The existence of n-particle n-hole deformed yrare bands in the N=28 isotones is explored using full \( pf \)-shell diagonalizations and the Lanczos Strength Function method. We find different 2p-2h and 4p-4h collective bands that, when allowed to mix, more often disappear. Only the 2p-2h yrare band in \(^{52}\text{Cr}\) and the 4p-4h yrare band in \(^{56}\text{Ni}\) survive, and only in this latter case, due to the reduced density of 2p-2h states, can the band be seen as a \( \gamma \)-cascade.

**Key words:** Shell Model, Effective interactions, Full \( pf \)-shell spectroscopy, Level schemes and transition probabilities.

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The occurrence of yrare bands of enhanced collectivity, with a well defined particle-hole structure on top of the ground state, has been recently documented by experiments in \(^{56}\text{Ni}\) [1], \(^{36}\text{Ar}\) [2] and \(^{40}\text{Ca}\) [3]. In the Ni and Ar cases the bands are dominantly made of 4p-4h excitations while in the \(^{40}\text{Ca}\) the leading structure is 8p-8h [4]. In \(^{56}\text{Ni}\) the band is classified as highly deformed \( \beta = 0.3/0.4 \), while in \(^{36}\text{Ar}\) and \(^{40}\text{Ca}\) they are characterised as superdeformed with \( \beta = 0.4/0.5 \) and \( \beta = 0.5/0.6 \) respectively. In a recent study [5], Mizusaki and co-workers have carried out a theoretical search for this kind of bands in the N=28 isotopes, using the Monte Carlo shell model approach. In this article we examine the same topic, in the framework of full \( pf \)-shell diagonalizations using the Lanczos method.

The \( pf \)-shell has been the locus of a lot of activity in nuclear structure since the advent of the exact \( 0h\omega \) calculations in \(^{48}\text{Cr}\) [6]. In a recent article [7] we have extend the full \( pf \)-shell calculations up to \( A=52 \) and we have introduced
the interaction KB3G, the one used in this work. The diagonalizations are performed in the \( m \)-scheme using a fast implementation of the Lanczos algorithm through the code ANTOINE \([8]\) or in J-coupled scheme using the code NATHAN \([9]\). Some details may be found in ref. \([10]\). The Lanczos Strength Function (LSF) method, following Whitehead’s prescription \([11]\), is explained and illustrated in refs. \([12,13,14]\).

The calculation of yrare bands in nuclei with large shell model dimensionalities, poses serious computational problems. The reason is that, most often, the interesting states lie at excitation energies where the level density is high. This represents a real challenge for all the shell model approaches, because it requires the calculation of many states of the same spin and parity. While this can be easily done for \( m \)-scheme dimensions of a few millions, the task becomes formidable for dimensions of tens of millions. The method of ref \([5]\) relies in the existence of local minima in the projected energy surface resulting of a constrained Hartree-Fock calculation. The Slater determinants corresponding to these minima are then fed into the quantum Monte Carlo diagonalization method (\textit{qmcd}). While this method is reasonably under control for the yrast states and other states originating in well defined minima, it is not clear how would it work in less clear-cut situations. As an example, ref \([5]\) claims that the \textit{qmcd} method is unpractical to describe a possible 4p-4h band in \(^{54}\text{Fe}\), which is then studied at a lower level of approximation, doing variation after projection (VAP) on the cranked Hartree-Fock solution.

Our method proceeds by three steps:

I) The space of solutions is explored by means of diagonalizations restricted to configurations with a fixed number of particle-hole excitations on the top of the reference one \((1f_{7/2})^N\), searching for collective bands.

II) If such bands are found, we proceed to immerse the bandhead state in the full space by means of the Lanczos Strength Function method, i.e. we take the np-nh ground state and use it as starting vector for the Lanczos iterations in the full space, in order to know whether it stands the mixing or not.

III) If it survives to the mixing, we try to build the physical band acting repeatedly upon it with the quadrupole operator and using again the LSF method as described below.

Let’s proceed with the first step in the four cases of interest, \(^{50}\text{Ti}, \(^{52}\text{Cr}, \(^{54}\text{Fe} \) and \(^{56}\text{Ni}\). In tables 1, 2, 3 and 4 we list the excitation energies and the BE2’s corresponding to the fixed 2p-2h and 4p-4h bands. In \(^{50}\text{Ti}\) none of the bands appear to be really collective, even though there is a certain quadrupole linking among the states. In \(^{52}\text{Cr}\) both are quite regular, with large BE2’s in the 4p-4h case. For \(^{54}\text{Fe}\) the situation is more complex; the 2p-2h band is clearly less collective than the corresponding one in \(^{52}\text{Cr}\), with a neat bifurcation at
J=6, while the 4p-4h band mimics perfectly a well deformed rotor. The same is valid for the 4p-4h band of $^{56}$Ni; in this nucleus the 2p-2h band shows no collectivity at all.

