EPJ Web of Conferences **324**, 00027 (2025) https://doi.org/10.1051/epjconf/202532400027
NSD2024

The enhancement of deformation in odd-even nuclei around A = 100

E. Maya-Barbecho[1,*] and *J.E.* García-Ramos[1,3,**]

[1]Departamento de Ciencias Integradas y Centro de Estudios Avanzados en Física, Matemática y Computación, Universidad de Huelva, 21071 Huelva, Spain
[2]Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, Fuentenueva s/n, 18071 Granada, Spain

Abstract. In this contribution, the shape coexistence phenomenon near the Z=40 proton sub-shell closure is analyzed for both even-even and odd nuclei around neutron number N=60. The onset of deformation is compared in even and odd nuclei using the intrinsic state formalism of the Interacting Boson Fermion Model with configuration mixing, which is presented for the first time in this contribution. The Nb isotopes are studied in detail showing that the onset of deformation can be explained in terms of the crossing of two configurations leading to a Type II Quantum Phase Transition.

1 Introduction

Shape coexistence is a phenomenon observed not only in many regions of the nuclear mass table but also in other systems, such as certain molecules, where it is manifested as molecular isomerism. In the atomic nuclei, shape coexistence is mainly associated to the areas near neutron as well as proton shell or sub-shell closures [1, 2], but recently it has been suggested to be present in many other areas [3].

The most traditional explanation for shape coexistence is based on the fact that in nuclei near a shell closure, there is a tendency to sphericity, and, therefore, particle-hole excitations (p-h) will become energetically costly because of the existence of a large energy gap. However, the energy of these excitations can be significantly reduced due to the enhanced quadrupole and pairing residual interactions, brought about by the presence of more effective valence nucleons [1]. Consequently, these excitations correspond to more deformed states. This effect becomes particularly significant when protons are near a shell closure, while neutrons are situated in the middle of a shell, or vice versa. In this scenario, shape coexistence arises in nuclei due to the coexistence of regular states (0p-0h excitations) with intruder ones (2p-2h excitations) within the same energy range despite having distinct deformations. Particularly interesting are the extreme cases where intruder states can even have lower energies than regular states [4].

In this contribution, we will approach what is the effect of adding an unpaired proton to an even nuclei around Z=40 and N=60. First, we will analyze the experimental systematics of radii and two-neutron separation energies (S_{2n}), setting apart odd and even neutron number cases. Secondly, we will present the so called intrinsic state formalism of the Interacting Boson Fermion Model (IBFM) [5] with configuration mixing (IBFM-CM), which is introduced here for the first time. This new formalism will be applied to the positive parity states of the Nb isotopes.

2 The onset of deformation: differences between even and odd nuclei

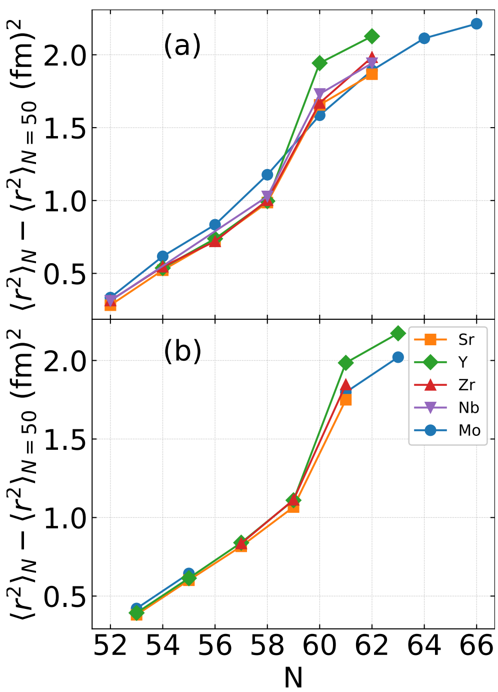

Figure 1. Experimental mean-square radii for Sr, Y, Zr, Nb, and Mo isotopes as a function of the neutron number. a) Even number of neutrons. b) Odd number of neutrons.

