The contribution of chiral three-body forces to the monopole component of the effective shell-model Hamiltonian

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We present a study of the role played by realistic three-body forces in providing a reliable monopole component of the effective shell-model Hamiltonian. To this end, starting from a nuclear potential built up within the chiral perturbation theory, we derive effective shell-model Hamiltonians with and without the contribution of the three-body potential and compare the results of shell-model calculations with a set of observables that evidence shell-evolution properties. The testing ground of our investigation are nuclei belonging to fp shell, since the shell-evolution towards shell closures in 48Ca and 50Ni provides a paradigm for shell-model Hamiltonians. Our analysis shows that only by including contributions of the three-body force the monopole component of the effective shell-model Hamiltonian is then able to reproduce the experimental shell evolution towards the closure at \( N = 28 \).

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I. INTRODUCTION

The evolution of the nuclear spectroscopic properties along isotopic and isotonic chains, towards the formation of magic numbers, is the feature that reveals the central role of the nuclear shell model (SM) and its success during the past 70 years [1-3]. Consequently, it is very desirable that effective Hamiltonians, which are employed to study the nuclear structure in the framework of the shell model, should be able to reproduce the observed shell evolution and closures.

Zuker and coworkers have extensively investigated the properties of the two-body matrix elements (TBMEs) of the residual interaction derived from realistic potentials by way of many-body perturbation theory [4], and, having performed a multipole decomposition of realistic SM Hamiltonians, have shown that their monopole component needs to be modified in order to reproduce the evolution of shell closures as a function of the number of valence nucleons [5]. They inferred that this should trace back to the lack of a three-nucleon force (3NF) in the nuclear realistic potentials employed to derive the effective SM Hamiltonian \( H_{\text{eff}} \), affecting its monopole component that, consequently, has to be corrected [8].

Extensive direct investigations about the role of 3NFs in realistic \( H_{\text{eff}} \)s have been carried out by Schwenk and coworkers, who have performed studies of oxygen [9,12] and calcium [11,13,14] isotopic chains. In the aforementioned works, the \( H_{\text{eff}} \)s were derived starting from nuclear potentials built up within the chiral perturbative expansion and softened by way of \( V_{\text{low-k}} \) technique [15,16] or the similarity renormalization-group (SRG) approach [17,18], and the results support the need of introducing three-body forces to reproduce the experimental behavior of the ground-state and yrast excitation energies as a function of the valence-nucleon number.

In order to tackle the long-standing problem of the role played by three-body forces in driving the shell evolution, we have found inspiration from the calculation of the effective single-particle energies (ESPEs) for \( p \)-shell nuclei, whose results we have presented in Ref. [19]. More precisely, we have found that the ESPEs calculated from the \( H_{\text{eff}} \) that includes contributions from both two- and three-body chiral potentials, provide a constant energy-splitting of the spin-orbit partners \( 0p_{1/2},0p_{1/2} \) as a function of the mass number \( A \). This splitting characterizes the correct reproduction of the subshell closure at \( Z,N = 6 \) observed in \( ^{12}\text{C} \), at variance with the result we have obtained omitting the contribution of the 3NF. As a matter of fact, the relative ESPE rapidly drops down if only the two-nucleon force (2NF) is included, and becomes even negative around \( A = 8 \). Then, the reproduction of the shell closure deteriorates, namely the observed energy of \( ^{12}\text{C} \) yrast \( J^+ = 2^+ \) is underestimated by \( \sim 1 \) MeV.

Since the ESPE of a level is calculated in terms of the bare single-particle (SP) energy and the monopole part of the TBMEs [20], it is clear that the above mentioned results point to an intimate relationship between 3NF and the monopole component of \( H_{\text{eff}} \).

On the above grounds, we devote the present paper to studying this connection choosing, as a testing ground, the nuclei belonging to the fp shell, namely nuclei that can be described in terms of the degrees of freedom of valence nucleons outside doubly-closed 40Ca, interacting in the model space composed by 0f1p orbitals. This region represents a paradigm to investigate the shell evolution within the shell model, since, as is well-known, the spin-orbit component of the SM mean field separates the 0f7/2 orbital from the others leading to the appearance of the
The starting point of our calculation is a nuclear potential based on chiral perturbation theory (ChPT) [21, 22], a choice that is motivated by two main considerations.

a) First, within this class of potentials long-range forces are ruled by the symmetries of low-energy quantum chromodynamics (QCD) - in particular the spontaneously broken chiral symmetry - and the short-range dynamics is absorbed into a complete basis of contact terms that are proportional to low-energy constants (LECs) fitted to two-nucleon data.

b) The second major characteristic of ChPT is that nuclear 2NF and many-body forces are generated on an equal footing [22, 24], since most interaction vertices that appear in the 3NF and in the four-nucleon force (4NF) also occur in the 2NF.

