Ab initio shell model with a core

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Abstract. The No Core Shell Model (NCSM) has been successful in describing the properties of light nuclei, \(A \leq 16\), starting from the fundamental interactions among the \(A\) nucleons, but it is currently difficult to extend the NCSM to heavier nuclei, because of the extremely large model spaces involved in the calculations. We present a new procedure, based on performing two unitary transformations on the Hamiltonian, so as to obtain the core, one-body, two-body and perhaps three-body input necessary for performing Standard Shell Model (SSM) calculations for nuclei. Such SSM calculations can be easily performed for \(sd\)- and \(pf\)-shell nuclei. We demonstrate the accuracy of our approach by applying it to nuclei within the \(0p\)-shell.

1. Introduction

The No Core Shell Model (NCSM) has had considerable success in describing the binding energies, excitation spectra and other physical properties of light nuclei, \(A \leq 16\), e.g., [1, 2, 3]. One of the principle reasons for these successes is that one can exactly calculate the effective interactions and operators to be used in a given model space, using a unitary transformation approach [4, 5]. The unitary matrix employed in this transformation is composed of the eigensolutions for the interacting system of a few nucleons \(n\), where \(n\) is usually only two or three. This is referred to as a cluster approximation but is perhaps more clearly defined as an \(n\)-body correlation, given by the eigensolutions for the fully correlated system of \(n\) nucleons. This unitary transformation is used to truncate the full space solution to a smaller model space. The \(n\)-body matrix elements obtained from this truncation are used as input to the many-body Hamiltonian for all \(A\) nucleons, which is then diagonalized in the model space. As the size of the model space increases, the cluster Hamiltonian approaches the full-space Hamiltonian, yielding the converged, (i.e., exact) solution. This procedure works well for lighter nuclei, \(A \leq 16\), whose many-body Hamiltonians can be diagonalized in sufficiently large model spaces, so as to obtain converged results. For heavier mass nuclei, existing computer technology does not allow calculations in the very large model spaces that they require in order to yield converged results. In this contribution, we outline a new approach for obtaining higher-order correlations, i.e., clusters, in smaller model spaces, so that microscopic calculations based on the NCSM can be extended to heavier nuclei, e.g., nuclei in the \(sd\)- and \(pf\)-shells.

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2. The NCSM Formalism and Its Extension

2.1. The NCSM Approach

One can outline the NCSM procedure as follows:

1. Start with a translationally invariant Hamiltonian for the $A$-nucleon system, which contains a realistic nucleon-nucleon (NN) potential and perhaps a complementary theoretical NNN potential.

2. Add to this the center-of-mass (COM) harmonic-oscillator (HO) Hamiltonian, so as to bind the COM of the $A$-nucleon system. This defines a basis, i.e., HO, for performing our calculations and also allows for the exact projection of spurious COM components from our final wave functions.

3. Solve this combined Hamiltonian [Steps 1 and 2] in an extremely large space, e.g., 300 or more HO configurations, so as to obtain fully converged solutions for the two-(or three-)nucleon system.

4. Using a unitary transformation constructed from the components of the eigensolutions in step 3, which span a smaller two-(or three-)nucleon model space, obtain the matrix elements of the effective two-(or three-)body Hamiltonian in the smaller model space.

   This procedure is similar to the earlier technique of taking a subset $d$ of the eigensolutions obtained in step 3 and explicitly projecting them into a smaller two-(or three-)nucleon model space of dimension $d$. In that case the exact two-(or three-)nucleon effective interaction in the $d \times d$ model space is given by a sum over $d$ of all terms of the form of a projected eigensolution times its corresponding full-space eigenenergy times the corresponding biorthogonal of the projected eigensolution. The truncating of the unitary matrix in step 4 is a straightforward technique for performing this truncation and summation.

5. Use these effective Hamiltonian matrix elements to construct the $A$-nucleon Hamiltonian matrix, which is then diagonalized in the $A$-nucleon model space.

6. Repeat steps 4 and 5 as the $A$-nucleon model-space size is increased, so as to obtain converged results.

2.2. Our Extension of the NCSM Approach

To extend the NCSM approach to heavier nuclei, for which the $A$-nucleon model spaces become unmanageable with existing computers, a new technique will be necessary. One such procedure [6] is to reintroduce a core into the NCSM approach, by performing a second unitary transformation, so as to include the effects of all $A$ nucleons into a single major shell, as proposed by Navrátil et al. [7].

This extension, which we call the “ab initio Shell Model with a Core,” adds additional steps to the ones given above.

7. Use the converged $A$-nucleon eigensolutions of step 6 to construct a second unitary transformation matrix, so as to project the converged $A$-nucleon model-space results in step 6 into the space, in which all $A$ nucleons occupy the lowest HO configuration allowed by the Pauli Exclusion Principle.
Figure 1. The g.s. energy of $^7\text{Li}$ as a function of $N_{\text{max}}$. The dots connected with a solid line are the full NCSM results. The squares connected with a dashed line are the SSM results without the three-body component. The dots connected with a dashed line are SSM results using a constant, bare $^4\text{He}$ g.s. energy. See the text for more details.