The region around N=60 and Z=40 is highly known for the sudden appearance of deformation. This fact was

*e-mail: esperanza.maya@alu.uhu.es
**e-mail: enrique.ramos@dfaie.uhu.es

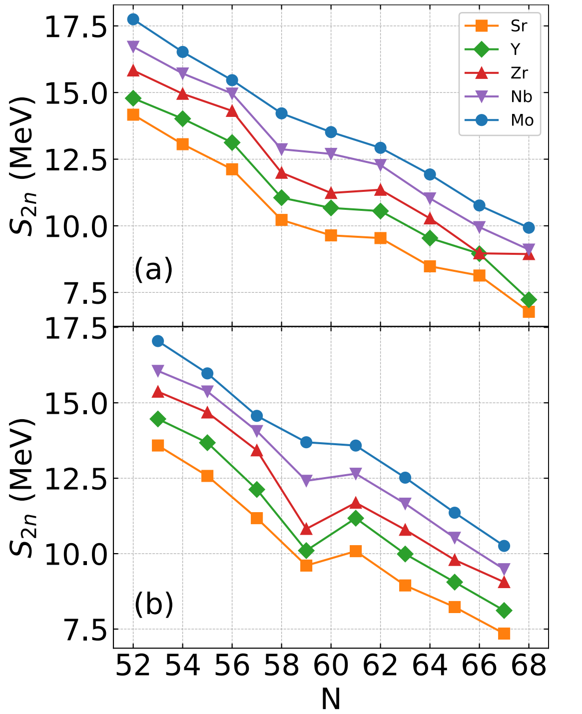

Figure 2. Experimental S_{2n} for Sr, Y, Zr, Nb, and Mo isotopes as a function of the neutron number. a) Even number of neutrons. b) Odd number of neutrons.

nicely explained in [6] in terms of the simultaneous occupation of neutrons and protons of spin-orbit partners, namely $1g_{9/2}$ for protons and $1g_{7/2}$ for neutrons, leading to proton 2p-2h excitations highly favored thanks to the spin-orbit partner interaction. This phenomenon has been also explained more recently in [7] in terms of the nuclear tensor interaction.

Nuclear deformation is not a direct observable but it can be extracted, on the one hand, in a quite direct way studying the systematics of the nuclear radii. On the other hand, the study of the S_{2n} also provides an indirect way to analyze the evolution of the nuclear deformation over an isotope chain. Because of the strong pairing component of the nuclear deformation, it is expected that odd and even nuclei will behave distinctly, hence, we have decided to present results for radii and S_{2n} separately for even and odd neutron number.

In Fig. 1, the radii are presented. In the case of even number of neutrons, panel a), it is clearly marked N=60, where there is a sudden increase in the radius. This is remarkable in Sr and Zr (even proton number) but specially in Y and Nb (odd proton number). Finally, in Mo a smooth trend is observed, which marks the end of the area of the onset of deformation [8]. When moving into the odd neutron number case, panel b), one observes a remarkable resemblance with the even case, with a rapid increase of the radius at N=60. Note that in the case of Y and Nb the nuclei are odd-odd and that for Mo there is no data for the central area. In summary, there are not noticeable differences differences between the even and the odd neutron number cases in the case of the radius.

In Fig. 2, the S_{2n} is depicted, separating, once more, the cases of even and odd neutron numbers. In both panels, one can easily note a sudden change in the slope of S_{2n} at N=60, being much more abrupt in the case of odd neutron number (panel b)). As a matter of fact, even in the case of Mo it is observed the flattening of the slope at N=60 for odd neutron number. In general, no differences are observed between the even and odd proton cases.

Hence, the onset of deformation in this area is a little more strong in the odd neutron case. Note that this is also so in Y and Nb isotopes that are also odd in the proton number. In other words, nuclei with either even or odd neutron number behave similarly regardless their proton character. This suggests that in this mass region the fastest changes appear for odd number of neutrons.

It is worth noting that this behavior observed in S_{2n} is also connected with the existence of a Quantum Phase Transition (QPT) [9]. The nature of the QPT can be connected with coexistence of two minima in an energy surface (Type I QPT) [9] or to the crossing of two different configurations (Type II QPT) [10].

