

# Perspectives on Nuclear Structure and Scattering with the *Ab Initio* No-Core Shell Model

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Nuclear structure and reaction theory are undergoing a major renaissance with advances in many-body methods, strong interactions with greatly improved links to Quantum Chromodynamics (QCD), the advent of high performance computing, and improved computational algorithms. Predictive power, with well-quantified uncertainty, is emerging from non-perturbative approaches along with the potential for new discoveries such as predicting nuclear phenomena before they are measured. We present an overview of some recent developments and discuss challenges that lie ahead. Our focus is on explorations of alternative truncation schemes in the harmonic oscillator basis, of which our Japanese–United States collaborative work on the No-Core Monte-Carlo Shell Model is an example. Collaborations with Professor Takaharu Otsuka and his group have been instrumental in these developments.

**KEYWORDS:** No-Core Shell Model, Monte-Carlo methods, Truncation methods, JISP16, Daejeon16

## 1. Introduction

With continuing advances in Leadership-Class computing and plans for further developments leading to Exascale systems (defined as having capabilities for  $10^{18}$  floating-point operations per second (flops)), computational scientists are developing quantum many-body approaches that portend a new era of research and discovery in physics as well as in other disciplines. In particular, the nuclear physics quantum many-body problem presents unique challenges that include the need to simultaneously develop (1) strong inter-nucleon interactions with ties to QCD in order to control the concomitant freedoms; (2) non-perturbative many-body methods that respect all the underlying symmetries; and (3) new algorithms that prove efficient in solving the quantum many-body problem on Leadership-Class supercomputers. This triad of forefront requirements impels multi-disciplinary collaborations that include theoretical physicists, applied mathematicians and computer scientists. These requirements also foster international collaborations, such as the Japan–United States collaboration, that can catalyze and incubate new ideas while sharing the workload among the participating teams.

While the physics goals for computational nuclear structure and reactions may seem obvious — i.e., retaining predictive power and quantifying the uncertainties — the opportunities and challenges presented with the continuing rapid development of supercomputer architectures are less obvious to the broader community. Simply put, with the need to develop and apply fully microscopic approaches to heavier nuclei as well as the need to include multi-nucleon interactions and the coupling to the continuum, even Exascale computers will be insufficient to meet all our plans. We therefore must also work to develop truncation schemes that reduce the computational burden without loss of fidelity to the underlying theory. In this work, we will focus on the second part of the triad mentioned above — the development of non-perturbative many-body methods that respect the underlying symmetries.

## 2. *Ab Initio* No-Core Monte Carlo Shell Model

Several years ago, teams of theorists from Japan and the United States initiated a joint research program aimed at benchmarking the No-Core Monte Carlo Shell Model (NC-MCSM) with the No-Core Shell Model (NCSM) using the same realistic interactions to define the nuclear Hamiltonian. This led to a series of projects [1–8] that provided results for light nuclei while developing improved methods for both approaches. We investigated light nuclei up through  $A = 12$  with both approaches and compared their predictions for the ground state energies.

In order to provide a perspective on this overview of benchmark results as well as some exploratory work in the next section, we will focus here on the similarities and differences in the Hamiltonian basis spaces in the different approaches. Both methods are applied within a single-particle harmonic oscillator (HO) basis, and in both methods the basis includes single-particle states up to a finite number of HO shells designated by  $N_{\text{shell}} = 1 + 2n + l$ , where  $n$  is the radial quantum number and  $l$  is the orbital angular momentum quantum number. Thus we count the  $0s$  shell as the first shell.

With a finite number of single-particle states, the most general basis for a many-body problem contains all possible many-body states (configurations) that can be constructed from these single-particle states, limited only by symmetry constraints. Diagonalizing the Hamiltonian in such a basis that contains all possible configurations for a given single-particle basis is referred to as a Full Configuration Interaction (FCI) calculation, and is considered the 'gold standard' in quantum chemistry.

