Ab Initio Shell Model Calculations with Three-Body Effective Interactions for *p*-Shell Nuclei

Petr Navrátil and W. Erich Ormand

Lawrence Livermore National Laboratory, L-414, P.O. Box 808, Livermore, California 94551

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We present a qualitative improvement of the *ab initio* no-core shell model (NCSM) approach by implementing three-body interaction capability for p-shell nuclei. We report the first calculations using three-body effective interactions derived from realistic nucleon-nucleon potentials for ^{6}Li, ^{8}Be, and ^{10}B and demonstrate that the use of three-body effective interactions speeds up the convergence of the NCSM approach. For ^{10}B, we predict $J^\pi T = 1^+0$ ground state, contrary to the experimental observation of 3^+0, when the AV8′ potential is used, indicating the need for true three-body forces.

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Various methods can be used to solve systems of more than two nucleons interacting by realistic interactions [1,2]. For $A > 4$ systems, a prominent approach has been the Green's function Monte Carlo (GFMC) method [2]. An alternative, and complementary, approach is the no-core shell model (NCSM) [3–8], which is based on effective interactions within the framework of the nuclear shell model. In this case, one derives an effective interaction for the A-body system within a computationally tractable model space that is designed to converge towards the exact result. One of the most important features of these effective interactions is that they are composed of two-, three-, up to A-body components even if the fundamental interaction is only pairwise. In practical applications, a compromise between the size of the model space and the number of clusters in the effective interaction must be made.

Until now, applications of NCSM for $A > 4$ have been based on two-body effective interactions. The first used G-matrix-based two-body interactions [3], while later, the Suzuki-Lee procedure [9] was implemented to derive two-body effective interactions for the NCSM [4]. This resulted in the elimination of the purely phenomenological parameter Δ used to define G-matrix starting energy. A truly *ab initio* formulation of the formalism was presented in Ref. [5] where convergence to exact solutions was demonstrated for the $A = 3$ system. The same was later accomplished for the $A = 4$ system [6], where it was also shown that a three-body effective interaction can be introduced to improve the convergence of the method.

An extension to three-body components in the effective interaction is important for two reasons. First, formally the inclusion of a three-body effective interaction within a given model space should improve the overall convergence of the method [6]. Although calculations up to $N_{\max} = 10$, with $N_{\max}$ the maximum many-body harmonic-oscillator (HO) excitation energy defining the model space, have been carried out for $A \leq 8$ [8], and near convergence has been achieved for $A = 6$, for $A > 10$ it is essentially impossible to extend the basis size to such an extent as to achieve convergence using just two-body effective interactions. Hence, it is crucial to test the alternative approach where convergence is sought by using higher-order terms in the effective interaction. The second reason is that there is ample evidence from exact solutions of three- and four-body systems that "true" three-body interactions are present in nuclei [1,2]. Given that the techniques in the many-body shell model calculation are the same for both the effective and "true" three-body interactions it is only logical to include the effective three-body interaction in the NCSM. In this Letter, we present the formalism and the first application of three-body effective interactions to *ab initio* studies of the structure of p-shell nuclei.

In the NCSM, we start from the intrinsic A-nucleon Hamiltonian $H_A = T_{\rm rel} + \mathcal{V}$, where $T_{\rm rel}$ is the relative kinetic energy and $\mathcal{V}$ is the sum of two-body or possibly higher-body nuclear and Coulomb interactions. To facilitate our calculations, we add a center-of-mass HO Hamiltonian, whose effect will be eventually subtracted in the final many-body calculation, and for a two-body interaction obtain the HO frequency-dependent Hamiltonian $H_A^\Omega = \sum_i^A h_i + \sum_{i<j}^A V_{ij}^{\Omega,A}$. The h_i is a one-body HO term and the two-body interaction $V_{ij}^{\Omega,A}$ contains a term proportional to $\frac{1}{A}(\vec{r}_i - \vec{r}_j)^2$ [4–8]. Since we solve the many-body problem in a finite HO basis space, it is necessary that we derive a model-space dependent effective Hamiltonian. For this purpose, we perform a unitary transformation [4–10] on the Hamiltonian, which accommodates the short-range correlations. In general, the transformed Hamiltonian is an A-body operator. The first-order approximation is to develop a two-particle cluster effective Hamiltonian, while the next improvement is to include three-particle clusters, and so on. The effective interaction is obtained from the decoupling condition between the model space and the excluded space for the two- or three-nucleon transformed Hamiltonian. On the two-body cluster level, we solve $h_1 + h_2 + V_{12}^{\Omega,A}$, and from the transformation we obtain $V_{2-\mathrm{eff},12}^{\Omega,A}$ and then solve the A-body problem using $\sum_i^A h_i + \sum_{i<j}^A V_{2-\mathrm{eff},ij}^{\Omega,A}$. On the three-body cluster level, we solve $h_1 + h_2 + h_3 + V_{12}^{\Omega,A} + V_{13}^{\Omega,A} + V_{23}^{\Omega,A}$ to obtain $V_{3-\mathrm{eff},123}^{\Omega,A}$ and then use $\sum_i^A h_i + \frac{1}{A-2}\sum_{i<j<k}^A V_{3-\mathrm{eff},ijk}^{\Omega,A}$ for the A-body problem. The resulting two- or three-body effective Hamiltonian depends on the nucleon number A, the HO frequency Ω,

