# HYBRID MULTIDETERMINANT CALCULATION OF ENERGY LEVELS OF CARBON ISOTOPES WITH A CHIRAL EFFECTIVE NUCLEON–NUCLEON INTERACTION

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We perform calculations for the binding energies and low-lying levels of $^{10,11,12,13,14,15,16,17,18,19,20,21,22}$C nuclei starting from the chiral N3LO nucleon–nucleon potential within the framework of the Hybrid Multideterminant scheme. The effective interaction is obtained using the Lee–Suzuki renormalization scheme applied to 4 and in some cases to 5, major harmonic oscillator shells. The results are compared with the experimental data.

## 1. Introduction

With the advent of modern accurate nucleon–nucleon interactions and modern many-body computational schemes, nuclear structure calculations starting from the nucleonic degrees of freedom have become possible in the recent years. A major advancement has been the systematic construction of realistic nucleon–nucleon potential using chiral effective field theories which start from the most general Lagrangian, consistent with the symmetries of QCD and the spontaneously broken chiral symmetry, appropriate for low energy nucleons and pions (Refs. [1,2,3,4]). Using these nucleon–nucleon interactions and sometimes even the three nucleon interaction derived from chiral effective field theory several nuclear structure calculations have been performed (Refs. [5,6,7,8]). Typically these calculations are limited to light nuclei ($A \simeq 16$) and, in some cases, to closed shell medium mass nuclei (Ref. [8]). The nuclear structure methods mostly used are the no-core shell model (Refs. [9,10,11,12]) which pioneered *ab initio* nuclear structure calculations, the coupled cluster method (Refs. [13,14,15]), the hyperspherical harmonics method (Refs. [16,17]) and, to a lesser extent, the hybrid multideterminant method (HMD) (Refs. [18,19,20]). The no-core shell model

method is limited by the size of the Hilbert space which become gigantic as the particle number is increased and is used for $A \simeq 16$. The coupled-cluster method is used typically at or around shell closure, but it has been applied also to medium mass nuclei (Ref. [15]). The hyperspherical harmonics method has been used for very light systems. The HMD method, which is utilized in this work, is not limited by the size of the Hilbert space as it can be easily used for medium mass nuclei, and it is equally applicable to closed and open shell nuclei (Ref. [21]). Using realistic nucleon–nucleon interactions, so far it has been used only in few cases. It is our goal to systematically apply this method to nuclei in several mass regions. This method belongs to the same family of the VAMPIR methods (Refs. [22, 23, 24]), except that the HMD uses a linear combination of particle Slater determinants instead of quasi-particle Slater determinants as in the VAMPIR methods. It is similar to the Quantum Monte Carlo method (Refs. [25, 26, 27]), except that the variational method is not stochastic. It utilizes quasi-Newtonian methods (Ref. [28]), and the Slater determinants are parametrized differently. In this work we take the N3LO nucleon–nucleon interaction (Ref. [4]), and study the carbon isotopes, both even and odd, and evaluate ground state energies and few excited states for all isotopes under study. Because of the large amount of calculations involved, especially for the odd isotopes, we limit ourselves to few harmonic oscillator frequencies, and renormalize the interaction up to 4, and in some cases up to 5, harmonic oscillator shells using the Lee–Suzuki (Refs. [28, 29, 30, 31]) renormalization procedure. In an *ab initio* approach, one considers several harmonic oscillator frequencies and an increasing number of harmonic oscillator major shells until the results are independent from the frequency and the number of major shells. In practice, at least for this chain of isotopes, this has never been done so far. Such an approach would be necessary if both accurate binding energies and excitation energy are required. Here we focus mostly on excitation energies and energy differences for which convergence is faster.

Some carbon isotopes have been considered in the framework of the UMOA renormalization prescription and shell model diagonalization (Ref. [32]) with a truncation in the number of allowed excitations. More recently they have been considered in Ref. [33], although the renormalization method is applied in momentum space (with a sharp cutoff at 2.1 fm$^{-1}$) rather than in the harmonic oscillator space. Moreover, an inert $^{14}$C has been assumed and the neutron single-particle space is restricted to the $sd$ shell. In contrast, we use a no-core approach up to the $fp$ shell included, and in some case up to $sdg$ shell, with the effective interaction constructed for this space. The heaviest of the carbon isotopes $^{22}$C has been recently found to be a borromean nucleus (Ref. [34]), that is, stable for particle emission although $^{21}$C is particle unstable. All calculations discussed in this work have

been performed using personal computers, two quad-core and four dual-core processors. The outline of this work is the following. In Sec. 2 we give a brief recap of the HMD method. In Sec. 3 and subsections we discuss the results and compare with the experimental data. In Sec. 4 we summarize the results.