3 The formalism

The IBFM [5] is a natural extension of the Interacting Boson Model (IBM) [11], where the nuclear system, described in terms of bosons with angular momentum L=0 (s) and L=2 (d), is coupled to the unpaired nucleon, either neutron or proton. The number of bosons, N, will correspond to half the number of valence nucleons (excluding the unpaired one). Here, we will deal with IBFM enlarged with the integration of 2p-2h excitations, i.e., with configuration mixing (IBFM-CM) [12, 13].

The Hamiltonian of the IBFM is written is terms of a boson, a fermion and a boson-fermion part,

$$\hat{H} = \hat{H}_B + \hat{H}_F + \hat{V}_{BF}. \tag{1}$$

The inclusion of 2p-2h excitations implies the use of a boson space $[N] \oplus [N+2]$ and, therefore,

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

where $\hat{H}^N$ stands for the regular Hamiltonian, $\hat{H}^{N+2}$ for the intruder one, $\hat{V}^{N,N+2}_{\text{mix}}$ is the mixing term and Δ^{N+2} the offset between both configurations. $\hat{P}_X$ ($\hat{P}^{\dagger}_X$) stands for the projector into the corresponding space. For a detailed description of the IBFM-CM Hamiltonian terms, we refer to [14, 15].

The proposed intrinsic state formalism of the IBFM-CM is constructed in terms of the original intrinsic state of the IBM [9, 16, 17],

$$\begin{aligned} |N;\beta,\gamma\rangle = \frac{1}{\sqrt{N!}} \Bigg(& \frac{1}{\sqrt{1+\beta^2}} \Big(s^{\dagger} + \beta \cos\gamma \, d^{\dagger}_{0} \\ & + \frac{1}{\sqrt{2}} \beta \sin\gamma \, (d^{\dagger}_{2} + d^{\dagger}_{-2}) \Big) \Bigg)^{N} |0\rangle, \end{aligned} \tag{3}$$

but adding a fermion that can be in any of the available shells, therefore, for taking into account the fermion degree of freedom, a matrix form is introduced,

$$\mathcal{H}_{IBFM}(N,\beta,\gamma) = \sum_{j,m}(E_B(N,\beta,\gamma)+\epsilon_j)a^\dagger_{j,m}a_{j,m} + \sum_{j_1,m_1,j_2,m_2} E_{BF}(N,\beta,\gamma)_{j_1,m_1,j_2,m_2} \times (a^\dagger_{j_1,m_1}a_{j_2,m_2} + a^\dagger_{j_2,m_2}a_{j_1,m_1}). \quad (4)$$

Where $a_{j,m}(a^\dagger_{j,m})$ are the fermion operators, ϵ_j the fermion single-particle energies, $E_B(N,\beta,\gamma)$ stands for the matrix element of $\hat{H}_B$ with the intrinsic state (3) (see [16]), and $E_{BF}(N,\beta,\gamma)_{m_1,m_2}$ is the matrix element of $\hat{V}_{BF}$ (see [18] although only for a single j shell). This formalism needs to be expanded to consider the regular and the intruder configurations as was introduced for the case of bosons in [19, 20],

$$\mathcal{H}^{CM}_{IBFM}(N,\beta,\gamma) = \begin{pmatrix} \mathcal{H}_{IBFM}(N,\beta,\gamma) & \Omega_{BF}(\beta) \\ \Omega_{BF}(\beta) & \mathcal{H}_{IBFM}(N+2,\beta,\gamma) \end{pmatrix}, \quad (5)$$

where $\Omega_{BF}(\beta)$ is written as

$$\Omega_{BF}(\beta) = \sum_{j_1,m_1} V_{mix}(\beta)\, a^\dagger_{j_1,m_1}a_{j_1,m_1}, \quad (6)$$

the expression of $V_{mix}(\beta)$ can be found in [19] and the matrix (6) is diagonal with a dimension of $\sum_j(2j+1)$. The matrix (5) has a dimension of $2\times\sum_j(2j+1)$. Its diagonalization provides $2\times\sum_j(2j+1)$ eigenvalues that depend on β and γ. Each of them should be minimized having, in principle, a different set of equilibrium deformation parameters (β_0,γ_0).

