

On **shape coexistence** and **quantum phase transitions:** Lead and Zirconium regions

J.E. García-Ramos and **K. Heyde**

Departamento de Ciencias Integradas y
Centro de Estudios Avanzados en Física, Matemáticas y Computación,
Universidad de Huelva, Spain
Department of Physics and Astronomy, University of Ghent, Belgium



FÍSICA
MATEMÁTICAS
COMPUTACIÓN



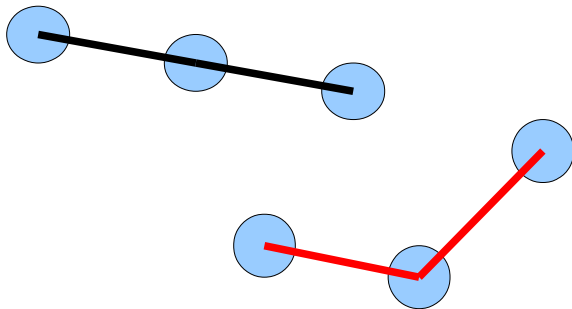
Universidad
de Huelva

What is shape coexistence?

It appears in quantum systems where eigenstates with very different density distribution coexist.

Therefore, the existence of a geometric interpretation is implicit .

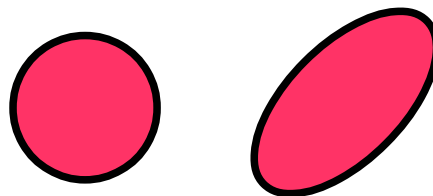
Molecules



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

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

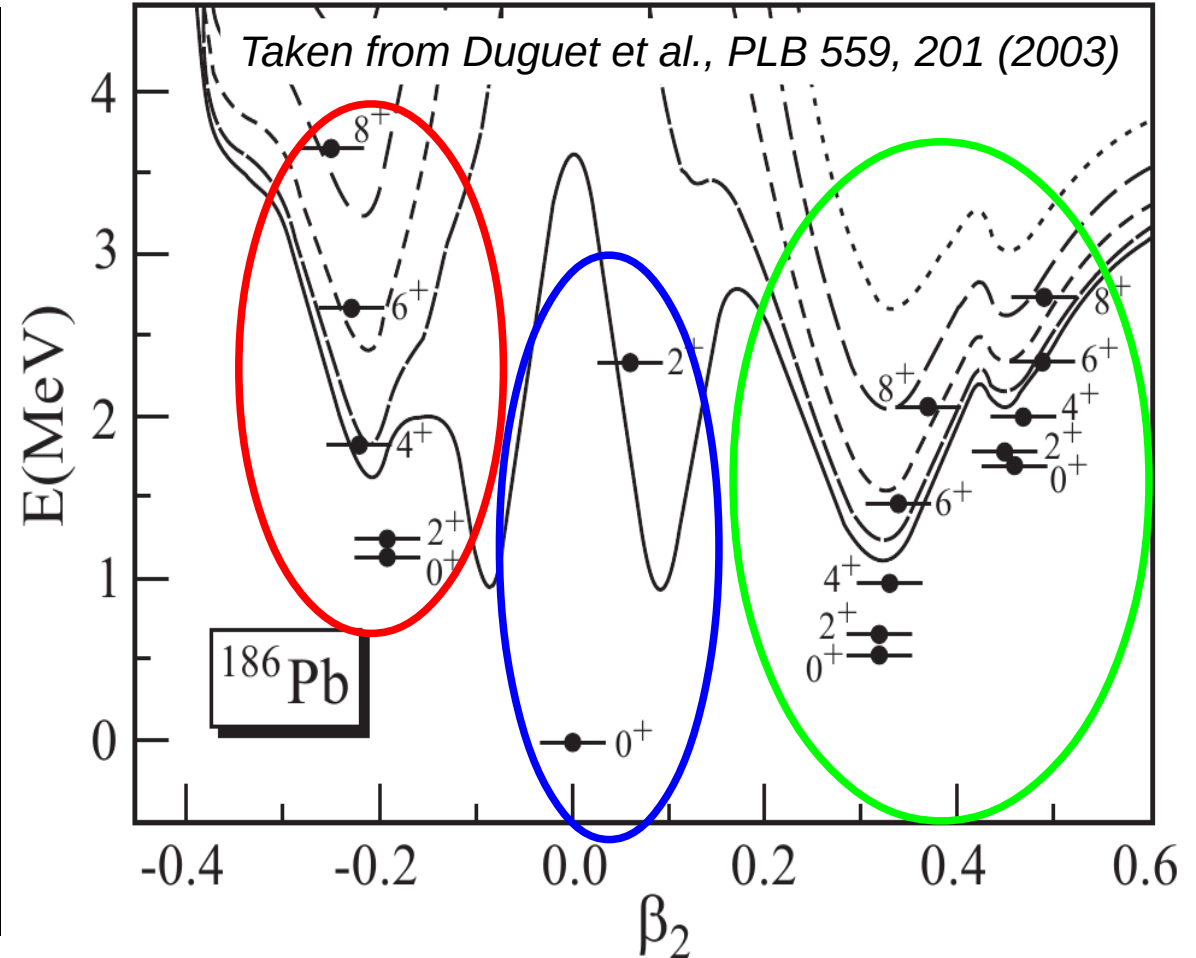
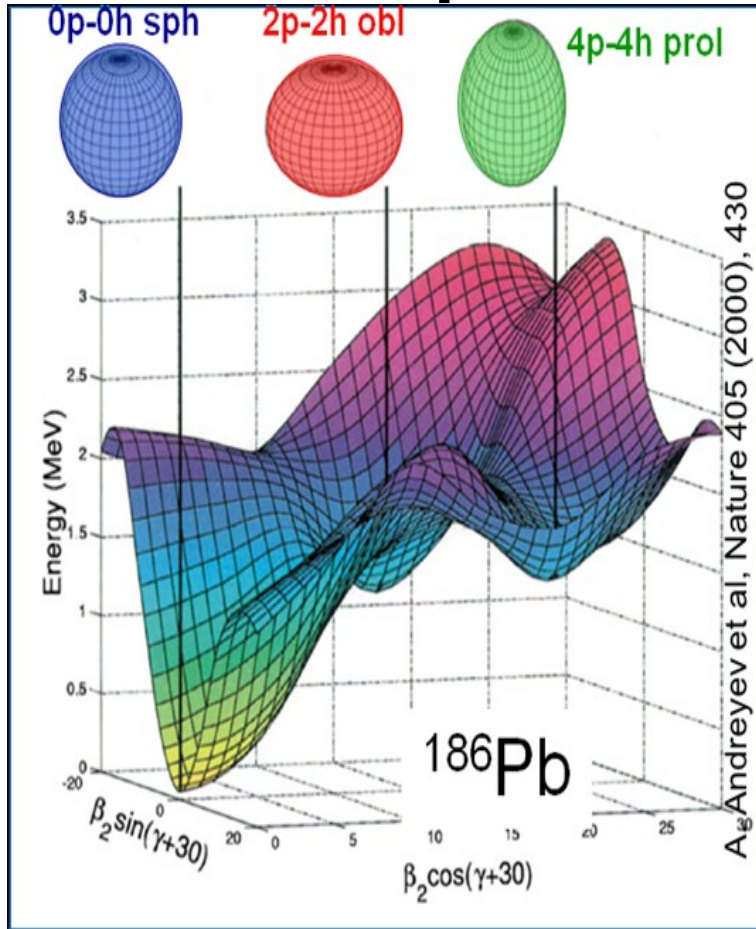
Nuclei



$$q_2 = q^2,$$

$$q_3 = q^3 \cos 3\delta,$$

Shape coexistence example

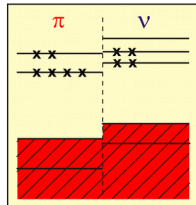


The angular momentum projected mean field plus the Generator Coordinate Method generates different bands with very different deformation.

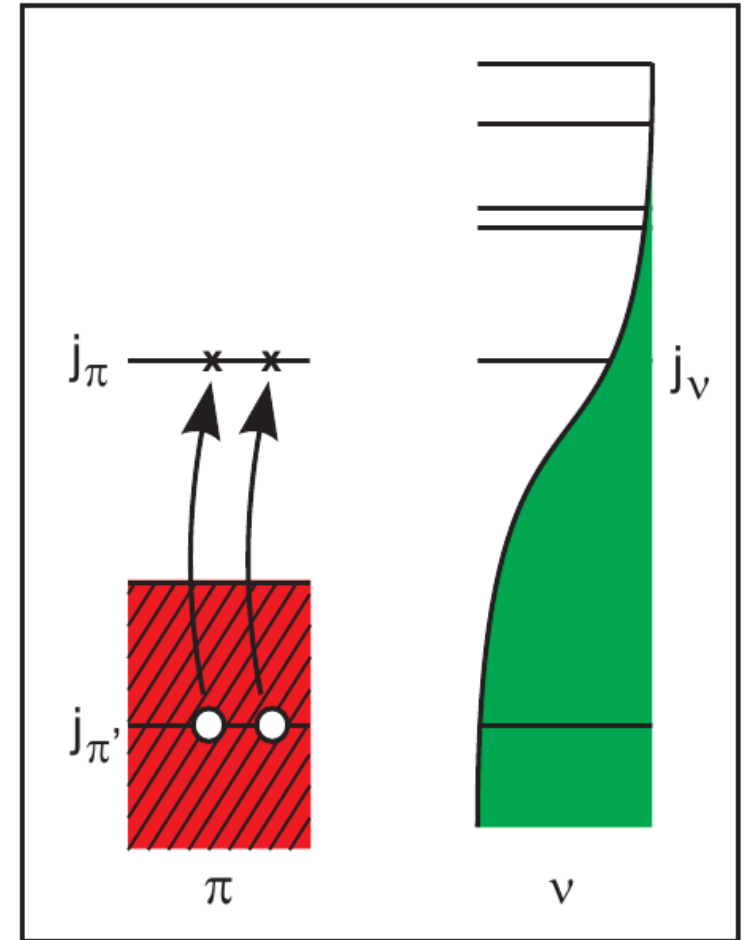
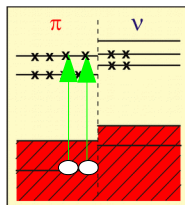
Shell Model/Interacting Boson Model

- 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 quadrupole correlations.
- Restricted to light and medium-heavy nuclei, at present.

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



$$+ b(J, M)$$

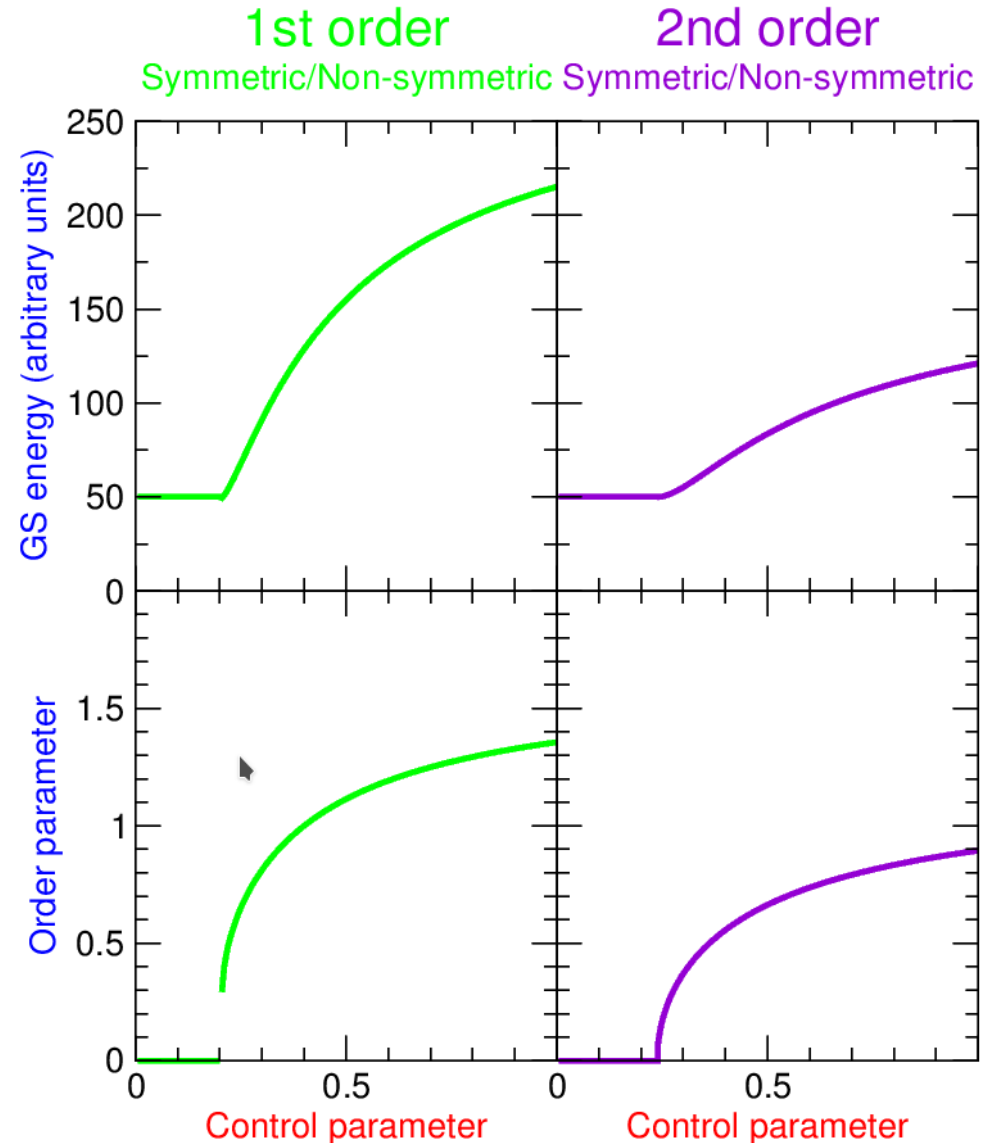


In heavy nuclei the huge model space imposes some kind of truncation: symmetry dictated truncation (IBM).

What is a Quantum Phase Transition?

A QPT appears when 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**. These transitions are assumed to occur at zero temperature.

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



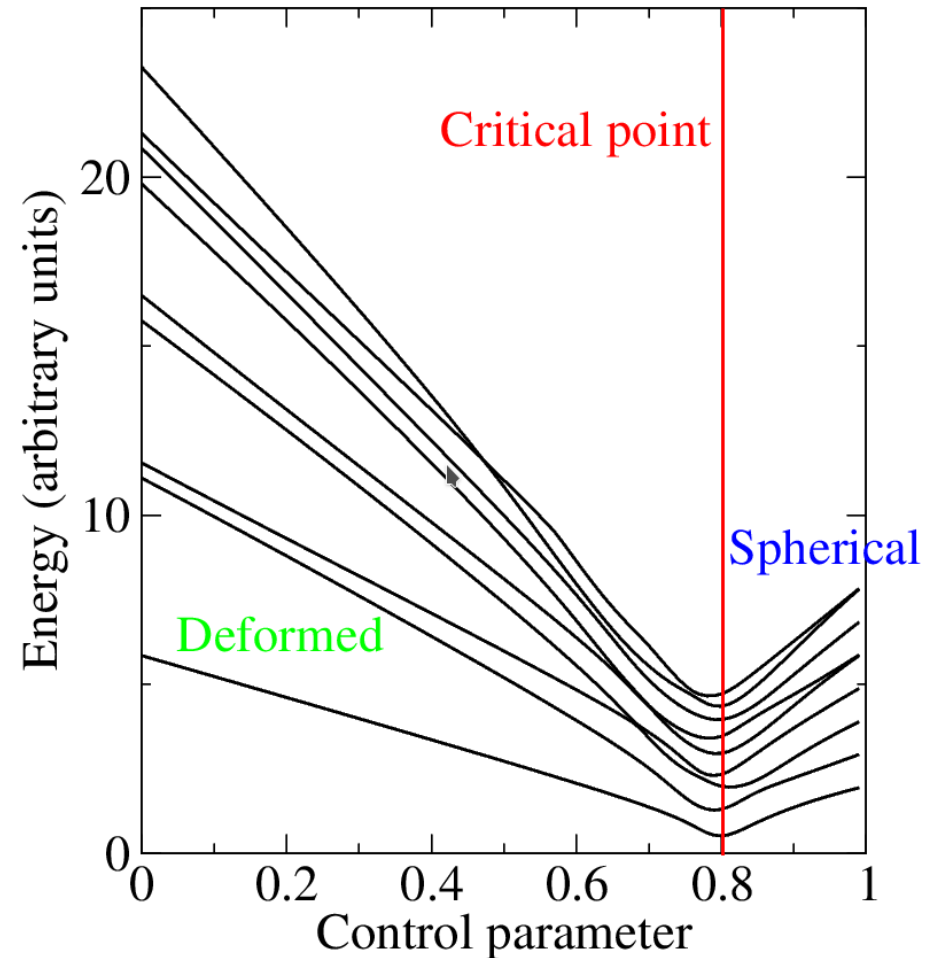
What is a Quantum Phase Transition?

