# On the nature of shape coexistence and quantum phase transition phenomena

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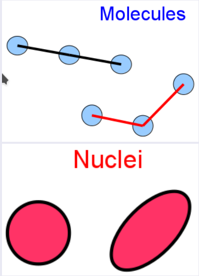
Supported by MCIN/AEI/10.13039/501100011033
PID2022-136228NB-C21

LASNPA XIV, Facultad de Ciencias, UNAM (México), June 17-21 2024

# Table of contents

# 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

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

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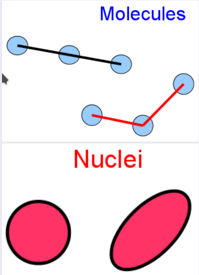


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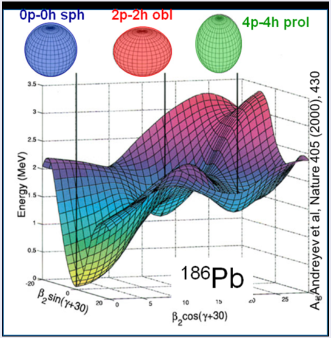
## Mean field: example of triple coexistence



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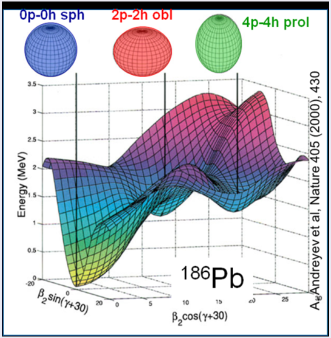
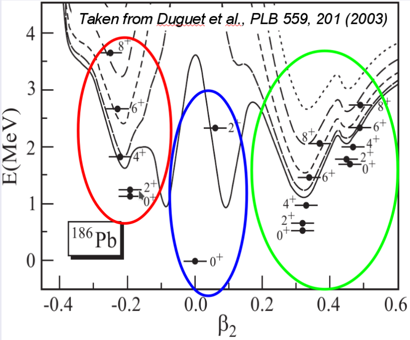
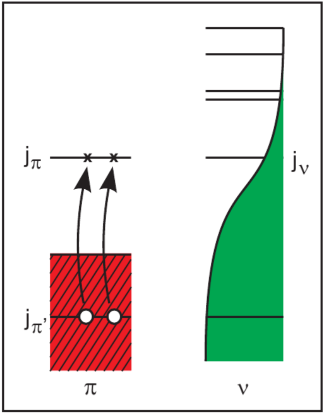



The angular momentum projected mean field plus the Generator Coordinate Method generates different bands with very different deformation.

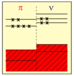
## Shell model. Where to be used

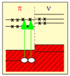
- For nuclei near to closed shells, either for neutrons or for protons, it can be energetically favorable to have excitations of 2p-2h, 4p-4h . . . crossing the energy gap.
- The np-nh excitations have a lower excitation energy than expected due to the correlation energy: pairing and deformed correlations.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




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

## "Sum" of configurations

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

$+ \; b(J,M)$ 

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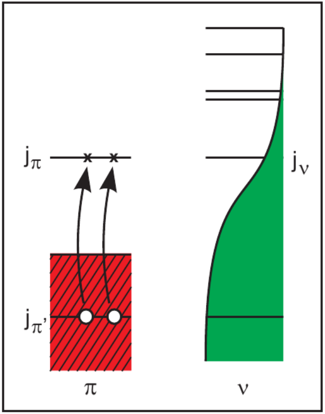


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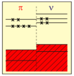
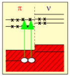
$\phi(J,M) = a(J,M)$  $+\ b(J,M)$ 

## 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.

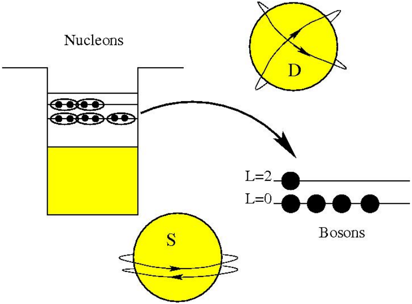
$$s^\dagger, d_m^\dagger (m = 0, \pm 1, \pm 2)$$
$$s, d_m (m = 0, \pm 1, \pm 2)$$

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

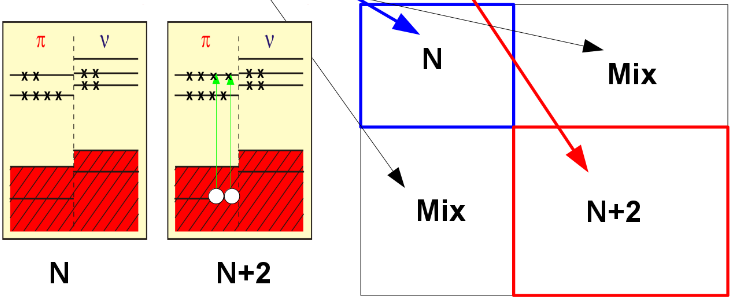
$$\hat{H}_{ECQF} = \varepsilon \hat{n}_d + \kappa \hat{Q} \cdot \hat{Q} + \kappa' \hat{L} \cdot \hat{L}$$




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

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




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

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

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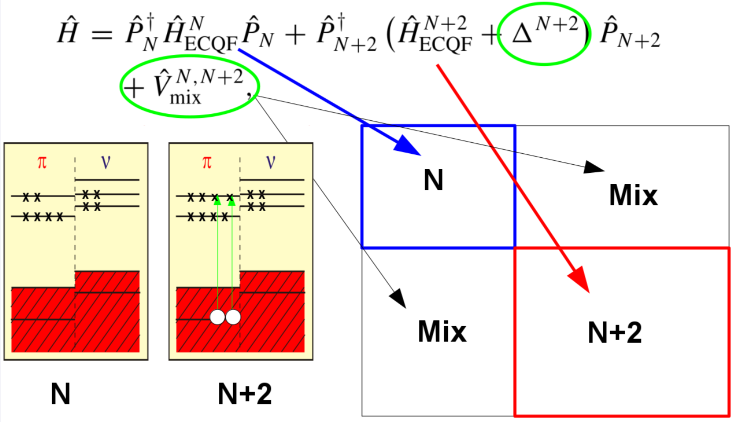


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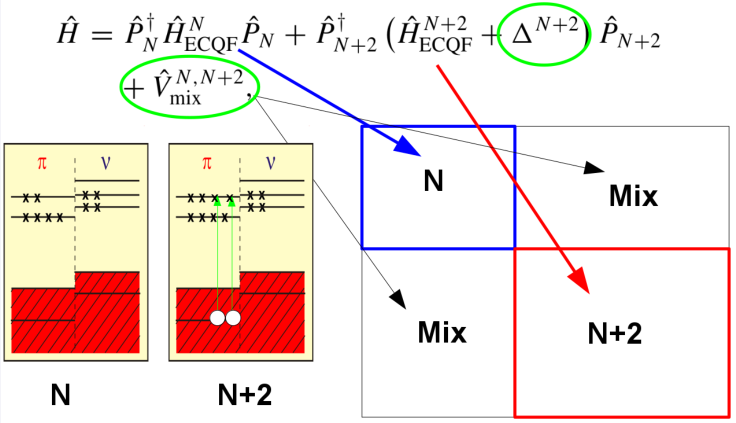