For the sake of completeness, we point out that, as in Ref. [19], a high-precision 2NF potential derived within the framework of chiral perturbation theory (ChPT) [21, 22], a choice that is motivated by two main considerations.

For the sake of consistency, the $c_1$, $c_3$, and $c_4$ LECs appearing in $V_{3\text{NF}}$, are the same as those in the N$^3$LO 2NF, their values being determined by the renormalization procedure that fits the nucleon-nucleon (NN) data [23].

Moreover, the 3NF 1π-exchange and contact terms are characterized by two extra LECs (known as $c_D$ and $c_E$, respectively), which cannot be constrained by two-body observables, but need to be determined by reproducing observables in systems with mass $A > 2$.

We adopt the same $c_D$, $c_E$ values employed in Ref. [19], namely $c_D = -1$ and $c_E = -0.34$, that have been determined by way of no-core shell model (NCSM) calculations [27, 28]. More precisely, in Ref. [27] it has been identified a set of observables in light $p$-shell nuclei that are strongly sensitive to the $c_D$ value in order to fix it, then $c_E$ has been constrained to reproduce the binding energies of the $A = 3$ system.

Details about the calculation of our 3NF matrix elements in the harmonic-oscillator (HO) basis are reported in Appendix of Ref. [19]. Note that the Coulomb potential is explicitly taken into account in our calculations.

In the same paper, a comprehensive description of the derivation of our effective SM Hamiltonians for one- and two-valence nucleon systems, starting from 2NF and 3NF, can also be found, while in the following we present only a short summary.

As mentioned before, our $H_{\text{eff}}$ is derived in the model space spanned by the four $0f_{1p}$ proton and neutron orbitals outside doubly-closed $^{40}\text{Ca}$. To this end, an auxiliary one-body potential $U$ is introduced in order to break up the Hamiltonian $H$ for a system of $A$ nucleons as the sum of a one-body term $H_0$, which describes the independent motion of the nucleons, and a residual interaction $H_1$:

\begin{equation}
H = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j=1}^{A} V_{ij}^{2\text{NF}} + \sum_{i<j<k=1}^{A} V_{ijk}^{3\text{NF}} = (1)
\end{equation}

In our calculation we use the HO potential, $U = \frac{1}{2}m\omega^2r^2$, with an oscillator parameter $\hbar\omega = 11$ MeV, according to the expression [29] $\hbar\omega = 45A^{-1/3} - 25A^{-2/3}$ for $A = 40$.

Once $H_0$ has been introduced, the reduced model space is defined in terms of a finite subset of $H_0$’s eigenvectors. The diagonalization of the many-body Hamiltonian in Eq. (1) within the infinite Hilbert space, that it is obviously unfeasible, is then reduced to the solution of an eigenvalue problem for an effective Hamiltonian $H_{\text{eff}}$ in a finite space.
Our approach to the derivation of \( H_{\text{eff}} \) is the time-dependent perturbation theory. Namely, \( H_{\text{eff}} \) is expressed through the Kuo-Lee-Ratcliff (KLR) folded-diagram expansion in terms of the vertex function \( Q \)-box, which is composed of irreducible valence-linked diagrams. We include in the \( Q \)-box one- and two-body Goldstone diagrams through third order in \( H_{2NF}^{1}\) and up to first order in \( H_{3NF}^{1} \). We stress that the input chiral 2NF and 3NF have not been modified by way of any renormalization procedures, and the perturbative properties of the \( Q \)-box from N3LO 2NF potential have been discussed in Ref. \[31\]. The folded-diagram series is then summed up to all orders using the Lee-Suzuki iteration method \[34\].

It is worth pointing out that, owing to the presence of the \(-U\) term in \( H_{2NF}^{1} \), \( U \)-insertion diagrams arise in the \( Q \)-box, and they are responsible for getting rid of the \( k\omega \) dependence introduced by the auxiliary potential \( U \) \[31\].

The \( H_{\text{eff}} \) derived for one-valence nucleon systems contains only one-body contributions and provides the SP energies for the SM calculation, while the two-body matrix elements are obtained from \( H_{\text{eff}} \) derived from the two-valence nucleon systems once the theoretical SP energies are subtracted from its diagonal matrix elements.

We have derived two \( H_{\text{eff}} \); one has been obtained calculating \( Q \)-box diagrams with 2NF vertices only, dubbed as \( H_{2NF}^{1} \). The other, indicated as \( H_{3NF}^{1} \), has been built up including also \( H_{2NF}^{1} \) first-order contributions in the collection of the \( Q \)-box diagrams (see Fig. 3 in Ref. \[19\]). In the Supplemental Material \[35\] the TBMEs of \( H_{2NF}^{1}, H_{3NF}^{1} \) can be found, while the proton and neutron SP energies calculated with respect to \( 0f_{7/2} \) orbital - \( \epsilon_{p} \) and \( \epsilon_{n} \), respectively - are reported in Table I.

