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Ab initio calculation of energies of light nuclei with the Hybrid Multideterminant scheme

G. Puddu[a]

Dipartimento di Fisica dell'Università di Milano, and INFN sezione di Milano, Via Celoria 16, I-20133 Milano, Italy

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Abstract. We use the AV8' nucleon-nucleon potential renormalized with the Lee-Suzuki prescription with the Hybrid Multideterminant scheme to evaluate energies of some light nuclei. The Lee-Suzuki prescription is used to evaluate the the two-body matrix elements up to 6 major oscillator shells in the lab frame. The Hybrid Multideterminant scheme is used to deal with the nuclear-structure problem. The results obtained for ^{6}Li, ^{12}C and ^{16}O are compared with the results obtained with other methods. The results suggest a reasonable convergence of the renormalization prescription for 6 major shells.

PACS. 21.60.Cs Shell model – 21.30.Fe Forces in hadronic systems and effective interactions – 27.20.+n $6 \leq A \leq 19$

1 Introduction

A major problem in nuclear physics is the understanding of the structure of nuclei starting from nucleon-nucleon potentials that reproduce the nucleon-nucleon scattering data and the properties of the deuteron. There are nowadays many high-accuracy nucleon-nucleon potentials that reproduce these data, such as the Argonne V18 (ref. [1]), the Nijmegen Nij93 (ref. [2]), the CD-Bonn (ref. [3]), the Idaho (ref. [4]) potentials, to mention a few. Several theoretical methods have been used, and are currently in use, to solve the problem of the Schroedinger equation. Among the others, the Green's Function Monte Carlo method (ref. [5]), by which expectation values are evaluated exactly within a statistical uncertainty, has been shown to be applicable up to $A = 12$. The coupled cluster method (refs. [6,7]), and the No-Core Shell Model method (NCSM) (refs. [8–11]). With this last method, first, the nucleon-nucleon potential (and in many cases a genuine three-nucleon potential) is renormalized so as to be able to work within a reasonably small shell model space (ref. [8]), shell model techniques are then used to extract low-energy properties of nuclei.

The key idea of NCSM is to use a truncated harmonic-oscillator basis. An effective Hamiltonian, appropriate for this truncated basis, must therefore be derived. In order to derive the effective Hamiltonian, an harmonic-oscillator potential acting on the center of mass is added to the Hamiltonian $\hat{H}$, without affecting the intrinsic properties of the nucleus. The infinite shell model space is divided into a finite active model space (the P-space) and the excluded space (the Q-space) with the aid of projectors P and Q. A unitary transformation X is then applied to the Hamiltonian that decouples the P-space from the Q-space, that is, $QX^{\dagger}\hat{H}XP = 0$, in the same spirit of the Lee-Suzuki method (refs. [12–14]). The effective Hamiltonian is then $PX^{\dagger}\hat{H}XP$. Once the effective Hamiltonian has been derived, energies and expectation values of low-energy eigenstates are evaluated with standard shell model diagonalization techniques.

Recently, we have studied a scheme to determine the low-energy eigenstates (applied however only to the first $J = 0$ and $J = 2$ eigenstates) of a shell model Hamiltonian (ref. [15]). This scheme is a hybrid method between the Quantum Monte Carlo Diagonalization method (refs. [16–18]) and the VAMPIR method (refs. [19,20]). With this method, the eigenstates of a shell model Hamiltonian $\hat{H}$ are written as a linear combination of Slater determinants,

$$|\psi\rangle = \sum_{\alpha=1}^{N_w} g_{\alpha} |\phi, \alpha, n\rangle |\phi, \alpha, p\rangle. \tag{1}$$

The labels n and p refer to neutrons and protons, respectively, and $|\phi, \alpha, \tau = n, p\rangle$ is a "deformed" Slater determinant built from the "deformed" creation operators

$$c_n^{\dagger}(\alpha, \tau) = \sum_{i=1}^{N_s} U_{i,n}(\alpha, \tau) a_{i,\tau}^{\dagger}. \tag{2}$$

