Microscopic approach to the shell model: study of nuclei north-east of $^{48}$Ca

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Abstract. We report on shell-model calculations for nuclei with valence nucleons outside $^{48}$Ca wherein a fully microscopic approach is adopted. Namely, the single-particle energies and the matrix elements of the two-body interaction are derived theoretically starting from the high-precision CD-Bonn nucleon-nucleon potential, renormalized by way of the $V_{\text{low-k}}$ approach. This has been done within the framework of the time-dependent degenerate linked-diagram perturbation theory. Our results compare satisfactorily with a large amount of experimental data.

1. Introduction

In the last decade interest has grown in so-called ab initio calculations for nuclear structure. What is usually meant by an ab initio calculation [1] is to start from a realistic nucleon-nucleon ($NN$) potential and possibly a three-body one and employ them within a many-body framework well suited to handle the short-range correlations induced by the nuclear force. A major requirement is the accuracy of the approximations involved, which should be kept under control by way of convergence checks.

Owing also to the considerable increase in computer power, substantial progress has been achieved in microscopic approaches to the nuclear many-body problem, such as the Green’s function Monte Carlo method (GFMC) [2], no-core shell model (NCSM) [3, 4], and coupled-cluster method (CCM) [5, 6].

Despite great efforts to extend the domain of applicability of these approaches, only a limited class of nuclei has been investigated up to now owing to the computational complexity. As a matter of fact, the GFMC and NCSM are presently able to describe nuclei with mass $A \leq 16$, while the CCM has been employed to study closed-shell and one-valence-nucleon systems only.

On the other hand, the advances in experimental techniques to produce exotic beams make now possible to explore the structure of nuclei at and close to the driplines. This is a major challenge of today’s nuclear physics, since these studies may reveal new features, such as shell modifications, that go beyond our present knowledge of nuclear structure. There is, consequently, a clear need to study open-shell nuclei in different mass regions, and the realistic shell model is the most advanced tool to perform microscopic calculations for these nuclei. In this approach, the basic ingredients of the shell-model hamiltonian, namely the single-particle energies and
two-body matrix elements, should be derived in the framework of a many-body theory (see for instance [7, 8]) starting from a free $NN$ potential.

These fully realistic shell-model calculations with no adjustable parameters have already proved to be successful in reproducing the spectroscopic properties of the $p$-shell nuclei [9] and $N = 82$ isotones [10], as well as the neutron dripline for the oxygen and carbon isotopes [11, 12].

In the present work, we focus our attention on nuclei that can be described in terms of valence protons and neutrons outside doubly-magic $^{48}$Ca, employing as model space the $0f_{7/2}$ level for protons and the four levels of the $28–50$ shell for neutrons. In this context, it should be mentioned that an issue of current interest is the role played, within the shell-model framework, by the neutron $0g_{9/2}$ orbital in the description of the experimental behavior of the yrast $J^\pi = 2^+$ states in heavy Cr and Fe isotopes [13–18]. We find worthwhile investigating this problem by performing shell-model calculations without adjustable parameters.

We have derived the shell-model effective hamiltonian starting from a low-momentum realistic potential derived from the high-precision CD-Bonn potential [19] by way of the well-known $V_{\text{low-}k}$ approach [20]. As pointed out in [10, 21] a three-body force should be added to our two-body $V_{\text{low-}k}$. In this case, our effective hamiltonian would consist of one- and two-body components, including also core-polarization effects arising from the three-body force, and of an effective three-body force that should be explicitly taken into account in the shell-model calculation. The derivation of such a hamiltonian is a very hard task, since we should treat three-body forces up to third-order in perturbation theory, as we usually do for the two-body ones. In this paper, therefore, we neglect the contributions of three-body forces. However, our previous experience with realistic shell-model calculations [8] makes us confident that the spectroscopic properties of these nuclei can be mainly ascribed to the effects of the two-body $NN$ interaction.

In the following section, we outline the perturbative approach to the derivation of our shell-model hamiltonian. In section 3, we present results of calculations for calcium, titanium, chromium, iron, and nickel isotopes. A brief summary is given in the last section.