This new IBFM-CM intrinsic state formalism allows to analyze energy surfaces in nuclei with an odd number of nucleons including two different 2p-2h configurations, being possible to consider fermions in a single- or a multiple-j shell. The triaxial degree of freedom, γ, is explicitly taken into account. In section 4, this formalism will be used to study the onset of deformation and the mean-field energy surfaces in the Nb isotopes.

4 The results

Nb isotopes have been studied in detail in the framework of the laboratory frame of the IBFM-CM in Refs.[14, 15], where a complete quantum analysis was carried out obtaining the values of the Hamiltonian parameters and providing a global description of the isotope chain $^{93-103}$Nb (see [14, 15] for the parameter values). We will use those Nb Hamiltonian parameters as well as apply the IBFM-CM intrinsic state formalism. In this contribution, the focus will be on the axial case of the positive parity states while the general case will be presented elsewhere [21]. The positive parity states correspond to placing the odd proton in the $1g_{9/2}$ shell.

To start the analysis, it is very convenient to study the eigenstates of (5) corresponding to the unmixed case, i.e., using $V_{mix}=0$. In Fig. 3a, the energy of the states is depicted, separating between regular (full lines) and intruder states (dashed lines) as a function of the projection of the

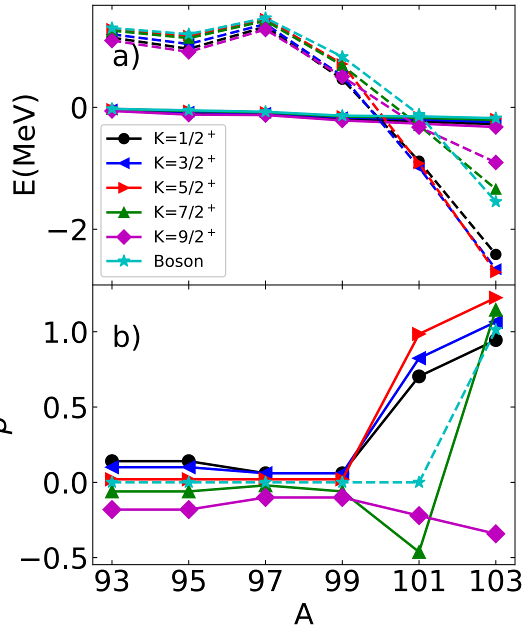

Figure 3. a) Unperturbed axial energies as a function K^π, full lines for regular while dashed ones for intruder states. b) β value for the lowest states of each K^π value. In both panels the boson curves are depicted

angular momentum, K, over the symmetry axis, assuming axial symmetry. As a reference, it is also plotted the regular and the intruder boson energies (cyan line with stars). In Fig. 3b the value of β that minimizes the energy of the lowest state for each projection K is plotted regardless of its regular or intruder nature. This figure clearly confirm the crossing in the ground state of two configurations with rather different deformation. As a matter of fact, the sudden onset of deformation is due to such a crossing. Note that for $K^\pi = 1/2^+, 3/2^+, 5/2^+, 7/2^+$ the onset of deformation appears before than for the boson system, while for $K^\pi = 9/2^+$ the deformation remains quite stable along all the isotope chain.

In Fig. 3a, it is also noticeable that the lowest state for $^{93-99}$Nb has $K^\pi = 9/2^+$, which is in agreement with the experimental ground state $j = 9/2^+$. In $^{101-103}$Nb, the lowest state has $K^\pi = 5/2^+$, but it is almost degenerated with $K^\pi = 3/2^+$ and $1/2^+$, once more in correspondence with the experimental ground state $j = 5/2^+$. Note that this calculation does not include the mixing term.

In Fig. 4, the axial energy surfaces in term of K^π are detailed, considering in this case $V_{mix} \neq 0$. The regular and intruder unmixed boson energy surfaces are provided as a reference. Note that the presented energy curves have a certain mixing between regular and intruder components. In the lightest isotopes there is a clear separation in two groups that can be proved to correspond to essentially pure regular (the lowest ones) and pure intruder states (the highest ones). When moving to heavier nuclei, clearly the two sets of configurations start mixing and crossing. When the heaviest isotopes ($^{101-103}$Nb) are reached, the lowest state for each K value presents a deformed minimum, having a large intruder character.