Table 1
Properties of the fixed 2p-2h and 4p-4h bands in $^{50}$Ti. Energies in MeV, B(E2)'s in $e^2 fm^4$, Q's in $e fm^2$.

| J  | ΔE  | B(E2)↓ | ΔE  | B(E2)↓ |
|----|-----|--------|-----|--------|
| 0  | 0.00|        | 0.00|        |
| 2  | 0.54| 78     | 0.59| 126    |
| 4  | 1.28| 106    | 1.79| 153    |
| 6  | 1.99| 103    | 2.42| 1      |
| 8  | 2.87| 86     | 3.49| 122    |
| 10 | 4.15| 66     | 4.67| 80     |
| 12 | 5.59| 40     | 5.97| 51     |

Table 2
Properties of the fixed 2p-2h and 4p-4h bands in $^{52}$Cr. Energies in MeV, B(E2)'s in $e^2 fm^4$, Q's in $e fm^2$.

| J  | ΔE  | B(E2)↓ | ΔE  | B(E2)↓ |
|----|-----|--------|-----|--------|
| 0  | 0.00|        | 0.00|        |
| 2  | 0.39| 112    | 0.46| 242    |
| 4  | 1.08| 157    | 1.21| 313    |
| 6  | 2.00| 162    | 1.97| 322    |
| 8  | 3.12| 156    | 2.92| 325    |
| 10 | 4.31| 105    | 4.33| 304    |
| 12 | 5.60| 96     | 6.10| 241    |

In our second step, we take the 0$^+$ band-head and allow it to mix with all the states. To optimize the calculation as well as to keep track of the initial state, we take it as starting vector (“pivot”) in the Lanczos construction in the full space (or in a large enough one). After N iterations, we compute its overlaps with the N quasi-physical states. For the fixed np-nh bandhead to be representative of a “physical” bandhead, there must be a single state that has a large overlap with it. As a bonus, this state is converged in very few
Table 3
Properties of the fixed 2p-2h and 4p-4h bands in $^{54}$Fe. The numbers in parenthesis correspond to non-yrast states that appear to be more strongly related to the band. Energies in MeV, $B(E2)$’s in $e^2 fm^4$, $Q$’s in $fm^2$.

| J   | $\Delta E$ | $B(E2)_{\downarrow}$ | $\Delta E$ | $B(E2)_{\downarrow}$ |
|-----|------------|----------------------|------------|----------------------|
| 0   | 0.00       | 0.00                 | 0.00       |                      |
| 2   | 0.45       | 101                  | 0.35       | 320                  |
| 4   | 1.35       | 138                  | 1.07       | 447                  |
| 6   | 2.36(2.51) | 11(125)              | 2.09       | 479                  |
| 8   | 3.61(3.82) | 44(91)               | 3.36       | 478                  |
| 10  | 4.79       | 1                    | 4.86       | 466                  |
| 12  | 4.92       | 11                   | 6.56       | 416                  |

Table 4
Properties of the fixed 2p-2h and 4p-4h bands in $^{56}$Ni. Energies in MeV, $B(E2)$’s in $e^2 fm^4$, $Q$’s in $fm^2$.

| J   | $\Delta E$ | $B(E2)_{\downarrow}$ | $\Delta E$ | $B(E2)_{\downarrow}$ |
|-----|------------|----------------------|------------|----------------------|
| 0   | 0.00       | 0.00                 | 0.00       |                      |
| 2   | 0.74       | 25                   | 0.43       | 313                  |
| 4   | 1.50       | 13                   | 1.37       | 439                  |
| 6   | 1.79       | 24                   | 2.70       | 467                  |
| 8   | 1.82       | 1                    | 4.30       | 459                  |
| 10  | 2.74       | 3                    | 6.07       | 418                  |
| 12  | 4.99       | 0                    | 7.90       | 283                  |

