Many-body calculations with deuteron based single-particle bases and their associated natural orbits

G Puddu

Dipartimento di Fisica dell’Università di Milano, Via Celoria 16, I-20133 Milano, Italy

E-mail: giovanni.puddu@mi.infn.it

Received 20 December 2017, revised 21 March 2018
Accepted for publication 5 April 2018
Published 25 April 2018

Abstract

We use the recently introduced single-particle states obtained from localized deuteron wave-functions as a basis for nuclear many-body calculations. We show that energies can be substantially lowered if the natural orbits (NOs) obtained from this basis are used. We use this modified basis for $^{10}$B, $^{16}$O and $^{24}$Mg employing the bare NNLO$_{eq}$ nucleon–nucleon interaction. The lowering of the energies increases with the mass. Although in principle NOs require a full scale preliminary many-body calculation, we found that an approximate preliminary many-body calculation, with a marginal increase in the computational cost, is sufficient. The use of natural orbits based on an harmonic oscillator basis leads to a much smaller lowering of the energies for a comparable computational cost.

Keywords: nuclear many-body problems, $ab$ initio methods, single-particle bases

1. Introduction

In $ab$ initio nuclear structure methods, the most formidable problem is the evaluation of properties of nuclei starting from the nucleon–nucleon interaction (even more challenging if the NNN interaction is included). One of the most fundamental approaches is the no core shell model (NCSM) [1–4], whereby the nuclear Hamiltonian is diagonalized using the Lanczos method by constructing a basis up to $N_{\text{max}}$ many-body excitations above the lowest configuration in an harmonic oscillator (h.o.) basis. This approach has been applied to light nuclei due to the explosive increase of the size of the Hilbert space with the number of particles. Other approaches like the coupled-cluster approach [5–8] scale polynomially with the size of the single-particle space and have been used also for medium-mass nuclei. The similarity renormalization group (SRG) [9–13] and especially its in medium extensions (IM-SRG) have been shown to be particularly promising for medium-mass nuclei for constructing valence space effective Hamiltonians as input to traditional shell model diagonalization techniques, hence leading to low-lying spectra [14–19].

Most of these approaches use as a single-particle basis h.o. orbits since they allow an exact separation between intrinsic and center of mass motion. It has been recognized that for weakly bound systems the asymptotic behavior at large distances of the h.o. single-particle wave-functions is not appropriate (e.g. halo nuclei). For weakly bound systems the convergence of observables, sensitive to the tail of the single-particle wave-functions, is far from optimal even using a large single-particle basis [20].

Recently in order to overcome this limitation of the h.o. basis, the use of other bases have been explored. Most importantly the natural orbits (NOs) have been implemented and a much more satisfactory convergence has been obtained in the study of the halo nucleus $^4$He [21]. NOs [22–26] can be defined as follows. Once a spherical single-particle basis of quantum numbers $nljm$ has been selected one can perform a preliminary many-body calculation to determine a good approximation to the exact ground-state wave-function $|\psi\rangle$. One can construct the one-body density matrix $\rho_{n,n'} = \langle \psi | \sum_m a_{n'ljm}^\dagger a_{nljm} | \psi \rangle$ for each partial wave $lj$, $a^\dagger/a$ being the creation/annihilation operators. We then diagonalize the matrix $\rho$. The eigenvectors obtained in this way will define a new single-particle basis $\nu$, $l$, $j$ called NOs. These orbitals can be used to redo the many-body calculation. In [21] this method showed improved convergence properties. Very recently NO basis have been used also for open systems [27].
Recently we have introduced a basis which has the desired asymptotic behavior at large distances and gives better binding energies [28]. This basis called localized deutereron basis (LDB), has been obtained by diagonalization of the S-wave of the deutereron wave function multiplied by a localizing center of mass wave-function. In this work we use the LDB to construct the corresponding NO basis. We are, in this work, primarily interested in increasing binding energies of nuclei thereby decreasing the need to work with large single-particle basis, which are the core of the computational cost of many-body calculations. As in [21] we do need a preliminary many-body calculation, however the increase in the computational cost is minor.

As a many-body technique we use the hybrid-multi-determinant (HMD) method [29], which expands nuclear eigenstates as a linear combination of Slater determinants of the most generic type, symmetries being restored with projectors to good many-body quantum numbers. Quasi-Newtonian optimization methods [30, 31] are then used to determine the many-body wave function. The projectors we commonly use are projectors to good z-component of the angular momentum and parity ($J_z$). We can use projectors to good angular momentum, but we decided to keep the computational cost reasonably low. Broadly speaking, our method consists in the following steps. First we construct the Hamiltonian for $A$ nucleons in the LDB basis, and run a preliminary many-body calculation. We use a large number of major shells and a small number of Slater determinants, typically $15 \div 25$, (note that a full scale many-body calculation needs the construction of at least few hundreds $J_z$ projected Slater determinants). We then construct the approximate density matrix and diagonalize it in order to obtain the new basis. Next we rewrite the Hamiltonian in this basis (which we call LDBNO) and redo the many-body calculations.

