New developments within the no-core shell model

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Abstract. We review recent developments in the ab initio no-core shell model, such as the influence of 3NFs on the binding energies and excitation spectra of light nuclei. Our calculations permit us to compare the effect of different choices for the theoretical 3NF on the properties of light nuclei. This is of particular interest in determining the best choice of the values for the contact terms in 3NFs derived from Chiral Perturbation Theory. Other recent developments in the NCSM include an investigation of the renormalization properties of physical operators, besides the nuclear Hamiltonian, as well as the Lorentz integral transform approach to the description of select reaction observables in light nuclei.

1. Introduction
The goal of the nuclear structure theory is to start with the fundamental interactions among the nucleons, e.g., nucleon-nucleon (NN) plus three-nucleon forces (NNN or 3NF), etc., and calculate the properties of atomic nuclei utilizing many-body quantum mechanical techniques. Besides the pioneering work of the Green’s function Monte Carlo group [1, 2], other powerful techniques such as the no-core shell model (NCSM) [3] and hyperspherical harmonics [4, 5] have been developed, allowing for a precise description of properties of light nuclei. Among all the many-body techniques, the NCSM is the most flexible, allowing calculations of nuclei up to $^{16}$O and beyond [6]. In this paper, we review the latest applications of the no-core shell model to the description of select structure and reaction observables.

2. Formalism
Unlike the phenomenological shell model, the NCSM allows all the nucleons to interact. One starts with the relative Hamiltonian for the $A$ nucleons interacting through NN and possibly theoretical NNN forces, i.e.,

$$H_{rel} = \frac{1}{A} \sum_{i>j=1} \frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i<j} V_{ij}^{NN} + \sum_{i<j<k} V_{ijk}^{NNN}. \quad (1)$$
For computational reasons, discussed in our previous publications, we add an HO center of mass Hamiltonian $H = P^2/(2m) + mA\Omega^2 R^2/2$ to the intrinsic Hamiltonian (1) to obtain

$$H^0_A = \sum_{i=1}^{A} \left[ \frac{\vec{p}_i^2}{2m} + \frac{1}{2} m \Omega^2 \vec{r}_i^2 \right] + \sum_{i>j=1}^{A} \left[ V_{ij}^{NN} - \frac{m \Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right] + \sum_{i<j<k} V_{ijk}^{NNN},$$

(2)

As the center-of-mass Hamiltonian is subtracted from the final results, it has no net influence on the intrinsic properties.

In principle, one would like to solve the $A$-nucleon Schrödinger equation for the interaction Hamiltonian $H_A$, but numerically this is not possible in the infinite dimensional Hilbert space. Consequently, one must truncate to a finite model space, where a large scale numerical calculation can be performed, which means that one must determine the appropriate “effective” Hamiltonian (or, equivalently, interaction) to utilize in the chosen restricted space.

One can show, by using, e.g., a Feshbach projection operator approach [7], that if one designs a unitary transformation

$$\mathcal{H} = e^S H_A e^{-S},$$

(3)

which exactly decouples the model space $P$ from the excluded space $Q$ ($P + Q = 1$), i.e., $PHQ = 0$ or $QHP = 0$, one obtains an energy-independent effective interaction in the model space $H_{eff} = PHP$. The diagonalization of $H_{eff}$ in the model space exactly reproduces a set of eigenvalues of the original problem; if both decoupling conditions are satisfied, one also obtains energy-independent effective operators corresponding to the other observables. In Eq. (3), $S$ is an anti-Hermitian operator having the properties $PSP = 0$, and $QSQ = 0$. In general, the operator $S$, as well as the effective Hamiltonian $H_{eff}$, is an $A$-body operator induced by the space truncation. Consequently, solving exactly for $H_{eff}$ is equivalent, and equally difficult, as solving for the full $A$-body Schrödinger equation in the infinite Hilbert space. Hence, one must determine $H_{eff}$ at a lower order of collectivity $a < A$. This is known as a cluster approximation, where in most previous investigations one has taken $a = 2$ (the two-body cluster approximation).

The cluster approximation introduces a residual dependence on the HO parameter $\hbar \Omega$, which will vanish as $P \to 1$. In this limit, $V_{eff} \to V$, so that the exact result is obtained. Thus, for light nuclei, in the largest model spaces accessible for numerical computation, many observables manifest only a weak dependence upon the HO frequency used in the calculation. Note that the space $P$ is defined by the maximum number of HO quanta, $N_{max} \hbar \Omega$, above the ground state configuration of the nucleus under study, i.e., this is an energy truncation. This allows an exact separation of the spurious CM motion in the wave function in the case that one uses a Slater determinant basis which is not translationally invariant.