For example, for $^6\text{Li}$ this would be four nucleons in the $0s_{1/2}$-shell and two nucleons in the $0p$-shell. Similar to Standard Shell Model (SSM) terminology, we call this the space of $0\hbar\Omega$ excitation energy, i.e., no energy is available to any of the $A$ nucleons for excitations to any higher HO shells. Thus, in our example of $^6\text{Li}$, the four nucleons in the $0s_{1/2}$-shell are effectively frozen into this configuration (like an inert core!) and only the two nucleons in the $0p$-shell can move around in that shell. Consequently, the two nucleons in the $0p$-shell yield a full set of $0p$-shell two-nucleon matrix elements, which by construction now contain all the correlations of the six-nucleon system. Note that this is equivalent to calculating the six-body cluster! When diagonalized in the $0p$-shell, this six-body-cluster result yields exactly the same eigenenergies as the full NCSM calculations for states with parentage predominately within the $0p$-shell.

8. For NCSM solutions involving $A$ nucleons, such that $A$ can be separated into $A-2$ core nucleons and two-valence nucleons, e.g., $^6\text{Li}$ going to a $^4\text{He}$ core and a valence proton and a valence neutron, one can then calculate the core, one-body and two-body parts of the solutions in step 7.

These core, one-body and two-body components are simply the input for a SSM calculation and can then be used to perform SSM calculations for heavier mass nuclei in the same major shell. For example, in the $0p$-shell, the results obtained for the $A = 5, 6$ and $7$ nuclear systems in steps 7 and 8 can be used to perform SSM calculations for $A = 8, 9, 10...16$ nuclear systems.

3. Applications to 0p-shell Nuclei
Figures 1 and 2 compare the results of full NCSM calculations (INOY NN potential [8, 9] as the $A$-nucleon model-space size, $N_{\text{max}}\hbar\Omega$, is varied from $N_{\text{max}} = 2$ to 12 with $\hbar\Omega = 14$ MeV) for the ground-state (g.s.) energy and excited-state energies of $^7\text{Li}$, respectively, with the results of SSM calculations, using the core, one-body and two-body components, computed as described above [steps 7 and 8], using the $^7\text{Li}$ NCSM two-body matrix elements.

The energy of the $^4\text{He}$ core inside the $^7\text{Li}$ nucleus is computed to be $-63.336$ MeV, significantly
Figure 2. NCSM (solid lines) and SSM without the three-body component (dashed lines) for the excited-state spectrum of $^7$Li. The states with spin $J$ are marked by $2J$.

larger than that for a bare $^4$He nucleus, being $-28.296$ MeV. This should not be a surprising result, because the two protons and the two-neutrons of the $^4$He core are in lower-lying $0s_{1/2}$ levels inside the $^7$Li mean field (e.g., a phenomenological Woods-Saxon potential), than in the mean field for a bare $^4$He nucleus.

The single-particle energies are then obtained by calculating the five-body clusters inside the $^7$Li nucleus, i.e., $^5$He and $^5$Li, and subtracting the above $^4$He core energy. The two-body matrix elements are found by subtracting the previous five-body cluster results from the earlier six-body cluster results, e.g., $^6$He, $^6$Li and $^6$Be. For $A = 7$ it is also possible to obtain the seven-body cluster results, from which effective three-body matrix elements can be obtained.

For the test calculations in the $0p$-shell we have performed such calculations, as described above, for the $A = 6$ and $A = 7$ nuclear systems and determined the core, one-body and two-body (and three-body for $A = 7$) components. For $A = 7$, SSM calculations performed in the $0p$-shell with the core, one-, two- and three-body components exactly reproduce (by construction) the results of a full NCSM calculation for $A = 7$ for eigenstates predominately in the $0p$-shell.

These components can also be used for performing SSM calculations in the $0p$-shell for nuclear systems with $A > 7$. For example, Fig. 3 shows results for $^8$He, $^9$He and $^{10}$He calculated with the CD Bonn NN potential [10] for $N_{\text{max}} = 6$ and $\hbar\Omega = 20$ MeV. At least for these maximal isospin cases, including the effective three-body contribution improves agreement with the exact NCSM results and appears to leave very limited room for effective four- or higher-body contributions.

The same double unitary transformation approach outlined previously for obtaining the effective components of the shell-model Hamiltonian in a single major shell, e.g., the $0p$-shell, can also be utilized for computing the effective components of any physical operator in the same major shell [11].

It should be noted that the double unitary transformation technique developed here is similar in philosophy to the work of Fujii, et al., [12] using the unitary-model-operator approach. However, in their work the second unitary transformation is to a single-particle basis, while in our case the second unitary transformation is based on a truncation to a smaller total energy for the $A$-nucleon model space.
Figure 3. Comparison of spectra for $^8$He, $^9$He and $^{10}$He from SSM calculations using up to two-body components (2BVC) and up to three-body components (3BVC) with exact NCSM results, all calculated for $N_{\text{max}} = 6$ and $\hbar \Omega = 20$ MeV using the CD-Bonn NN potential [10].

4. Conclusions
The purpose of the present investigations was to demonstrate the feasibility of using our double unitary transformation technique for determining the input components for SSM calculations in a single major shell. This was done by performing calculations for nuclei in the $0p$-shell, for which exact NCSM calculations can also be performed, thereby providing a check on our proposed procedure.

The good agreement obtained between our exact NCSM calculations and our SSM calculations encourages us to extend this procedure to $sd$- and $pf$-shell nuclei. Because the second unitary transformation is always made to the lowest energy model space, i.e., $0\hbar \Omega$, the final results will always look like an inert core plus a few valence nucleons. Work on the extension of this approach to $sd$- and $pf$-shell nuclei is currently in progress.

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