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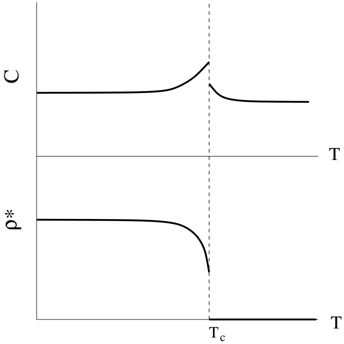
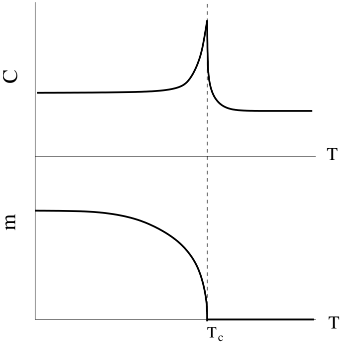
# Examples of Macroscopic Phase Transitions



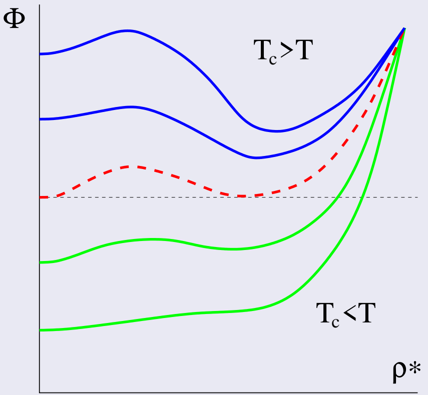

First order phase transition.
Liquid-gas



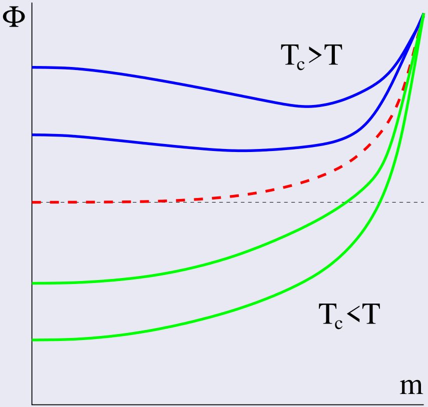

Second order phase transition.
Paramagnetic-ferromagnetic

# Inside a Quantum Phase Transition

## First order




## Second order

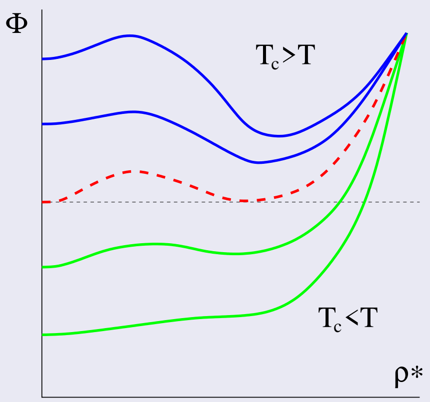



## Φ in the Landau theory

$$\Phi = A(T,...)\beta^4 + B(T,...)\beta^2 + C(T,...)\beta$$

# Inside a Quantum Phase Transition

## First order

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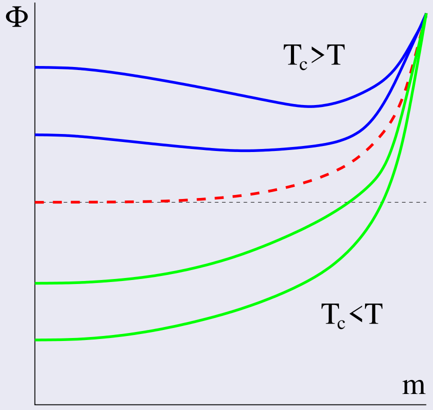


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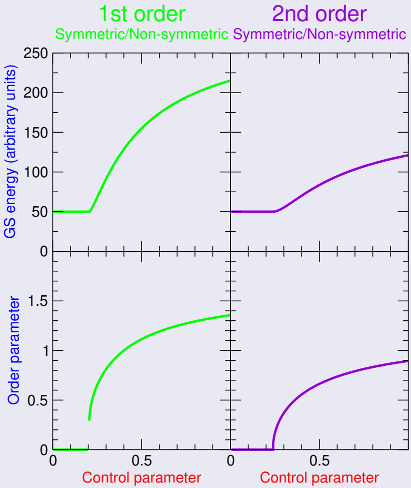
# What a Quantum Phase Transition (QPT) is?

A QPT appears when the ground state a quantum system experiences a sudden change in its structure (order parameter) when a parameter that affects the Hamiltonian (control parameter) slightly changes around its critical value. This transitions are assumed to occurs at zero temperature.

$$\hat{H} = (1-\xi)\hat{H}_1 + \xi \hat{H}_2$$



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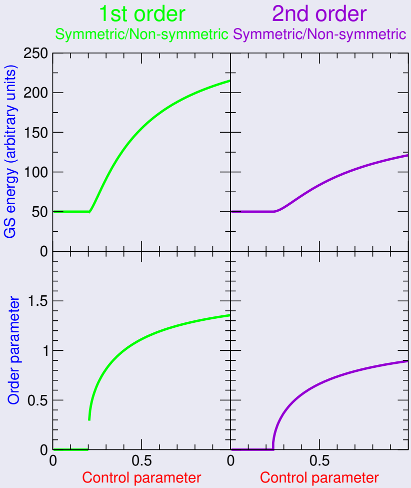
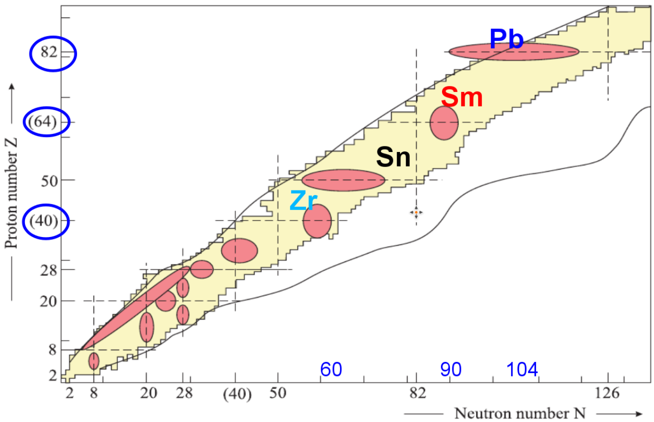


## Regions of interest



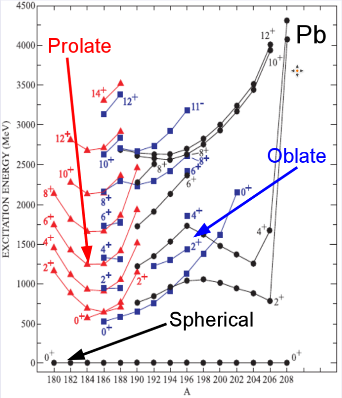

Pb and Sn regions are ideal regions to study the importance of Shape Coexistence (SC).

