Deriving the nuclear shell model from first principles

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Abstract. A procedure for calculating microscopically the input for standard shell-model calculations, *i.e.,* the core and single-particle energies plus the two-body effective model-space interactions, is presented and applied to nuclei at the start of the *sd*-shell. Calculations with the JISP16 and Idaho χEFT N^{3}LO nucleon-nucleon interactions are performed and yield consistent results, which also are similar to phenomenological results in the *sd*-shell as well as with other theoretical calculations, utilizing other techniques. All results show only a weak A-dependence.

1. Introduction

Tremendous progress has been made in the last 15 to 20 years in the constructing of a unified microscopic formalism capable of describing the properties of nuclei and nuclear reactions. This has been achieved: 1.) by a better understanding of the fundamental interactions among the nucleons, mainly through the use of Chiral Effective Field Theory (χEFT) [1, 2, 3] and 2.) by the development of new approaches or by the improvement of existing methods, for solving the nuclear many-body problem, such as, the Greens Function Monte Carlo (GFMC) [4, 5], No-Core Shell Model (NCSM) [6, 7, 8, 9] and Coupled Cluster (CC) [10, 11, 12, 13] approaches, among others. The success of these approaches is well-documented, especially for light nuclei, *e.g.,* $A \leq 16$ (see the above references).

However, the main problem facing most of these techniques is how to extend them to heavier mass nuclei, because of the rapid growth of the model spaces required to obtain a converged result or other computational problems related to the increase in A. Consequently, there is currently much interest in developing a method for computing microscopically the input for Standard Shell Model (SSM) calculations, *i.e.,* the inert core energy, the single-particle (s.p.) energies and the effective two-body interactions in the valence space, using one of the successful, existing many-body methods, *e.g.,* those mentioned above. Such a procedure was put forward by Navrátil *et al.* in 1998 [14] and applied successfully to a calculation of the effective charges and gyromagnetic ratios for 0p-shell nuclei. This approach was expanded by Lisetskiy *et al.* [15, 16] to all nuclei in the 0p-shell. Their results exhibited a strong A-dependence, which arose from specific choices made in the definition of the core and s.p. energies. We note that there is considerable freedom in the definitions of the contributions to the effective valence-space Hamiltonian.

This contribution presents the approach with another choice of the core and valence-space energies, along with its application to nuclei at the start of the *sd*-shell. This modified method exhibits only a very weak A-dependence and produces results, which are consistent with two recent, but different theoretical approaches to this problem [17, 18, 19].

2. Formalism

The basic formalism is well-described in Refs. [15, 16] and the reader is referred to these publications for the details of this method. The procedure can be outlined as follows:

(i) Start with a nucleus, such as, ^{18}F, which has the SSM structure of an *inert* core, (*e.g.*, ^{16}O) with two valence nucleons in the first major shell outside of the core, in this case, the *sd*-shell.

(ii) Pick some existing many-body method, such as the NCSM or the CC approach, to calculate the eigenvalues and eigenfunctions for this nucleus. In the case of the NCSM the nucleon-nucleon (NN) interaction used in performing the numerical calculations is truncated, *i.e.,* renormalized, into a tractable two-nucleon model space using the Okubo-Lee-Suzuki (OLS) transformation [20, 21, 22]. This procedure is referred to as determining the two-nucleon (2N) cluster in a finite model (*i.e.,* basis) space.

(iii) Use this 2N-cluster to construct the A-nucleon Hamiltonian in the model space, which is then diagonalized in the model space to obtain the A-nucleon eigenenergies and eigenfunctions.

(iv) Perform a second OLS transformation of these converged eigenenergies and eigenfunctions into the $0\hbar\Omega$ space, which is, by definition, the space of the inert core plus two-valence nucleons in the first major shell outside of the core. Because this space has zero excitation energy available to it, the nucleons in the core are *energetically frozen* and, hence, do indeed behave like an inert core. Thus, all of the A-body correlations obtained by solving the A-nucleon problem in the large model space are now fully contained in the matrix elements of the two-nucleons in the valence space.

(v) Now separate the obtained two-body matrix elements into a core energy, s.p. energies and effective two-body interactions, as described in Refs. [15, 16], except that the A-dependence for the kinetic energy is taken to be A_{core} instead of A, when calculating the core energy, and $A_{core}+1$ for the s.p. energies.

(vi) These core and s.p. energies and two-body effective interactions can now be used for performing SSM calculations for the rest of the nuclei in that major shell, *e.g.,* the *sd*-shell.

