Shell Model Far From Stability: Island of Inversion Mergers

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Abstract. In this study we propose a common mechanism for the disappearance of shell closures far from stability. With the use of Large Scale Shell Model calculations (SM-CI), we predict that the region of deformation which comprises the heaviest Chromium and Iron isotopes at and beyond N=40 will merge with a new one at N=50 in an astonishing parallel to the N=20 and N=28 case in the Neon and Magnesium isotopes. We propose a valence space including the full pf-shell for the protons and the full sdg shell for the neutrons, which represents a come-back of the harmonic oscillator shells in the very neutron rich regime. Our calculations preserve the doubly magic nature of the ground state of ⁷⁸Ni, which, however, exhibits a well deformed prolate band at low excitation energy, providing a striking example of shape coexistence far from stability. This new Island of Inversion (IoI) adds to the four well documented ones at N=8, 20, 28 and 40.

1. Introduction
The limits of the nuclear stability and the origin of the chemical elements in the universe are burning issues in nuclear physics. These fundamental questions pose a major challenge to our theoretical understanding of nuclei, in particular towards the neutron drip line. The link between the nuclear structure of neutron-rich nuclei and nucleosynthesis is well established; for instance, the modeling of the composition of neutron-star crusts requires the knowledge of the binding energies and the structure of the nuclides near the N=50 and N=82 shell closures [1]. Intense experimental programs are devoted to structure studies of neutron-rich exotic nuclei and recently the details of the shape coexistence in ⁶⁸Ni and the existence of a new IoI surrounding ⁶⁴Cr have been explored [2, 3, 4, 5, 6, 7, 8, 9, 10, 11] and theoretical described [13, 14]. In this study, we describe the occurrence of a new Island of Inversion (IoI) at N=50 and an equivalent phenomenon of IoI’s merging occurring for N=40 and N=50 similar to the one observed between N=20 and N=28 [12]. In the meantime, there have been new experimental studies on the chromium and iron isotopes up to N=42 and N=46 respectively, which seem to support it as well [15], and interesting theoretical an experimental explorations of the physics close to ⁷⁸Ni [16, 17, 18], which have helped us a lot in the present investigation. The trends in the evolution of the
spherical mean field which favour the appearance of the IoI’s have also been discussed in ref. [19].

2. Model space and interaction

The valence designed for the study of \( ^{78}\text{Ni} \) region is defined of the \( pf \) shell for protons and the \( sdg \) shell for neutrons using an inert core of \( ^{60}\text{Ca} \). When full space calculations are not feasible, the configurational space is extended up to eight particle-hole excitations across the \( Z = 28 \) and \( N = 50 \) gaps ensuring convergence of the wave functions. The dimensions of the matrices to be diagonalized are at the edge of present computer capabilities for solving the problem exactly, in several cases reaching \( 2 \times 10^{10} \) Slater determinants, using Antoine and Nathan shell model codes [20, 21]. The effective interaction is based on realistic Two-Body Matrix Elements (TBME) with phenomenological constrains to incorporate missing three body effects. These constrains of monopole type are chosen to monitor

- cross-shell excitations across the proton \( Z = 28 \) gap through reproduction of the E2 strength in \( ^{80}\text{Zn} \)
- and for the neutrons to reproduce the zirconium two-neutron separation energies \( S_{2n} \).

In Fig. 1, we show the comparison between calculations and experimental \( S_{2n} \) energies including recent ISOLTRAP measurements [22]. The quality of the obtained spectroscopic known data can also be seen in 2 energies for neutron rich zinc and germanium isotopes (Fig. 2) including most recent data[23, 24] from RIKEN. We name the interaction PFSDG-U hereafter and more details can be obtained in [25]. In order to assess more clearly the deformation properties in our study, we will complement our results, prior to full diagonalisation with Constrained Hartree-Fock Calculations (CHF) within the same valence space and effective interaction.

![Figure 1](image-url)

**Figure 1.** Two-neutron separation energies compared to PFSDG-U calculations (blue points are from [22]).

3. \( ^{78}\text{Ni} \): shape coexistence

Fig. 3 shows the Potential Energy Surface obtained from CHF calculations and the low-lying spectrum resulting from the diagonalisation. At the mean field level, \( ^{78}\text{Ni} \) has a double closed structure characterized by a spherical minimum corresponding to the closed shell configuration but several minima appear at relatively low excitation energy. From the diagonalisation, the structure is much more complex, with a deformed structure with a \( 0^+ \) band-head around 2.5
Figure 2. Systematics of $2^+$ and $4^+$ excitation energies compared to PFSDG-U calculations (blue points are from [23, 24]).

MeV. The Yrast sequence also belongs to this rotationnal band up to spin $6^+$ where the crossing appears with “normal” $1p1h$ states. for this band (Tab. 1) shows the necessity to go beyond ab-initio or standard “LNPS” ($pf_g^9d^9/2_d^5/2$) space for the description of low-lying states in $^{78}\text{Ni}$ which do not predict deformed intruder states as Yrast states. On the other hand the $2^+_2$ state of “$1p1h$” nature lies around 3.1 MeV, in the energy range of recent ab-initio predictions [26].

Figure 3. Potential energy Surface and Energy spectrum for $^{78}\text{Ni}$ with the PFSDG-U effective interaction. The low-lying deformed structure is emphasized with a blue rectangle.

