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Shape Coexistence in $^{78}$Ni as the Portal to the Fifth Island of Inversion

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Large Scale Shell Model calculations (SM-CI) 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 the harmonic oscillator shells in the very neutron rich regime. The onset of deformation is understood in the framework of the algebraic SU3-like structures linked to quadrupole dominance. Our calculations preserve the doubly magic nature of the ground state of $^{78}$Ni, which, however, exhibits a well deformed prolate band at low excitation energy, providing a striking example of shape coexistence far from stability. This new IoI adds to the four well documented ones at N=8, 20, 28 and 40.

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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, given the important role played by the structure of neutron-rich nuclei in numerous astrophysical processes [1]. A peculiar manifestation of the nuclear dynamics, absent in most interacting fermionic systems, is the phenomenon of shape coexistence, i.e., the appearance of quantum states of very different shapes very close in energy, typically much smaller than what could be anticipated in a mean field description [2]. This is a major consequence of the dominant role of the correlations in the nucleus. The experimental exploration of regions of very neutron rich nuclei has recently unveiled the presence of a rich variety of shape coexistence scenarios in this sector of the nuclear chart. They are particularly frequent at the edge of the so called Islands of Inversion, (IoI’s) which appear close to semi-magic or even doubly magic nuclei. The IoI’s are formed when a group of nuclei, expected to be spherical in their ground states, become deformed, precisely because the strong nuclear quadrupole-quadrupole interaction produces a shape transition in which highly correlated many particles many holes configurations dubbed “intruders” turn out to be more bound than the spherical ones. These intruder deformed bands often appear at low excitation energy in the magic nuclei close to the IoI’s, hence, shape coexistence acts in fact as a portal to the IoI’s. An intense experimental program [3-12] has recently explored the details of the shape coexistence in $^{68}$Ni and the existence of a new IoI surrounding $^{64}$Cr. Large scale shell model calculations predicted first, and later explained in detail this behaviour [13,14], with particular emphasis in the strong similarity of the mechanisms driving the onset of deformation and the collapse of the shell closures at N=20 and N=40. Another recent experimental and theoretical finding is the merging of the IoI’s at N=20 and N=28 [15, 17]. In view of these precedents, we wondered if a new IoI might exist at N=50 and if an equivalent phenomenon of IoI’s merging occurs for N=40 and N=50, and these questions prompted this study, whose results support fully both conjectures. In the meantime, there have been new experimental measures on the chromium and iron isotopes up to N=42 and N=46 respectively, which seem to support it as well [18], and interesting theoretical an experimental explorations of the physics close to $^{78}$Ni [19,21], 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 been discussed in ref. [22].

The valence space. Why should intruder configurations produce shape coexistence in $^{78}$Ni and deformed ground states in $^{76}$Fe and $^{74}$Cr? Because of the interplay of the spherical mean field and the quadrupole-quadrupole correlations. Therefore, we must ensure that the chosen valence space can incorporate the latter properly. Due to the similarity between the N=20-28 and the N=40-50 regions, we chose to define an interaction covering the $pf$-$sdg$ valence space which parallels what we did successfully for the sd-$pf$ case [16, 17]. It is well known that quadrupole collectivity is maximised when the orbits close to the Fermi level permit the realisation of two variants of Elliott’s SU(3) [24, 26]: Pseudo-SU(3) which occurs when all the orbits of a major oscillator shell except the one with the largest j are quasi-degenerated, and Quasi-SU(3) when the orbit with the largest j and its $\Delta j=2, \Delta l=2$ partners are quasi-degenerated. For the protons, the natural space beyond Z=20 and up to Z=32-34...
is indeed the full pf shell, which will bring-in quadrupole collectivity of Quasi or Pseudo-SU(3) type depending on the number of protons and the value of the Z=28 gap. In the neutron side, as we add neutrons in excess of N=40, the role of the neutron pf-shell orbits is slowly transferred to the companions of the 0g7/2 orbit in the sdg major oscillator shell. Unfortunately, size prevents us to following the transition from N=40 to N=50 keeping both sets of neutron orbits in our valence space, but we expect a smooth transit from one space to another. The border line between the space of ref. [18] and the new valence space corresponds to closing the 1p1/2 neutron orbit as well. In the N=40 valence space, the neutron collectivity is provided by the Pseudo-SU(3) coherence of the holes below N=40 and the Quasi-SU(3) coherence of the particles above it, and the mean field regulator is the N=40 gap. Close to N=50 the build-up of collectivity is different. Neutrons above N=50 can develop Pseudo-SU(3) coherence, whereas neutron holes in the 0g7/2 neutron orbit help with their single shell prolate quadrupole moment. The mean field regulator is now the N=50 gap. In brief, the valence space proposed in this article comprises the p=3 harmonic oscillator (HO, \( E(p)=\hbar \omega(p+1/2) \)) shell (pf) for the protons and the p=4 HO shell (sdg) for the neutrons. Thus, compared to that of ref. [13] the new valence space corresponds to closing the pf shell and including the missing sdg shell orbits for the neutrons, using an inert core of \(^{60}\)Ca.

