Realistic Effective Interactions and Nuclear Structure Calculations

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Abstract. We address the two main questions relevant to microscopic nuclear structure calculations starting from a free NN potential. These concern the accuracy of these kinds of calculations and the extent to which they depend on the potential used as input. Regarding the first question, we present some results obtained for nuclei around doubly magic 132Sn and 208Pb by making use of an effective interaction derived from the Bonn A potential. Comparison shows that our results are in very good agreement with the experimental data. As for the second question, we present the results obtained for the nucleus 134Te by making use of four different NN potentials. They indicate that nuclear structure calculations may help in understanding the off-shell nature of the NN potential.

INTRODUCTION

The shell model is the basic framework for nuclear structure calculations in terms of nucleons. Since the early 1950s many hundreds of shell-model calculations have been carried out, most of them being very successful in describing a variety of nuclear structure phenomena. In any standard shell-model calculation one has to start by defining a model space, namely by specifying a set of active single-particle (s.p.) orbits. The choice of the model space is of course conditioned by the size of the matrices to be set up and diagonalized. The rapid increase in computer power and the development of high-quality codes in the last decade has greatly extended the feasibility of large-scale calculations [1]. While these technical improvements add to the practical value of the shell model, much uncertainty still exists for what concerns the model-space effective interaction $V_{\text{eff}}$.

In most of the existing calculations to date either empirical effective interaction containing several adjustable parameters have been used or the two-body matrix elements have been treated as free parameters, this latter approach being limited to small model spaces.

This uncertainty in shell model work can only be removed by taking a more fundamental approach, namely by deriving the effective interaction from the free nucleon-nucleon (NN) potential. As is well known, the first step in this direction was taken in the mid 1960s by Kuo and Brown [2] who derived an $s$-$d$ shell effective interaction from the Hamada-Johnston potential [3]. Since that time there has been substantial progress towards a microscopic approach to nuclear structure calculations starting from a free NN potential. On the one hand, high-quality NN potentials have been constructed which reproduce quite accurately all the known NN data. On the other hand, the many-body methods for calculating the matrix elements of the effective interaction have been largely improved. A review of modern NN potentials is given in Ref. [4] while the main aspects of the derivation of $V_{\text{eff}}$ are discussed in Ref. [5]. These improvements have brought about renewed interest in shell-model calculations with realistic effective interactions. In this context, the two crucial questions are: i) how accurate is an effective interaction derived from the NN potential? ii) to which extent can nuclear structure calculations distinguish between different NN potentials?

Recent calculations for nuclei in the 100Sn and 132Sn regions [6–11] have achieved very good agreement with experiment indicating the ability of realistic effective interactions to provide a description of nuclear structure properties at least as accurate as that provided by traditional, empirical interactions. To our knowledge, no systematic investigation concerning the second question has been carried out thus far. The main interest in
trying to answer this question stems from the fact that two potentials which fit equally well the NN data up to the inelastic threshold may differ substantially in their off-shell behavior. Thus, from microscopic nuclear structure calculations we may learn something about the off-shell properties of the nuclear potential.

The main aim of this paper is to report on some achievements of our current work relevant to both the above questions. We shall first present some results of realistic shell-model calculations for nuclei having either few protons outside doubly magic $^{132}\text{Sn}$ or few neutron holes in doubly magic $^{208}\text{Pb}$. They are $^{135}\text{I}$, $^{136}\text{Xe}$ and $^{206,205,204}\text{Pb}$. In all of these calculations we have made use of a realistic effective interaction derived from the Bonn A free $NN$ potential [12]. Then we shall present the results obtained for the two proton-nucleus $^{134}\text{Te}$ by making use of four different potentials, Paris [13], Nijmegen93 [14], Bonn A and CD Bonn [15], which are all based on the meson theory of nuclear force.

We shall see that while the former study confirms what was learned from our previous calculations with the Bonn potential, the latter indicates a dependence of nuclear structure results on the kind of potential used as input.