## 2. A brief recap of the HMD method

The HMD method (Refs. [18, 19, 20]) consists in solving the many-body Schrodinger equation using as ansatz for the yrast eigenstates $|\psi\rangle$ a linear combination of Slater determinants, *i.e.*

$$|\psi\rangle = \sum_{\alpha=1}^{N_{\mathrm{w}}} g_\alpha \hat{P} |\phi, \alpha\rangle . \tag{1}$$

The operator $\hat{P}$ restores the desired exact quantum numbers (angular momentum and parity), $\alpha$ labels the Slater determinants and $|\phi, \alpha\rangle$ is a general Slater determinant (that is, no symmetries are imposed). Each Slater determinant is built from the generalized creation operators

$$c_n^\dagger(\alpha) = \sum_{i=1}^{N_{\mathrm{s}}} U_{i,n}(\alpha) a_i^\dagger . \tag{2}$$

$a_i^\dagger$ is the creation operator in the harmonic oscillator single-particle state $i$, and $N_{\mathrm{s}}$ is the dimension of the single-particle basis. The complex numbers $g_\alpha$ and $U_{i,n}$ are determined by minimizing the expectation values of the Hamiltonian with quasi-Newtonian methods (*cf.* Refs. [28, 35] and references in there). Clearly the larger the number of Slater determinants $N_{\mathrm{w}}$ the more $|\psi\rangle$ will approach the exact yrast eigenstate. The ansatz of Eq. (1) is valid for yrast eigenstates, for excited eigenstates having the same quantum numbers we must in addition add terms containing the lower eigenstates with the same quantum numbers and the linear combination must preserve orthogonality with the previously determined eigenstates (Ref. [23]).

The degree of accuracy of the ansatz of Eq. (1) for finite $N_{\mathrm{w}}$ has been recently analyzed in Ref. [36] in order to construct extrapolation techniques, using the phenomenological $fpd6$ realistic effective interaction. We have tested the accuracy and effectiveness of our quasi-Newtonian variational method for $^{56}$Ni. Using 15 angular momentum projected Slater determinants we obtained for the ground state energy $-203.157$ MeV, with 25 Slater determinants we obtained $-203.175$ MeV and using 35 Slater determinants $-203.182$ MeV. This is to be compared with the exact shell model value of $-203.198$ MeV quoted in Ref. [36], and with the Quantum Monte Carlo result (prior extrapolation) of $-203.161$ MeV which was obtained with 150 Slater determinants (Ref. [36]).

In practice, for *ab initio* no-core calculations, we avoid the use of the full angular momentum projector since experience shows that, in such cases, we need a rather large number of fully angular momentum and parity projected Slater determinants to obtain good approximations to the eigenstates and therefore, in order to reduce the computational cost, we proceed as follows.

We add to the Hamiltonian a term $\gamma(\hat{J}^2 - J(J+1))$, where $\hat{J}$ is the angular momentum operator and $J$ is the desired value and we use, instead of the full angular momentum projector only the projector to good projection onto the $z$-axis $J_z = J$, much in the same way it is done in standard shell model calculations. This device is very useful especially for odd and odd–odd mass nuclei. The wave functions obtained in this way are used to evaluate observables with the full three-dimensional angular momentum projector. Experience shows that few hundreds Slater determinants are relatively easy to obtain and the full re-projection of the wave function obtained this way is much less expensive than the use of the full projector from the beginning. However, if we desire excited states with the same exact quantum numbers, the use of the full projector seems necessary so far.

As discussed in the next section, for no-core calculations, we need several hundreds $J_z^{\pi}$ projected Slater determinants to reach a reasonable convergence to the energies, however the convergence to the excitation energies is much faster, provided wave functions with different $J_z^{\pi}$ undergo exactly the same sequence of computational steps. The number of Slater determinants necessary to achieve convergence increases with the number of major shells. Hence for 5 major shells calculations we only evaluate excitations energies.

The intrinsic Hamiltonian used in the calculations is obtained in the following way. First an harmonic oscillator potential is added to the $A$-particle Hamiltonian, the resulting Hamiltonian is $A$-dependent. The two-body interaction is obtained by renormalizing the two-particle $A$-dependent Hamiltonian with the Lee–Suzuki procedure, much in the same way it is done in the no-core shell model (*cf.* Ref. [9] for a detailed description). The two-particle interaction is restricted to some number of relative coordinate harmonic oscillator shells $N_{\mathrm{r}} + 1$. The two-body matrix elements of the intrinsic Hamiltonian for the $A$-particle system can then be constructed. Using the Talmi–Moshinski transformations brackets, the matrix elements of this intrinsic Hamiltonian are evaluated up to $N_{\mathrm{r}}/2+1$ major shells in the frame of the single-particle coordinates. This is the HMD-a version of the method (*cf.* Ref. [20] for more details). Usually, in order to prevent center of mass excitations in the evaluation of excited states a term proportional to the harmonic oscillator Hamiltonian for the center of mass $\beta(\hat{H}_{\mathrm{cm}} - 3/2\hbar\Omega)$ is added at the end.

The variational calculation is carried out progressively. That is, we start with a single Slater determinant and add trial Slater determinant one at a time and always optimize the last added Slater determinant. At specific numbers of Slater determinants we vary anew all Slater determinants one at a time. For example, when $N_w = 5$ all Slater determinants are varied anew, and after we reach, say, $N_w = 10, 15, 25, 35, 50$ we re-optimize all Slater determinants *etc.* The numbers $5, 10, 15, 25, 35, 70, 100, 150 \ldots$ are somewhat a free choice. By far this is the most expensive part of the calculation, especially if we consider the full angular momentum and parity projector, hence the choice to replace it with a partial projector and only after a sufficiently large number of Slater determinants has been constructed, we use the full projector to evaluate expectation values.