### Table I: Theoretical proton and neutron SP energies (in MeV) from \( H_{2NF}^{1} \) and \( H_{3NF}^{1} \).

| Energy (MeV) | \( H_{2NF}^{1} \) | \( H_{3NF}^{1} \) |
|-------------|------------------|------------------|
| \( 0f_{7/2} \) | 0.0              | 0.0              |
| \( 0f_{5/2} \) | 4.2              | 5.1              |
| \( 1p_{3/2} \) | 0.0              | 0.5              |
| \( 1p_{1/2} \) | 1.0              | 2.0              |

In order to accomplish our goal to investigate the shell evolution of spectroscopic properties of \( fp \) nuclei, we have performed a multipole decomposition of \( H_{2NF}^{1} \) and \( H_{3NF}^{1} \), focussing our interest on their monopole components. It is worth recalling that the angular-momentum-averaged monopole component of the shell-model Hamiltonian is defined as follows:

\[
\langle i, j | H_{\text{eff}}^{\text{mon}} | i, j \rangle = \epsilon_{i} + \epsilon_{j} + \frac{\sum_{J}(2J+1)\langle i, j | V_{\text{eff}} | i, j \rangle_{J}}{\sum_{J}(2J+1)} = \epsilon_{i} + \epsilon_{j} + V_{ij}^{\text{mon}} ,
\]

where \( V_{\text{eff}} \) is the two-body component of \( H_{\text{eff}} \), \( i \) and \( j \) indicate the quantum numbers of the SP states, and the \( \epsilon_{i} \) are the SP energies. Consequently, we have also studied the evolution of the proton and neutron ESPEs as a function of the valence nucleons, that are defined as:

\[
\text{ESPE}(j) = \epsilon_{j} + \sum_{j'} V_{jj'}^{\text{mon}} n_{j'} ,
\]

where the sum runs over the model-space levels \( j \), \( n_{j} \) being the number of particles in the level \( j \).

### III. RESULTS

#### A. Monopole components of the effective SM Hamiltonians

Before we start our discussion about the characteristics of the monopole component of \( H_{2NF}^{1} \) and \( H_{3NF}^{1} \), it is worth coming back to the calculated SP energies of both effective Hamiltonians, which can be found in Fig. 1 as single-particle spectra of \( ^{41}\text{Sc} \) and \( ^{41}\text{Ca} \). We do not show in this figure any experimental counterparts, because the experimental information about the spectroscopic factors of both nuclei is rather scanty, and consequently we have no clear indications on the SP nature of the observed low-energy levels \[38\].

![FIG. 1: Calculated SP spectra of \( ^{41}\text{Sc} \) and \( ^{41}\text{Ca} \), as obtained from \( H_{2NF}^{1} \) and \( H_{3NF}^{1} \). They represent the proton and neutron SP energies, respectively, employed in our calculations.](image)

From the inspection of Fig. 1, we observ that \( H_{2NF}^{1} \) does not provide enough spin-orbit splitting between the \( 0f_{7/2}, 0f_{5/2} \) orbitals in both \( ^{41}\text{Sc} \) and \( ^{41}\text{Ca} \). Moreover, the \( 0f_{7/2} \) and \( 1p_{3/2} \) orbitals are not well-separated and, consequently, it can be inferred that calculations with \( H_{2NF}^{1} \) might not be able to describe the shell closure that is observed at \( Z, N = 28 \). On the other hand, the contribution coming from the 3NF is able to heal this defect of the SM Hamiltonian, and in the SP spectrum of \( H_{3NF}^{1} \) the \( 0f_{7/2} \) orbital is lowered enough with respect to the \( 1p_{3/2}, 1p_{1/2}, 0f_{5/2} \) orbitals to lay the foundation of a better shell closure at \( N, Z = 28 \).

Actually, a shell closure cannot be guaranteed only by the SP energy spacings, since the TBMEs of \( H_{\text{eff}} \) play a
crucial role in their evolution as a function of the valence-nucleon number. As a matter of fact, in Ref. [19] the SP energies of p-shell nuclei, calculated with and without 3NF contributions, start both from a sufficient spin-orbit splitting to provide, in principle, the $Z, N = 6$ sub-shell closure. However, we have found that the monopole component of $H_{\text{eff}}^{3\text{NF}}$ compresses the separation between the $0p_{3/2}$ and $0p_{1/2}$ orbitals when increasing the valence-nucleon number, at variance with the $H_{\text{eff}}^{2\text{NF}}$ monopole term that preserves a constant energy spacing.

On the above ground, a study of the evolution of the ESPEs of $H_{\text{eff}}^{2\text{NF}}$ and $H_{\text{eff}}^{3\text{NF}}$ in terms of the valence-nucleon number is highly desirable to understand how to obtain a sound description of their shell closure properties. This evolution of the ESPEs depends only on the TBMEs, and in the following we decide to report, without loss of generality, the neutron and proton ESPEs calculated employing the TBMEs of $H_{\text{eff}}^{2\text{NF}}$ and $H_{\text{eff}}^{3\text{NF}}$, but starting from the same set of SP energies, namely those of $H_{\text{eff}}^{2\text{NF}}$. This is done to evidence the relevant features of the $H_{\text{eff}}^{2\text{NF}}, H_{\text{eff}}^{3\text{NF}}$ monopole components, and to infer their different shell-evolution properties.

