Properties of ^{12}C in the *Ab Initio* Nuclear Shell Model

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We obtain properties of ^{12}C in the *ab initio* no-core nuclear shell model. The effective Hamiltonians are derived microscopically from the realistic CD Bonn and the Argonne V8′ nucleon-nucleon (NN) potentials as a function of the finite harmonic oscillator basis space. Binding energies, excitation spectra, and electromagnetic properties are presented for model spaces up to $5\hbar\Omega$. The favorable comparison with available data is a consequence of the underlying NN interaction rather than a phenomenological fit.

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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] applied 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 $A \leq 8$, interacting by realistic potentials, have been obtained [4].

For more complex nuclei, treated as systems of nucleons interacting by realistic NN interactions, we apply the no-core shell model (SM) approach [6–9]. To date, this *ab initio* method has been successfully applied to solve the three-nucleon as well as the four-nucleon bound-state problem [8,9]. Here, we address a vastly more complex system, ^{12}C, and present first results for an illustrative set of observables with two realistic NN interactions.

There are several pressing reasons to investigate ^{12}C in a way that preserves as much predictive power as possible. The ^{12}C nucleus plays an important role [10] 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}C, to measure the strangeness content of the nucleon [11,12]. For these and many other reasons, there have been multi-$\hbar\Omega$ SM studies of ^{12}C in the past [13–15]. However, unlike our approach, phenomenological effective interactions were used.

We start from the two-body Hamiltonian for the A-nucleon system, which depends on the intrinsic coordinates alone, $H_A = T_{\rm rel} + \mathcal{V}$, where $T_{\rm rel}$ is the relative kinetic energy operator and $\mathcal{V}$ is the sum of two-body nuclear and Coulomb interactions, $\mathcal{V} = V_{\rm N} + V_{\rm C}$. There is no phenomenological one-body term. We neglect many-body interactions at present. To facilitate our work, we add an A-nucleon harmonic oscillator (HO) Hamiltonian acting solely on the center-of-mass (CM), $H_{\rm CM} = T_{\rm CM} + U_{\rm CM}$, where $U_{\rm CM} = \frac{1}{2}Am\Omega^2\vec{R}^2$, $\vec{R} = \frac{1}{A}\sum_{i=1}^{A}\vec{r}_i$, and m is the nucleon mass. The effect of this HO CM Hamiltonian will be subtracted in the final many-body calculation. The Hamiltonian, with a pseudodependence on Ω, can be cast into the form

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

Since we solve the many-body problem in a finite HO model space, the realistic nuclear interaction in (1) will yield pathological results unless we derive a model-space dependent effective Hamiltonian. For this purpose, we adopt approaches presented by Suzuki and Lee [16], Da Providencia and Shakin [17], and Suzuki and Okamoto [18], which yield an Hermitian effective Hamiltonian.

According to Da Providencia and Shakin [17], a unitary transformation of the Hamiltonian H_A^Ω, which is able to accommodate the short-range two-body correlations, can be introduced by choosing a two-body, in our case translationally invariant, anti-Hermitian operator $S = \sum_{i<j=1}^{A} S_{ij}$, such that $\mathcal{H} = e^{-S}H_A^\Omega e^S$. The transformed Hamiltonian can be expanded in terms of up to A-body clusters $\mathcal{H} = \mathcal{H}^{(1)} + \mathcal{H}^{(2)} + \mathcal{H}^{(3)} + \ldots$, where the one-body and two-body pieces are given as $\mathcal{H}^{(1)} = \sum_{i=1}^{A} h_i$, $\mathcal{H}^{(2)} = \sum_{i<j=1}^{A}\tilde{V}_{ij}$, with

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

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_{12} from the decoupling condition

$$Q_2 e^{-S_{12}}(h_1 + h_2 + V_{12})e^{S_{12}}P_2 = 0. \quad (3)$$

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 [18], $S_{12} = \operatorname{arctanh}(\omega - \omega^\dagger)$, with the operator ω satisfying $\omega = Q_2\omega P_2$. This is the same

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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 $\langle\alpha_P\,|\,k\rangle$. Here $|\alpha_P\rangle$ 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 $\tilde{V}_{12}$ 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 $\mathcal{H}^{(1)} + \mathcal{H}^{(2)} - H_{\rm CM}$ is translationally invariant and that $\tilde{V}_{12} \to V_{12}$ for $N_{\max} \to \infty$. A significant consequence of preserving translational invariance is the factorization of our wave function into a product of a CM $\frac{3}{2}\hbar\Omega$ component times an internal component, which allows exact correction of any observable for CM effects. This feature distinguishes our approach from most phenomenological SM studies that involve multiple HO shells.