Both the method and the set of computer codes have been extensively tested.

## 3. Carbon isotopes

For all the cases discussed below the coefficient of the center of mass Hamiltonian is fixed to $\beta = 0.7$, the harmonic oscillator frequency is for most of the cases $\hbar\Omega = 14$ MeV. The coefficient $\gamma$ of the $\hat{J}^2 - J(J+1)$ term is set to 0 for the even–even isotopes to 2 MeV or 4 MeV for the odd-mass isotopes. In the following, the experimental values of the binding energies are taken from Ref. [37] and the excitation energies form Ref. [38]. For $^{17}$C and $^{19}$C the experimental data is taken from Ref. [39], for $^{18}$C from Ref. [40] and for $^{20}$C from Ref. [41]. In what follows we also discuss the variation of the number of nucleons in the single particle shells and define $\delta n(E_x, a, t) = n(E_x, a, t) - n(E_{gs}, a, t)$, where $E_x$ is any of the excited states, $E_{gs}$ is the ground state energy, $a$ is any of the single-particle shells and $t = n, p$ denotes the type of particles (neutrons or protons). Only the largest variations will be given, the ones that are omitted are too small compared with the others. This is a very simple way to classify the type of excitation, *e.g.* neutron excitation, proton excitation or both.

As previously mentioned, in some cases we have performed calculations also with 5 major shells. We find that the absolute binding energies are different from the ones obtained with 4 major shells, however the excitation energies are rather similar. This reflects the fact that energy differences converge much better than the energies. Also the value of $\hbar\Omega = 14$ MeV is close to the energy minimum as a function of $\hbar\Omega$, thereby decreasing the dependence of the energies on $\hbar\Omega$. A systematic calculation for several values of $\hbar\Omega$, for 4 and 5 major shells, for all these isotopes is too lengthy on personal computers. Unless explicitly stated we consider $\hbar\Omega = 14$ MeV and 4 major shells.

### 3.1. $^{10}C$

The experimental binding energy of $^{10}$C is 60.320 MeV. Using 250 Slater determinants, optimized as explained in the previous section with $J_z^\pi = 0^+$ and then re-projecting to $J^\pi = 0^+$, in order to evaluate the expectation values, we obtained a binding energy of 53.438 MeV. The behavior of the ground state energy as a function of the inverse of the number of Slater determinants, $N_{SD}$, is shown in Fig. 1. The behavior of the energies in Fig. 1 is typical if the number of Slater determinants is large enough. It is reasonable, due to the linear behavior of the energy as a function of $1/N_{SD}$ to extrapolate in order to estimate the uncertainty of the calculation. The extrapolated value for the ground-state energy is $-53.808$ MeV, hence our result has an uncertainty of 0.7%. We found this $1/N_{SD}$ behavior in most of the cases. Only in few cases the number of Slater determinants was not sufficiently large. We use anyway a linear extrapolation in order to have an estimate of the uncertainty of the calculations. These uncertainties should not be confused with the statistical uncertainties as in Monte Carlo calculations. They are simply an estimate of the possible decrease of the energies if we would increase the number of Slater determinants, that is, how far we are from the exact values.
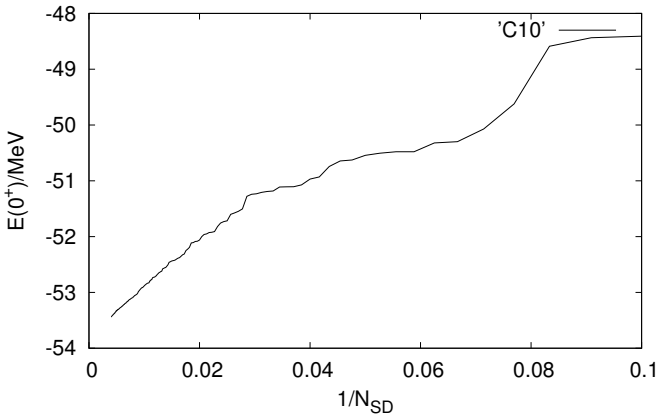


Fig. 1. Ground-state energy of $^{10}$C as a function of the inverse of the number of Slater determinants.

For the light carbon isotopes we find that theoretical binding energies are underestimated compared to the experimental values, while for the heavy carbon isotopes the theoretical values overestimate the corresponding experimental values. The experimental value of the excitation energy of the $2_1^+$ state is 3.354 MeV. Our calculation gives $E(2_1^+) = 3.764$ MeV. In Fig. 2 we show the behavior of the excitation energy as a function of the number of the Slater determinants. As it can be seen the value of the excitation
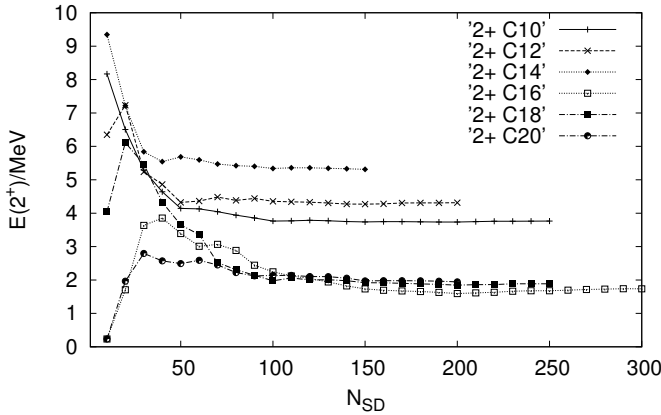
Fig. 2. Excitation energy of the $2_1^+$ state as a function of the number of Slater determinants for the even carbon isotopes.