Sm region is the paradigm of Quantum Phase Transition (QPT) region.

Zr region seems to be the ideal region to study the interplay between SC and QPT.

# Shape coexistence

## Pb isotopes




Three families of states are present.

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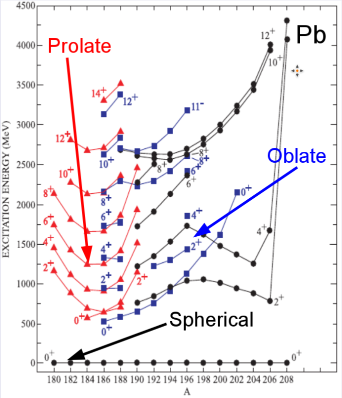


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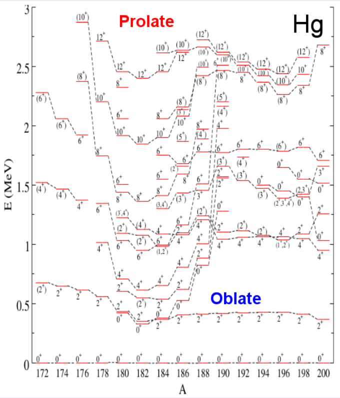
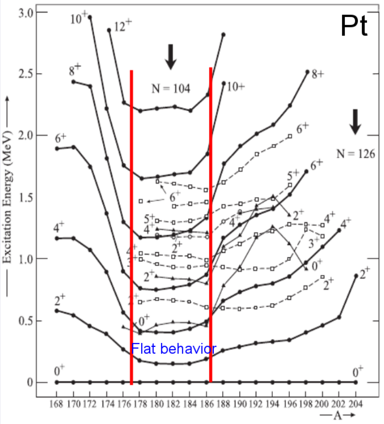



The presence of two families of states is self-evident.

# Lead region

## Pt isotopes

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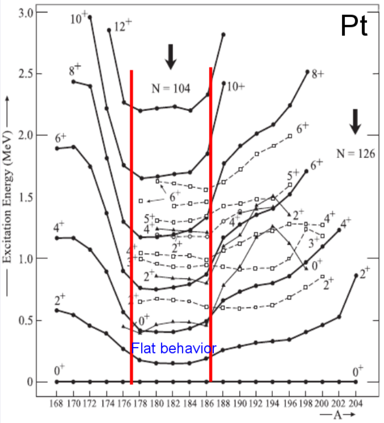


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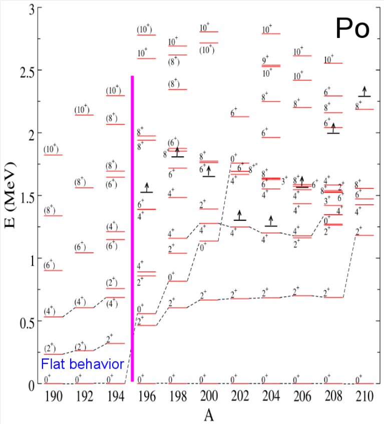
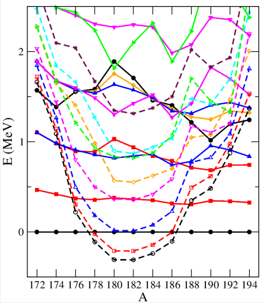



Here, we hardly reach the midshell and no clear conclusions can be obtained.

# Unperturbed energies

## Pt isotopes




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

JEGR and K. Heyde, NPA **825**, 39 (2009).

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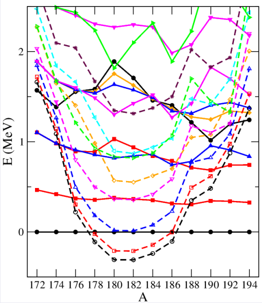


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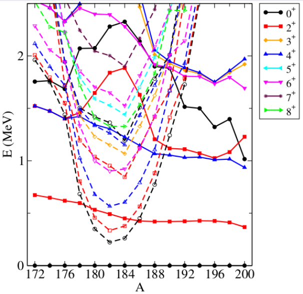


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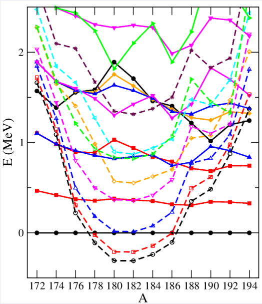


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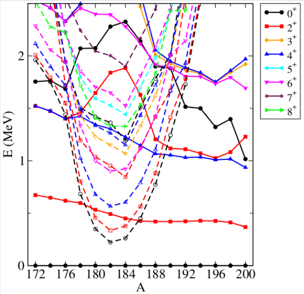


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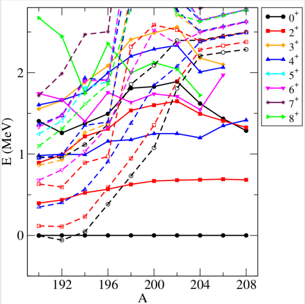


Intruder and regular configurations are almost degenerated at midshell. JEGR and K. Heyde, PRC **92**, 034309 (2015).

# Radii

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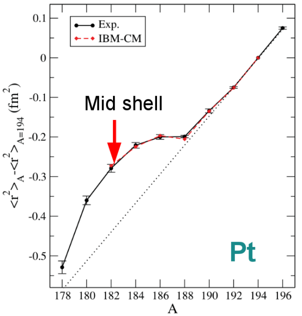


The three cases show a clear departure from the spherical trend.

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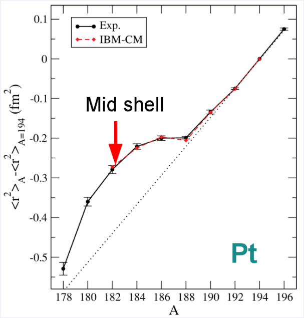


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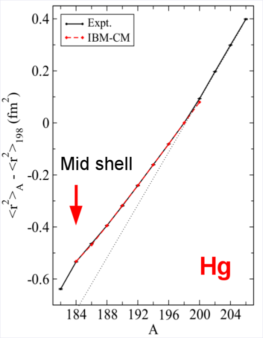


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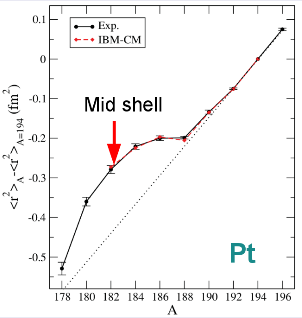


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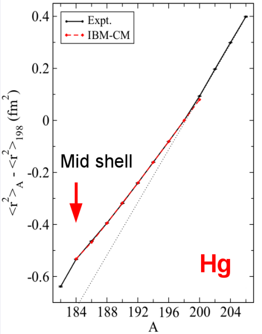