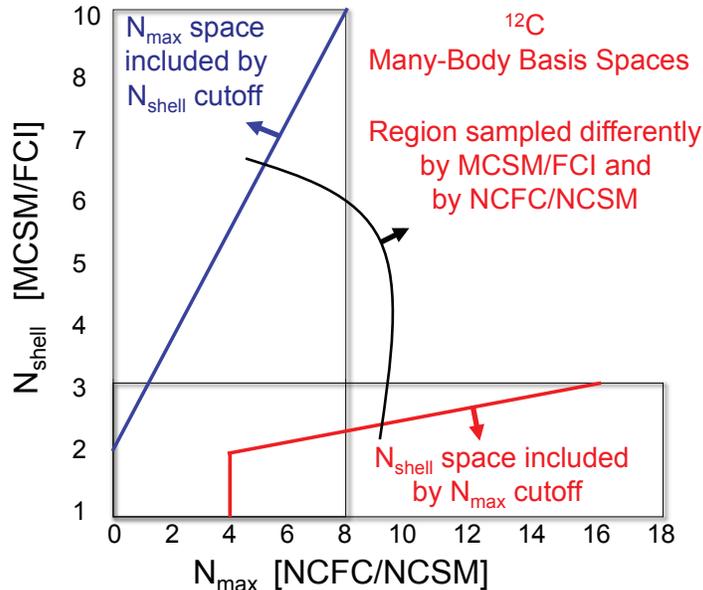
However, the (naive) basis size  $D$  of an FCI calculation grows like

$$D = \binom{N_{\text{sp}}}{Z} \binom{N_{\text{sp}}}{N}$$

for an  $A$ -body calculation with  $Z$  protons,  $N$  neutrons, and  $N_{\text{sp}}$  single-particle states. With only four HO shells ( $N_{\text{shell}} = 4$ ) we have  $N_{\text{sp}} = 40$  and the FCI basis size for  $^{12}\text{C}$  is of the order of  $10^{16}$ . Even after applying symmetry constraints, that will still be several orders of magnitude beyond what can be diagonalized on current Leadership-Class computing systems. In addition,  $N_{\text{shell}} = 4$  is not actually sufficient for converging a calculation for  $^{12}\text{C}$ , as can be seen from Fig. 2 below. Hence the need to further truncate the many-body basis.

The NCSM uses a many-body basis truncation defined by  $N_{\text{max}}$ , the number of HO quanta summed over all nucleons above the lowest possible number of quanta for that nucleus [9]. Such a truncation scheme includes configurations with e.g. one nucleon in a highly excited HO state and all others in the lowest HO states, as well as configurations in which several nucleons (or even all nucleons if  $N_{\text{max}} \geq A$ ) are excited by one quantum. When the NCSM results are extrapolated to the infinite matrix limit, we refer to the results as obtained in the No-Core Full Configuration (NCFC) method [10]. In addition to drastically reducing the basis size compared to an FCI calculation with the same highest single-particle HO state, this particular truncation also leads to an exact factorization of the center-of-mass motion and the intrinsic motion of the self-bound nuclei [11–13] — and ultimately, it is the intrinsic wavefunction that is required for reaction calculations [14, 15].

In the NC-MCSM, the many-body basis states are selected from the underlying FCI basis defined by a single-particle truncation parameter  $N_{\text{shell}}$ . It is a generalization of the Monte Carlo Shell Model (MCSM), in which many-body states are constructed from linear combinations of non-orthogonal angular-momentum and parity projected deformed Slater determinants. (For a review on the MCSM, see Ref. [16].) With increasing dimension of the Monte Carlo basis space, the ground state energy of a NC-MCSM calculation converges from above to the corresponding FCI value. The energy, therefore, always gives the variational upper bound for the exact ground state energy. Typically only a few hundred Monte Carlo basis states are kept, though the underlying FCI basis can be of the order of  $10^{20}$ . If needed, the ground state energy (and other observables) can be extrapolated by the energy variance method [2].