We find a sizable increase in the binding energies. We considered in this work three nuclei, $^{10}$B, $^{16}$O and $^{24}$Mg. Remarkably, the gain in binding energies compared to the h.o. basis, increases with the mass, at least in the cases we have considered. The NN interaction we have used is the ‘bare’ NNLO$_{\text{opt}}$ interaction [32]. The outline of this work is as follows. In section 2 we describe the method, in section 3 we discuss the numerical results. Particular emphasis is placed to the cases of small number of major shells, since for large single-particle spaces we expect all bases to give essentially the same results. In section 4 we give some concluding remarks.

2. Computational method and choice of the single-particle basis

2.1. The LDB

Consider the Hamiltonian in the center of mass system for $A$ particle interacting with a potential $V_p$,

$$ H = \sum_{i=1}^{A} \frac{\mathbf{p}_i^2}{2m} + V_p, $$

where $\mathbf{p}_i$ is the momentum of particle $i$. In [28] we took $A = 2$, although in principle we could consider $A$ as a variational parameter in order to construct an efficient single-particle basis. Let us diagonalize $H_{12}$ and discard the D-wave of the ground-state wave-function. The S-wave depends on the relative momentum of the neutron and proton and it is not localized in coordinate space. We achieve localization by multiplying this two-particle wave function by a center of mass wave-function in an S state. The full wave function depends on the momenta $\mathbf{p}_1, \mathbf{p}_2$ through $|\mathbf{p}_1 - \mathbf{p}_2|$ and $|\mathbf{p}_1 + \mathbf{p}_2|$. The cosine dependence can be expanded in terms of Legendre polynomials which can then be expanded in terms of spherical harmonics of the angular coordinates of particle 1 and 2. The coefficients of this expansion depend on the momenta $p_1$ and $p_2$. These coefficients (for each single-particle angular momentum value $l$) can be diagonalized on a mesh. Thus the full two-particle wave-function is written as a linear combination of products of spherical single-particle wave-functions $Q_{n_1}(\mathbf{p}_1) Y_{l_1}^{m_1}(\mathbf{p})$ for particle 1 and 2. The quantum number $n$ labels the eigenvalues properly reordered so that the largest absolute values of the coefficients in this linear combination correspond to the smallest values of $n$. The aforementioned center of mass wave function must be such that in coordinate space the single-particle radial part decays as $\exp(-\alpha r)$, $\alpha$ being a free positive parameter. Its role is to ‘squeeze’ or extend the size of the system. The $n, l$ space orbits are augmented with the spin degrees of freedom giving the single-particle basis $n, l, j, m$. A full discussion of the properties of this single-particle basis, as well as its nodal structure, is given in [28].

The evaluation of the matrix elements of the interaction in this basis needs some discussion. In principle we could use the vector brackets formalism of [33–36] in order to evaluate the matrix elements $\langle a, b, J|V|c, d, J'\rangle$ for the $nn$, $np$, $pp$ cases, for the single-particle states $a = (n_a, l_a, j_a)$, $b = (n_b, l_b, j_b)$, $c = (n_c, l_c, j_c)$, $d = (n_d, l_d, j_d)$, $J = j_a + j_b$. This is the optimal method for strong interactions at large relative momentum transfer. In this work we use the NNLO$_{\text{opt}}$ interaction which is sufficiently soft so that we can expand the above matrix elements in terms of the corresponding ones in an h.o. basis [37]. Therefore, we first evaluate the matrix elements $\langle a', b', J|V|c', d', J\rangle$ in a sufficiently large h.o. basis, then we evaluate the sums

$$ \langle a, b, J|V|c, d, J\rangle = \sum_{a' b' c' d'} \langle a|a'\rangle \langle b|b'\rangle \langle c'|c'\rangle \langle d'|d'\rangle \langle a', b', J|V|c', d', J\rangle $$

and the overlaps are given by

$$ \langle a'|a\rangle = \delta_{a',a} \int dpQ_{n_a}(p)P_{n_a}(p) $$

$P_{n_a}(p)$ being the h.o. radial wave functions. We considered the h.o. matrix elements in a basis satisfying $2n_a' + l_a' + 2n_b' + l_b' \leq N_{2\text{max}}$ for $N_{2\text{max}} = 26$. Softer interactions can presumably be dealt with smaller values of $N_{2\text{max}}$. We found that binding energies increase with increasing values of $N_{2\text{max}}$. This is the reason why we had to consider 27 major h.o. shells. Also note that if $N_{2\text{max}}$ is sufficiently large the matrix elements of equation (1) become independent of frequency of the h.o. basis because of completeness.
Moreover the frequency which appears in the overlaps of equation (2) has no relation with the frequency of the Hamiltonian of the center of mass (see below). The single-particle space spanned by the LDB, to be used in many-body calculations, satisfies the restriction

\[ 2n_\alpha + l_\alpha \leq \epsilon_{\text{max}}. \tag{3} \]

The comparison between many-body calculations, using the LDB and the ones obtained with the h.o. representation is meaningful if the h.o. quantum numbers satisfy the same restriction of equation (3), i.e.