The effective interaction. Our starting effective interaction matrix elements are based on the free nucleon-nucleon interaction of reference [27], regularised and renormalised with the G-matrix techniques of reference [28]. We modify their monopole part in order to reproduce the experimental evolution of the regulating gaps in the model space. Following the previous study of \(^{78}\)Ni in [14] we have left unchanged most of the monopoles of the LNPFS interaction and, to fix the remaining ones, we have adjusted the neutron ESPE’s to reproduce the experimental binding energies of the nickel isotopes \( (S_n \text{ for } A=69 \text{ and } S_{2n} \text{ for } A=68-72) \), the binding energies of the zirconium isotopes \( A=90-98 \) and the neutron gaps in the N=50 isotones. The size of the Z=28 proton gap is controlled by the B(E2)’s from the first excited 2\(^+\) states to the 0\(^+\) ground states of the zinc and germanium isotopes around N=50. We adopt for \(^{79}\)Cu the single particle spectrum of the \( \text{jun45} \) interaction [29]. Finally, the \(^{79}\)Ni single particle spectrum and the cross-shell pf-sdg proton-neutron monopoles are constrained to reproduce the N=49 and N=51 available data. In particular the relative location of the 9/2\(^+\), 5/2\(^+\) and 1/2\(^+\) states in the N=49 isotones and their evolution from Z=30 [21] to Z=32-40 [22]. The final values of the Effective Single Particle Energies are gathered in Figure 1. We name the resulting interaction PFSDG-U. 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.

Projected Energy Surfaces. To unveil the presence of intrinsic structures underlying our SM-CI results in the laboratory frame, we have performed Constrained Hartree Fock (CHF) calculations in the pf – sdg valence space using the PFSDG-U interaction. We solve the Hartree-Fock equations constrained by the quadrupole deformation parameters \( \beta \text{ and } \gamma \) which break rotational invariance and thus produce deformed shapes – to obtain the energy as a function of these parameters. The results are displayed as contour plots in the (mass) \( \beta-\gamma \) plane (aka Projected Energy Surfaces PES) in Fig 2. It is seen that at the mean field level, \(^{78}\)Ni is an spherical doubly-magic nucleus in its ground state with local deformed oblate and prolate minima. \(^{76}\)Fe has instead three minima, spherical, prolate and oblate, the latter two connected by the \( \gamma \) degree of freedom. In the case of \(^{74}\)Cr,
whereas for the 4p-4h one we get $E(2^+)=555$ eV.