At the critical point:

- The ground state energy is non-analytical.
- Energy gap between the ground and the first excited states goes to zero.

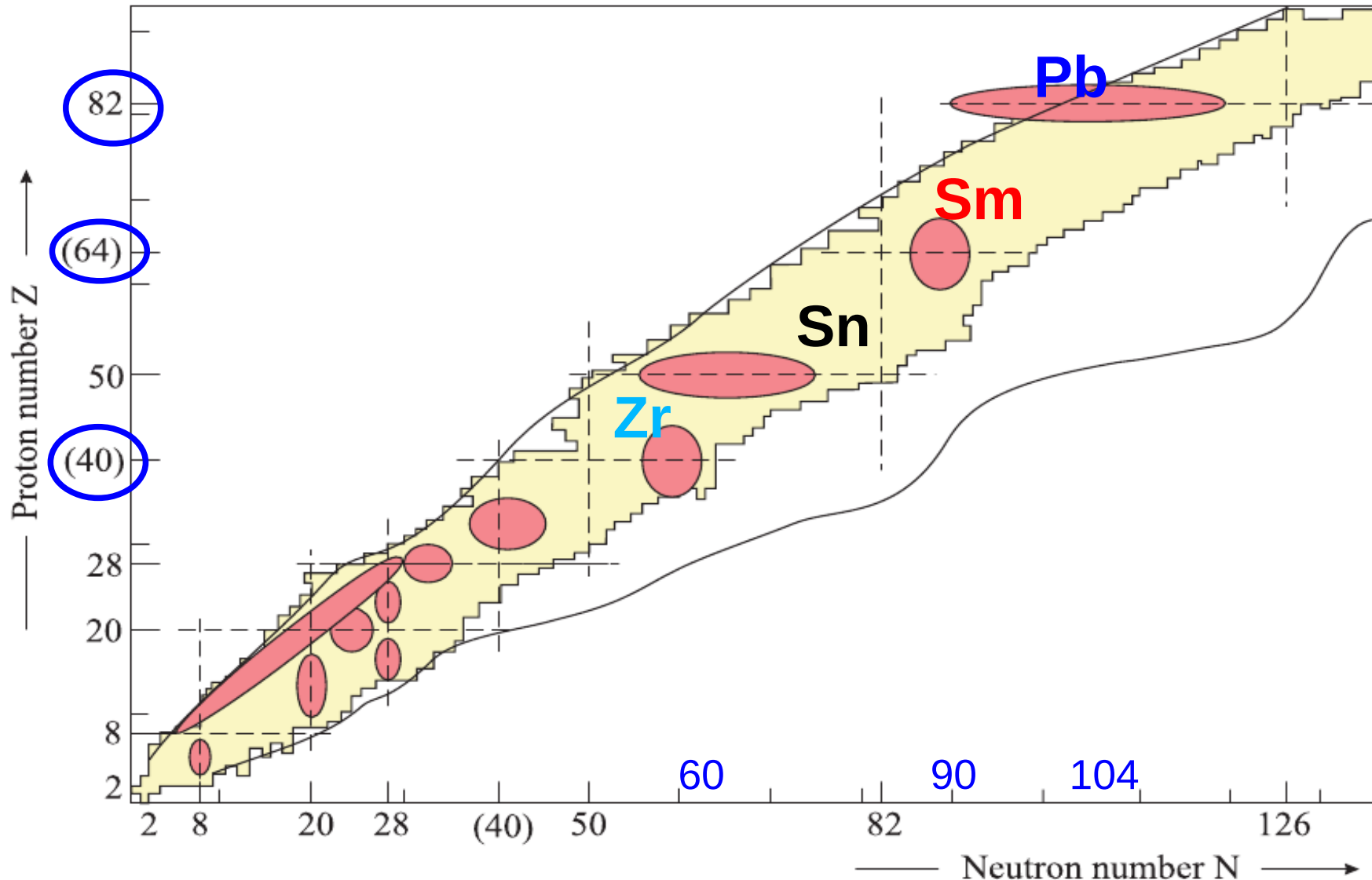
Challenges when dealing with QPTs in atomic nuclei

- It is a finite system, therefore abrupt changes, if any, are smoothed out.
- **There is not a true control parameter.**
- How can we define an order parameter?
- **How can we define the phases of the system?**
- The phase transition does not characterize a single nucleus, but it is a property of an entire region.



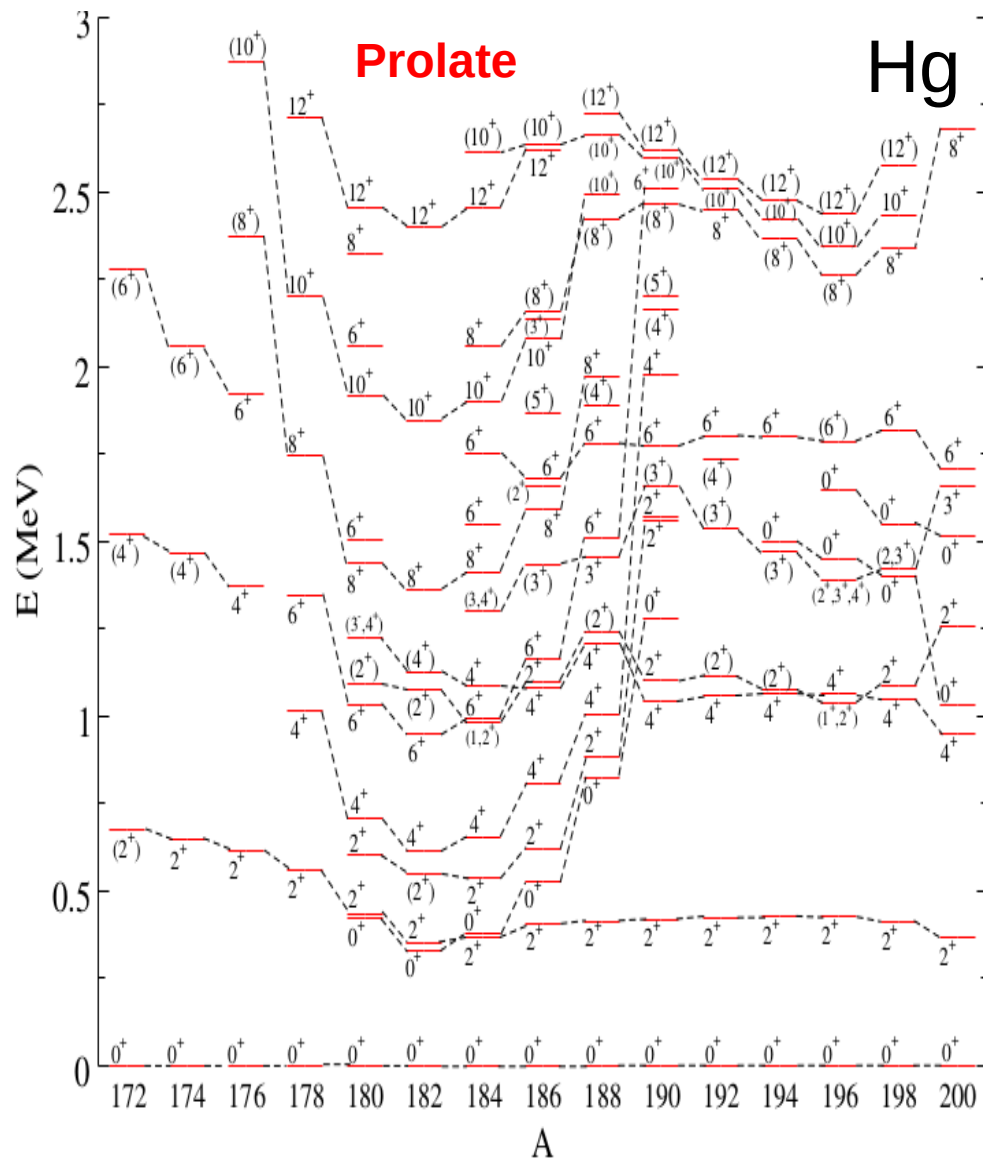
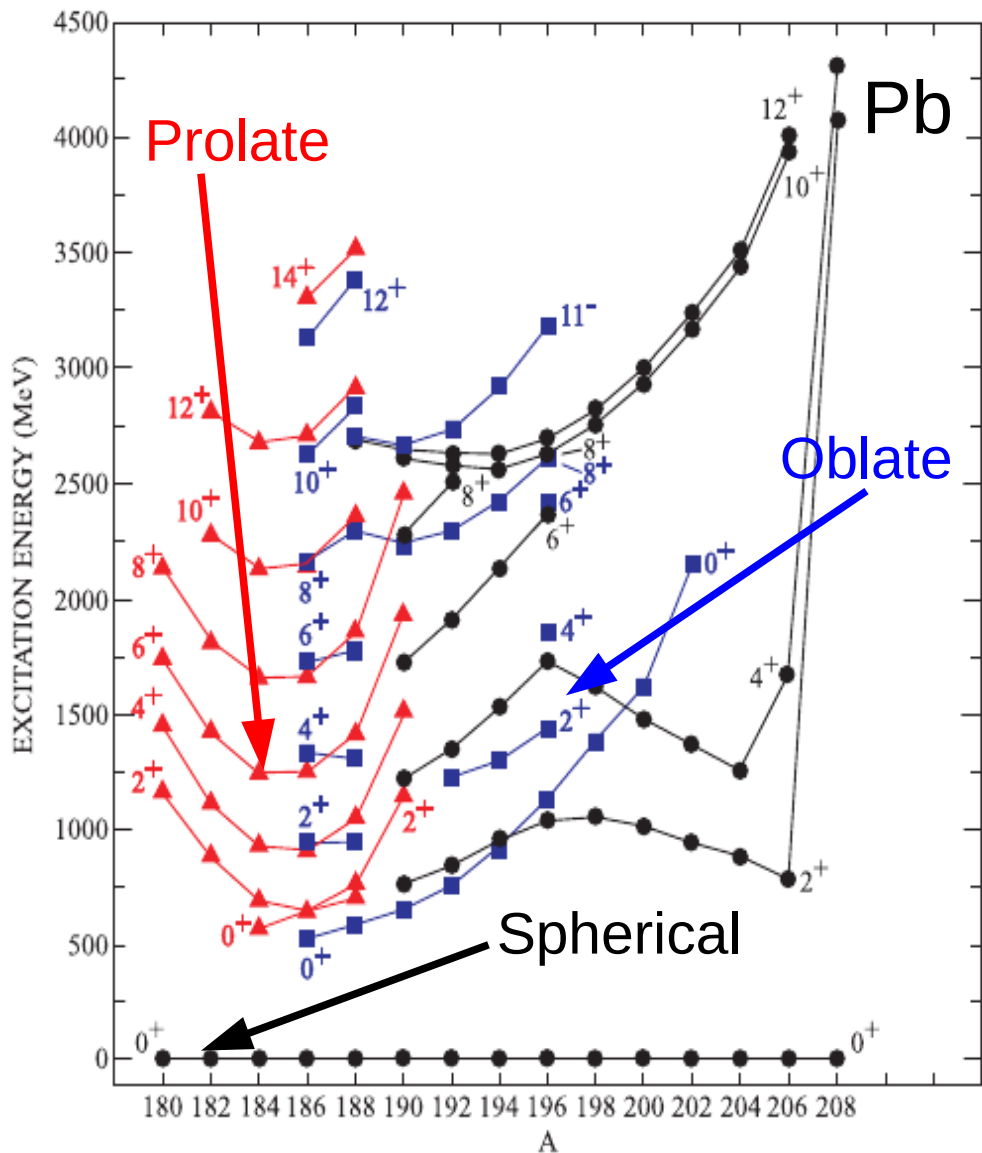
Low lying 0^+ states of an IBM calculation with $N=20$ between the $U(5)$ and $SU(3)$ limits

Many regions to be understood



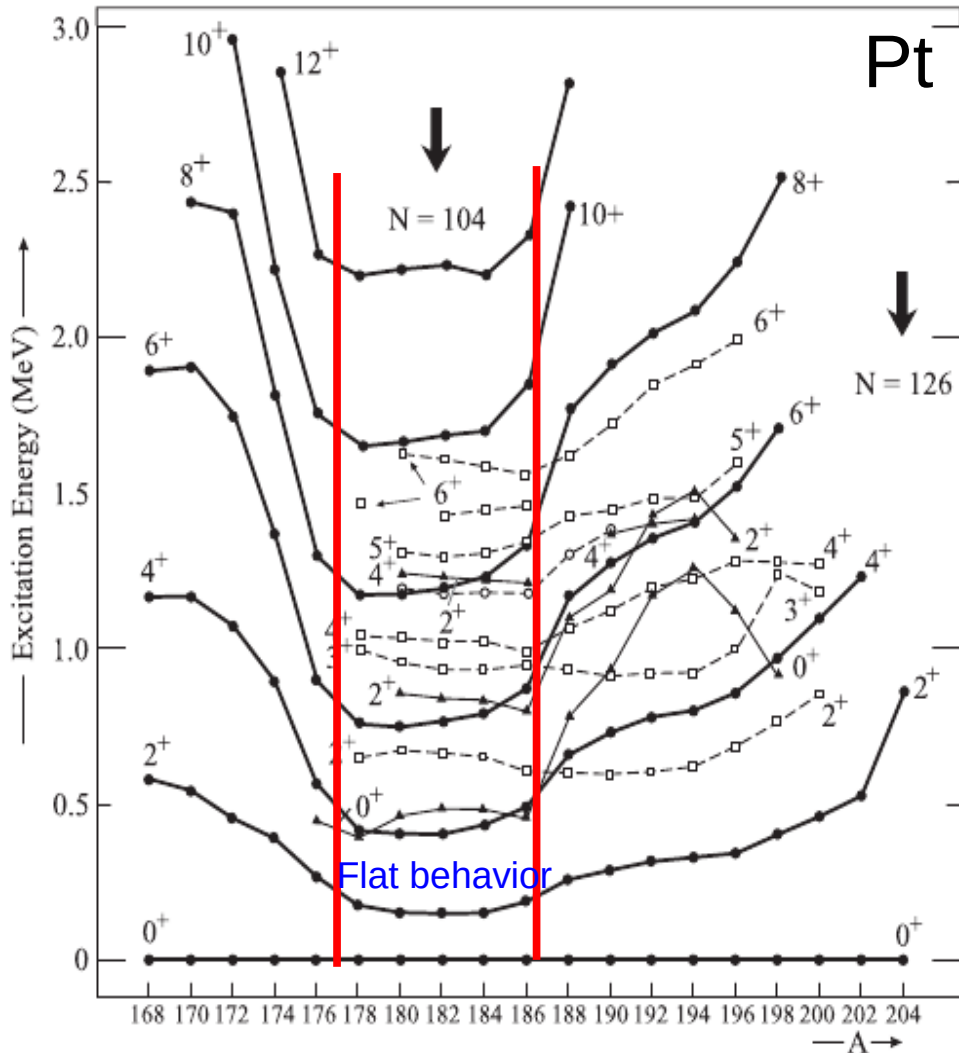
K. Heyde and J. L. Wood, Rev. Mod. Phys. 83, 1467 (2011).

