Microscopic calculations of nuclear structure beyond the 0p-shell

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Abstract. Significant progress has been made in our microscopic understanding of the properties of light nuclei, starting from the basic nucleon-nucleon and three-nucleon interactions among the particles inside the nucleus. The main challenge now is to extend these successes for light nuclei ($A \leq 16$) to heavier mass nuclei. Here we discuss three recent approaches within the No Core Shell Model for possibly going beyond the 0p-shell.

1. Introduction
Over the last twenty years significant advances have been made in our ability to perform ab initio calculations for describing the properties of atomic nuclei. These advances have come in the form of 1.) a better understanding of how to construct consistent nucleon-nucleon (NN), three-nucleon (NNN) and higher-nucleon interactions based on QCD, using Effective Field Theory (EFT) and Chiral Perturbation Theory (CPT) [1, 2]; 2.) the development of new and/or improved nuclear many-body techniques, such as the Green Function Monte Carlo (GFMC) approach [3], the No Core Shell Model (NCSM) formalism [4], the Coupled Cluster (CC) method [5], etc., for performing the many-nucleon calculations; and 3.) tremendous advances in computer hardware and software, which allow for much larger and more complicated numerical calculations to be performed. Although important progress has been made in our understanding of the interactions among nucleons based on QCD, an analytical form for these interactions has not yet been obtained, so that the NN, NNN and higher-N interactions, both phenomenological and QCD-based, that are currently available for use in numerical calculations, still contain parameters, which must be fitted to experimental data or results based on such data, e.g., the NN phase shifts, etc. The QCD based interactions do have the advantage of consistently showing the evolution of higher-nucleon forces, but have continuing problems regarding regulators, ultraviolet cutoffs, power counting, and renormalization group invariance. These are all issues beyond the scope and subject of this presentation, which deals with the many-body techniques that use such interactions as input. In particular, this talk deals with the question of how the NCSM can be modified, extended and/or improved, so as to handle heavier-mass nuclei beyond the 0p-shell.

2. Understanding nuclei beyond the 0p-shell
One of the major problems facing most nuclear many-body methods for calculating the properties of atomic nuclei microscopically is the rapid growth of the model space, in which the calculations must be performed so as to obtain converged results, with the increasing number of nucleons in...
the nucleus, \( A \). So far, this has restricted most techniques to calculations for nuclei within the 0\( p \)-shell.

A great deal of time and effort is presently being devoted to this problem. Some of these new approaches are 1.) the \textit{ab initio} Shell Model with a Core [6, 7], 2.) the Importance Truncation method [8], 3.) the NCSM in an EFT Framework [9, 10, 11], 4.) the Monte Carlo-NCSM [12], 5.) the In-Medium Similarity Renormalization Group (SRG) [13], the Symmetry-adapted NCSM [SP(3,R)] [14], and a number of other techniques. Here we will limit our discussion to topics 1.) to 3.), because of our involvement in these three efforts.

### 3. Extending the NCSM to Heavier-Mass Nuclei

#### 3.1. The \textit{ab initio} Shell Model with a Core

The basic idea of this approach is to use the usual NCSM method to calculate microscopically the input for standard Shell Model calculations, \textit{i.e.}, the energy of the inert core, the single-particle (s.p.) energies, and the two-nucleon effective-interaction matrix elements within the major shell of interest [6].

#### 3.1.1. Formalism

The formalism for the \textit{ab initio} Shell-Model-with-a-Core approach can be outlined as follows:

(i) Perform a NCSM calculation in a sufficiently large model space for a nucleus with two nucleons outside of a doubly magic closed shell, such as, \( ^6 \text{Li} \) or \( ^6 \text{He} \), so as to obtain converged results for the ground state (g.s.) and first few excited states.

(ii) Project the six-nucleon wave functions and energies, obtained in the above NCSM calculation, into the 0\( h \)\( \Omega \) model space, \textit{i.e.}, by using an unitary transformation. This produces what we call the six-body cluster results, that is, six-body matrix elements in the restricted model space, which contain all the six-body correlations from the full (or large) model space. Because we have restricted the energy in the smaller model space to be 0\( h \)\( \Omega \), the four nucleons in the 0\( s \)-shell do not have enough energy to be excited into the 0\( p \)-shell and, thus, essentially form a \textit{frozen} or \textit{inert} \( ^4 \text{He} \) core. The remaining two-body matrix elements of the two nucleons in the 0\( p \)-shell now contain all the correlation information of the six-nucleon system.