energy is rather stable and the oscillation for large $N_{SD}$ have an amplitude of about 10 keV for this nucleus. The reason for this remarkable stability is that both calculations for the $0^+$ and the $2^+$ energy have almost the same error and of the same sign (these are variational calculations) and this error cancels out in the evaluation of the excitation energy. This is the reason why excitation energies converge much better than the absolute value of the energies. It should be stressed however that the relative uncertainty in the binding energy is small. It is interesting to look at the variation of the population of nucleons as we go from the ground-state to the excited state. We have $\delta n(2^+, 0p, n) = 0.08$ and $\delta n(2^+, 0p, p) = 0.07$. Although small, the number of neutrons (protons) excited above the $s$ and $p$ shells is nonzero: $\delta n(2^+, sd, n) = 0.17$, $\delta n(2^+, sd, p) = 0.21$ and $\delta n(2^+, fp, n) = 0.12$ and $\delta n(2^+, fp, p) = 0.15$.

For this nucleus, we performed also a calculation with $\hbar\Omega = 11$ MeV with 4 major shells. The binding energy becomes 51.372 MeV (compared with 53.438 MeV for $\hbar\Omega = 14$ MeV), however the excitation energy of the $2_1^+$ is $E(2_1^+) = 3.72$ MeV and it is well converged as a function of the number of Slater determinants, and it is almost the same as the one obtained for $\hbar\Omega = 14$ MeV, which is 3.764 MeV. For $\hbar\Omega = 17$ MeV, the excitation energy of the $2_1^+$ state obtained with 300 Slater determinants, becomes $E(2_1^+) = 3.73$ MeV. It is quite remarkable that although the energies have a non negligible $\hbar\Omega$ dependence, the excitation energies are nearly constant.

Using $\hbar\Omega = 14$ MeV we have also performed a calculation with 5 major shells. However, we used only 200 Slater determinants, and obtained $E(2_1^+) = 3.67$ MeV. The calculation is not entirely converged since the excitation energy has a small increase with the number of Slater determinants

(about 70 KeV in the last 30 Slater determinants), but it is consistent with and it approaches the values obtained with 4 major shells. This shows that working with 4 major shells and $\hbar\Omega = 14$ MeV, gives reliable results for the excitation energies for this nucleus.

At this point a few comments are in order about the convergence of our method. The HMD method is applicable regardless of the dimensionality of the Hilbert space, however we do not know yet how many Slater determinants we have to optimize in order to obtain the energies within, say 1% accuracy. We do know however that larger Hilbert spaces require a larger number of Slater determinants. Using 4 major shells, we need a few hundreds Slater determinants (perhaps even 500), for calculations utilizing 5 major shells this number is higher, hence it is not so surprising that the excitation energy for the $2_1^+$ state in the case of 5 major shells is not entirely converged with 200 Slater determinants. Presumably, the optimal way to calculate binding energies is to evaluate differences of binding energies and to perform an accurate binding energy calculation on just one isotope. An other possibility is to explore, in the context of *ab initio* calculations, the extrapolation method of Ref. [36].

### 3.2. $^{11}C$

The experimental value of the binding energy of $^{11}$C is 73.44 MeV and the ground state has $J^\pi = 3/2^-$, which is reproduced by our calculation. The theoretical value is 67.842 MeV. As before for large $N_{\mathrm{SD}}$ the energy is linear as a function of $1/N_{\mathrm{SD}}$ and the extrapolated value is 68.546 MeV giving a theoretical uncertainty of 1%. The energy of the first excited state $(1/2^-)$ is not well reproduced. The experimental value is 2 MeV, while our calculation gives 0.58 MeV. The first $5/2^-$ state has an experimental excitation energy of 4.32 MeV, our calculation gives 3.38 MeV. In Fig. 3 we show the behavior of the excitation energies as a function of the number of Slater determinants. The number of neutrons (protons) for the ground-state in the $s$, $p$, $sd$ and $fp$ shells are 1.81(1.83), 2.79(3.75), 0.21(0.22), 0.19(0.2), respectively. Moreover, for the $1/2^-$ state

$$\delta n(1/2^-, 0p3/2, n) = -0.19, \qquad \delta n(1/2^-, 0p1/2, n) = 0.19,$$
$$\delta n(1/2^-, 0p3/2, p) = -0.25, \qquad \delta n(1/2^-, 0p1/2, p) = 0.24.$$

