On the nature of the shape coexistence and the quantum phase transition phenomena in the zirconium and lead region

José-Enrique García-Ramos

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What Shape Coexistence (SC) is?

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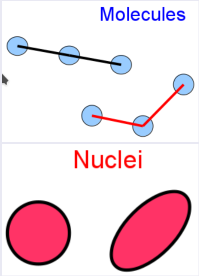
Therefore, the existence of a geometric interpretation is implicit.



Quadrupole shape invariants

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

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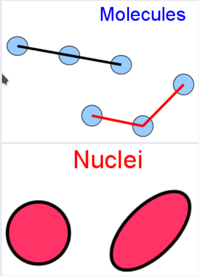

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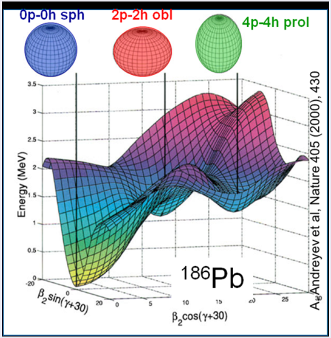
Mean field: example of triple coexistence



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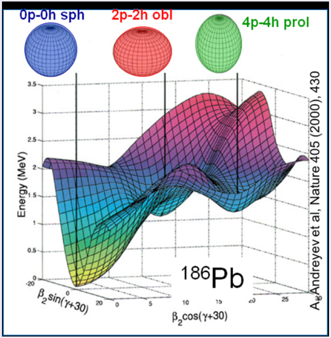
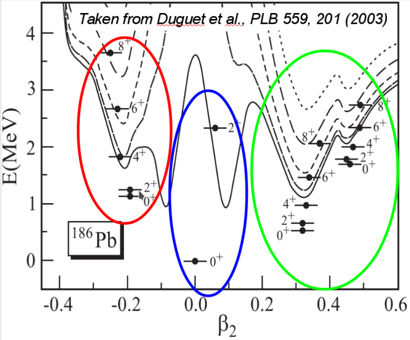


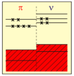


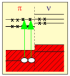
The angular momentum projected mean field plus the Generator Coordinate Method generates different bands with very different deformation.

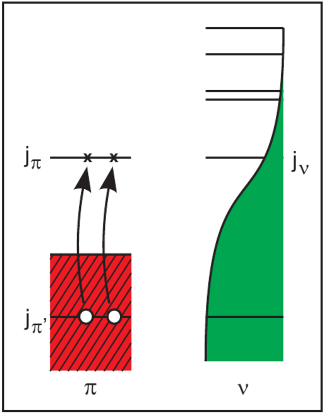
Shell model. Where to be used

- 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.

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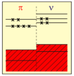
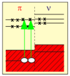
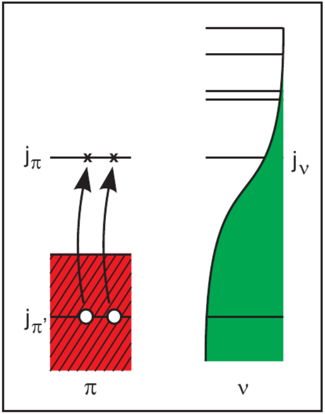
$\phi(J,M) = a(J,M)$  $+\ b(J,M)$ 



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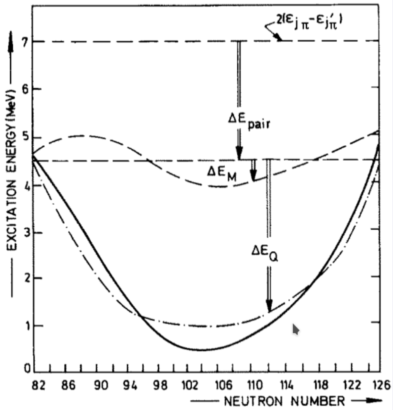
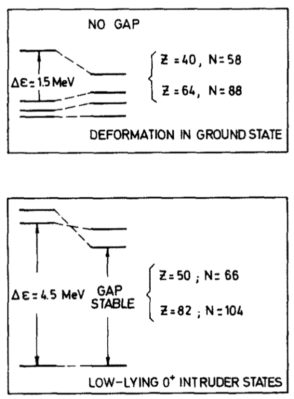
Competition of interactions

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.

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.

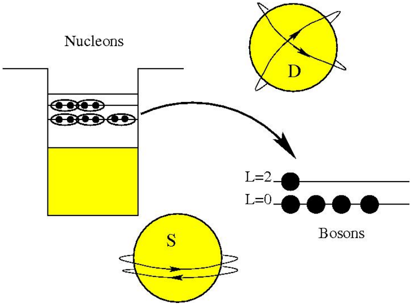
$$s^\dagger, d_m^\dagger (m = 0, \pm 1, \pm 2)$$
$$s, d_m (m = 0, \pm 1, \pm 2)$$

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

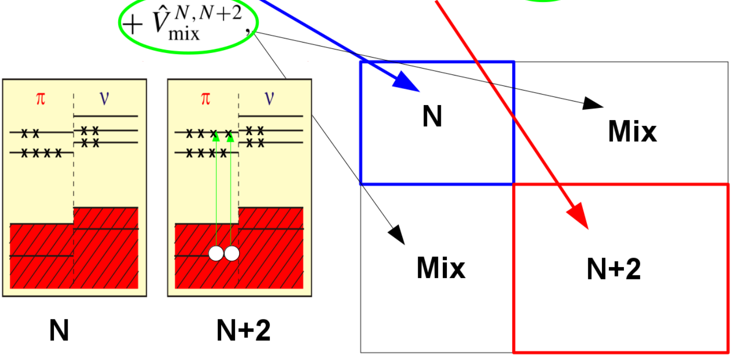
$$\hat{H}_{ECQF} = \varepsilon \hat{n}_d + \kappa \hat{Q} \cdot \hat{Q} + \kappa' \hat{L} \cdot \hat{L}$$



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

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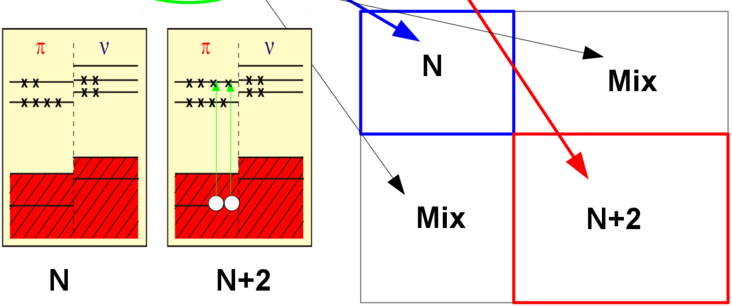

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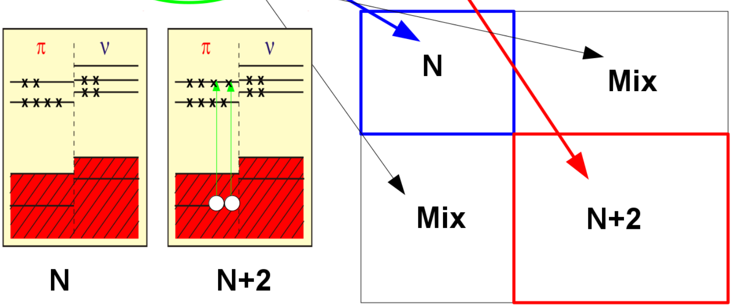

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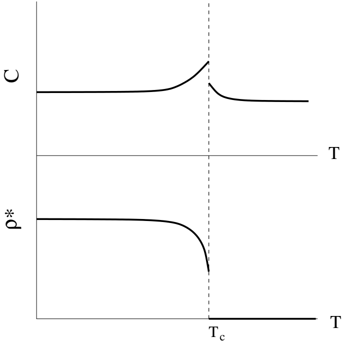
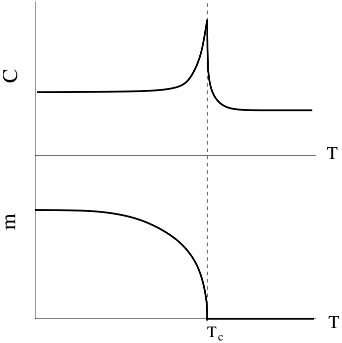
Examples of Macroscopic Phase Transitions



