Description of nuclei around $N = 20$ starting from the Argonne V18 interaction.

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Abstract

Using the Argonne V18 interaction, renormalized with the Lee-Suzuki method, we study nuclei around the $N = 20$ island of inversion. We include 5 major oscillator shells, in a no-core approach, using the Hybrid Multi-Determinant method reaching up to few hundreds Slater determinants. Although qualitatively in agreement with the experimental levels, the calculated BE2 do not show the same amount of collectivity seen experimentally.

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1 Introduction.

The evolution of the shell structure and magic numbers for extreme $N/Z$ ratios has become one of the major topics both in experimental and theoretical nuclear physics (for a review see for example ref.[1]). Magic numbers may not be the same as we move away from the stability line. The first instance was found in ref. [2] where it has been shown that the experimental data for Na isotopes was inconsistent with the $N = 20$ shell closure. In ref. [3] it has been predicted that Na isotopes for $N \approx 20$ develop large deformation and that the orbitals coming from the $f$ shell becomes occupied (the basis used in ref.[3] is a deformed harmonic oscillator basis). Since then, many experimental and theoretical studies in this island of inversion region have been performed (cf. ref.[1]). Among the others, shell model calculations have been performed using the (sd) and (fp) spherical major shells, ref.[4], and Monte Carlo shell model (ref.[5]). In these calculations an inert core has been assumed and a realistic effective interaction has been adapted to the region (not to be confused with the renormalized interactions discussed below).

To the author knowledge, no calculations starting from a bare nucleon-nucleon interaction have been performed. In this work we consider the Argonne V18 interaction (ref. [6]) and study Ne, Mg and Si isotopes with neutron number $N = 18, 20, 22$. Experimentally, Neon and Magnesium display the disappearance of the neutron shell closure at $N = 20$, however Silicon at $N = 20$ and heavier isotones have an increased excitation energy of the $2^+_1$ state, compared to the neighboring isotopes, pointing out to a restoration of the neutron shell closure. Our approach is based on the Lee-Suzuki (refs.[7]-[10]) renormalization prescription, whereby the bare NN interaction is replaced by an effective interac-
tion adapted to the large no core shell model space (cf. also ref.[11]). We consider only the effective two-body interaction and ignore the many-body interactions induced by the renormalization prescription. We limit our study to 5 spherical major harmonic oscillator shells, although the real features of interaction are seen only with a large number of major shells. Once we determine the effective interaction, we use the Hybrid-Multi-Determinant method (HMD) (ref. [12]-[14]) to expand the nuclear wave functions in terms of the most generic Slater determinants (i.e. no special symmetries are imposed). The results we obtained are mixed. From one hand the trend of the experimental excitation energies of the first $2^+_1$ (ref.[15]) is reproduced, that is the energy of the $2^+_1$ decreases from $N = 18$ to $N = 22$ for $Ne$ and $Mg$ isotopes and it increases at $N = 20$ for $Si$, however a good quantitative agreement is lacking. Also the BE2 are too small compared to the experimental data (cf. ref.[16] for a recent compilation), pointing out to an insufficient collectivity for $Ne$ and $Mg$. As discussed in the next sections, we evaluated also the average occupation numbers of the neutrons in the various orbits. The occupation numbers we obtained are very different from the ones obtained with realistic effective interactions. This is probably due to the very different nature of the effective interactions used in our context and in the MCSM and shell model context. This can be understood by considering that an increase of the single-particle space in the LS renormalization scheme, would make the LS effective interaction harder and harder at short distances. A “hard” interaction would scatter nucleons to all majors shell of the single-particle space, while in shell model calculations at the most one considers the $sd$ and $fp$ major shells. Very likely, this does not depend on the renormalization prescription.

Also we do not renormalize the transition operators nor any other. Following
the results of ref. [17], we renormalize only operators that are very strong at short
distances. We do not take the translational invariant quadrupole operator, rather
we take the usual one in the lab frame with bare charges. The outline of this paper
is the following. In section 2 we recall the HMD method. In section 3 we discuss
the results. Since there are several ways that have been used to renormalize the
NN interaction we give in the appendix a detailed description of the method we
have used.