**OUTLINE OF CALCULATIONS**

As already mentioned in the Introduction, for all the six nuclei considered in this paper we have employed an effective interaction derived from the Bonn A potential. For $^{134}\text{Te}$ we have also performed calculations employing three other effective interactions derived from the Paris, Nijmegen93 and CD Bonn potential, respectively. These effective interactions were all obtained using a $G$-matrix folded-diagram formalism, including renormalizations from both core polarization and folded diagrams. For the $N=82$ isotones $^{134}\text{Te}$, $^{135}\text{I}$ and $^{136}\text{Xe}$ we have considered $^{132}\text{Sn}$ as an inert core and let the valence protons occupy the five single-particle (s.p.) orbits $0g_{7/2}$, $1d_{5/2}$, $2s_{1/2}$, $1d_{3/2}$, and $0h_{11/2}$. For the Pb isotopes, we have treated neutrons as valence holes with respect to the $^{208}\text{Pb}$ closed core and included in the model space the six single-hole (s.h.) orbits $2p_{1/2}$, $1f_{5/2}$, $2p_{3/2}$, $0i_{13/2}$, $1f_{7/2}$, and $0h_{9/2}$. A description of the derivation of our $V_{\text{eff}}$ for the $N=82$ isotones and for the Pb isotopes can be found in Refs. [16] and [17], respectively. For the shell-model oscillator parameter $\hbar\omega$ we have used the value 7.88 MeV for the $N=82$ isotones and 6.88 MeV for the Pb isotopes, as obtained from the relationship $\hbar\omega = 45A^{-1/3} - 25A^{-2/3}$ for $A=132$ and $A=208$, respectively.

As regards the s.p. energies, for the $N=82$ isotones we have taken three s.p. spacings from the experimental spectrum of $^{133}\text{Sb}$ [18,19]. In fact, the $g_{7/2}$, $d_{5/2}$, $d_{3/2}$, and $h_{11/2}$ states can be associated with the ground state and the 0.962, 2.439 and 2.793 MeV excited levels, respectively. As for the $s_{1/2}$ state, its position has been determined by reproducing the experimental energy of the $\frac{1}{2}^+$ level at 2.15 MeV in $^{137}\text{Cs}$. This yields the value $\epsilon_{s_{1/2}} = 2.8$ MeV. Regarding the Pb isotopes, the s.h. energies have all been taken from the experimental spectrum of $^{207}\text{Pb}$ [20]. They are (in MeV) $\epsilon_{p_{1/2}} = 0$, $\epsilon_{f_{5/2}} = 0.570$, $\epsilon_{p_{3/2}} = 0.898$, $\epsilon_{i_{13/2}} = 1.633$, $\epsilon_{f_{7/2}} = 2.340$, and $\epsilon_{h_{9/2}} = 3.414$.

**RESULTS**

In Fig. 1 we report the experimental [21,22] and theoretical spectra of the three-proton nucleus $^{135}\text{I}$. As regards the two-proton nucleus $^{134}\text{Te}$, the results obtained by using the Bonn A potential are to be found in Fig. 6. The spectra of both these nuclei have already been presented in a previous paper [16], where a detailed comparison between theory and experiment is made. In that paper we also reported the calculated $E2$ and $E3$ transition rates in $^{134}\text{Te}$ and compared them with the available experimental data. While we refer the reader for details to the above paper, we emphasize here the very good agreement between the calculated spectra and the experimental ones, as is shown by the value of the rms deviation $\sigma$ [23], which are 106 keV and 58 keV for $^{134}\text{Te}$ and $^{135}\text{I}$, respectively.
FIGURE 1. Experimental and calculated spectrum of $^{135}$I.

The experimental [24] and calculated spectra of the four-proton nucleus $^{136}$Xe are compared in Fig. 2, where all the calculated and experimental levels up to about 2.5 MeV excitation energy are reported. Excluding the three states with $J^\pi = 3^-, 4^+, J^\pi = (4^+, 4^+$), at 2.13, 2.46, and 2.56 MeV, respectively, each level in the observed spectrum can be unambiguously identified with a level predicted by the theory. The quantitative agreement between theory and experiment is quite satisfactory. In fact, a rather large discrepancy (248 keV) occurs only for the 0$^+$ state, the calculated excitation energies of all other states differing by less than 110 keV from the experimental values. The rms deviation relative to the eight identified excited states is 107 keV. As regards the three above-mentioned states, for which we have not attempted to establish a correspondence between theory and experiment, a firm spin assignment to the levels at 2.13 and 2.46 MeV is needed to clarify the situation.

Let us now come to the Pb isotopes. The experimental [25–27] and theoretical spectra of $^{206}$Pb, $^{205}$Pb and $^{204}$Pb are compared in Figs. 3, 4 and 5, where we report all the calculated and experimental levels up to 2.5, 1.5 and 2.0 MeV, respectively. In the high-energy regions we only compare the calculated high-spin states with the observed ones. From Figs. 3-5 we see that a very good agreement with experiment is obtained for the low-energy spectra. In particular, in each of the three nuclei the theoretical level density reproduces remarkably well the experimental one.
FIGURE 2. Experimental and calculated spectrum of $^{136}\text{Xe}$.

