Shell evolution and nuclear forces

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\textbf{A B S T R A C T}

We present a quantitative study of the role played by different components characterizing the nucleon–nucleon interaction in the evolution of the nuclear shell structure. It is based on the spin–tensor decomposition of an effective two-body shell-model interaction and the subsequent study of effective single-particle energy variations in a series of isotopes or isotones. The technique allows to separate unambiguously contributions of the central, vector and tensor components of the realistic effective interaction. We show that while the global variation of the single-particle energies is due to the central component of the effective interaction, the characteristic behavior of spin–orbit partners, noticed recently, is mainly due to its tensor part. Based on the analysis of a well-fitted realistic interaction in the \textit{sd pf} shell-model space, we analyze in detail the role played by the different terms in the formation and/or disappearance of \(N = 16\), \(N = 20\) and \(N = 28\) shell gaps in neutron-rich nuclei.

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The shell structure is a common feature of finite quantum systems. Amongst them, atomic nuclei represent unique objects characterized by the appearance of a specific shell structure. In particular, the magic numbers which correspond to the shell closures, will change depending on the \(N/Z\) ratio, i.e. when we move from nuclei in the vicinity of the \(\beta\)-stability line towards the particle driplines. This has attracted a lot of attention nowadays because an increasing number of nuclei far from stability have become accessible experimentally (e.g., [1] and references therein). The hope to reach even more exotic nuclei demands for an improved modeling, i.e. in the context of nuclear astrophysics. Since the underlying shell structure determines nuclear properties in a major way, changes of nuclear shell closures and the mechanisms responsible for that should be much better understood.

Recently, the role of different components of the nucleon–nucleon (NN) interaction in the evolution of the shell structure has been actively discussed. Based on the analysis of the origin of a shell closure at \(N = 16\), Otsuka et al. [2] have suggested that a central spin–isospin-exchange term, \(f(\pi)(\delta \cdot \bar{\delta})(\vec{r} \cdot \vec{\bar{r}})\) of the NN interaction plays a decisive role in the shell formation.

However, from a systematic analysis of heavier nuclei, another conjecture has been put forward, namely, the dominant role played by the tensor force [3]. The evidence is based on the comparison of the position of experimental one-particle or one-hole states in nuclei adjacent to semi-magic configurations with the so-called effective single-particle energies (ESPE’s). Within the shell-model framework, the latter ESPE’s are defined [4] as one-nucleon separation energies for an occupied orbital (or extra binding gained by the addition of a nucleon to an unoccupied orbital) evaluated from a Hamiltonian containing nucleon single-particle energies (the bare single-particle energies with respect to a closed-shell core) plus the monopole part of the two-body residual interaction [5,6], i.e.

\[
\hat{H}_{\text{mon}} = \sum_{j,\rho}^p \epsilon_j^\rho \hat{n}_j^\rho + \sum_{j,\rho,\rho'} V_{jj}^{\rho\rho'} \hat{n}_j^\rho \hat{n}_j^{\rho'} (1 + \delta_{jj'} \delta_{\rho\rho'}) \tag{1}
\]

where \(j\) denotes a set of single-particle quantum numbers (\(nlj\)) and \(\rho\) refers to a proton (\(\pi\)) or to a neutron (\(\nu\)), \(\hat{n}_j^\rho\) are particle-number operators. \(V_{jj}^{\rho\rho'}\) are centroids of the two-body interaction defined as [5–7]

\[
V_{jj}^{\rho\rho'} = \frac{\sum_j |J\pi_\rho J\pi'_{\rho'}| V_{J\pi_\rho J\pi'_{\rho'}} |J\pi_\rho J\pi'_{\rho'}\rangle_M (2J + 1) \left( (\delta_{J\pi'} + 1) \delta_{\rho\rho'} - (\delta_{\rho\rho'} + 1) \delta_{J\pi'} \right)}{(2J + 1)(2J'_{\rho} + 1 - \delta_{\rho\rho'})} \tag{2}
\]

where the total angular momentum of a two-body state \(J\) runs over all possible values.