2. Outline of calculations

Within the framework of the shell model, an auxiliary one-body potential $U$ is introduced in order to break up the hamiltonian 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 $H_1$:

$$H = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j=1}^{A} V_{ij}^{NN} = T + V = (T + U) + (V - U) = H_0 + H_1. \quad (1)$$

Once $H_0$ has been introduced, it is possible to define a reduced model space in terms of a finite subset of $H_0$’s eigenvectors. In this space, an effective hamiltonian $H_{\text{eff}}$ may be constructed and the diagonalization of the many-body hamiltonian (1) in an infinite Hilbert space is then reduced to the solution of an eigenvalue problem in a finite space.

As mentioned in the Introduction, we want to derive an effective shell-model hamiltonian $H_{\text{eff}}$ for a model space spanned by the single-proton level $0f_{7/2}$ and the four single-neutron levels $0f_{5/2}, 1p_{3/2}, 1p_{1/2}, 0g_{9/2}$ outside $^{48}$Ca core. This has been done in the framework of the time-dependent perturbation theory by way of the Kuo-Lee-Ratcliff (KLR) folded-diagram expansion [22]. More precisely, we first renormalize the high-momentum repulsive components of the CD-Bonn $NN$ potential by way of the $V_{\text{low-}k}$ approach [20, 23], which provides a smooth potential preserving exactly the on-shell properties of the original $NN$ potential. Next, we express $H_{\text{eff}}$ in terms of the vertex function $Q$-box, which is composed of irreducible valence-linked diagrams [24, 25]. In the derivation of the $Q$-box we have included one- and two-body Goldstone diagrams through third order in $H_1$. Since it is computationally prohibitive to perform calculations beyond
the third order in perturbation theory, we have calculated the Padé approximant \([2\,|\,1]\) \([26, 27]\) of the \(\hat{Q}\)-box, so as to obtain a value to which the perturbation series should converge, as suggested in \([28]\). The folded-diagram series is then summed up to all orders using the Lee-Suzuki iteration method \([29]\).

The hamiltonian \(H_{\text{eff}}\) contains one-body contributions, whose collection is the so-called \(\hat{S}\)-box \([30]\). In realistic shell-model calculations a subtraction procedure is commonly used, so as to retain only the two-body terms of \(H_{\text{eff}}(V_{\text{eff}})\) while the SP energies are taken from experiment. Instead, in this work we have employed the SP energies obtained from the \(\hat{S}\)-box calculation.

A discussion of the convergence properties of \(H_{\text{eff}}\) is now in order. For the sake of clarity, we first consider the SP energies and then the two-body matrix elements (TBME) of \(V_{\text{eff}}\).

In figure 1 we report the neutron SP spectrum calculated as a function of the maximum allowed excitation energy of the intermediate states expressed in terms of the oscillator quanta \(N_{\text{max}}\). The results obtained at third order in perturbation theory are reported with black symbols, while those obtained using the Padé approximants \([2\,|\,1]\) are represented by red symbols. We see that an \(N_{\text{max}} \geq 22\) calculation yields converged values for the SP energies.

Since the comparison between the third-order results and those obtained by means of the Padé approximant is an indicator of the dependence of our results on the higher-order perturbative terms, we conclude that higher-order contributions are not very relevant, and should only slightly affect the relative spectrum.

![Figure 1](image1.png)

**Figure 1.** (Color online) Theoretical single-neutron energies as a function of \(N_{\text{max}}\). The black symbols refer to third-order results, the red ones to those obtained with Padé approximants. See text for details.

![Figure 2](image2.png)

**Figure 2.** Diagonal neutron-neutron \(J^{\pi}=0^+\) matrix elements of \(V_{\text{eff}}\) as a function of \(N_{\text{max}}\). See text for details.

In figure 2, we report the diagonal neutron-neutron \(J^{\pi}=0^+\) matrix elements of \(V_{\text{eff}}\) as a function of \(N_{\text{max}}\). We have chosen these matrix elements because they are the largest ones in the entire set of \(V_{\text{eff}}\) TBME and the most sensitive to increases in the number of intermediate states. From figure 2 it is clear that our results have practically achieved convergence at \(N_{\text{max}} = 18\).