(iii) Separate these two-body matrix elements into a \( ^4 \text{He} \)-core contribution, s.p. energies for the 0\( p_{1/2} \) and 0\( p_{3/2} \) configurations and residual two-nucleon effective interactions in the 0\( p \)-shell. Using the core and s.p. energies along with the residual two-nucleon matrix elements in a standard Shell Model calculation for two-particles in the 0\( p \)-shell will reproduce the same results as those for the same configurations in the full NCSM calculation, by construction.

(iv) Calculate, in a similar manner, the seven-body cluster for \( A = 7 \) nuclei, which will yield the 3N matrix elements.

(v) The \( A \)-dependence of these terms can be found by performing six-body-cluster calculations for all 0\( p \)-shell nuclei with \( A > 7 \).

#### 3.1.2. Results for 0\( p \)-shell nuclei

As stated above, the 0\( p \)-shell results for \( A = 6 \) nuclei are exact by construction. The results for \( A = 7 \) nuclei, using only the six-body-cluster terms, are close to the exact NCSM determinations, suggesting that the three-nucleon contributions are small. As Fig. 1 indicates, these three-nucleon contributions are also small for nuclei with \( A > 7 \), at least when the CD-Bonn NN potential is used [15]. Other physical quantities can also be computed, besides the binding energies and excitation spectra, such as EM moments and transition strengths [7].
3.2. The Importance Truncated NCSM

The basic idea of the Importance Truncation (IT) approach is to decrease the size of the model space required in a given NCSM calculation by eliminating configurations based on an importance criterium. This approach was pioneered in the NCSM by Roth and Navrátil [16] and is referred to as the IT-NCSM. This initial formulation used a multiparticle-multihole (e.g., \(2p - 2h\), etc.) approach to generate the basis states coming from the next larger \(N_{\text{max}}\) space. However, this approach was criticized for possibly having size-extensive issues [17, 18]. Thus, an improved approach to generate the basis states coming from the next larger \(N_{\text{max}}\) space was developed [8, 19], which includes all basis states in the truncation space, but in a sequential manner, as discussed below. The most complete description of this IT-NCSM method is given in [19].

The IT-NCSM procedure is based on multi-configuration perturbation theory (PT), as originally conceived in quantum chemistry [20, 21, 22]. The basic idea centers around a size parameter \(\kappa\) that determines, which many-body basis states are kept in a certain \(N_{\text{max}}\) model space. One wants to calculate the first-order PT contributions to the total wave function, coming from components in the next larger model space, i.e., \(N_{\text{max}} \Rightarrow N_{\text{max}} + 2 \Rightarrow N_{\text{max}} + 4 \Rightarrow \text{etc.}\), namely,

\[
|\psi^{(1)}_{N_{\text{max}} + 2, \text{IT}}\rangle = \sum_{\nu \in N_{\text{max}} + 2} \frac{\langle \phi_{\nu}|W|\Psi_{\text{ref},N_{\text{max}}}\rangle}{\epsilon_{\nu} - \epsilon_{\text{ref},\text{sp}}} |\phi_{\nu}\rangle
\]  

(1)

In Eq. (1) \(|\psi^{(1)}_{N_{\text{max}} + 2, \text{IT}}\rangle\) denotes the approximate wave function of the full space \(N_{\text{max}} + 2\) wave function; \(|\phi_{\nu}\rangle\), the \(N_{\text{max}} + 2\) many-body basis states; \(|\Psi_{\text{ref},N_{\text{max}}}\rangle\), the previously calculated reference state in the \(N_{\text{max}}\) space; and \(W\), the perturbation operator. The two terms in the denominator refer to the single-particle energies of the states \(\phi_{\nu}\) and \(|\Psi_{\text{ref},N_{\text{max}}}\rangle\), respectively. The energy \(\epsilon_{\text{ref},\text{sp}}\) is always taken to be the lowest unperturbed energy configuration of the nucleus. For example, in the case of \(^6\text{Li}\), this would correspond to taking \(\epsilon_{\text{ref},\text{sp}} = 2\hbar\Omega\), because there are two valence nucleons in the \(N = 1\) shell. We neglect the zero-point motion of the HO, i.e., \((3/2)\hbar\Omega\), since we only require the difference in energy of the s.p. energies. Furthermore, for \(^6\text{Li}\) \(\epsilon_{\nu} = (6 + 2)\hbar\Omega\) for the basis states in \(N_{\text{max}} = 4\). It is convenient to define the \(W\) as \(W = H - H_0\), where \(H\) is the initial Hamiltonian and \(H_0\) is that part of \(H\), which connects only many-body basis states that lie in the initial basis space, i.e., from 0 up to \(N_{\text{max}}\). Thus, \(H_0\) does not connect basis states from the reference space to the \(N_{\text{max}} + 2\) space. Consequently, we can rewrite Eq. (1) in the form