[a] e-mail: Giovanni.Puddu@mi.infn.it

That is,

$$|\psi\rangle = \sum_{\alpha=1}^{N_w} g_\alpha \prod_{\tau=n,p} c_1^\dagger(\alpha,\tau) c_2^\dagger(\alpha,\tau)\dots c_{N_\tau}^\dagger(\alpha,\tau)|0\rangle = \sum_{\alpha=1}^{N_w} g_\alpha \prod_{\tau=n,p} \sum_{i_1 i_2 \dots i_{N_\tau}} U_{i_1,1}(\alpha,\tau) U_{i_2,2}(\alpha,\tau)\dots \times U_{i_{N_\tau},N_\tau}(\alpha,\tau) a_{i_1,\tau}^\dagger a_{i_2,\tau}^\dagger \dots a_{i_{N_\tau},\tau}^\dagger |0\rangle, \quad (3)$$

with $|0\rangle$ being the particle vacuum, N_τ the number of particles for each species. The label i refers to the N_s spherical single-particle states and the complex coefficients $U_{i,n}(\alpha,\tau)$ are determined by minimizing the energy. No *a priori* assumptions are made concerning the structure of the Slater determinants. Some constraints to the arbitrary form of eq. (1) can be imposed, provided the Hubbard-Stratonovich Transformation (HST) (ref. [21]) applied to $\exp(-\beta\hat{H})|\text{ref.}\rangle$ ($|\text{ref.}\rangle$ being some starting Slater determinant and $\hat{H}$ being the Hamiltonian) does not violate such constraints, in the same spirit of the QMCD method. As it can easily be seen, for large β, the HST applied to a starting Slater determinant gives the ground state of $\hat{H}$ as a sum of Slater determinants. A projector to exact quantum numbers (*e.g.*, angular momentum, parity) can be conveniently applied (and usually is) to eq. (1). As the number of wave functions N_w in eq. (1) is increased, the HST implies that eq. (1) converges to the ground state (for specified projected quantum numbers). If the state of eq. (1) is kept orthogonal to the previously determined eigenstate, eq. (1) will converge to the first excited state, in the same spirit of the EXCITED VAMPIR approach (ref. [19]).

Rather than parameterizing the set of Slater determinants in eq. (2) with the integration variables of the Hubbard-Stratonovich transformation, we choose the general parametrization of eq. (3) in terms of the complex variables $U_{i,n}(\alpha,\tau)$ and determine these coefficients with the powerful energy minimization methods typical of the VAMPIR methods, with some variants discussed in ref. [15].

As well known, direct shell model diagonalization methods are limited by the huge dimensionality of the Hamiltonian matrix to be diagonalized (see for example table 1 below). However, eqs. (1)-(3) do not depend on the dimensionality of the Hilbert space. For a given single-particle space, all possible spherical Slater determinants $a_{i_1,\tau}^\dagger a_{i_2,\tau}^\dagger \dots a_{i_{N_\tau},\tau}^\dagger|0\rangle$ appear. If the amplitude of these spherical Slater determinants were completely arbitrary (and not products) a single term of the type of eq. (3) would be sufficient to solve the problem exactly. Equation (3) implies instead that these coefficients are of product type $(U_{i_1,1}(\alpha,\tau)\dots U_{i_{N_\tau},N_\tau}(\alpha,\tau))$ hence the need to take several "deformed" Slater determinants. The HST, however, ensures that if their number N_w is large enough, eq. (1) converges to the ground state. The number of deformed Slater determinants necessary to reach reasonable convergence does not depend on the dimensionality of the Hilbert space. It strongly depends on whether the projector to good quantum numbers is applied. If eq. (10) is used as a variational ansatz without the projectors, the number N_w can easily reach several thousands. If a partial projector is used (for example the projector to good z-projection of the angular momentum and good parity), N_w is of the order of few hundreds, and if the projector to good angular momentum and parity is applied in eq. (1), only several tens are necessary. Of course the number N_w also depends on the desired degree of accuracy. If mathematically exact energies are computed, N_w would equal the size of the Hilbert space. A reasonable level of accuracy is $\sim 100\,\text{KeV}$.

The ansatz eq. (1) is sufficiently powerful to allow even for the description of short-range correlations. In ref. [22] the method has been applied to a schematic model of fermions interacting with a short-range strongly repulsive potential and it has been shown that the probability of having any two particles at distances comparable or smaller than the range of the core, is negligible. This is due to nearly complete cancellation of direct and exchange contributions to the two-particle probability. In the cases studied in this work, however, we use microscopically derived two-body effective potentials, and this capability is not essential.

These considerations provide a strong motivation to apply this scheme to the nuclear-structure problem starting from bare nucleon-nucleon potentials. In this work we use the potential AV8' (ref. [23]), which is the isospin-conserving version of AV18 (of the electromagnetic part only the isoscalar part of the Coulomb potential is retained and the isovector and isotensor parts are discarded).