Shape coexistence key indicators

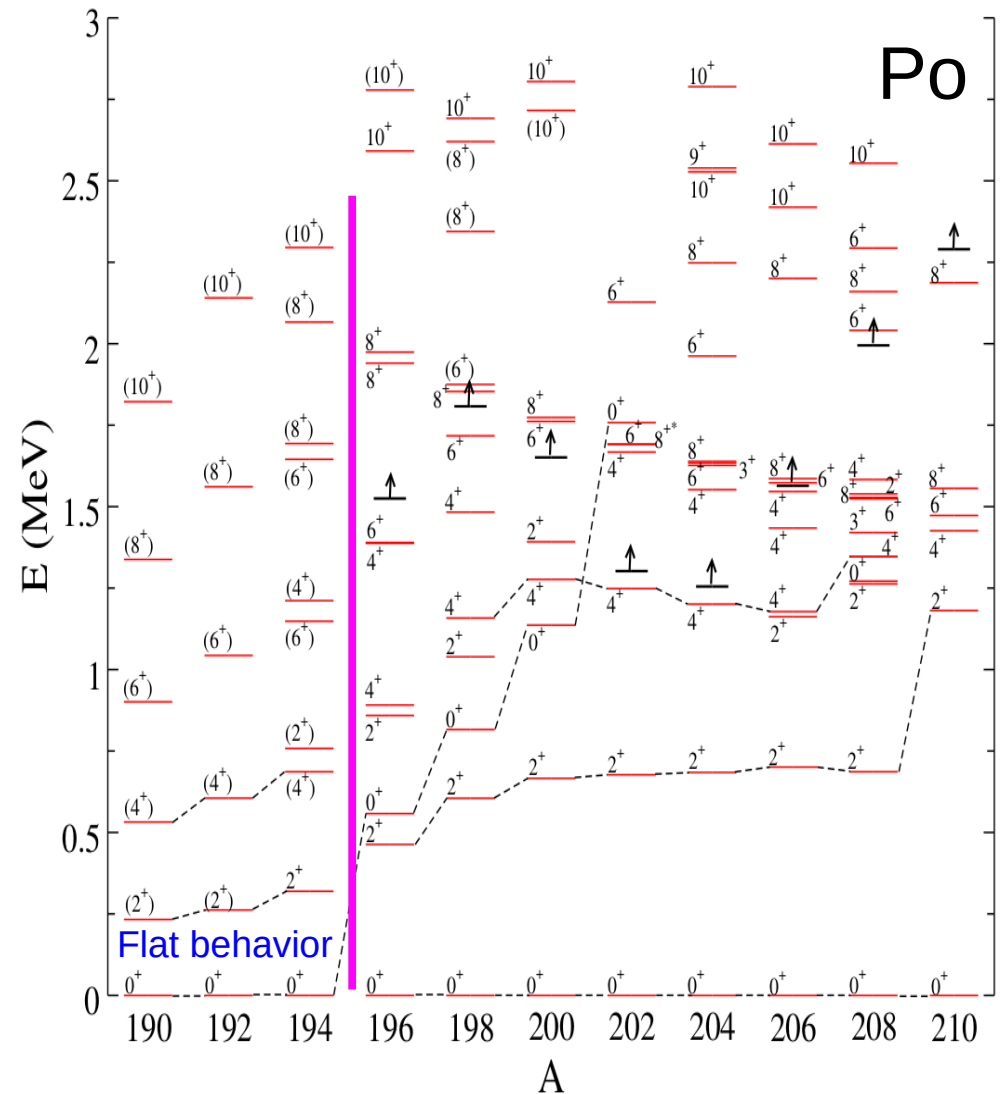


JEGR and K. Heyde, PRC 89, 014306 (2014)

Pt and Po isotopes



JEGR and K. Heyde, NPA 825, 39 (2009),
 JEGR, V. Hellemans, and K. Heyde, PRC 84, 014331 (2011).

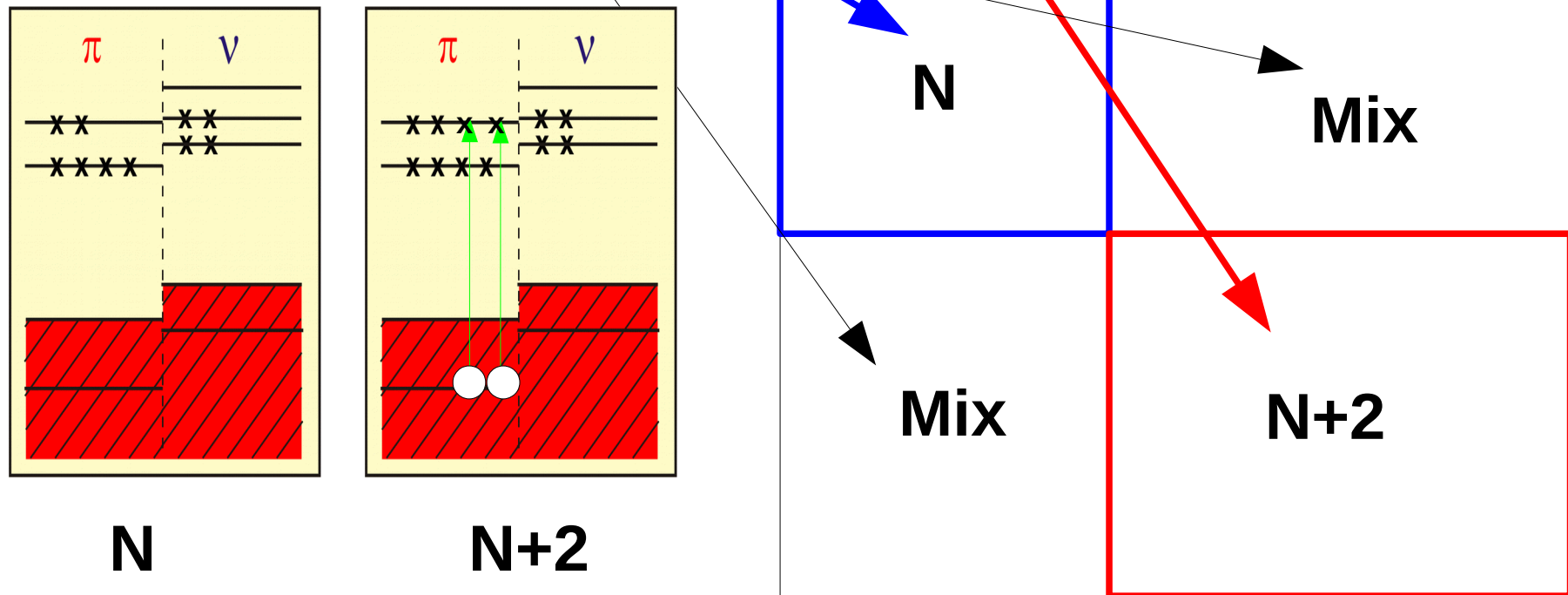


JEGR and K. Heyde, PRC 92, 034309 (2015).

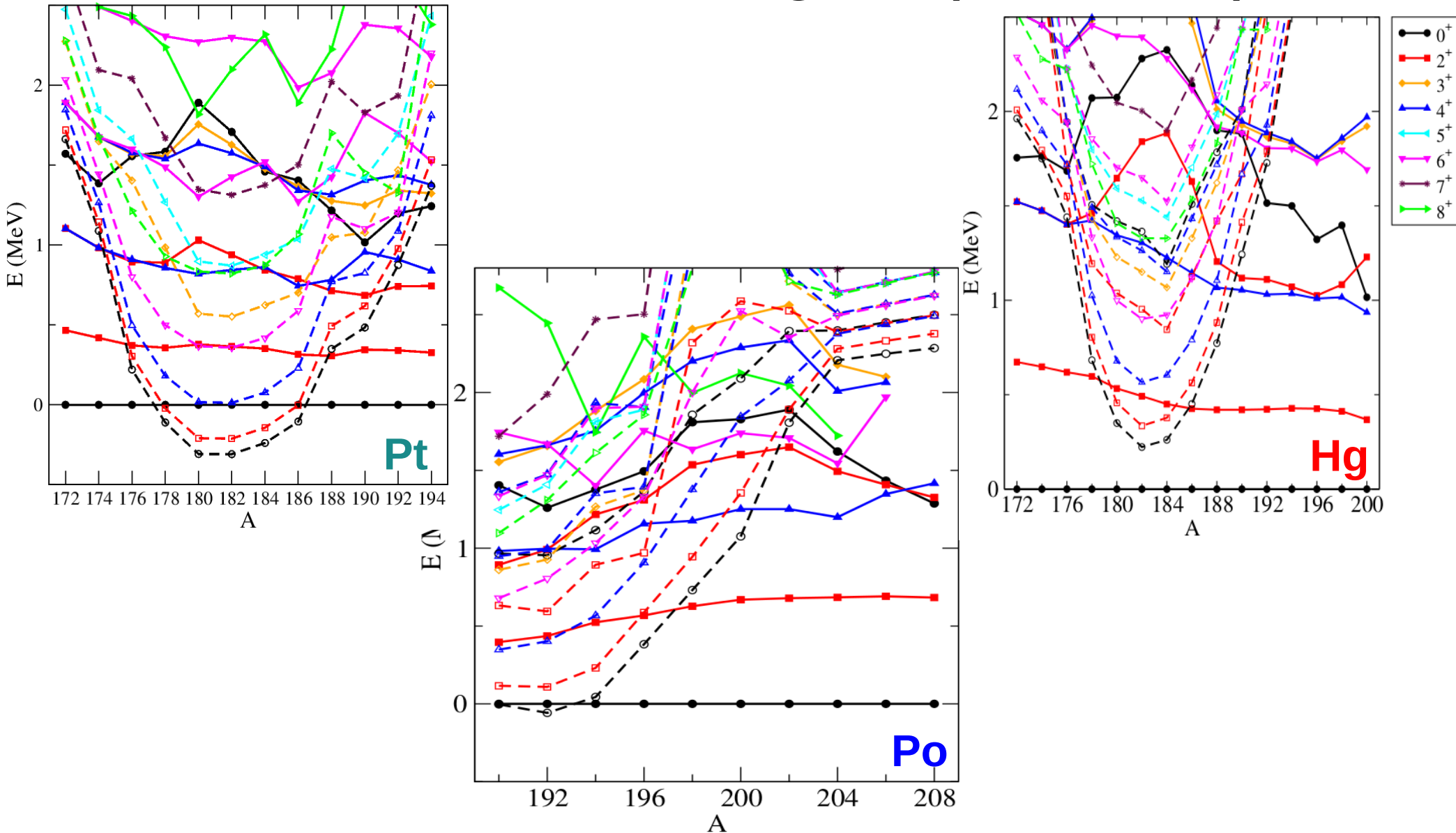
Interacting Boson Model

(configuration mixing)

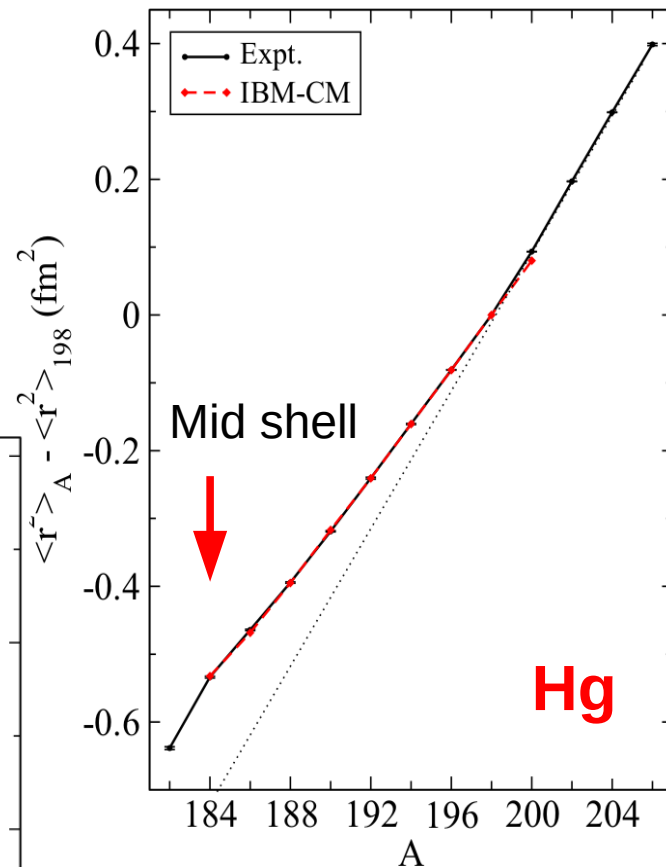
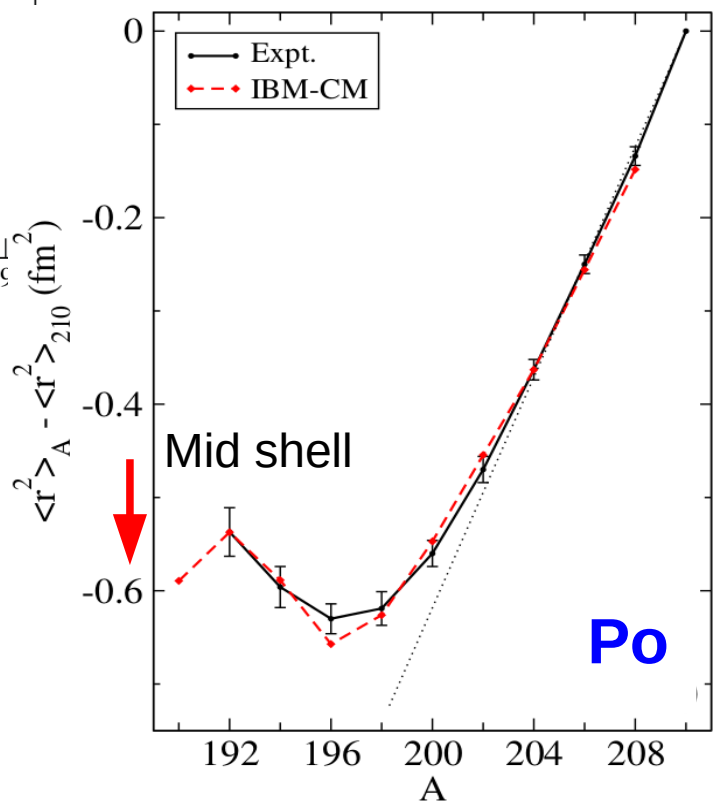
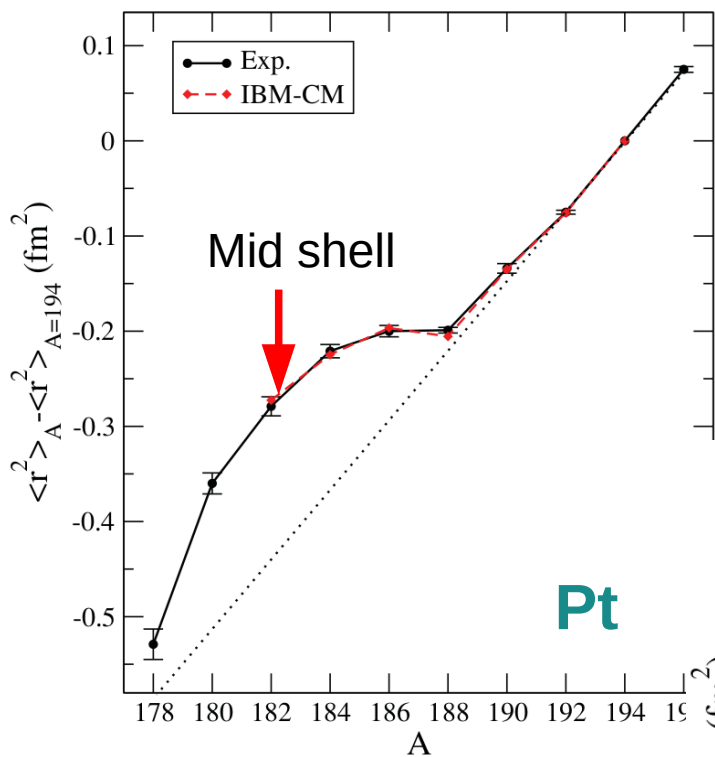
$$\hat{H} = \hat{P}_N^\dagger \hat{H}_{\text{ECQF}}^N \hat{P}_N + \hat{P}_{N+2}^\dagger (\hat{H}_{\text{ECQF}}^{N+2} + \Delta^{N+2}) \hat{P}_{N+2} + \hat{V}_{\text{mix}}^{N,N+2}$$