\[ 2n_\alpha' + l_\alpha' \leq \epsilon_{\text{max}}. \tag{4} \]

As before \( n_\alpha', l_\alpha' \) are the h.o. quantum numbers. Note that the large h.o. space is used only to evaluate the matrix elements of the interaction in the LDB basis. The expansion method of equations (1), (2) is widely used, however for ‘harder’ interactions the vector brackets formalism is presumably the most appropriate one. Note however that the necessary number of h.o. shells to be used in the expansion of equations (1) and (2) has some relation to the number of h.o. necessary to properly take into account the ‘hardness’ of the NN interaction. For interactions ‘harder’ than NNLO-opt a much larger value of \( N_{2\text{max}} \) is necessary. The intrinsic kinetic energy matrix elements are evaluated directly with the LDB orbits. We always add to the Hamiltonian the center of mass term \( \beta(H_{\text{cm}} - \beta \omega / 2) \), where \( H_{\text{cm}} \) is the h.o. Hamiltonian for the center of mass, in order to suppress center of mass excitations. Its frequency, \( \omega \), is not necessarily related to the frequency used in the aforementioned expansion. Before summarizing the HMD variational method, let us assume that we have constructed the full Hamiltonian both in the LDB and h.o. representation for a specified value of \( \epsilon_{\text{max}} \). The h.o. frequency in the h.o. representation is selected so as to minimize the ground-state energy obtained with few Slater determinants. Afterwards we keep the same value of \( \omega \) for all values of \( \epsilon_{\text{max}} \). In principle we could re-determine the optimal value of \( \omega \) for every value of \( \epsilon_{\text{max}} \). Similarly the value of \( \alpha \) specifying the LDB is selected such that it minimizes the ground-state energy obtained with few Slater determinants for a specified value of \( \epsilon_{\text{max}} \).

The NOs corresponding to either the h.o. or to the LDB representation are constructed as follows. Let us select a sufficiently large value of \( (2n + l) = \epsilon_0 \). In the calculations discussed in the next section we took \( \epsilon_0 = 7 \) (that is, 8 major shells). Let us consider an approximate eigenstate \( \langle \psi \rangle \) obtained as a linear combination of \( N_D \) variationally determined Slater determinants (typically \( N_D = 15 \) at the most \( N_D = 25 \)) and let us evaluate the density matrix

\[ \rho_{n,m} = \langle \psi | \sum_m a_{n,m}^{\dagger} a_{n,m} | \psi \rangle \tag{5} \]

for all \( n, j \) quantum numbers. We actually use the sum of neutron and proton densities. We diagonalize \( \rho_{n,m} \) and obtain the eigenvectors \( \psi_{n,m} (l, j) \) where \( \nu \) labels the eigenvalues. For both the h.o. and the LDB representation we construct the new single-particle basis (the same for neutrons and protons)

\[ |\nu, l, j\rangle = \sum_{n=0}^{(\epsilon_0 - l)/2} v_{n,\nu}(l, j)|n, l, j\rangle. \tag{6} \]

The expansion of equation (6) is useful only if

Table 1. Expectation values of the energy for \(^{10}\text{B} \) for \( J^z = 1^+ \). All energies are in MeV’s. The harmonic oscillator calculation used \( \hbar \omega = 18 \), while the LDB value for \( \alpha = 2.7 \, \text{fm}^{-1} \) and \( \hbar \omega = 16 \). After each column the corresponding values of \( \langle \beta(H_{\text{cm}} - \beta \omega / 2) \rangle \) for \( \beta = 0.5 \) are given. Two different rows give the results for two different numbers of Slater determinants. Some values are omitted. The LDBNO values for \( \epsilon_{\text{max}} = 7 \) are essentially the same for LDB with \( \epsilon_{\text{max}} = 7 \). See the text for more explanations and discussions.

| \( \epsilon_{\text{max}} \) | \( N_D \) | \( \langle \epsilon(\text{ho}) \rangle \) | \( E(\text{CM}) \) | \( E(\text{LDB}) \) | \( E(\text{CM}) \) | \( E(\text{LDBNO}) \) | \( E(\text{CM}) \) |
|---|---|---|---|---|---|---|---|
| 4 | 150 | -40.35 | -43.63 | -46.25 |
| 4 | 200 | -41.33 | 0.23 | -44.49 | 0.40 | -47.11 | 0.35 |
| 5 | 150 | -45.05 | 0.25 | -46.93 | 0.38 | -49.15 | 0.33 |
| 5 | 200 | -47.99 | 0.38 | -49.81 | 0.35 | -50.03 | 0.33 |
| 6 | 150 | -47.46 | 0.25 | -48.53 | 0.35 | -49.81 | 0.32 |
| 6 | 200 | -49.57 | 0.35 | -50.66 | 0.32 |
| 7 | 150 | -49.21 | 0.26 | -49.63 | 0.34 |
| 7 | 200 | -50.54 | 0.34 |

Figure 1. Energy versus variance for \(^{10}\text{B} \) and \( J^z = 1^+ \) for several \( \epsilon_{\text{max}} \) values. A quadratic fit has also been obtained with the LDBNO orbits has also been included.
new bases of equation (6) are the NO corresponding to the h.o. or the LDB representation depending on the initial basis. We can now re-derive the matrix elements of the Hamiltonian in this new basis (both h.o and LDB) using the expansion method. We stress that we do not obtain any improvement in the binding energies if \( e_{\text{max}} = e_0 \). In the case of NNLOopt, we always use \( e_0 = 7 \) and, at the most \( e_{\text{max}} \leq 6 \). The advantage of using NO orbits is that we need to perform a partial many-body calculation with \( e_0 + 1 \) major shells with a small number of Slater determinants, hence with a small additional computational cost.