The calculation discussed in this work consists of several steps. We first renormalize the nucleon-nucleon potential along similar lines of the NCSM. Then we first solve the angular momentum (either full or only J_z projected) and/or parity projected Hartree-Fock problem, then we increase the number of wave functions in eq. (1) and determine the new ones with the energy minimization requirement. To end up with a small number of wave functions at the end of the calculation, we often redetermine the previous ones since these were determined with a smaller number of Slater determinants, for example for $N_w = 5$ we replace the Hartree-Fock wave function with a new Slater determinant, and so on. Experience with this, and with other potentials not reported in this work, has led us to exclude single-particle wave functions with orbital angular momentum larger than 4 from the single-particle space, at least for the nuclei we studied and for the values of the oscillator frequency $\hbar\Omega$ we have used. This is computationally very useful since large l values contribute the most to the size of the single-particle space and, as a consequence, to the size of the Hilbert space. The correctness of this assumption is justified also (rather than repeat the calculation for the energy) by looking at the fractional number of particles in a given n, l orbit.

We stress that the calculations reported in this work are not fully equivalent to the NCSM approach. In the NCSM approach the many-body basis consists of all $N\hbar\Omega$ excitations above the lowest unperturbed configuration, in

order to ensure the exact separation between intrinsic and center-of-mass spectrum. Instead, we work with a specified number of harmonic-oscillator major shells. Hence, we consider a rather large number of $N\hbar\Omega$ excitations above the lowest spherical configuration, but not all $N\hbar\Omega$ excitations are included. Solely the ones that can be built with a specified number of major shells. Moreover, we consider only the intrinsic Hamiltonian $\hat{H}_{int}$, rather than $\hat{H}_{int}+\beta\hat{H}_{cm}$, where the center-of-mass Hamiltonian $\beta\hat{H}_{cm}$ is added in order to shift at high energy the excitations of the center of mass. Because of this approach to the center-of-mass motion, we expect some differences in the results compared to the NCSM approach. Once we fix the single-particle space and the harmonic-oscillator potential, the matrix elements of the intrinsic Hamiltonian are determined by the Lee-Suzuki procedure and by the Talmi-Moshinski transformation.

The outline of this paper is as follows. In sect. 2 we give the details of the renormalized Hamiltonian and discuss a subtle consequence of the treatment of the center of mass and in sect. 3 we discuss the results.

2 The effective potential and the Lee-Suzuki method

The first task is to evaluate the matrix elements of the Hamiltonian once a set of major oscillator shells has been selected. The single-particle space is comprised of all harmonic-oscillator (HO) wave functions with orbital quantum numbers n, l satisfying $2n+l \leq N_{lab}$. We stress at the outset that although the effective potential is extracted from the Hamiltonian containing an HO potential acting on the center of mass (c.m.) as done in ref. [9] in the NCSM approach, the Hamiltonian we use in the actual variational calculation is the intrinsic Hamiltonian. We follow closely the notations and the method of ref. [9]. However, as explained in the introduction, we do not impose any restriction on the number of excitations across harmonic-oscillator shells as normally done in the NCSM. More precisely, we take into account all possible excitations that can be obtained with the selected single-particle space.

The Hamiltonian for A particles is

$$\hat{H} = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j} V_N\big(r_{ij}\big) = \hat{H}_{int} + \frac{P_{cm}^2}{2mA}\,, \qquad (4)$$

m being the nucleon mass, V_N the nucleon-nucleon potential, r_{ij} is the distance between particles, P_{cm} is the total momentum and $\hat{H}_{int}$ is the intrinsic Hamiltonian. As in ref. [9], we add an harmonic potential to the center of mass. That is, we take for the renormalization procedure

$$\hat{H}_{\Omega} = \hat{H}_{int} + \hat{H}_{cm} = \hat{H} + \frac{1}{2}mA\Omega^2 R_{cm}^2 = \sum_{i=1}^{A} h_i + \sum_{i<j} V_{ij}^{(A)}, \qquad (5)$$

with

$$V_{ij}^{(A)} = V_N\big(r_{ij}\big) - \frac{m\Omega^2}{2A} r_{ij}^2, \qquad (6)$$

and

$$h_i = \frac{p_i^2}{2m} + \frac{1}{2}m\Omega^2 r_i^2. \qquad (7)$$

$\hat{H}_{cm}$ in eq. (5) is the harmonic-oscillator Hamiltonian of the center of mass. The renormalization prescription of Lee and Suzuki consists in replacing the Hamiltonian of eq. (5) with an effective Hamiltonian in the many-body shell model space (the so-called P-space), which has the same spectrum of the original Hamiltonian in the full Hilbert space. A necessary condition is that the effective Hamiltonian should not have matrix elements between the model space and the excluded part of the Hilbert space (the so-called Q-space). This is usually done with a cluster approximation. At the level of two-particle cluster approximation (ref. [9]), the Hamiltonian which is renormalized is the A-dependent two-particle Hamiltonian