3. Results

3.1. Three-body forces

A uniform feature of all NCSM calculations with only NN interactions, as well as for other microscopic approaches for calculating the spectra of light nuclei [1, 2], is that they consistently underbind the ground states of nuclei and do not converge to the excited state energies [8, 9]. The general consensus is that one needs additional 3NF’s, or perhaps even more-nucleon forces, to explain these discrepancies. This seems like a reasonable assumption, because three- and more-nucleon forces naturally arise in the determination of the nuclear force from effective field theory using a chiral perturbation theory (CPT) approach [10, 11].

At the present time ad hoc combinations of NN and 3NF’s can provide the correct binding energies for the three- and four-nucleon systems [12, 13], but some fail for $p$-shell nuclei and
some 3N scattering observables. Although the application of CPT provides consistent NN and 3NF models [10, 11], this approach yields so-called contact terms, i.e., constant terms in the momentum space, which must presently be determined by fitting experimental data. In the CPT approach 3NF’s first appear at next-to-next-lowest order (N2LO) and have two contact terms, with two strength constants called \( c_D \) and \( c_E \). When these two strength constants are determined for the Idaho-N3LO interaction,[14] by fitting to the binding of \(^3\)H and \(^3\)He [15], we find that two sets of values, called 3NF-A and 3NF-B, can be found, which determine these data exactly.

We note that the NCSM offers a way to test these different theoretical 3NF’s by performing nuclear-structure calculations at the three-body cluster level for \( p \)-shell nuclei. The mere presence of 3NF’s requires in the lowest order that we must use the three-body cluster approximation, that is the transformation \( S \) must be computed for \( a = 3 \). The effect of adding the theoretical 3NF can be determined by performing the three-body cluster calculation first with only the NN interaction and then a second time, including the 3NF.

![Figure 1.](image)

We have performed the first such calculations for \(^6\)Li[16] and \(^7\)Li[15], so as to test the feasibility of this concept. Details of this approach along with numerous results are given in Ref. [15]. In Fig. 1 we show the results for the low-energy spectrum of \(^7\)Li, which are marginally better for the choice 3NF-B over 3NF-A. Clearly, more calculations for other \( p \)-shell nuclei need to be carried out before a more definitive conclusion can be drawn.

However, it seems fairly obvious at this time that one possibility for determining the unknown terms in theoretical 3NF’s will come from the comparison of results of nuclear-structure calculations with experimental spectra of \( p \)-shell nuclei. In this regard, the NCSM offers a straightforward method for performing these calculations and making these comparisons.

### 3.2. Electromagnetic operators

Because, in general, non-scalar operators can connect different two-body channels, the application of the unitary transformation to transition operators is much more involved than for the Hamiltonian. Recent investigations have shown that the renormalization in the lowest-cluster approximation is strongly dependent on the range of the operator under consideration. Thus, for long-range operators, such as the quadrupole transition operator, it has been shown that the renormalization in the two-body cluster approximation has little effect.[17] For example, for \(^6\)Li, \( B(E2) = 2.183 \, e^2 \, fm^4 \) was obtained using the bare quadrupole operator in the \( 2\Omega \) model space for the \( 2^+ 0 \to 1^+ 0 \) transition, and \( B(E2) = 2.269 \, e^2 \, fm^4 \) [17], when the corresponding effective operator is employed, i.e., it is only a negligible renormalized. However, in \( 10\Omega \),
using bare operator one obtains $B(E2) = 4.502 \, e^2 \, fm^4$. In principle, since one expects larger renormalization in the smaller model space (which takes into account a larger excluded space), the value obtained with the effective operator in $2\hbar \Omega$ model space should be significantly closer to the result in the $10\hbar \Omega$ model space. Since this is obviously not the case, one concludes that the effect of the renormalization for long-range operators is very small. This has been demonstrated in the case of the longitudinal-longitudinal distribution function, [18], where a considerable model independence can be obtained even in the smaller model space for large momentum transfer (short range). Therefore, short-range operators can be reliably calculated in the two-body cluster approximation (the lowest approximation) even in small spaces, when using the appropriate effective operator.[18] On the other hand, long-range operators, are only weakly renormalized at the two-body cluster level. In order to accommodate the long-range correlations, one has to increase the model-space size and/or use a higher-order cluster approximation.

3.3. Total photo-disintegration of $^4$He in a test case

In an inclusive reaction, the response function

$$R(\omega) = \int d\omega |\langle \Psi_f | \hat{O} | \Psi_0 \rangle|^2 \delta(E_f - E_0 - \omega),$$

contains the relevant information on the dynamics of the nuclear target under the influence of external electromagnetic probes. In Eq. (4), $\omega$ is the energy transferred by the probe, and $\hat{O}$, the excitation operator, while $|\Psi_{0/f}\rangle$ and $E_{0/f}$ are the wave functions and energies of the ground and final states of the perturbed system, respectively.