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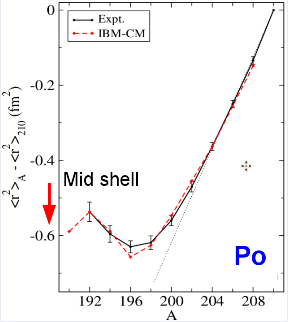


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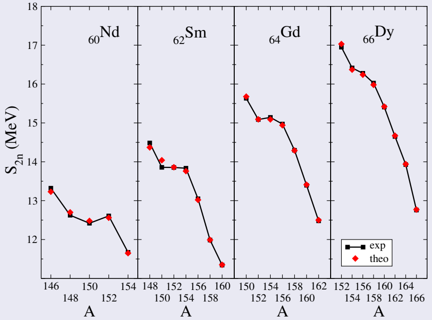
# Quantum Phase Transition indicators in the rare-earth region: Type I

## Two-neutron separation energy. Why?

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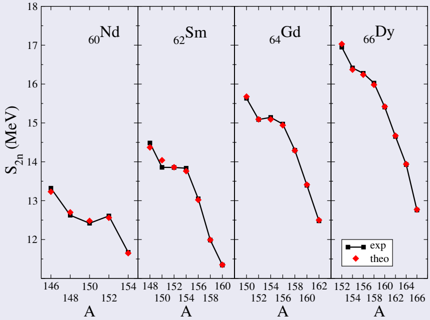


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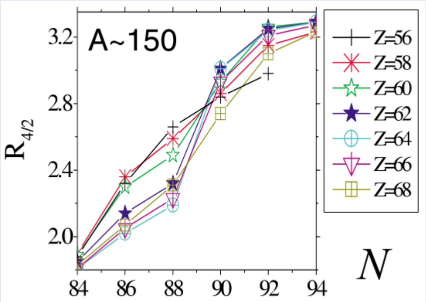
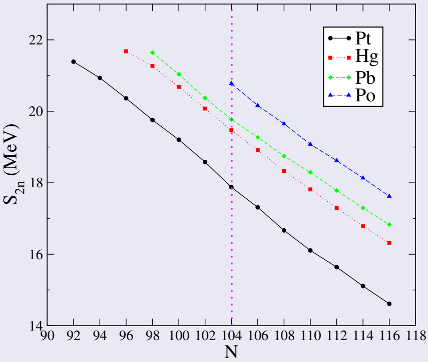
## $E(4_1^+)/E(2_1^+)$




$E(4_1^+)/E(2_1^+)$ can be used as an order parameter and, therefore, it is a key observable to find where a QPT develops.

# Hints for QPTs in lead region?

## Two-neutron separation energy

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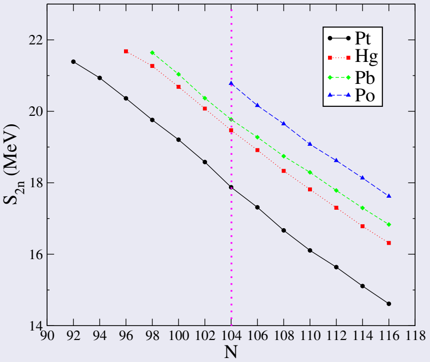


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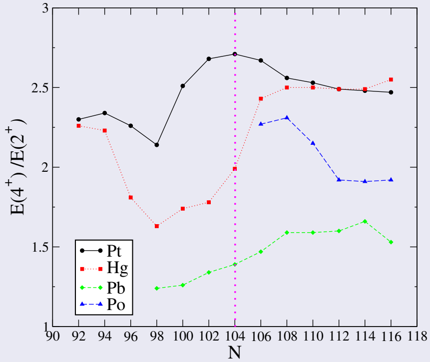


$E(4_1^+)/E(2_1^+)$ does not present neither the typical behaviour of an order parameter. Only Pt isotopes resemble the expected trend for an order parameter when approaching midshell from the left.

# Something in common?

- Rapid change in the structure of certain states, including the ground-state.
- Lowering of certain $0^+$ states.
- At the mean-field level several minima coexist.
- Onset of deformation: radii and isotopic shift.

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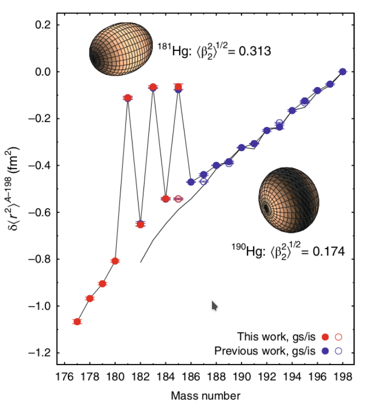
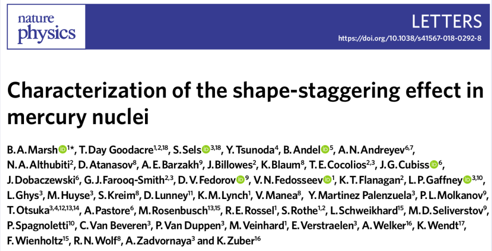



Nature Physics, October 2018



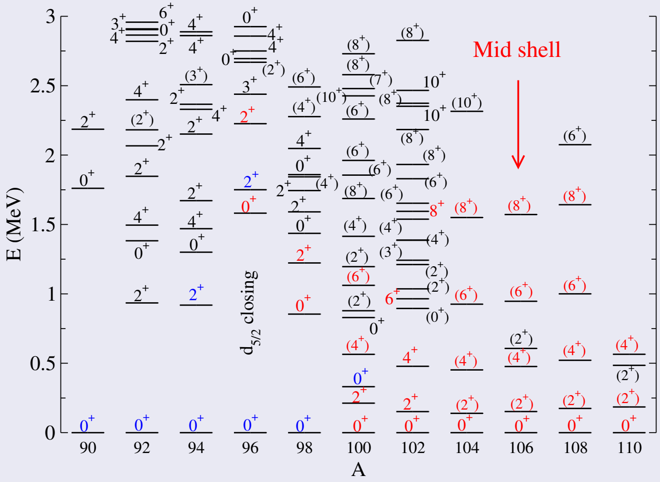
nature physics
LETTERS
https://doi.org/10.1038/s41567-018-0292-8

## Characterization of the shape-staggering effect in mercury nuclei

B. A. Marsh[1*], T. Day Goodacre[1,2,18], S. Sels[3,18], Y. Tsunoda[4], B. Andel[5], A. N. Andreyev[6,7], N. A. Althubiti[2], D. Atanasov[8], A. E. Barzakh[9], J. Billowes[2], K. Blaum[8], T. E. Cocolios[2,3], J. G. Cubiss[6], J. Dobaczewski[6], G. J. Farooq-Smith[2,3], D. V. Fedorov[9], V. N. Fedosseev[1], K. T. Flanagan[2], L. P. Gaffney[3,10], L. Ghys[3], M. Huyse[3], S. Kreim[8], D. Lunney[11], K. M. Lynch[1], V. Manea[8], Y. Martinez Palenzuela[3], P. L. Molkanov[9], T. Otsuka[3,4,12,13,14], A. Pastore[6], M. Rosenbusch[13,15], R. E. Rossel[1], S. Rothe[1,2], L. Schweikhard[15], M. D. Seliverstov[9], P. Spagnoletti[10], C. Van Beveren[3], P. Van Duppen[3], M. Veinhard[1], E. Verstraelen[3], A. Welker[16], K. Wendt[17], F. Wienholtz[15], R. N. Wolf[8], A. Zadvornaya[3] and K. Zuber[16]