2.2. A brief recap of the variational method

We start with Hamiltonians of the form

\[
\hat{H} = \frac{1}{2} \sum_{i,j,k,l} H_{ijkl} a_i^\dagger a_j^\dagger a_l a_k,
\]

where \( i, j, k, l \) are the single-particle quantum numbers \((n_i, l_i, j_i, m_i)\), ... for both neutrons and protons and for a specified \( e_{\text{max}} \). The sum runs from 1 up to the total number of single-particle states \( N_i \). The HMD method [29] expands eigenstates as

\[
|\psi\rangle = \sum_{d=1}^{N_d} P(U_d),
\]

where \( P \) is a projector to good quantum numbers, \( |U_d\rangle \) is a generic Slater determinant for \( A \) particles written as

\[
|U_d\rangle = \tau_1 \tau_2 \ldots \tau_A |0\rangle,
\]

where \( |0\rangle \) is the vacuum and the generalized creation operators \( \tau_a, (a = 1, 2, \ldots, A) \) are of the type

\[
\tau_a = \sum_i U_{ia} a_i^\dagger.
\]

The complex numbers \( U_{ia} \) are determined using the quasi-Newtonian method of rank-3 described in detail in [31] in order to minimize the expectation value of the energy. In equation (8), \( N_d \) should be as large as possible. For a given \( e_{\text{max}} \) we start with a small number of Slater determinants and we progressively increase \( N_d \) to larger and larger values. Since the computational cost can be large for large \( N_d \) (especially for large \( e_{\text{max}} \)), we resort to the energy variance extrapolation method (EVE) which we briefly describe below. This method has been introduced in [38] and progressively improved in [39–43]. The basic idea is that if \( |\psi\rangle \) is sufficiently close to an exact eigenstate of eigenvalue \( E_0 \), then

\[
\langle \psi | \hat{H} | \psi \rangle = E_0 + a \langle \psi | \hat{H}^2 | \psi \rangle - \langle \psi | \hat{H} | \psi \rangle^2,
\]

where \( a \) is a constant. Hence we have to plot \( \langle \psi | \hat{H} | \psi \rangle \) versus the energy variance and extrapolate to 0 variance. The intercept with the energy axis will give the eigenvalue. If \( |\psi\rangle \) is not sufficiently close to an eigenstate, there are correction terms in equation (11). In practice we use the reordering technique developed in [44]. Briefly, this technique is as follows. Let us assume that we have collected \( N_D \) Slater determinants in a specified order. We can construct many-

---

**Figure 2.** Energy versus variance for \(^{10}\text{B}\) and \(J^e_i = 1^+ \) for several \( e_{\text{max}} \) values. A quadratic fit obtained with the LDB orbits has also been included.

**Figure 3.** Energy versus variance for \(^{10}\text{B}\) and \(J^e_i = 1^+ \) for several \( e_{\text{max}} \) values. A quadratic fit obtained with the h.o. orbits has also been included.
body states

$$|\psi_N\rangle = \sum_{d=1}^{N} c_d |U_d\rangle \quad (N = 1, 2, \ldots, N_D),$$

(12)

where the complex numbers $c_d$ are obtained by minimizing the energy. For each $N$ we can evaluate equation (11). However the order of the Slater determinants is arbitrary. The reordering technique consists in reordering the Slater determinants so that equation (11) applied to equation (12) gives an EVE plot as linear as possible. We have applied this

| $\epsilon_{\text{max}}$ | $N_D$ | $E(\text{ho})$ | $E_{\text{CM}}$ | $E(\text{LDB})$ | $E_{\text{CM}}$ | $E(\text{LDBNO})$ | $E_{\text{CM}}$ |
|-----------------------|-------|----------------|----------------|----------------|----------------|----------------|----------------|
| 4                     | 150   | -39.39         | -42.81         | -45.54         |                |                |                |
| 4                     | 200   | -40.07 0.24    | -43.43 0.33    | -46.24 0.26    |                |                |                |
| 5                     | 150   | -44/34 0.21    | -46.76         | -48.79         |                |                |                |
| 5                     | 200   | -47.46 0.28    | -49.66 0.24    |                |                |                |                |
| 6                     | 150   | -47.02 0.20    | -48.58         | -49.51         |                |                |                |
| 6                     | 200   | -49.31 0.23    | -50.30 0.22    |                |                |                |                |
| 7                     | 150   | -48.96 0.20    | -49.82         |                |                |                |                |
| 7                     | 200   | -50.36 0.21    |                |                |                |                |                |

