Shell-Model Calculations with Realistic Effective Interactions

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Abstract. In this paper, we present some results of shell-model calculations employing effective interactions derived from the CD-Bonn free nucleon-nucleon potential. These concern $^{18}$O, $^{134}$Te, and $^{210}$Po, and are part of a comprehensive study of nuclei around doubly closed shells. Comparison of the calculated results with experimental data illustrates the degree of accuracy of modern realistic shell-model calculations.

INTRODUCTION

A basic ingredient in nuclear shell-model calculations is the model-space effective interaction. The most popular approach to the determination of $V_{eff}$ relies on the use of empirical effective interactions, which leads in general to a very successful description of nuclear structure properties. While this approach is certainly of great practical value for the interpretation of experimental data, it is not satisfactory from a first-principle point of view. In fact, a fundamental goal of nuclear structure theory is to understand the properties of complex nuclei in terms of the nucleon-nucleon (NN) interaction. This implies the derivation of $V_{eff}$ from the free NN potential.

Over the last decade there has been substantial progress towards a microscopic approach to nuclear structure calculations starting from a free NN potential. This has concerned both the two basic ingredients which come into play in this approach, namely the NN potential and the many-body methods for deriving the model-space effective interaction.

As regards the first point, several NN potentials have been constructed, which give a very accurate description of the NN scattering data and are suitable for application in nuclear structure. These are the Nijmegen potentials [1], the Argonne $V_{18}$ potential [2], and the very recent high-precision CD-Bonn potential [3] which, according to the analysis made in [3], gives the most accurate reproduction of the presently available $NN$ data.

As for the second point, an accurate calculation of the Brueckner $G$-matrix has become feasible while the so-called $\hat{Q}$-box folded-diagram series for the effective interaction $V_{eff}$ can be summed up to all orders using iterative methods. An outline of the derivation of $V_{eff}$ will be given in section 2.

Based on these improvements, in recent years there has been a renewed interest...
in shell-model calculations employing effective interactions derived from the free \( NN \) potential. In this context, a key issue is how accurate a description of nuclear structure properties can be provided by these “realistic” effective interactions.

On this problem, we have concentrated our efforts during the last few years [4-9]. We have focused attention on nuclei with few valence particles or holes, since they provide the best testing ground for the basic ingredients of shell-model calculations, especially as regards the matrix elements of the effective \( NN \) interaction.

It is our aim here to present some selected results of our calculations, which have been obtained by making use of the CD-Bonn \( NN \) potential, and the main conclusions of our study.

**THE SHELL-MODEL EFFECTIVE INTERACTION**

Let us now outline our derivation of \( V_{\text{eff}} \). Because of the strong repulsive core, which is a feature common to all modern \( NN \) potentials, the model-space \( G \) matrix corresponding to the chosen \( V_{NN} \) must be calculated first. The \( G \) matrix is defined [10] by the integral equation:

\[
G(\omega) = V + VQ_2\frac{1}{\omega - Q_2TQ_2}Q_2G(\omega),
\]

where \( V \) represents the \( NN \) potential, \( T \) denotes the two-nucleon kinetic energy, and \( \omega \) is an energy variable (the so-called starting energy). The two-body Pauli exclusion operator \( Q_2 \) prevents double counting, namely the intermediate states allowed for \( G \) must be outside the chosen model space. Thus the Pauli operator \( Q_2 \) is dependent on the model space, and so is the \( G \) matrix. The operator \( Q_2 \) is specified, as discussed in Ref. [10], by a set of three numbers \((n_1,n_2,n_3)\) each representing a single-particle orbital. Note that in Eq.(1) the Pauli exclusion operator \( Q_2 \) is defined in terms of harmonic oscillator wave functions while plane-wave functions are employed for the intermediate states of the \( G \) matrix.

Our procedure for calculating the \( G \) matrix goes as follows. We first calculate the free \( G \) matrix \( G_F \) in a proton-neutron representation, \( G_F \) being defined by

\[
G_F = V + V\frac{1}{e}G_F,
\]

with \( e \equiv (\omega - T) \). Note that \( G_F \) does not contain the Pauli exclusion operator and hence its calculation is relatively convenient. Then we calculate the Pauli correction term [10, 11],

\[
\Delta G = -G_F\frac{1}{e}P_2\frac{1}{P_2(\frac{1}{e} + \frac{1}{e}G_F\frac{1}{e})}P_2\frac{1}{e}G_F,
\]

where \( P_2 = 1 - Q_2 \), separately for protons and for neutrons. Finally, the full \( G \) matrix as defined by Eq.(1) is obtained as

\[
G = G_F + \Delta G.
\]
For the harmonic oscillator parameter $\hbar \omega$ we use the value obtained from the expression $\hbar \omega = (45A^{-1/3} - 25A^{-2/3})$ MeV.