The monopole Hamiltonian represents a spherical mean field extracted from the interacting shell model. Its spherical single-particle states, or ESPE’s, provide an important ingredient for the

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formation of shells and interplay between spherical configurations and deformation in nuclei. Large shell gaps obtained from a monopole Hamiltonian are a prerequisite to obtain certain magic numbers. A reduction of the spherical shell gaps may lead to formation of a deformed ground state, if the correlation energy of a given excited configuration and a decrease in the monopole part are large enough to make such an intruder excitation energetically favorable.

For example, the ESPE of the v0f5/2 orbital at Z = 8, N = 20 is the difference between total energy obtained, using Eq. (1), for 28O in its ground state and 29O with an extra neutron in the 0f5/2 state assuming normal filling of the orbits (normal filling is used throughout this work). Considering a series of isotopes or isotones, it is clear that ESPE’s will experience a shift provided by the monopole part of the proton–neutron matrix elements, mainly. The bigger the overlap of the proton and neutron radial wave functions and the higher the j-values of the orbitals considered will lead, in general, to more drastic changes. In the present study we take into account the mass dependence of the two-body matrix elements of the effective interaction according to the rule:

\[ V(A) = (A_{core}/A)^{1/3} V(A_{core}). \]

From the analysis of the experimental data and the ESPE’s it has been noticed [38] that systematically

\[ |V^{\pi \nu}_{j,j'}| > |V^{\pi \nu}_{j,j'}|, \quad |V^{\pi \nu}_{j,j'}| > |V^{\pi \nu}_{j,j'}|, \]

where \( j_s = l + 1/2 \) and \( j_v = l - 1/2 \) are proton orbitals and \( j_s' = l + 1/2 \) and \( j_v' = l - 1/2 \) are neutron orbitals. Thus, an extra attraction is manifested between generalized spin–orbit partners (proton \( j = l + 1/2 \) and neutron \( j' = l - 1/2 \) with \( l \neq l' \) or vice versa).

This remarkable property is in line with the analytic relation valid for a pure tensor force [3], i.e. using the above notation,

\[ (2j_s + 1)V^{\pi \nu}_{j,j'} + (2j_v + 1)V^{\pi \nu}_{j,j'} = 0. \]

To strengthen this idea, Otsuka et al. [3] have compared changes of the ESPE’s in Ca, Ni and Sb isotopes, as due to the tensor force only and estimating its strength.

et al. [3] have compared changes of the ESPE’s in Ca, Ni and Sb isotopes, as due to the tensor force only and estimating its strength. The procedure allows to separate the central, vector and tensor parts of the effective interaction. The monopole properties of each component can be studied separately, elucidating unambiguously its role in the shell evolution. The method has already been applied in a similar context [32,33], however, the authors used different effective interactions in smaller model spaces, concluding on a second-order tensor effect only. Contrary to these results, we put into evidence an important first-order tensor effect in the present study.

A spin–tensor decomposition of the two-particle interaction has been known for many years [34–40]. In a given model space, a complete set of two-body matrix elements determines the properties of nuclei ranging within this space. For spin 1/2 fermions (nucleons), one can construct from their spin operators a complete set of linear operators in a two-particle spin space:

\[ S_1^{0} = 1, \quad S_2^{0} = |\sigma_1 \times \sigma_2|^{0}, \quad S_3^{1} = \sigma_1 + \sigma_2, \quad S_4^{2} = |\sigma_1 \times \sigma_2|^{2}, \quad S_5^{1} = |\sigma_1 \times \sigma_2|^{1}, \quad S_6^{1} = \sigma_1 - \sigma_2. \]

By coupling the spin tensor operators with the corresponding rank tensors in the configuration space one can construct scalar interaction terms. The most general two-body interaction can then be written as

\[ V(1,2) \equiv V = \sum_{k=0,1,2} \langle S^{(k)}, Q^{(k)} \rangle = \sum_{k=0,1,2} V^{(k)}. \]

