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Monte Carlo Shell Model for *ab initio* nuclear structure

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Abstract. We report on our recent application of the Monte Carlo Shell Model to no-core calculations. At the initial stage of the application, we have performed benchmark calculations in the *p*-shell region. Results are compared with those in the Full Configuration Interaction and No-Core Full Configuration methods. These are found to be consistent with each other within quoted uncertainties when they could be quantified. The preliminary results in $N_{\rm shell} = 5$ reveal the onset of systematic convergence pattern.

1 Introduction

One of the major challenges in nuclear theory is to reproduce and to predict nuclear structure and reactions from *ab initio* calculations with realistic nuclear forces. Among the *ab initio* nuclear many-body approaches for $A \geq 4$ [1], the No-Core Shell Model (NCSM) is one of the powerful methods for the study of nuclear structure and reactions in the *p*-shell nuclei [2].

As the NCSM treats all the nucleons on an equal footing, computational demands for the calculations explode exponentially as the number of nucleons increases. Current computational resources limit the direct diagonalization of the Hamiltonian matrix using the Lanczos algorithm to basis spaces with a dimension of around 10^{10}. In order to access heavier nuclei beyond the *p*-shell region with larger basis dimensions, much effort has been devoted to the NCSM calculations. One of these approaches is the Importance-Truncated NCSM (IT-NCSM) [3] where the basis spaces are extended by using an importance measure evaluated using perturbation theory. Another approach is the Symmetry-Adapted NCSM (SA-NCSM) [4] where the basis spaces are truncated by the selected symmetry groups. Similar to these attempts, the Monte Carlo NCSM (MC-NCSM) [5, 6] is one of the promising candidates to go beyond the Full Configuration Interaction (FCI) method which is a different truncation of the basis states that commonly used in the NCSM.

In these proceedings, we focus on the latest application of the MCSM toward the *ab initio* no-core calculations, which have become feasible recently with the aid of the major developments in the MCSM algorithm [7] and also a remarkable growth in the computational power of the state-of-the-art supercomputers. Most of the benchmark results in the MC-NCSM presented here are summarized in Ref. [6].

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2 MCSM

The MCSM has been developed mainly for conventional shell-model calculations with an assumed inert core [8]. Recently the algorithm and code itself have been heavily revised and rewritten so as to accommodate massively parallel computing environments [7]. Now we can apply the MCSM not only to conventional shell-model calculations but also to no-core calculations.

The MCSM approach proceeds through a sequence of diagonalization steps within the Hilbert subspace spanned by the deformed Slater determinants in the HO single-particle basis. Importance-truncated bases are stochastically sampled so as to minimize the energy variationally. With increasing the number of importance-truncated basis, the computed energy converges from above to the exact value and gives the variational upper bound. An exploratory no-core MCSM investigation of the proof-of-principle type has been done for the low-lying states of the Be isotopes by applying the existing MCSM algorithm with a core to a no-core problem [5].

Recent improvements on the MCSM algorithm have enabled significantly larger calculations [7]. The crucial developments for no-core calculations achieve (1) the efficient computation of matrix products for the most time-consuming part in the MCSM calculations, (2) the conjugate gradient method in the basis-search process, and (3) the energy-variance extrapolation for our MCSM (approximated) results into the FCI (exact) ones in the finite basis spaces. Because of space limitations, we refer for the details of these improvements to Ref. [7].

3 Benchmarks

The recent development of the MCSM algorithm [7] , together with significant computational resources, enables us to perform a benchmark of no-core MCSM calculations [6]. Figure 1 is the recent comparison of the energies for each state and basis space in the selected *p*-shell nuclei between the MCSM and FCI methods. The FCI gives the exact energies in the finite basis spaces, while the MCSM provides approximate energies. Thus the comparisons between them show how well the MCSM works in no-core calculations. Furthermore, we also plot the No-Core Full Configuration (NCFC) [9] results for the states of $4 \leq A \leq 10$ as the fully converged energies in the infinite basis space.

For this benchmark comparison, the JISP16 two-nucleon interaction [10] is adopted and the Coulomb force is turned off. The energies are evaluated for the optimal harmonic oscillator frequencies where the calculated energies are minimized for each state and basis space. Here the contributions from the spurious center-of-mass motion are ignored for simplicity. The basis space ranges from $N_{\rm shell} = 2$ to 5 where $N_{\rm shell}$ is the number of the major shell included in the basis space. Some energies in $N_{\rm shell} = 4$ and 5 are available only from the MCSM results, as the *M*-scheme dimensions for these states are already close to or above the current computational limitation in the FCI approach. We took 100 importance-truncated basis states and extrapolated the results by the energy variance.