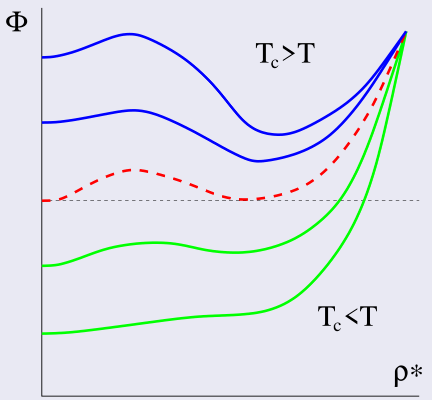
First order phase transition.
Liquid-gas



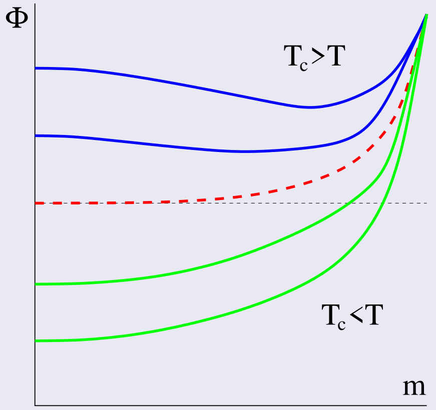
Second order phase transition.
Paramagnetic-ferromagnetic

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

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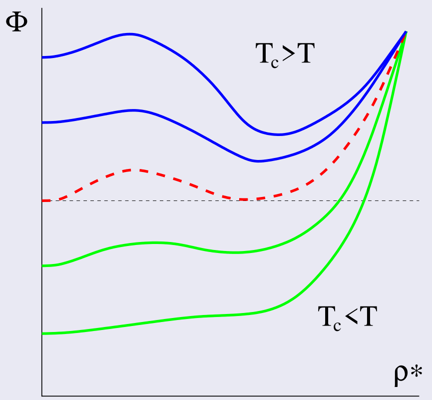

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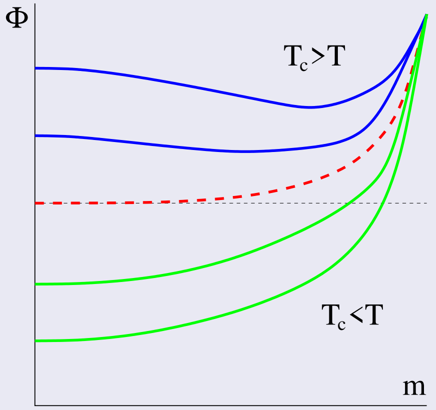

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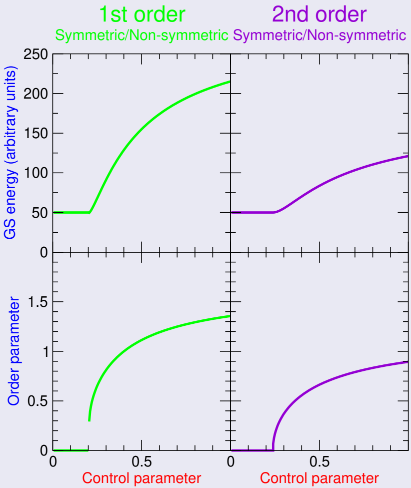
What a Quantum Phase Transition (QPT) is?

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. This transitions are assumed to occurs at zero temperature.

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



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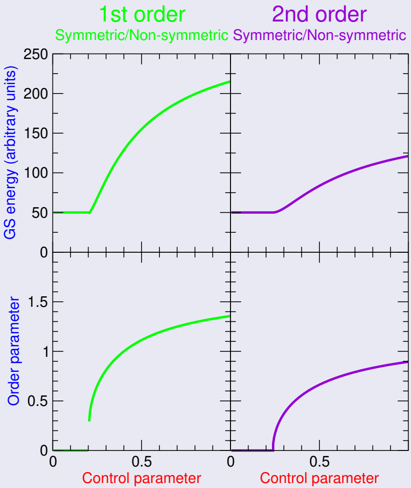


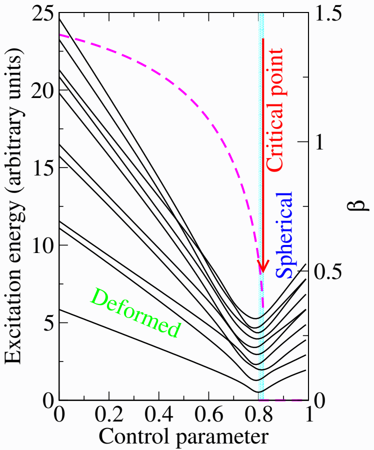
At the critical point

- The ground state energy is non-analytical (in the thermodinamic limit).
- 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.

Gap



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

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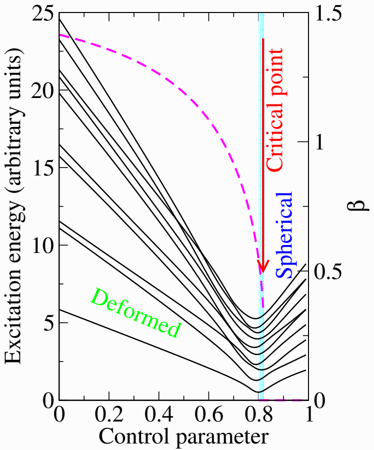

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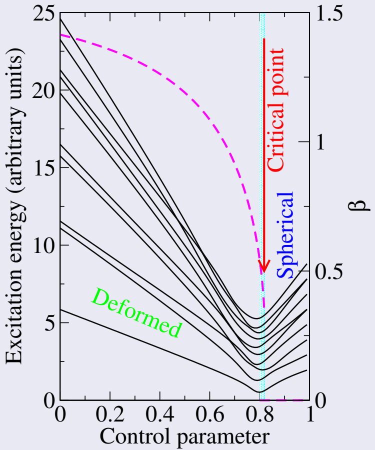

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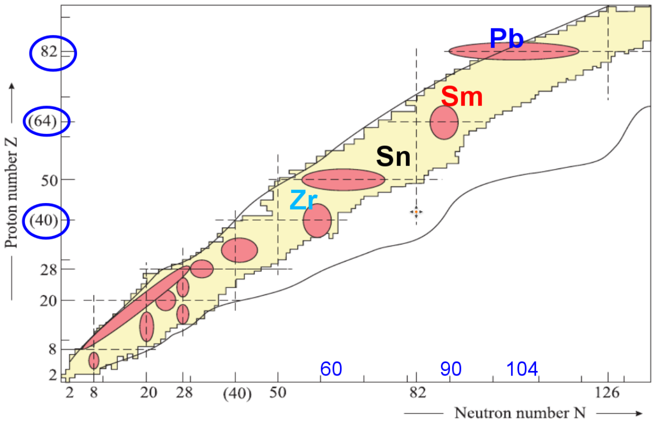
Regions of interest



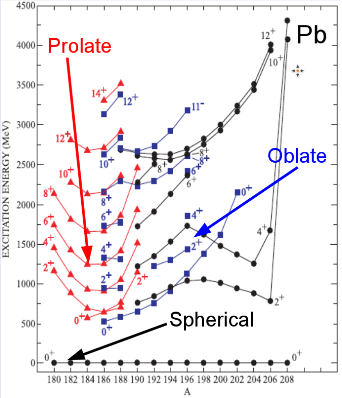
Pb and Sn regions are ideal regions to study the importance of Shape Coexistence (SC).

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.

