaces

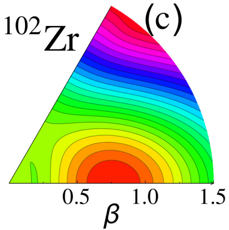
^{98}Zr



^{100}Zr



^{102}Zr



Mean field energy surface shows up a rapid evolution from a spherical to a well deformed shape. ^{100}Zr shows the coexistence of two minima.

Conclusions

- Lead region clearly shows up the onset of shape coexistence and, indeed, it is the paradigm of shape coexistence region.
- Even-even Zr isotopes present a very rapid change in their structure, with a clear change of *regime* in ^{100}Zr.
- The IBM-CM provides an accurate description of the observed rapid changes and of the different *shapes* present in the spectrum.
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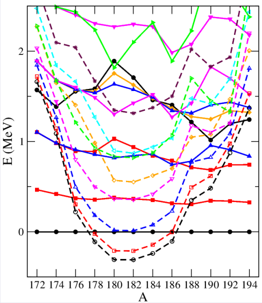
Thank you

Unperturbed energies

Pt isotopes



The parabolic energy systematics is clear and the intruder configuration becomes the ground state.

Unperturbed energies

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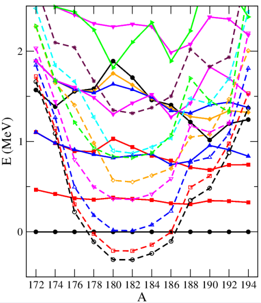

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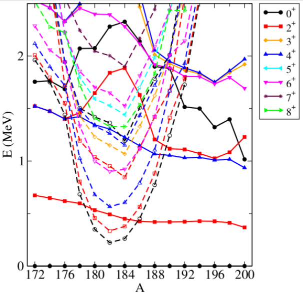
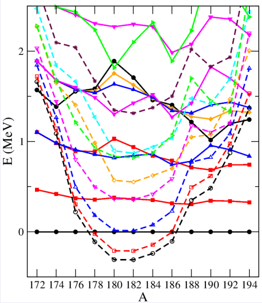
Hg isotopes



The parabolic energy systematics is obvious, but the ground state always presents a regular nature.

Unperturbed energies

Pt isotopes



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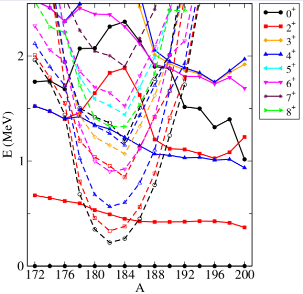

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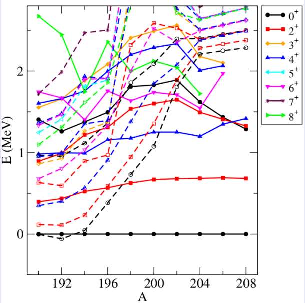
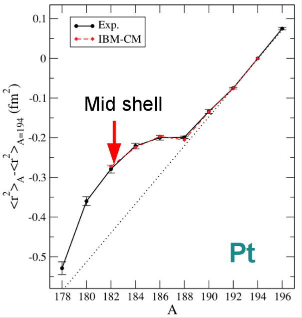
Po isotopes



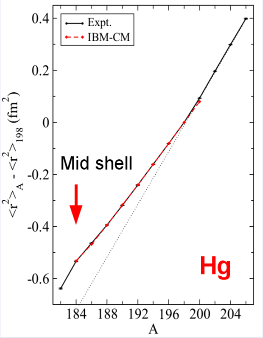
Intruder and regular configurations are almost degenerated at midshell.

Radii

Pt isotopes



Hg isotopes



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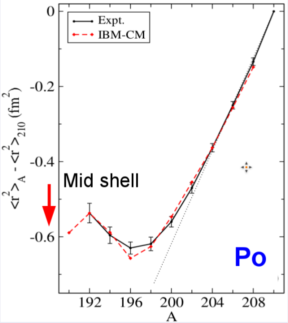
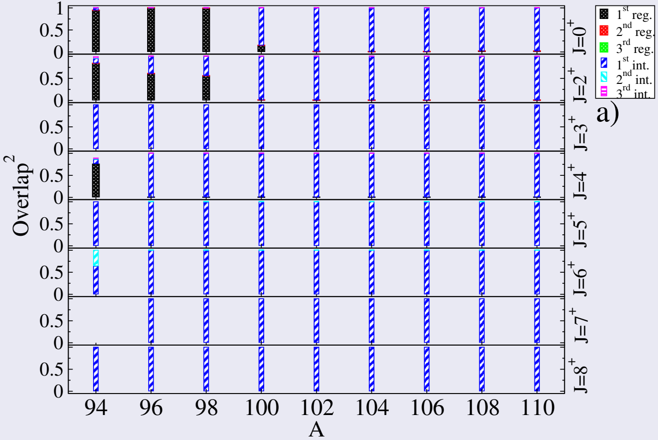


The three cases show a clear departure from the spherical trend.