The most significant approximation used in the present application is the neglect of higher than two-body clusters in the unitary transformed Hamiltonian expansion. Our method is not a variational approach so 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]. The method 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. Such a generalization leads to the derivation of the three-body effective interaction, which has been successfully applied in our calculations for the $A = 4$ system [8,9]. We learned that for an optimal HO frequency the contribution of higher-order clusters to the binding energy are about 10% in similar model spaces that we employ here.

To solve for the properties of ^{12}C, we employ the m-scheme Many-Fermion Dynamics code [19]. Because of the fast growing matrix dimensions, reaching 6 488 004 at the $N_{\max} = 5$ model space, we are restricted to $N_{\max} = 0, 2, 4$ for the positive-parity states and $N_{\max} = 1, 3, 5$ for the negative-parity states. Here, we utilize $\hbar\Omega = 15$ MeV which lies in the range where the largest model space results are least sensitive to $\hbar\Omega$. Full details will be reported elsewhere.

We present results for the CD Bonn [20] and the Argonne V8′ [4] NN potentials. Our positive-parity state results are presented in Table I and in Fig. 1, and the negative-parity state results are in Table II and Fig. 2. While the energy of the lowest eigenstate of each parity increases with increasing model space, the relative level spacings are less dependent on model-space size. As a gauge of trends with increasing model-space size, consider the rms changes in excitation energies of the first seven excited states of each parity in the CD Bonn case. For positive-parity states, the rms changes are 1.31 (0.22) MeV in going from 0 to 2 (2 to 4)$\hbar\Omega$. For negative parity states, the rms changes are 0.87 (0.20) MeV in going from 1 to 3 (3 to 5)$\hbar\Omega$. The difference between the $N_{\max} = 2(3)$ and 4(5) results is significantly smaller than that between the $N_{\max} = 0(1)$ and 2(3) results, which is similar to the convergence trends we saw in lighter systems [6,8,9]. Our obtained binding energy of about 88 MeV in the $4\hbar\Omega$ space is expected to decrease with a further model space enlargement. We estimate, however, that our result should be within 10% of the exact solution for the two-body NN potential used. In order to reach the experimental binding energy, likely a true three-body NN interaction is neccessary [4].

TABLE I. Experimental and calculated energies, ground-state point-proton rms radii, the 2_1^+-state quadrupole moments, as well as $E2$ transitions, in $e^2\,\mathrm{fm}^4$, and $M1$ transitions, in μ_N^2, of ^{12}C. A HO frequency $\hbar\Omega = 15$ MeV was employed. The experimental values are from Refs. [21,22].

	^{12}C	CD Bonn			AV8′		
Model space	⋯	$4\hbar\Omega$	$2\hbar\Omega$	$0\hbar\Omega$	$4\hbar\Omega$	$2\hbar\Omega$	$0\hbar\Omega$
$\lvert E_{gs}(0^+0)\rvert$ (MeV)	92.162	88.518	92.353	104.947	87.675	92.195	104.753
r_p (fm)	2.35(2)	2.199	2.228	2.376	2.202	2.228	2.376
Q_{2^+} ($e\,\mathrm{fm}^2$)	+6(3)	4.533	4.430	4.253	4.536	4.427	4.250
$E_x(2^+0)$ (MeV)	4.439	3.697	3.837	3.734	3.584	3.766	3.699
$E_x(1^+0)$ (MeV)	12.710	14.141	14.525	13.866	14.044	14.549	13.935
$E_x(4^+0)$ (MeV)	14.083	13.355	13.636	12.406	12.848	13.255	12.192
$E_x(1^+1)$ (MeV)	15.110	16.165	16.291	15.290	16.295	16.515	15.488
$E_x(2^+1)$ (MeV)	16.106	17.717	17.945	15.970	17.945	17.823	15.920
$E_x(0^+1)$ (MeV)	17.760	16.618	16.493	14.698	16.205	16.208	14.574
$B(E2; 2^+0 \to 0^+0)$	7.59(42)	4.625	4.412	4.092	4.612	4.397	4.091
$B(M1; 1^+0 \to 0^+0)$	0.0145(21)	0.0042	0.0032	0.0013	0.0026	0.0019	0.0008
$B(M1; 1^+0 \to 2^+0)$	0.0081(14)	0.0017	0.0013	0.0008	0.0013	0.0012	0.0008
$B(M1; 1^+1 \to 0^+0)$	0.951(20)	0.355	0.280	0.158	0.316	0.252	0.147
$B(M1; 1^+1 \to 2^+0)$	0.068(9)	0.0002	0.0028	0.0115	0.0023	0.0078	0.0167
$B(E2; 2^+1 \to 0^+0)$	0.65(13)	0.283	0.015	0.0018	0.104	0.000	0.002

