

AB INITIO LARGE-BASIS NO-CORE SHELL MODEL AND ITS APPLICATION TO LIGHT NUCLEI*

BRUCE R. BARRETT[†], PETR NAVRÁTIL[‡]

Department of Physics, University of Arizona
P.O. Box 210081, Tucson, AZ 85721, USA

W.E. ORMAND

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

AND JAMES P. VARY

Department of Physics and Astronomy, Iowa State University
Ames, IA 50011, USA

(Received December 11, 2001)

We discuss the *ab initio* No-Core Shell Model (NCSM). In this method the effective Hamiltonians are derived microscopically from realistic nucleon–nucleon (NN) potentials, such as the CD-Bonn and the Argonne AV18 NN potentials, as a function of the finite Harmonic Oscillator (HO) basis space. We present converged results, *i.e.*, up to $50\hbar\Omega$ and $18\hbar\Omega$ HO excitations, respectively, for the $A = 3$ and 4 nucleon systems. Our results for these light systems are in agreement with results obtained by other exact methods. We also calculate properties of ${}^6\text{Li}$ and ${}^6\text{He}$ in model spaces up to $10\hbar\Omega$ and of ${}^{12}\text{C}$ up to $6\hbar\Omega$. Binding energies, rms radii, excitation spectra and electromagnetic properties are discussed. The favorable comparison with available data is a consequence of the underlying NN interaction rather than a phenomenological fit.

PACS numbers: 21.60.-n, 21.60.Cs, 21.30.Fe, 21.45.+v

1. Introduction

While various methods have been developed to solve the three- and four-nucleon systems with realistic interactions [1–4], few approaches are suitable for heavier nuclei at this time. Apart from the coupled cluster method [5]

* Presented at the XXVII Mazurian Lakes School of Physics, Krzyże, Poland, September 2–9, 2001.

[†] e-mail: bbarrett@physics.arizona.edu

[‡] On leave of absence from Nuclear Physics Institute, AS CR, 250 68 Řež near Prague, Czech Republic.

applied typically to closed shell and near-closed shell nuclei, the Green's function Monte Carlo method is the only approach for which exact solutions of systems with $A \leq 8$ have been obtained [4].

For both few nucleon systems and p -shell nuclei, treated as systems of nucleons interacting by realistic NN interactions, we apply the no-core shell model approach [6–12]. Application of this technique requires that effective interactions appropriate for a given finite model space be employed. In the standard formulation of this approach, utilizing a single-particle (s.p.) coordinate HO basis, the effective interaction is determined for a system of two nucleons bound in a HO well and interacting by the NN potential. We note that the use of a HO basis is crucial for insuring that the center of mass (c.m.) motion of the nucleus does not mix with the internal motion of the nucleons. This approach is limited by the model space as well as by the fact that only a two-body effective interaction is used, despite the fact that higher-body effective interactions might not be negligible. Although the practical applications depend on the HO frequency and the model space, our results are guaranteed to converge to an exact solution once a sufficiently large model space is reached [8,9].

Recently, we combined the NCSM approach to the three- and four-nucleon systems with the use of an antisymmetrized, translationally invariant HO basis [8,9], as an alternative formulation of the shell model problem for very light nuclei. Due to the omission of the c.m. and to the use of a coupled basis, this method allows us to extend the shell model calculations to significantly larger model spaces, *e.g.*, up to $50\hbar\Omega$ for $A = 3$ and $18\hbar\Omega$ for $A = 4$ systems. In addition, this approach makes it possible to develop the three-body effective interactions for applications to $A > 3$ systems.

In this contribution, we discuss both formulations and present results for $A = 3, 4$ and 6 systems as well as our recent results for ^{12}C . For all discussed systems we consider several realistic, or semi-realistic, NN interactions.

2. No-core shell model approach

2.1. Hamiltonian

In the no-core shell model approach we start with the one- plus two-body Hamiltonian for the A -nucleon system, *i.e.*,

$$H_A = \sum_{i=1}^A \frac{\vec{p}_i^2}{2m} + \sum_{i<j=1}^A V_N(\vec{r}_i - \vec{r}_j), \quad (1)$$

where m is the nucleon mass and $V_N(\vec{r}_i - \vec{r}_j)$, the NN interaction. In the next step we modify the Hamiltonian (1) by adding to it the c.m. HO potential $\frac{1}{2}Am\Omega^2\vec{R}^2$, $\vec{R} = (1/A)\sum_{i=1}^A\vec{r}_i$. This potential will be subtracted in the final many-body calculation. This added and later subtracted potential permits the use of the convenient HO basis and provides a mean field that facilitates the calculation of the effective interactions. The modified Hamiltonian, with a pseudo-dependence on the HO frequency Ω , can be cast into the form

$$H_A^\Omega = \sum_{i=1}^A \left[\frac{\vec{p}_i^2}{2m} + \frac{1}{2}m\Omega^2\vec{r}_i^2 \right] + \sum_{i<j=1}^A \left[V_N(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A}(\vec{r}_i - \vec{r}_j)^2 \right]. \quad (2)$$

Since we solve the many-body problem in a finite HO model space, the realistic nuclear interaction in Eq. (2) will yield unreasonable results unless we employ a model-space dependent effective Hamiltonian. In general, for an A -nucleon system, an A -body effective interaction is needed. As we will discuss later, the effective interaction is, in the present calculations, approximated by a two-body or a three-body effective interaction. Large model spaces are desirable to minimize the role of neglected effective many-body terms. In fact, large model spaces are desirable for the evaluation of any observable, *i.e.*, the larger the model space is, the smaller the renormalization contributions to any effective operator.