Here, \( V^{(0)} \) and \( V^{(2)} \) represent the central and tensor parts of the effective NN interaction. The \( V^{(k=1)} \) term contains the so-called symmetric \( (S^{(1)}_{i=j}) \) and antisymmetric \( (S^{(1)}_{i\neq j}) \) spin–orbit operators [37], which we will denote as LS and ALS, respectively. To obtain the matrix elements for the different multipole components in \( jj \) coupling, one transforms two-body matrix elements between normalized and antisymmetrized states from \( jj \) coupling to LS coupling in the standard way. The LS-coupled matrix elements of \( V^{(k)} \) can be calculated from the LS coupled matrix elements of \( V^{(k)} \) as

\[ \langle ab : LS, JMTM_T \rangle V^{(k)} |cd : L'S', JMTM_T \rangle = (2k + 1)(-1)^J \left\{ \begin{array}{ccc} L & S & J \\ S' & L' & k \end{array} \right\} \times \sum_J (-1)^J (2J' + 1) \left\{ \begin{array}{ccc} L & S & J' \\ S' & L' & k \end{array} \right\} \times \langle ab : LS, J'MTM_T \rangle |cd : L'S', J'MTM_T \rangle, \]

where \( a = (n_a, l_a) \). Finally, starting from the LS coupled matrix elements of \( V^{(k)} \), for each \( k \), we arrive at a set of \( jj \) coupled matrix elements to be used for further investigation. It is important to
We start with the "classical" case of the properties of stable as well as nuclei further away from stability [29]. But less pronounced behavior is noticed for the neutron 1(d from S to Ca), i.e., the corresponding splitting increases. A similar components of the effective interaction that connect two-nucleon using the realistic interaction [29] and its components separately.

The opposite effect is observed when protons fill the 0(d/2) orbital with protons (from 28O to 34Si), due to the change in the spin-to-orbital orientation with respect to the proton 0(d/2) orbital. The tensor contribution remains large but changes its sign (1.96 MeV). This enforces the central contribution (2.17 MeV) and reduces the tensor contribution (1.96 MeV).

Similarly, the increase of the gap between the neutron 0(d/2) and 0(f/2) orbitals when going from 35S to 34Si and onwards from 35S to 40Ca (columns 3 and 4 of Table 1) is a joint effect of the central and tensor component of the effective interaction. This is an important manifestation of the tensor force in this region. Due to the fact that at N = 20 the above two neutron orbitals have (i) the same radial quantum number, and, (ii) a different spin-to-orbital orientation, a large and negative tensor contribution of ~1.93 MeV results for the variation of the gap between the 0(d/2) and 0(f/2) orbitals when filling the 0(d/2) orbital with protons (from 36S to 40Ca). This large tensor shift, however, is almost fully cancelled by the central contribution of 1.99 MeV. The combined effect results in only a slight overall decrease of the N = 20 shell gap from 40Ca to 36S and 34Si, thereby preserving the semi-magic nature of the latter nuclei. At the same time, while filling the 0(d/2) orbital with protons (from 28O to 34Si), due to the change in the spin-to-orbital orientation with respect the proton 0(d/2) orbital, the tensor contribution remains large but changes its sign (1.96 MeV). This enforces the central contribution (2.17 MeV) and results in a rapid decrease of the N = 20 shell gap below 34Si which is at the origin of the so-called 'island of inversion' around 32Mg (deformed ground state).

The position of the 0(d/2) orbital and the possible shell gaps between this orbital and either the 1s1/2 or 0f/2 orbital plays an important role in the formation of N = 16 as a magic number at Z = 8. This was formerly ascribed to result from the spin-isospin-exchange part of the central force component [2] and sometime later to be due to mainly a pure tensor force [41]. The present results support the important role of both a central part (in its spin-isospin-exchange channel) and a tensor part in changing the shell structure between O and Si.