3. Applications

We have performed NCSM calculations in the *sd*-shell for nuclei with $A = 18$ and 19 using the JISP16 [23] and Idaho χEFT N^{3}LO [24] NN interactions. The maximum model-space size that we could handle in these calculations was $N_{max} = 4$, *i.e.,* all configurations up to energies of $4\hbar\Omega$, where $\hbar\Omega$ is the harmonic-oscillator energy.

The eigenenergies and eigenfunctions obtained in our calculations for the ground and excited states of $A = 18$ and $A = 19$ nuclei were then projected into the $0\hbar\Omega$ space, utilizing the OLS transformation. For example, for $A = 18$ this yields 18-body matrix elements for four nucleons in the 0*s*-shell, 12 nucleons in the 0*p*-shell and two nucleons in the *sd*-shell. Because of the restriction to a total excitation energy of $0\hbar\Omega$ the lowest-lying 16 nucleons form an ^{16}O core, because they are *energetically frozen* against excitations into the *sd*-shell. Thus, all the 18-body correlations of the large model-space results are now contained within the two-body matrix elements (TBMEs) of the two nucleons in the *sd*-shell, *i.e.,* the valence nucleons.

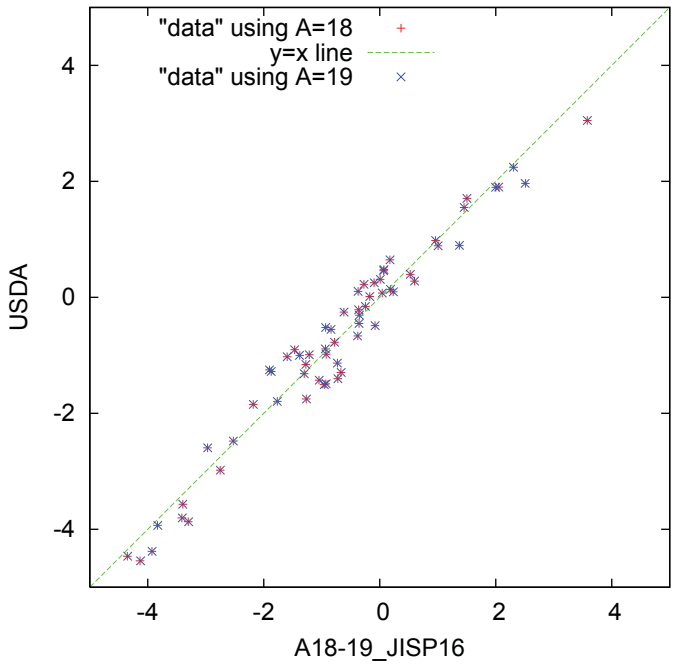

Figure 1. Comparison of our two-body effective shell-model interactions, *i.e.,* after the OLS transformation into the $0\hbar\Omega$ space, for A=18 (red +) and A=19 (blue x) nuclei with the phenomenological USDA two-body matrix elements of Brown and Richter [26].

These highly correlated TBMEs can now be separated into an inert ^{16}O core energy, s.p. energies for each of the two nucleons in the *sd*-shell and residual effective two-body shell-model interactions. This is done by first calculating the g.s. energy of the ^{16}O using the TBMEs generated for the original $A = 18$ calculation, *i.e.,* this is an ^{16}O core *inside* of ^{18}O or ^{18}F. Note that the relative kinetic-energy operator used in the ^{16}O calculations should be for only 16 nucleons. The *sd*-shell s.p. energies are then obtained by calculating the low-lying spectra of ^{17}O and ^{17}F and subtracting the previously calculated ^{16}O core energy. Finally, the two-body effective shell-model interactions are found by subtracting the ^{16}O core energy plus the appropriate s.p. energies for the two *sd*-shell valence nucleons from the original, highly correlated TBMEs obtained by the second OLS transformation. Thus, we now have all the input necessary for performing SSM calculations for other nuclei within the *sd*-shell.

To study the A-dependence of our results, we can repeat the above calculations for the $A = 18$-cluster inside of nuclei with $A = 19, A = 20$, *etc.*

4. Results

Figure 1 compares our two-body effective shell-model interactions for $A = 18$ and $A = 19$ with the phenomenological two-body effective *sd*-shell matrix elements of Brown and Richter [26], for their so-called USDA interaction. First of all, one notes how closely these three sets of TBMEs are correlated. Secondly, one observes that our $A = 18$ and $A = 19$ results are essentially the same, *i.e.,* they are only weakly A-dependent.

Table 1 gives the ^{16}O core energies and the $A = 17$ s.p. energies for the $A = 18$ and $A = 19$ systems, calculated with the JISP16 NN interaction [23]. Again one notices the weak A-dependence. Calculations have also been carried out using the Idaho χEFT N^{3}LO

Table 1. ^{16}O core energies (E_{core}) and proton and neutron single-particle energies for the JISP16 NN interactions for the $A = 18$ and $A = 19$ systems.