Shape coexistence

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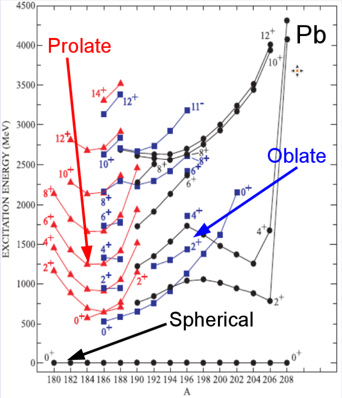

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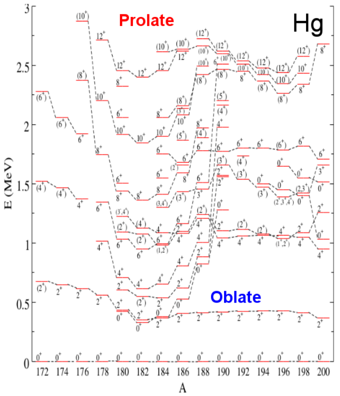
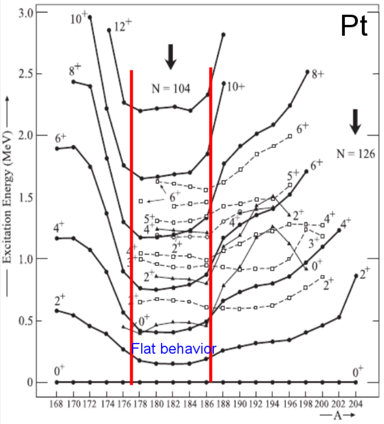


The presence of two families of states is self-evident.

Lead region

Pt isotopes



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

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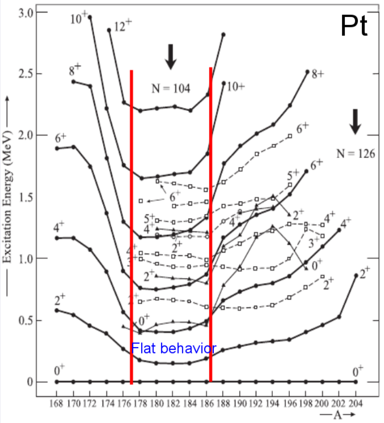

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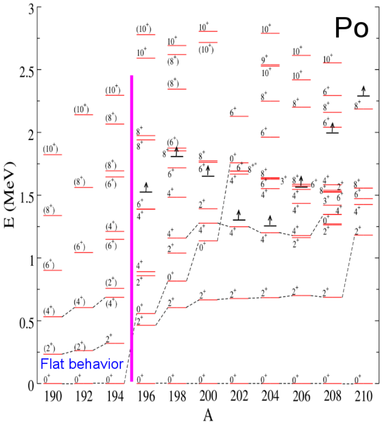
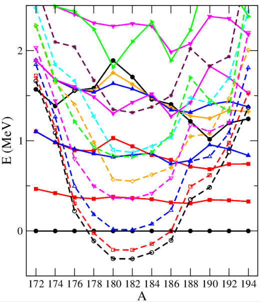


Here, we hardly reach the midshell and no clear conclusions can be obtained.

Unperturbed energies

Pt isotopes



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

Unperturbed energies

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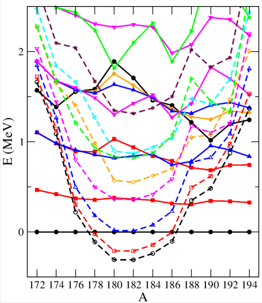

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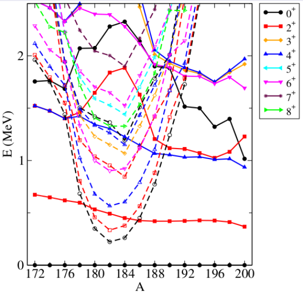

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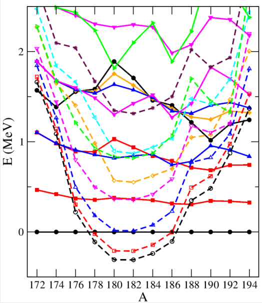

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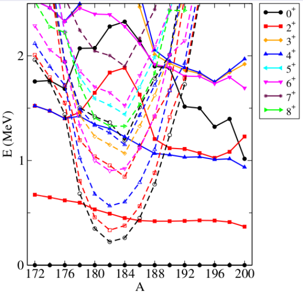

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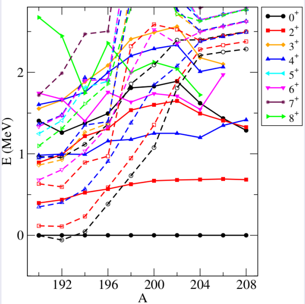
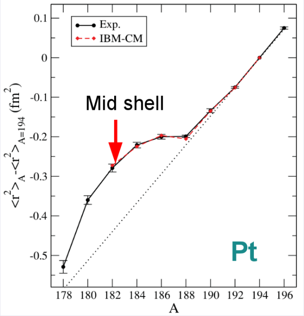


Intruder and regular configurations are almost degenerated at midshell.

Back

Radii

Pt isotopes



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

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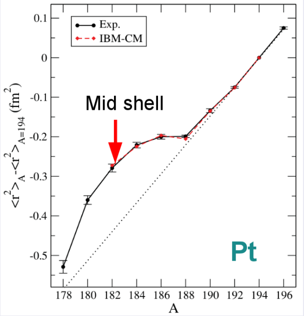

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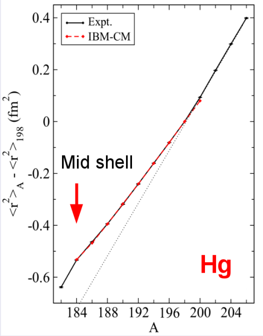

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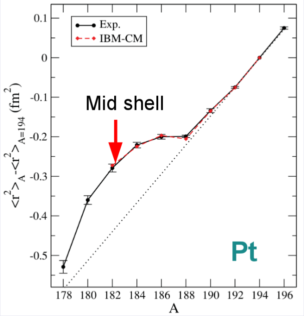

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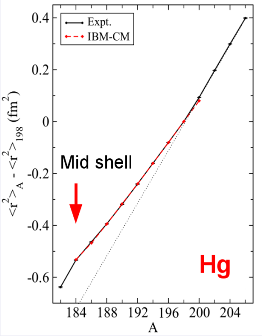

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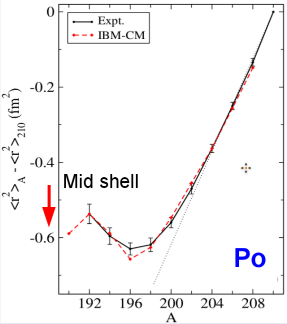

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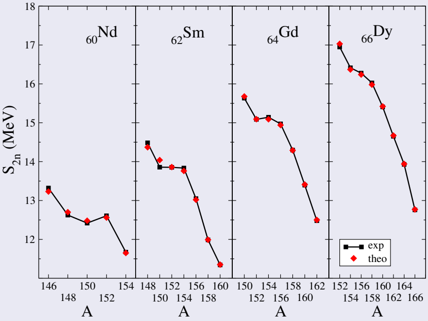
Quantum Phase Transition indicators in the rare-earth region

Two-neutron separation energy. Why?



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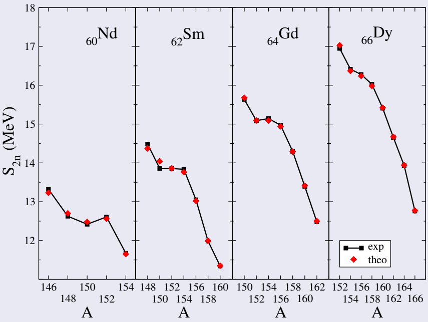
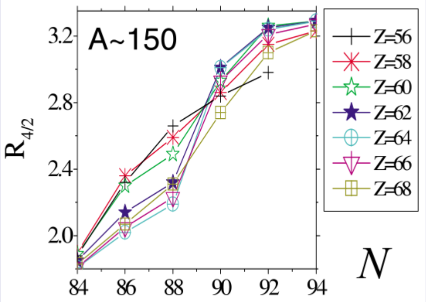


S_{2n} is connected with the first derivative of the binding energy. Its discontinuity is a hint for the onset a first order QPT.