As regards the order-by-order convergence, we compare in table 1 all the \(\hat{Q}\)-box neutron-neutron \(J^{\pi}=0^+\) matrix elements calculated at third order with those given by the \([2\,|\,1]\) Padé approximant \([26]\).
\[ [2|1] = V_{Qbox}^0 + V_{Qbox}^1 + V_{Qbox}^2 (1 - (V_{Qbox}^0)^{-1})^{-1} \]

where \( V_{Qbox}^n \) is the square non-singular matrix representing the \( n \)th-order contribution to the \( J^\pi = 0^+ \) \( Q \)-box in the perturbative expansion. From table 1 we see that our third-order results are in good agreement with those from the \([2|1]\) Padé approximant. This indicates a weak dependence of our results on higher-order \( Q \)-box perturbative terms.

**Table 1.** \( Q \)-box neutron-neutron \( J^\pi = 0^+ \) two-body matrix elements at third order in \( V_{low-k} \) (in MeV) compared with those obtained by calculating the Padé approximant \([2|1]\).

| Configuration | 3rd order | Padé \([2|1]\) |
|---------------|-----------|----------------|
| \( \langle 0f_{5/2}\rangle^2 \) \( V_{Qbox} \) \( \langle 0f_{5/2}\rangle^2 \) | -1.381 | -1.109 |
| \( \langle 0f_{5/2}\rangle^2 \) \( V_{Qbox} \) \( \langle 1p_{3/2}\rangle^2 \) | -1.096 | -0.979 |
| \( \langle 0f_{5/2}\rangle^2 \) \( V_{Qbox} \) \( \langle 1p_{1/2}\rangle^2 \) | -0.521 | -0.491 |
| \( \langle 0f_{5/2}\rangle^2 \) \( V_{Qbox} \) \( \langle 0g_{9/2}\rangle^2 \) | 2.698 | 2.444 |
| \( \langle 1p_{3/2}\rangle^2 \) \( V_{Qbox} \) \( \langle 1p_{3/2}\rangle^2 \) | -1.083 | -1.028 |
| \( \langle 1p_{3/2}\rangle^2 \) \( V_{Qbox} \) \( \langle 1p_{1/2}\rangle^2 \) | -1.742 | -1.407 |
| \( \langle 1p_{3/2}\rangle^2 \) \( V_{Qbox} \) \( \langle 0g_{9/2}\rangle^2 \) | 1.747 | 1.567 |
| \( \langle 1p_{1/2}\rangle^2 \) \( V_{Qbox} \) \( \langle 1p_{1/2}\rangle^2 \) | -0.089 | -0.236 |
| \( \langle 1p_{1/2}\rangle^2 \) \( V_{Qbox} \) \( \langle 0g_{9/2}\rangle^2 \) | 1.312 | 1.174 |
| \( \langle 0g_{9/2}\rangle^2 \) \( V_{Qbox} \) \( \langle 0g_{9/2}\rangle^2 \) | -1.254 | -1.305 |

3. Results

In this section, we report the results of our shell-model calculations for calcium, titanium, chromium, iron and nickel isotopes with mass number \( A > 48 \). The calculations have been performed by using the Oslo shell-model code [31].

First, it is worth commenting on our theoretical SP energies as compared to the experimental low energy spectra of \(^{48}\)Sc and \(^{49}\)Ca. The former are reported in table 2. Since we employ the sole SP level \( 0f_{7/2} \) as proton model space, we can compare the theoretical value, -8.2 MeV, with the experimental \(^{48}\)Sc ground-state (g.s.) energy with respect to \(^{48}\)Ca, -9.63 MeV. The observed energy spacings in \(^{49}\)Ca are \( E_{1/2^-} - E_{3/2^-} = 2.023 \) NeV , \( E_{5/2^-} - E_{3/2^-} = 3.585 \) MeV and \( E_{9/2^+} - E_{3/2^-} = 4.017 \) MeV, while the g.s. energy with respect to \(^{48}\)Ca is -5.147 MeV.