	$A = 18$ ($E_{core} = -115.529$)			$A = 19$ ($E_{core} = -115.319$)		
a	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$
ϵ_a^n	-3.068	6.262	-2.270	-3.044	6.289	-2.248
ϵ_a^p	0.603	9.748	1.398	0.627	9.774	1.419

Table 2. ^{16}O core energies (E_{core}) and proton and neutron single-particle energies for the chiral N3LO NN interactions for the $A = 18$ and $A = 19$ systems.

	$A = 18$ ($E_{core} = -118.469$)			$A = 19$ ($E_{core} = -118.306$)		
a	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$
ϵ_a^n	-3.638	3.763	-3.042	-3.625	3.770	-3.031
ϵ_a^p	0.044	7.299	0.690	0.057	7.307	0.700

NN interaction [24]. These results are shown in Table 2. The results for both interactions are similar and again show only a weak A-dependence.

In a recent paper, Jansen *et al.* [17] report on investigations similar to ours but using the Coupled Cluster approach for performing their large model-space calculations and including the Idaho χEFT 3NF at N^{2}LO with the χEFT NN interaction at N^{3}LO [24]. They find $E_{^{16}O,A=18}$ = -130.462 MeV and $E_{^{16}O,A=19}$ = -130.056 MeV, for the ^{16}O core energies for $A = 18$ and $A = 19$, respectively. One observes a slightly lower ^{16}O core energy, by about 10%, due to the inclusion of the 3NF, and a weak A-dependence, similar to ours. The input for SSM calculations can also be obtained using the In-Medium Similarity Renormalization Group (IM-SRG) approach [18, 19]. Preliminary results, obtained using this method [25], are consistent with our results given here.

Finally, columns 1 and 2 of Fig. 2 compare, respectively, the SSM calculation for $A = 18$ with the exact NCSM calculation for $A = 18$. By construction these two results must be the same. Columns 3 and 4 compare, respectively, the results of SSM calculations performed for $A = 19$ using the $A = 18$ input and the $A = 19$ input. These are compared with the full NCSM results for $A = 19$ in column 5. The strong similarity of these results again demonstrates the weak A-dependence of the SSM input. The close agreement with the full NCSM results suggests that the effective three-body interactions in the $A = 19$ systems are small. However, this point needs to be tested by performing calculations for larger A systems in the *sd*-shell.

5. Conclusions

We have performed *ab initio* NCSM calculations for $A = 18$ and $A = 19$ nuclei, which were then projected into the *sd*-shell, using the OLS transformation. These projected results were then used to determine the ^{16}O core energy, *sd*-shell s.p. energies and two-body effective *sd*-shell interactions. Our results correlate well with both phenomenological results and theoretical results obtained using the CC and IM-SRG methods. The results are found to be weakly A-dependent, so that they should be appropriate for performing SSM calculations for nuclei throughout the *sd*-shell.

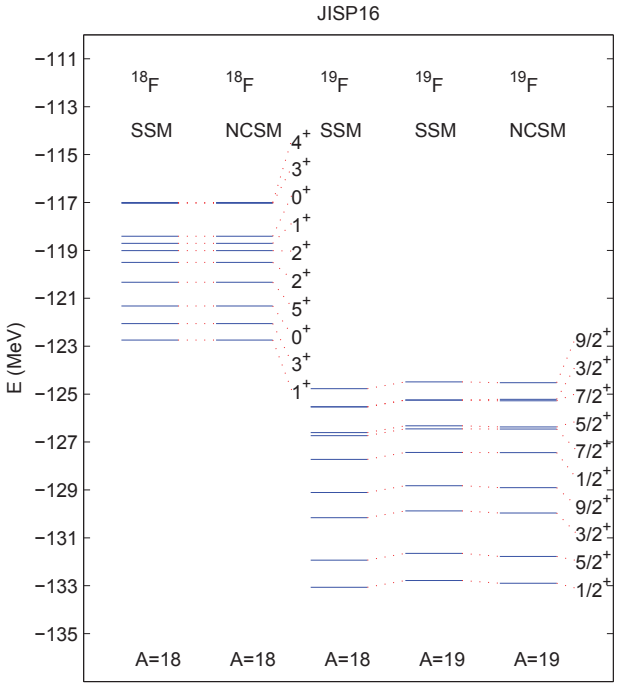

Figure 2. The ground and low-lying excited-state energies of ^{18}F and ^{19}F obtained by SSM and NCSM calculations, using the shell-model input for ^{18}F and ^{19}F, respectively, and generated as described in the text. All calculations are based on the JISP16 NN interaction [23].

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