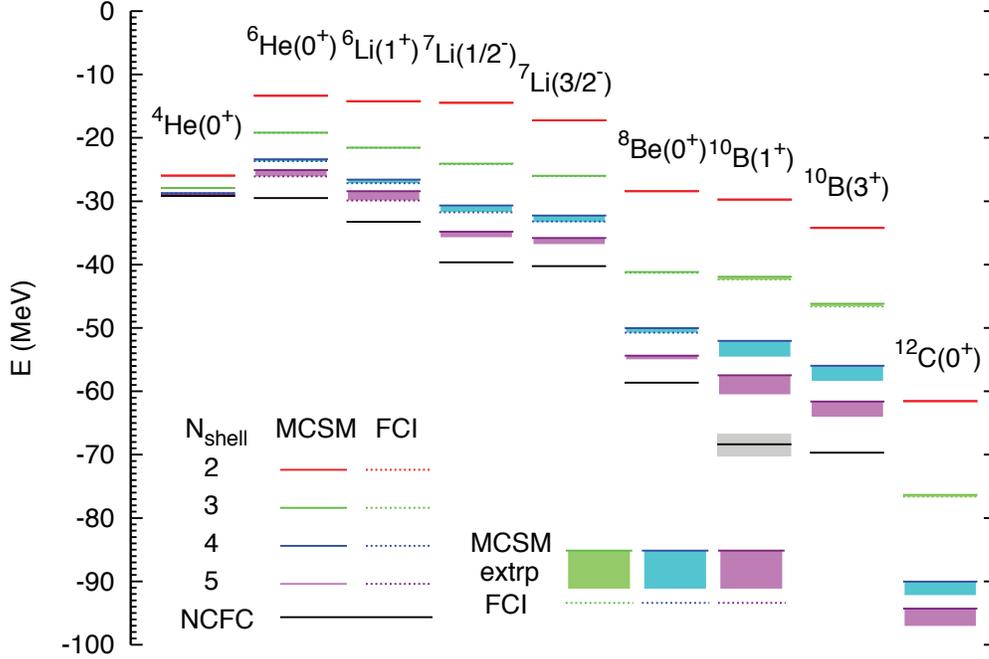
**Fig. 1.** (Color online) Overview of the bases covered with the NC-MCSM and NCSM methods for the case of  $^{12}\text{C}$  (adapted from Ref. [2]).

Figure 1 sketches the topography of many-body bases adopted in the different methods: the NC-MCSM (and also the FCI method) and the NCSM method (with extrapolation for the NCFC method). This illustrates the different regions of the single-particle space emphasized in the different approaches. Of course, the full (infinite dimensional) space is covered with increasing either  $N_{\text{shell}}$  or  $N_{\text{max}}$  and it becomes a practical issue of the respective rates of convergence.

One of the advantages offered by the NC-MCSM approach is its computational scaling with increasing number of nucleons  $A$ . We presented a study of the advantageous scaling properties of the NC-MCSM in Ref. [2] where we found that the rate of increased demand on computational resources (for increasing  $A$  at fixed  $N_{\text{shell}}$ ) is orders of magnitude slower than for the NCSM (for increasing  $A$  at fixed  $N_{\text{max}}$ ). The question then turns to the adequacy of extrapolation techniques for each method and the resulting quantified uncertainties. These issues have been addressed in our subsequent efforts [5–8].

Note that the rate of convergence depends on the observable so each method is likely to have its advantages for certain observables. One may imagine that, qualitatively, the NC-MCSM/FCI approach is advantageous for observables dominated by contributions from multiparticle correlations in higher basis configurations while the NCSM/NCFC favors observables that are sensitive to short-range nucleon-nucleon ( $NN$ ) correlations, though this is only a rough picture.