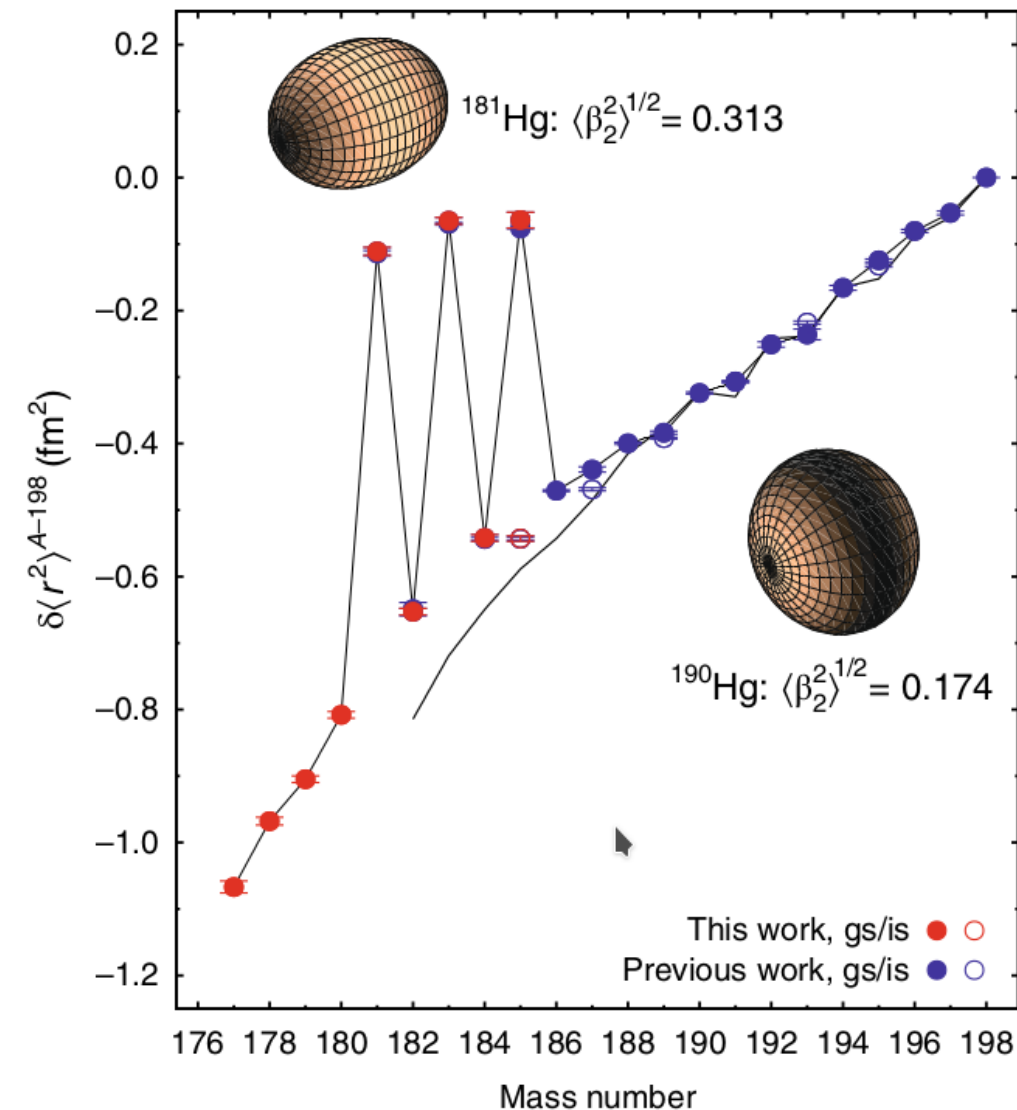
Unperturbed energies (IBM-CM)



Radii in shape coexistence regions



Radii in shape coexistence regions



nature
physics

LETTERS

<https://doi.org/10.1038/s41567-018-0292-8>

Characterization of the shape-staggering effect in mercury nuclei

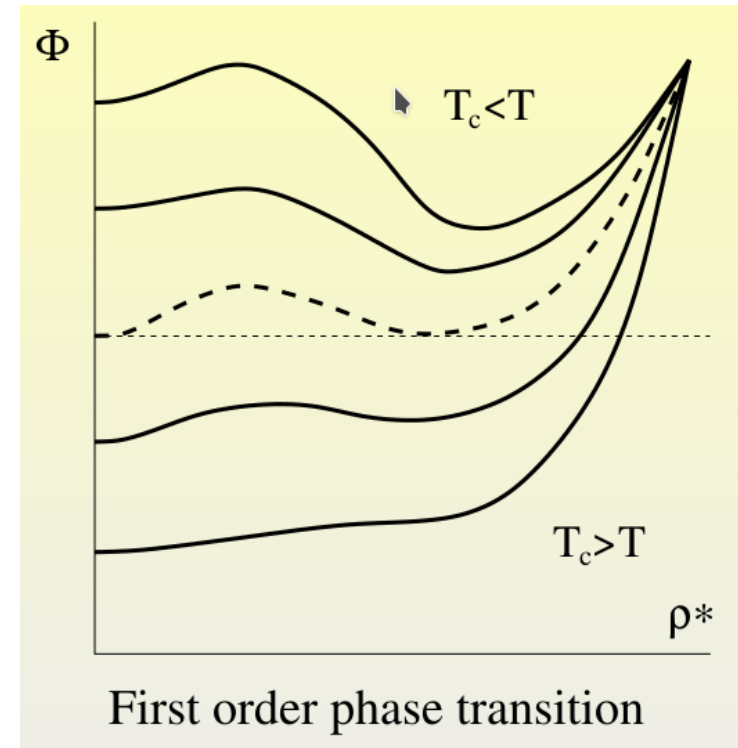
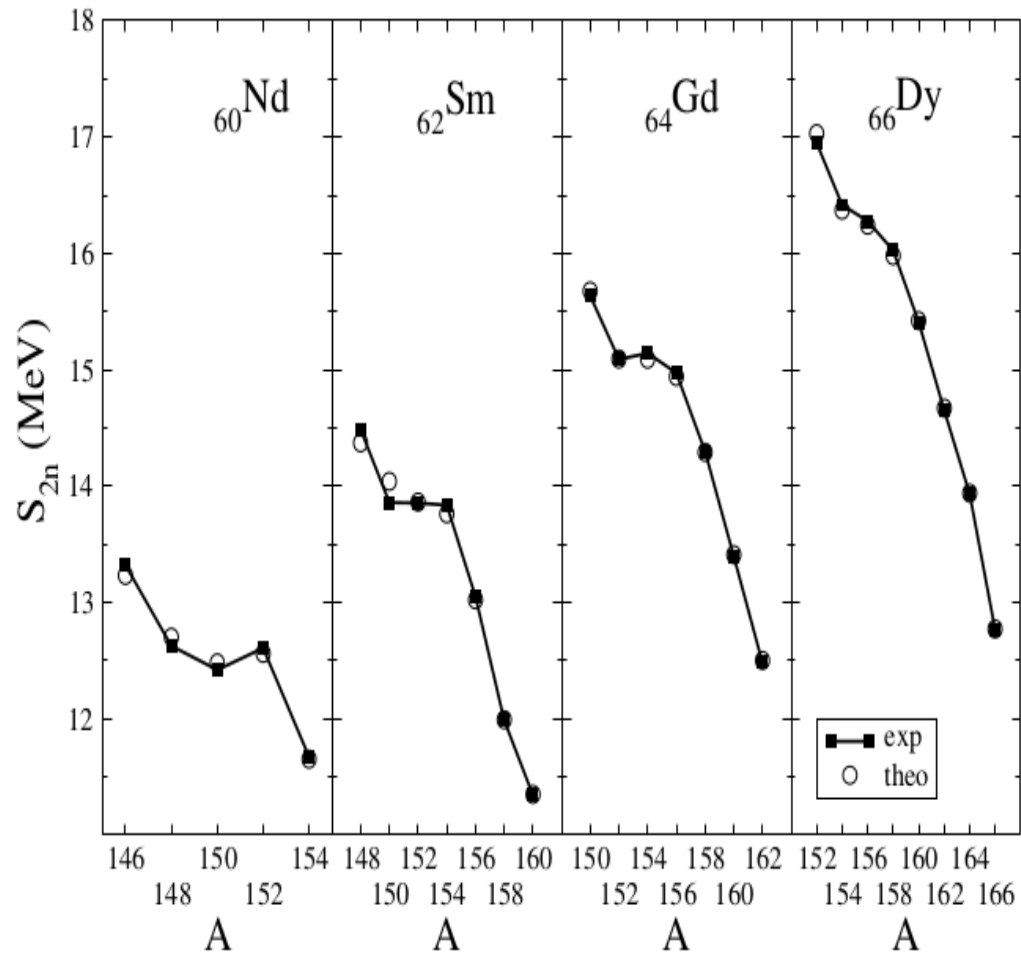
B. A. Marsh^{1*}, T. Day Goodacre^{1,2,18}, S. Sels^{3,18}, Y. Tsunoda⁴, B. Andel⁵, A. N. Andreyev^{6,7},
 N. A. Althubiti², D. Atanasov⁸, A. E. Barzakh⁹, J. Billowes², K. Blaum⁸, T. E. Cocolios^{2,3}, J. G. Cubiss⁶,
 J. Dobaczewski⁶, G. J. Farooq-Smith^{2,3}, D. V. Fedorov¹⁰, V. N. Fedosseev¹¹, K. T. Flanagan², L. P. Gaffney^{3,10},
 L. Ghys³, M. Huyse³, S. Kreim⁸, D. Lunney¹¹, K. M. Lynch¹, V. Manea³, Y. Martinez Palenzuela³, P. L. Molkanov⁹,
 T. Otsuka^{3,4,12,13,14}, A. Pastore⁶, M. Rosenbusch^{13,15}, R. E. Rossel¹, S. Rothe^{1,2}, L. Schweikhard¹⁵, M. D. Seliverstov⁹,
 P. Spagnoletti¹⁰, C. Van Beveren³, P. Van Duppen³, M. Veinhard¹, E. Verstraelen³, A. Welker¹⁶, K. Wendt¹⁷,
 F. Wienholtz¹⁵, R. N. Wolf⁸, A. Zadornaya³ and K. Zuber¹⁶

October 2018

The shape staggering effect manifests characteristic features of a quantum phase transition^{15–17}: in a given nucleus, different phases—a near spherical and a strongly deformed nuclear shape—appear at almost the same energy without mixing. By making small changes in the control parameter, which in this case is the neutron number, the system alternates between the two phases. In the case of the mer-

Clear cut example of a delicate balance between monopole, quadrupole and pairing interaction.

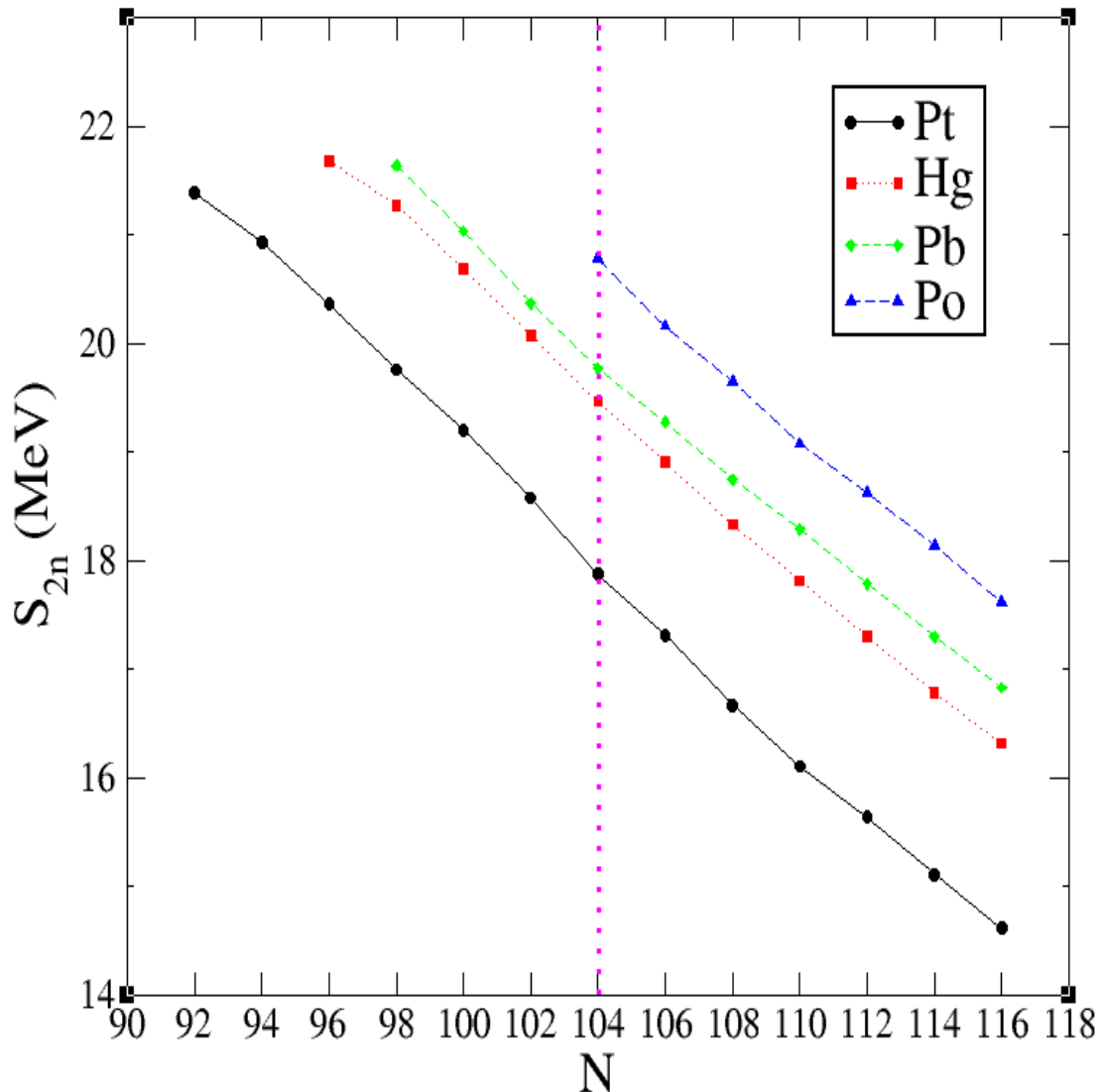
QPT key indicators: 2n separation energies



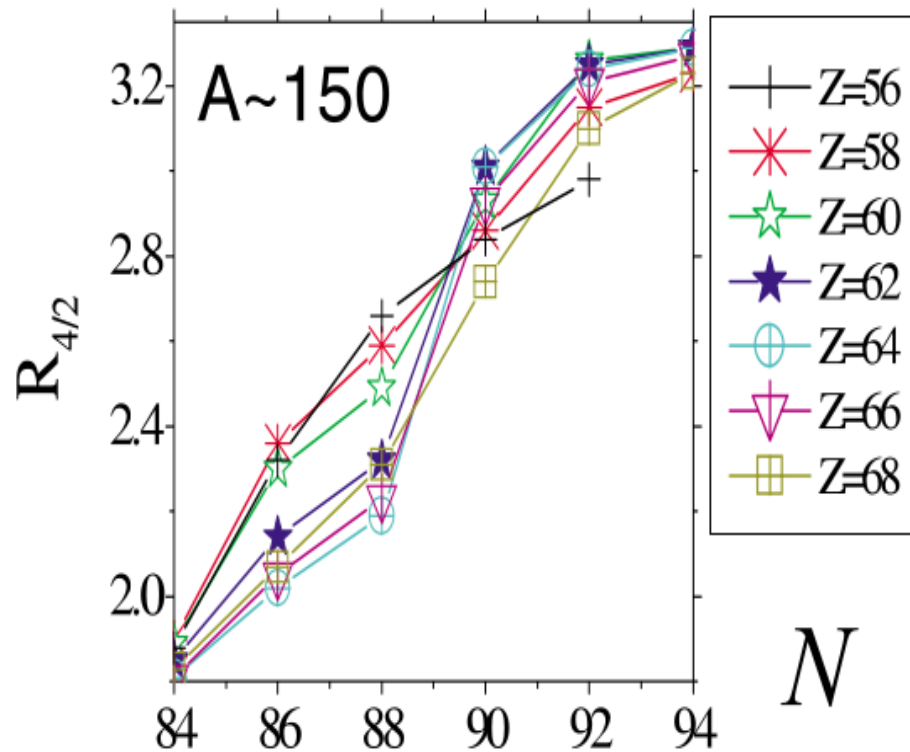
Discontinuity in the first derivative of the energy

No indication of QPT in lead region

The linear trend is observed all the way, therefore, the structure of the ground state remains stable.