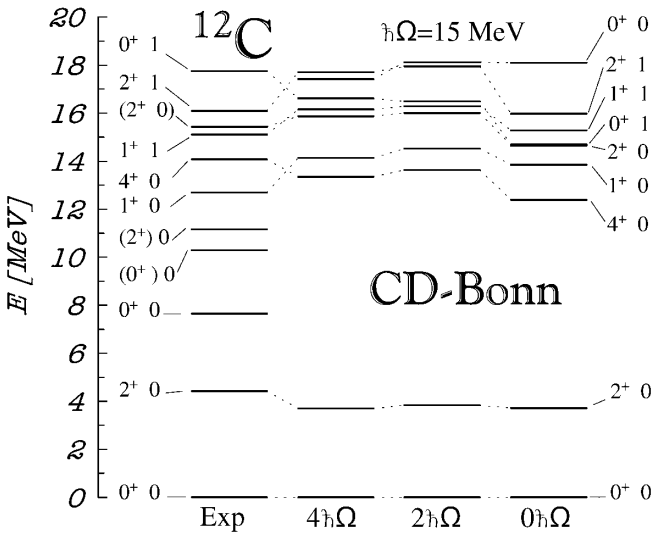

FIG. 1. Experimental and theoretical positive-parity excitation spectra of ^{12}C. Results obtained in $4\hbar\Omega$, $2\hbar\Omega$, and $0\hbar\Omega$ model spaces are compared. The effective interaction was derived from the CD Bonn *NN* potential in a HO basis with $\hbar\Omega = 15$ MeV. The experimental values are from Ref. [21].

In general, we obtain a reasonable agreement of the states dominated by $0\hbar\Omega$ and $1\hbar\Omega$ configurations with experimental levels. We also observe a general trend of improvement with increasing model-space size. We obtain a reasonable set of excitation energies for the $T = 1$ states relative to the lowest $T = 0$ state of each parity. In addition, our lowest 0^+ $T = 2$ state lies between 27 and 29 MeV, depending on the *NN* potential and the model space, in good agreement with the experimental 0^+2 state at 27.595 MeV. We note that the favorable comparison with available data is a consequence of the underlying *NN* interaction rather than a phenomenological fit. Our ground-state wave function in the $4\hbar\Omega$ calculation contains 61% of the $0\hbar\Omega$ component. The occupancy of the $0p3/2$ level is 5.74 nucleons, while the occupancy of the $0p1/2$ level is 1.90 nucleons. From Tables I and II, it is clear that the excitation energies of the negative-parity states relative to the positive-parity states decrease rapidly with the model-space enlargement. Still, even in our largest spaces the 3^-0 state is more than 5 MeV too high compared to the experiment.

In order to achieve a more realistic excitation energy a still larger HO expansion is needed, especially for states with significant cluster structure. The two- and higher-$\hbar\Omega$ dominated states, such as the 7.65 MeV 0^+0 state that is known to be a three-alpha cluster resonance [23], 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 as we observed in ^{4}He calculations performed in the present formalism [8,9]. Also, an optimal HO frequency for the convergence of the ground state will differ from the optimal frequency for the $2\hbar\Omega$ states. We investigated the position of the lowest $2\hbar\Omega$ dominated states and the giant quadrupole resonance (GQR) $E2$ distribution. Our lowest $2\hbar\Omega$ 0^+ state lies at about 40 MeV excitation energy and the GQR $E2$ strength is fragmented between 43 to 50 MeV in the $2\hbar\Omega$ calculation. In the $4\hbar\Omega$ model space the excitation energy of the lowest $2\hbar\Omega$ 0^+ state drops by 5 MeV to about 35 MeV and similarly the GQR strength position is lowered to 37–47 MeV, while the experimental is observed in the range 18–28 MeV [24].

There is little difference between the results from the two *NN* interactions, although the overall agreement with experiment is slightly better for the CD Bonn potential, e.g., stronger binding and the $T = 1$ state ordering.

Our radius and $E2$ results, based on the bare radius operator and bare nucleon charges, are smaller than the experimental values. The underestimation of the rms radius, the quadrupole moment, and the $E2$ transitions is linked with the overestimation of the position of the GQR strength and suggests that even in the $N_{\max} = 4$ space we still miss significant clustering effects. Clearly, there is

TABLE II. Experimental and calculated negative-parity state energies, the 3^-0-state point-proton rms radii, and quadrupole moments are shown. The calculated excitation energy of 3^-0 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 $\hbar\Omega = 15$ MeV was employed.