2 A brief recap of the method.

The HMD method (ref.[12]-[14]) is a variational approach to obtain eigenfunc-
tions of an Hamiltonian. Given a spherical basis of $N_s$ single-particle states (e.g.
an harmonic oscillator basis) the Hamiltonian is written as

$$\hat{H} = \frac{1}{2} \sum_{ijkl} H_{ij,kl} a_i^\dagger a_j^\dagger a_l a_k$$

(2.1)

where $ijkl$ label single-particle states ($i = 1, 2, ... N_s$) and the one-body part has
been included in the two-body interaction. We antisymmetrize from the start the
matrix elements of the Hamiltonian $H_{ij,kl} = -H_{ij,kl}$, since exchange contribu-
tions are the opposite of direct terms. We describe eigenstates as a linear superpo-
sition of Slater determinants of the most generic type

$$|\psi> = \sum_{S=1}^{N_D} g_S \hat{P} |U_S>$$

(2.2)

where $\hat{P}$ is a projector to good quantum numbers (e.g. good angular momentum
and parity) $N_D$ is the number of Slater determinants $|U_S>$ expressed as

$$|U_S> = \tau_1(S)\tau_2(S)...\tau_A(S)|0>$$

(2.3)
the generalized creation operators $\bar{c}_\alpha(S)$ for $\alpha = 1, 2, ..., A$ are a linear combination of the creation operators $a_i^\dagger$

$$\bar{c}_\alpha(S) = \sum_{i=1}^{N_s} U_{i,\alpha}(S) a_i^\dagger \quad \alpha = 1, ... A$$  \hspace{1cm} (2.4)

The complex coefficients $U_{i,\alpha}(S)$ represent the single-particle wave-function of the particle $\alpha = 1, 2, ..., A$. We do not impose any symmetry on the Slater determinants (axial or other) since the $U_{i,\alpha}$ are variational parameters. These complex coefficients are obtained by minimizing the energy expectation values

$$E[U] = \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle}$$  \hspace{1cm} (2.5)

The coefficients $g_S$ are obtained by solving the generalized eigenvalue problem

$$\sum_S < U_S | \hat{P} \hat{H} | U_S > g_S = E \sum_S < U_{S'} | \hat{P} | U_S > g_{S'}$$  \hspace{1cm} (2.6)

for the lowest eigenvalue $E$.

Few comments are in order about this method. If we expand eq.(2.3) in terms of the of spherical single-particle creation operators, we include all possible contributions of the spherical basis of the Hilbert space. However these contributions are not independent from each other, and this is the reason why we must consider a large number of them (even several hundreds). Second, the projector to good quantum numbers ideally should be the exact one (see for example ref.[18]) in terms of integrals over the Euler angles. However, our experience with the exact 3-dimensional projectors, tells us that the number of mesh points of the Euler angles has to be rather large, making the numerical integration computationally very expensive. If we were looking for the best approximation to eigenstates in terms of few Slater determinants, this would be unavoidable (actually in such a case we would prefer quasi-particle states), but we are looking for a sequence
of states which approximate better and better the exact eigenstates. In order to make the calculations feasible, we prefer to consider projectors to good parity and \(z\)-component of the angular momentum. This way we can generate hundreds of Slater determinants. The resulting approximation for an eigenstate has the lowest energy for a given \(J_z\) value. This is appropriate for low energy eigenstates of even-even systems. The method would be inadequate for odd-even and odd-odd systems. In these cases we prefer to add to the Hamiltonian a term \(\gamma \hat{J}^2\), with \(\gamma > 0\), so that all states with \(J \neq J_z\) would be moved to high energy and all states with \(J < J_z\) are canceled by the \(J_z\) projector. This is particularly useful if we have a large single-particle basis and large number of particles. In order to improve the wave-functions, at the end of the calculation we reevaluate the energies or transition probabilities replacing the \(J_z\) projector with the exact projector to good angular momentum. We have done this in the case of \(^{33}\text{Mg}\). For large systems, the full angular momentum projector has to be nearly exact, otherwise the variational method breaks down.

We consider a quasi-Newton minimization method. It is a generalization of the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method (cf. for example ref.[19] and references in there). It is described in detail in ref. [20]. Quasi-Newton methods minimize the functional using the energy gradients \(\partial E/\partial U\). Using this method, we vary one Slater determinant at a time, not all Slater determinants simultaneously. The reason is that with this method we determine a direction and a step of descent in the energy hyper-surface. However Slater determinants have different step sizes and therefore a simultaneous variation of all Slater determinants might need small step sizes, slowing down the convergence to the energy minimum.