As the Hamiltonian H_A^Ω (2) differs from the Hamiltonian H_A (1) only by a c.m. dependent term, no dependence on Ω should exist for the intrinsic properties of the nucleus. However, because of the neglect of many-body terms in the effective-interaction derivation, a dependence on Ω appears in our calculations. This dependence decreases as the size of the model-space is increased.

2.2. Unitary transformation of the Hamiltonian and the two-body effective interaction

For the derivation of the effective interaction, we adopted approaches presented by Lee, Suzuki [13], Da Providencia, Shakin [14], and Suzuki, Okamoto [15], which yield an Hermitian effective Hamiltonian.

In the spirit of the above mentioned papers, we introduce a unitary transformation of the Hamiltonian, by choosing an anti-Hermitian operator S , such that

$$\mathcal{H} = e^{-S} H_A^\Omega e^S. \quad (3)$$

In our approach, S is determined by the requirements that \mathcal{H} and H_A^Ω have the same symmetries and eigenspectra over the subspace \mathcal{K} of the full Hilbert space. In general, both S and the transformed Hamiltonian are A -body operators. Our simplest, non-trivial approximation to \mathcal{H} is to develop a two-body

effective Hamiltonian. The next improvement is to develop a three-body effective Hamiltonian. This approach consists then of an approximation to a particular level of clustering:

$$\mathcal{H} = \mathcal{H}^{(1)} + \mathcal{H}^{(a)}, \quad (4)$$

where the one-body and a -body ($a \leq A$) pieces are given as

$$\mathcal{H}^{(1)} = \sum_{i=1}^A h_i, \quad (5)$$

$$\mathcal{H}^{(a)} = \frac{\binom{A}{2}}{\binom{a}{2}} \sum_{i_1 < i_2 < \dots < i_a} \tilde{V}_{i_1 i_2 \dots i_a}, \quad (6)$$

with

$$\tilde{V}_{12 \dots a} = e^{-S^{(a)}} H_a^\Omega e^{S^{(a)}} - \sum_{i=1}^a h_i, \quad (7)$$

where $S^{(a)}$ is an a -body operator;

$$H_a^\Omega = h_1 + h_2 + h_3 + \dots + h_a + V_a, \quad (8)$$

and

$$V_a = \sum_{i < j}^a V_{ij}. \quad (9)$$

Note that there is no sum over a in Eq. (4). In the above equations, it has been assumed that the basis states are eigenstates of the one-body, in our case HO, Hamiltonian $\sum_{i=1}^A h_i$. We now introduce our present application, in which we take $a = 2$, so that the interaction, \tilde{V}_{12} , is given by Eq. (7)

$$\tilde{V}_{12} = e^{-S^{(2)}} (h_1 + h_2 + V_{12}) e^{S^{(2)}} - (h_1 + h_2). \quad (10)$$

The full space is divided into a model or P -space, and a Q -space, using the projectors P and Q with $P + Q = 1$. It is then possible to determine the transformation operator $S^{(2)}$ from the decoupling condition

$$Q_2 e^{-S^{(2)}} (h_1 + h_2 + V_{12}) e^{S^{(2)}} P_2 = 0. \quad (11)$$

The two-nucleon-state projectors (P_2, Q_2) follow from the definitions of the A -nucleon projectors P, Q . The solution for this approach [15] is given by

$$S^{(2)} = \operatorname{arctanh}(\omega - \omega^\dagger), \quad (12)$$

with the operator ω satisfying $\omega = Q_2\omega P_2$. This is the same operator, which we previously employed [7–9]. It can be directly obtained from the eigensolutions $|k\rangle$ of $h_1+h_2+V_{12}$ as $\langle\alpha_Q|\omega|\alpha_P\rangle = \sum_{k\in\mathcal{K}}\langle\alpha_Q|k\rangle\langle\tilde{k}|\alpha_P\rangle$, where we denote by tilde the inverted matrix of $\langle\alpha_P|k\rangle$. In the above relation, $|\alpha_P\rangle$ and $|\alpha_Q\rangle$ are the two-particle model-space and Q -space basis states, respectively, and \mathcal{K} denotes a set of d_P eigenstates, whose properties are reproduced in the model space, with d_P equal to the model-space dimension.