	^{12}C	CD Bonn			AV8′		
Model space	⋯	$5\hbar\Omega$	$3\hbar\Omega$	$1\hbar\Omega$	$5\hbar\Omega$	$3\hbar\Omega$	$1\hbar\Omega$
$\lvert E(3^-0)\rvert$ (MeV)	82.521	72.952	75.331	83.390	72.300	75.360	83.459
r_p (fm)		2.309	2.316	2.425	2.310	2.315	2.425
Q_{3^-} (e fm^2)		−7.942	−7.596	−6.936	−7.920	−7.575	−6.933
$E(3^-0) - E_{gs}$ (MeV)	9.641	15.566	17.022	21.557	15.375	16.835	21.294
$E_x(3^-0)$ (MeV)	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$E_x(1^-0)$ (MeV)	1.203	2.093	2.256	1.561	2.112	2.274	1.552
$E_x(2^-0)$ (MeV)	2.187	3.722	4.051	3.582	3.722	4.057	3.567
$E_x(4^-0)$ (MeV)	3.711	4.866	5.084	4.768	4.741	4.993	4.710
$E_x(0^-0)$ (MeV)		7.148	7.062	5.712	7.148	7.156	5.777
$E_x(2^-1)$ (MeV)	6.929	7.671	7.783	7.340	7.949	8.237	7.574
$E_x(3^-0)$ (MeV)		7.877	8.151	6.886	7.651	7.983	6.745
$E_x(1^-1)$ (MeV)	7.589	8.048	7.951	7.042	8.117	8.096	7.184

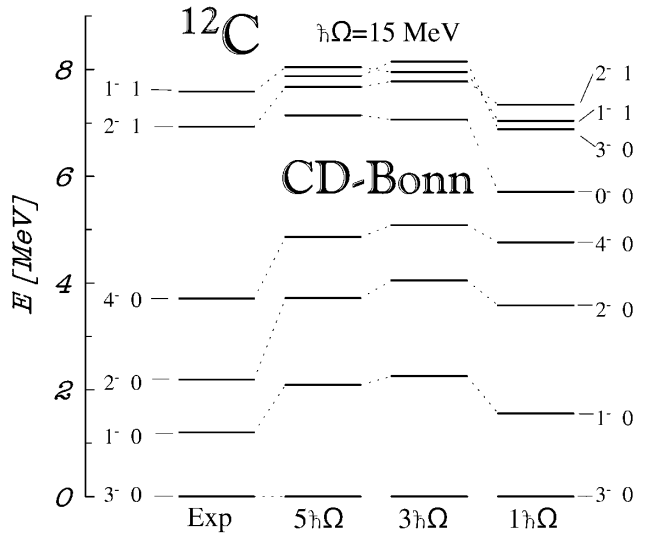

FIG. 2. Experimental and theoretical negative-parity spectra of ^{12}C. Results obtained in $5\hbar\Omega$, $3\hbar\Omega$, and $1\hbar\Omega$ model spaces are compared. Other factors are the same as in Fig. 1.

still a need for effective operators, which are calculable within our theoretical framework. In general, to compute a two-body correction to a one-body operator in our formalism is more involved than the evaluation of the effective interaction. But, it is easy to study the lowest order renormalization for a two-body operator depending on the relative position of two nucleons as, e.g., the point-nucleon rms radius operator. Then, $O_{\text{eff}} \approx \sum_{i<j=1}^{A} e^{-S_{ij}} O_{ij} e^{S_{ij}}$. We computed this term for the point-proton rms radius operator and found that the renormalization leads to an increase of the radius and that the size of this increase drops as the model-space size increases. The r_p results presented in Table I that were obtained without renormalization should be increased due to the renormalization by about 0.06, 0.02, and 0.01 fm for the $N_{\max} = 0$, 2, and 4 model spaces, respectively. This does not imply that the renormalization of other operators, e.g., the $E2$ operator, cannot be substantially higher. Similarly, as observed in our ^{3}H calculations [9], we anticipate that, in contrast with the energies, the higher-order corrections will be more significant and the overall convergence slower for other observables.

We present these results as a useful description of the 0 and $1\hbar\Omega$-dominated states of ^{12}C. Our wave functions along with the one-body and two-body densities may also be used to predict cross sections for neutrino and muon reactions with ^{12}C. The trends are encouraging and we will carry out larger model-space investigations in order to achieve greater convergence.

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