![Figure 1. Comparison of spectra for $^8\text{He}$, $^9\text{He}$ and $^{10}\text{He}$ 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 $\hbar\Omega = 20\text{ MeV}$ using the CD-Bonn NN potential [15].](image-url)
\begin{equation}
|\psi_{N_{\text{max}}+2,\text{IT}}^{(1)}\rangle = \sum_{\nu \in N_{\text{max}}+2} \frac{\langle \phi_\nu | H | \Psi_{\text{ref},N_{\text{max}}} \rangle}{\epsilon_\nu - \epsilon_{\text{ref},\text{sp}}} |\phi_\nu\rangle,
\end{equation}

so that the importance measure, \(\kappa_\nu\), of a basis state \((\phi_\nu)\) can be defined as

\begin{equation}
\kappa_\nu = \frac{|\langle \phi_\nu | H | \Psi_{\text{ref},N_{\text{max}}} \rangle|}{\epsilon_\nu - \epsilon_{\text{ref},\text{sp}}}.
\end{equation}

The importance measure \(\kappa_\nu\) can now be used to set a threshold limit, on which basis states are included in the truncated \(N_{\text{max}} + 2\) space. If the threshold value for \(\kappa_\nu\) is taken to be a few \(10^{-5}\), say \(2 \times 10^{-5}\), then only basis states \((\phi_\nu)\) in the \(N_{\text{max}} + 2\) space with \(\kappa_\nu \geq 2 \times 10^{-5}\) are kept. Basis states \((\phi_\nu)\) with \(\kappa_\nu\) lower than this threshold will be discarded, starting the truncation of the \(N_{\text{max}} + 2\) space. Once the truncated \(N_{\text{max}} + 2\) basis has been formed, it can be used to diagonalize the Hamiltonian \(H\) in this truncated space. This yields a new g.s. wave function, \(|\Psi_{\text{ref},(N_{\text{max}}+2)}\rangle\), which is then used as the reference state for evaluating all the basis states in the \(N_{\text{max}} + 4\) basis space, using the same method as described above, and so on.

This sequential method has the advantage that it automatically generates all basis states in the evaluated \(N_{\text{max}}\) space, so it only needs to be done once per basis space. Furthermore, one can generate a sequence of g.s. energies for each truncated \(N_{\text{max}}\) basis space, which can be easily extrapolated to obtain the g.s. energy at \(N_{\text{max}} = \infty\).

In practice, the calculations must be done for several values of \(\kappa_\nu\), because it is not possible, by definition, to do the calculations for \(\kappa_\nu = 0\). This would be equivalent to performing the NCSM calculation in the full \(N_{\text{max}} + 2\) space. If we could do this, then there would be no need to truncate the \(N_{\text{max}} + 2\) space. Thus, we need results for several values of \(\kappa_\nu\), which will guide us in constructing extrapolation procedures for going to the limit \(\kappa_\nu \rightarrow 0\).

Our research group is currently investigating refinements of this method, for which preliminary results in the \(0p\)-shell are yielding encouraging results. One of these refinements is to include one or more excited states as additional reference states. Doing this, we find a much improved rate of convergence in the IT-NCSM process, as shown in Fig. 2 [8].

### 3.3. The NCSM in an EFT framework

For many years, the standard procedure in nuclear many-body theory has been to start with a given free-space NN potential (and NNN potential) and then to use this potential to construct an appropriate effective interaction in a model space for calculating nuclear properties. However, it is also possible to use the philosophy of Effective Field Theory (EFT), i.e., a separation of the relevant physics based on different physical scales, e.g., high-momentum physics versus low-momentum physics, to construct effective interactions in model spaces without going through the intermediate step of first constructing a free-space NN potential (and NNN potential) [9, 10, 11]. Not only would such a procedure be more efficient, but it would also have the possibility of yielding effective interactions that would converge more rapidly in the different many-body techniques, thereby allowing calculations to be performed for heavier-mass nuclei.

#### 3.3.1. Formalism

Effective Field Theory (EFT) [1, 2] is based on a separation of scales, such as the nucleon mass or the pion mass, where the details of the physics at energies greater than the separation energy (representing the short-distance physics) are irrelevant for understanding the physics below the separation energy (representing the long-distance physics). In EFT the low-energy degrees of freedom are explicitly included, while the high-energy degrees of freedom are integrated out.