Spectroscopic results. Let’s move now to the predictions of the full fledged diagonalizations using the interaction PFSDG-U, starting with the results at fixed number of neutron excitations across the N=50 closure. For this calculations we do not impose any truncation in the proton space. The structure of the 2p-2h and 4p-4h bands are very similar for all the isotopes (except for $^{70}$Ca) and correspond to well deformed rotors with a nearly perfect J(J+1) spacing and $B(E2)$’s consistent with deformations very close to the ones obtained in the SU3 limit (we use standard effective charges $q_π=1.31$ and $q_ν=0.46$). For the 2p-2h yrast band of $^{74}$Cr we have $E(2^+)=0.27$ MeV and $B(E2)(2^+_1 \rightarrow 0^+_2)=360$ e²fm⁴, whereas for the 4p-4h one we get $E(2^+)=0.17$ MeV and $B(E2)(2^+_1 \rightarrow 0^+_2)=555$ e²fm⁴. We have estimated the correlation energies of the 2p-2h and 4p-4h neutron configurations, diagonalizing a properly normalized quadrupole interaction in the $sdg$ space for the neutrons and the $Quasi-pf$ doublet for the protons. The results are displayed in Table I. It is seen that both for the 2p-2h and 4p-4h cases the largest correlation energies correspond to $^{74}$Cr and $^{76}$Fe followed by those of $^{78}$Ni and $^{72}$Ti. Notice that removing protons from $^{78}$Ni, the intruder configurations will benefit from the gain in correlation energy and from the reduction of the N=50 neutron gap, therefore we may expect an abrupt shape change producing an IoI.

For the full diagonalizations we use a truncation scheme in terms of the sum of the number of neutron excitations across N=50 and proton excitations across Z=28 (t). We perform full space calculations for Ca, Ti and Cr and we are limited to t=8 for Ni and Fe, but the calculations seem to be converged. For $^{78}$Ni (see Fig. 3) we predict a doubly magic ground state at 65%, with a first $2^+$ excited state at 2.88 MeV, which belongs to the (prolate) deformed band based in the intruder 0⁺ which appears at an excitation energy of 2.65 MeV and a second $2^+$ of 1p-1h nature at 3.15 MeV, connected to the ground state with $B(E2)=110$ e²fm⁴. We have plotted the landscape is fully dominated by the prolate solution. These deformed structures have typically $β∼0.3$.

![FIG. 2. (color online) Projected Energy Surfaces for $^{78}$Ni, $^{76}$Fe, and $^{74}$Cr with the interaction PFSDG-U.](image)

![FIG. 3. (color online). Theoretical spectra of the N=50 isotones with the PFSDG-U interaction. In red the deformed intruder band of $^{73}$Ni.](image)

### Table I. Quadrupole correlation energies of the neutron intruder configurations, relative to the N=50 closure (in MeV).

<table>
<thead>
<tr>
<th>Component</th>
<th>$^{78}$Ni</th>
<th>$^{76}$Fe</th>
<th>$^{74}$Cr</th>
<th>$^{72}$Ti</th>
<th>$^{70}$Ca</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2p-2h$</td>
<td>5.3</td>
<td>6.5</td>
<td>7.0</td>
<td>5.3</td>
<td>2.2</td>
</tr>
<tr>
<td>$4p-4h$</td>
<td>9.3</td>
<td>10.9</td>
<td>11.3</td>
<td>9.1</td>
<td>4.8</td>
</tr>
</tbody>
</table>

### Table II. Some $E2$ properties of the N=50 isotones. Energies in MeV, $B(E2)$’s in e²fm⁴, Q’s in efm².

<table>
<thead>
<tr>
<th>Isotope</th>
<th>$\Delta E$</th>
<th>$B(E2)_{2^+ \rightarrow 0^+}$</th>
<th>$Q_π$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{78}$Ni</td>
<td>2.88</td>
<td>3.45</td>
<td>-39</td>
</tr>
<tr>
<td>$^{76}$Fe</td>
<td>0.43</td>
<td>1.05</td>
<td>-45</td>
</tr>
<tr>
<td>$^{74}$Cr</td>
<td>0.24</td>
<td>0.72</td>
<td>-51</td>
</tr>
<tr>
<td>$^{72}$Ti</td>
<td>0.41</td>
<td>1.02</td>
<td>-34</td>
</tr>
<tr>
<td>$^{70}$Ca</td>
<td>0.01</td>
<td>1.80</td>
<td>-3</td>
</tr>
</tbody>
</table>
ted as well the yrast 4+ which belongs to the deformed band, its 6+ member, and several states of particle-hole nature. The B(E2)(2_1^+ → 0_2^+) goes up to 516 e²fm⁴. The location of the intruder band depends of the competition of the monopole losses whose linear part is given by the neutron ESPE's and the correlation gains (see Table I). In 78Ni the balance favours the closed shell, with the intruder 2p-2h (neutron) band below 3 MeV. Removing two protons, in 76Fe, the N=50 gap is reduced and the correlation energy increased. This produces an abrupt lowering of the intruder configurations whose band-heads become nearly degenerated with the 0p-0h N=50 closure. Hence, the ground state of 76Fe turns out to be a very complicated mixture of np-nh configurations, including 21% of 0p-0h and 33% of neutron 2p-2h. The yrast 2+ appears at 0.43 MeV and it is rather of 2p-2h plus 4p-4h nature. This mismatch produces a certain quenching of the deformation and of the entrance in the IoI’s. The distortion of the spectrum is due to the mixing of the spherical and the deformed superfluid, with its ground state wave function evenly spread (24/24/21/16)% between the (0/2/4/6)p-h configurations, and a first excited 0+ state at about 500 keV of doubly magic, N=50, Z=20, character.