In Fig. 2, we present recent benchmarks of the ground state energies of several light nuclei using the JISP16  $NN$  interaction [17]. We selected this interaction since it produced a high-quality description of the  $NN$  scattering data and was known to provide a good description of the properties of light nuclei up to about  $A = 12$  [18, 19]. For the purposes of our benchmark we neglected the Coulomb interaction between the protons. We find that the NC-MCSM results with energy variance extrapolation are nearly identical with the FCI results. The differences between the extrapolated NC-MCSM results and the NCFC results provide a measure of the need for increasing  $N_{\text{shell}}$ . Fortunately, addi-



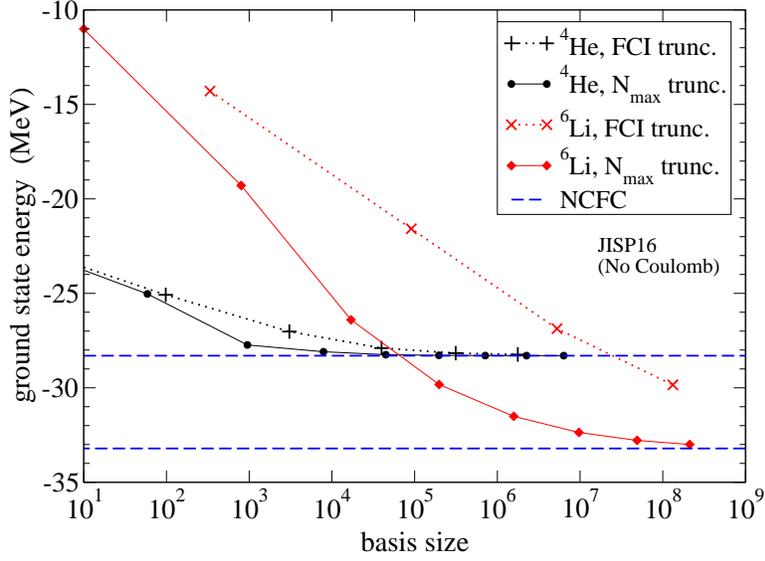
**Fig. 2.** (Color online) Comparisons of the energies between the NC-MCSM and FCI along with the fully converged NCFC results where available. The NCFC result for the  $^{10}\text{B}(1^+)$  state has a large uncertainty indicated by the grey band. The NC-MCSM (FCI) results are shown as the solid (dotted) lines. The extrapolated NC-MCSM results are illustrated by colored bands. The NC-MCSM results, with extrapolation to their full  $N_{\text{shell}}$  basis [7], nearly coincide with the FCI results. From top to bottom, the truncation of the basis is  $N_{\text{shell}} = 2$  (red), 3 (green), 4 (blue), and 5 (purple). Note that some results with  $N_{\text{shell}} = 4$  and 5 were obtained only with the NC-MCSM (adapted from Ref. [7]).

tional improvements to the NC-MCSM methods are under development and larger  $N_{\text{shell}}$  values are already achievable [7].

In order to understand better the benchmark results, it is helpful to have a comparison of convergence versus many-body basis size rather than by comparing results directly between an FCI truncation and an  $N_{\text{max}}$  truncation. In Fig. 3, we present comparisons of the convergence rates for the ground states of  $^4\text{He}$  and  $^6\text{Li}$  as a function of the many-body basis size using the FCI truncation and the  $N_{\text{max}}$  truncation schemes [20]). Both truncations approach the exact answer from above in concert with the variational property of these approaches. Clearly, the  $N_{\text{max}}$  truncation provides faster convergence as a function of the dimensionality. One should keep in mind, however, the discussion above concerning the very different computational scaling properties with increasing  $A$  of the NC-MCSM and the NCSM/NCFC approaches. Good computational scaling with increasing  $A$  becomes overwhelmingly more important at sufficiently large  $A$ .