The $5/2^-$ state is primarily a neutron excitation. In fact

$$\delta n(5/2^-, 0p3/2, n) = -0.38, \qquad \delta n(5/2^-, 0p1/2, n) = 0.38,$$
$$\delta n(5/2^-, 0p3/2, p) = -0.1, \qquad \delta n(5/2^-, 0p1/2, p) = 0.09.$$

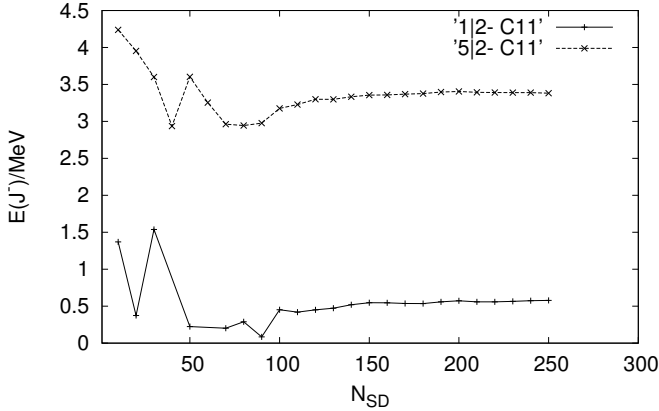Fig. 3. Excitation energy of the $1/2^-$ and $5/2^-$ states as a function of the number of Slater determinants for $^{11}C$.

## 3.3. $^{12}C$

$^{12}C$ has been extensively investigated, both experimentally and theoretically because of its astrophysical importance. As in the no-core shell model calculations the $0_2^+$ state (the Hoyle state), is missing at low energy. A small number of harmonic oscillator major shells is not sufficient to reproduce the position of this state. The experimental binding energy is 92.16 MeV, the calculated value with 200 Slater determinants is 90.154 MeV and the extrapolated value is 90.773 MeV. We performed another calculation using 400 Slater determinants and obtained 90.503 MeV and a corresponding extrapolated value of 90.940 MeV. In this case the $1/N_{SD}$ behavior seen in the previous cases is not entirely correct. This example shows that the extrapolated values give simply an uncertainty of the calculated ones. Also in this case the uncertainty is about 1%. The calculated excitation energy of the $2_1^+$ state is 4.31 MeV to be compared with the experimental value of 4.44 MeV. The behavior of the excitation energy as a function of the number of Slater determinants is shown in Fig. 2. The occupation numbers for the ground state are nearly equal for neutrons and protons, and a small number of neutrons and protons is moved from the $0p3/2$ to the $0p1/2$ shell ($< 0.1$) for the $2^+$ state.

## 3.4. $^{13}C$

Odd-mass isotopes allow to study whether the single-particle properties of the Hamiltonian are correct. The experimental binding energy of $^{13}C$ is 97.11 MeV and the ground-state has $J^\pi = 1/2^-$. Some low-lying yrast levels of negative parity are (in MeV) $E(3/2^-) = 3.68$, $E(5/2^-) = 7.55$. Our calcu-

lation reproduces the correct $J^\pi = 1/2^-$ of the ground-state with a binding energy of 97.58 MeV (with 250 Slater determinants and an uncertainty of 0.5%). For the above negative parity levels we obtained $E(3/2^-) = 2.6$ MeV and $E(5/2^-) = 5.89$ MeV (cf. Fig. 4). Regarding the nature of these states, we have

$$\delta n(3/2^-, 0p3/2, n) = -0.34, \qquad \delta n(3/2^-, 0p1/2, n) = 0.35,$$
$$\delta n(3/2^-, 0p3/2, p) = -0.33, \qquad \delta n(3/2^-, 0p1/2, p) = 0.33,$$

and for the $5/2^-$ state

$$\delta n(5/2^-, 0p3/2, n) = 0.14, \qquad \delta n(5/2^-, 0p1/2, n) = -0.16,$$
$$\delta n(5/2^-, 0p3/2, p) = -0.46, \qquad \delta n(5/2^-, 0p1/2, p) = 0.47.$$

These variations show that the $5/2^-$ is primarily a proton excitation.
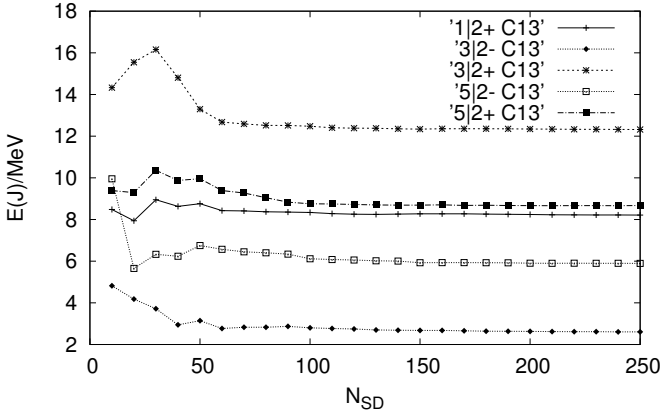


Fig. 4. Excitation energies of the selected states as a function of the number of Slater determinants for $^{13}$C.