The resulting two-body effective interaction $P_2\tilde{V}_{12}P_2$ depends on A , on the HO frequency Ω and on N_{\max} , the maximum many-body HO excitation energy (above the lowest configuration) defining the P -space. It follows that $\mathcal{H}^{(1)} + \mathcal{H}^{(2)} - H_{\text{c.m.}}$ is translationally invariant and that $\tilde{V}_{12} \rightarrow V_{12}$ for $N_{\max} \rightarrow \infty$.

2.3. Three-body effective interaction

The most significant approximation used in the present application is the neglect of higher than two-body clusters in the unitary transformed Hamiltonian expansion. Because our method is not a variational approach, the neglected clusters can contribute either positively or negatively to the binding energy. Indeed, we find that the character of the convergence depends on the choice of Ω [6,8,9]. Our approach can be readily generalized in order to include, *e.g.*, three-body clusters, and to demand the model-space decoupling on the three-body cluster level. A method for deriving the three-body effective interaction was presented in our papers [8,9], which can be obtained by setting $a = 3$ in Eqs. (4)–(9).

In this case, our Hamiltonian formally consists only of one-body and three-body terms. We next calculate the three-body effective interaction that corresponds to $V_{ij} + V_{ik} + V_{jk}$ from the three-nucleon condition

$$Q_3e^{-S^{(3)}}(h_1 + h_2 + h_3 + V_{12} + V_{13} + V_{23})e^{S^{(3)}}P_3 = 0, \quad (13)$$

in complete analogy to Eq. (11). The three-body effective interaction $P_3\tilde{V}_{123}P_3$ is then obtained utilizing the solutions of the three-nucleon system for the Hamiltonian

$$H_3^\Omega = h_1 + h_2 + h_3 + V_{12} + V_{13} + V_{23}, \quad (14)$$

in a manner similar to that discussed after Eq. (12). As the interaction depends only on the relative positions of nucleons 1, 2 and 3, the three-nucleon c.m. can be separated, when solving the Schrödinger equation with H_3^Ω . As for the two-nucleon Hamiltonian, $h_1 + h_2 + V_{12}$, the c.m. term is not considered in the effective-interaction calculation. We obtain the three-nucleon solutions corresponding to the Hamiltonian (14) by, first, introducing Jacobi

coordinates, and, second, introducing for the interactions V_{12}, V_{13}, V_{23} , the two-body effective interactions corresponding to a large space, characterized by $N_{3\max} \approx 30$, which defines the size of the three-nucleon model space, and derived according to the procedure described in the previous subsection. A space of this size is sufficient for obtaining exact or almost exact solutions of the three-nucleon problem [8, 9].

As for two-body effective interaction $P_2 \tilde{V}_{12} P_2$, $P_3 \tilde{V}_{123} P_3$ is a function of the nucleon number A and depends on the HO frequency Ω and on the model-space defining-parameter N_{\max} . In addition, it also depends on the choice of $N_{3\max}$. Obviously, $N_{3\max}$ must be sufficiently large, in order to make this dependence negligible. The limiting properties of \tilde{V}_{123} are as follows:

$$P_3 \tilde{V}_{123} P_3 \rightarrow P_3 \sum_{i<j=1}^3 \tilde{V}_{ij} P_3 \quad \text{for } N_{\max} \rightarrow N_{3\max}$$

and

$$\tilde{V}_{123} \rightarrow \sum_{i<j=1}^3 V_{ij} \quad \text{for } N_{\max}, N_{3\max} \rightarrow \infty.$$

We have applied this approach successfully to the $A = 4$ system [8, 9].

2.4. Standard and translationally-invariant approaches

As discussed in the previous subsections, by using the effective interaction theory, we arrive at a Hamiltonian that has the following structure

$$\begin{aligned} \{H_A^\Omega\}_{\text{eff}} = & \sum_{i=1}^A \left[\frac{\vec{p}_i^2}{2m} + \frac{1}{2} m \Omega^2 \vec{r}_i^2 \right] \\ & + \left\{ \sum_{i<j=1}^A \left[V_N(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right] \right\}_{\text{eff}}, \quad (15) \end{aligned}$$

with the interaction term depending on relative coordinates (and/or relative momenta) only. The notation $\{\}_{\text{eff}}$ on the right-hand side means that the interaction within the curly braces is utilized in the calculation of the effective interaction for a given model-space size. The c.m. dependence appears only in the one-body HO term. There are two possibilities for solving the many-body Schrödinger equation with the Hamiltonian (15).

First, we may work with s.p. coordinates and the Slater-determinant for the complete $N\hbar\Omega$, HO basis. In this case, we employ the m -scheme Many-Fermion Dynamics (MFD) shell model code [16] to perform the Hamiltonian-matrix evaluation and diagonalization. A significant consequence of preserving translational invariance of the interaction term is the factorization of our

wave function into a product of a c.m. $(3/2)\hbar\Omega$ component times an internal component, which allows exact correction of any observable for c.m. effects. This feature distinguishes our approach from most phenomenological shell model studies that involve multiple HO shells.