In addition, we have performed a spin-tensor decomposition (see, for instance, Ref. [39] and references therein) of the $H_{\text{eff}}^{2\text{NF}}$ and $H_{\text{eff}}^{3\text{NF}}$ monopole terms to understand the role played by the central, vector, and tensor components of the interaction in determining the evolution of the neutron and proton ESPEs when the nucleons fill the $0f_{7/2}$ orbital. At the end of this Section, we report the results of our analysis for the neutron-neutron and proton-neutron matrix elements of the monopole component $V_{\text{eff}}^{\text{mon}}$ involved in the formation of the $Z, N = 28$ shell closures.

In the following, we examine the proton and neutron ESPEs as a function of the number of valence neutrons. It is worth mentioning that our final considerations would be the same if we consider the evolution of proton and neutron ESPEs as a function of the number of valence protons, because the isospin invariance of our $H_{\text{eff}}$ is broken only by the Coulomb potential.

Figures 2 and 3 show the neutron and proton ESPEs obtained with $H_{\text{eff}}^{2\text{NF}}$ TBMEs, respectively, starting from $H_{\text{eff}}^{3\text{NF}}$ SP energies, evolved as a function of the valence neutrons up to $N = 28$. Black dots, blue squares, green diamonds, and indigo triangles indicate the $0f_{7/2}, 0f_{5/2}, 1p_{3/2}$, and $1p_{1/2}$ ESPE, respectively.

We start to comment the results of the neutron ESPE evolution. As shown in Fig. 2 the spacings between the $fp$ orbitals remain almost constant with respect to the evolution of the valence-neutron number, with $0f_{7/2}$ well separated from the other ones. This feature seems to point to a reasonable shell closure in doubly-closed $^{48}$Ca when employing SP energies obtained from $H_{\text{eff}}^{3\text{NF}}$. The results of the full SM calculation will be presented in the next Section.

Figure 3 shows the evolution of the proton ESPEs with respect to the valence-neutron number, and we see that the $0f_{7/2} - 0f_{5/2}$ spin-orbit energy splitting remains constant, as well as the $1p_{3/2} - 1p_{1/2}$ one. However, at variance with the evolution of the neutron ESPEs, we observe that the gap between the $1p_{3/2}, 1p_{1/2}$ and $0f_{7/2}, 0f_{5/2}$ proton ESPEs is not constant, resulting in an increasing separation in energy between the $0f_{7/2}$ and $1p_{3/2}$ proton ESPEs, and a collapse of the $0f_{5/2}$ proton ESPE onto the $1p_{1/2}$ one at $N = 28$. The first of these two features should drive to a stronger shell closure of the proton $0f_{7/2}$ orbital, when the number of neutrons is evolved. However, the grouping of the $0f_{5/2}, 1p_{3/2}, 1p_{1/2}$ orbitals favors the configuration mixing and, consequently, enhances the collectivity leading to a quenching of this shell closure.

These observations point to a different behavior of the proton-neutron monopole component of $H_{\text{eff}}$ with respect to the one of the identical-particle channel. As a matter of fact, the shell closure of $^{56}$Ni is less strong than that observed in $^{48}$Ca, evidenced by the fact that, experimentally, the excitation energy of the yrast $J^\pi = 2^+$ is about
1 MeV smaller than the one in $^{48}\text{Ca}$.

We now begin to examine the calculated neutron and proton ESPEs of $H_{\text{eff}}^{3\text{NF}}$, as a function of the valence-neutron number.

In Fig. 4 we report the neutron ESPEs up to $N = 28$. As can be seen, the neutron monopole component of $H_{\text{eff}}^{3\text{NF}}$ enlarges at $N = 28$ the $0f_{7/2} - 0f_{5/2}$ spin-orbit splitting and the $0f_{7/2} - 1p_{3/2}$ gap by $\sim 1$ MeV and 0.7 MeV, respectively, while leaves the $1p_{1/2} - 1p_{3/2}$ splitting almost unchanged.

![Neutron ESPE](image)

**FIG. 4:** Same as in Fig. 2 but for $H_{\text{eff}}^{3\text{NF}}$.

From the inspection of Fig. 5 we see that the behavior of the $H_{\text{eff}}^{3\text{NF}}$ proton ESPEs, as a function of the valence-neutron number, is very similar to that obtained with the $H_{\text{eff}}^{2\text{NF}}$ proton-neutron monopole component as reported in Fig. 2. However, it should be pointed out that now at $N = 28$ we observe a $0f_{7/2} - 0f_{5/2}$ spin-orbit splitting that is $\sim 1$ MeV larger, and a larger gap ($\sim 0.4$ MeV) between $1p_{3/2}$ and $0f_{7/2}$ orbitals, with respect to the one obtained with the $H_{\text{eff}}^{2\text{NF}}$ proton-neutron monopole component.