In Fig. 2, we show the two-body contribution to the binding energy from the monopole part of the realistic interaction and its different components. For the analysis we choose the N = 19 isotones 27O, 33Si, 35S and 39Ca with a neutron hole (relative to N = 20) in the 0(d/2) state. As is seen, the global shift is due to

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Table 1

| Energy gap | (ν0Ωl/2, ν1ςl/2) | (ν0f2/2, νΩl/2) | (ν0f2/2, νΩl/2) | (ν0Ωl/2, πΩl/2) | (πΩl/2, πΩl/2) | (ν0Ωl/2, ν1ςl/2) | (ν0f2/2, νΩl/2) | (ν0f2/2, νΩl/2) |
|------------|------------------|-----------------|-----------------|-----------------|-----------------|------------------|-----------------|-----------------|
| Filling orbital | πΩl/2 | πΩl/2 | πΩl/2 | VΩl/2 | VΩl/2 | πΩl/2 | πΩl/2 | πΩl/2 |
| 28O → 28Si | | | | | | | | |
| Total | -2.57 | 3.68 | 0.21 | -2.33 | -3.156 | 1.60 | 1.81 |
| Central | -1.87 | 2.17 | 1.99 | -0.21 | -1.58 | 2.03 | 1.31 |
| TE | -1.58 | 2.23 | 2.48 | 0.62 | -1.19 | 2.03 | 1.02 |
| TO | -0.68 | -0.31 | -0.11 | -0.03 | 0.25 | -0.25 | -0.14 |
| SE | 0.71 | -0.45 | 0.01 | -0.50 | -0.57 | -0.02 | 0.18 |
| SO | -0.32 | 0.70 | -0.39 | -0.30 | -0.07 | 0.28 | 0.25 |
| Vector | 0.36 | -0.45 | 0.15 | 0.61 | 0.06 | 0.23 | -0.18 |
| even | -0.12 | -0.06 | 0.25 | 0.60 | 0.25 | 0.22 | -0.27 |
| odd | 0.07 | -0.04 | -0.41 | -0.51 | -0.40 | -0.11 | 0.41 |
| AL5 | 0.41 | -0.35 | 0.31 | 0.52 | 0.21 | 0.12 | -0.33 |
| Tensor | -1.06 | 1.96 | -1.93 | -2.73 | -1.64 | -0.67 | 0.68 |
| even | -0.78 | 1.31 | -1.28 | -1.59 | -0.96 | -0.43 | 0.43 |
| odd | -0.28 | 0.66 | -0.65 | -1.14 | -0.68 | -0.24 | 0.26 |

**Fig. 3.** Variation of proton single-hole states in Ca-isotopes using the realistic interaction [29].

the central part of the effective interaction when adding up to 12 protons to the 16O core. This contrasts with the results, presented before, in which we studied the local relative variations in the single-particle energy in which the tensor force component plays a major role.

More evidence results from the single-proton holes in Ca-isotopes i.e. studying the K isotopes. There is a crossing of the 1ςl/2 and the 0d3/2 orbitals when approaching 48Ca and, in addition, a lowering of the energy gap between the 0d3/2 and the 0d5/2 orbitals when going from 40Ca to 48Ca, confirmed experimentally [1,42,43]. In Fig. 3, we show the variation of the proton ESPE’s in Ca-isotopes obtained from the same effective interaction, while in Table 1 we present a detailed analysis of the role of different components in the evolution of the gaps. It is seen (columns 5) that the lowering of the gap between proton 0d3/2 and 0d5/2 orbitals as neutrons fill the 0f5/2 orbital is mainly due to the tensor force. However, it is the central part, combined with the contribution from the tensor force, which reduces the gap between proton 0d3/2 and 1ςl/2 orbitals when approaching 48Ca (column 6).

Finally, we explore evolution of neutron ESPE’s in N = 28 isotones, from O to Ca, as a function of proton number. The characteristic trends of spin–orbit partners, generic for a pure tensor force, are well manifested when using the same realistic interaction (see Fig. 4); approaching neutron 0f5/2 and 0f3/2 spin-orbit partners, and likewise for the 1p3/2 and 1p1/2 spin-orbit partners, when filling the proton 0d5/2 orbital. An opposite effect results when filling the 0d3/2 orbital and fingerprints the contribution from a tensor term.