The minimization strategy consists in the following steps. We first generate
the Hartree-Fock solution ($N_D = 1$) then we add one Slater determinant at a time and optimize the last Slater determinant in order to minimize the energy. After we reach a specified number of Slater determinants we vary all Slater determinants anew. We repeat this addition-refinement step several times. Each time increasing $N_D$ by several Slater determinants.

The energies obtained with this method approach more and more, but are not, the exact energies. This however is not a severe problem. We are mostly interested in excitation energies. In the region of the island of inversion, the excitation energy of the first $2^+$ gives an indication of the breaking of shell closure. Both $E(0^+)$ and $E(2^+)$ approach the exact values from above and contain comparable errors of the same sign which mostly cancel in the difference. That is, excitation energies converge much faster than the energies themselves.

For many-particle systems the nucleon-nucleon interaction is very strong at small distances (or large relative momenta) and therefore the interaction must be renormalized. There are many prescriptions for the renormalization which necessarily give different effective Hamiltonians. We add in the appendix a detailed description of the adopted renormalization procedure based on the UMOA of refs.[7]-[10], since this method has been implemented in several ways, together with a numerical test. In the next section we shall discuss the results obtained for $^{30,32,33,34}\text{Mg}$, $^{28,30,32}\text{Ne}$ and $^{32,34,36}\text{Si}$ isotopes using 5 major harmonic oscillator shells.
3 Excitation energies around the $N = 20$ island of inversion.

Our main focus is on the excitation energy of the first $2^+$ state for $Z = 10, 12, 14$ around $N = 18, 20, 22$. We consider only one harmonic oscillator frequency $\hbar \omega = 12\text{MeV}$. The NN interaction is the Argonne $v18$ potential (ref.[6]). In all cases we add to the renormalized Hamiltonian a center of mass term $\beta (H_{cm} - 3\hbar \omega / 2)$ with $\beta = 1$, $H_{cm}$ being the center of mass harmonic oscillator Hamiltonian, in order to prevent spurious center of mass excitations. Typical size of the Hilbert space are $10^{29} \div 10^{30}$. For all nuclei we build in sequence wave functions consisting of $N_D = 1, 2, 5, 10, 15, 25, 35, 50, 70, 100, 150, 200, ..$ Slater determinants (these numbers are somewhat arbitrary). Every time we reach the above numbers we re-optimize anew all Slater determinants. The energies require a very large number of Slater determinants to converge. Consider for example the energies of the first $0^+$ and of the first $2^+$ for $^{32}\text{Mg}$ shown in fig.1. Although the pattern of convergence for both states is the same, the energies are themselves not fully converged. A very rough estimate (assuming an approximate $1/N_D$ behavior for the energies) indicates that the ground state is about $1 \div 1.5\text{MeV}$ lower. From fig.1 we can see that 5 major shells do not describe well the energies: the binding energies are too large. Improved values can be obtained by increasing the number of major shells (the interaction is renormalized to a specific number of major shells). However calculations with 6 or 7 major shells are computationally much more involved (for 6 major shells we have 112 single-particle states for both neutrons and protons and for 7 major shells this number becomes 168). In fig.2, we show the convergence of the excitation energy for $Ne$ isotopes. The $N = 20$ shell closure is absent,
Figure 1: Energies of $^{32}Mg$ for $J = 0^+$ and $J = 2^+$ as a function of the number of Slater determinants.
Figure 2: Convergence of the excitation energy of $2^+_1$ as a function of the number of Slater determinants for Ne isotopes.

although not to the same extent seen experimentally. In fig.3 and fig.4 we show the convergence of the excitation energy for Mg and Si isotopes respectively. For Mg a pattern similar to Ne can be seen.

Notice the different behavior of Si isotopes, where one can see an increase in the energy of the $2^+$ state for $N = 20$, again not to the same extent seen experimentally. We summarize the results of the calculations in table 1 together with the corresponding experimental values of refs.[15],[16]. It seems that the calculated values do not show enough collectivity. This is confirmed also by the calculated BE2 values which are systematically lower than the experimental values. There could be several reasons for this, not necessarily related to the V18 interaction. First we renormalized to 5 major shells only. Moreover the harmonic oscilla-
Figure 3: Convergence of the excitation energy of $2^+_1$ as a function of the number of Slater determinants for Mg isotopes.
Figure 4: Convergence of the excitation energy of $2_1^+$ as a function of the number of Slater determinants for Si isotopes.
tor basis has the wrong large distance behavior instead of the proper exponential falloff. For medium nuclei the h.o. representation might not be appropriate.