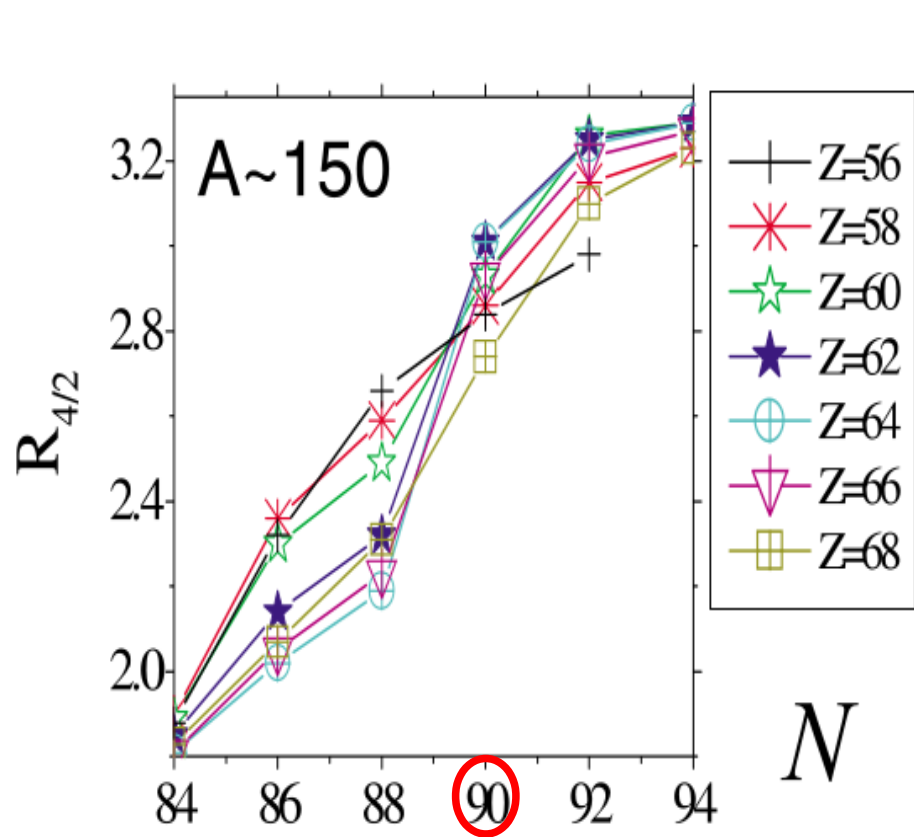
QPT key indicators: energy ratios



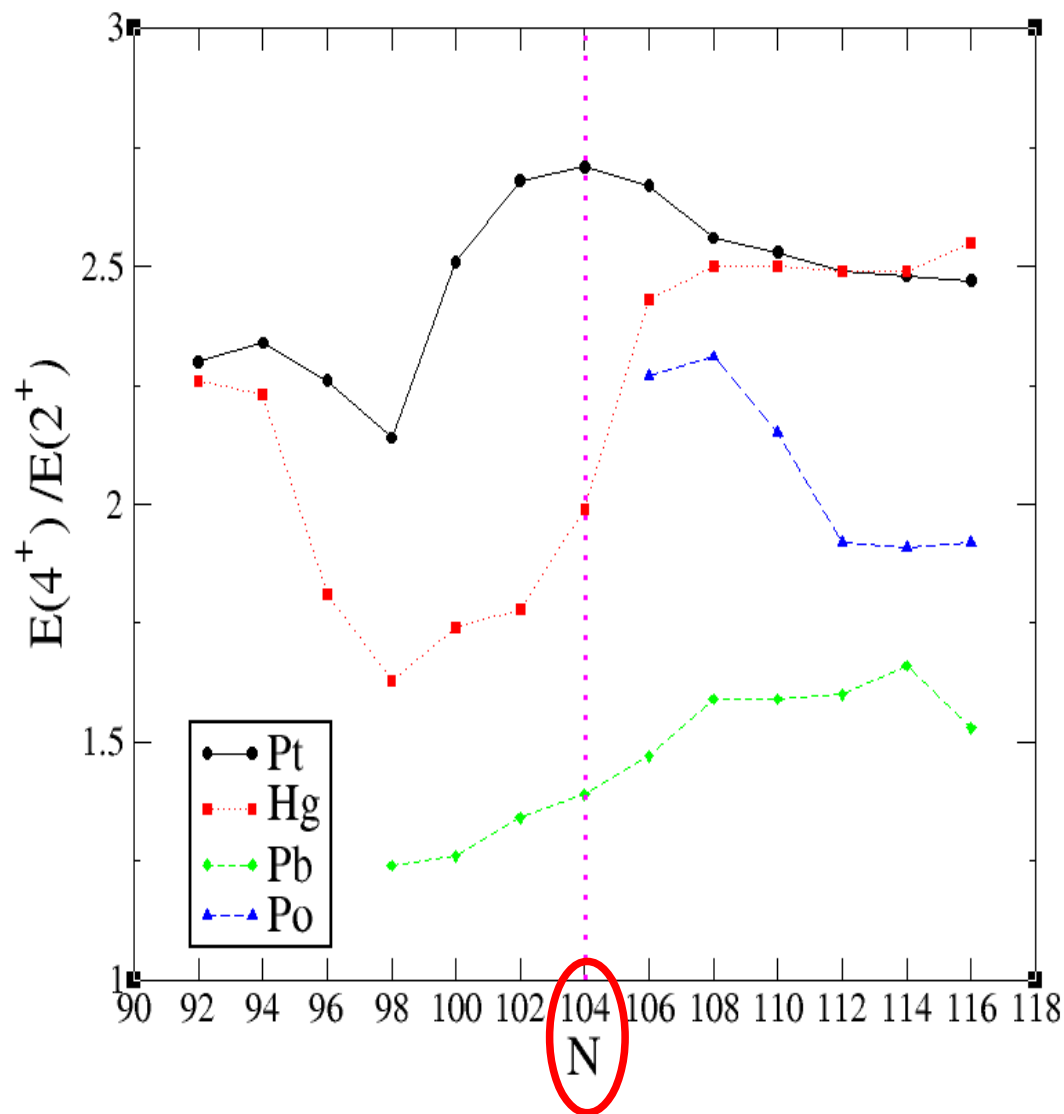
$E(4+)/E(2+)$ can be used as an order parameter and, therefore is a key observable to find where QPT develop

P. Cejnar, J. Jolie, and R.F. Casten,
RPM 82, 2155 (2010)

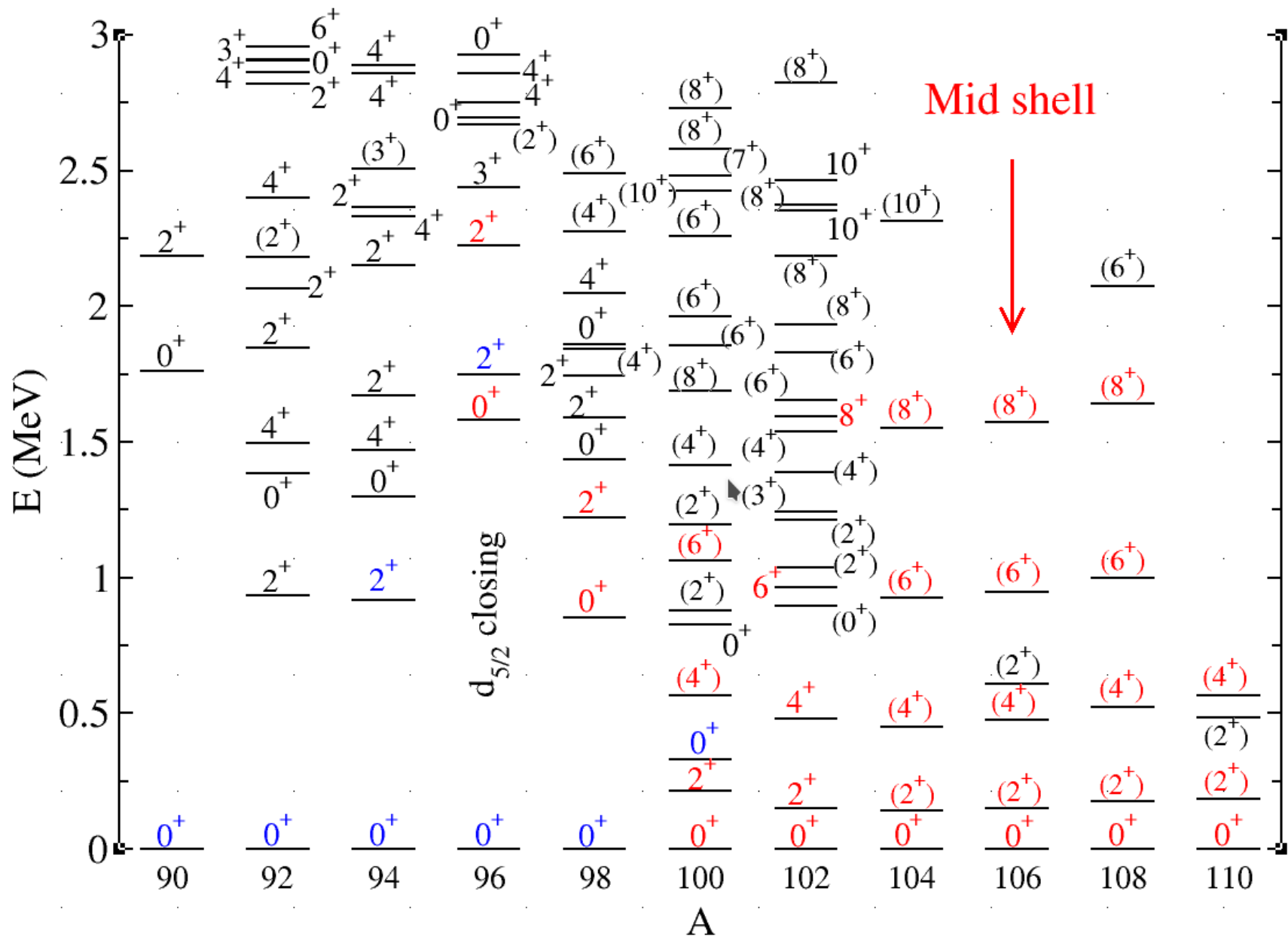
No clear indication of a QPT in lead region



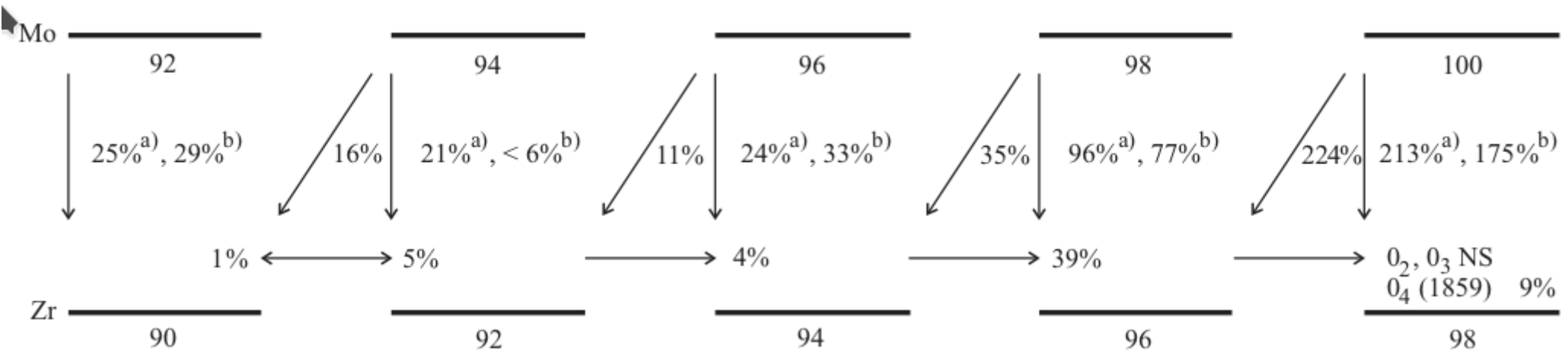
P. Cejnar, J. Jolie, and R.F. Casten, RPM 82, 2155 (2010)