Based on these results, we may infer that the $H_{\text{eff}}^{3\text{NF}}$ monopole component could provide better closure properties than $H_{\text{eff}}^{2\text{NF}}$. This will be explored in Section III B, where the diagonalization of the full Hamiltonians $H_{\text{eff}}^{2\text{NF}}$ and $H_{\text{eff}}^{3\text{NF}}$ will be performed, and the results for $fp$-shell isotopic chains will be compared with experiment.

As mentioned above, we conclude this Section showing the results of a spin-tensor decomposition of the $H_{\text{eff}}^{2\text{NF}}$ and $H_{\text{eff}}^{3\text{NF}}$ monopole terms to understand the formation of the $\mathcal{Z}$, $N = 28$ shell closures in terms of the different components of the interaction.

![Proton ESPE](image)

**FIG. 5:** Same as in Fig. 2 but for $H_{\text{eff}}^{3\text{NF}}$ proton ESPEs.

In Tables II and III we show the central, vector, tensor contents of the neutron-neutron centroids of $H_{\text{eff}}^{2\text{NF}}$ and $H_{\text{eff}}^{3\text{NF}}$, respectively, involved in the evolution of the neutron ESPEs when neutrons fill the $0f_{7/2}$ orbital. We have also reported the differences between centroids, calculated with respect to the $0f_{7/2}$ centroid, and dubbed as $\Delta$, that are most relevant in determining the shell gaps. The same quantities are shown in Tables IV, V for the proton-neutron centroids involved in the evolution of the proton ESPEs when neutrons fill the $0f_{7/2}$ orbital.

Let us start discussing neutron-neutron interaction. We see in Tables II and III that, except for the neutron-neutron $0f_{7/2}0f_{5/2}$ centroid, the tensor content is rather small with respect to the central and vector ones. This is true for both $H_{\text{eff}}^{2\text{NF}}$ and $H_{\text{eff}}^{3\text{NF}}$. However, while in $H_{\text{eff}}^{2\text{NF}}$ the central and vector forces are both attractive and contribute to push down all the neutron orbitals, this does not happen for $H_{\text{eff}}^{3\text{NF}}$. The inclusion of the 3NF brings a repulsive contribution to the central component of the monopole term so that 3 out of 4 central $V_{\text{mon}}$ matrix elements change their sign. On the other side, the nature

### TABLE II: Spin-tensor contributions (in keV) to $V_{\text{mon}}$ and $\Delta$ for the neutron-neutron matrix elements of $H_{\text{eff}}^{2\text{NF}}$ (see text for details). The subscripts refer to the SP orbital by way of their $2\cdot j$ value, where $j$ is the total angular momentum.

| $V_{f7/2}^{\text{mon}}$ | $V_{f5/2}^{\text{mon}}$ | $\Delta_{7/2}$ | $V_{7/3}^{\text{mon}}$ | $V_{7/3}^{\text{mon}}$ | $\Delta_{7/3}$ | $V_{1/2}^{\text{mon}}$ | $V_{1/2}^{\text{mon}}$ | $\Delta_{1/2}$ |
|------------------|------------------|--------------|------------------|------------------|--------------|------------------|------------------|--------------|
| Central          | -36              | -68          | -12              | -42              | 14           | -63              | -7               |              |
| Vector           | -56              | -4           | 52               | -64              | -8           | -51              | 5                |              |
| Tensor           | 21               | -88          | -109             | 10               | -11          | -20              | -41              |              |
| Total            | -91              | -160         | -69              | -96              | -5           | -134             | -43              |              |

### TABLE III: Same as in Table II but for the $H_{\text{eff}}^{3\text{NF}}$ (see text for details).

| $V_{f7/2}^{\text{mon}}$ | $V_{f5/2}^{\text{mon}}$ | $\Delta_{7/2}$ | $V_{7/3}^{\text{mon}}$ | $V_{7/3}^{\text{mon}}$ | $\Delta_{7/3}$ | $V_{1/2}^{\text{mon}}$ | $V_{1/2}^{\text{mon}}$ | $\Delta_{1/2}$ |
|------------------|------------------|--------------|------------------|------------------|--------------|------------------|------------------|--------------|
| Central          | -36              | 8            | 44               | 108              | 144          | 93               | 129              |              |
| Vector           | -63              | 119          | 182              | -110             | -47          | -101             | -38              |              |
| Tensor           | 22               | -72          | -94              | 7                | -15          | -13              | -35              |              |
| Total            | -77              | 55           | 132              | 5                | 82           | -21              | 56               |              |
of the vector component does not change but is enhanced by the 3NF. It is worth noting that the tensor content is about the same when employing 2NF or 3NF.