It is instructive to evaluate the occupation numbers of neutrons that reveal which single-particle states are occupied. In tables 2-4, we show these occupation numbers for Ne, Mg and Si isotopes respectively. Notice that the \( N_{ho} = 4 \) major shell is populated for all isotopes under consideration. The single-particle state \( 1d5/2 \) has one neutron in all nuclei under consideration. Also the state \( 0p3/2 \) has one neutron less than expected (the \( N_{ho} = 1 \) core shell is excited). The \( 0f7/2 \) orbital is nearly empty for neutron number \( N = 18, 20 \), and it is occupied (about 0.5) only for \( N = 22 \). This is the opposite of what has been found using realistic effective interactions assuming an inert \(^{16}\text{O} \) core and valence nucleons in the \( sd - pf \) shells (ref. [5]). This is not necessarily in contradiction with the findings of ref.[3], since our basis is spherical while in ref. [3] a deformed basis has been used. A less detailed information can be obtained by evaluating the total number of neutrons in each major h.o. shell \( N_{ho} \). The result is given

| Nucleus | \( E(2^+)_{exp} \) | \( E(2^+)_{th} \) | \( N_D \) | \( BE2(th) \) | \( BE2(exp) \) |
|---------|-------------------|-------------------|---------|-------------------|-------------------|
| \(^{28}\text{Ne}\) | 1.304 | 1.733 | 200 | 62.1 | 136(23) |
| \(^{30}\text{Ne}\) | 0.792 | 1.250 | 200 | 48.0 | 226(35) |
| \(^{32}\text{Ne}\) | 0.722 | 1.036 | 250 | 74.2 | - |
| \(^{31}\text{Mg}\) | 1.4828 | 1.747 | 200 | 16.6 | 273(26) |
| \(^{32}\text{Mg}\) | 0.8853 | 1.171 | 200 | 57 | 434(52) |
| \(^{34}\text{Mg}\) | 0.660 | 1.160 | 250 | 93.2 | 573(79) |
| \(^{32}\text{Si}\) | 1.941 | 1.373 | 150 | 120.8 | 122(+36 − 21) |
| \(^{34}\text{Si}\) | 3.327 | 2.316 | 150 | 37.9 | 85(33) |
| \(^{36}\text{Si}\) | 1.408 | 1.445 | 200 | 20.5 | 193(59) |

Table 1: Experimental and calculated \( E(2^+) \) in MeV and \( BE2(0^+ \rightarrow 2^+) \) in \( e^2 fm^4 \) for Ne, Mg and Si isotopes. Experimental values are taken from refs. [15][16].
Table 2: Neutron occupation numbers for Ne isotopes.

| n  | l   | j   | $^{28}$Ne | $^{30}$Ne | $^{32}$Ne |
|----|-----|-----|-----------|-----------|-----------|
| 0  | 0   | 1/2 | 1.96      | 1.99      | 1.99      |
| 0  | 1   | 3/2 | 3.31      | 3.32      | 3.47      |
| 0  | 1   | 1/2 | 1.82      | 1.84      | 1.85      |
| 0  | 2   | 5/2 | 5.00      | 4.99      | 5.03      |
| 0  | 2   | 3/2 | 2.06      | 3.74      | 3.76      |
| 1  | 0   | 1/2 | 1.64      | 1.72      | 1.73      |
| 0  | 3   | 7/2 | 0.08      | 0.08      | 0.50      |
| 0  | 3   | 5/2 | 0.06      | 0.07      | 0.13      |
| 1  | 1   | 3/2 | 0.65      | 0.66      | 1.77      |
| 1  | 1   | 1/2 | 0.14      | 0.14      | 0.38      |
| 0  | 4   | 9/2 | 0.04      | 0.03      | 0.05      |
| 0  | 4   | 7/2 | 0.03      | 0.03      | 0.05      |
| 1  | 2   | 5/2 | 0.83      | 0.93      | 0.89      |
| 1  | 2   | 3/2 | 0.13      | 0.20      | 0.17      |
| 2  | 0   | 1/2 | 0.26      | 0.26      | 0.25      |