⁴⁰Zr spectra



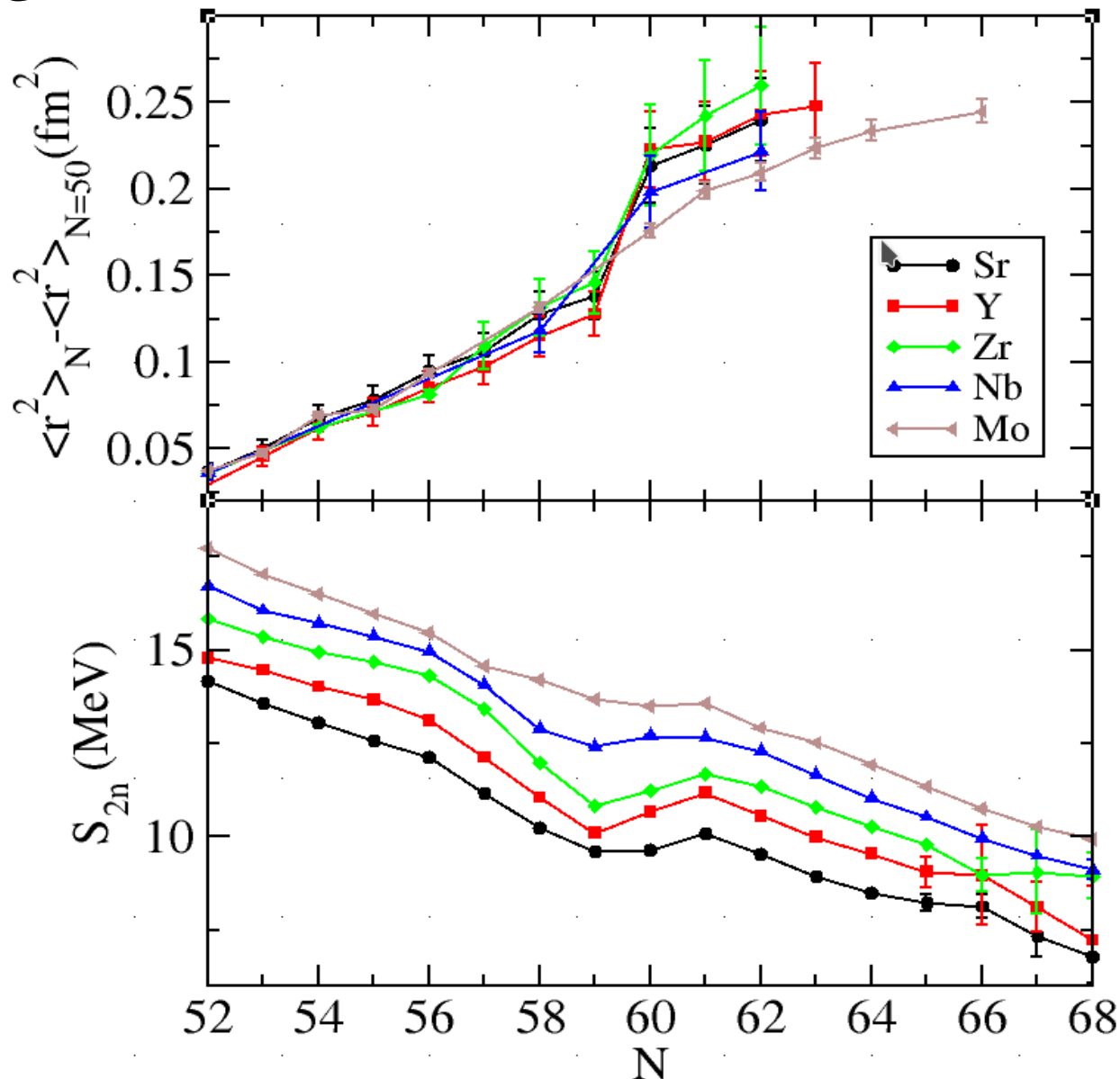
Multiparticle transfer strengths



K. Heyde and J. L. Wood, Rev. Mod. Phys. 83, 1467 (2011).

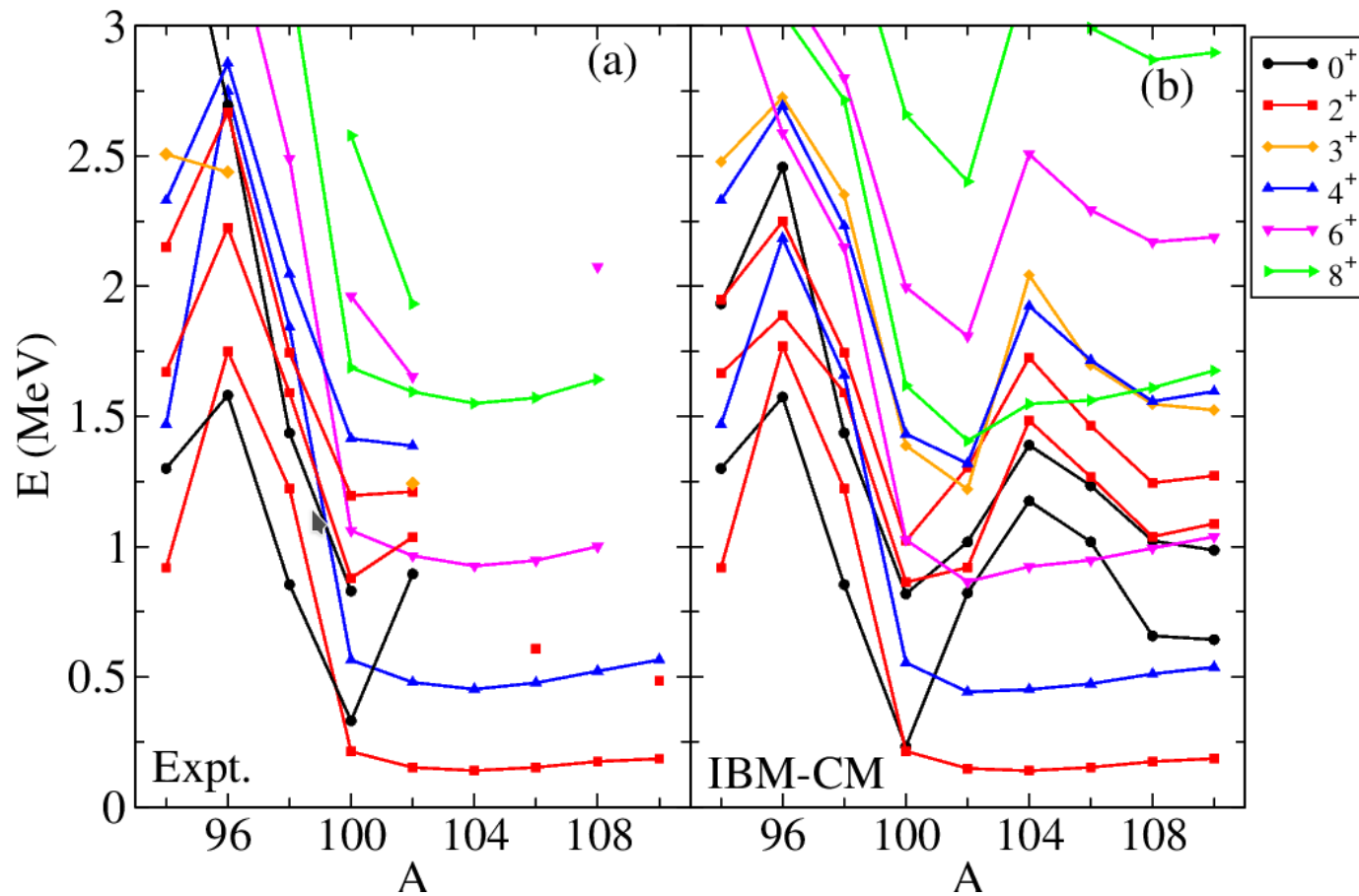
"... reveal that pairing collectivity for the 0^+ ground states and first excited states for some of these isotopes exhibits a "coexisting" character, i.e., transfer strength goes strongly to more than one "condensate"..."

Shape Coexistence or Quantum Phase Transition?

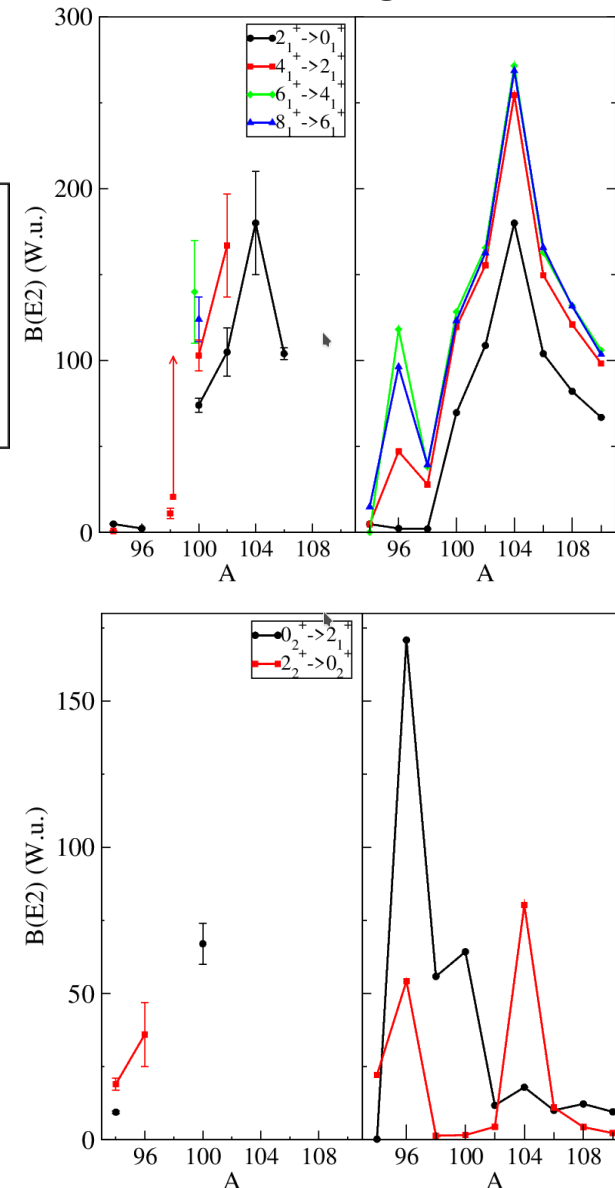


The IBM calculation

Excitation energies

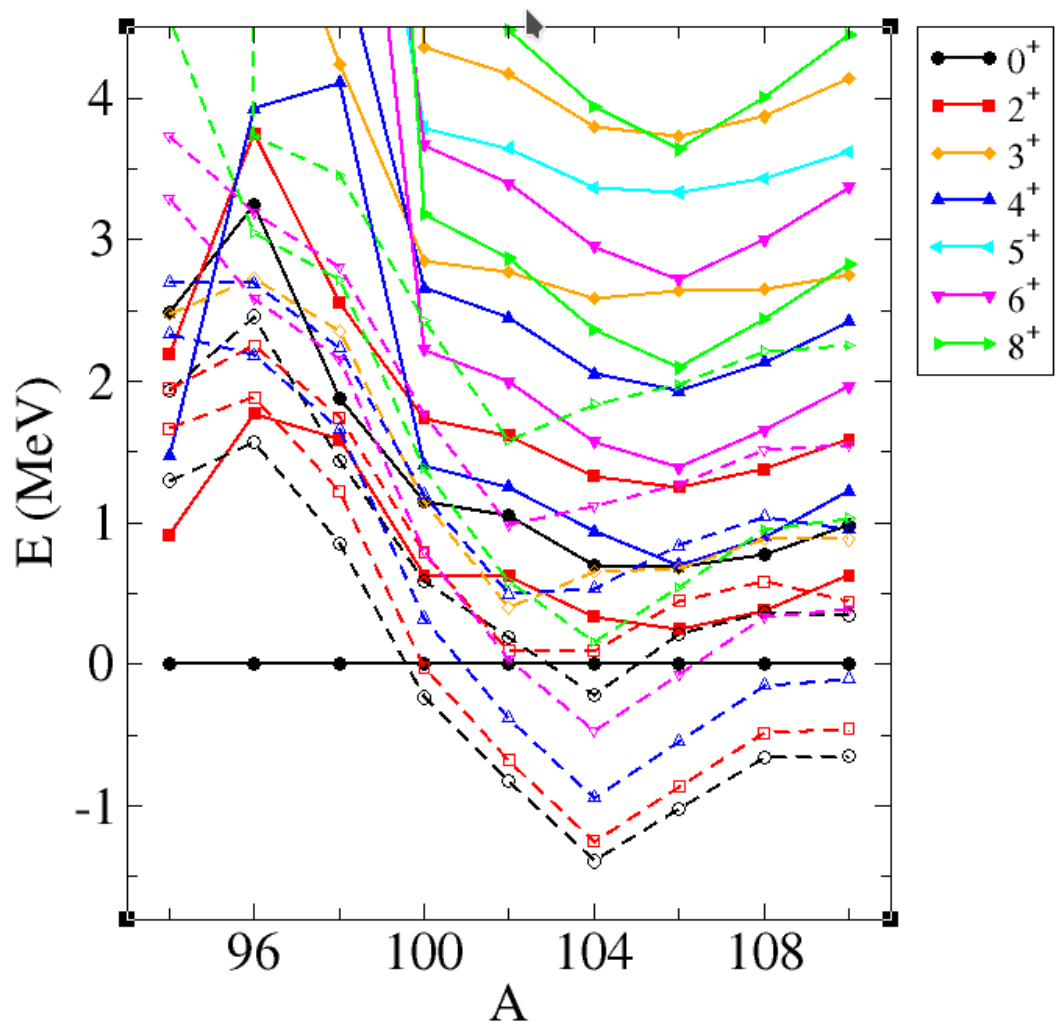
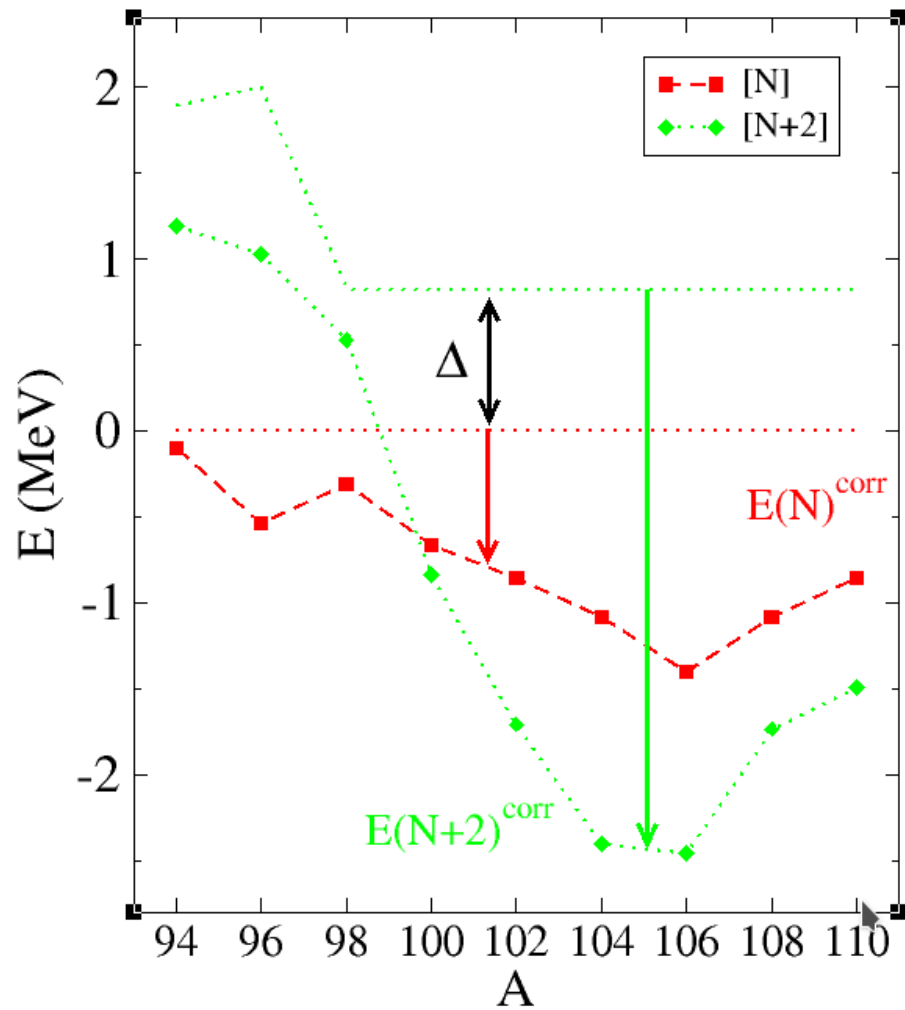


BE2's



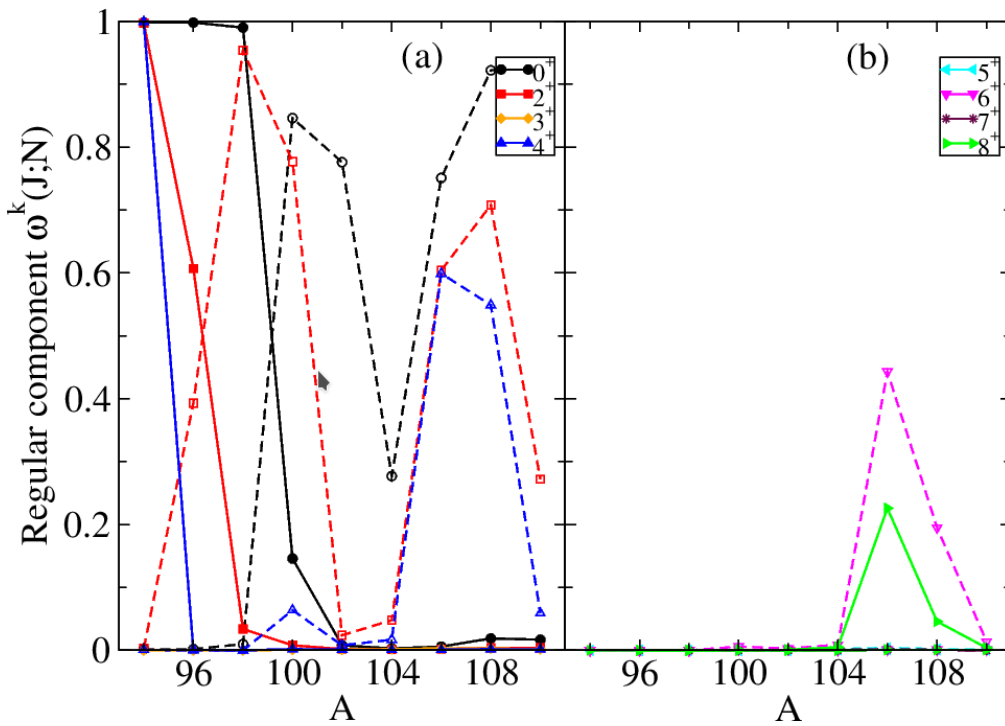
See also Noam Gabrielov's talk, today before lunch