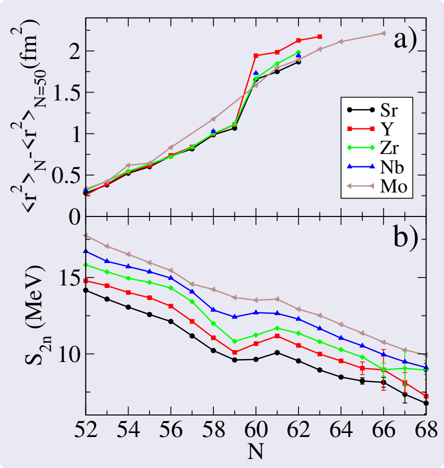
"The shape staggering effect manifests characteristic features of a quantum phase transition: in a given nucleus, different phases ... By making small changes in the control parameter, which in this case is the neutron number, the system alternates between the two phases..."

# Energy systematics for even-even Zr nuclei



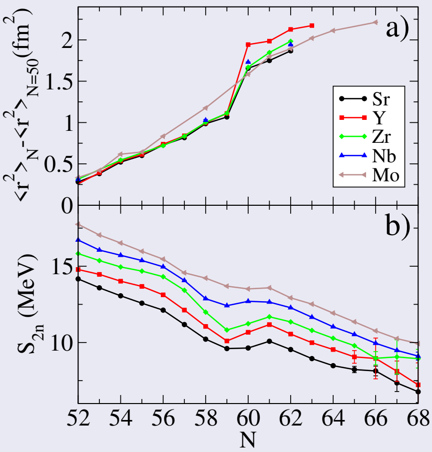

Blue labels for spherical states while red labels for deformed ones.

# Radii and two-neutron separation energies




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

# Radii and two-neutron separation energies

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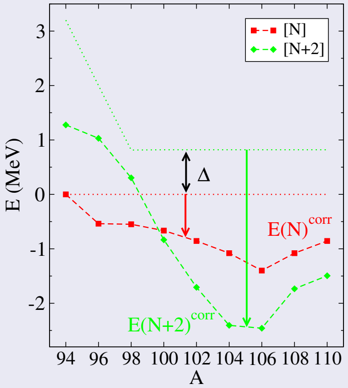
# Unperturbed energies

## Correlation energies (Zr case)




The intruder configuration becomes theground state for $A = 100$ and onwards. JEGR and K. Heyde, PRC **100**, 044315 (2019).

# Unperturbed energies

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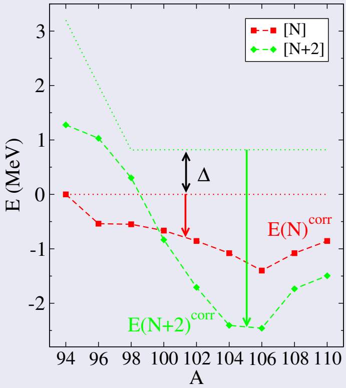
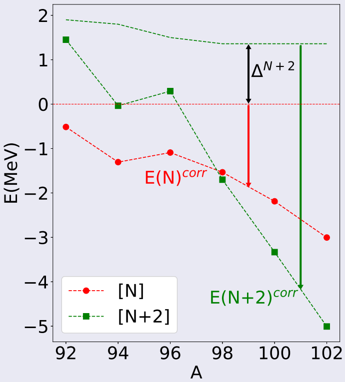



The intruder configuration becomes theground state for $A = 100$ and onwards. JEGR and K. Heyde, PRC **100**, 044315 (2019).

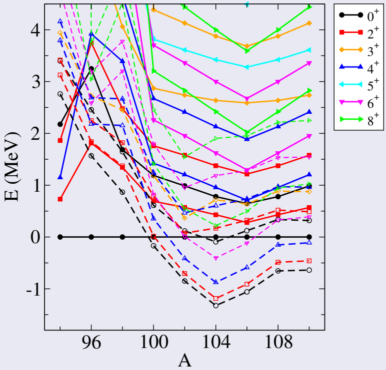
## Correlation energies (Sr case)




The intruder configuration becomes the ground state for $A = 98$ and onwards. E. Maya-Barbecho and JEGR, PRC **105**, 034341 (2022).

# Unperturbed energies

## Unperturbed spectra (Zr case)




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

# Unperturbed energies

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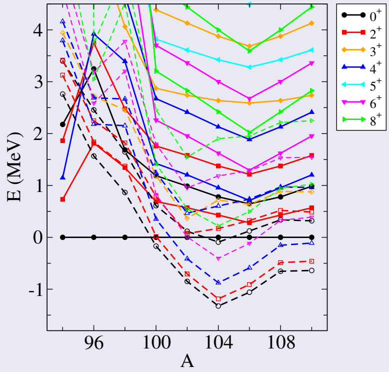
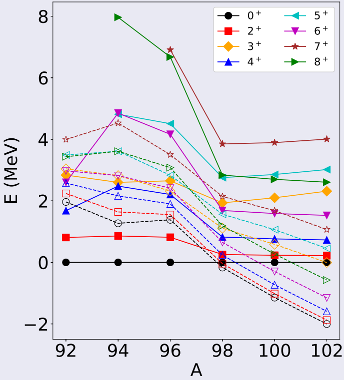



Intruder states present a *parabolic* behaviour while regular ones *flat*.

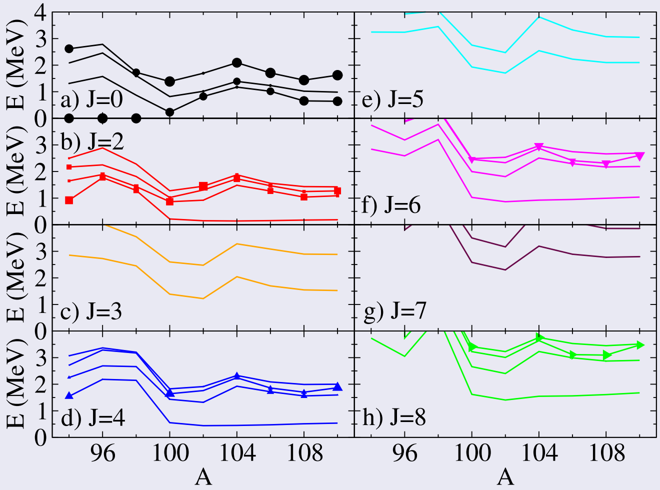
## Unperturbed spectra (Sr case)