TABLE IV: Same as in Table [I] but for the proton-neutron matrix elements of $H_{\text{eff}}^{2\text{NF}}$ (see text for details).

|   | $V_{7,5}^{\text{eff}}$ | $V_{5,3}^{\text{eff}}$ | $\Delta_{7,5}$ | $V_{7,3}^{\text{eff}}$ | $V_{5,1}^{\text{eff}}$ | $\Delta_{7,3}$ | $V_{7,1}^{\text{eff}}$ | $\Delta_{7,1}$ |
|---|------------------------|------------------------|----------------|------------------------|------------------------|----------------|------------------------|----------------|
| Central | -563 | -1083 | -480 | -246 | 134 | -162 | 141 |
| Vector | -92 | 174 | 266 | -50 | 42 | -14 | 78 |
| Tensor | -24 | 65 | 89 | 26 | 50 | -52 | -28 |
| Total | -719 | -844 | -125 | -493 | 226 | -528 | 191 |

TABLE V: Same as in Table [IV] but for the proton-neutron matrix elements of $H_{\text{eff}}^{3\text{NF}}$ (see text for details).

|   | $V_{7,5}^{\text{eff}}$ | $V_{5,3}^{\text{eff}}$ | $\Delta_{7,5}$ | $V_{7,3}^{\text{eff}}$ | $V_{5,1}^{\text{eff}}$ | $\Delta_{7,3}$ | $V_{7,1}^{\text{eff}}$ | $\Delta_{7,1}$ |
|---|------------------------|------------------------|----------------|------------------------|------------------------|----------------|------------------------|----------------|
| Central | -562 | -988 | -426 | -361 | 201 | -351 | 211 |
| Vector | -117 | 234 | 351 | -83 | 34 | -41 | 76 |
| Tensor | -27 | 72 | 99 | 24 | 51 | -48 | -21 |
| Total | -706 | -682 | 24 | -420 | 286 | -440 | 266 |

As regards the proton-neutron monopole, we see in Tables [IV] [V] that the effects of the 3NF on the central, vector and tensor components are quite similar to those observed for the neutron-neutron monopole. However, in this case the central components are significantly more attractive, becoming on the overall much more relevant with respect to the vector and tensor ones.

We can say that the ESPEs are mainly determined by the central and vector components, and in particular by the central one for the proton-neutron interaction. However, when looking at the differences in the ESPs or at the spin-orbit splittings, that involve differences between centroids (see $\Delta$ in the Tables), we see that the central contributions, having essentially the same sign for all centroids, lose in part their dominant role, and consequently the energy gaps result from the subtle interplay between all three components of the monopole interaction. In particular, for the proton shell gaps of $H_{\text{eff}}^{3\text{NF}}$, a small $\Delta_{7,5}$ is found because of an almost complete balancing of the central component by the vector plus tensor ones, which leads to small changes in the evolution of the $0f_{7/2} - 0f_{5/2}$ spin-orbit splitting as a function of the neutron number, as shown in Fig. 6. The increase of the $1p_{3/2} - 0f_{7/2}$ gap is instead clearly related to the positive interference of all the components of the monopole term.

Summing up the above discussion, we can say that while the repulsive or attractive nature of the vector component is enhanced by the inclusion of 3NF, the activity of the central content is reduced by repulsive corrections and no significant changes are produced in the tensor component.

B. Shell-model calculations

There are some spectroscopic features which reveal the shell closure properties, and among them two of the most important ones they are the behavior of excitation energy of yrast $J^\pi = 2^+$ states and the evolution of the ground-state (g.s.) energy in even mass isotopic/isotonic chains, with respect to the number of valence neutrons/protons.

These properties will be investigated diagonalizing the Hamiltonians $H_{\text{eff}}^{2\text{NF}}$ and $H_{\text{eff}}^{3\text{NF}}$, and employing for both of them the set of SP energies provided by $H_{\text{eff}}^{3\text{NF}}$. In addition to these two effective SM Hamiltonians, we have built another one, that we dub $H_{\text{eff}}^{\text{mon}}$, by summing the monopole component of $H_{\text{eff}}^{3\text{NF}}$ and the multipole ones belonging to $H_{\text{eff}}^{2\text{NF}}$. The scope of this operation is to evidence the interplay of the monopole and multipole components through the diagonalization of the effective SM Hamiltonian, and will be better clarified in the discussion of the results of our calculations.

The experimental and theoretical results obtained with $H_{\text{eff}}^{2\text{NF}}$, $H_{\text{eff}}^{3\text{NF}}$, and $H_{\text{eff}}^{\text{mon}}$ will be indicated in the figures with red dots, blue triangles, black diamonds, and indigo squares, respectively.

We start our study with calcium isotopes, and in Fig. 6 they are shown their $J^\pi = 2^+$ excitation energies from $N = 22$ up to $N = 30$.