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and $N_{\max}$. The effective interaction approaches the bare interaction for $N_{\max} \to \infty$.

The three-body effective interaction is derived as described above and in Ref. [6] by solving $h_1 + h_2 + h_3 + V_{12}^{\Omega,A} + V_{13}^{\Omega,A} + V_{23}^{\Omega,A}$ in a large Jacobi-coordinate HO basis in all possible three-nucleon channels that contribute to the model space defined by $N_{\max}$. To speed up convergence of the three-body solutions, we use two-body effective interactions for $V_{ij}^{\Omega,A}$ corresponding to a sufficiently large three-body space, e.g., $N_{3\max} = 30$–40. From these solutions we then construct the three-body effective interaction corresponding to $N_{\max} < N_{3\max}$ using the Suzuki-Lee approach. The resulting three-body effective interaction is given in an antisymmetrized HO Jacobi-coordinate basis and can readily be applied in $A > 3$ Jacobi-coordinate calculations such as ^{4}He [6,11].

For p-shell nuclei, it turns out that the single-particle Slater-determinant (SD) HO basis is more efficient to use. In order to utilize our three-body effective interaction with the SD HO basis, we need to transform it first. At the two-body level, this transformation is very well known and depends on HO Brody-Moshinsky brackets. For our three-body case, we used m-scheme three-body SD basis states with definite parity and third component of angular momentum and isospin. The transformation from the Jacobi basis is complex and depends on products of two HO Brody-Moshinsky brackets (one for two particles with mass ratio 1 and a second for two particles with mass ratio 1/2) and the parentage coefficients obtained by antisymmetrization of the Jacobi coordinate HO basis. The full details of the transformation will be described elsewhere.

Once the three-body interaction is transformed, it is ready for an input to a standard shell model code. Typically, shell model codes are designed to handle only one- and two-body interactions. Therefore, we had to extend or develop new codes capable of including three-body interactions. In particular, we extended the many-fermion dynamics (MFD) code [13]. In addition, we developed a completely new parallel code, REDSTICK, specifically for this purpose, using a different algorithm for evaluating the Hamiltonian matrix. The m-scheme SD basis is used and the matrix diagonalization is performed using the Lanczos algorithm in both codes. We cross-checked the results obtained by both codes and obtained identical results. In addition, we performed $4\hbar\Omega$ ($N_{\max} = 4$) ^{6}Li calculations within the Jacobi-coordinate formalism [6] and obtained identical results to the shell model codes, thereby validating the transformation from Jacobi coordinate basis to the single-particle SD basis.

Before describing our results for p-shell nuclei, we illustrate the power of effective interaction theory in Fig. 1, where we show results obtained for ^{4}He using the QCD-based, effective-field theory (EFT) [14], Idaho-A [15] two-nucleon (NN) potential. The figure contrasts the results obtained with the bare and two-body and three-body effective interactions. We note that the three-body correlations in the effective interaction dramatically improve the convergence, and quite reasonable results are obtained already for $N_{\max} \approx 4$–6. Further, unlike for the standard NN potentials, it is clear that for $N_{\max} \geq 10$, the three-body correlations dominate the two-body correlations. These EFT potentials are a new development for NN interactions and are not only nonlocal, but tend to have softer cores, which leads to faster overall convergence. In addition, for complex systems they are also comprised of three-nucleon (NNN) interactions that are systematically derived along with the two-body terms. It is an important question for the future as to how well these potentials describe the properties of complex nuclei. These interactions are particularly well suited to the NCSM method provided that the three-body correlations are included in the computations.