The positive parity levels involve the $sd$ shell. The experimental locations in MeV are (we consider only few yrast levels) $E(1/2^+) = 3.09$, $E(5/2^+) = 3.85$ and $E(3/2^+) = 7.69$. The corresponding theoretical values are $E(1/2^+) = 8.2$, $E(5/2^+) = 8.67$ and $E(3/2^+) = 12.32$, nearly 5 MeV too high. The variations of the occupation numbers reveal the nature of these levels. We have

$$\delta n(1/2^+, 0p3/2, n) = -0.53,$$
$$\delta n(1/2^+, 0p1/2, n) = -0.35,$$
$$\delta n(1/2^+, 1s1/2, n) = 0.83,$$
$$\delta n(1/2^+, 0p3/2, p) = -0.25,$$
$$\delta n(1/2^+, 0p1/2, p) = 0.30.$$

The neutron $1s1/2$ orbital contains one extra neutron. All others $\delta n$ are small. For the $5/2^+$ state we have

$$
\begin{aligned}
\delta n(5/2^+, 0p3/2, n) &= -0.53\,, \\
\delta n(5/2^+, 0p1/2, n) &= -0.34\,, \\
\delta n(5/2^+, 0d5/2, n) &= 0.94\,, \\
\delta n(5/2^+, 0p3/2, p) &= -0.29\,, \\
\delta n(5/2^+, 0p1/2, p) &= 0.34\,.
\end{aligned}
$$

Almost one extra neutron in the $0d5/2$ orbital. For the $3/2^+$ state we have

$$
\begin{aligned}
\delta n(3/2^+, 0p3/2, n) &= -0.59\,, \\
\delta n(3/2^+, 0p1/2, n) &= -0.28\,, \\
\delta n(3/2^+, 0d3/2, n) &= 0.78\,, \\
\delta n(3/2^+, 0p3/2, p) &= -0.34\,, \\
\delta n(3/2^+, 0p1/2, p) &= 0.38\,.
\end{aligned}
$$

Almost one extra neutron in the $0d3/2$ orbital. In all cases there is a strong proton excitation. For this nucleus different value of $\hbar\Omega$ were not considered. The rather large excitation energy across major shells remains to be understood, that is, whether it is an artifact of the restriction to 4 major shells, or it is a feature of this $NN$ interaction. Eventually, this nucleus will be studied in the future in a more detailed way (*i.e.* a larger number of major shells and several values of $\hbar\Omega$).

### 3.5.  $^{14}C$

The experimental binding energy of this nucleus is 105.284 MeV and the excitation energy of the $2_1^+$ state is 7.01 MeV. The first excited state is a $1^-$ state at 6.09 MeV. This high excitation energy is considered as a motivation for model assumptions that take $^{14}$C as an inert core. We considered 150 Slater determinants. Our result for the binding energy is 109.976 with an uncertainty of 0.37%. As in the previous cases, the energy shows a $1/N_{\text{SD}}$ behavior for large $N_{\text{SD}}$. Our values for the excitation energies are $E(2_1^+) = 5.31$ MeV and $E(1^-) = 12.3$ MeV. As expected the $2^+$ state is a proton excitation and $\delta n(2^+, 0p3/2, p) = -0.68$ and $\delta n(2^+, 0p1/2, p) = 0.69$. The number of neutrons in the $0s$ and $0p$ shells is 7.3 indicating that the closure of the neutron shell is partially broken. One can see this more explicitely by comparing the final ground-state results with the ones obtained with a Hartree–Fock calculation using the full angular momentum projector. The HF binding energy is 106.33 MeV, close to the HMD value. However, the proton occupation numbers for the $p$ shell are different and, to a less extent,

also the neutron occupation numbers. The calculated $1^-$ state is mostly a neutron excitation, in fact

$$\delta n(1^-, 0p3/2, n) = -0.17,$$
$$\delta n(1^-, 0p1/2, n) = -0.67,$$
$$\delta n(1^-, 1s1/2, n) = 0.82,$$
$$\delta n(1^-, 0p3/2, p) = -0.21,$$
$$\delta n(1^-, 0p1/2, p) = -0.25.$$

Both the structure of this state and the high energy of the $1^-$ state again indicate that the distance between the $p$ and $sd$ major shells is too large.

For this nucleus we performed also a calculation of the excitation energy of the $2_1^+$ state using $\hbar\Omega = 11$ MeV and 200 Slater determinants. We obtained $E(2_1^+) = 4.36$ MeV. Using $\hbar\Omega = 17$ MeV with 200 Slater determinants we obtained $E(2_1^+) = 5.6$ MeV (we did not in this case reevaluate the excitation energy with the full angular momentum projector). These results show a dependence of $E(2_1^+)$ on $\hbar\Omega$. We therefore performed for this nucleus a calculation using 5 major shells. Again no reprojection was performed at the end of the calculation for this case. For $\hbar\Omega = 11$ MeV, 14 MeV, 17 MeV we obtained $E(2_1^+) = 4.23$ MeV, 4.8 MeV, 4.7 MeV, respectively. The uncertainty of the calculation is about 0.1 MeV. There is still a residual $\hbar\Omega$ dependence of the excitation energy, but it is smaller than the one obtained with 4 major shells.