As seen in Fig. 1, the energies are consistent with each other to within $\sim$ 100 keV where both results are available. Furthermore the $N_{\rm shell} = 5$ results begin to show the trend of the convergence to the NCFC results obtained by extrapolating the $N_{\rm max}$ truncated results to the infinite basis space. The next step is to extrapolate the $N_{\rm shell}$ results to the infinite basis space by using the extrapolation techniques in the $N_{\rm max}$ truncation [9, 11, 12]. In principle, the results extrapolated to the infinite basis space should be consistent with each other in spite of how the basis spaces are truncated. It is interesting to examine whether the extrapolated results in the $N_{\rm shell}$ and $N_{\rm max}$ truncations converge to the same value within quantified uncertainties. The detailed comparisons among the MCSM, FCI, and NCFC methods are discussed in Ref. [6].

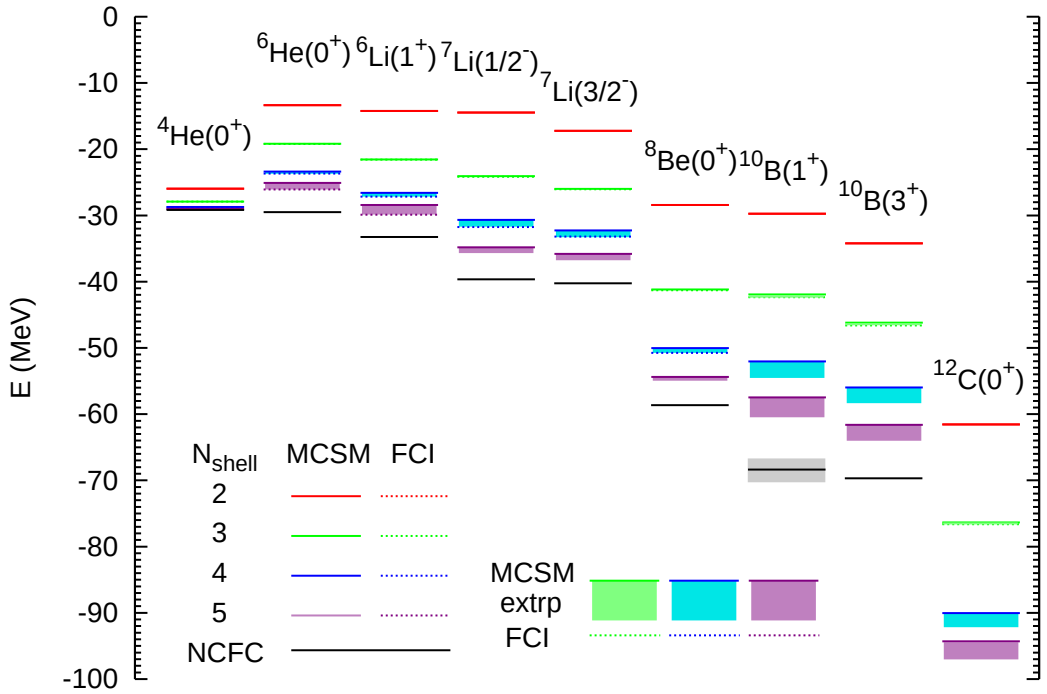

Figure 1. Comparisons of the energies between the MCSM and FCI along with the fully converged NCFC results where available. The NCFC result for the ^{10}B(1$^+$) state has a large uncertainty indicated by the grey band. The MCSM (FCI) results are shown as the solid (dotted) lines that nearly coincide where both are available. The extrapolated MCSM results are illustrated by bands. From top to bottom, the truncation of the basis space is $N_{\rm shell}$ = 2 (red), 3 (green), 4 (blue), and 5 (purple). Note that the MCSM results are extrapolated by the energy variance with second-order polynomials. Also note that some results in $N_{\rm shell}$ = 4 and 5 were obtained only with MCSM.

4 Summary

By exploiting the recent development in the MCSM algorithm, no-core calculations with the MCSM algorithm can be achieved on massively parallel supercomputers. From the benchmark calculations, the observables give good agreement between the MCSM and FCI results in the *p*-shell nuclei. The $N_{\rm shell}$ = 5 results reveal the onset of systematic convergence pattern. Further work is needed to investigate the extrapolation to the infinite basis space in the $N_{\rm shell}$ truncation.

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