### 3. No-Core Shell Model with Alternative Truncation Schemes

When we compare the FCI and the NCSM results above, we are comparing different truncations of the many-body basis formed with HO single-particle states. It is natural to investigate whether alternative truncation schemes are valuable in that they could provide better converged results with comparable demand on computational resources. For example, we could examine alternatives to trun-



**Fig. 3.** (Color online) Convergence of the ground state energy for  ${}^4\text{He}$  and  ${}^6\text{Li}$  with JISP16 (without the Coulomb interaction) as function of the many-body basis size. NCSM results with  $N_{\text{max}}$  truncation are connected by solid lines. FCI results with  $N_{\text{shell}}$  truncation are connected by dotted lines. Both methods appear to converge from above, in accord with the variational principle, to the extrapolated NCFC result (adapted from Ref. [20]).

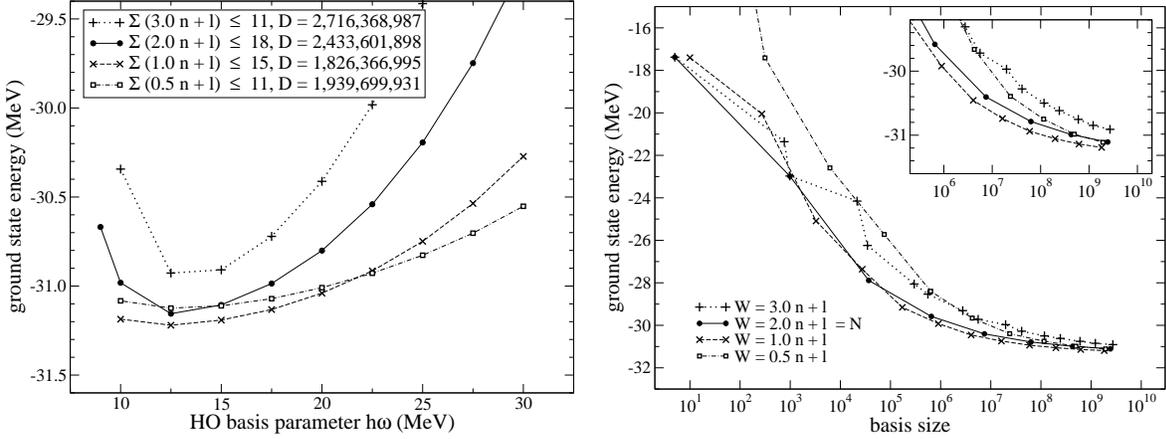
cating on the sum of the number of HO quanta in a many-body basis configuration [21]. Instead, we could also apply specific weights to each single-particle orbital, characterized by  $n$ ,  $l$ , and  $j$ , and truncate the basis based on the sum of these assigned weights in a many-body basis configuration. In this approach, the  $N_{\text{max}}$  truncation of a conventional NCSM calculation is recovered by choosing the weights to be  $(2n + l)$ . Furthermore, there is no reason for the underlying spatial single-particle wavefunctions to be HO wavefunctions. Indeed, alternative single-particle basis functions such as the Laguerre functions [13, 22, 23] and the natural orbital basis [24] do both provide a modest improvement of the convergence rates.

Here we explore possible improvements when we simply use  $W = (\alpha n + \beta l)$  but retain the HO single-particle basis. The coefficients  $\alpha$  and  $\beta$  define a weight  $W$  for each orbital and the many-body basis is truncated by a cutoff in the sum over all nucleons of these weights for the orbitals in a many-body basis configuration

$$\sum_{i=1}^A W_i \leq W_{\text{max}}.$$

One can easily see that varying the coefficients  $\alpha$  and  $\beta$  allows a tradeoff between radial and orbital basis functions. We will examine only the ground state energies and root mean square (RMS) point-proton radius here for a few selected cases for  $\alpha$  and set  $\beta = 1$  without loss of generality. Similar convergence studies for other single-particle basis functions, as well as other observables, will be addressed in the future. In addition, we could consider using the total angular momentum  $j$  in place of, or in addition to, the orbital angular momentum  $l$  in determining the weight, to give different emphases to spin-orbit partner orbitals; and furthermore, we could differentiate the weights for proton and neutron orbitals.