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

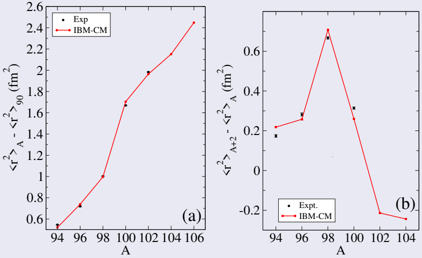
# Wave function

## Regular component and energy (Zr case)

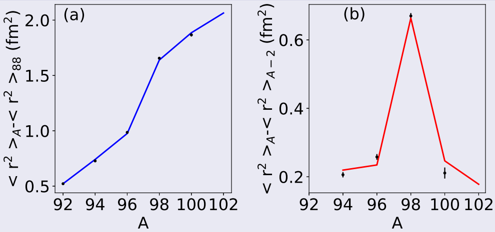


# Radii and isotope shift

## Zr isotopes

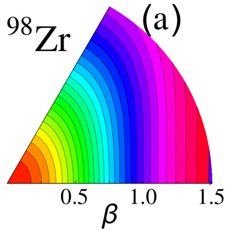



## Sr isotopes

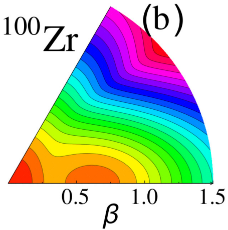


# Mean-field energy surfaces

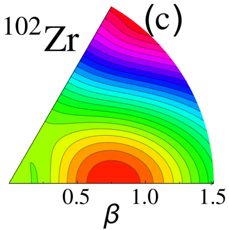
### $^{98}$Zr




### $^{100}$Zr



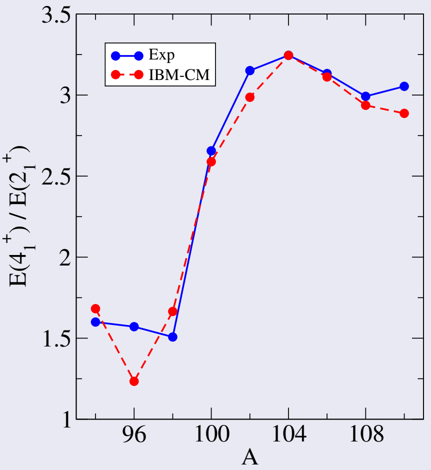

### $^{102}$Zr




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.

# Hints pointing to a QPT: Type II

## $E(4_1^+)/E(2_1^+)$ (Zr case)



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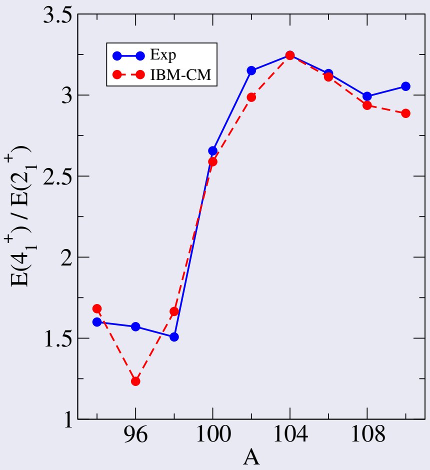
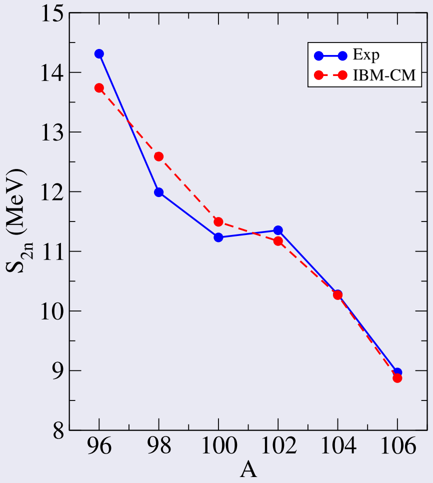
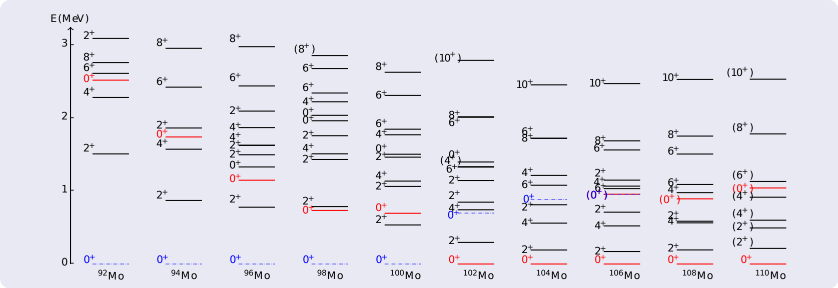
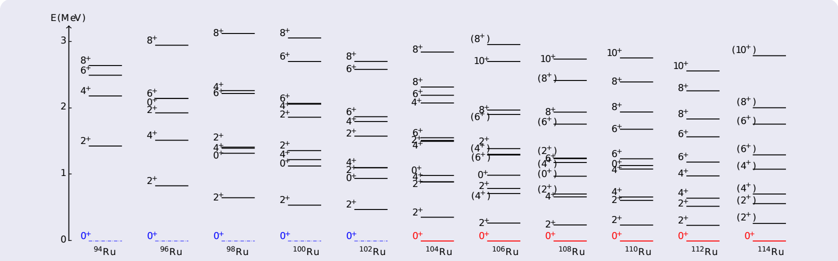



## Two-neutron separation energy (Zr case)



# Energy systematics of Mo and Ru isotopes

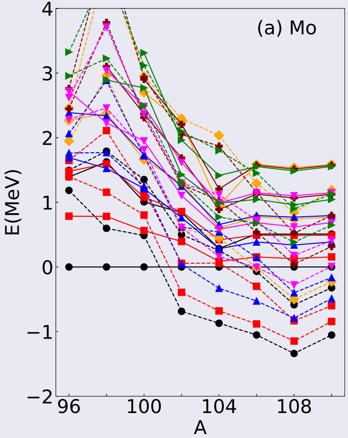



Blue labels for spherical states while red labels for deformed ones.

# Crossing or not

## Mo




Intruder states present a *parabolic* behaviour while regular ones *flat*. E. Maya-Barbecho, S. Baid, J.M. Arias, and JEGR, PRC **108**, 034316 (2023).

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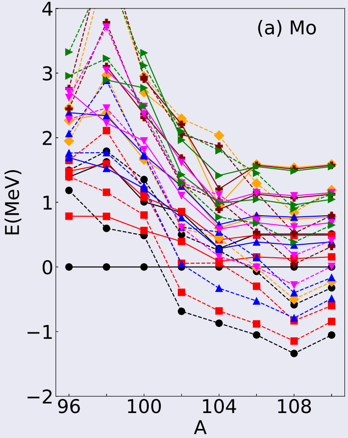
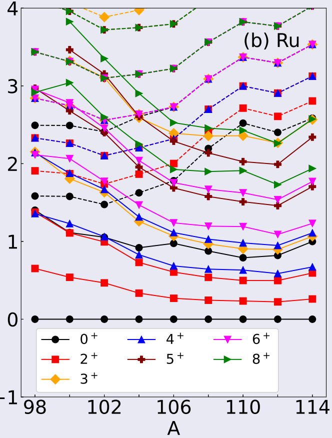



Intruder states present a *parabolic* behaviour while regular ones *flat*. E. Maya-Barbecho, S. Baid, J.M. Arias, and JEGR, PRC **108**, 034316 (2023).

