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AB-INITIO NO-CORE SHELL MODEL

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We discuss the no-core shell model approach, an *ab initio* method with effective Hamiltonians derived from realistic nucleon-nucleon (NN) potentials as a function of the finite harmonic-oscillator (HO) basis space. We present results for three and four nucleon systems in model spaces that include up to $50\hbar\Omega$ and $18\hbar\Omega$ HO excitations, respectively. For these light systems we are in agreement with results obtained by other exact methods. Also, we calculate the properties of ^{6}Li and ^{6}He in model spaces up to $10\hbar\Omega$, and of ^{12}C for model spaces up to $6\hbar\Omega$.

1 Introduction

While various methods have been developed to solve the three- and four-nucleon systems with realistic interactions [1,2,3,4], few approaches are suitable for heavier nuclei at this time. Beyond $A = 4$ 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 the p-shell nuclei, treated as systems of nucleons interacting by realistic NN interactions, we apply the no-core shell-model (NCSM) approach [5,6,7,8]. In this method, effective interactions apropriate for a given finite model space are utilized. In its new formulation [7,8] the calculation depends only on the HO frequency and the model space size and is guaranteed to converge to an exact solution once a sufficiently large size of the model space is reached.

In the standard approach of this method, with the single-particle coordinate HO basis utilized, the effective interaction is determined for a system of two nucleons bound in a HO well and interacting by the NN potential. We present our results for $A = 6$ systems as well as for ^{12}C obtained in this way.

Alternatively, for very light systems, it is possible to re-formulate the shell-model problem in a translationally-invariant way. Recently, we combined the NCSM approach to the three- and four-nucleon systems with the use of anti-symmetrized translationally invariant HO basis [7]. This allows us to extend the

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shell-model calculations to achieve convergence for $A = 3$ and 4.

2 No-core shell-model approach

We start from the one- plus two-body Hamiltonian for the A-nucleon system, i.e., $H_A = \sum_{i=1}^{A} \frac{\vec{p}_i^2}{2m} + \sum_{i<j=1}^{A} V_{\rm N}(\vec{r}_i - \vec{r}_j)$, where m is the nucleon mass and $V_{\rm N}$, the NN interaction. In the next step, we modify this Hamiltonian by adding to it the center-of-mass HO potential $\frac{1}{2}Am\Omega^2\vec{R}^2$, $\vec{R} = \frac{1}{A}\sum_{i=1}^{A}\vec{r}_i$. The effect of this potential will be subtracted in the final many-body calculation and it does not influence the intrinsic properties of the many-body system. It permits the use of the convenient HO basis and provides a mean field that facilitates the calculation of the effective interaction. The modified Hamiltonian, with a pseudo-dependence on the HO frequency Ω, can be cast into the form

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

Since we solve the many-body problem in a finite HO model space, the realistic nuclear interaction in Eq. (1) will yield pathological results unless we derive a model-space dependent effective Hamiltonian. In general, for an A-nucleon system, an A-body effective interaction is needed. As discussed further, we approximate this effective interaction by a two- or a three-body effective interaction. Large model spaces are then desirable to minimize the role of neglected effective many-body terms.

For the derivation of the effective interaction, we adopt the approach presented by Lee and Suzuki [9]. We make use of a unitary transformation of the Hamiltonian by choosing a translationally invariant, antihermitian operator S such that $\mathcal{H} = e^{-S}H_A^{\Omega}e^{S}$. 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. In the two-body approximation, the transformed interaction is obtained as $\tilde{V}_{12} = e^{-S_{12}}(h_1 + h_2 + V_{12})e^{S_{12}} - (h_1 + h_2)$. The terms h_i and V_{12} correspond to the one- and two-body terms in Eq. (1). The full space is then divided into a model, or P-space, and an excluded, or Q-space, using the projectors P and Q, $P + Q = 1$. It is then possible to determine the transformation operator S_{12} from the decoupling condition $Q_2e^{-S_{12}}(h_1 + h_2 + V_{12})e^{S_{12}}P_2 = 0$. The two-nucleon-state projectors (P_2, Q_2) follow from the definitions of the A-nucleon projectors P, Q. This approach has a solution, $S_{12} = \mathrm{arctanh}(\omega - \omega^{\dagger})$, with the operator ω satisfying $\omega = Q_2\omega P_2$. It can be directly obtained from the eigensolutions $|k\rangle$ of $h_1 + h_2 + V_{12}$ [6,7,8].

Table 1: NCSM results for the ground-state energies of ^{3}H, ^{3}He and ^{4}He.

^{3}H					
NN potential	MN	MT-V	CD-Bonn	AV18	AV8′
E_{gs} [MeV]	-8.385(2)	-8.239(4)	-8.002(4)	-7.61(1)	-7.75(2)

^{3}He		
NN potential	CD-Bonn	AV18
E_{gs} [MeV]	-7.249(4)	-6.90(1)

^{4}He				
NN potential	MN	MT-V	CD-Bonn	AV8′
E_{gs} [MeV]	-29.94(1)	-31.28(8)	-26.30(15)	-25.80(20)

The resulting two-body effective interaction $\tilde{V}_{12}$ depends on A, the HO frequency Ω and $N_{\max}$, the maximum many-body HO excitation energy (above the lowest configuration) defining the P-space. It follows that $\tilde{V}_{12} \to V_{12}$ for $N_{\max} \to \infty$.