Second, we may introduce Jacobi coordinates and a HO basis that depends on these coordinates [8,9]. Then the c.m. degrees of freedom can be completely removed. This approach has the advantage that larger model spaces can be utilized. In addition, due to the flexibility of the HO basis depending on the Jacobi coordinates, three- or even higher-body interactions can be employed. On the other hand, it is rather demanding to antisymmetrize such a basis. This limits applicability of this approach to very light nuclei. Here we present results only for $A = 3$ and 4 systems solved in this way. The results given for $A = 6$ systems and for ^{12}C are obtained in the standard way using the MFD shell model code. It should be stressed, however, that the two alternative approaches are completely equivalent and lead to the same results.

3. Results

3.1. ^3H , ^3He

We performed calculations for the $A = 3$ systems interacting by several realistic and semi-realistic NN potentials in model spaces up to $50\hbar\Omega$ ($N_{\text{max}} = 50$), *i.e.*, in still larger model spaces than in our previous published papers [8,9]. We employed the semi-realistic Minnesota (MN) [17] and MT-V

TABLE I

Results for the ground-state energies (in MeV) obtained for ^3H , ^3He and ^4He using the Minnesota (MN), Malfliet–Tjon V (MT-V), CD-Bonn, AV18 and AV8' NN potentials are presented. Shown values are based on the results calculated in the model spaces up to $N_{\text{max}} = 50$ for ^3H , ^3He , and $N_{\text{max}} = 18$ for ^4He , respectively. The errors were estimated from the dependences on the HO frequency Ω and on the model-space size characterized by N_{max} .

| | NN potential | | | | |
|---------------|----------------|-----------|------------|----------|------------|
| | MN | MT-V | CD-Bonn | AV18 | AV8' |
| ^3H | -8.385(2) | -8.239(4) | -8.002(4) | -7.61(1) | -7.75(2) |
| ^3He | — | — | -7.249(4) | -6.90(1) | — |
| ^4He | -29.94(1) | -31.28(8) | -26.30(15) | — | -25.80(20) |

[18] NN potentials as well as modern, realistic CD-Bonn [19], AV18 and AV8' [4] NN potentials. Our ${}^3\text{H}$ and ${}^3\text{He}$ results are summarized in Table I. The MN and MT-V potentials include no tensor force, while the non-local CD-Bonn NN potential has a weaker tensor force than the local AV18 and AV8'. In general, we observe that the stronger the tensor force is, the stronger the HO frequency dependence and the slower the convergence with N_{max} . In particular, our MN potential results are the fastest to converge. On the other hand, even for the AV18 NN potential, the $N_{\text{max}} = 50$ models space is sufficient for obtaining a converged result with an error less than 10 keV, as shown in Fig. 1. The AV8' NN potential is more difficult and some HO frequency dependence remains even at $50\hbar\Omega$. Our overall $A = 3$ results, however, are in excellent agreement with other exact methods, as can be judged by comparing numbers from Table I with results presented in Refs. [17,20,21] and references therein.

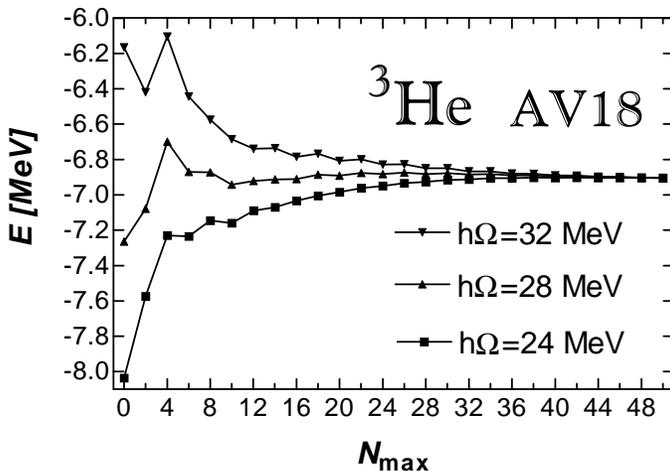


Fig. 1. Ground-state energy dependence on the model-space size for ${}^3\text{He}$ interacting by the AV18 NN potential.