In Table 1 (columns 7 and 8), we analyze in detail the reduction of the N = 28 shell gap, i.e. the change in the neutron 1p3/2-0f7/2 energy difference from 48Ca to the lighter isotones. To start with, these two orbitals have different radial quantum numbers. Therefore, the radial overlap contributing to the Vπνπν0d3/20f3/2 centroid is larger than the radial overlap contributing to the Vπνπν0d3/21p1/2 centroid. As can be seen from the table, the contributions from the central and tensor terms are dominating. Since both the 0f3/2 and 1p3/2 orbital are ‘spin-up’ oriented (jz = l + 1/2), the tensor term contributes in a similar way to the energy shift when protons fill the 0d3/2 orbital (Vπνπν0d3/20f3/2 and Vπνπν0d3/21p1/2 are both positive). The same happens when protons fill the 0d3/2 orbital (Vπνπν0d3/20f3/2 and Vπνπν0d3/21p1/2 are both negative). The overall difference in sign is due to the different relative spin to orbital orientation of the neutron orbitals (both (jz = l + 1/2) relative to the proton orbitals (jz = l ± 1/2)). Due to the difference in absolute value of the centroids, in particular, due to different radial overlaps for
ν0f−π0d versus ν1p−π0d, the positive and negative tensor contributions to the energy centroid do not cancel. They result in a shift of 0.68 MeV and −0.67 MeV filling the 0d3/2 or 0d5/2 orbital, respectively. Adding this tensor energy shift to the central plus vector energy shift results in a reduction of the N = 28 shell gap going from 48Ca to 44S and from 42Si to 36O. This situation contrasts the N = 20 shell gap evolution discussed before.

These examples illustrate that in the discussion of shell gap evolution, it is mandatory to take into account what particular orbitals are considered. Both the central and tensor term represent important ingredients, together with the magnitude of the radial overlaps involved.

To summarize, we have proposed a quantitative study of the shell structure evolution in series of isotopes or isotones, based on a spin–tensor decomposition of the two-body matrix elements. The method has allowed us to clarify the role played by the different terms of the effective interaction in the variation of the single-particle energy of different orbitals.

Based on the analysis of the best realistic interaction in the 1s0d1p0f shell-model space [29], we show that the evolution of the N = 16, N = 20 and N = 28 shell gaps is a combined effect of different spin–tensor terms, of which the central term in its triplet-even channel and the tensor term are of overwhelming importance. This conclusion partially supports the results of Refs. [32,33] regarding the importance of the triplet even channel but evidences the crucial role of the first-order tensor term as conjectured in Refs. [3,8]. The tensor term plays a dominant role, with increasing role of the vector term in the single-particle energy difference for spin–orbit partners. However, from the examples discussed here, one cannot assign unambiguously a dominating role to the tensor mechanism in cases when no explicit spin–orbit partners are considered. For example, the increase in energy splitting between proton 0h11/2 and 0g7/2 when filling neutron 0h11/2 in heavy Sb isotopes, or in the energy splitting between neutron 0h11/2 and 0g7/2 when filling proton 0g9/2 in N = 51 isotones, discussed in Ref. [3], may be a result of different parts of the effective interaction. To clarify the observed situation, a corresponding quantitative analysis should be performed.

The decomposition is a suitable tool only for the model spaces when all spin–orbit partners are present. This does not allow, at the present moment, to analyze heavier nuclei and check the hypothesis of the tensor force action in heavy systems, until a realistic determination of the position of relevant spin–orbit partners is established. As can be seen from the present work, the vector term of the effective interaction typically counter-acts the tensor term. The increasing role of the vector term could form a plausible scenario for a reduction of the tensor effect in heavy nuclei and explain the results obtained from shell-model studies of Ref. [31]. This requires more data on key heavy nuclei and the availability of extremely large-scale shell-model calculations.

Note added

The authors have noticed that just recently Otsuka et al. [44] have come to very much the same conclusions as presented in our paper with respect to the need of considering both a central and tensor force to describe the variation in shell structure in a correct and consistent way.

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