Table 2. Expectation values of the energy for $^{10}$B for $J^P = 3^+$. All energies are in MeV’s. The harmonic oscillator calculation used $\hbar \omega = 18$, while the LDB value for $\alpha$ is 2.7 fm$^{-1}$ and $\hbar \omega = 16$. After each column the corresponding values of $\langle \beta (H_{\text{CM}} - 3\hbar \omega/2) \rangle$ are given. Two different rows give the results for two different numbers of Slater determinants. Some values are omitted. The LDBNO values for $\epsilon_{\text{max}} = 7$ are essentially the same for LDB with $\epsilon_{\text{max}} = 7$. See the text for more explanations and discussions.

| $\epsilon_{\text{max}}$ | $N_D$ | $E(\text{ho})$ | $E_{\text{CM}}$ | $E(\text{LDB})$ | $E_{\text{CM}}$ | $E(\text{LDBNO})$ | $E_{\text{CM}}$ |
|-----------------------|-------|----------------|----------------|----------------|----------------|----------------|----------------|
| 4                     | 150   | -97.88         | -101.89        | -112.82        |                |                |                |
| 4                     | 200   | -99.10 0.22    | -102.61 0.51   | -113.84 0.25   |                |                |                |
| 5                     | 150   | -105.65 0.27   | -112.17        | -118.00        |                |                |                |
| 5                     | 200   | -113.02 0.31   | -118.65 0.19   |                |                |                |                |
| 6                     | 150   | -108.44 0.26   | -116.75        | -118.97        |                |                |                |
| 6                     | 200   | -117.47 0.21   | -119.70 0.16   |                |                |                |                |
| 7                     | 150   | -110.57 0.27   | -119.20        |                |                |                |                |
| 7                     | 200   | -119.91 0.16   |                |                |                |                |                |

Table 3. Expectation values of the energy for $^{16}$O. All energies are in MeV’s. The harmonic oscillator calculation used $\hbar \omega = 24$, while the LDB value for $\alpha$ is 2.5 fm$^{-1}$ and $\hbar \omega = 20$. After each column the corresponding values of $\langle \beta (H_{\text{CM}} - 3\hbar \omega/2) \rangle$ are given.

Figure 4. Energy versus variance for $^{14}$O for several $\epsilon_{\text{max}}$ values. A quadratic fit has also been included obtained with the LDBNO orbits.

Figure 5. Energy versus variance for $^{16}$O for several $\epsilon_{\text{max}}$ values. A quadratic fit has also been included obtained with the LDB orbits.
In this section we discuss the calculations for the binding energies of $^{10}$B, $^{16}$O and $^{24}$Mg. The experimental data for the binding energies are from [45]. The ground-state spin of $^{10}$B has been a problem in ab initio calculations using chiral NN interactions, both the N3LO and NNLO opt. In [46] within the NCSM, using the N3LO interaction [47] the experimental spin ($3^+$) and the binding energy of 64.75 MeV, within a few tens of KeV’s, have been reproduced with the essential addition of the NNN interaction. In the case of the NNLO opt (used in all calculations of this work) the lowest $1^+$ and $3^+$ states are nearly degenerate [32] in the NCSM, however the obtained binding energy is too low. In table 1 we show the results of our calculation for $J_l^z = 1^+$ using the h.o., the LDB and the LDBNO representations. The LDBNO has been constructed from an approximate LDB calculation at $\epsilon_0 = 7$ and $N_D = 15$. Several comments are in order. First the LDB basis produced better energies than the h.o. representation. However for large $\epsilon_{\text{max}}$ the three representations give nearly the same results. This is not very surprising since for large single-particle spaces we expect on general grounds the results to be compatible with each other. The LDBNO representation for a given $\epsilon_{\text{max}}$ is almost equivalent to the LDB results with $\epsilon_{\text{max}} + 1$, except for $\epsilon_{\text{max}} = \epsilon_0$. We have to construct the LDBNO basis from a much larger LDB space, otherwise we get essentially the same results. All LDBNO bases discussed here have been obtained from an approximate LDB calculations at $\epsilon_0 = 7$. The most relevant comparison is with the smallest space. We stress that our goal is not to do a one-to-one comparison between the results obtained with the h.o. representation and the corresponding ones obtained with the LDB and their associated NO’s. Our goal is to obtain a single-particle basis that outperforms the h.o. and once this representation is identified we mostly work with this better representation. If we would redo all calculations with both bases, there would be no point in trying to construct an optimal one, since it would double the computational cost. This is the reason why some entries are missing in the tables. In table 1, notice that the gain in energy with the LDBNO compared to the h.o. is about 14%. Moreover note that the results obtained with $N_D = 200$ are about 1 MeV lower than the ones obtained with $N_D = 150$. This points out that a much larger number of Slater determinants is needed to reach satisfactory convergence. The $J_l^z = 1^+$ results obtained with the LDBNO basis has also been dealt with the reordered EVE method. In figures 1–3 we show the data obtained with the HMD method, the EVE extrapolations (linear and quadratic) for the LDBNO, the LDB and the h.o. bases respectively for the $1^+$ state of $^{10}$B.