Note too that each state of a given $J^\pi$ in any of three calculated spectra has its experimental counterpart, with a few exceptions. In fact, as may be seen in Fig. 4, the $\frac{9}{2}^-$, $\left( \frac{9}{2}, \frac{5}{2} \right)^-$, and $\left( \frac{9}{2}, \frac{7}{2} \right)^-$ states observed at 1.265, 1.374 and 1.499 MeV in $^{205}\text{Pb}$ cannot be safely identified with levels predicted by the theory. As regards $^{204}\text{Pb}$, we find the $0^+_4$ state at 1.954 MeV while the experimental one, which is not reported in Fig. 5, lies at 2.433 MeV. It should be mentioned, however, that the theory predicts four more $0^+$ states in the energy interval 2.2–2.6 MeV. Aside from these uncertainties, the agreement between calculated and experimental spectra is such as to allow us to identify experimental states with no firm or without spin-parity assignment. For $^{206}\text{Pb}$ our results suggest that the observed levels at 2.197 and 2.236 MeV have $J^\pi = 3^+$ and $1^+$, respectively. As for $^{205}\text{Pb}$, we predict $J^\pi = \frac{1}{2}^-$ and $\frac{3}{2}^-$ for the experimental levels at 0.803 and 0.998 MeV.

Regarding the quantitative agreement between our results and experiment, the rms deviation $\sigma$ is 207 and 216 keV for $^{206}\text{Pb}$ and $^{204}\text{Pb}$, respectively. For $^{205}\text{Pb}$ the $\sigma$ value is 74 keV, excluding the three above mentioned states, for which we have not attempted any identification. Concerning the high-spin states in $^{206}\text{Pb}$ and $^{205}\text{Pb}$, from Figs. 3 and 4 we see that they are also well described by the theory. In $^{204}\text{Pb}$ the agreement between theory and experiment is rather worse for the states lying above 4.3 MeV excitation energy, the largest discrepancy being about 400 keV for the $16^2_2$ state.
We have also calculated the electromagnetic properties for each of the three isotopes. For the sake of brevity we do not report these results in the present paper, but refer the reader to Ref. [17], where a detailed comparison with the available experimental data is also made. We only mention here that a very good overall agreement is obtained.

As already mentioned in the Introduction, we are currently investigating the dependence of nuclear structure results on the $NN$ potential used to derive the model space effective interaction. Here we present the results obtained for the nucleus $^{134}$Te which provides a very good testing ground for this investigation. In fact, this nucleus has only two valence protons and thus offers the opportunity to test directly the matrix elements of the calculated effective interactions. Furthermore, all the s.p. energies, except $\epsilon_{s_1/2}$, are known from experiment. The uncertainty in the position of the $s_{1/2}$ level, however, has practically no influence on the low-energy spectrum.
FIGURE 4. Experimental and calculated spectrum of $^{205}$Pb.
In Fig. 6 we report the four theoretical spectra obtained by using the Paris, Nijmegen93, CD Bonn and Bonn A potentials together with the experimental one [28,29]. We see that the best agreement with experiment is produced by the Bonn A effective interaction. The rms deviation $\sigma$ is 106, 160, 211, and 346 keV for Bonn A, CD Bonn, Nijm93 and Paris, respectively. These results show that different $NN$ potentials produce somewhat
different nuclear structure results. Of course, the significance of these differences, which do not exceed 100 keV if we exclude the Paris potential, may be a matter of discussion. The following remark is, however, in order. The four potentials considered differ in the strength of the tensor-force component as measured by the predicted $D$-state probability of the deuteron $P_D$. This is 4.4% for Bonn A, 4.83% for CD Bonn, 5.76% for Nijm93, and 5.8% for Paris. Our results suggest that potentials with a weak tensor force may lead to a better description of nuclear structure properties. This is quite an interesting point since differences in $P_D$ may in turn be traced to off-shell differences.
CLOSING REMARKS

As pointed out in the Introduction, in this paper we have been concerned with the two main problems related to microscopic nuclear structure calculations starting from a free NN potential. On the one hand, we have shown some recent results of shell-model calculations for nuclei around $^{132}$Sn and $^{208}$Pb obtained by employing an effective interaction derived from the Bonn A nucleon-nucleon potential. The success achieved by these calculations confirm the conclusion reached in our earlier works [6–8,16] that this effective interaction is able to describe with quantitative accuracy the spectroscopic properties of nuclei around closed shells.