3.2. ${}^4\text{He}$

In this paper, we present our ${}^4\text{He}$ results obtained in model spaces up to $18\hbar\Omega$, as also shown in Table I. This extension of the model-space size from earlier work allowed us to reduce errors on our CD-Bonn ${}^4\text{He}$ result published in Ref. [9] and bring our results into even better agreement with the recent Faddeev–Yakubovsky calculations by Nogga *et al.* [21]. As for the $A = 3$ systems, the MN potential calculations are the fastest to converge. In Fig. 2 we show the basis-space dependence for different HO frequencies. The effective two-body interaction determined with this potential is sufficient

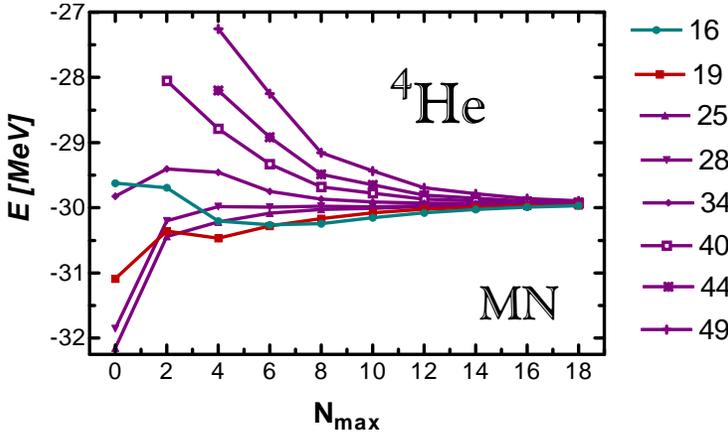


Fig. 2. Ground-state energy dependence on the model-space size for ${}^4\text{He}$ interacting by the MN potential.

for obtaining convergence in the $18\hbar\Omega$ model space to an accuracy of 10 keV. For the CD-Bonn potential our results are essentially converged, while for the AV8' or AV18 potentials, convergence is slower. For AV8' we used the three-body effective interaction, which improved the convergence. In Fig. 3 we present the model-space size dependence for the CD-Bonn NN potential. Results obtained using the three-body effective interaction, in model spaces up to $16\hbar\Omega$, are also displayed in Fig. 3.

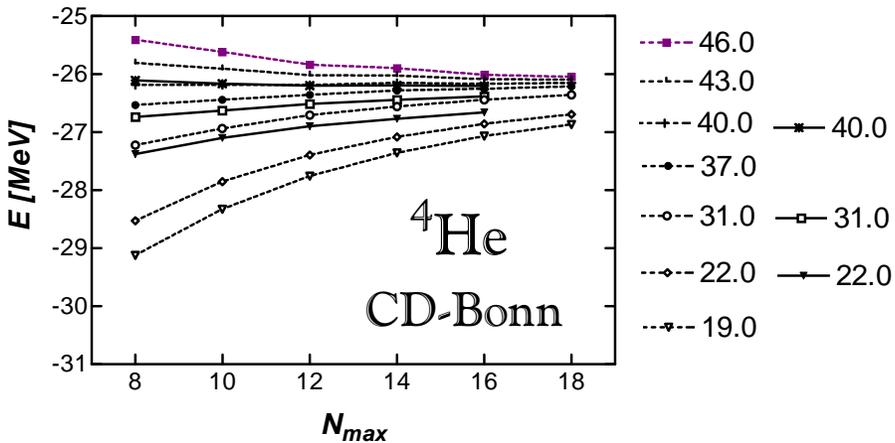


Fig. 3. Ground-state energy dependence on the model-space size for ${}^4\text{He}$ interacting by the CD-Bonn NN potential. The solid lines correspond to calculations with the three-body effective interaction.

3.3. ${}^6\text{Li}$, ${}^6\text{He}$

We performed calculations for ${}^6\text{Li}$ and ${}^6\text{He}$ [11], utilizing the m -scheme MFD code [16], in model spaces up to $10\hbar\Omega$ for the MN, AV8' and the CD-Bonn NN potentials. For the semi-realistic MN potential we achieve convergence and our ground-state energy result, $-34.48(26)$ MeV, is in good agreement with the result, -34.59 MeV, obtained by the stochastic variational method [17]. For the AV8' (without Coulomb) NN potential, convergence is more difficult to achieve. In the frequency dependence minimum, we obtain a result of -30.30 MeV in the $10\hbar\Omega$ space compared with the GFMC result of -29.47 MeV. We again emphasize that no Coulomb interaction is included. As our calculation is not variational, our binding energy may decrease with the model space enlargement. In Fig. 4, we compare our energy levels with those obtained by the GFMC for the AV8'. We obtain quite reasonable agreement, and the spectrum exhibits good stability for the low-lying states. states are broad resonances and, therefore, their movement is not surprising.

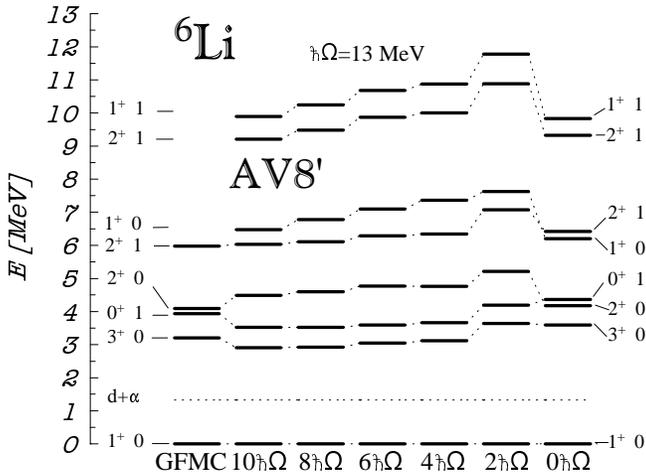


Fig. 4. ${}^6\text{Li}$ excitation spectra obtained in the NCSM and in the GFMC.