As it can be seen from figure 1, the linear regime is reached especially for $\epsilon_{\text{max}} = 6$. Keeping in mind that the correction to the energy is sizable the extrapolated value for the $J_l^z = 1^+$ energy is $-60.1$ MeV, to be compared with the NCSM results of $-54.35$ MeV [32] obtained for $N_{\text{max}} = 10$. Of course we must keep in mind that the correction given by the EVE is quite large and that the presence of additional terms in equation (11) can modify the extrapolated value. That is, although in principle the EVE technique is conceptually very robust, we must be close to 0 variance. The uncertainty can be reduced using the full angular momentum projector. Note that for $\epsilon_{\text{max}} = 4$ there are some overtones in figure 1. Note that the clattering in the figure is only apparent. Consider for example figure 1 obtained for the $1^+$ state of $^{10}$B. Figure 1 consists of three ‘lines’. Each ‘line’ represents the calculations for a specified $\epsilon_{\text{max}}$. The lower the energies of the lines the larger $\epsilon_{\text{max}}$. The dots on each line represent the actual computations. The upper line is for $\epsilon_{\text{max}} = 4$ and the lower is for $\epsilon_{\text{max}} = 6$ or $\epsilon_{\text{max}} = 7$, depending on the case. Each data

3. Numerical results

In this section we discuss the calculations for the binding energies of $^{10}$B, $^{16}$O and $^{24}$Mg. The experimental data for the binding energies are from [45]. The ground-state spin of $^{10}$B has been a problem in ab initio calculations using chiral NN interactions, both the N3LO and NNLO opt. In [46] within the NCSM, using the N3LO interaction [47] the experimental spin ($3^+$) and the binding energy of 64.75 MeV, within a few tens of KeV’s, have been reproduced with the essential addition of the NNN interaction. In the case of the NNLO opt (used in all calculations of this work) the lowest $1^+$ and $3^+$ states are nearly degenerate [32] in the NCSM, however the obtained binding energy is too low. In table 1 we show the results of our calculation for $J_l^z = 1^+$ using the h.o., the LDB and the LDBNO representations. The LDBNO has been constructed from an approximate LDB calculation at $\epsilon_0 = 7$ and $N_D = 15$. Several comments are in order. First the LDB basis produced better energies than the h.o. representation. However for large $\epsilon_{\text{max}}$ the three representations give nearly the same results. This is not very surprising since for large single-particle spaces we expect on general grounds the results to be compatible with each other. The LDBNO representation for a given $\epsilon_{\text{max}}$ is almost equivalent to the LDB results with $\epsilon_{\text{max}} + 1$, except for $\epsilon_{\text{max}} = \epsilon_0$. We have to construct the LDBNO basis from a much larger LDB space, otherwise we get essentially the same results. All LDBNO bases discussed here have been obtained from an approximate LDB calculations at $\epsilon_0 = 7$. The most relevant comparison is with the smallest space. We stress that our goal is not to do a one-to-one comparison between the results obtained with the h.o. representation and the corresponding ones obtained with the LDB and their associated NO’s. Our goal is to obtain a single-particle basis that outperforms the h.o. and once this representation is identified we mostly work with this better representation. If we would redo all calculations with both bases, there would be no point in trying to construct an optimal one, since it would double the computational cost. This is the reason why some entries are missing in the tables. In table 1, notice that the gain in energy with the LDBNO compared to the h.o. is about 14%. Moreover note that the results obtained with $N_D = 200$ are about 1 MeV lower than the ones obtained with $N_D = 150$. This points out that a much larger number of Slater determinants is needed to reach satisfactory convergence. The $J_l^z = 1^+$ results obtained with the LDBNO basis has also been dealt with the reordered EVE method. In figures 1–3 we show the data obtained with the HMD method, the EVE extrapolations (linear and quadratic) for the LDBNO, the LDB and the h.o. bases respectively for the $1^+$ state of $^{10}$B.

As it can be seen from figure 1, the linear regime is reached especially for $\epsilon_{\text{max}} = 6$. Keeping in mind that the correction to the energy is sizable the extrapolated value for the $J_l^z = 1^+$ energy is $-60.1$ MeV, to be compared with the NCSM results of $-54.35$ MeV [32] obtained for $N_{\text{max}} = 10$. Of course we must keep in mind that the correction given by the EVE is quite large and that the presence of additional terms in equation (11) can modify the extrapolated value. That is, although in principle the EVE technique is conceptually very robust, we must be close to 0 variance. The uncertainty can be reduced using the full angular momentum projector. Note that for $\epsilon_{\text{max}} = 4$ there are some overtones in figure 1. Note that the clattering in the figure is only apparent. Consider for example figure 1 obtained for the $1^+$ state of $^{10}$B. Figure 1 consists of three ‘lines’. Each ‘line’ represents the calculations for a specified $\epsilon_{\text{max}}$. The lower the energies of the lines the larger $\epsilon_{\text{max}}$. The dots on each line represent the actual computations. The upper line is for $\epsilon_{\text{max}} = 4$ and the lower is for $\epsilon_{\text{max}} = 6$ or $\epsilon_{\text{max}} = 7$, depending on the case. Each data
Table 4. Expectation values of the energy for \(^{24}\text{Mg}\). All energies are in MeV’s. The harmonic oscillator calculation used \(\hbar \omega = 20\), while the LDB value for \(\alpha\) is \(2.9\text{ fm}^{-1}\) and \(\hbar \omega = 16\). After each column the corresponding values of \((3/2)(\text{CM} – \text{LDB}/2)\) are given. We included also a result for 5 natural orbits major shells built from the h.o. \(\epsilon_{\text{max}} = 7\) representation using the expansion method \((E(\text{h.o} – \text{no}))\).

