Can Realistic Shell-Model Calculations be Predictive?

N Itaco\textsuperscript{1,2}, L Coraggio\textsuperscript{2}, A Covello\textsuperscript{1} and A Gargano\textsuperscript{2}

\textsuperscript{1} Dipartimento di Fisica, Università di Napoli Federico II, Complesso Universitario di Monte S. Angelo, Via Cintia - I-80126 Napoli, Italy
\textsuperscript{2} Istituto Nazionale di Fisica Nucleare, Sezione di Napoli Complesso Universitario di Monte S. Angelo, Via Cintia - I-80126 Napoli, Italy
E-mail: nunzio.itaco@unina.it

Abstract. A major requirement for a nuclear model is, not only to reproduce and describe accurately the available experimental data, but also to provide reliable predictions for physical quantities not yet measured. Over the past two decades, we have performed various realistic shell-model calculations for nuclei in different mass regions, which have all yielded results in good agreement with the available experimental data. In this paper we present some selected results illustrating their predictive power.

1. Introduction

The advances in experimental techniques to produce exotic beams make nowadays possible to plan new experiments to explore the structure of nuclei at and close to the driplines. This is a major challenge of today nuclear physics, since these studies may reveal new features that go beyond our present understanding of nuclear structure. In such a context, a key point is to ascertain the capability of the available nuclear models of providing reliable predictions for physical quantities not yet measured, whose knowledge may be of stimulus and guidance for upcoming experiments.

The shell model is an invaluable theoretical tool to understand the structure of nuclei, giving a framework for a microscopic description of nuclear properties based essentially on the use of effective Hamiltonians. In particular, during the last two decades the realistic shell model, that makes use of effective Hamiltonians derived from the bare nucleon-nucleon (NN) potential in the framework of the many-body theory, has proved to lead to an accurate description of the structure of nuclei in various mass regions both close to and far from the valley of stability (see [1–4] for some recent examples). A major merit of this microscopic approach is that no adjustable parameter is introduced, which makes more interesting to wonder about its predictivity through the examination of the results so far obtained.

Here we shall present some selected cases which clearly evidence the good predictive power of realistic shell-model calculations. These cases will be discussed in section 3, after a brief description of the theoretical framework (section 2). A brief summary is given in the last section.
2. Theoretical framework

As mentioned in the Introduction, a basic ingredient for realistic shell-model calculations is the effective Hamiltonian $H_{\text{eff}}$, which is constructed starting from a $NN$ potential $V^{NN}$ that gives a very accurate description of the experimental data of the two nucleon problem. This is the case of all modern $NN$ potentials, as for instance CD-Bonn [5], Argonne V18 [6], Nijmegen [7]. All these potentials, however, exhibit a strong short-range repulsive behavior thus preventing their direct use in the derivation of $H_{\text{eff}}$, which is based on a perturbative approach. In the past, this problem has been faced renormalizing the potential by way of the Brueckner reaction matrix, while a new approach is provided today by the availability of low-momentum $NN$ potentials. As a matter of fact, one can start from a realistic model for $V^{NN}$ and integrate out its high-momentum components thus obtaining a smooth potential $V_{\text{low}-k}$ that preserves exactly the onshell properties of the original $V^{NN}$ [8, 9]. Alternatively, one can recur directly to a chiral potential based upon the effective field theory (EFT) [10, 11]. In both cases, these low-momentum potentials may be used as input in the derivation of $H_{\text{eff}}$ without the need of any further renormalization.

The starting point is the $A$-nucleon system Hamiltonian. By introducing an auxiliary one-body potential $U$, this may be written as the sum of a one-body term $H_0$, describing the independent motion of the nucleons, and a residual interaction $H_1$:

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

In the shell model, the nucleus is schematized as an inert core plus $n$ interacting valence nucleons, and a reduced space, the so-called model space, is defined in terms of a finite subset of $d$ eigenvectors of $H_0$

$$|\Psi_i\rangle = [a_1^\dagger a_2^\dagger \ldots a_n^\dagger]|c\rangle \ , \quad (2)$$

where $|c\rangle$ represents the inert core, the subscripts $1, 2, \ldots, n$ denote the single-particle (SP) valence states and $i$ stands for all the quantum numbers needed to specify the state. In this model space, an effective Hamiltonian may be constructed so as to reduce the diagonalization of the Hamiltonian (1) in an infinite Hilbert space to the solution of the eigenvalue problem:

$$H_{\text{eff}} P |\Psi_\alpha\rangle = E_\alpha P |\Psi_\alpha\rangle \ , \quad (3)$$

where $\alpha = 1, \ldots, d$, the $E_\alpha$ and the corresponding $|\Psi_\alpha\rangle$ being a subset of the eigenvalues and eigenvectors of the original Hamiltonian.