### 3.6.  $^{15}C$

The experimental binding energy of $^{15}$C is 106.5 MeV and the ground state has $J^\pi = 1/2^+$. The first excited state has $E(5/2^+) = 0.74$ MeV and the first $3/2^+$ state is at 4.78 MeV. The first few negative parity levels are $E(1/2^-) = 3.10$ MeV, $E(5/2^-) = 4.22$ MeV and $E(3/2^-) = 4.66$ MeV. Our results are the following. The binding energy obtained with 250 Slater determinants is 110.586 MeV with an uncertainty of 0.46%. The ground-state spin and parity are properly reproduced. Heavy carbon isotopes overbind compared to the experimental data while the light ones underbind. Our results for the yrast positive parity levels are: $E(5/2^+) = 0.79$ MeV and $E(3/2^+) = 5.43$ MeV (*cf.* Fig. 5). If we compare the occupation numbers of the $1/2^+$ state of $^{15}$C with the occupation numbers of the ground-state of $^{14}$C we find that mostly they differ because of the population of the $1s1/2$ neutron shell. The difference in the number of neutrons for this shell is 0.88. The remaining 0.12 neutrons are accounted for small difference in the population of the other neutron shells. The largest differences in the occupation
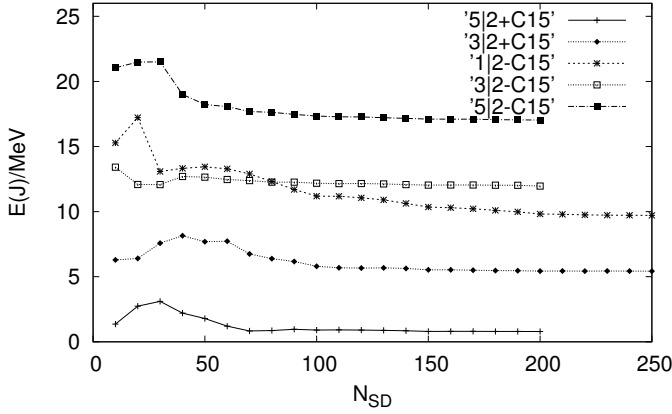
Fig. 5. Excitation energies of the selected states as a function of the number of Slater determinants for $^{15}$C.

numbers of the $5/2^+$ state and the $1/2^+$ state are the following

$$\delta n(5/2^+, 0d5/2, n) = 0.91, \qquad \delta n(1/2^+, 1s1/2, n) = -0.88,$$
$$\delta n(5/2^+, 0p3/2, p) = -0.13, \qquad \delta n(1/2^+, 0p1/2, p) = 0.13.$$

That is, the $5/2^+$ state is predominantly, but not entirely a neutron excitation. The $3/2^+$ state is not a neutron excitation built on the ground state. In fact the dominant differences in the occupation numbers are

$$\delta n(3/2^+, 0d3/2, n) = 0.14, \qquad \delta n(1/2^+, 1s1/2, n) = -0.12,$$
$$\delta n(3/2^+, 0p3/2, p) = -0.56, \qquad \delta n(1/2^+, 0p1/2, p) = 0.58.$$

Therefore, this state is predominantly a proton excitation. The first negative parity yrast levels have high excitation energy compared with the corresponding experimental values. We obtained $E(1/2^-) = 9.7$ MeV $E(3/2^-) = 11.97$ MeV (this state was obtained with 200 Slater determinants and is not fully converged). The calculated $5/2^-$ is so high in energy that we cannot rule out a center of mass excitation. The variations of the occupation numbers compared with the ground state are

$$\delta n(1/2^-, 0p3/2, n) = -0.16, \qquad \delta n(1/2^-, 0p1/2, n) = -0.7,$$
$$\delta n(1/2^-, 0d5/2, n) = 1.02, \qquad \delta n(1/2^-, 1s1/2, n) = -0.14,$$
$$\delta n(1/2^-, 0p3/2, p) = -0.27, \qquad \delta n(1/2^-, 0p1/2, p) = 0.33,$$
$$\delta n(3/2^-, 1s1/2, n) = -0.84, \qquad \delta n(3/2^-, 1p3/2, n) = 0.86.$$

Therefore, the $3/2^-$ state is a neutron excitation from the $sd$ shell to the $fp$ shell, while the $1/2^-$ is mostly an excitation from the $p$ shell to the $sd$ shell.

### 3.7. $^{16}C$, $^{18}C$, $^{20}C$

The experimental binding energy of $^{16}$C is 110.75 MeV and the first excited state is $E(2^+) = 1.766$ MeV. For this nucleus we used 300 Slater determinants and obtained a binding energy of 114.707 MeV with a 0.6% uncertainty. The theoretical $2^+$ has an excitation energy of 1.74 MeV, in good agreement with the experimental value. This state is predominantly a neutron excitation since

$$\delta n(2^+, 0d5/2, n) = 0.12, \qquad \delta n(2^+, 1s1/2, n) = -0.12.$$

The $fp$ shell is appreciably populated by 0.43 neutrons and 0.33 protons. It seems that intrashell excitations are overall in agreement with the experimental values (*cf.* the discussion of the other isotopes) but intershell excitations are too high compared with the experimental data.