**Table 2.** Theoretical SP energies (in MeV). See text for details.

| nlj   | Single-particle energies |
|-------|--------------------------|
| \( \pi 0f_{7/2} \) | -8.2 |
| \( \nu 0f_{5/2} \) | -5.4 |
| \( \nu 1p_{3/2} \) | -9.7 |
| \( \nu 1p_{1/2} \) | -8.0 |
| \( \nu 0g_{9/2} \) | -6.2 |
From table 2, we see that our relative single-neutron energies are not in good agreement with experiment. In particular the theoretical $0g_{9/2}^{\pi}$ SP state is about 0.5 MeV lower than the observed yrast $J^\pi = \frac{9}{2}^+$ state in $^{49}$Ca, while the theoretical $0f_{5/2}^{\pi}$ SP energy is about 0.7 MeV greater than the experimental excitation energy of the yrast $J^\pi = \frac{5}{2}^+$ state. Moreover, a large discrepancy occurs when comparing the experimental g.s. energies with respect to $^{48}$Ca with our calculated ones. Since, as shown in the previous section, the convergence properties of our $H_{\text{eff}}$ seem to leave very little room for improvement of our calculation of SP energies and TBME, the above discrepancies can be probably traced to the lack of a three-body force in addition to the two-body $V_{\text{low-k}}$ potential.

In the following, besides presenting the results obtained with theoretical SP energies (labelled as I), we also report on calculations performed using, as in Ref. [16], SP energies deduced from the experimental spectra of $^{49}$Sc and $^{49}$Ca (labelled as II). In this way, we should empirically take into account three-body force effects in the one-body component of our effective hamiltonian.

3.1. Calcium isotopes

In figure 3, we report the calculated excitation energies of the yrast $2^+$ states as a function of the neutron number up to $N = 36$. It can be seen that the available observed energies are well reproduced.

![Figure 3](image1.png)

**Figure 3.** (Color online) Experimental [32] and calculated excitation energies of the yrast $J^\pi = 2^+$ states in calcium isotopes from $N = 30$ to 36.

In figure 4, the experimental and calculated energy spectra of the odd-mass nucleus $^{51}$Ca up to 3 MeV excitation energy are shown. In this connection it should be mentioned that calculations I and II provide a seniority-one yrast $J^\pi = \frac{9}{2}^+$ state at excitation energies of 3.603 and 4.131 MeV, respectively. Experimentally, a $J^\pi = \frac{9}{2}^+$ state has been observed at 4.155 MeV, which has been interpreted in Ref. [34] as a $1p - 1h \ Z = 20$ cross-shell excitation.

![Figure 4](image2.png)

**Figure 4.** Experimental [33, 34] and calculated low-energy spectra of $^{51}$Ca. See text for details.

3.2. Titanium isotopes

The calculated excitation energies of the yrast $2^+$ states in titanium isotopes are reported in figure 5 up to $N = 34$. It can be seen that the observed excitation energies are well reproduced by both calculations I and II up to $N = 34$. The drop of the experimental $2^+$ excitation energy in $^{56}$Ti evidences the lack of a $N = 34$ shell closure in titanium isotopes, which is well reproduced by both calculations.
In figure 6, we report the two calculated energy spectra of the odd-mass nucleus $^{51}$Ti up to 2.5 MeV excitation energy. We see that the agreement with the experimental spectrum is quite satisfactory for both calculations. It should be mentioned that I and II predict a yrast $J^\pi = \frac{9}{2}^+$ state of single-particle nature at excitation energies of 3.096 and 3.620, respectively. Experimentally, a $J^\pi = \frac{9}{2}^+$ state has been observed at 3.771 MeV.

### 3.3. Chromium isotopes

The excitation energies of the yrast $2^+$ states for the chromium isotopes are reported in figure 7 up to $^{64}$Cr.

It is worth noting that the observed lowering of the yrast $2^+$ states is interpreted as a signature of the development of a pronounced collectivity near $N = 40$ [14]. Both calculations

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**Figure 5.** (Color online) Same as in figure 3, but for titanium isotopes from $N = 28$ to 34.

**Figure 6.** Experimental [32] and calculated low-energy spectra of $^{51}$Ti. See text for details.

**Figure 7.** (Color online) Same as in figure 3, but for chromium isotopes from $N = 28$ to 40.

**Figure 8.** Experimental [32] and calculated low-energy spectra of $^{53}$Cr. See text for details.
I and II reproduce qualitatively the experimental behavior of the observed $J^\pi = 2^+_1$ energies, even if from $^{62}\text{Cr}$ on there is a sizeable overestimation of the experimental data. This may be a consequence of our limited model space, which is spanned only by one single-proton level and does not take into account explicitly the $1d_{5/2}$ single-neutron state, whose inclusion has been recently suggested to reproduce the large quadrupole collectivity in this mass region [15].