Because the number of discrete states in light nuclei is very small and it is very difficult to calculate scattering states for $A > 3$, a direct numerical calculation of the response function (4) is extremely challenging. The Lorentz integral transform (LIT) approach [19] was introduced in order to overcome these difficulties. In this approach one first calculates the integral transform of the response function with a Lorentzian kernel

$$L(\sigma_R, \sigma_I) = \int d\omega \frac{R(\omega)}{(\omega - \sigma_R)^2 + \sigma_I^2} = \langle \tilde{\Psi} | \tilde{\Psi} \rangle,$$

and then inverts numerically $L$, obtaining $R$ [20, 21]. The finite imaginary part $\sigma_I$ guaranties that the state $\tilde{\Psi}$ is the unique solution of the inhomogeneous “Schrödinger-like” equation

$$(H - E_0 - \sigma_R + i\sigma_I)|\tilde{\Psi}\rangle = \hat{O}|\Psi_0\rangle.$$  

Moreover, the right-hand side of the previous equation is localized, as $|\Psi_0\rangle$ is a bound state. Therefore, the solution $\tilde{\Psi}$ has an asymptotic boundary condition similar to a bound state. Hence, one can apply bound-state techniques for its solution, and, in particular, expansions over basis sets of localized functions. From this point of view, the NCSM is very well suited, as it uses bound-state basis to expand the solution of the Schrödinger equation and the presence of the imaginary part does not introduce any additional difficulty.

We present results for the response function to the isovector dipole excitation in Fig. 2. This response represents the leading contribution to low-energy photo-disintegration cross sections. In this calculation we have used the semirealistic Minnesota (MN) interaction as input, and the effective interaction was calculated in the three-body cluster approximation. We have chosen the MN force, because it provides very good convergence for the nuclear properties. Details of the calculation can be found in Ref. [22].

Among the four different HO frequencies adopted to investigate the dependence of the resulting response on this parameter, $\hbar \Omega = 12, 19$ and $28$ MeV show very good agreement. The
result for $\hbar \Omega = 40$ MeV, not yet completely in convergence, shows a slightly larger discrepancy with respect to the other curves, although mainly in the low-energy part of the response. Indeed, the numerical inversion procedure is very sensitive to the accuracy of the calculation of the LIT, especially in the low-$\sigma_R$ region. We find that for $\hbar \Omega = 40$ MeV [or “for higher HO frequencies”] bigger model spaces are needed in order to reach an equally good sampling of the complex-energy continuum. Nevertheless, in the energy range $60$ MeV $\leq \omega \leq 80$ MeV all four responses agree within 7% or better.

![Figure 2. The dipole response function calculated by means of the LIT, using the semirealistic Minnesota (MN) two-body interaction. The results show a very weak dependence upon the HO frequency used in the calculation. We show only the results obtained in the largest model space we can handle, $16\hbar \Omega$ for positive-parity states, and $17\hbar \Omega$ for negative-parity states](image)

The MN force has been also used as input for a calculation of the same properties by means of the effective interaction hyperspherical harmonics (EIHH) method. While we do not show here the EIHH results, the two methods are in very good agreement [22].

In this calculation, the NCSM results reached the level of precision required by the LIT calculation (for details regarding the numerical inversion procedure and the level of accuracy required, we refer the reader to Refs. [20, 21]). However, the caveat is that the force used in this calculation was not a very realistic one and more investigations have to be performed in order to assess the reliability of the method, when using more realistic forces. Moreover, the present investigation has shown a reasonable HO frequency independence only when using very large model spaces, which suggests that the description of such processes via the LIT for heavier nuclei would require much more numerical effort.

4. Summary
We have reviewed some of the latest applications of the NCSM to the description of nuclear properties, namely NNN interactions, extension of the effective operator formalism to other observables, and the response function in the case of the total disintegration of $^4$He.

The NCSM plays a special role in nuclear physics. While, in general, not as accurate as other $ab$-$initio$ methods, its main advantage is its flexibility to handle both local and non-local interactions on the same footing. Moreover, it can also be applied to heavier nuclei than any other method. Finally, the same techniques can be used to construct effective interactions for heavier nuclei in one shell. Coming entirely from $ab$-$initio$ principles, such effective interactions should be more reliably extended to heavier nuclei, including those outside the region of stability.

For the LIT investigation, we acknowledge our collaborator C. W. Johnson, Physics Department, San Diego State University. B.R.B, S.Q, and I.S. acknowledge partial support by NFS grants PHY0070858 and PHY0244389. This work was performed in part under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48. P.N. and W.E.O. received support from LDRD contract 04-ERD-058. J.P.V. acknowledges partial support by USDOE grant No DE-FG-02-
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