Wave function

Overlap with the intermediate basis: first state



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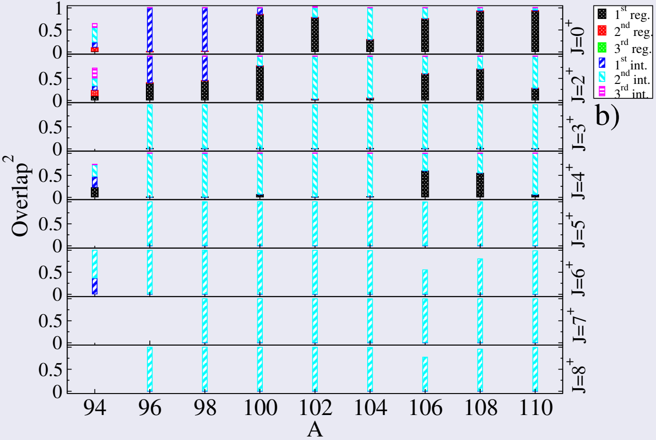
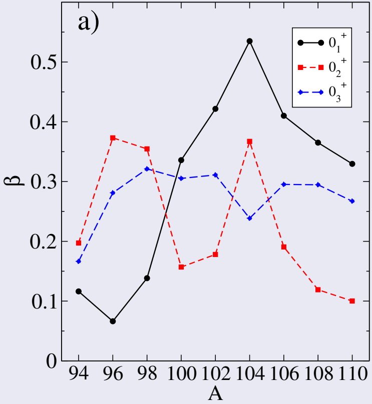
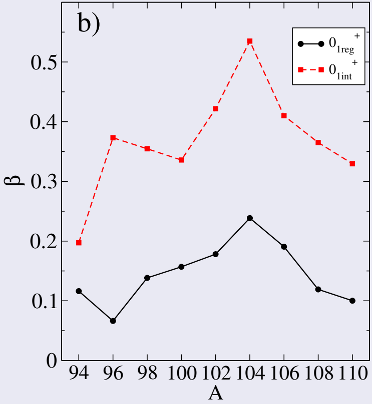


Deformation from quadrupole shape invariants

0_1^+, 0_2^+, and 0_3^+



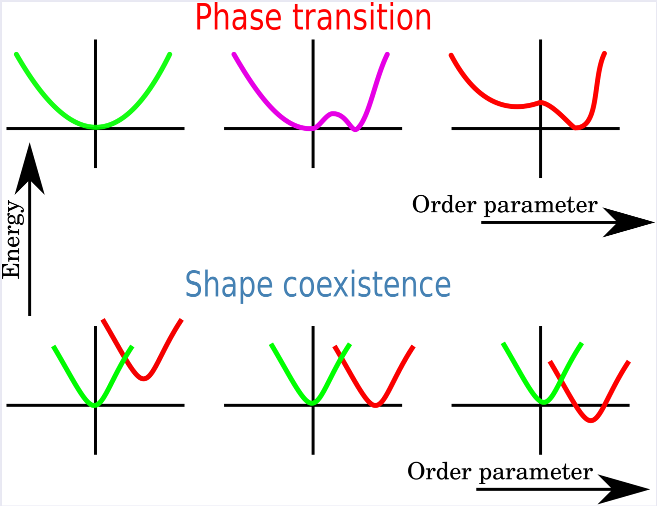
0_{1reg}^+, 0_{1int}^+



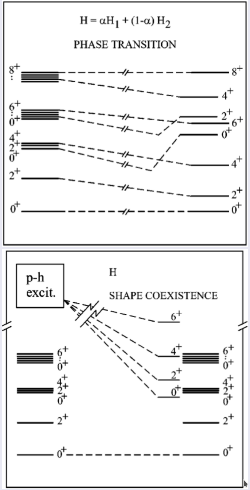
Value of β extracted from the quadrupole moment, $\beta = \frac{4\pi\sqrt{q_2}}{3\,Z\,e\,r_0^2\,A^{2/3}}$.

Schematic view

Two minima

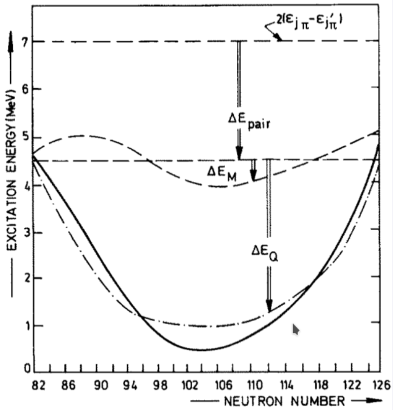


PRC 69, 054304 (2004)