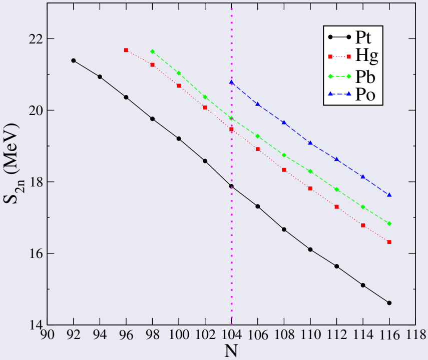
$E(4_1^+)/E(2_1^+)$



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



The linear trend of S_{2n}, even at midshell, does not suggest any sign of QPT.

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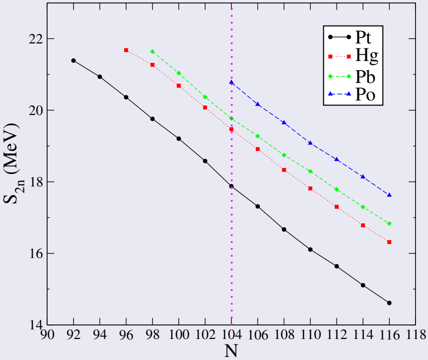

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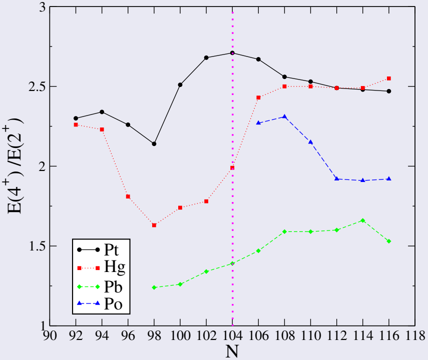

$E(4_1^+)/E(2_1^+)$ does not present neither the typical behaviour of an order parameter. Only Pt isotopes resemble the expected trend for an order parameter when approaching midshell from the left.

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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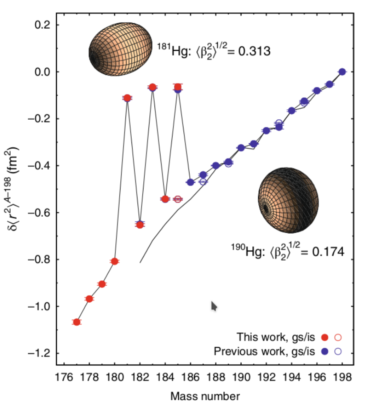


Nature Physics, October 2018

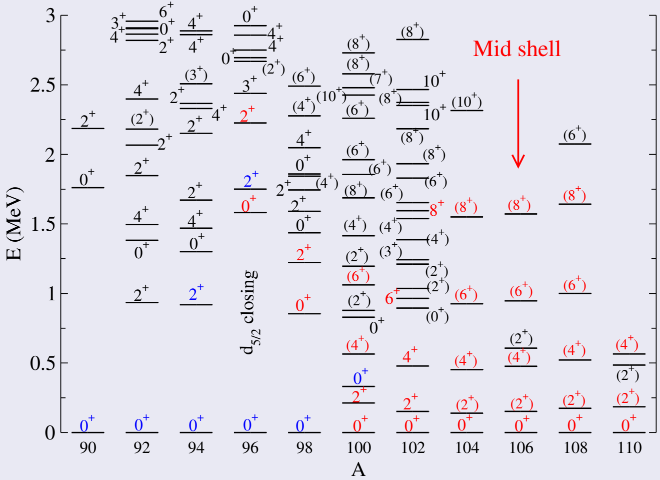
nature physics LETTERS
https://doi.org/10.1038/s41567-018-0292-8

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]

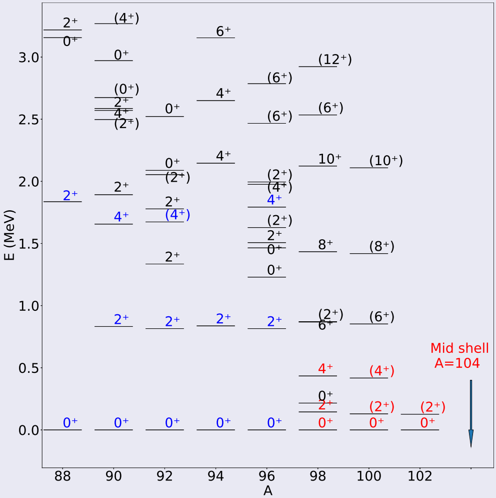
"The shape staggering effect manifests characteristic features of a quantum phase transition: in a given nucleus, different phases ... By making small changes in the control parameter, which in this case is the neutron number, the system alternates between the two phases..."

Energy systematics for even-even Zr nuclei



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

Energy systematics for even-even Sr nuclei



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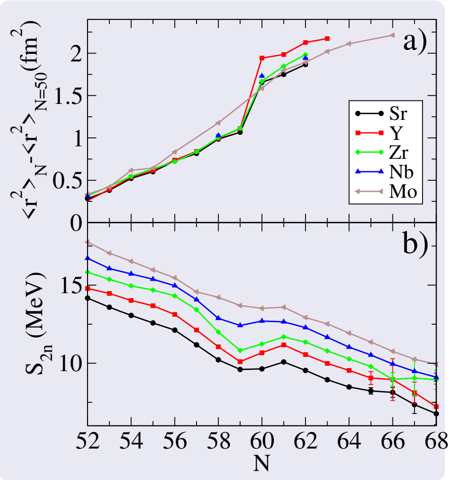
Radii and two-neutron separation energies



- 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 that the observed one in rare-earth region, although, once more, the *discontinuity* is smoothed out for Mo.

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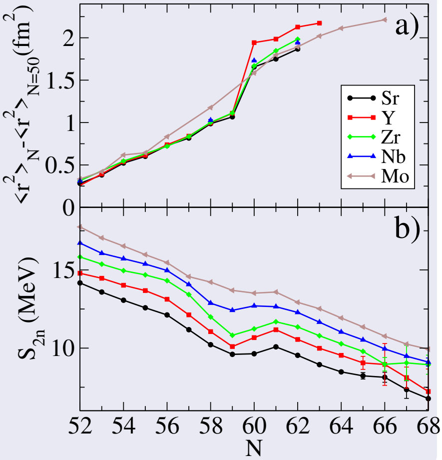

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The fitting procedure

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

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

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

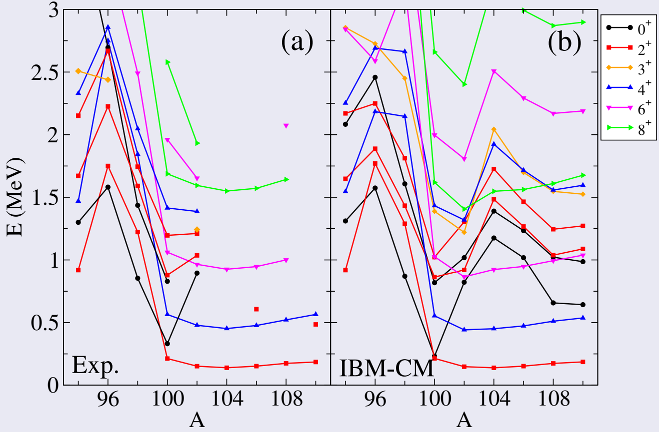
The parameters (for Zr isotopes)

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 $\sqrt{\mathrm{W.u.}}$

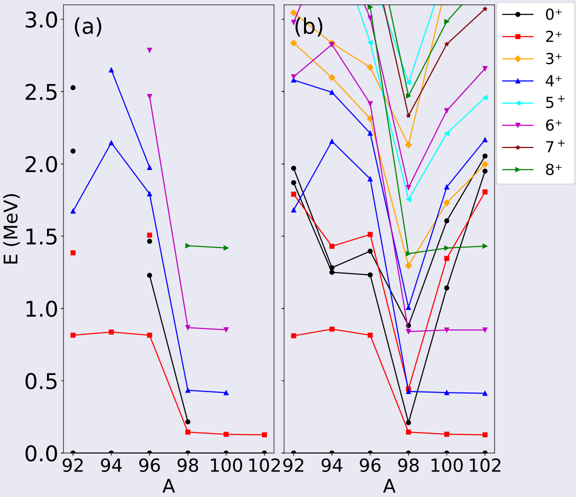
Comparing theory and experimental data

Energies (Zr case)