## Ru




Intruder states present a *parabolic* behaviour while regular ones *flat*. E. Maya-Barbecho, S. Baid, J.M. Arias, and JEGR, PRC **108**, 034316 (2023).

# Radii and $S_{2n}$

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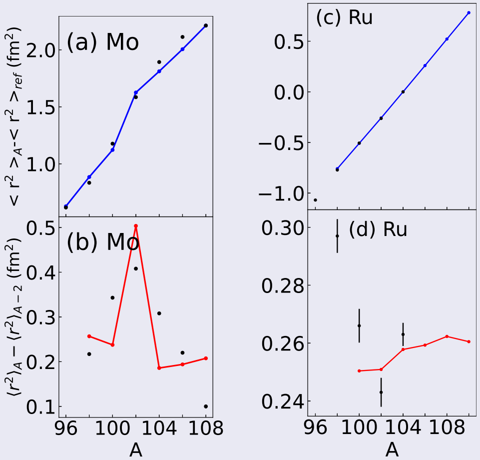
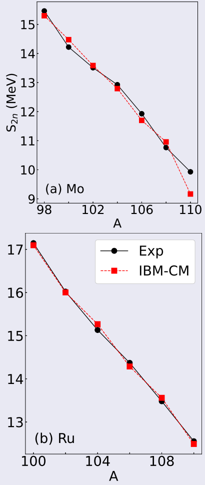
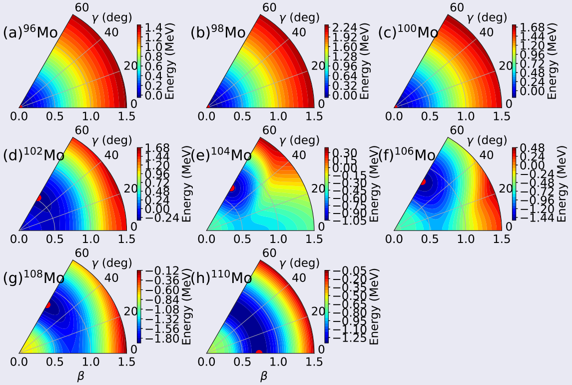



## $S_{2n}$



# Mean-field energy surfaces

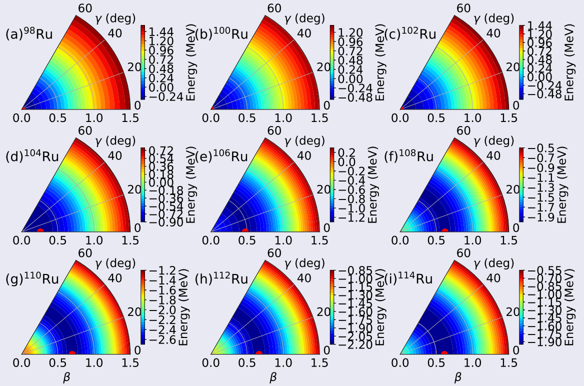
## Mo isotopes




Mean field energy surface shows up a rapid evolution from a spherical to a well deformed shape. $^{102-104}$Mo shows the coexistence of two minima.

# Mean-field energy surfaces

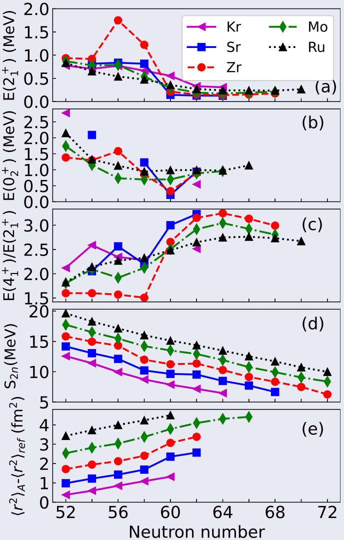
## Ru isotopes




Mean field energy surface shows up a slow evolution from a spherical to a well deformed shape. $^{104}$Ru shows a rather flat minimum.

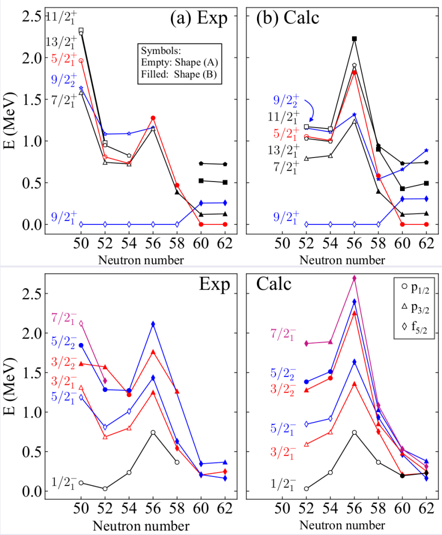
# Global view

## Relevant systematics




The different systematics points toward a QPT/Shape coexistence area in Sr, Zr, and Mo, being Kr and Ru at the border of this area.

# Nb energy systematics and IBFM-CM results




N. Gavrielov, Phys. Rev. C 108, 014320 (2023); N. Gavrielov, A. Leviatan, and F. Iachello, Phys. Rev. C 106, L051304 (2022) introduced the IBFM with configuration mixing (IBFM-CM) in two seminal works.

$g_{9/2}$ for positive parity and $p_{1/2}$, $p_{3/2}$, and $f_{5/2}$ for negative parity.

# The IBFM-CM intrinsic state: the shape of odd-even nuclei

## The extension of the IBM-CM intrinsic state

$$H_{CM}^{IBM} = \begin{pmatrix} E^B(N,\beta,\gamma) & \Omega^B(\beta) \\ \Omega^B(\beta) & E^B(N+2,\beta,\gamma) \end{pmatrix} \rightarrow$$

Energy surface and equilibrium value of deformation parameters

A. Frank, O. Castaños, P. Van Isacker, and E. Padilla, AIP Conf. Proc. 638, 23 (2002); A. Frank, P. Van Isacker, and F. Iachello, PRC **73**, 061302(R) (2006).