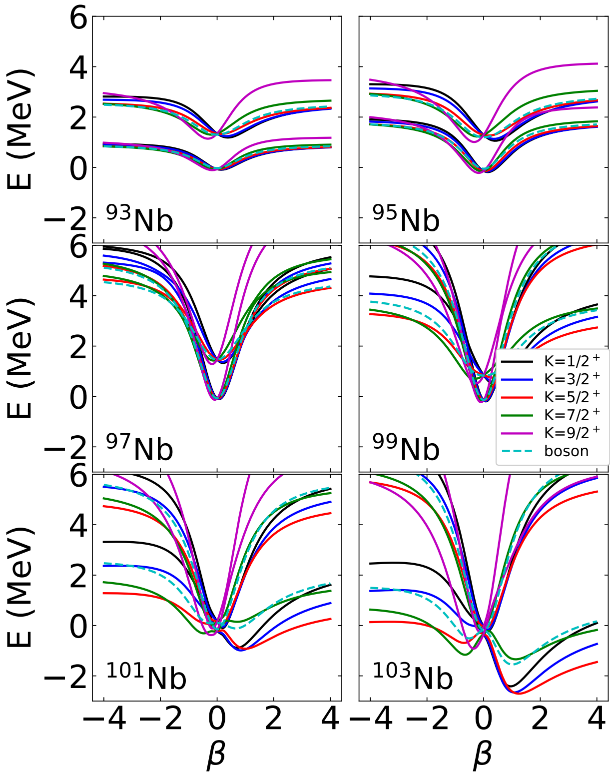

Figure 4. Axial energy curves as a function of K^{+} for $^{93-103}$Nb isotopes, including $V_{mix} \neq 0$. The unperturbed boson energy curves are depicted as a reference.

5 Conclusions

In this contribution we have explored the experimental values of nuclear radii and S_{2n} of nuclei around Z=40 and N=60 in order to see whether there is a difference in systematics when studying separately even and odd number of neutrons. In the case of radii, only tiny differences are observed between odd- and even-neutron numbers, but in the case of S_{2n}, more drastic changes are observed in the slope of S_{2n} in the odd-neutron case, showing even a clear dip at N=60.

Furthermore, we have presented the new intrinsic state formalism of the IBFM-CM and we have shown some results using realistic Hamiltonians for Nb isotopes. We have proved that there is a crossing of two configurations at N=60, that finally is at the origin of a QPT [10, 22] of Type II in Nb, also known in Zr. The odd Z value in Nb seems to enhance the abruptness of the QPT.

6 Acknowledgements

The authors thank N. Gavrielov and J.M. Arias for useful discussions and also thank N. Gavrielov for providing Nb parameters. This work was partially supported by grant PID2022-136228NB-C21 funded by MCIN/AEI/10.13039/50110001103 and “ERDF A way of making Europe”. EMB thanks economical support from grant AST22-00001-X funded by EU "NextGenerationEU", by MCIN/AEI/10.13039/50110001103, by Consejería de Universidad, Investigación e Innovación de la Junta de Andalucía and by University of Huelva. Resources supporting this work were provided by the CEAFMC and Universidad de Huelva High Performance Computer (HPC@UHU) funded by ERDF/MINECO project UNHU-15CE-2848.