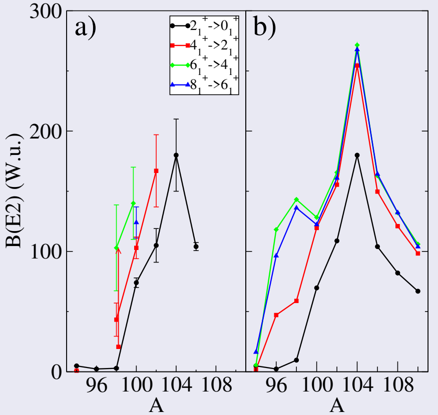
Comparing theory and experimental data

Energies (Sr case)



B(E2) transition rates

Intraband (Zr case)



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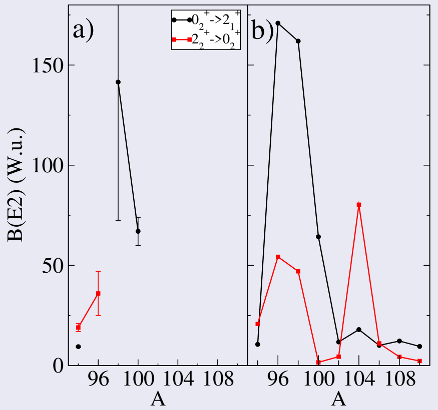

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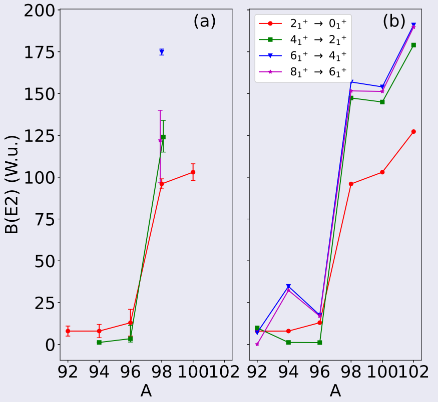

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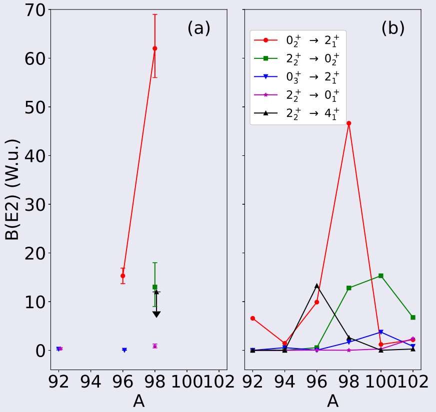
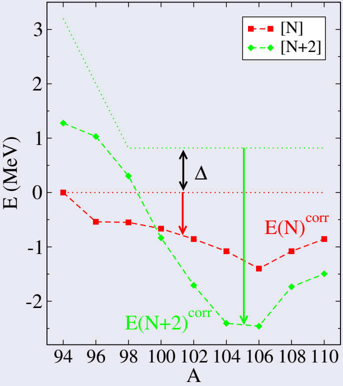


Unperturbed energies

Correlation energies (Zr case)



The intruder configuration becomes theground state for $A = 100$ and onwards.

Unperturbed energies

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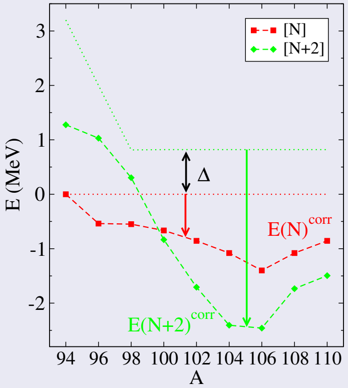

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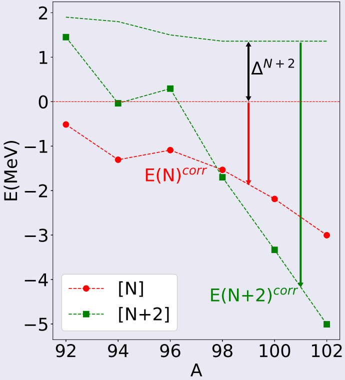
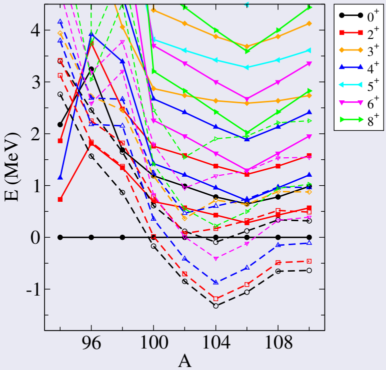


The intruder configuration becomes the ground state for $A = 98$ and onwards.

Unperturbed energies

Unperturbed spectra (Zr case)



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

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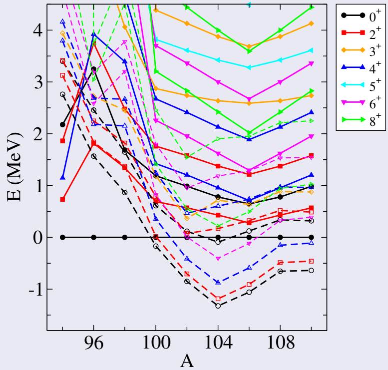

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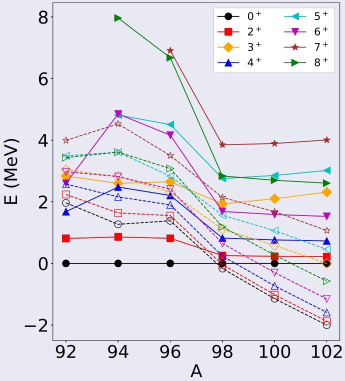
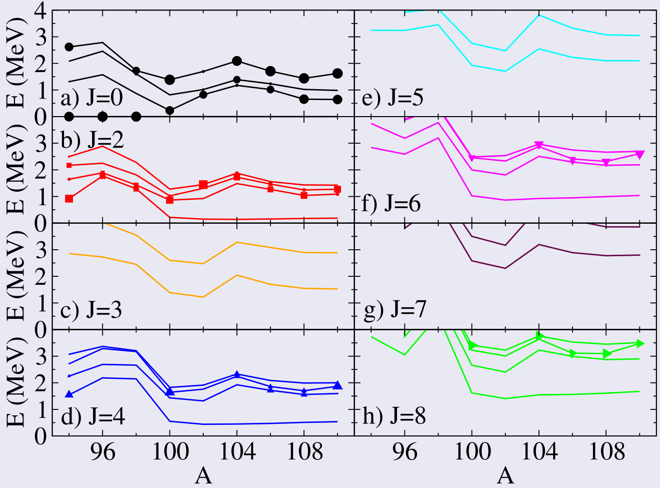


Intruder states present a *parabolic* behaviour while *flat* the regular ones.