Finally, we gather in Figure 4 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 in the IoI’s. The same is indeed true for the iron chain. The agreement of the SM-CI description with experiment may soon extend to full chains of isotopes from the proton to the neutron drip lines, for instance from 48Ni and 44Cr (N=20) in the pf-shell with the KB3G interaction, to 80Ni and 76Cr (N=52) using PFSDG-U.

In conclusion, it looks as if Nature would like to replicate the N=40 physics at N=50. Shape coexistence in doubly magic 78Ni turns out to be the portal to a new Io 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 Io’s in the neutron rich shores of the nuclear chart counts now five members: N=8, 20, 28, 40, and 50.

Note. A paper describing the heaviest Nickel isotopes with “ab initio” methods has been posted in arXiv [30].

TABLE III. Average number of p-h excitations and occupancies of the neutron and proton orbits above N=50 and Z=28 for several intruder states

<table>
<thead>
<tr>
<th></th>
<th>(n^h)</th>
<th>(n^p)</th>
<th>(\sigma_{3/2}^h)</th>
<th>(\sigma_{3/2}^p)</th>
<th>(\sigma_{1/2}^h)</th>
<th>(\sigma_{1/2}^p)</th>
<th>(\sigma_{1/2}^p)</th>
<th>(\Omega_{1/2}^h)</th>
<th>(\Omega_{1/2}^p)</th>
</tr>
</thead>
<tbody>
<tr>
<td>78Ni</td>
<td>0.2</td>
<td>2.7</td>
<td>2.3</td>
<td>1.1</td>
<td>0.8</td>
<td>0.4</td>
<td>0.4</td>
<td>0.3</td>
<td>0.4</td>
</tr>
<tr>
<td>76Fe</td>
<td>2.5</td>
<td>3.0</td>
<td>1.4</td>
<td>1.2</td>
<td>0.8</td>
<td>0.6</td>
<td>0.4</td>
<td>0.8</td>
<td>0.4</td>
</tr>
<tr>
<td>74Cr</td>
<td>0.3</td>
<td>4.9</td>
<td>1.6</td>
<td>1.8</td>
<td>1.1</td>
<td>1.2</td>
<td>0.8</td>
<td>1.1</td>
<td>0.3</td>
</tr>
<tr>
<td>72Ti</td>
<td>0.2</td>
<td>4.8</td>
<td>0.9</td>
<td>2.2</td>
<td>0.7</td>
<td>0.6</td>
<td>1.3</td>
<td>0.7</td>
<td>0.1</td>
</tr>
<tr>
<td>70Ca</td>
<td>0.1</td>
<td>3.5</td>
<td>0.0</td>
<td>1.9</td>
<td>0.3</td>
<td>0.2</td>
<td>1.1</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

FIG. 4. (color online) 2+ energy systematics in the nickel and chromium isotopic chains. Experimental data compared with calculations using the LNPS [13] and PFSDG-U interactions.
very recently. Whereas both calculations agree in many aspects, they differ in the absence in the latter of the intruder, deformed, np-nh excited band, coexisting with the particle-hole states built upon the doubly magic ground state of $^{78}$Ni.

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