3 Results

3.1 ^3H, ^3He, ^4He

Our results for $A = 3$ and $A = 4$ systems are summarized in Table 1. We performed calculations using the semi-realistic Minnesota (MN) and MT-V [10] NN potentials as well as modern realistic CD-Bonn [11], AV18 and AV8′ NN potentials. For the $A = 3$ systems, we used model spaces up to $50\hbar\Omega$ ($N_{\max} = 50$). Our $A = 4$ results were obtained in model spaces up to $18\hbar\Omega$ using two-body effective interactions. In addition, we also performed calculations using three-body effective interactions in model spaces up to $16\hbar\Omega$. This is particularly important for the AV8′ NN potentials, as the two-body effective interation approximation is insufficient in this case.

Overall, our $A = 3$, as well as $A = 4$, results are in excellent agreement with other exact methods, as can be judged by comparing with results presented in Refs. [10,12,13] and references therein.

3.2 ^6Li, ^6He

We performed calculations for ^{6}Li and ^{6}He in model spaces up to $10\hbar\Omega$ using the MN, AV8′ and the CD-Bonn NN potentials. For the semi-realistic MN potential we almost 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 [10]. For the AV8′ (without Coulomb) NN

potential, the convergence is much harder 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. As our calculation is not variational, our binding energy may decrease with the model space enlargement. In Fig. 1, we compare our energy levels with those obtained by the GFMC for the AV8′. We have a very reasonable agreement and the spectrum exhibits good stability for the low-lying states. The higher lying states are broad resonances, and therefore, their movement is not surprising.

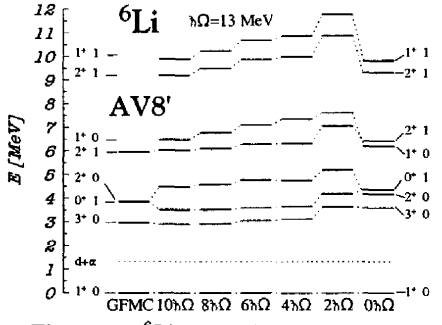

Figure 1: ^{6}Li excitation spectra obtained in the NCSM and in the GFMC.

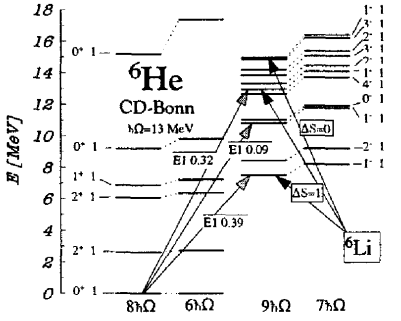

Figure 2: Positive and negative-parity excitation spectra of ^{6}He.

Recently, it was argued that a soft-dipole mode in ^{6}He has been observed in a charge exchange reaction on ^{6}Li [14]. In Fig. 2, we present our ^{6}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 fm^2, as well as the strong spin flip and spin non-flip transitions from the ^{6}Li ground state. Our results are in a qualitative agreement with the experimental observation in the sense that the lowest 1^-1 state collects a substantial E1 strength and the transition from ^{6}Li is spin flip dominated. On the other hand, the spin non-flip transition goes to a higher lying 1^-1 state in agreement with experiment [14].

3.3 ^{12}C

Here we discuss an extension of our ^{12}C study published in Ref. [8]. 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 $\hbar\Omega$ [8].

In Table 2 and Fig. 3, we present the ground-state energy, excitation spectra as well as several other observable results calculated with the CD-

Table 2: The experimental and calculated ground-state energies, point-proton rms radii, and 2_1^+-state quadrupole moments of ^{12}C.

	^{12}C	CD-Bonn			
model space	-	$6\hbar\Omega$	$4\hbar\Omega$	$2\hbar\Omega$	$0\hbar\Omega$
$\lvert E_{\rm gs}(0^+0)\rvert$ [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 fm^2]	+6(3)	4.717	4.533	4.430	4.253

Bonn NN potential. While the energy of the ground-state eigenstate increases with increasing model space, the relative level spacings are less dependent on model-space 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.

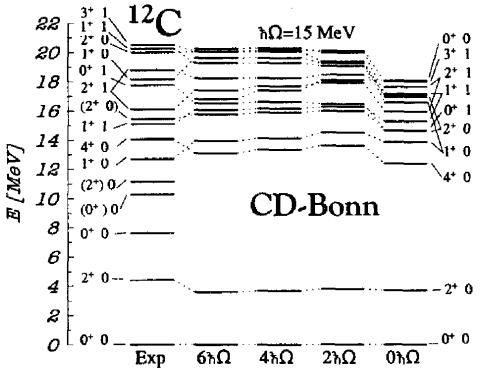

Figure 3: Experimental and theoretical excitation spectra of ^{12}C.

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. 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.

4 Conclusions

In the present contribution, we described the *ab initio* no-core shell-model approach and discussed its application to the lightest nuclei, ^{3}H, ^{3}He and ^{4}He, for which we obtain converged results. Also, we showed our results for ^{6}Li,

^{6}He and ^{12}C. 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.

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