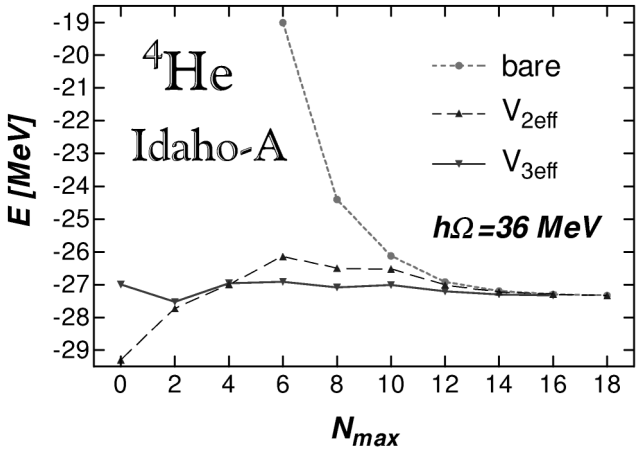

FIG. 1. Calculated ground-state energy of ^{4}He using the EFT two-body Idaho-A NN potential (no Coulomb). Results obtained with the bare (short-dashed line), two-body effective (long-dashed line), and three-body effective (full line) interactions in $0\hbar\Omega$–$18\hbar\Omega$ basis spaces with the HO frequency of $\hbar\Omega = 36$ MeV are presented. Our converged ground-state energy is $-27.34(3)$ MeV.

We performed calculations for ^{6}Li, ^{8}Be, and ^{10}B using the Argonne V8′ NN potential [2] including Coulomb. Results for these nuclei obtained by the GFMC method are available for a comparison [2,16]. Our calculations for ^{6}Li were performed up to the $6\hbar\Omega$, while those for ^{8}Be and ^{10}B only up to the $4\hbar\Omega$ due to increased complexity. In Fig. 2, we present the frequency dependence of the ^{6}Li, ^{8}Be, and ^{10}B ground state for both two-body and three-body effective interactions. We can see that the three-body effective interaction calculation has a weaker dependence on both the frequency and basis size, and, thus, has a better convergence rate. We note that the method is not variational so higher-cluster components may contribute with either sign to the total binding energy. We seek a region where the ground state is approximately independent of the HO frequency. Our calculated energy results are summarized in Table I where we note that convergence at the level of approximately 500 keV is achieved for the ground states of all three nuclei with the three-body effective interaction. Of the three cases,