$H_{\text{eff}}$ may be derived by way of a similarity transformation constructing a new Hamiltonian $H = X^{-1} H X$ that satisfies the decoupling equation between the model space $P$ and its complement $Q$:

$$Q H P = 0 \ , \quad (4)$$

so that the desired effective Hamiltonian is $H_{\text{eff}} = P H P$. A detailed description of the approach for deriving $H_{\text{eff}}$ by way of perturbation theory can be found in [12, 13].

Before concluding this section, it is worth spending few words about the issue regarding the choice of the model-space SP energies. The effective Hamiltonian constructed within the above outlined approach contains one- and two-body contributions. However, a subtraction procedure is commonly used in realistic shell-model calculations, so as to retain only the two-body terms of $H_{\text{eff}}$, while the SP energies are taken from experiment. This approach, although less fundamental, enables to take into account implicitly the effects of three-body forces on the SP energies.
3. Results
We present some selected results of realistic shell-model calculations, performed in previous works, for nuclei belonging to different mass regions, namely heavy calcium isotopes, neutron deficient tin isotopes, and Sn isotopes beyond $N = 82$.

3.1. Heavy calcium isotopes
In 2009 we published a paper reporting the results of realistic shell-model calculations for neutron-rich Ca isotopes [14]. We performed calculations for calcium isotopes with mass ranging from $A = 49$ to $A = 56$ by employing the $fp$ shell as model space for the valence neutrons outside the doubly magic nucleus $^{40}$Ca and the effective interaction derived from the CD-Bonn $NN$ potential. Some predictions for the $^{53–56}$Ca isotopes, that were completely unknown at that time, were shown in [14].

![Figure 1.](image1.png)

**Figure 1.** (Color online) Experimental [15, 16] and calculated $S_{2n}$ for calcium isotopes with $N = 22 − 34$.

![Figure 2.](image2.png)

**Figure 2.** Experimental [17, 18] and calculated excitation energies of the yrast $J^\pi = 2^+$ states for calcium isotopes with $N = 22 − 34$.

During the past few years, there has been a great interest in the study of heavy calcium isotopes from both the experimental and theoretical point of view. This interest is testified, for instance, by two letters that have recently appeared in Nature. One of them, published in June 2013, reports the results of an experiment performed at the ISOLDE/CERN facility with ISOLTRAP leading to first mass measurement for $^{53}$Ca and $^{54}$Ca [16]. These new mass-data reveal a pronounced decrease in the two-neutron separation energy ($S_{2n}$), quite similar to that observed beyond $^{40}$Ca, which was interpreted as a clear signature of the $N = 32$ shell closure.

Few months later, in October 2013, another very interesting letter on the results of a experimental spectroscopic study of $^{54}$Ca was published [18]. In this experiment, performed by proton knockout reactions with fast radioactive projectiles, the yrast $2^+$ state was identified at an excitation energy of 2.043 MeV. This large value, comparable with that of $^{52}$Ca evidences the onset of a sizable subshell closure at $N = 34$ in calcium isotopes.

In figures 1 and 2 we report our calculated $S_{2n}$ for even Ca isotopes and the $2^+$-states excitation energies, respectively, as shown in reference [14]. The theoretical values are compared with the presently available data and with the results obtained using the phenomenological shell-model Hamiltonian GXPF1A [19]. As it can be seen, in both cases our predictions turn out to be
in quite good agreement with the new data. This is especially noteworthy for the $2^+$ excitation energy in $^{54}$Ca, for which the two theoretical predictions were remarkably different. This point was discussed in detail in reference [14], where it was shown that the difference between the results of the two shell-model calculations is related to the different $T = 1$ monopole properties of the two effective interactions.

3.2. Neutron-deficient Sn isotopes

The nucleus $^{100}$Sn is the heaviest particle-bound doubly magic nucleus with an equal number of neutrons and protons. Therefore its neighboring provide the opportunity to investigate the effective interaction for nuclei in the vicinity of the proton drip line with protons and neutrons filling the same orbitals. In particular, the study of Sn isotopes has attracted a special interest, since it may give direct information on neutron pairing correlations.

The work of reference [20], which dates back to almost 20 years ago, may be placed in this context. The $^{102,103,104,105}$Sn nuclei were studied within the framework of the shell model using two effective interactions derived from the Bonn A [21] and the Paris [22] $NN$ potentials. The aim was essentially to assess the role of realistic effective interactions in the mass region around $^{100}$Sn. At that time, in fact, the practical value of these interactions was still not completely assessed. The calculations were performed using as model space the five neutron orbitals of the 50-82 shell with $SP$ energies determined through an analysis of the low-energy spectra of the tin isotopes with $105 \leq A \leq 111$. No information on the spectrum of the single-neutron nucleus $^{101}$Sn was in fact available. Now we know the position of the $\frac{5}{2}^+$ state at 0.171 MeV excitation energy with respect to the $\frac{7}{2}^+$ ground state. This value is not far from the adopted one in [20] for the $\epsilon_{g7/2} - \epsilon_{d5/2}$ single-particle spacing, namely 0.2 MeV.