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## The IBFM-CM formalism for multiple $j$'s (preliminary)

$$H_{CM}^{IBFM} = \begin{pmatrix} \left[E^{IBFM}(N,\beta,\gamma)\right] & [\Omega(\beta)] \\ [\Omega(\beta)] & \left[E^{IBFM}(N+2,\beta,\gamma)\right] \end{pmatrix}$$

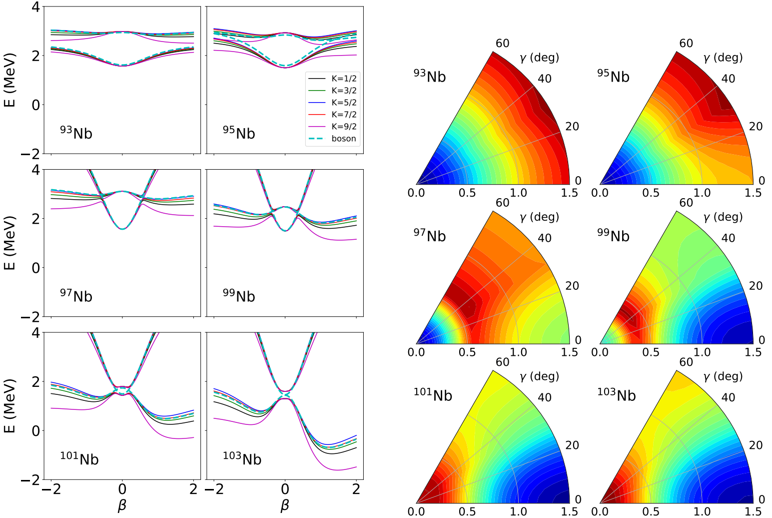
$$E^{IBFM}(N,\beta,\gamma)_{jmj'm'} = \delta_{jj'}\delta_{mm'}(E^B(N,\beta,\gamma)+\epsilon_j) + V^{BF}(N,\beta,\gamma)_{jmj'm'}$$

$$\Omega(\beta)_{jmj'm'} = \delta_{jj'}\delta_{mm'}\Omega^B(\beta)$$

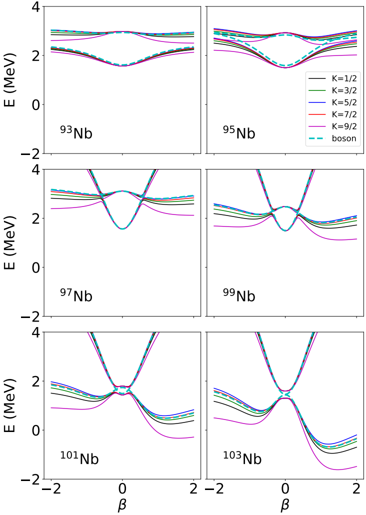
$\sum_i(2j_i+1)$ energy surfaces and corresponding equilibrium parameters

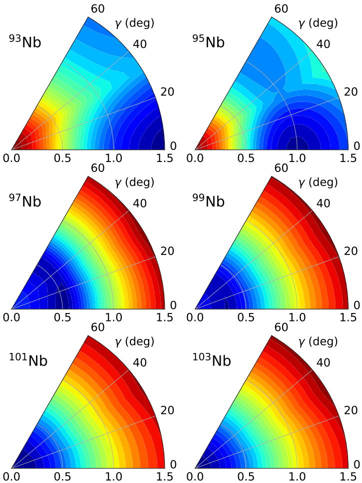
(A. Leviatan, PLB **209**, 415 (1988); C.E. Alonso, J.M. Arias, F. Iachello, and A. Vitturi, NPA **539**, 59 (1992).)

# Nb positive parity: ground state energy surface (preliminary)

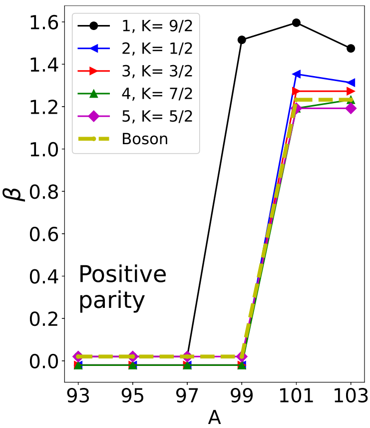


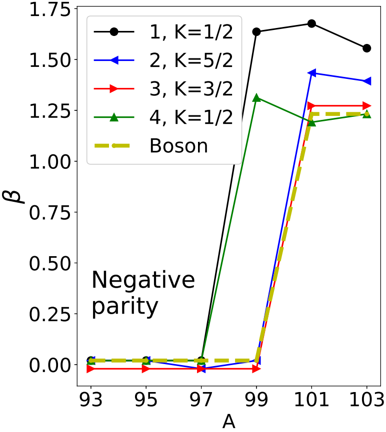
# Nb positive parity: first intruder energy surface (preliminary)



# Quantum Phase Transitions in Nb: the onset of deformation (preliminary)

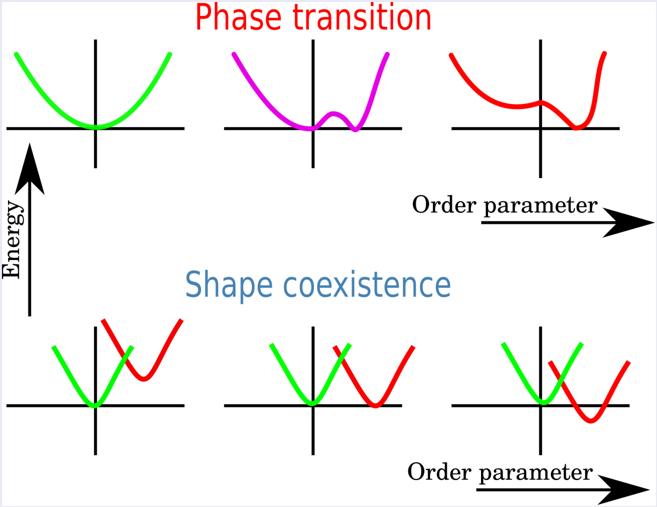


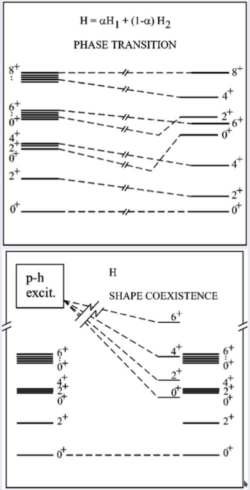

(Studied in the case of a single configuration in D. Petrellis, A. Leviatan b, F. Iachello, PLB **705**, 379 (2011); Ann. Phys. **326**, 926 (2011).)

# Schematic view

## Two minima




## PRC 69, 054304 (2004)



# Conclusions or rather open questions

- Lead region clearly shows up the onset of shape coexistence. Large mixing and relative energies hinder the onset of a Quantum Phase Transition.
- Rare-earth region is the most clear cut example of *critical region*, but without clear influence of shape coexistence, although the SU3-proxy symmetry supports the presence of neutron particle-hole excitations (Bonatsos et al).
- Are both descriptions compatible? The answer is in Zr region: type I and type II QPT introduced by Gavrielov, Leviatan and Iachello
- Can a Quantum Phase Transition be described in terms of the onset of intruder configurations?
- How things change in odd-even nuclei?
- Is shape coexistence always present *before* a Quantum Phase Transition sets in, or are they fully disconnected?

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# Thanks for your attention

Also to my collaborators:
Kris Heyde (U. Gent),
Esperanza Maya-Barbacho and Pablo Martín-Higueras (U. Huelva),
Samira Baid and Pepe Arias (U. Sevilla)

Supported by MCIN/AEI/10.13039/501100011033, project number PID2022-136228NB-C21