See Pb case

Wave function

Regular component and energy (Zr case)



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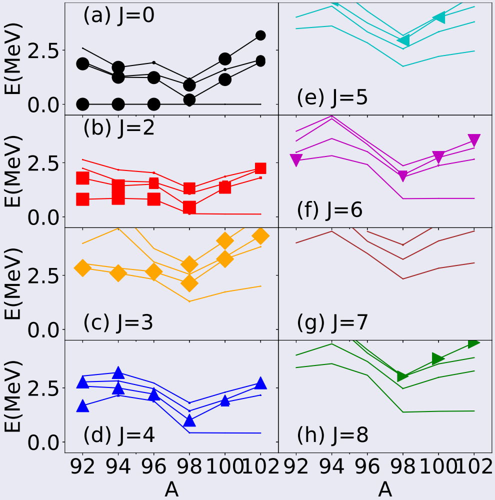
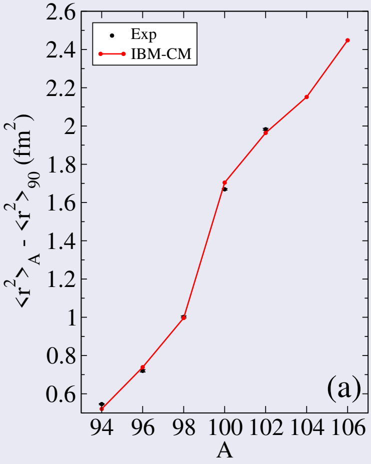
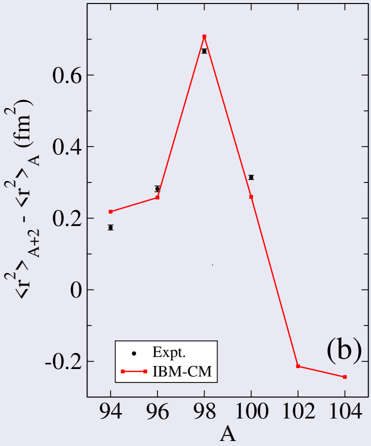


Radii

Radii (Zr case)

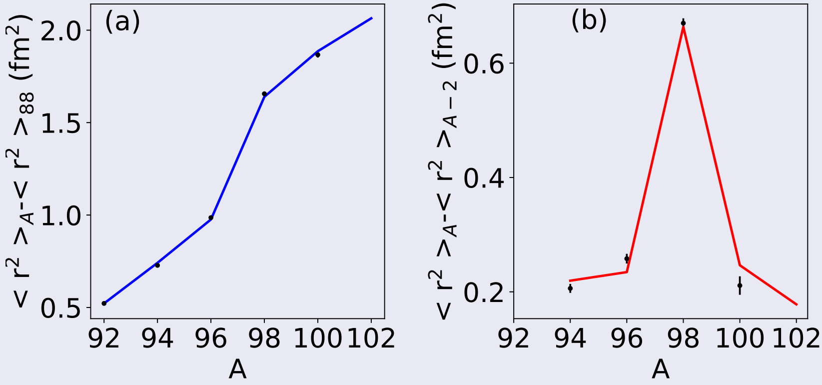


Isotopic shift (Zr case)



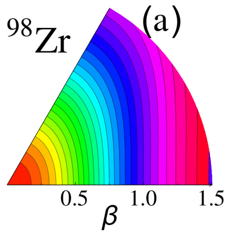
Radii

Radii ans isotopic shift (Sr case)

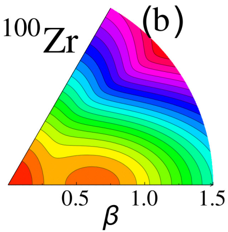


Mean-field energy surfaces

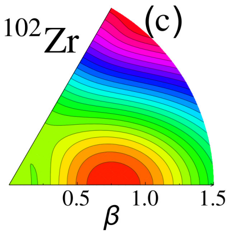
^{98}Zr



^{100}Zr



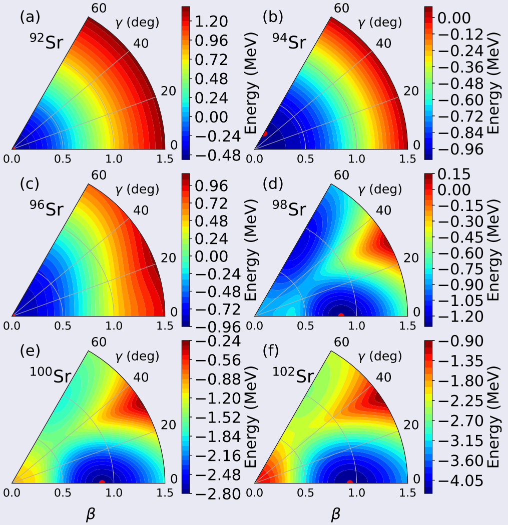
^{102}Zr



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.

Mean-field energy surfaces

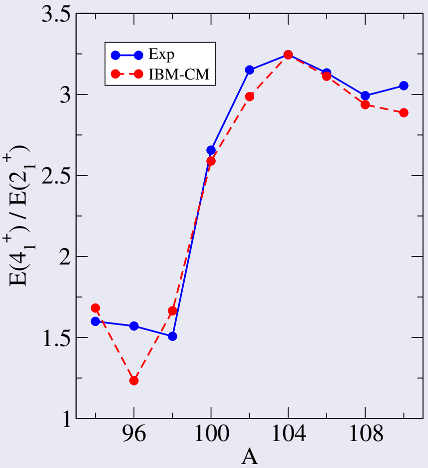
Sr isotopes



Mean field energy surface shows up a rapid evolution from a spherical to a well deformed shape. ^{98}Sr shows the coexistence of two minima.

Hints pointing to a QPT

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



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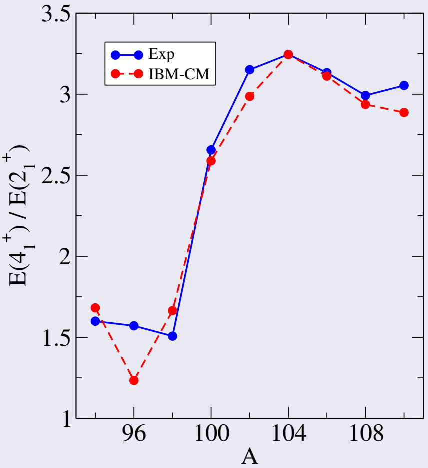

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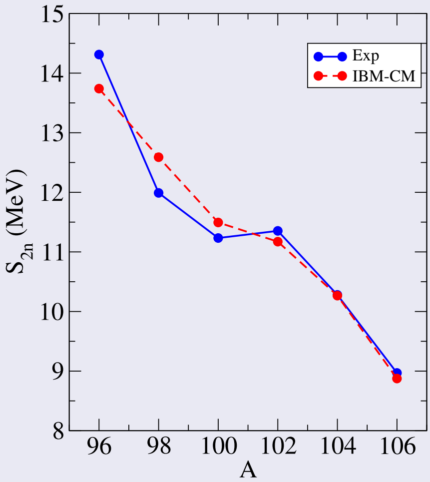

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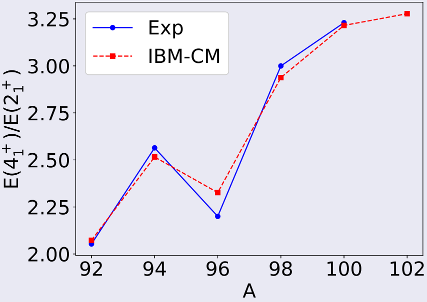

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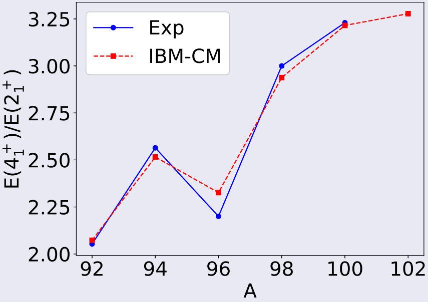

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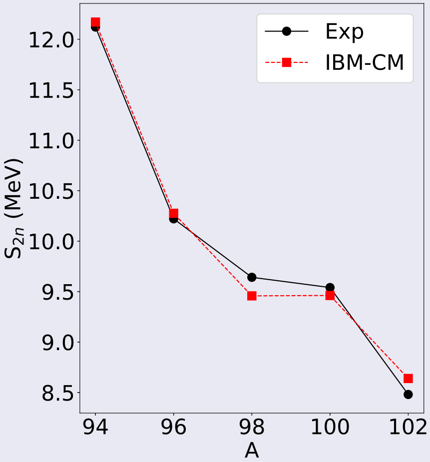

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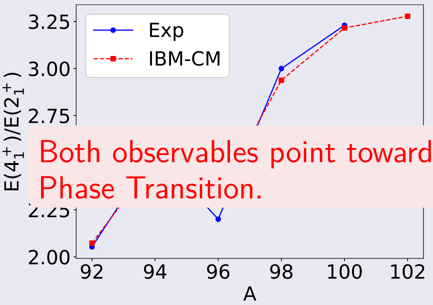