![Calcium isotopes](image)

FIG. 6: Experimental and calculated excitation energies of the yrast $J^\pi = 2^+$ states for calcium isotopes from $N = 22$ to 30. See text for details.

We observe that the results obtained with all three Hamiltonians are very similar. The shell closure at $N = 28$ is very-well reproduced by $H_{\text{eff}}^{3\text{NF}}$ and $H_{\text{eff}}^{\text{mon}}$, while the $J^\pi = 2^+$ excitation energy obtained with $H_{\text{eff}}^{2\text{NF}}$ is about 0.7 MeV lower than the experimental one [38].

The different results of the $^{48}\text{Ca}$ shell-closure trace back to the different energy gap between the $1p_{3/2}$ and $0f_{7/2}$ neutron ESPEs when we employ the monopole term of $H_{\text{eff}}^{2\text{NF}}$ and $H_{\text{eff}}^{3\text{NF}}$, as can be seen in Figs. 1 and 2.
These different closure properties, related to whether 3NF are included or not in the derivation of the effective SM Hamiltonian, are present also in the calculation of the two-neutron separation energies ($S_{2n}$) that are shown in Fig. 7 for the calcium isotopes up to $N = 34$. To this end, we have shifted the SP energies in Table I in order to reproduce the experimental g.s. energy of $^{41}$Ca and $^{41}$Sc with respect to $^{40}$Ca.

We have reported the results up to $N = 34$ since in Refs. [14, 40] the comparison between experimental and calculated masses of neutron-rich calcium isotopes has been spotted as a way to pin down the role of 3NF in nuclear structure calculations.

As can be seen, both experimental [40, 41] and theoretical $S_{2n}$ show a rather flat behavior up to $N = 28$, then a sudden drop occurs at $N = 30$ that is a signature of the shell closure due to the $0f_{7/2}$ filling. Another decrease appears at $N = 34$ because at that point the valence neutrons start to occupy the $1p_{1/2}$ and $0f_{5/2}$ orbitals.

The results obtained with $H_{\text{eff}}^{3\text{NF}}$ and $H_{\text{eff}}^{\text{mon}}$ follow closely the behavior of the experimental $S_{2n}$, while those obtained with $H_{\text{eff}}^{2\text{NF}}$ provide a less satisfactory energy drop between $N = 28$ and 30. This supports the crucial role of 3NF contributions to reproduce the observed shell evolution.

Now we move from systems with identical valence particle to those with both valence protons and neutrons, in order to investigate the changes in the shell evolution and closure properties originating from the collectivity ignited by the $T = 0$ channel of the residual interaction.

In Fig. 8 the calculated $J^\pi = 2^+_1$ excitation energies of titanium isotopes are reported and compared with data [38]. We observe that the experimental behavior is, overall, well reproduced by all three SM Hamiltonians, the largest discrepancies occurring for $^{42}$Ti and $^{52}$Ti.

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From the inspection of Fig. 9, we observe that also the $S_{2n}$ experimental behavior [41] is well reproduced by $H_{\text{eff}}^{3\text{NF}}$ and $H_{\text{eff}}^{\text{mon}}$, while calculations with $H_{\text{eff}}^{2\text{NF}}$ underestimate the drop of two-neutron separation energy between $N = 28$ and 30. The latter feature evidences that also when the $T = 0$ channel is involved, the contribution of 3NF helps to obtain a better comparison with experiment.

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The collective behavior increases with the number of interacting proton and neutrons, as can be observed for the chromium and iron isotopes. In Figs. 10, 11 we report the experimental [38] and calculated excitation energies of the yrast $J^\pi = 2^+$ up to $N = 30$ for both isotopic chains. We observe in both cases that the calculations with $H^{2NF}_{\text{eff}}$ underestimate the experimental value at $N = 28$ providing too much collectivity, while effective SM Hamiltonians, whose monopole component includes 3NF contributions, are able to reproduce the experimental behavior rather well.

![Iron isotopes](image1)

**FIG. 11:** Same as in Fig. 8 but for iron isotopes. See text for details.

![Chromium isotopes](image2)

**FIG. 12:** Same as in Fig. 9 but for chromium isotopes. See text for details.

Similar considerations follow from the inspection of Figs. 12, 13, where the experimental [41] and calculated $S_{2n}$ for chromium and iron isotopes up to $N = 30$ are shown, respectively. We point out that empty red circles refer to estimated values reported in Ref. [41].

As can be seen, for these isotopes the observed $S_{2n}$ decrease from $N = 28$ to $N = 30$ is no longer as steep as in the calcium and titanium isotopes, evidencing the quenching of the $N = 28$ shell closure.

Once again the 3NF contribution, which is included in the monopole component of $H^{3NF}_{\text{eff}}$ and $H^{\text{mon}}_{\text{eff}}$, provides a better reproduction of the experimental drop from $N = 28$ to 30.