Table 3: Neutron occupation numbers for Mg isotopes.

| n  | l   | j   | $^{30}$Mg | $^{32}$Mg | $^{34}$Mg |
|----|-----|-----|-----------|-----------|-----------|
| 0  | 0   | 1/2 | 1.93      | 1.99      | 1.99      |
| 0  | 1   | 3/2 | 3.29      | 3.31      | 3.46      |
| 0  | 1   | 1/2 | 1.80      | 1.82      | 1.83      |
| 0  | 2   | 5/2 | 4.86      | 4.90      | 4.93      |
| 0  | 2   | 3/2 | 2.20      | 3.64      | 3.66      |
| 1  | 0   | 1/2 | 1.48      | 1.67      | 1.68      |
| 0  | 3   | 7/2 | 0.08      | 0.08      | 0.57      |
| 0  | 3   | 5/2 | 0.06      | 0.07      | 0.12      |
| 1  | 1   | 3/2 | 0.66      | 0.68      | 1.76      |
| 1  | 1   | 1/2 | 0.16      | 0.16      | 0.35      |
| 0  | 4   | 9/2 | 0.04      | 0.03      | 0.05      |
| 0  | 4   | 7/2 | 0.03      | 0.03      | 0.05      |
| 1  | 2   | 5/2 | 0.92      | 1.02      | 0.99      |
| 1  | 2   | 3/2 | 0.19      | 0.30      | 0.26      |
| 2  | 0   | 1/2 | 0.29      | 0.32      | 0.30      |
### Table 4: Neutron occupation numbers for $Si$ isotopes.

| $n$ | $l$ | $j$ | $^{32}Si$ | $^{34}Si$ | $^{36}Si$ |
|-----|-----|-----|--------|--------|--------|
| 0   | 0   | 1/2 | 1.86   | 1.99   | 1.99   |
| 0   | 1   | 3/2 | 3.29   | 3.29   | 3.49   |
| 0   | 1   | 1/2 | 1.80   | 1.80   | 1.81   |
| 0   | 2   | 5/2 | 4.76   | 4.82   | 4.85   |
| 0   | 2   | 3/2 | 2.50   | 3.54   | 3.57   |
| 1   | 0   | 1/2 | 1.21   | 1.62   | 1.63   |
| 0   | 3   | 7/2 | 0.07   | 0.06   | 0.53   |
| 0   | 3   | 5/2 | 0.06   | 0.06   | 0.11   |
| 1   | 1   | 3/2 | 0.68   | 0.70   | 1.85   |
| 1   | 1   | 1/2 | 0.17   | 0.19   | 0.30   |
| 0   | 4   | 9/2 | 0.04   | 0.02   | 0.03   |
| 0   | 4   | 7/2 | 0.03   | 0.03   | 0.04   |
| 1   | 2   | 5/2 | 0.99   | 1.12   | 1.09   |
| 1   | 2   | 3/2 | 0.25   | 0.40   | 0.36   |
| 2   | 0   | 1/2 | 0.30   | 0.37   | 0.35   |