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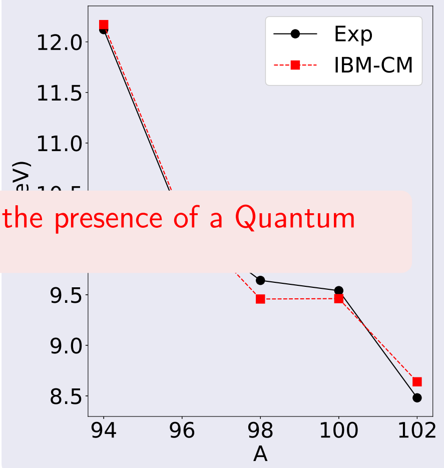
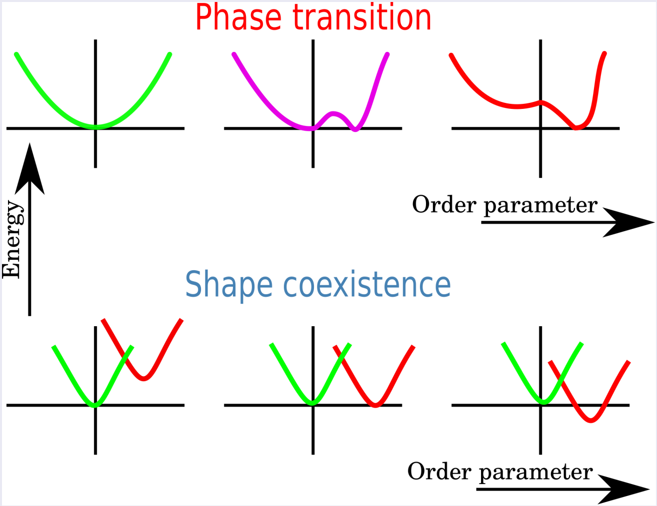


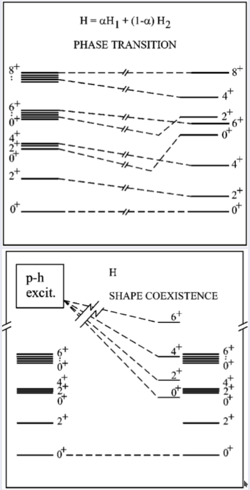
Both observables point towards the presence of a Quantum Phase Transition.

Schematic view

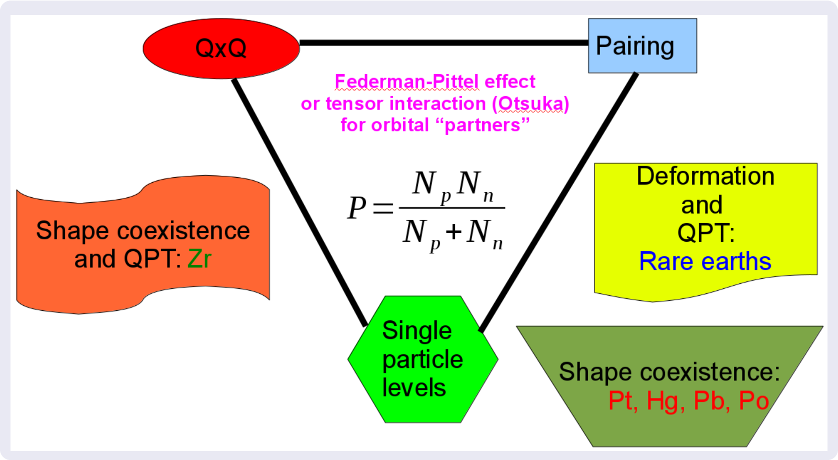
Two minima



PRC 69, 054304 (2004)



Competition of interactions

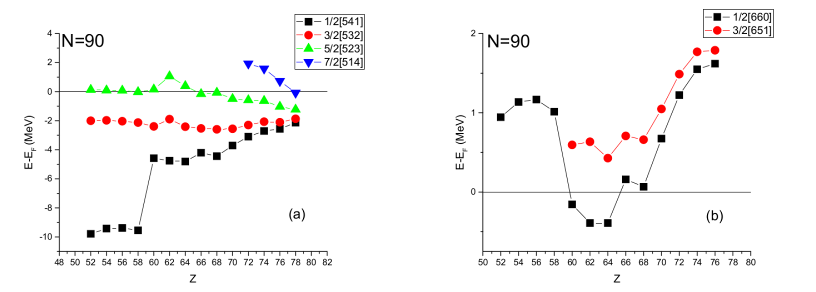


A novel approach: Proxy-SU(3) symmetry

- Proposed in PRC **95**, 064325 (2017), Eur. Phys. J. A **56**, 239 (2020), Eur. Phys. J. A **57**, 84 (2021), by Andriana Martinou, Dennis Bonatsos, I. E. Assimakis, K. Karakatsanis, et al.
- This mechanism is based on the interplay between the Harmonic Oscillator (HO) magic numbers and spin-orbit (SO) like magic numbers. The main element of the new mechanism are particle excitations occurring between the HO and SO sets of shells.
- According to this mechanism shape coexistence cannot appear everywhere on the nuclear chart, but only within specific regions, called islands of shape coexistence, the shores of which are determined through group theoretical arguments in a parameter independent way.
- The islands predicted by the present mechanism are fully compatible with the regions of the nuclear chart in which the particle–hole mechanism has been applied.

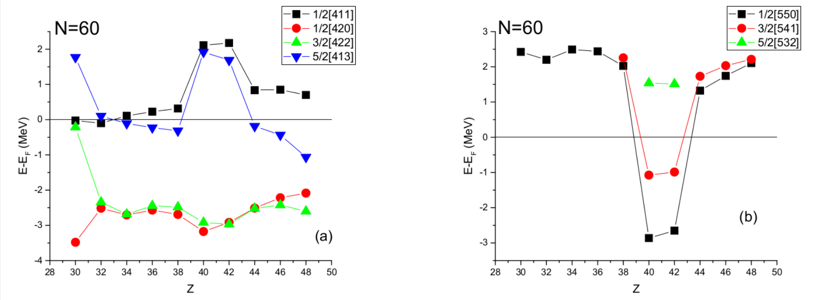
Proxy-SU(3) symmetry

Rare-earth region. Neutron single particle orbitals energies relative to the Fermi energy obtained by a relativistic density functional. https://arxiv.org/abs/2204.00805



Proxy-SU(3) symmetry

Zr region. Proton single particle orbitals energies relative to the Fermi energy obtained by a relativistic density functional.
https://arxiv.org/abs/2204.00805



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.
- Are both descriptions compatible? Maybe the answer is in Zr region.
- 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?

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- 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.
- Are both descriptions compatible? Maybe the answer is in Zr region.
- 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?