In figure 8, the calculated energy spectra of the odd-mass nucleus $^{53}\text{Cr}$ are shown and compared with the experimental one up to 2.5 MeV excitation energy. It can be seen that the agreement is quite good for both calculations.

3.4. Iron isotopes

In figure 9 the $2^+_1$ excitation energies of even iron isotopes are shown as a function of the neutron number $N$.

![Figure 9](Image)

**Figure 9.** (Color online) Same as in figure 3, but for iron isotopes from $N = 28$ to 42.

As for chromium isotopes, the results with calculations I and II are very similar. We see that the observed decreasing trend, which may be interpreted as the onset of collectivity around $Z = 24$, is reproduced by our calculations, although, owing to the limited size of our model space, from $N = 36$ on our results systematically overestimate the observed $2^+_1$ excitation energies.

3.5. Nickel isotopes

Our model space allows to describe the spectroscopic properties of Ni isotopes with mass $A > 56$. It is worth noting that in this case only the neutron degrees of freedom are explicitly taken into account, the eight valence protons being frozen in the $f_{7/2}$ orbital. This means that the effective proton-neutron interaction comes into play only via its monopole component that makes the $^{49}\text{Ca}$ SP spectrum evolve into the $^{57}\text{Ni}$ SP one. This of course reduces the scope of our description. In figure 10 we report the SP energy levels of $^{57}\text{Ni}$ obtained with calculations I and II, and compare them with the corresponding observed ones. As can be seen, the agreement is rather satisfactory, which indicates the reliability of the proton-neutron monopole components of our effective hamiltonian.

In figure 11 the $2^+_1$ excitation energies of even nickel isotopes are shown as a function of the neutron number $N$. The agreement of the calculated $J^\pi = 2^+_1$ excitation energies with the experimental ones is rather unsatisfactory. In particular, both calculations provide a subshell closure at $N = 32$, which has no experimental counterpart, while the observed $N = 40$ subshell closure is not well reproduced. This is mainly due to the fact that our effective hamiltonian does not take explicitly into account $Z = 28$ cross-shell excitations, which indeed may be not negligible.
3.6. Ground-state energies

In figure 12 the calculated g.s. energies relative to $^{48}$Ca of the even Ca, Ti, Cr and Fe isotopes are reported and compared with the available experimental (continuous red line) and estimated (dashed red line) data [36].

As can be observed, a common feature of all figures is that calculation I fails to reproduce the experimental behavior, providing a collapse of the g.s. energies as function of $N$. This is not the case of calculation II, whose results are always in a quite good agreement with experiment, apart from a certain overbinding that becomes sizeable only for $N > 36$.

From the comparison of the results of the two calculations, it can be deduced that the monopole component of our effective shell-model interaction is not responsible for the collapse with calculation I and can be therefore considered quite reliable. Furthermore, it is worth pointing out that the main responsibility of this collapse cannot be traced back to a deficiency of the whole theoretical SP spectrum. As a matter of fact, if the theoretical proton and neutron SP spectra are shifted so as to reproduce the experimental $^{49}$Sc and $^{49}$Ca binding energies respectively, the experimental g.s. energies are well reproduced (black dotted line) as in calculation II.

4. Summary

We have presented here an extensive shell-model study of nuclei north-east of $^{48}$Ca within the framework of a fully microscopic approach. This means that, starting from a $V_{\text{low-k}}$ derived from the CD-Bonn $NN$ potential, an effective hamiltonian has been derived by way of perturbation theory and then employed in shell-model calculations without any adjustable parameters.

On the whole, when compared with experiment our results exhibit an agreement that may be considered quite good, especially if one takes into account that our effective hamiltonian consists only of five single-particle energies and less than one hundred two-body matrix elements. In this connection, it should be noted that our choice of a proton model space including only the $0f_{7/2}$ level reduces the scope of a detailed description of spectroscopic properties, especially when approaching the filling of the $\pi 0f_{7/2}$ level.
Figure 12. (Color online) Experimental [36] and calculated ground-state energies for calcium, titanium, chromium and iron isotopes as a function of the number of neutrons $N$. See text for details.

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