### Table 5: Number of neutrons in the major h.o. shells for all cases.

| $N_{ho}$ | $^{28}Ne$ | $^{30}Ne$ | $^{32}Ne$ | $^{30}Mg$ | $^{32}Mg$ | $^{34}Mg$ | $^{32}Si$ | $^{34}Si$ | $^{36}Si$ |
|----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 0        | 1.96      | 1.99      | 1.99      | 1.93      | 1.99      | 1.99      | 1.86      | 1.99      | 1.99      |
| 1        | 5.13      | 5.16      | 5.32      | 5.09      | 5.13      | 5.29      | 5.09      | 5.09      | 5.20      |
| 2        | 8.7       | 10.45     | 10.51     | 8.54      | 10.21     | 10.27     | 8.47      | 9.98      | 9.95      |
| 3        | 0.93      | 0.95      | 2.78      | 0.96      | 0.99      | 2.8       | 0.98      | 1.01      | 2.79      |
| 4        | 1.29      | 1.45      | 1.41      | 1.47      | 1.7       | 1.65      | 1.61      | 2.39      | 1.87      |
in table 5. In all Ne isotopes, the \( N_{ho} = 4 \) major shell has about one neutron. Both \(^{28}\text{Ne}\) and \(^{30}\text{Ne}\) have one neutron in the \( N_{ho} = 3 \) fp shell and the added two neutrons occupy the \( N_{ho} = 2 \) major shell. Adding two more neutrons, they mostly occupy the \( N_{ho} = 3 \) shell. A similar pattern is seen also in \( Mg \) isotopes. Silicon isotopes show a different behavior. Going from \(^{32}\text{Si}\) to \(^{32}\text{Si}\) one neutron occupies the \( N_{ho} = 3 \) shell and the other one occupies the \( N_{ho} = 4 \) shell and two more neutrons occupy the \( N_{ho} = 3 \) shell. Consider now the \( N = 20 \) isotone chain. As we increase the number of protons the number of neutrons in the \( N_{ho} = 3 \) shell does not change, instead the \( N_{ho} = 4 \) becomes more populated at the expenses of the \( N_{ho} = 2 \) shell. Let us remark that in this approach there are no single-particle energy levels. Moreover from fig.1, one can see that the amount of correlation energy is rather large, being about 15 MeV's for \(^{32}\text{Mg}\).

We have not performed a systematic study of even-odd nuclei. We studied only the case of \(^{33}\text{Mg}\). For this nucleus we added a term \( \gamma \hat{J}^2 \) to the Hamiltonian with \( \gamma = 1 \)MeV. Our calculation suggests that the spin of the ground state is \( 3/2^- \). The first excited state has \( J^\pi = 7/2^- \) at an excitation energy of 0.1MeV followed by a \( 1/2^- \) state at 0.49MeV. The convergence curve as a function of the number of Slater determinants is shown in fig. 5. The spin of the ground state of this nucleus has been subject to some debate (cf. ref.[21]).
Figure 5: Low energy levels of $^{33}Mg$ as a function of the number of Slater determinants.
4 Appendix

The Lee-Suzuki renormalization.

The nuclear Hamiltonian is

\[ H = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j} V_{ij}^{NN} \]  (A1)

where \( m \) is the nucleon mass which we take equal to twice the reduced mass and \( V_{ij}^{NN} \) is the Argonne \( v18 \) interaction. To this Hamiltonian, similarly to what is done in the no core shell model approach (NCSM) (ref. [11]), we add a center of mass harmonic potential

\[ V_{cm} = \frac{1}{2} m A \omega^2 R_{cm}^2 \]  (A2)

The resulting Hamiltonian \( H^{\omega,A} \) can be rewritten as

\[ H^{\omega,A} = \sum_{i=1}^{A} h_i + \sum_{i<j} V_{ij}^{\omega,A} \]  (A3)

where

\[ h_i = \frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 r_i^2 \]  (A4a)

and

\[ V_{ij}^{\omega,A} = V_{ij}^{NN} - \frac{m \omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \]  (A4b)

At the cluster-2 approximation we consider the 2-particle Hamiltonian

\[ H_2^{\omega,A} = h_1 + h_2 + V_{12}^{\omega,A} \]  (A5)

This Hamiltonian separates into a center of mass Hamiltonian for the 2 particles plus a Hamiltonian in the relative coordinates \( r, p \)

\[ H_r = \frac{p^2}{m} + \frac{1}{4} m \omega^2 r^2 + V_{12}^{\omega} \equiv H_0 + V_{12}^{\omega} \]  (A6)
which defines $H_{0r}$. The Hamiltonian $H_r$ of relative motion is the one that is renormalized using the Lee-Suzuki procedure. For all values of the spin, the angular momentum, the isospin and the z-projection of the isospin, $s, j, t$ and $t_z$ all matrix elements of this bare Hamiltonian are evaluated (the radial quantum number can reach $200 \div 250$). The radial quantum number must be large enough so that the single-particle space is complete for all practical purposes. Let us call $H_{ij}$ the resulting matrix. The indices $i, j$ are defined in the full single-particle space of relative coordinates. The renormalization procedure consists in separating the full space in two parts with the aid of projectors $P$ (model space) and $Q$ (excluded space, such that $P + Q = 1$). According to the UMOA prescription a unitary transformation is performed on $H$ such that there is no coupling between the $P$ space and the $Q$ space. Briefly summarized the method consists in the following steps. Let $p, p'$ be indices in the model space and $q, q'$ be the indices of the excluded space. First we diagonalize the bare Hamiltonian and let $H = V \epsilon \tilde{V}$ the corresponding eigenvalue equation ($\epsilon$ and $V$ are the energy eigenvalues and eigenvectors). Let us call $U_{p,p'} = V_{p,p'}$ and $W_{q,p} = V_{q,p}$ the P-part and the QP-part of the matrix of the eigenvectors $V$, respectively, and let