iterations, what makes the method computationally efficient. In figure 1 we have plotted the overlaps for the 2p-2h (upper panel) and 4p-4h (lower panel) band-heads in $^{52}$Cr. The calculations are carried out in the full $pf$-shell (m-scheme dimension 45 millions) using the coupled code Nathan ($0^+ \times 10^5$) and 150 iterations are made. Notice how the 2p-2h state is concentrated at 45% in one “physical” state with no other one taking any relevant share. The excitation energy of this state, 2.43 MeV, is in correspondence with the experimental $0^+_2$ at 2.65 MeV. It has a 46% content of 2p-2h, 26% of 3p-3h, 18% of 4p-4h and minor percentages of the other components. The fact that the mixing takes place with components of higher p-h rank should result in
an increase of collectivity with respect to the fixed 2p-2h band. Besides the “coherent” 2p-2h state, the next four $0^+$ states produced by the calculation are also in correspondence with the experimental $0^+$'s:

$0_2^+$; exp. 4.74 MeV; th. 5.15 MeV,
$0_4^+$; exp. 5.60 MeV; th. 5.47 MeV,
$0_5^+$; exp. 5.75 MeV; th. 6.04 MeV,
$0_6^+$; exp. 6.10 MeV; th. 6.30 MeV,

a rather spectacular achievement of the shell model spectroscopy!!

![Graph](image)

Fig. 1. Overlaps of the 2p-2h(a) and 4p-4h(b) band-heads in $^{52}$Cr with the physical states.

On the contrary, the much more collective 4p-4h band-head is completely dissolved in the full space; no physical state carries a dominant fraction of the overlap. According to that, no 4p-4h band exists in $^{52}$Cr. Whether the 2p-2h band has any experimental relevance or not, will be discussed below.

Very much the same occurs in $^{50}$Ti; the 2p-2h bandhead survives at 61% in the full space $0_2^+$ at 4.08 MeV (exp. at 3.87 MeV); the 4p-4h bandhead is fully dispersed among many physical states.

For $^{54}$Fe the full space calculations of the overlap distribution become unaffordable. However, we think that it is sufficiently safe to compute the np-nh mixing at a level of truncation $t=n+4$. In figure 2 we present the results of
these calculations (t=6 for the 2p-2h -upper panel- and t=8 for the 4p-4h -lower panel-). In this last case, the m-scheme dimension is 177 millions. Using the coupled code Nathan we deal with a $0^+$ dimension of $2.5 \times 10^6$ and make 150 iterations. The situation resembles that of $^{52}$Cr; the coherent 2p-2h state represents 43% of the $0^+_2$ at 2.77 MeV (exp. at 2.56 MeV) and no other state carries a significant fraction of it. In the 4p-4h case the fragmentation is complete, no residue of a band is left. According to this result, the claim in ref. [5] of the existence of a 4p-4h band in this nucleus, based on a VAP-CHF calculation, has to be taken with some skepticism.

![Fig. 2](image)

Fig. 2. Overlaps of the 2p-2h(a) and 4p-4h(b) band-heads in $^{54}$Fe with the physical states.

For $^{56}$Ni we refer to our calculations in [1] and to the experimental results to state the existence of a 4p-4h band. The reason why it survives in this nucleus and not in $^{54}$Fe, is clearly the very different level density in both nuclei. In $^{56}$Ni, because it is doubly magic, the number of 2p-2h states is nearly an order of magnitude smaller than in $^{54}$Fe, whose 4p-4h bands wreck in a sea of 2p-2h states.

This brings us to step III. We have now several candidates to bandheads, but, do they develop a real band? The answer is “yes” in the well known case of the 4p-4h band in $^{56}$Ni. We shall now proceed to examine the situation in the other cases. It could be done “brute force” by computing many states of each spin and their E2 transition probabilities and looking for band-like patterns, but this approach is only realistic (from the computational point of view) in $^{50}$Ti, where we have actually used it to check our approximations. The
method we use is, once again, an application of the Lanczos strength function technique. We start with the bandhead \(0^+\) and apply the quadrupole operator on it: \(Q|0^+\rangle\). This operation generates a threshold vector that we take as the “pivot” in the Lanczos procedure. We perform \(N \sim 100\) iterations to produce an approximate strength function. At this stage, either there is one state that carries most of the strength, signaling its pertenence to the band, or not, in which case there is no band. In the positive case the resulting \(|2^+\rangle\) state is retained as a band member and we proceed to act with \(Q\) on it. Now there are several possible angular momentum couplings, but we follow the \(\Delta J=2\) path in the even-even nuclei. The procedure is repeated until the strength bifurcates, dilutes or plainly disappears.