The experimental binding energy of $^{18}$C is 115.67 MeV and $E(2^+) = 1.59$ MeV. With 250 Slater determinants we obtained a binding energy of 119.73 MeV and $E(2^+) = 1.89$ MeV. The $2^+$ state is predominantly a neutron excitation with a 0.12 increase in the population of the $0d5/2$ orbital at the expenses of the $0d3/2$ and $1s1/2$. Also here we have 0.44 neutrons and 0.3 protons in the $fp$ shell.

The experimental binding energy of $^{20}$C is 119.17 MeV and $E(2^+) = 1.59$ MeV. With 200 Slater determinants we obtained a binding energy of 124.43 MeV and $E(2^+) = 1.94$ MeV. The $2^+$ state is mostly a neutron excitation with a 0.11 decrease in the population of the $1s1/2$ orbital in favor of the $0d3/2$ and $0d5/2/2$. The only appreciable change in the number of proton is a 0.03 decrease in the $0p3/2$ population in favor of the $0p1/2$ orbit. Also here we have 0.46 neutrons and 0.29 protons in the $fp$ shell. We repeated this calculation using 400 Slater determinants in order to see whether $^{22}$C is more bound than $^{20}$C. Absolute values for the energies have a slower convergence with the number of Slater determinants than excitation energies, and 400 Slater determinants are not sufficient to determine unambiguously whether $^{22}$C is bound in this approach. We obtained $E_{gs}(^{22}C) - E_{gs}(^{20}C) = 0.2$ MeV and this energy difference is slowly decreasing with the number of Slater determinants. The model space used in this work can hardly properly describe halo nuclei. The isotope $^{21}$C is unbound by few MeVs.

### 3.8. $^{17}C$, $^{19}C$

The experimental binding energy for $^{17}$C is 111.48 MeV. The ground state has $J^\pi = 3/2^+$ and the known excited states have $E(1/2^+) = 0.21$ MeV and $E(5/2^+) = 0.331$ MeV. For this nucleus we considered only 150 Slater

determinants and therefore the calculated binding energy is not well determined (we did not see in this case a linear behavior as a function of $1/N_{SD}$. The calculated binding energy is 114.48 MeV. More importantly the ground-state has $J^\pi = 1/2^+$ in disagreement with the experimental value. Although less accurate than the excitation energies in the previous cases, we have $E(3/2^+) = 0.4$ MeV and $E(5/2^+) = 1.9$ MeV. The experimental binding energy for $^{19}$C is 115.8 MeV and the ground-state has $J^\pi = 1/2^+$, the first excited state has $E(3/2^+) = 0.196$ MeV and the second excited state has $E(5/2^+) = 0.269$ MeV. The calculated binding energy is 120.05 MeV with an estimated uncertainty of 0.4%. The ground-state has $J^\pi = 3/2^+$ in disagreement with the experimental value.

### 3.9. Separation energies

Although we have seen, in this model space, a systematic underbinding for light isotopes and overbinding for the heavy ones, it is interesting to extract the neutron separation energies and to compare them with the experimental data. This is done in Fig. 6. The overall trend is rather well
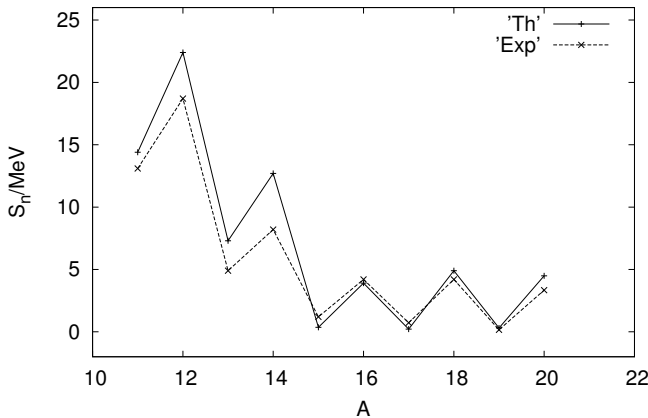


Fig. 6. Neutron separation energies for carbon isotopes.

reproduced, especially the even–odd effect. In all these calculations the binding energies are not fully converged, that is, we need a larger number of Slater determinants. However, this does not represent a problem as previously mentioned, since these calculations are variational. In other words, the theoretical errors have all the same sign and such errors tend to cancel out in the evaluation of the separation energies. This seems to be especially true for the evaluation of the excitation energies. As a final point, let us mention that the sizes of the Hilbert spaces with 4 major shells, range from $3 \times 10^{10}$ in the case of $^{10}$C to about $10^{16}$ in the case of $^{22}$C.

## 4. Summary

In this work we have studied carbon isotopes in a fully microscopic way using the chiral N3LO interaction properly renormalized to 4 (in some cases 5) major shells. In this treatment there are no adjustable parameters. We have evaluated binding energies, separation energies and few low energies levels. There seems to a systematic discrepancy with the experimental data whenever energy levels involve cross-shell excitation. Moreover, although by a small amount, $^{22}$C is not bound. This is not very surprising since the model space is not well suited to describe loosely bound systems. The first $2^+$ state of heavy even isotopes are dominated by neutron excitation and for light odd isotopes the proper spin of the ground state is reproduced.

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