$$S_{q,p} = \sum_{p'} W_{q,p'} U_{p'p}^{-1}$$

(A7)

where the sum runs over the P-indices. We avoid the use of the traditional symbol $\omega$ for this matrix, in order not to confuse it with the h.o. frequency. Let us also construct the P-space matrix

$$N_{p,p'} = \delta_{p,p'} + \sum_{q} S_{q,p} S_{q,p'}$$

(A8)

$\delta$ being the Kronecker $\delta$. Further, let us build the matrix

$$\Omega_{p,p'} = N_{pp'}^{-1/2}, \quad \Omega_{q,p} = \sum_{p'} S_{q,p'} N_{p'p}^{-1/2}$$

(A9)
which connects the $P + Q$ space with the $P$ space. Then the renormalized Hamiltonian is then given by

$$H_{pp'}^{\text{ren}} = \sum_{ij} \Omega_{i,p} H_{ij} \Omega_{j,p'}$$  \hspace{1cm} (A10)

where in the above equation the sum is over the full space. The eigenvalues of $H^{\text{ren}}$ coincide (almost to machine accuracy) with the P-part of the eigenvalues of the bare $H$. The full details of the proof can be found in ref. [7]-[10].

Note however that recently the above prescription has been recast in a more simplified and transparent form in ref. [22]. The two formulations can be shown identical using the property $VPV^\dagger P = PV PV^\dagger P + QVPV^\dagger P = UU^\dagger + WU^\dagger$. This renormalization prescription can be formulated in terms of the singular value decomposition of the matrix $U$ (ref. [23]), which is numerically very robust. The main point of ref.[22] and ref. [23] is to rewrite the renormalized Hamiltonian as

$$H^{\text{ren}} = (UU^\dagger)^{-1/2}U(P\epsilon)U^\dagger(UU^\dagger)^{-1/2}$$  \hspace{1cm} (A11)

and (cf. ref. [23])

$$(UU^\dagger)^{-1/2}U = XY^\dagger$$  \hspace{1cm} (A12)

where $X$ and $Y^\dagger$ are the left and right singular eigenvectors of $U$.

The P-indices are relative to major harmonic oscillator shells. Typically we renormalize to $N_{\text{ren}} = 8$ major shells in the intrinsic frame. We point out that these are not the major shells used in the variational calculation as discussed later.

Once we obtain the renormalized 2-particle Hamiltonian we can define an effective potential for two particles from $H^{\text{ren}}$ as

$$V^{\text{ren}} = H^{\text{ren}} - H_0$$  \hspace{1cm} (A13)

This interaction replaces $V_{ij}^{\omega,A}$ in eq.(A3). Next we subtract from eq(A3) the Hamiltonian of the center of mass in order to obtain the intrinsic Hamiltonian
and the final result is, for the 2 particle system,

$$H_{1,2}^{\text{int}} = H_0 + V_{\text{ren}} + \left( \frac{2}{A} - 1 \right) H_0$$

(A14a)

and

$$H^{\text{int}} = \sum_{i<j} H_{i,j}^{\text{int}}$$

(A14b)

for the A-particle system. We are now in a position to transform these matrix elements from the intrinsic frame to the lab frame, using the Talmi-Moshinsky (cf. ref. [24] for a very efficient implementation) transformation brackets.