4. Chromium and Iron isotopes: deformation

We move now to open proton shell nuclei and investigate the chromium and iron isotopes. The PES here reflects the transition from the nickel spherical cases to clear prolate deformed minima for the chromium chain with an intermediate situation in the iron chain. From the full diagonalisation results, the deformation is present in both isotopic chains. The most deformed case is the one of $^{74}\text{Cr}$ were the $\beta$ deformation parameter extracted from the intrinsic quadrupole moment derived from the Bohr-Mottelson model [27] amounts to almost 0.4 signing a clear strong deformation regime.
Table 1. Occupancies of the low-lying deformed structure in $^{78}$Ni

|          | $f_{7/2}$ | $f_{5/2}$ | $p_{3/2}$ | $p_{1/2}$ |
|----------|-----------|-----------|-----------|-----------|
| $^p$     | 5.4       | 1.0       | 1.0       | 0.5       |
| $^n$     | 7.0       | 1.2       | 0.8       | 0.5       | 0.4       |

Figure 4. Potential Energy Surfaces for $^{70-74}$Cr (upper panel) and $^{72-76}$Fe (lower panel).

Table 2. E2 properties of the yrast states of the N=50 isotopes. Energies in MeV, B(E2)'s in e$^2$.fm$^4$, Q's in e.fm$^2$.

|          | $E^*$ ($2_1^+$) | $Q_s$ | BE2$_+^+$ | $Q_m^+$ | $\beta^m$ |
|----------|----------------|-------|------------|---------|-----------|
|          | (MeV)          | (e.fm$^2$) | (e$^2$.fm$^4$) | (e.fm$^2$) |          |
| $^{70}$Cr| 0.30           | -41   | 420        | 340     | 0.26      |
| $^{72}$Cr| 0.23           | -48   | 549        | 407     | 0.30      |
| $^{74}$Cr| **0.24**       | **-51** | **630**   | **552** | **0.39**  |
| $^{72}$Fe| 0.44           | -36   | 316        | 289     | 0.21      |
| $^{74}$Fe| 0.47           | -39   | 330        | 308     | 0.22      |
| $^{76}$Fe| 0.35           | -39   | 346        | 320     | 0.25      |

Finally, we show in Figure 5 (right panel) the evolution of the $2^+$ excitation energies for the nickel and chromium chains. The present calculations are complemented towards N=40 with the results obtained using the LNPS interaction and valence space [13]. It is seen that the magic peaks at N=40 and N=50 in the nickels disappear completely in the chromiums; the fingerprint of the onset of deformation and of the entrance into the IoI’s. The same is indeed true for the iron chain. In this figure, we also compare this evolution with the one for the calcium, silicon and magnesium chains from our previous study, using the SDPF-MIX Hamiltonian [12]. The profiles
observed between N=20-28 and N=40-50 indicates strong similarities in the physics developing far from stability. The transitions from magicity with shape coexistence to deformation appear to be a common scenario for the IoI’s.

5. Conclusions
In conclusion, the deformation mechanism observed at N=40 is predicted to extend up to N=50. Shape coexistence in doubly magic $^{78}$Ni turns out to be the portal to a new IoI at N=50, which merges with the well established one at N=40 for the isotopes with Z≤26. With this new addition, the archipelago of IoI’s in the neutron rich shores of the nuclear chart counts now five members: N=8, 20, 28, 40, and 50.

Figure 5. The chart of nuclides below $^{100}$Sn showing the Islands of Inversion and their mergers.

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References
[1] R. N. Wolf, et al. 2013 Phys. Rev. Lett. 110 041101
[2] O. Sorlin, et al. 2002 Phys. Rev. Lett. 88, 092501
[3] M. Hannawald, et al. 1999 Phys. Rev. Lett. 82 1391
[4] W. Rother, et al. 2011 Phys. Rev. Lett. 106 022502
[5] J. Ljungvall, et al. 2010 Phys. Rev. C 81 061301
[6] A. Gade, et al. 2010 Phys. Rev. C 81 051304
[7] A. Dijon, et al. 2012 Phys. Rev. C 85 031301
[8] F. Recchia, et al. 2013 Phys. Rev. C 88 041302(R)
[9] S. Suchyta, et al. 2014 Phys. Rev. C 89 021301(R)
[10] T. Baugher, et al. 2014 Phys. Rev. C 86 011305(R)
[11] H. L. Crawford, et al. 2013 Phys. Rev. Lett. 110 242701
[12] E. Courir, F. Nowacki, and A. Poves 2014 Phys. Rev. C 90 014302
[13] S. M. Lenzi, F. Nowacki, A. Poves, and K. Sieja 2010 Phys. Rev. C 82 054301
[14] L. Coraggio, A. Covello, A. Gargano, and N. Itaco 2014 Phys. Rev. C 89 024319
[15] C. Santamaria, et al. 2015 Phys. Rev. Lett. 115 192501
[16] K. Sieja, and F. Nowacki 2012 Phys. Rev. C 85 051301
[17] A. Gottardo, et al. 2016 Phys. Rev. Lett. 116 182501
[18] X. F. Yang, et al. 2016 Phys. Rev. Lett. 116 182502
[19] O. Sorlin 2014 EPJ Web of Conferences 66 01016
[20] Caurier E, Martinez-Pinedo G, Nowacki F, Poves A and Zuker A P 2005 Rev. Mod. Phys 77 427
[21] Caurier E and Nowacki F 1999 Acta. Phys. Polonica B 30 705
[22] A. Welker et al. 2017 Phys. Rev. Lett. 115 192502
[23] C. Shand et al. 2017 Phys. Lett. B 773 492
[24] M. Lettman et al. 2017 Phys. Rev. C 96 011301(R)
[25] F. Nowacki, A. Poves, E. Caurier, B. Bounthong 2016 Phys. Rev. Lett. 117 272501
[26] G. Hagen, G. R. Jansen, and T. Papenbrock 2016 Phys. Rev. Lett. 117 172501
[27] Bohr A and Mottelson B 1953 Math. Fis. Medd. Dan. Vid. Selsk 27 n° 16