We also investigated the transitions from the ground states of ${}^6\text{He}$ and ${}^6\text{Li}$ to the negative parity states of ${}^6\text{He}$ [11]. Recently, it was argued that a soft-dipole mode in ${}^6\text{He}$ has been observed in a charge exchange reaction on ${}^6\text{Li}$ [22]. In Fig. 5, we present our ${}^6\text{He}$ excitation spectra obtained in $6-9\hbar\Omega$ model spaces. We indicate the strong E1 transitions together with the $B(E1)$ values, in $e^2 \text{fm}^2$, as well as the strong spin flip and spin non-flip transitions from the ${}^6\text{Li}$ ground state. Our results are in qualitative agreement with the experimental observation in the sense that the lowest

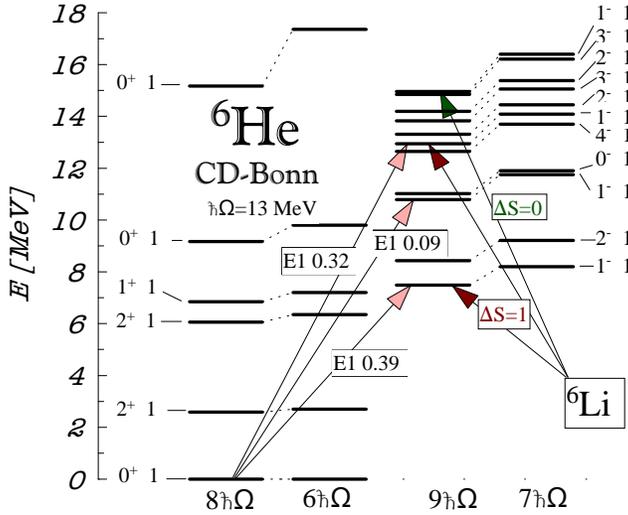


Fig. 5. Positive and negative-parity excitation spectra of ${}^6\text{He}$ obtained in the NCSM. Strong E1 transitions as well as the spin flip and spin non-flip transitions from ${}^6\text{Li}$ are indicated.

1^-1 state collects a substantial E1 strength and the transition from ${}^6\text{Li}$ is spin flip dominated. Also, the spin non-flip transition goes to a higher lying 1^-1 state in agreement with experiment [22].

3.4. ${}^{12}\text{C}$

In this subsection we address a vastly more complex system, ${}^{12}\text{C}$. There are several pressing reasons to investigate ${}^{12}\text{C}$ in a way that preserves as much predictive power as possible. The ${}^{12}\text{C}$ nucleus plays an important role [23] in neutrino studies using liquid scintillator detectors. Also, there has been considerable interest recently in parity-violating electron scattering from $(J^\pi, T) = (0^+, 0)$ targets, like ${}^{12}\text{C}$, to measure the strangeness content of the nucleon [24, 25].

To solve for the properties of ${}^{12}\text{C}$, we employ the m -scheme MFD code [16]. Here we discuss an extension of our ${}^{12}\text{C}$ study published in Ref. [10]. In particular, we show our first results obtained in the $6\hbar\Omega$ space, where the dimensions reach 32 million. We utilize $\hbar\Omega = 15$ MeV, which lies in the range where the largest model-space results are least sensitive to $\hbar\Omega$ [10].

In Table II and Fig. 6, we present the g.s. energy, excitation spectra as well as several other observable results calculated with the CD-Bonn NN potential. While the energy of the g.s. eigenstate increases with increasing model space, the relative level spacings are less dependent on model-space

TABLE II

Experimental and calculated g.s. and 3^- -state energies, point-proton rms radii, the 2_1^+ -state and the 3^- -state quadrupole moments of ^{12}C . Results obtained in different model spaces, *i.e.*, $N_{\text{max}} = 6, 4, 2, 0$ for the positive-parity and $N_{\text{max}} = 5, 3, 1$ for the negative-parity states and using effective interactions derived from the CD-Bonn NN potential are given. The calculated excitation energy of the 3^- state is obtained by comparing its energy in the $N\hbar\Omega$ space with the ground state in the $(N-1)\hbar\Omega$ space. A HO frequency of $\hbar\Omega = 15$ MeV was employed. The experimental values are from Refs. [26, 27].