In Fig. 4 we present the ground state energy of  ${}^8\text{He}$  with the Daejeon16  $NN$  interaction [25] at specific choices of  $\alpha$  (with  $\beta = 1$ ). The conventional  $N_{\text{max}}$  truncation is recovered for  $\alpha = 2$ , in which case  $W_{\text{max}} = 18$  corresponds to  $N_{\text{max}} = 14$  for  ${}^8\text{He}$ . In order to make these comparisons at



**Fig. 4.** Ground state energy of  ${}^8\text{He}$  with Daejeon16 as function of the HO basis parameter  $\hbar\omega$  (left) and as function of the basis size at  $\hbar\omega = 15$  MeV (right) for using different single-particle weights ( $\alpha n + l$ ).

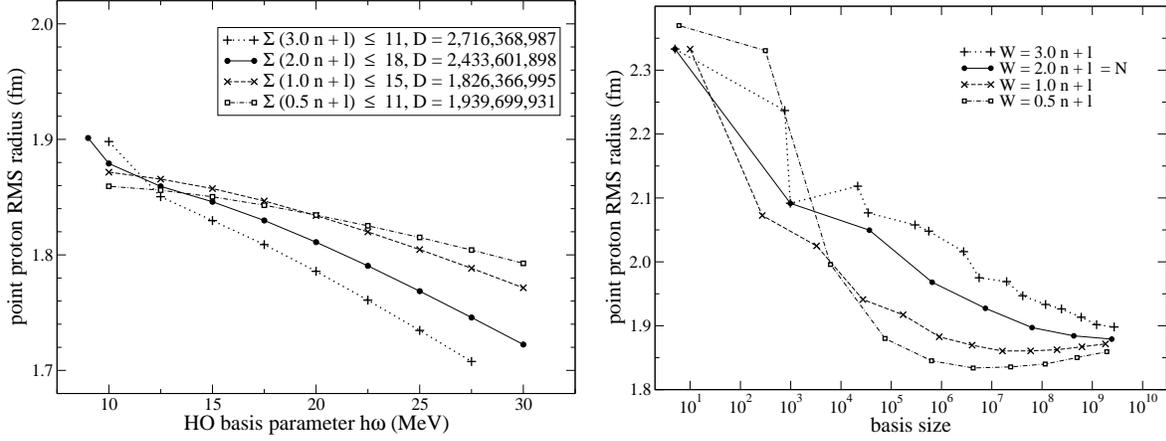
approximately constant computational effort, we select a cutoff  $W_{\text{max}}$  for each calculation (quoted in the legend) such that it produces similar matrix dimensions of about two billion. We observe in the left panel of Fig. 4 that, as we decrease the weight of radial excitations compared to angular excitations, the dependence of the ground state energy on the HO parameter  $\hbar\omega$  decreases. Furthermore, we see that  $\alpha = 1.0$ , i.e. an orbital weight of  $W = (n + l)$ , gives the lowest upper bound near the variational minimum even though it has the smallest dimension among the cases in this comparison set.

In the right panel of Fig. 4 we examine the convergence rate of the ground state energy of  ${}^8\text{He}$  as a function of the many-body basis size for the same set of choices for  $\alpha$  as in the left panel at a fixed value of the basis parameter  $\hbar\omega$ . As expected, all choices of weights produce convergence from above with increasing basis size in concert with the variational principle. As the separate curves approach the same asymptotic value, the differences among the curves may seem small on this scale, but in the inset we can clearly see that for basis sizes between a million and a few billion the calculations with  $\alpha = 1.0$  are closer to convergence than the other calculations with comparable basis sizes. For bases of 10 billion or more,  $\alpha = 0.5$  might be an even better choice.