Using the above $G$ matrix we then calculate the irreducible vertex function $\hat{Q}$-box, which is composed of irreducible valence-linked $G$-matrix diagrams through second order. These are precisely the seven first- and second-order diagrams considered by Shurpin et al. [12]. The effective interaction can be written in operator form as

$$V_{\text{eff}} = \hat{Q} - \hat{Q}' \int \hat{Q} + \hat{Q}' \int \hat{Q} - \hat{Q}' \int \hat{Q} \int \hat{Q} \int \hat{Q} + \ldots,$$

where $\hat{Q}$ is the $\hat{Q}$-box, and the integral sign represents a generalized folding operation [13]. $\hat{Q}'$ is obtained from $\hat{Q}$ by removing terms of first order in the reaction matrix $G$.

After the $\hat{Q}$-box is calculated, the energy-independent $V_{\text{eff}}$ is obtained by summing up the folded-diagram series of Eq.(5) to all orders using the Lee-Suzuki iteration method [14]. This last step can be performed in an essentially exact way for a given $\hat{Q}$-box.

RESULTS

To illustrate the degree of accuracy to which realistic shell-model calculations can describe the spectroscopic properties of nuclei near closed shells, we report here some results we have obtained for light-, medium- and heavy-mass nuclei having two valence particles. They have been obtained by using the OXBASH shell-model code [15].

| $E$(MeV) | $J^\pi$ | Exp. | Calc. |
|----------|--------|------|------|
| 0$^+$    | 0.000  | 0.000|
| 2$^+$    | 1.982  | 1.824|
| 4$^+$    | 3.555  | 3.269|
| 0$^+$    | 3.634  | 3.720|
| 2$^+$    | 3.920  | 3.889|

As already mentioned in the Introduction, we have made use of effective interactions derived from the CD-Bonn NN potential. Regarding the single-particle energies, we have taken them from the experimental spectra of the corresponding single-particle valence nuclei.

In Tables 1-3 we compare the experimental [16] and calculated low-energy levels of $^{18}$O, $^{134}$Te, and $^{210}$Po. We see that the observed excitation energies in all the three nuclei are very well reproduced by our calculations, the discrepancy being less than 150 keV for most of the states.

We refer the reader to papers [5, 8], where we have made use of the Bonn-A NN potential [17], for a more complete analysis of the spectroscopic properties of $^{134}$Te and $^{210}$Po.
| E(MeV)       | J^π  | Exp. | Calc. |
|-------------|------|------|-------|
| 0^+         | 0.000| 0.000|
| 2^+         | 1.279| 1.188|
| 4^+         | 1.576| 1.472|
| 6^+         | 1.691| 1.605|
| 6^+         | 2.398| 2.249|
| 2^+         | 2.462| 2.438|

TABLE 3. Experimental and calculated low-energy levels in $^{210}$Po.

| E(MeV)       | J^π  | Exp. | Calc. |
|-------------|------|------|-------|
| 0^+         | 0.000| 0.000|
| 2^+         | 1.181| 1.076|
| 4^+         | 1.427| 1.342|
| 6^+         | 1.473| 1.435|
| 8^+         | 1.557| 1.498|
| 8^+         | 2.188| 2.123|
| 2^+         | 2.290| 2.250|

SUMMARY

In this paper, we have presented some recent results of realistic shell-model calculations, which are part of a comprehensive study aimed to assess the role of realistic effective interactions in nuclear structure theory.

The main conclusion of our study is that this kind of calculations is able to provide a quantitative description of nuclear structure properties. It should be noted, however, that most of our calculations have until now concerned nuclei with identical valence nucleons. A careful test of the $T = 0$ matrix elements is of course equally important. In this regard, we may mention that in the study [7] of the doubly odd nucleus $^{132}$Sb we have obtained results which are as good as those regarding like nucleon systems. Along the same lines we are currently studying other nuclei with both neutrons and protons outside closed shells.

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