On the other hand, we have presented some preliminary results of a study aimed at ascertaining how much nuclear structure results depend on the NN potential one starts with. As a first testing ground, we have chosen the two valence-proton nucleus $^{134}$Te, making use of the Paris, Bonn A, CD Bonn and Nijm93 NN potentials. Since this study is still in the initial stage, it is premature to draw any definite conclusion. We plan to extend this kind of calculations to several other nuclei and to other modern high-quality potentials, like Argonne $v_{18}$ [30], Nijm I and Njim II [14], which have not been considered here. The results obtained so far, however, indicate that microscopic nuclear structure calculations may provide valuable information on the off-shell behavior of the NN potential.

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REFERENCES

1. Caurier, E., Martínez-Pinedo, G., Nowacki, F., Poves, A., Retamosa, I., and Zuker, A. P., to be published in Phys. Rev. C, and references therein.
2. Kuo, T. T. S., and Brown, G. E., Nucl. Phys. 85 40 (1966).
3. Hamada, T., and Johnston, I. D., Nucl. Phys. 34 382 (1962).
4. Machleidt, R., contribution to these Proceedings
5. Kuo, T. T. S., in New Perspectives in Nuclear Structure (Ravello 1995), edited by A. Covello (World Scientific, Singapore, 1996), p. 159.
6. Andreozzi, F., Coraggio, L., Covello, A., Gargano, A., Kuo, T. T. S., Li, Z. B., and Porrino, A., Phys. Rev. C 54, 1636 (1996).
7. Andreozzi, F., Coraggio, L., Covello, A., Gargano, A., Kuo, T. T. S., and Porrino, A., Phys. Rev. C 56, R16 (1997).
8. Covello, A., Andreozzi, F., Coraggio, L., Gargano, A., Kuo, T. T. S., and Porrino, A. Prog. Part. Nucl. Phys. 38, 165 (1997).
9. Holt, A., Engeland, T., Osnes, E., Hjorth-Jensen, M., and Suhonen, J., Nucl. Phys. A618, 107 (1997).
10. Suhonen, J., Toivanen, J., Holt, A., Engeland, T., Osnes, E., and Hjorth-Jensen, M., Nucl. Phys. A628, 41 (1998).
11. Holt, A., Engeland, T., Hjorth-Jensen, M., and Osnes, E., Nucl. Phys. A634, 41 (1998).
12. Machleidt, R., Holinde, K., and Elster, Ch., Phys. Rep. 149, 1 (1987).
13. Lacombe, M., Loiseau, B., and Richard, J. M., Vinh Mau, R., Côté, J., Pires, P., and de Torreil, R., Phys. Rev. C 21, 861 (1980).
14. Stoks, V. G. J., Kloppm, R. A. M., Terheggen, C. P. F., and de Swart, J. J., Phys. Rev. C 49, 2950 (1994).
15. Machleidt, R., Sammarruca, F., and Song, Y., Phys. Rev. C 53, R1483 (1996).
16. Covello, A., Coraggio, L., and A. Gargano, in Proceedings of the SNEC98 Intern. Conference (Padova 1997), Nuovo Cimento A, in press.
17. Coraggio, L., Covello, A., Gargano, A., Itaco, N., and Kuo, T. T. S., Phys. Rev. C, 58 (1998).
18. Sergeenkov Yu., V., and Sigalov, V. M., Nucl. Data Sheets 49, 39 (1986).
19. Sanchez Vega, M., Fogelberg, B., Mach, H., Taylor, R. B. E., Lindroth, A., and Blomqvist, J., Phys. Rev. Lett. 80, 5504, (1998).
20. Martin, M. J., Nucl. Data Sheets 70, 313 (1993).
21. Zhang, C. T., et al. Phys. Rev. Lett. 77, 3743 (1996).
22. Sergeenkov, Yu. V., Nucl. Data Sheets 52, 205 (1987).
23. We define $\sigma = \left( \frac{1}{N_d} \sum_{i} [E_{\text{exp}}(i) - E_{\text{calc}}(i)]^2 \right)^{1/2}$, where $N_d$ is the number of data.
24. Tuli, J. K., *Nucl. Data Sheets* **71**, 1 (1994).
25. Helmer, R. G., and Lee, M. A., *Nucl. Data Sheets* **61**, 93 (1990).
26. Rab, S., *Nucl. Data Sheets* **69**, 679 (1993).
27. Schmorak, M. R., *Nucl. Data Sheets* **72**, 409 (1994).
28. Omtvedt, J. P., Mach, H., Fogelberg, B., Jerrestam, D., Hellström, M., Spanier, L., Erokhina, K. I., Isakov, V. I., *Phys. Rev. Lett.* **75**, 3090 (1995).
29. Sergeenkov, Yu. V., *Nucl. Data Sheets* **71**, 557 (1994).
30. Wiringa, R. B., Stoks, V. G. J., and Schiavilla, R., *Phys. Rev. C* **51**, 38 (1995).