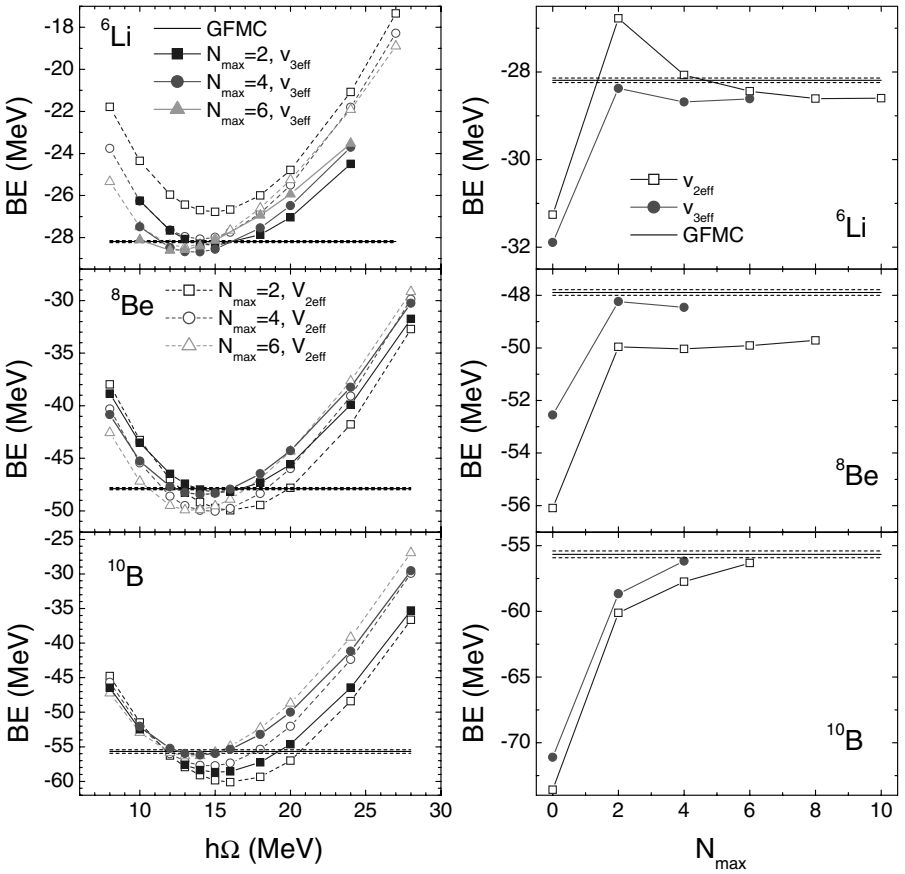

FIG. 2. Calculated ground-state energy of ^{6}Li (upper panel), ^{8}Be (middle panel), and ^{10}B (lower panel) using the AV8′ *NN* potential with Coulomb. Results using the two-body effective interaction and the three-body effective interaction in basis spaces up to $6\hbar\Omega$ in the range of HO frequencies of $\hbar\Omega = 8-28$ MeV are shown and compared to the GFMC results from Refs. [2,16]. On the right-hand side, the energies at the HO frequency minima as a function of $N_{\max}$ are plotted.

perhaps the most notable is ^{8}Be, where the ground-state energy is substantially improved with the three-body effective interaction. In particular, the $4\hbar\Omega$ results are within 570 keV of the GFMC calculation, whereas the deviation with the two-body effective interaction even in the $8\hbar\Omega$ space is in excess of 1.8 MeV. The agreement between our calculations and the GFMC worsens for the higher-lying excited states, in particular, for broad states like the 4^+0 ^{8}Be. In general, we find that unbound states that are characterized by broad resonances tend to converge more slowly in our approach. Further, it is likely that higher-order clustering effects may be present in ^{8}Be, which might be improved with a four-body effective interaction.

TABLE I. Calculated energies, in MeV, of ^{6}Li, ^{8}Be and ^{10}B, using the AV8′ *NN* potential including the Coulomb interaction. The NCSM results corresponding to the Ω-dependence minimum for a given $N_{\max}$ and $J^\pi T$ using $V_{3-\mathrm{eff}}$ and $V_{2-\mathrm{eff}}$ are compared to the GFMC results [2,16].

	GFMC	NCSM $V_{3-\mathrm{eff}}$	NCSM $V_{2-\mathrm{eff}}$
^{6}Li $E(1^+0)$	−28.19(5)	−28.61 ($6\hbar\Omega$)	−28.60 ($10\hbar\Omega$)
^{6}Li $E(3^+0)$	−24.98(5)	−25.54 ($6\hbar\Omega$)	−25.58 ($10\hbar\Omega$)
^{6}Li $E(0^+1)$	−24.15(4)	−24.76 ($6\hbar\Omega$)	−25.20 ($10\hbar\Omega$)
^{6}Li $E(2^+0)$	−24.12(4)	−23.97 ($6\hbar\Omega$)	−24.23 ($10\hbar\Omega$)
^{8}Be $E(0^+0)$	−47.89(11)	−48.46 ($4\hbar\Omega$)	−49.72 ($8\hbar\Omega$)
^{8}Be $E(2^+0)$	−45.62(11)	−44.80 ($4\hbar\Omega$)	−46.09 ($8\hbar\Omega$)
^{8}Be $E(4^+0)$	−38.69(11)	−36.05 ($4\hbar\Omega$)	−37.25 ($8\hbar\Omega$)
^{8}Be $E(1^+0)$	−32.77(15)	−31.13 ($4\hbar\Omega$)	−32.80 ($8\hbar\Omega$)
^{8}Be $E(3^+0)$	−31.23(15)	−29.58 ($4\hbar\Omega$)	−30.99 ($8\hbar\Omega$)
^{8}Be $E(2^+1)$	−32.7(1)	−31.84 ($4\hbar\Omega$)	−33.40 ($8\hbar\Omega$)
^{10}B $E(1^+0)$	−55.67(26)	−56.19 ($4\hbar\Omega$)	−56.32 ($6\hbar\Omega$)
^{10}B $E(3^+0)$	−53.23(26)	−54.83 ($4\hbar\Omega$)	−54.96 ($6\hbar\Omega$)

In Figs. 3 and 4, we present the ^{8}Be and ^{10}B excitation spectra. Here, the $4\hbar\Omega$ three-body effective interaction excitation spectra are compared to the results with two-body effective interaction at $4\hbar\Omega$ and $8\hbar\Omega$ for ^{8}Be and $6\hbar\Omega$ for ^{10}B. We note the general agreement between the three-body effective interaction spectrum and that obtained with $V_{2-\mathrm{eff}}$ in the largest space, in particular, for the $T = 0$ states. For ^{8}Be, we also show the position of the $T = 0$ intruder states that we investigated in Ref. [8] using just the two-body effective interaction. It is remarkable how the use of the three-body effective interaction strongly influences these states in contrast to the $0\hbar\Omega$ dominated states. Nevertheless, the space enlargement lowers these states even more.