One then constructs a potential, in this case in the NCSM model space, which is consistent with the symmetries of the QCD Lagrangian and is expanded as a Taylor series in the momenta.
or as a contact gradient expansion in coordinate space. Each term in this potential expansion contains a constant. These constants are known as the low-energy constants (LECs). For now, the LECs are determined by fitting to experimental data.

In the case of the NCSM the calculations are performed in an harmonic-oscillator (HO) space for two-nucleons up to some maximum energy, $E_{\text{max}} = (N_{\text{max}} + \frac{3}{2})\hbar \omega$. Thus, the calculations are carried out in a truncated model space, so the interactions in this truncated space represent the renormalized effective interactions. In standard NCSM calculations one needs to repeat the calculations for increasing $N_{\text{max}}$ to check that the results are converging in an appropriate manner. In EFT one introduces a cutoff $\Lambda$, known as the Ultraviolet (UV) cutoff, which depends on $N_{\text{max}} \hbar \omega$. To obtain a correct EFT result, one must achieve Renormalization Group Invariance (RGI). This means that the LECs, which are redetermined as $\Lambda$ increases, become independent of $\Lambda$. In other words, for a high enough $\Lambda$, the LECs have absorbed the high-energy physics and the calculated physical observables are approximately independent of the cutoff $\Lambda$. The Taylor series expansion of the potential provides a power counting or hierarchy between the different contributions, which yield results that are improvable order by order, i.e., leading order (LO) > next-to-leading order (NLO) > next-to-next-to-leading order (NNLO) > etc.

3.3.2. Results  Our first investigation was for an EFT without pions, i.e., a separation-scale energy of $\approx 100$ MeV, which is known as the pionless EFT. In this case the Hamiltonian in the NCSM model space contains three potential terms consistent with the QCD symmetries, namely the NN potentials in the triple $S$ and single $S$ channels and a NNN potential in the $S = \frac{1}{2}$ channel. One then uses this Hamiltonian to compute the three LECs associated, respectively, with the three potential terms above. That is, the values of the LECs are adjusted until they reproduce, in our case, the binding energies of the deuteron, the triton and the $\alpha$ particle. Once these constants are determined, the Hamiltonian in the NCSM model space is completely known and can be used to compute other nuclear properties, such as the energy of the first-excited $0^+$ state of the $\alpha$ particle or the binding energy of $^6\text{Li}$. The determination of the Hamiltonian must be done for increasing values of $\Lambda$ to achieve RGI. Because the calculations are performed using HO wave functions, i.e., in an HO potential well, one must also take the limit as $\omega \rightarrow 0$ (the Infrared (IR) cutoff), since the nucleus is a self-bound system. Thus, the LECs are functions of both $\Lambda$ and $\omega$.

![Figure 2](image1.png)

**Figure 2.** The g.s. energy at $\hbar \Omega = 12$ MeV vs the number of basis states kept. The (+) signs are when only the g.s. is used as a reference states, whereas the (×) signs are the behavior, when the lowest three states are used.

![Figure 3](image2.png)

**Figure 3.** Energy of the first-excited $(0^+,0)$ state in $^4\text{He}$ as a function of the UV cutoff $\Lambda$ for different values of the frequency $\hbar \omega$ in MeV. The dashed curve marks the limit $\hbar \omega \rightarrow 0$. 
Figure 3 shows our results for the energy of the first-excited $0^+$ state in the $\alpha$ particle, for increasing $\Lambda$ and decreasing $\omega$, which yields $E(J^P,T,^4\text{He}) = E(0^+_2,0)_{\text{theor}} = 18.8$ MeV, in the limits $\Lambda \to \infty$ and $\omega \to 0$, compared with $E(0^+_2,0,^4\text{He})_{\text{expt}} = 20.21$ MeV. These agree within 10%, which is remarkable agreement for a LO calculation and indicates that the description of this level is insensitive to details of the short-range physics.

Following the same procedure, we also evaluated for the first time in the pionless EFT the binding energy of $^6\text{Li}$. For large values of the UV cutoff $\Lambda$ and small values of the IR cutoff $\omega$, we estimate the binding energy to be about 23 MeV, to be compared with the experimental result of 31.99 MeV. While not as precise as the first-excited-$0^+$-state energy in $^4\text{He}$, this agreement between the theoretical and experimental values for the binding energy of $^6\text{Li}$ to within 30% is consistent with the expected errors in LO in the pionless EFT.

Applications to two and three nucleons in a trap are made in Ref. [11]. Work is currently in progress for extending our formalism to the pionfull EFT, i.e., the EFT with pions.

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