![Nickel isotopes](image3)

**FIG. 14:** Same as in Fig. 8 but for nickel isotopes. See text for details.

Finally, we examine the nickel isotopes whose study is pivotal to understand the shell-closure properties of SM Hamiltonians. As we have discussed above, the proton closure at $Z = 28$ is eroded by the increment of the number of valence neutrons approaching doubly-closed $^{56}$Ni because of the collectivity induced by the proton-neutron interaction. Consequently, reproducing the evolution of the spectroscopic properties of nickel isotopes towards the shell closure may represent a challenging test for the theoretical SP energies and TBMEs.

In Fig. 14 we show the behavior of the calculated and experimental [38] $J^\pi = 2^+_1$ excitation energies of nickel isotopes up to $N = 30$.

As can be seen, the three effective Hamiltonians predict a shell closure at $N = 20$ ($^{48}$Ni), although less marked with $H^{3NF}_{\text{eff}}$, that confirms the ability of their monopole components to provide a similar behavior in the identical-particle channel.

Actually, both $H^{3NF}_{\text{eff}}$ and $H^{\text{mon}}_{\text{eff}}$ compare themselves quite well with $^{52,54,56}$Ni data, while the results obtained...
with $H_{2NF}^{\text{eff}}$ exhibit a too strong collective behavior, failing to reproduce the shell closure at $N = Z = 28$. As a matter of fact, the comparison between the results obtained with $H_{2NF}^{\text{eff}}$ and $H_{\text{mon}}^{\text{eff}}$ evidences very clearly that the correct shell evolution may be obtained only including 3NF contributions in the monopole component of the SM Hamiltonian, the SP energies being not sufficient to balance the collectivity induced by the $T = 0$ multipole component of the TBMEs.

where we have reported, for the $N = 28$ isotones, the experimental and calculated behavior of both $J^\pi = 2^-\nu$ excitation energies and $B(E2; 2^+ \rightarrow 0^+)$ transition rates. The proton and neutron effective charges to calculate the $B(E2)$s have been obtained by way of many-body perturbation theory using only 2NF vertices, and details of the derivation of effective SM one-body operators can be found in Ref. [42].

As can be seen, the filling of the proton $0f_{7/2}$ orbital tunes the collectivity at $N = 28$ between the doubly closed $^{48}\text{Ca}$ and $^{56}\text{Ni}$, and the evolution of such a collective behavior is well reproduced including 3NF contributions, but is a failure by considering only 2NF.

**IV. CONCLUDING REMARKS AND OUTLOOK**

In this paper we have presented the results of SM calculations for $fp$-shell nuclei in the framework of the realistic shell model, starting from chiral 2NF and 3NF, and deriving effective SM Hamiltonians within the many-body perturbation theory.

In particular, we have calculated the contribution at first order in perturbation theory of a N$^4$LO chiral 3NF potential to the $H_{\text{eff}}$, in order to study how it affects its monopole component and the ability to describe the observed shell-closure properties of $fp$ isotopic chains. To this end, starting from two different $H_{\text{eff}}$s - one including 3NF contributions and the other one not - we have first carried out an analysis of the proton and neutron effective single-particle energies as a function of the valence-neutron number. This study has provided information about shell-closure properties and their dependence on the 3NF effects included in the monopole components of $H_{\text{eff}}$.

We have also performed a spin-tensor decomposition of the monopole term to investigate the effects of the 3NF on the central, vector, and tensor components. We have found that the inclusion of 3NF strengthens the vector content, and quenches the attractivity of the central component, the tensor term being almost unaffected. Successively, we have performed a full diagonalization of our $H_{\text{eff}}$s for the calcium, titanium, chromium, iron, and nickel isotopes, and focussed our attention on the shell evolution of the excitation energies of the yrast $J^\pi = 2^+$ states and the two-neutron separation energies.

The conclusion of our study can be summarised as follows:

- Starting from realistic potentials, derived within the chiral perturbation theory, the role of the 3NF is fundamental to obtain SP energies and TBMEs that may reproduce the shell evolution as observed from experiment.
- The TBMEs of $H_{\text{eff}}$ derived from 2NF only own deficient monopole components, which cannot balance the collectivity induced by higher multipole components in the proton-neutron channel. The
result is an erosion of the $N = 28$ shell closure when the number of valence protons increases.

- The central role of the monopole component of the $H_{\text{eff}}$ is testified by the fact that when it is subtracted from $H_{\text{eff}}^{2\text{NF}}$, and substituted with the monopole of $H_{\text{eff}}^{3\text{NF}}$, the observed shell evolution and the $N = 28$ shell closure is restored.

The outlook of our future work points towards the improvement of the derivation of $H_{\text{eff}}^{3\text{NF}}$ by including higher-order contributions with 3N vertices in the perturbative expansion of the $Q$ box, and the investigation of heavier systems in order to assess the reliability of present approach in exotic neutron-rich nuclear systems.

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