| \(\epsilon_{\text{max}}\) | \(N_D\) | \(E(\text{ho})\) | \(E_{\text{CM}}\) | \(E(\text{ho} – \text{no})\) | \(E(\text{LDB})\) | \(E_{\text{CM}}\) | \(E(\text{LDBNO})\) | \(E_{\text{CM}}\) |
|-------------------|---------|----------------|----------------|------------------|----------------|----------------|----------------|----------------|
| 4                 | 150     | -121.58        | 0.26           | -128.06          | -136.76        | -146.84        | -145.58        | -146.84        |
| 4                 | 200     | -122.90        | 0.26           | -128.06          | -137.73        | 0.44           | 0.44           | 0.44           |
| 5                 | 150     | -149.26        | -156.58        | -150.35          | 0.47           | -157.63        | 0.53           |                |
| 5                 | 200     | -157.03        | 0.41           | -161.04          | 0.38           |                |                |                |
| 6                 | 150     | -150.35        | 0.47           | -157.63          | 0.53           |                |                |                |
| 7                 | 150     | -161.04        | 0.38           | -161.04          | 0.38           |                |                |                |

Figure 7. Energy versus variance for \(^{24}\text{Mg}\) for several \(\epsilon_{\text{max}}\) values. A quadratic fit has also been included obtained with the LDBNO orbits.

In table 2, we show the results for the \(^{3}\text{P}\) state of \(^{10}\text{B}\). For the \(J^\pi = 3^+\), the EVE plots do not show a linear behavior, in some cases not even monotonic. Presumably, the HMD calculations have to be carried out to better accuracy with a much larger number of Slater determinants.

In table 3 we show the results for \(^{16}\text{O}\). Note that binding obtained for \(\epsilon_{\text{max}} = 4\) is about 15% better than the one obtained with the h.o. basis. In figures 4–6 we show the EVE plots for \(^{16}\text{O}\) for the LDBNO, the LDB and the h.o. basis, respectively. Again we perform also a quadratic fit to have an idea about the uncertainties. Note for \(\epsilon_{\text{max}} = 7\) the extrapolated ground-state energies are consistent with each other for all bases. That is, the NNLO\(_{\text{opt}}\) interaction is rather soft. The extrapolated value for the ground state energy of \(^{16}\text{O}\) is about \(-137.6\text{ MeV}\). This value should be compared with the coupled-cluster value of about \(-131\text{ MeV}\) obtained with 15 major h.o. shells of \([32]\).

In table 4 we present the results for \(^{24}\text{Mg}\). In this case we did not perform all calculations with the h.o. basis. For Mg we constructed also a NO basis starting from the h.o. basis (under the heading \(E(\text{h.o} – \text{no})\)) for \(\epsilon_0 = 7\) and \(N_D = 15\) (as for the LDB). Note that the energy is higher than the one obtained with the LDB as shown in table 4.

Note that the increase in binding energy obtained with LDBNO is about 19% compared with the h.o. results. In figure 7 we show the LDBNO EVE plot. Some discrepancies between the linear and the quadratic fit can be seen. The extrapolation to 0 variance for the largest single-particle space, points out to overbinding by the NNLO\(_{\text{opt}}\) interaction for \(^{24}\text{Mg}\) with respect to the experimental binding energy.

4. Conclusions

In this work we have performed many-body calculations for three nuclei using a natural orbit single-particle basis constructed from the LDB single-particle states. We considered a ‘bare’ NN interaction (NNLO\(_{\text{opt}}\)). A better convergence in the binding energies has been obtained. The NOs based on the LDB basis outperform the standard h.o. representation. The energy gain is more pronounced for the heavier nucleus considered in this work.