| | ^{12}C | CD-Bonn | | | |
|---------------------------------|-----------------|----------------|----------------|----------------|----------------|
| Model space | – | $6\hbar\Omega$ | $4\hbar\Omega$ | $2\hbar\Omega$ | $0\hbar\Omega$ |
| $ E_{\text{gs}}(0^+0) $ [MeV] | 92.162 | 85.630 | 88.518 | 92.353 | 104.947 |
| r_p [fm] | 2.35(2) | 2.195 | 2.199 | 2.228 | 2.376 |
| Q_{2+} [$e\text{fm}^2$] | +6(3) | 4.717 | 4.533 | 4.430 | 4.253 |
| Model space | – | – | $5\hbar\Omega$ | $3\hbar\Omega$ | $1\hbar\Omega$ |
| $ E(3^-0) $ [MeV] | 82.521 | | 72.952 | 75.331 | 83.390 |
| r_p [fm] | | | 2.309 | 2.316 | 2.425 |
| Q_{3-} [$e\text{fm}^2$] | | | -7.942 | -7.596 | -6.936 |
| $E(3^-0) - E_{\text{gs}}$ [MeV] | 9.641 | | 15.566 | 17.022 | 21.557 |

size. In particular, the excitation spectrum is remarkably stable when the model space is changed from $4\hbar\Omega$ to $6\hbar\Omega$. In general, we obtain reasonable agreement of the states dominated by $0\hbar\Omega$ configurations with experimental levels. We note that the favorable comparison with available data is a consequence of the underlying NN interaction rather than a phenomenological fit. Our obtained binding energy of about 85.6 MeV in the $6\hbar\Omega$ space is expected to decrease with a further model-space enlargement. We estimate, however, that our result should be within better than 10% of the exact solution for the two-body CD-Bonn NN potential. In order to reach the experimental binding energy, likely a true three-body NN interaction is necessary [4].

The two- or higher- $\hbar\Omega$ dominated states, such as the 7.65 MeV 0^+0 state, are not seen in the low-lying part of our calculated spectra. In general, the convergence rate of the $2\hbar\Omega$ dominated states is quite different than that of the ground state. However, we observe a decreasing excitation energy of the second 0^+0 state. We expect this state eventually to change its structure and become the cluster state.

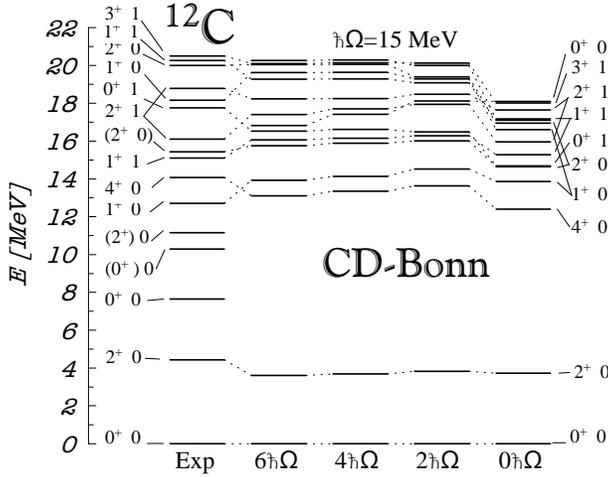


Fig. 6. Experimental and theoretical excitation spectra of ^{12}C .

4. Conclusions

In this contribution, we described the *ab initio* NCSM approach and discussed its application to the lightest nuclei, ^3H , ^3He and ^4He , for which we obtain well-converged results. Due to the utility of Jacobi coordinates in these few-nucleon calculations, we are able to reach very large model spaces, *i.e.*, $50\hbar\Omega$ for $A = 3$ and $18\hbar\Omega$ for $A = 4$. Also, we showed our results for ^6Li , ^6He and ^{12}C . For $A=6$, we performed calculations in model spaces up to $10\hbar\Omega$ with dimensions approaching 10^7 . In the case of ^{12}C , we were limited to model spaces up to $6\hbar\Omega$, where the dimensions reach 32 million. In these far more complex cases, we get close to convergence for $A = 6$. For ^{12}C we do not reach full convergence, but nonetheless we obtain a reasonable approximation for the lowest $0\hbar\Omega$ -dominated states. We note that we performed NCSM calculations for the $0s$ - and $0p$ -shell nuclei in the past [6, 7], using a similar approach to that discussed here. In those calculations, however, an additional adjustable parameter was present, contrary to the approach reported here. Our current technique allows us to obtain converged, exact solutions, as shown in our presented results.

B.R.B. and J.P.V. acknowledge partial support by the NSF grant no. PHY0070858 and USDOE grant no. DE-FG-02-87ER-40371, respectively. The 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 no. 00-ERD-028.