Unperturbed energies

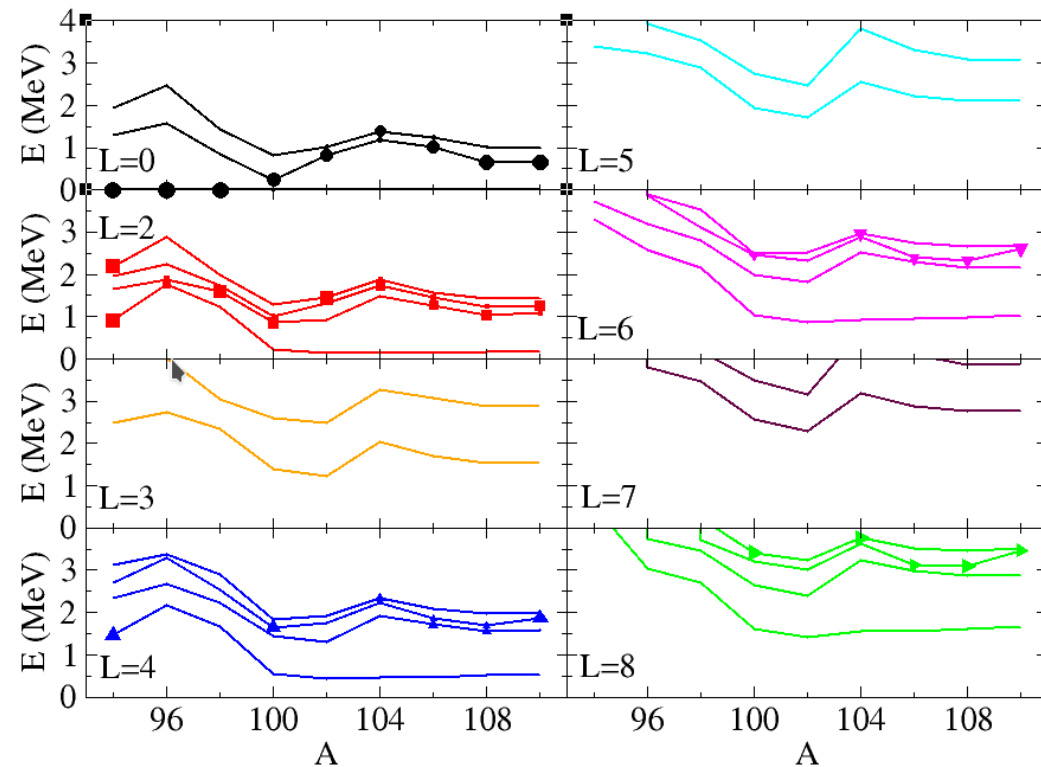


The wave function

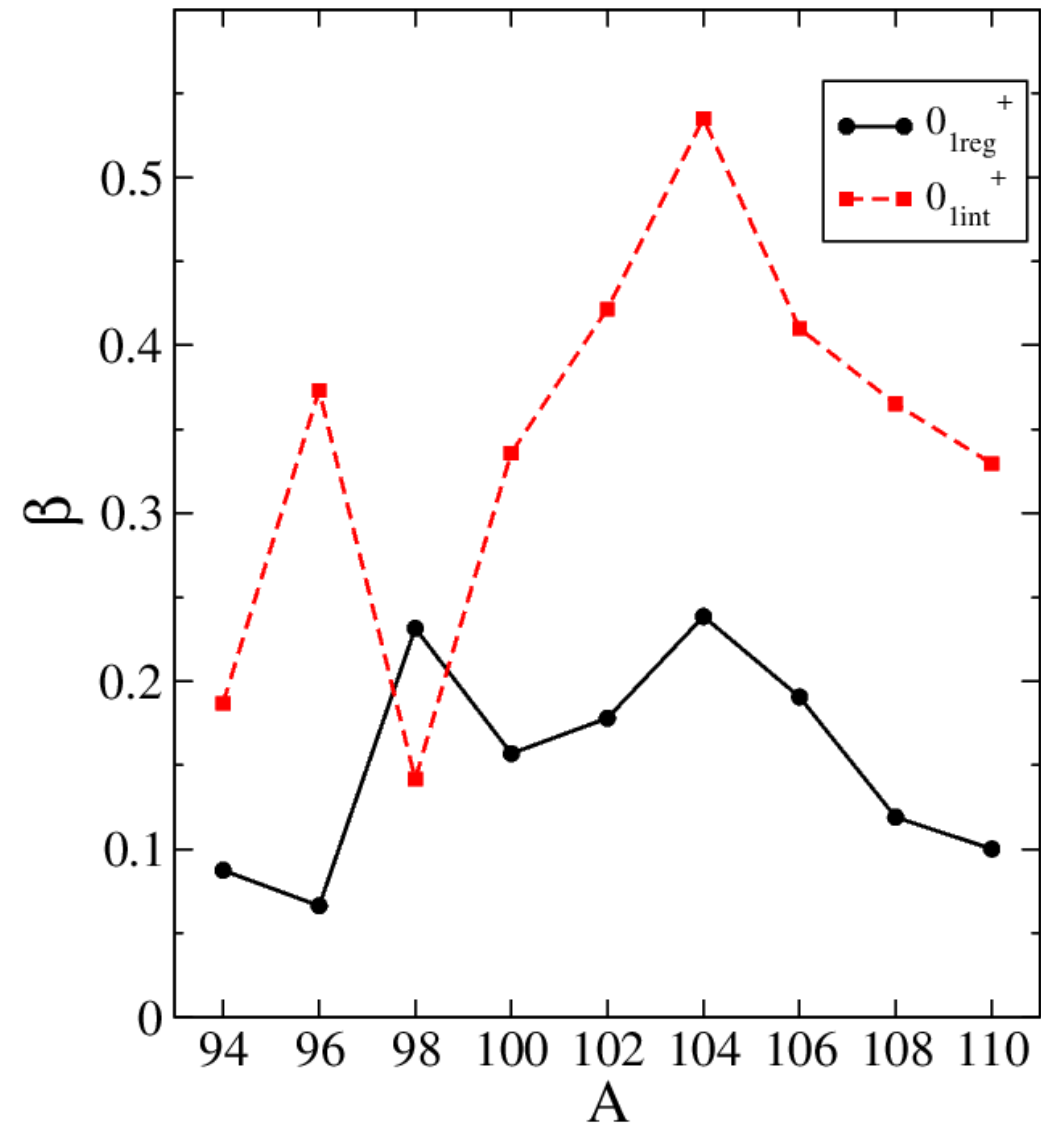
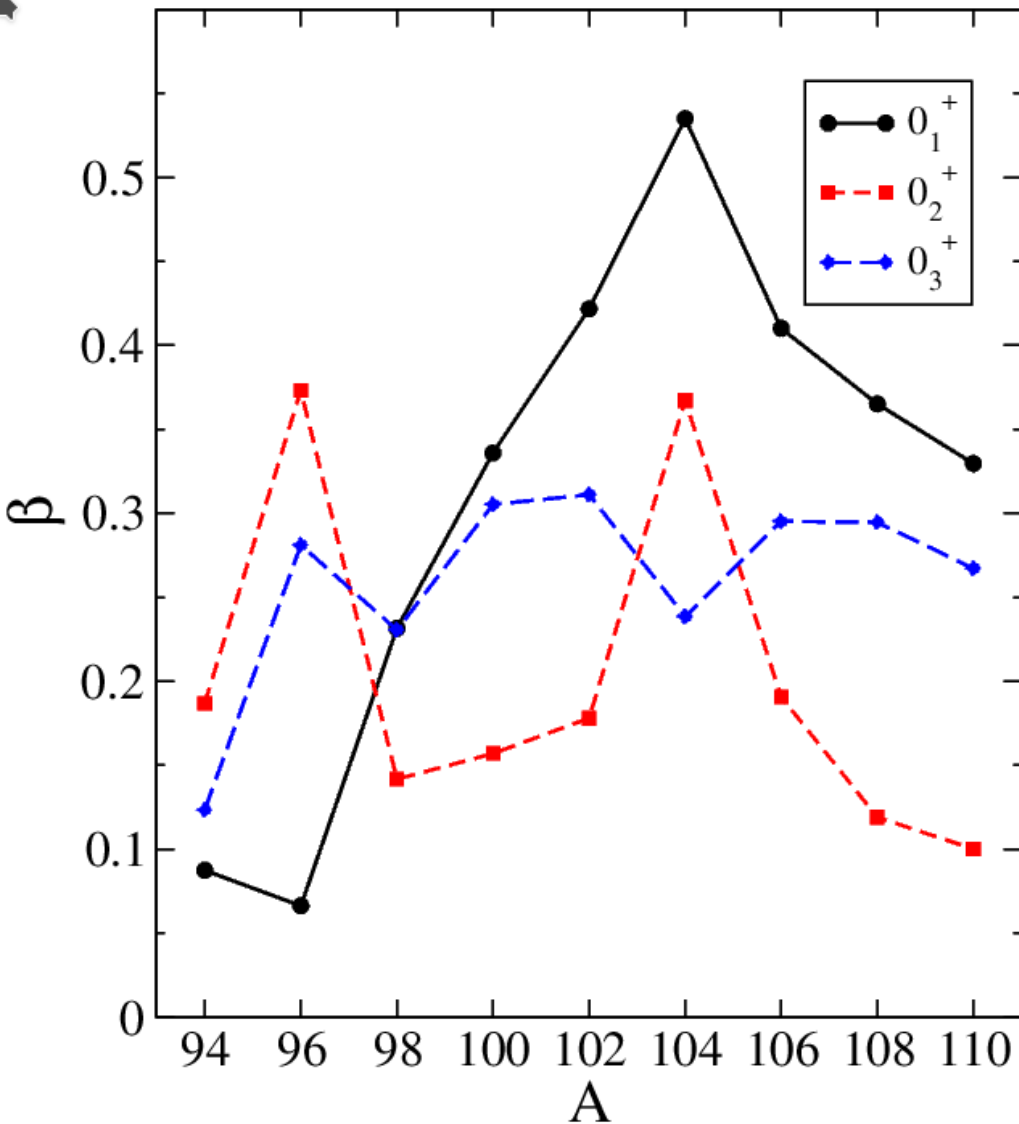
Regular component of selected states



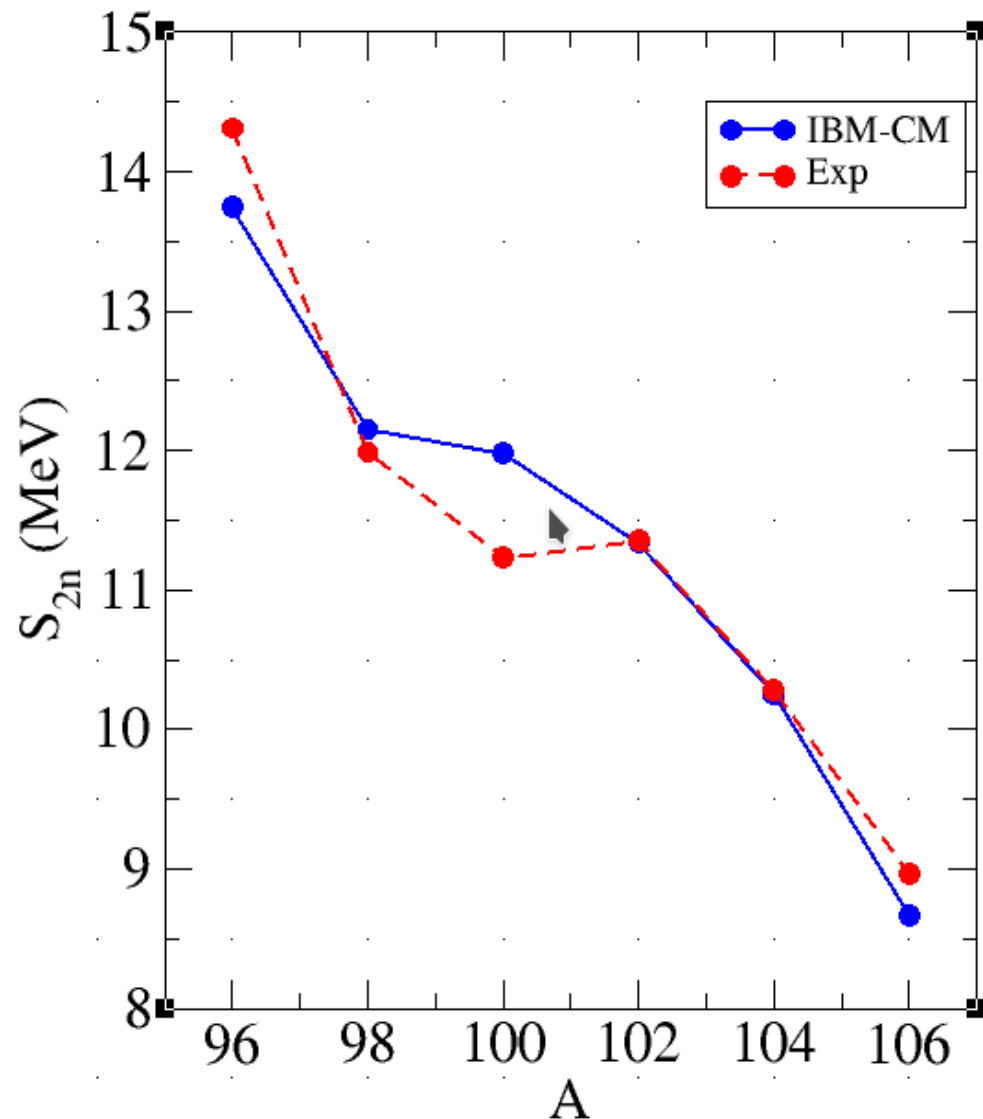
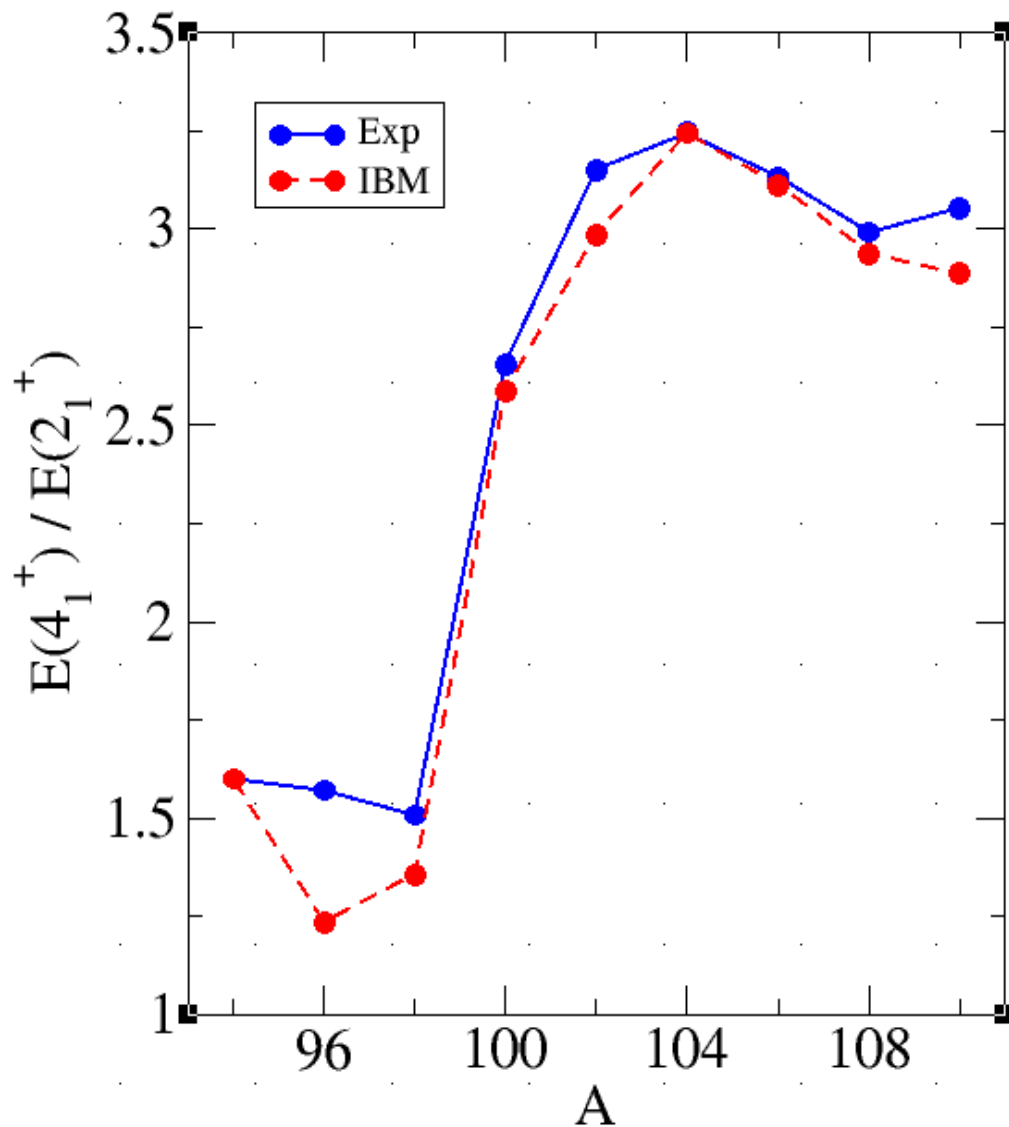
Distribution of the regular component