References

[1] K. Heyde, J.L. Wood, Shape coexistence in atomic nuclei, Rev. Mod. Phys. **83**, 1467 (2011). 10.1103/RevModPhys.83.1467

[2] P.E. Garrett, M. Zielińska, E. Clément, An experimental view on shape coexistence in nuclei, Progress in Particle and Nuclear Physics **124**, 103931 (2022). https://doi.org/10.1016/j.ppnp.2021.103931

[3] D. Bonatsos, K. Karakatsanis, A. Martinou, T. Mertzimekis, N. Minkov, Microscopic origin of shape coexistence in the N=90, Z=64 region, Physics Letters B **829**, 137099 (2022). https://doi.org/10.1016/j.physletb.2022.137099

[4] J.E. García-Ramos, K. Heyde, Quest of shape coexistence in Zr isotopes, Phys. Rev. C **100**, 044315 (2019). 10.1103/PhysRevC.100.044315

[5] F. Iachello, P. Van Isacker, The Interacting Boson-Fermion Model, Cambridge Monographs on Mathematical Physics (Cambridge University Press, 1991)

[6] P. Federman, S. Pittel, Towards a unified microscopic description of nuclear deformation, Phys. Lett. B **69**, 385 (1977). https://doi.org/10.1016/0370-2693(77)90825-5

[7] T. Togashi, Y. Tsunoda, T. Otsuka, N. Shimizu, Quantum Phase Transition in the Shape of Zr isotopes, Phys. Rev. Lett. **117**, 172502 (2016). 10.1103/PhysRevLett.117.172502

[8] E. Maya-Barbecho, S. Baid, J.M. Arias, J.E. García-Ramos, At the borderline of shape coexistence: Mo and Ru, Phys. Rev. C **108**, 034316 (2023). 10.1103/PhysRevC.108.034316

[9] A. Dieperink, O. Scholten, On shapes and shape phase transitions in the interacting boson model, Nucl. Phys. A **346**, 125 (1980). https://doi.org/10.1016/0375-9474(80)90492-3

[10] N. Gavrielov, A. Leviatan, F. Iachello, Intertwined quantum phase transitions in the Zr isotopes, Phys. Rev. C **99**, 064324 (2019). 10.1103/PhysRevC.99.064324

[11] F. Iachello, A. Arima, The interacting boson model (Cambridge University Press, Cambridge, 1987)

[12] P.D. Duval, B.R. Barrett, Configuration mixing in the interacting boson model, Phys. Lett. B **100**, 223 (1981). https://doi.org/10.1016/0370-2693(81)90321-X

[13] P.D. Duval, B.R. Barrett, Quantitative description of configuration mixing in the interacting boson model, Nucl. Phys. A **376**, 213 (1982). https://doi.org/10.1016/0375-9474(82)90061-6

[14] N. Gavrielov, A. Leviatan, F. Iachello, Mixed configurations and intertwined quantum phase transi-

tions in odd-mass nuclei, Phys. Rev. C **106**, L051304 (2022). 10.1103/PhysRevC.106.L051304

[15] N. Gavrielov, Configuration mixing and intertwined quantum phase transitions in odd-mass niobium isotopes, Phys. Rev. C **108**, 014320 (2023). 10.1103/PhysRevC.108.014320

[16] J. Ginocchio, M. Kirson, An intrinsic state for the interacting boson model and its relationship to the Bohr-Mottelson model, Nucl. Phys. A **350**, 31 (1980). https://doi.org/10.1016/0375-9474(80)90387-5

[17] A.E.L. Dieperink, O. Scholten, F. Iachello, Classical Limit of the Interacting-Boson Model, Phys. Rev. Lett. **44**, 1747 (1980). 10.1103/PhysRevLett.44.1747

[18] D. Petrellis, A. Leviatan, F. Iachello, Quantum phase transitions in Bose–Fermi systems, Annals of Physics **326**, 926 (2011). https://doi.org/10.1016/j.aop.2010.12.001

[19] A. Frank, O. Castaños, P.V. Isacker, E. Padilla, The Geometry of the IBM with Configuration Mixing, AIP Conf. Proc. **638**, 23 (2002). 10.1063/1.1517933

[20] A. Frank, P.V. Isacker, F. Iachello, Phase transitions in configuration mixed models, Phys. Rev. C **73**, 061302 (2006). 10.1103/PhysRevC.73.061302

[21] Maya-Barbecho, J.E. García-Ramos, work in progress (2024).

[22] J.E. García-Ramos, K. Heyde, Subtle connection between shape coexistence and quantum phase transition: The Zr case, Phys. Rev. C **102**, 054333 (2020). 10.1103/PhysRevC.102.054333