Thanks for your attention

Some references of interest

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- J.E. García-Ramos and K. Heyde, "Disentangling the nuclear shape coexistence in even-even Hg isotopes using the interacting boson model",*15th International Symposium on Capture Gamma-Ray Spectroscopy and Related Topics (CGS15)*, EPJ Web of Conferences **93**, 01004-4 (2015).
- J.E. García-Ramos and K. Heyde, "Nuclear shape coexistence in Po isotopes: An interacting boson model study", Physical Review C **92**, 034309-19pp (2015).
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- J.E. García-Ramos and K. Heyde, "On the nature of the shape coexistence and the quantum phase transition phenomena: lead region and Zr isotopes", *16th International Symposium on Capture Gamma-Ray Spectroscopy and Related Topics (CGS16)*, EPJ Web of Conferences **178**, 05005 (2018).
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- J.E. García-Ramos and K. Heyde, "Subtle connection between shape coexistence and quantum phase transition: The Zr case", Physical Review C 102, 054333-16p (2020).
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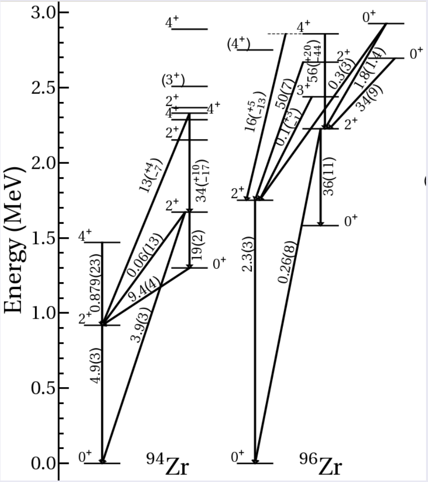
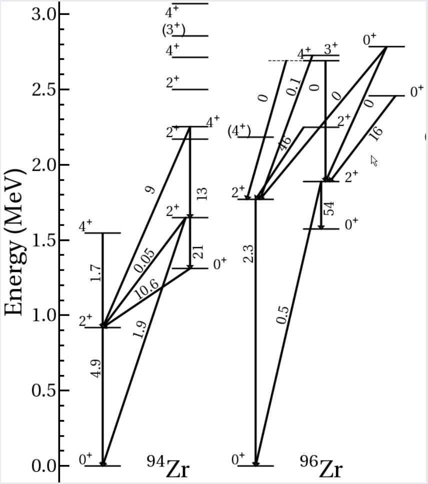
Comparing theory and experimental data

Experimental

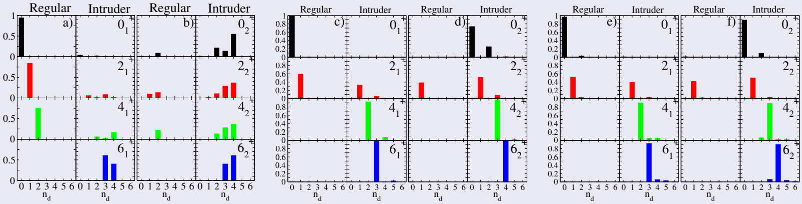


Theoretical

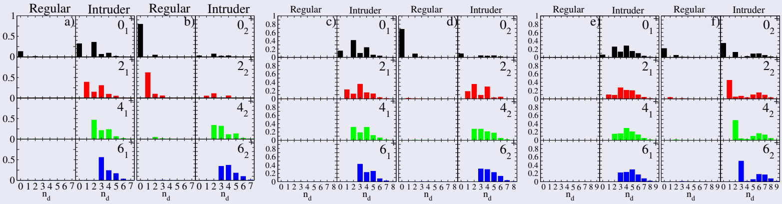


Wave function: U(5) decomposition

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

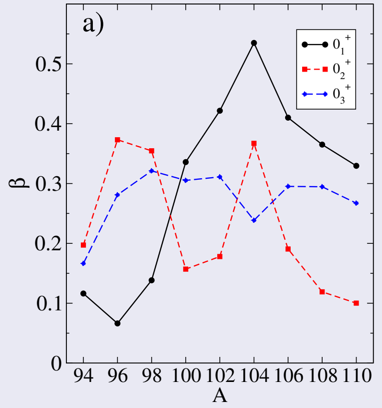


^{100}Zr, ^{102}Zr and ^{104}Zr

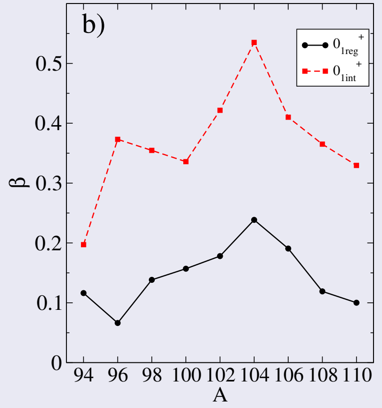


Deformation from quadrupole shape invariants

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



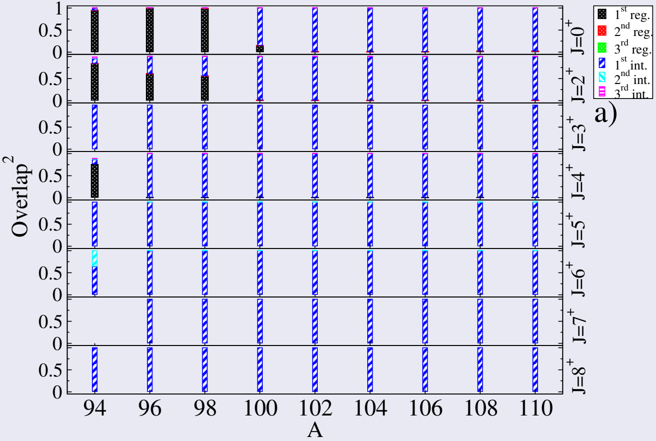
0_{1reg}^+, 0_{1int}^+



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

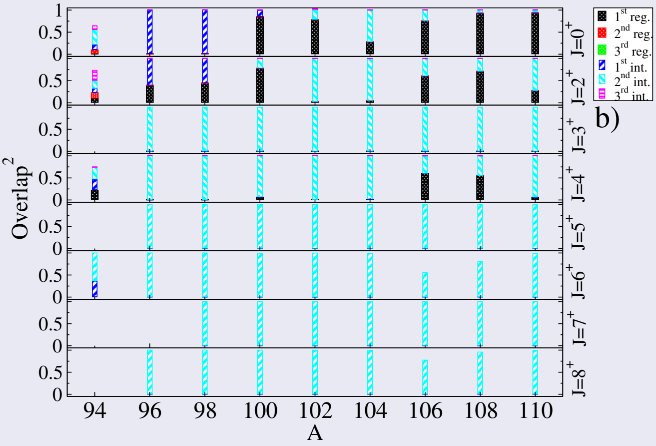
Wave function

Overlap with the intermediate basis: first state



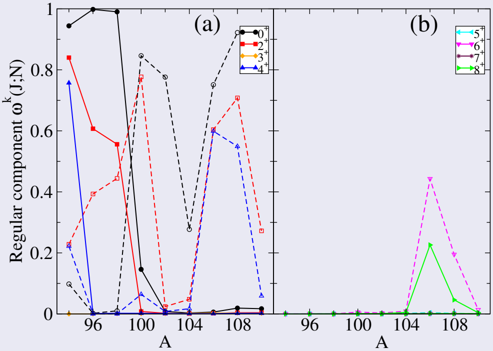
Wave function

Overlap with the intermediate basis: second state



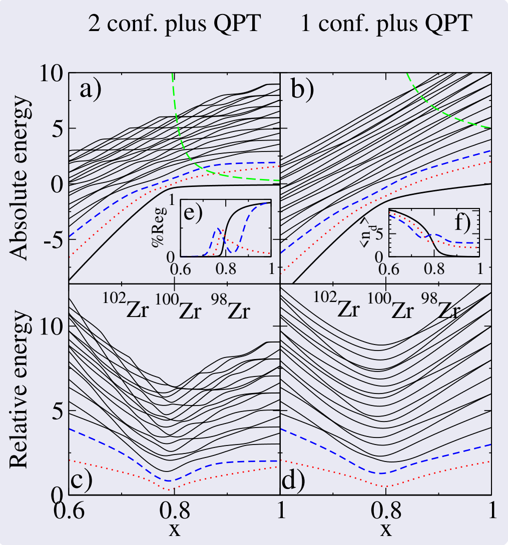
Wave function

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
$w^k(J,N) \equiv \sum_i \mid a_i^k(J;N) \mid^2$.

QPT plus configuration mixing



Two configurations:

$\varepsilon_N = 1$, $\varepsilon_{N+2} = x$,
$\kappa_{N+2} = \frac{x-1}{N+2}$,
$\chi = -\sqrt{7}/2$,
$\omega_0^{N,N+2} = \omega_2^{N,N+2} = 0.02$,
and $\Delta^{N+2} = 0.75$.
$N = 18$ $(N + 2 = 20)$

Single configuration:

$\varepsilon = x$, $\kappa = \frac{x-1}{N}$,
$\chi = -\sqrt{7}/2$. $N = 20$.