REFERENCES

- [1] L.D. Faddeev, *Zh. Eksp. Teor. Fiz.* **39**, 1459 (1960) *Sov. Phys. JETP* **12**, 1014 (1961); J.L. Friar, G.L. Payne, V.G.J. Stoks, J.J. de Swart, *Phys. Lett.* **B311**, 4 (1993).
- [2] O.A. Yakubovsky, *Sov. J. Nucl. Phys.* **5**, 937 (1967); W. Glöckle, H. Kamada, *Phys. Rev. Lett.* **71**, 971 (1993).
- [3] M. Viviani, A. Kievsky, S. Rosati, *Few-Body Systems* **18**, 25 (1995).
- [4] B.S. Pudliner, V.R. Pandharipande, J. Carlson, S.C. Pieper, R. B. Wiringa, *Phys. Rev.* **C56**, 1720 (1997); R.B. Wiringa, *Nucl. Phys.* **A631**, 70c (1998).
- [5] R.F. Bishop, M.F. Flynn, M.C. Boscá, E. Buendía, R. Guardiola, *Phys. Rev.* **C42**, 1341 (1990); J.H. Heisenberg, B. Mihaila, *Phys. Rev.* **59**, 1440 (1999).
- [6] D.C. Zheng, B.R. Barrett, L. Jaqua, J.P. Vary, R.L. McCarthy, *Phys. Rev.* **C48**, 1083 (1993); D.C. Zheng, J.P. Vary, B.R. Barrett, *Phys. Rev.* **C50**, 2841 (1994); D.C. Zheng, B.R. Barrett, J.P. Vary, W.C. Haxton, C.L. Song, *Phys. Rev.* **C52**, 2488 (1995).
- [7] P. Navrátil, B.R. Barrett, *Phys. Rev.* **C54**, 2986 (1996); *Phys. Rev.* **C57**, 3119 (1998).
- [8] P. Navrátil, B.R. Barrett, *Phys. Rev.* **C57**, 562 (1998), *Phys. Rev.* **C59**, 1906 (1999).
- [9] P. Navrátil, G.P. Kamuntavičius, B.R. Barrett, *Phys. Rev.* **C61**, 044001 (2000); e-print archive nucl-th/9907054.
- [10] P. Navrátil, J.P. Vary, B.R. Barrett, *Phys. Rev. Lett.* **84**, 5728 (2000); *Phys. Rev.* **62**, 054311 (2000).
- [11] P. Navrátil, J.P. Vary, B.R. Barrett, to be published in *Phys. Rev. Lett.* **87**, (2001).
- [12] C.P. Viazminsky, J.P. Vary, *J. Math. Phys.* **92**, 2055 (2001).
- [13] K. Suzuki, S.Y. Lee, *Prog. Theor. Phys.* **64**, 2091 (1980); K. Suzuki, *Prog. Theor. Phys.* **68**, 246 (1982). K. Suzuki, R. Okamoto, *Prog. Theor. Phys.* **70**, 439 (1983).
- [14] J. Da Providencia, C.M. Shakin, *Ann. Phys. NY* **30**, 95 (1964).
- [15] K. Suzuki, *Prog. Theor. Phys.* **68**, 1999 (1982); K. Suzuki, R. Okamoto, *Prog. Theor. Phys.* **92**, 1045 (1994).
- [16] J.P. Vary, *The Many-Fermion-Dynamics Shell Model Code*, Iowa State University, 1992 (unpublished); J.P. Vary, D.-C. Zheng, *The Many-Fermion-Dynamics Shell Model Code*, Iowa State University, 1994.
- [17] K. Varga, Y. Suzuki, *Phys. Rev.* **C52**, 2885 (1995) and references therein.
- [18] R.A. Malfliet, J.A. Tjon, *Nucl. Phys.* **A127**, 161 (1969).
- [19] R. Machleidt, F. Sammarruca, Y. Song, *Phys. Rev.* **C53**, 1483 (1996).
- [20] N. Barnea, W. Leidemann, G. Orlandini, *Phys. Rev.* **C61**, 054001 (2000).
- [21] A. Nogga, H. Kamada, W. Glöckle, *Phys. Rev. Lett.* **85**, 944 (2000).

- [22] S. Nakayama, T. Yamagata, H. Akimune, I. Daito, H. Fujimura, Y. Fujita, M. Fujiwara, K. Fushimi, T. Inomata, H. Kohri, N. Koori, K. Takahisa, A. Tamii, M. Tanaka, H. Toyokawa, *Phys. Rev. Lett.* **85**, 262 (2000).
- [23] A.C. Hayes, *Phys. Rep.* **315**, 257 (1999); P. Vogel, nucl-th/9901027; E. Kolbe, K. Langanke, P. Vogel, *Nucl. Phys.* **A652**, 91 (1999).
- [24] M.J. Musolf, *et al.*, *Phys. Rep.* **239**, 1 (1994).
- [25] W.E. Ormand, *Phys. Rev. Lett.* **82**, 1101 (1999).
- [26] F. Ajzenberg-Selove, *Nucl. Phys.* **A506**, 1 (1990).
- [27] I. Tanihata, T. Kobayashi, O. Yamakawa, S. Shimoura, K. Ekuni, K. Sugimoto, N. Takahashi, T. Shimoda, H. Sato, *Phys. Lett.* **B206**, 592 (1988).