Deformation from quadrupole shape invariants



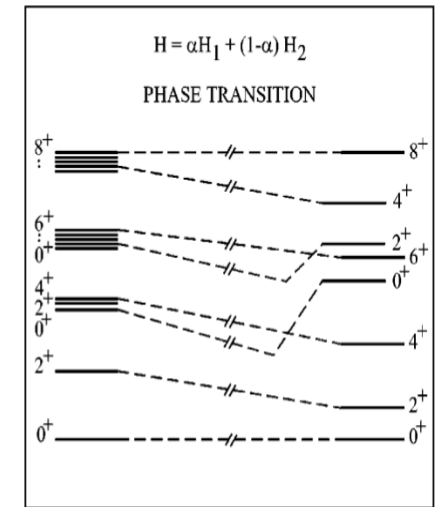
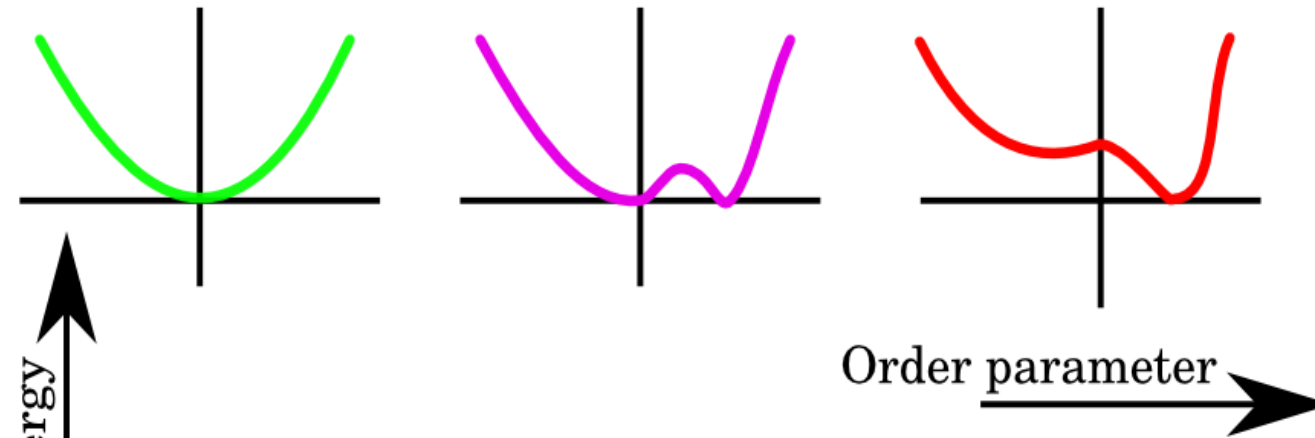
Hints pointing to a Quantum Phase Transition



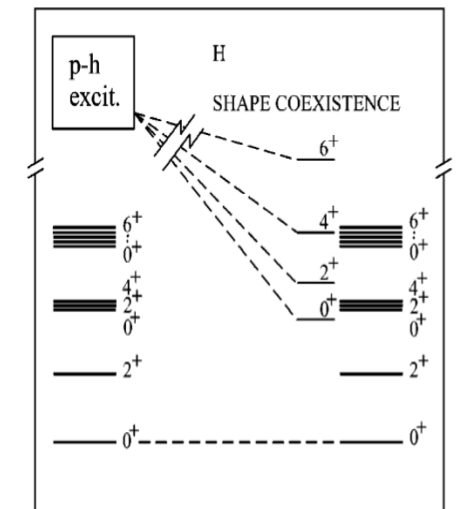
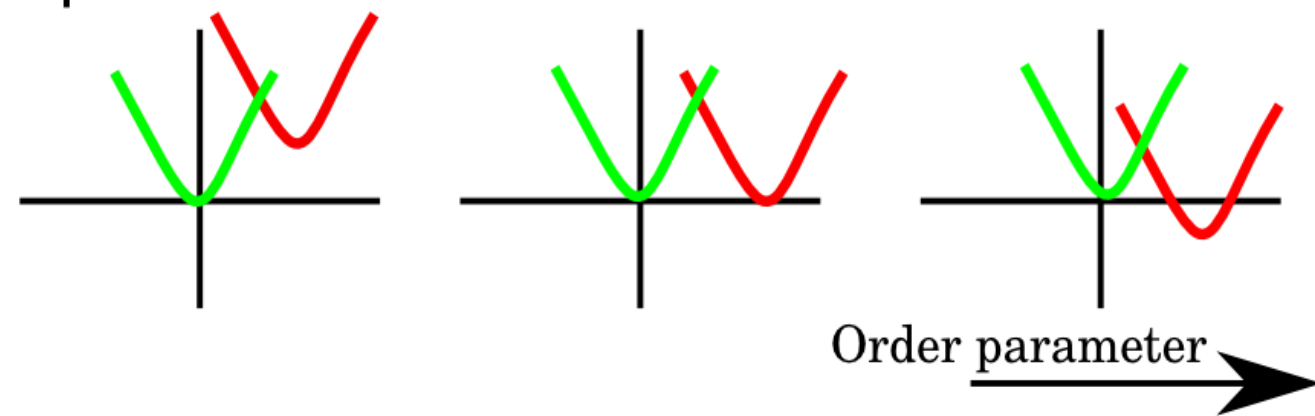
JEGR and K. Heyde, to be published

A schematic view

Phase transition

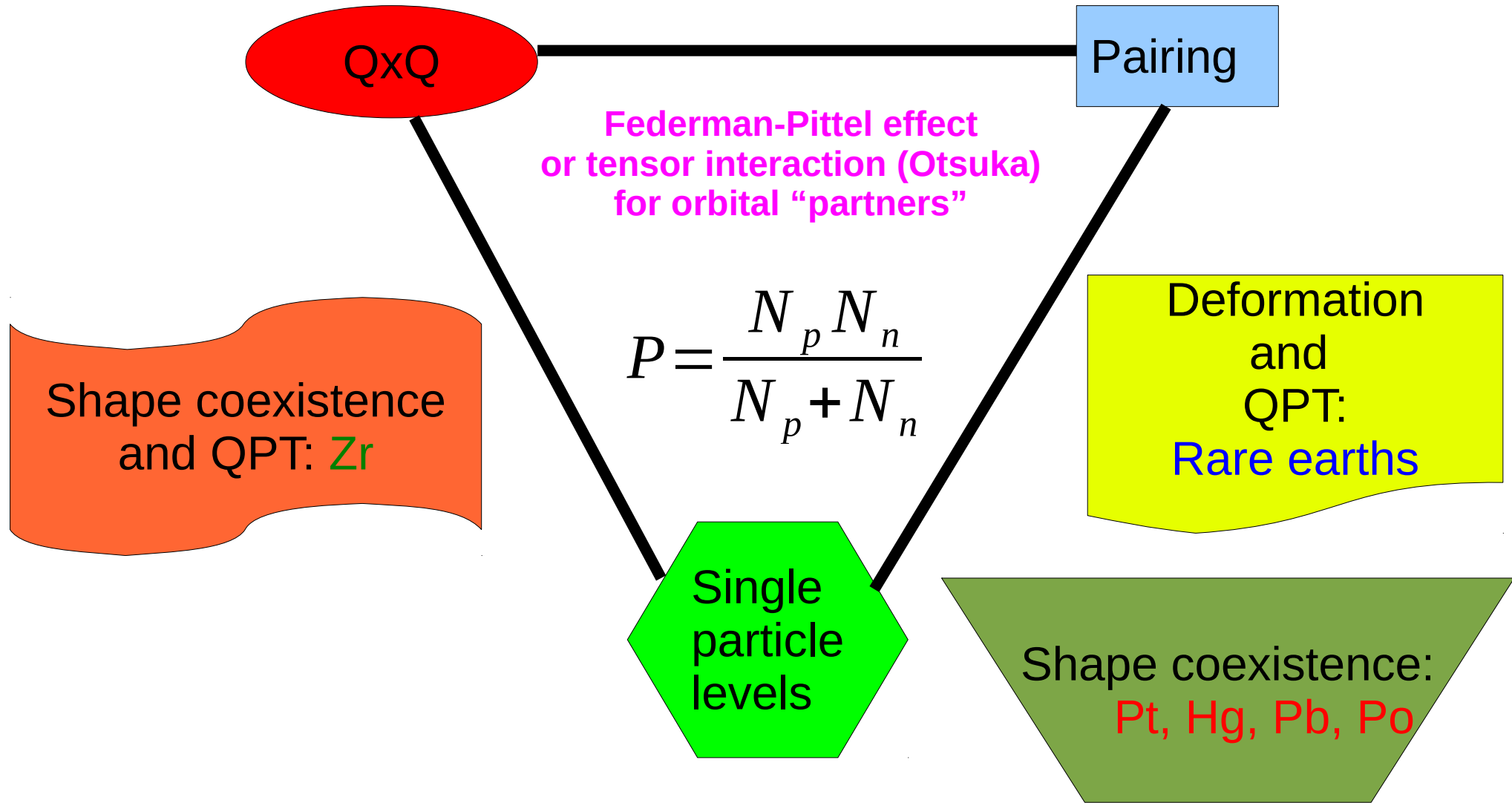


Shape coexistence



PRC 69, 054304 (2004)

Competition between interactions



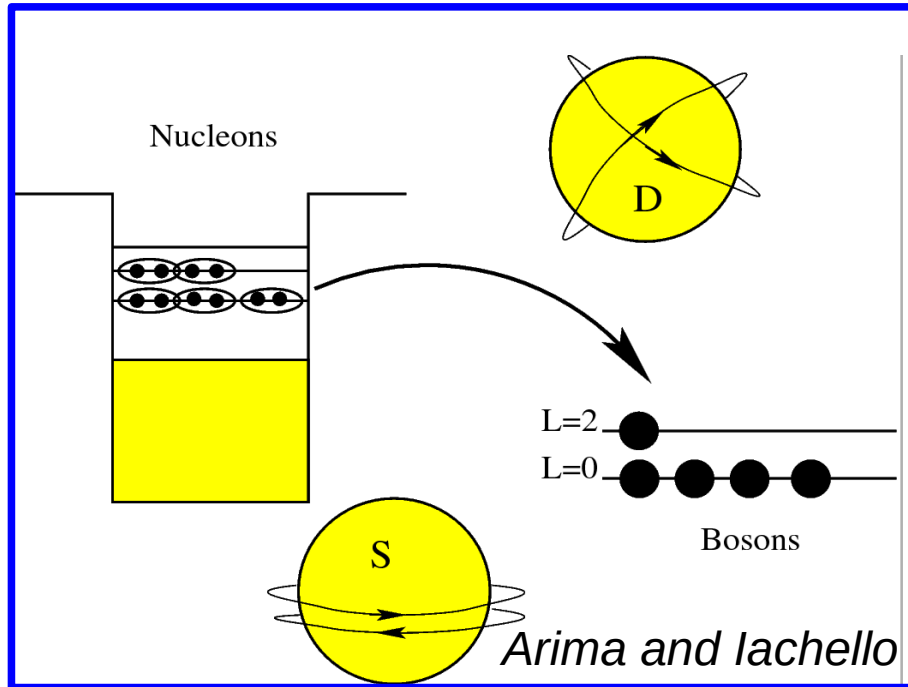
Some open questions

- Are both descriptions compatible?
- Can a Quantum Phase Transition be described in terms of the onset of intruder configurations?
- Is shape coexistence always present “before” a Quantum Phase Transition sets in, or are they fully disconnected?



Thank you

Interacting Boson Model (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**.

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

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

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

How to fix the parameters (IBM)

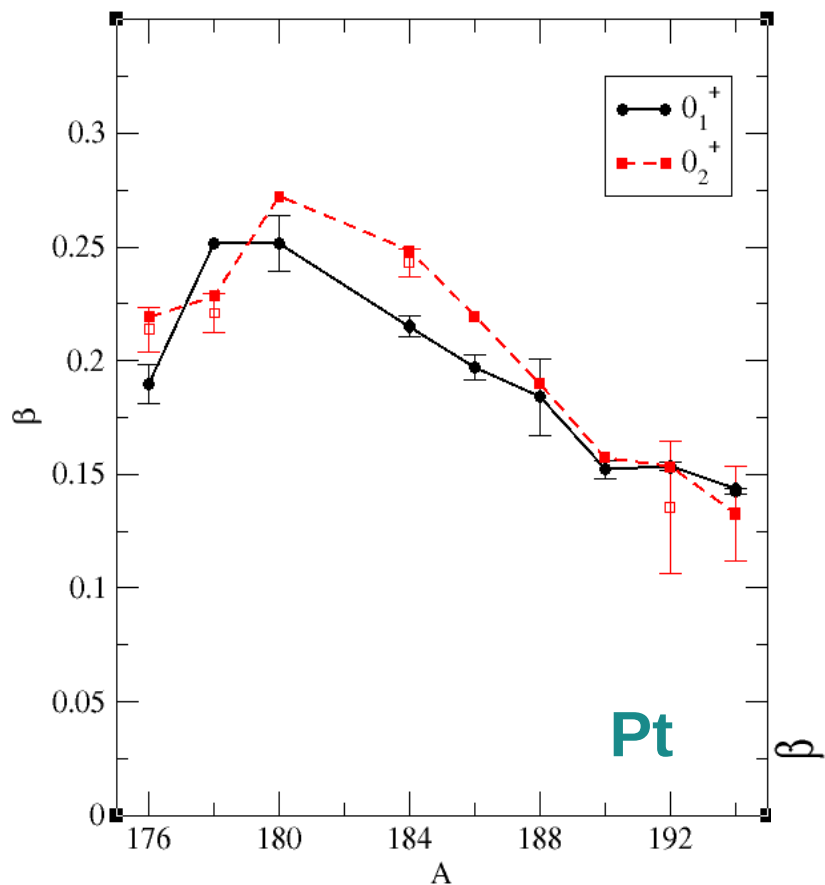
Least squares fit to the experimental data, including excitation energies and absolute B(E2) transitions.

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

Error (keV)	States
$\sigma = 0.1$	2_1^+
$\sigma = 1$	$4_1^+, 0_2^+, 2_2^+$
$\sigma = 10$	$2_3^+, 3_1^+, 4_2^+, 6_1^+, 8_1^+$
$\sigma = 100$	$2_4^+, 3_1^+, 4_3^+, 6_2^+$

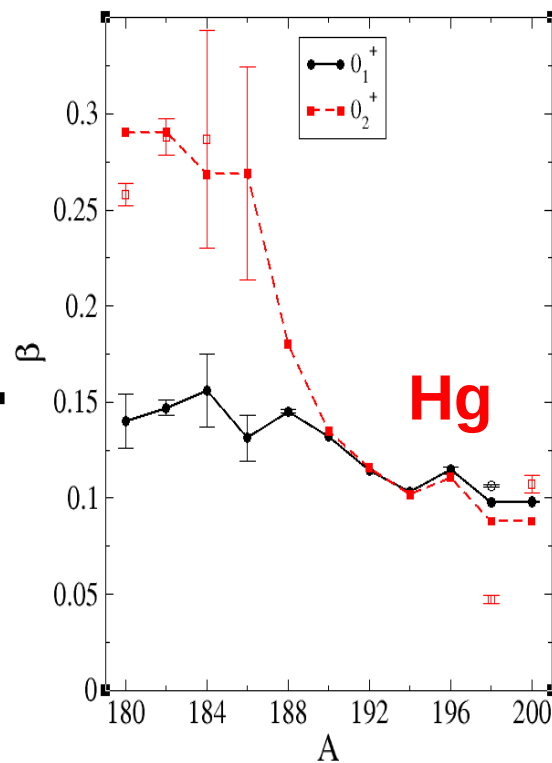
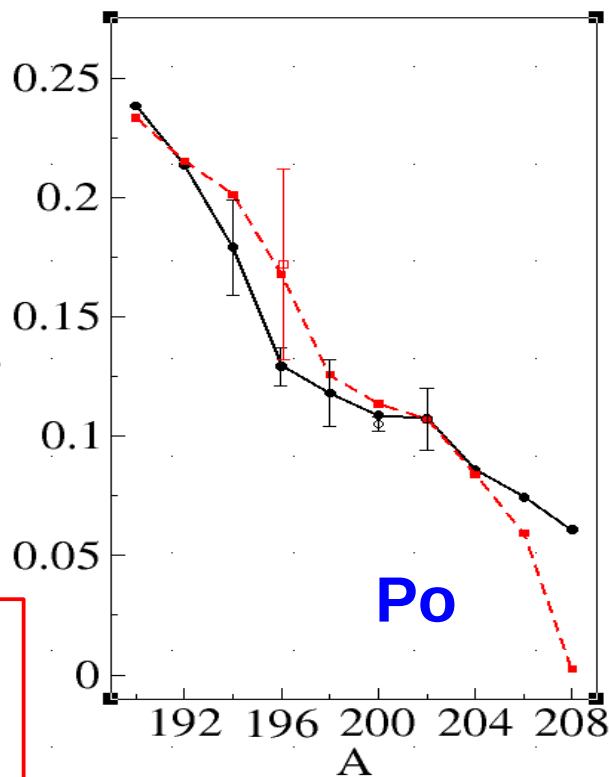
+ all the known B(E2) transitions

Deformation



Beta's from B(E2) values

$$\beta = \frac{4\pi \sqrt{B(E2; J \rightarrow J-2)}}{3Ze r_0^2 A^{2/3} \langle J020 | J-20 \rangle}$$



U(5) components