In \(^{50}\)Ti we obtain a sequence of states that fulfill the requirements discussed above. However, their energy spacings are not very much rotor-like and their \(B(E2)\)’s are only about \(100 \text{ e}^2 \text{ fm}^4\). These values are comparable to those of the yrast band. Some of these states have been measured, but they do not appear to show any band signature.

In \(^{52}\)Cr we can definitely speak of a “theoretical” yrare band. Our results for the excitation energies are very close to those of ref. [5]. In table 5 we list the excitation energies, the percentage of the \(B(E2)\) of the transition from \(J-2\) to \(J\) carried by each state, the amount of \(2p-2h\) components, the \(B(E2)\) and the spectroscopic quadrupole moments. All these numbers are consistent with a deformed band up to \(J=10\), afterwards a bifurcation and reduction of the strength takes place. Notice the large \(B(E2)\) values, similar to those of the yrast band of \(^{48}\)Cr, corresponding to \(\beta \sim 0.3\). Besides, the energy spacings are very close to those of a rigid rotor;

Table 5
Yrare \(2p-2h\) band in \(^{52}\)Cr. Excitation energies are relative to the \(0^+_2\) band-head, experimentally at 2.64 MeV and calculated at 2.43 MeV. Energies in MeV, \(B(E2)\)’s in \(\text{e}^2 \text{ fm}^4\), \(Q\)’s in \(\text{e} \text{ fm}^2\)

| J  | \(\Delta E\) | \% of \(B(E2)^{\uparrow}\) | \% of \(2p-2h\) | \(B(E2)^{\downarrow}\) | \(Q_{\text{spec}}\) |
|----|-------------|----------------|-------------|---------------|-------------|
| 0  | 0.00        | 46             |             |               |             |
| 2  | 0.44        | 77             | 43          | 238           | -27.7       |
| 4  | 1.32        | 82             | 43          | 323           | -39.3       |
| 6  | 2.51        | 77             | 42          | 329           | -39.3       |
| 8  | 4.14        | 83             | 44          | 331           | -39.2       |
| 10 | 6.03        | 66             | 39          | 239           | -25.5       |
| 12 | 8.02        | 27             | 51          | 66            | -13.7       |
| 12 | 8.31        | 28             |             |               |             |
\[ \frac{\Delta E(4^+)}{\Delta E(2^+)} = 3(3.33); \]
\[ \frac{\Delta E(6^+)}{\Delta E(4^+)} = 1.9(2.1); \]
\[ \frac{\Delta E(8^+)}{\Delta E(6^+)} = 1.65(1.71); \]
\[ \frac{\Delta E(10^+)}{\Delta E(8^+)} = 1.46(1.53); \]

(the values in parenthesis are those of the rigid rotor limit). The percentage of the 2p-2h components as well as the occupation numbers of the individual orbits are nicely constant too. The spectroscopic quadrupole moments correspond to a prolate rotor and are fully consistent with the B(E2)'s. The sequence of calculated states, 0\(^+\) at 2.43 MeV, 2\(^+\) at 2.87 MeV, 4\(^+\) at 3.75 MeV and 6\(^+\) at 4.94 MeV can be put in correspondence with the experimental ones at 2.64 MeV (0\(^+\)), 3.16 MeV (2\(^+\)), 4.04 MeV (4\(^+\)) and 5.14 MeV (6\(^+\)). However, there are no transitions experimentally observed linking these states. This means that, due to the presence of many other 2p-2h states to which to decay by M1 transitions and to the phase space enhancement of the E2 transitions to the yrast band, the “theoretical” yrare band does not show up experimentally as a \(\gamma\)-cascade. In \(^{54}\text{Fe}\) the situation is even worse. The bifurcation, already present at the fixed 2p-2h level, appears also in the “physical” band. Only the sequence 0\(^+\), 2\(^+\), 4\(^+\) behaves like a band, but with B(E2)'s substantially smaller than in the \(^{52}\text{Cr}\) yrare band.

In summary, we have found that yrare bands of a definite np-nh character exist in the N=28 isotones. When full mixing is permitted, only the 2p-2h bands survive in \(^{50}\text{Ti}, {52}\text{Cr}\) and \(^{54}\text{Fe}\), with different degrees of collectivity. In \(^{50}\text{Ni}\) it is the 4p-4h band which is physical. This is due to the difference in the 2p-2h level density in the doubly magic case. In addition, we find that the 2p-2h bands preferentially decay out, making their experimental identification very difficult.

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