To the final Hamiltonian we add the term

$$\beta \left( H_{\text{cm}} - 3\hbar\omega/2 \right)$$

(A15)

with $\beta > 0$ to prevent center of mass excitations. We end up with all possible matrix elements $\langle n_a l_a n_b l_b J|H|n_c l_c n_d l_d J \rangle$ in the lab frame for the $nn, np$ and $pp$ interaction. The quantum numbers in the lab frame, satisfy

$$2n_a + l_a + 2n_b + l_b \leq N_{\text{ren}}$$

(A16)

Most important, we consider quantum numbers $n, l$ such that

$$2n + l \leq N_{\text{ren}}/2$$

(A17)

That is, we use an energy truncation scheme, called HMD-a in ref. [14]. The use of condition (A16) is called HMD-b in ref.[14]

As discussed in ref. [25], there are many ways to renormalize the Hamiltonian. The one discussed above is the one adopted in all calculations of this work. Let us remark that instead of condition (A17) we could have adopted the condition (A16) for the quantum numbers in the lab frame. We prefer condition (A17) since (A16)
strongly overbounds unless we consider many major shells. Condition (A16) is useful as a numerical test for the deuterium. We have performed a numerical test using $N_{\text{ren}} = 6$ (7 major shells in the lab frame) with $\hbar \omega = 12 \text{MeV}$ for the deuterium. The HMD-b method for 5 Slater determinants gave a discrepancy from the exact binding energy of the deuterium of 0.27 KeV. Using 10 Slater determinants this discrepancy has been reduced to 1.3 eV and using 15 Slater determinants this discrepancy has been further reduced to 0.015 eV. By exact binding energy we mean the value obtained by diagonalizing the bare Hamiltonian matrix in the intrinsic frame with 480 major oscillator shells.
References

[1] O. Sorlin, M.-G. Porquet. Progress in Particle and Nuclear Physics 61, 602(2008).

[2] C. Thibault et al. Phys. Rev. C 12, 644(1975).

[3] X. Campi, H. Flocard, A.K. Kerman, and S. Koonin, Nucl. Phys. A251, 193(1975).

[4] E.K. Warburton, J.A. Becker, and B.A. Brown. Phys. Rev. C 41, 1147(1990).

[5] Y. Utsuno, T. Otsuka, T. Mizusaki, and M. Honma. Phys. Rev. C 60, 054315(1999).

[6] R.B. Wiringa, V.G.J. Stoks, and R. Schiavilla. Phys. Rev. C 51, 38(1995).

[7] K. Suzuki and S.Y. Lee. Prog. Theor. Phys. 64, 2091(1980).

[8] K. Suzuki. Prog. Theor. Phys. 68, 1627(1982).

[9] K. Suzuki. Prog. Theor. Phys. 68, 1999(1982).

[10] K. Suzuki and R. Okamoto. Prog. Theor. Phys. 92, 1045(1992).

[11] P. Navratil, J.P. Vary, and B.R. Barrett. Phys. Rev. C 62, 054311(2000).

[12] G. Puddu. J. Phys. G: Nucl. Part. Phys. 32 (2006) 321

[13] Eur. Phys. J. A 31, 163(2007).

   G. Puddu. Eur. Phys. J. A 34, 413(2007)

[14] G. Puddu Eur. Phys. J. A 45, 233(2010))

23
[15] Evaluated Nuclear Structure Data File. http://www.nndc.bnl.gov/ensdf/

[16] B.Pritychenko, M.Birch, B.Singh, M.Horoi. arXiv:1312.5975v4 [nucl-th]

[17] I.Stetcu, B.R.Barrett, P.Navratil, and J.P.Vary.
Phys. Rev. C71, 044325(2005).

[18] P. Ring and P. Schuck. The Nuclear Many-Body Problem. Springer-Verlag
New York 1980,

[19] W. Lederman ed. Handbook of Applicable Mathematics. Vol. III,
Numerical Methods, chapter 11. John Wiley and Sons, New York 1981.

[20] G.Puddu. Eur. Phys. J. A 42, 281(2009).

[21] D.T. Yordanov et al. Phys. Rev. Lett. 99, 212501(2007).

[22] A.F.Lisetskiy, B.R.Barrett, M.K.G. Kruse, P.Navratil, I.Stetcu, and J.P.Vary.
Phys. Rev C 78, 044302(2008).

[23] S.Kvaal. Phys. Rev.C 78,044330(2008).

[24] G.P.Kamuntavicius, R.K.Kalinauskas, B.R.Barrett, S.
Micevicius, D. Germanas, Nucl. Phys. A 695, 191 (2001).

[25] J.D.Holt, T.T.S.Kuo, and G.E.Brown. Phys.Rev. C 69,034329(2004).