![Figure 3](image-url)

**Figure 3.** Experimental [17] and calculated low-energy spectra of $^{102,103}$Sn.

A satisfactory agreement between theory and experiment was obtained for $^{104,105}$Sn by using the Bonn A potential. In particular, the calculated spectrum of $^{104}$Sn was very close to the experimental one, the only exception being the position of the $2^+$ state which was overestimated.
by about 250 keV. Analogously, in $^{105}$Sn the largest discrepancies were found for the energies of states arising from the coupling of single-particle states to the $2^+$ state of $^{104}$Sn.

In [20], the predictions for the two lighter nuclei $^{102}$Sn and $^{103}$Sn, for which only recently some spectroscopic information has become available, were also reported. In figure 3, the experimental spectra of $^{102,103}$Sn [17] are compared with the calculated ones. Note that we have included only theoretical states with the experimental counterpart.

It is worth noting that the quality of agreement between theory and experiment is similar to that found for $^{104,105}$Sn. Clearly we overestimate the energies of the $2^+$ state in $^{102}$Sn, which reflects on $^{103}$Sn. This may be traced back to $Z = 50$ cross-shell excitations which are not explicitly taken into account in the adopted model space [23].

3.3. Tin isotopes beyond $N = 82$

During the last two decades, there has been substantial progress in gaining experimental information on nucleon-rich nuclei far from the stability line, which has evidenced changes in the shell structure when approaching the neutron drip line. In this context, nuclei in the regions of the shell closures with a large $N/Z$ ratio, as for instance tin isotopes beyond $N = 82$, are a subject of great interest, opening the opportunities to better understand the forces that bind the nucleons together in very extreme conditions. The experimental information on heavy tin isotopes are, however, still very limited owing to the present experimental difficulties to access such short-lived nuclei. Further information, which may help us to gain insight into the structure these nuclei, will be provided in not a distant future thanks to the continuous advances in the experimental techniques. It is, therefore, challenging to make predictions which may stimulate and provide guidance to future experiments.

![Figure 4](image-url) (Color online) Experimental (red symbols) [17, 26] and calculated (black symbols) excitation energies of the yrast $J^\pi = 2^+, 4^+$ and $6^+$ states for tin isotopes with $A = 134 – 140$.

In 2011, we reported on a shell-model study of Sn isotopes with $N \geq 82$ employing a realistic effective interaction derived from the CD-Bonn $NN$ potential renormalized via the $V_{\text{low-k}}$
approach [24]. In these calculations, $^{132}$Sn was taken as closed core and the valence neutrons were let to move in the six orbitals of the 82-126 shell. Based on the very good agreement of our results with the observed energies for $^{134}$Sn, which was the only known nucleus, we investigated the evolution of the yrast $2^+$ state and of the other $J \neq 0$ members of the lowest-lying multiplet when adding neutron pairs up to $N = 90$. As a main outcome of our calculations, we predicted an almost flat behavior for the excitation energies of the yrast $2^+$, $4^+$, and $6^+$ states (see figure 4). We found only a slight increase at $N = 90$, due to the sub-shell closure of the $f_{7/2}$ orbital. As a matter of fact, our prediction for $^{140}$Sn excludes the possible existence of a $N = 90$ shell closure as suggested in [25].

Very recently, studying the projectile fission of a $^{238}$U beam at the RIKEN Radioactive Isotope Beam Factory, the delayed $\gamma$-ray cascades originating from the decay of $6^+$ isomeric states have been observed in $^{136,138}$Sn [26]. The observed excitation energies, reported in figure 4, are very well reproduced by calculated values of reference [24]. This supports our results for the hitherto unknown spectrum of $^{140}$Sn.

4. Summary

The predictive power of a nuclear model is a parameter of the utmost importance in the evaluation of its merits. It would be, in fact, highly desirable to know the capability of a nuclear model in providing reliable predictions as well as its limits. This is especially true nowadays, when, thanks to the availability of radioactive ion beams and the advances in detection techniques, experiments are being planned to explore the unknown structure of nuclei when moving towards the drip lines. In this paper we have studied the predictive power of realistic shell-model calculations, by reporting some selected results for heavy calcium isotopes, neutron deficient Sn isotopes and tin isotopes beyond $N = 82$. The results shown here were already the subject of previous works, where the comparison between theory and experiment was, obviously, limited to the data available at that time. In this contribution, we have shown that our predictions give an accurate description of quantities recently measured. This makes us confident in the good predictive power of our approach.

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