Next, let us consider a different observable, namely the point-proton RMS radius of  ${}^8\text{He}$ . Note that this observable is known to converge slowly with  $N_{\text{max}}$  in the conventional NCSM truncation, because the  $r^2$  operator is long-range and therefore sensitive to the asymptotic tail of the wave function. Our results are presented in Fig. 5, using these same weights for the single-particle states and the same cutoffs in the many-body basis as for the ground state energies.

First, we consider the dependence of the RMS point-proton radius on  $\hbar\omega$  in the left panel of Fig. 5. Again, as we decrease the weight of radial excitations compared to angular excitations, the dependence of the RMS radius on the HO parameter  $\hbar\omega$  decreases. However, without the benefit of a variational principle for this observable, it is more challenging to determine which truncation provides the most rapid convergence. Nevertheless, greater independence of  $\hbar\omega$  would be one favorable indicator of improved convergence. Among the cases examined, the  $(0.5n + l)$  case displays the smallest  $\hbar\omega$  dependence over the entire  $\hbar\omega$  range shown. Furthermore, the  $\hbar\omega$  dependence is weakest in the low  $\hbar\omega$  region where the ground state energies are near their minima with respect to  $\hbar\omega$  as seen in the left panel of Fig. 4 above. Based on this criterion alone, it would seem to suggest that the preferred weight for this observable is  $W = (0.5n + l)$  among the cases we examined, although that is not the preferred weight obtained by considering the ground state energy above.

Turning our attention to the right panel of Fig. 5 we present the RMS point-proton radius as a function of many-body basis size at a fixed value of the basis parameter, that is  $\hbar\omega = 10$  MeV. Here,



**Fig. 5.** Point-proton RMS radius of  ${}^8\text{He}$  with Daejeon16 as function of the HO basis parameter  $\hbar\omega$  (left panel) and as function of the basis size at  $\hbar\omega = 10$  MeV (right panel) for different single-particle weights ( $\alpha n + l$ ).

the case ( $n + l$ ) provides the RMS radius results with the least sensitivity to many-body basis size at higher dimensions. Note that this is the preferred weight for the convergence of the ground state energy. Clearly, it would be worthwhile continuing these investigations to larger many-body bases and different choices for the single-particle weights in order to map out the convergence with respect to the single-particle orbital weights and the many-body truncation.

#### 4. Conclusions and Outlook

By benchmarking the NC-MCSM and the NCSM approaches, we confirm that their respective extrapolated ground state energy results are in agreement with expectations. For the NC-MCSM, extrapolated ground state energies using the energy variance method agree with the FCI results where available. Furthermore, the NC-MCSM and the NCSM results for the ground state energy with increasing basis size are consistent with each other. However, the NC-MCSM results lie above the NCSM results at comparable many-body basis sizes. For progressing to heavier nuclei, the NC-MCSM shows superior computational scaling properties and is expected to provide valuable *ab initio* results in these heavier systems where the NCSM has limited utility at the present time.

We also explored different truncation schemes of the many-body basis in the NCSM framework and found encouraging results by including more harmonic oscillator single-particle states with higher radial quantum numbers than would be included with the traditional  $N_{\text{max}}$  truncation. The ground state energy of  ${}^8\text{He}$  converged more rapidly with increasing basis size using weights for the single-particle orbitals of  $W = (n + l)$ , in combination with a cutoff  $W_{\text{max}}$  on the sum of these weights for the many-body configurations in our basis. Furthermore, both the ground state energy and the RMS point-proton radius showed significantly improved independence of the basis parameter  $\hbar\omega$  with these single-particle weights.

There is much work to be done to more fully explore the opportunities of alternative truncation schemes. To list a few here, we mention: (1) adopting natural orbitals or other single-particle bases; (2) investigating additional nuclei; (3) adopting other Hamiltonians including those with three-nucleon interactions; (4) mapping out the convergence patterns of additional observables and (5) developing and applying extrapolation methods for all observables.

We look forward to continuing our joint efforts with our colleagues in Japan and we wish Takaharu Otsuka good health and many active and enjoyable years ahead.

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