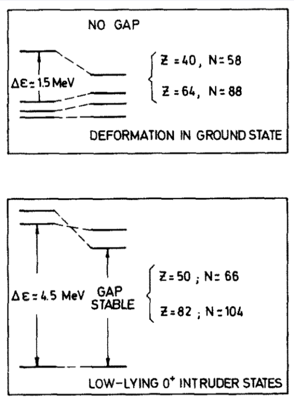
Competition of interactions

The effect of the different components



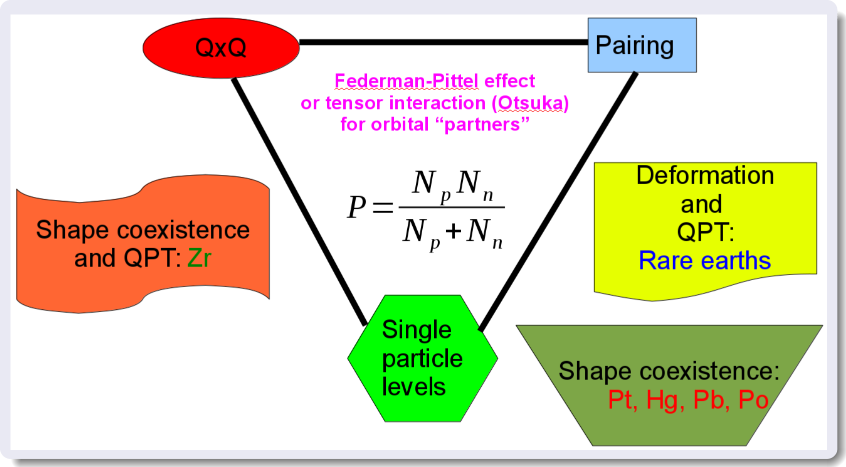
Figures taken from K. Heyde et al., Nuclear Physics A**466**, 189 (1987).

Gap versus deformation



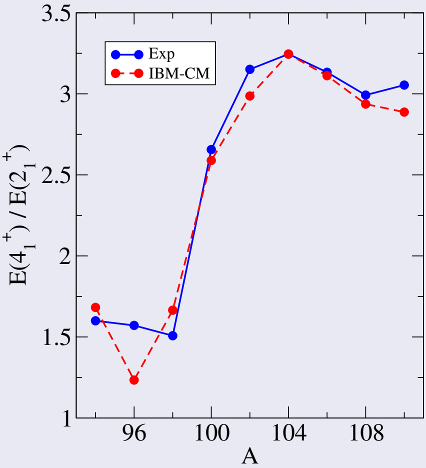
The precise balance between the gap size and the contribution of residual interaction will determine the shape of the nucleus.

Competition of interactions



Hints pointing to a QPT

$E(4_1^+)/E(2_1^+)$



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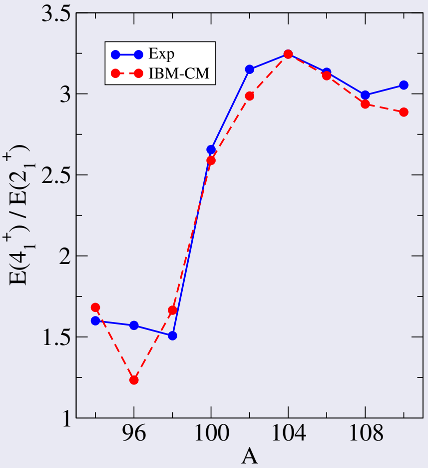
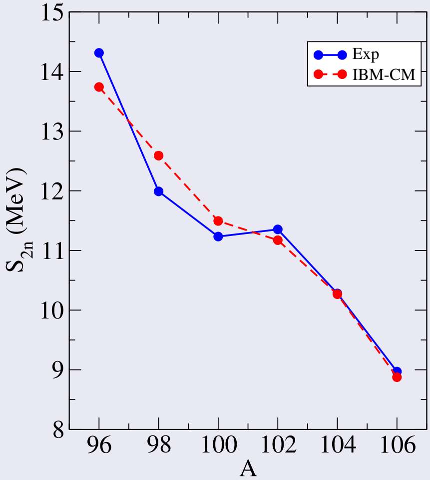


Two-neutron separation energy



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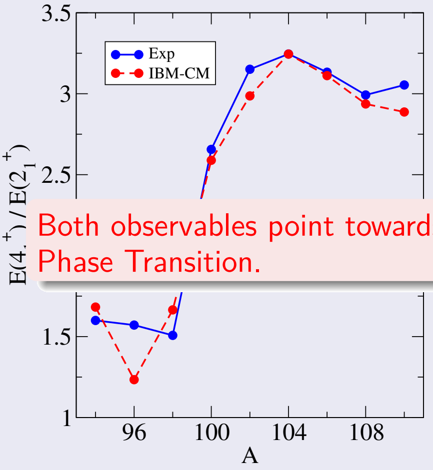

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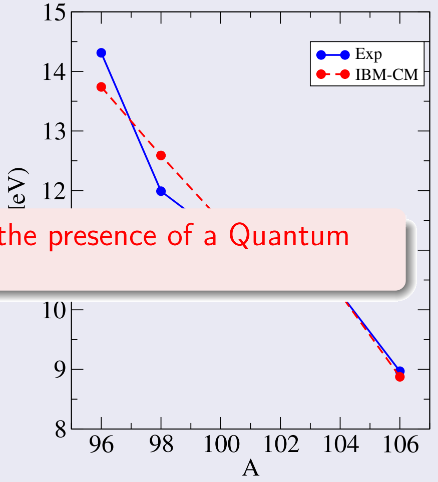

Both observables point towards the presence of a Quantum Phase Transition.