References

[1] Navratil P, Vary J P and Barrett B R 2000 Phys. Rev. Lett. 84 5728
[2] Navratil P, Vary J P and Barrett B R 2000 Phys. Rev. C 62 054311
[3] Navratil P, Quaglioni S, Stetcu I and Barrett B R 2009 J. Phys. G: Nucl. Part. Phys. 36 083101
[4] Barrett B R, Navratil P and Vary J P 2013 Prog. Part. Nucl. Phys. 69 131
[5] Wloch M, Dean D, Gour J R, Hjorth-Jensen M, Kowalski K, Papenbrock T and Piecuch P 2005 Phys. Rev. Lett. 94 212501
[6] Hagen G, Papenbrock T, Dean D J and Hjorth-Jensen M 2008
       Phys. Rev. Lett. 101 092502
[7] Hagen G, Hjorth-Jensen M, Jansen G R, Machleidt R and
       Papenbrock T 2012 Phys. Rev. Lett. 109 032502
[8] Hagen G, Papenbrock T, Dean D J and Hjorth-Jensen M 2010
       Phys. Rev. C 82 034330
[9] Bogner S K, Furnstahl R J and Schwenk A 2010 Prog. Part.
       Nucl. Phys. 65 94
[10] Bogner S K, Furnstahl R J, Ramanan S and Schwenk A 2007
      Nucl. Phys. A 784 79
[11] Bogner S K, Furnstahl R J and Perry R J 2007 Phys. Rev. C 75
      061001(R)
[12] Jurgenson E D, Navratil P and Furnstahl R J 2009 Phys. Rev.
      Lett. 103 082501
[13] Hebeler K 2012 Phys. Rev. C 85 021002
[14] Hergert H, Bogner S K, Morris T D, Schwenk A and
       Tsuchiyama K 2016 Phys. Rep. 621 165
[15] Bogner S K, Hergert H, Holt J D, Schwenk A, Binder S,
       Calci A, Langhammer J and Roth R 2014 Phys. Rev. Lett.
       113 142501
[16] Parzuchowski N M, Morris T D and Bogner S K 2017 Phys.
      Rev. C 95 044304
[17] Stroberg S R, Calci A, Hergert H, Holt J D, Bogner S K,
      Roth R and Schwenk A 2017 Phys. Rev. Lett. 118 032502
[18] Parzuchowski N M, Stroberg S R, Navratil P, Hergert H and
      Bogner S K 2017 Phys. Rev. C 96 034324
[19] Gebrerufael E, Vobig K, Hergert H and Roth R 2017 Phys.
      Rev. Lett. 118 152503
[20] Caprio M A, Maris P and Vary J P 2014 Phys. Rev. C 90
      034305
[21] Constantinou C, Caprio M A, Vary J P and Maris P
      arXiv:1605.04976 [nucl-th]
[22] Lowdin P-O 1955 Phys. Rev. 97 1474
[23] Lowdin P-O and Shull H 1956 Phys. Rev. 101 1730
[24] Davidson E R 1972 Rev. Mod. Phys. 44 451
[25] Mahaux C and Sartor R 1991 Adv. Nucl. Phys. 20 1
[26] Stoitsov M V, Antonov A N and Dimitrova S S 1993 Phys.
      Rev. C 48 74
[27] Jaganathan Y, Id Betan R M, Michel N, Nazarewicz W and
      Ploszajczak M 2017 Phys. Rev. C 96 054316
[28] Puddu G 2017 J. Phys. G: Nucl. Part. Phys. 44 105104
[29] Puddu G 2006 J. Phys. G: Nucl. Part. Phys. 32 321
[30] Puddu G 2007 Eur. Phys. J. A 31 163
[31] Puddu G 2010 Eur. Phys. J. A 45 233
[32] Lederman W (ed) 1981 Handbook of Applicable Mathematics.
      Vol III, Numerical Methods (New York: Wiley) ch 11
[33] Puddu G 2009 Eur. Phys. J. A 42 281
[34] Ekström A et al 2013 Phys. Rev. Lett. 110 192502
[35] Balian R and Brezin E 1969 Nuovo Cimento B 61 403
[36] Wong C W and Clement D M 1972 Nucl. Phys. A 183 210
[37] Kung C L, Kuo T T S and Ratcliff K F 1979 Phys. Rev. C 19
      1063
[38] Hagen G, Hjorth-Jensen M and Michell N 2006 Phys. Rev. C
      73 064307
[39] Caprio M A, Maris P and Vary J P 2012 Phys. Rev. C 86
      034312
[40] Imada M and Kashima T 2000 J. Phys. Soc. Japan 69 2723
[41] Mizusaki T and Shimizu N 2012 Phys. Rev. C 85 021301(R)
[42] Mizusaki T 2004 Phys. Rev. C 70 044316
[43] Mizusaki T, Utsuno Y, Mizusaki T, Otsuka T, Abe T and
      Honma M 2010 Phys. Rev. C 82 061305(R)
[44] Puddu G 2012 J. Phys. G: Nucl. Part. Phys. 39 085108
[45] Shimizu N, Utsuno Y, Mizusaki T, Honma M, Tsunoda Y and
      Otsuka T 2012 Phys. Rev. C 85 054301
[46] Audi G and Wapstra A H 1993 Nucl. Phys. A 561 1
[47] Navratil P, Gueorguiev V G, Vary J P, Ormand W E and
      Nogga A 2007 Phys. Rev. Lett. 99 042501
[48] Entem D R and Machleidt R 2003 Phys. Rev. C 68 044001