We also note that the ^{10}B results yield the 1^+0 state as the ground state with the AV8′ *NN* potential contrary to the experimental observation [17] of 3^+0. This is also observed in our calculations using the charge-dependent

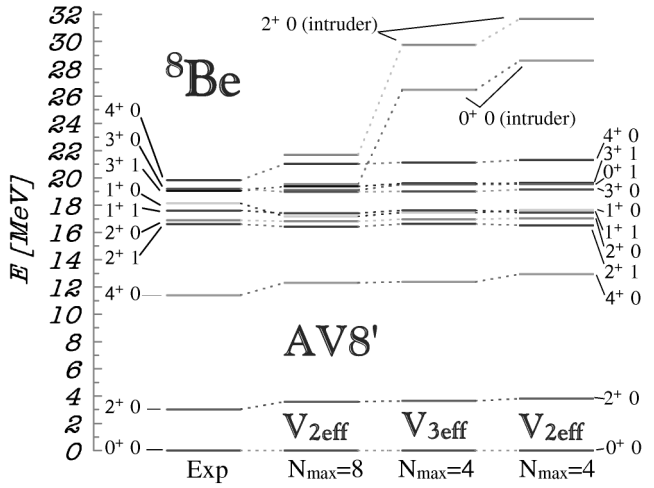

FIG. 3. Experimental and theoretical positive-parity excitation spectra of ^{8}Be using the AV8′ *NN* potential with Coulomb. The results for $V_{2-\mathrm{eff}}$ in $4\hbar\Omega$ and $8\hbar\Omega$ and $V_{3-\mathrm{eff}}$ in $4\hbar\Omega$ basis space using $\hbar\Omega = 14$ MeV are compared. The experimental values are from Ref. [17]

Bonn *NN* potential [18]. The incorrect ground-state spin prediction in ^{10}B shows the deficiency of the realistic *NN* potentials, in particular, an insufficient spin-orbit force, and, when combined with results for $A = 3$ and 4 systems, clearly indicates the need for a real three-body interaction. We note that for the Argonne potentials, this result has recently been confirmed by the GFMC calculations [16].

In the future, we will include the effects of the "true" three-body interaction. At that point, we will then carry out systematic investigations for p-shell nuclei ranging to ^{16}O, which are all computationally accessible with three-body interactions in the $4\hbar\Omega$ model space. For light p-shell nuclei, we will extend calculations to the $6\hbar\Omega$ model space. Another possibility to help increase the model-space size

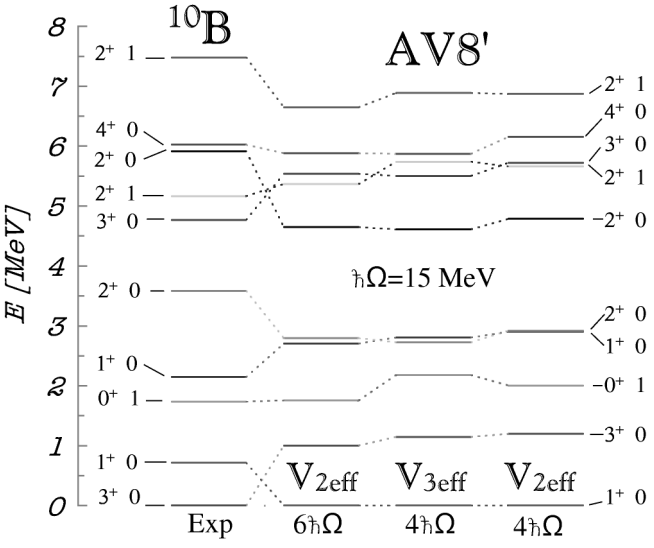

FIG. 4. The same as in Fig. 3 for ^{10}B using $\hbar\Omega = 15$ MeV. The largest space with $V_{2-\mathrm{eff}}$ was $6\hbar\Omega$.

for heavier p-shell nuclei is to utilize the interesting feature that the three-body effective interaction appears to act primarily as a density-dependent two-body interaction. Preliminary results indicate that only a small error, approximately 100 keV, is introduced when truncating the full three-body effective interaction by neglecting the pure three-body configurations. Still further in the future, we will explore the possibility to include four-body clusters in the effective interaction.

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