$$\hat{H}_{12} = h_1 + h_2 + V_{12}^{(A)}. \qquad (8)$$

At this level of approximation, the bare potential is replaced with an effective two-body potential which is dependent on the particle number A and the harmonic-oscillator frequency $\hbar\Omega$. Strictly, the exact procedure generates many-body forces. Since as the dimensionality of the P-space is increased one tends to recover the original bare Hamiltonian, these many-body forces become less and less important. Therefore the two-particle cluster approximation is sufficiently accurate if by increasing the size of the model space, the results for the energies remain constant. The effective potential is most easily determined by separating the center of mass and relative coordinates in eq. (8) as done in ref. [9]. The P-space for the two-particle system is comprised of all harmonic-oscillator wave functions in the center of mass having quantum numbers n, l satisfying $2n+l \leq 2N_{lab}$, while the Q-space of all HO states not included in the P-space, up to $2n+l \leq 200$. We included all possible j values, although $j > 6$ give a negligible contribution. The required radial integrals were evaluated using a large box of length up to 40 fm with typically 2500 integration points.

For a discussion and the details of the renormalization prescription we refer the reader to ref. [9] and references in there. As discussed in the next section, the two-particle cluster approximation seems to be reasonably accurate already at $N_{lab} = 5$, at least for the cases considered in this paper.

Once the matrix elements of the renormalized two-body Hamiltonian have been determined, we transform the matrix elements to the laboratory frame using the Talmi-Moshinky transformation brackets (TMB). We have used the recent implementation given in ref. [24]. The intrinsic Hamiltonian is

$$\hat{H}^{int} = \sum_{i<j} \left[V_{ij}^{eff} + \frac{1}{A}\left[\frac{\big(p_i - p_j\big)^2}{2m} + \frac{1}{2}m\Omega^2(\vec{r}_i - \vec{r}_j)^2 \right] \right]. \qquad (9)$$

The $(\vec{r}_i - \vec{r}_j)^2$ in the above equation cancels out the corresponding term in eq. (6). The relevant transformation law for the two-body matrix elements is the following. If we consider the L-S coupling scheme (the early versions of the computer programs used in this work were written in this scheme), the transformation reads

$$\begin{aligned}
&\langle n_a l_a n_b l_b L_{ab} S J T | \hat{H}^{int}_{1,2} | n_c l_c n_d l_d L_{cd} S J T \rangle = \\
&\sum_{nn'll'\lambda\mathcal{N}\mathcal{L}} \langle n_a l_a n_b l_b; L_{ab} | nl\mathcal{N}\mathcal{L}; L_{ab} \rangle \\
&\times \langle n_c l_c n_d l_d; L_{cd} | n'l'\mathcal{N}\mathcal{L}_{cd}; L_{cd} \rangle (-1)^{L_{ab}+L_{cd}} \\
&\times \sqrt{\hat{L}_{ab}\hat{L}_{cd}} \begin{Bmatrix} l & S & \lambda \\ J & \mathcal{L} & L_{ab} \end{Bmatrix} \begin{Bmatrix} l' & S & \lambda \\ J & \mathcal{L} & L_{cd} \end{Bmatrix} \\
&\times \langle nlS\lambda T | \hat{H}^{int}_{1,2} | n'l'S\lambda T \rangle. \qquad (10)
\end{aligned}$$

In the above equation $\hat{L} = 2L + 1$. The quantum numbers n, l are the radial quantum number in the relative coordinate and the relative orbital angular momentum, respectively. $\mathcal{N}$, $\mathcal{L}$ are the corresponding ones for the center of mass. λ is the angular momentum in the center of mass of the two particles.

In the j-j coupling scheme (implemented in the more efficient computer programs used in this work), the above matrix elements are transformed using the 9-j coupling coefficients.

As mentioned in the introduction the ansatz of eq. (1) is used with angular-momentum projectors (either partial projectors to good J_z values or the full projector to good values of J^2 and J_z) and with the projector to good parity (both not explicitly written down in eq. (1)). It is easy to work with the projectors written in the laboratory frame. However, since we use the intrinsic Hamiltonian, we should use the projectors in the center-of-mass frame. That is, the angular momentum we use, is the total angular momentum (intrinsic + center of mass). However, since we determine the lowest eigenstates of the intrinsic Hamiltonian, in the limit of a large number of Slater determinants, eq. (1) must give an eigenstate of the intrinsic Hamiltonian, that is, in this limit,

$$\psi(\vec{r}_1, \ldots, \vec{r}_A) = \psi_{int}(\vec{r}\,'_1, \ldots, \vec{r}\,'_A)\phi_{cm}\big(\vec{R}_{cm}\big), \qquad (11)$$

where $\vec{r}\,'_1, \ldots, \vec{r}\,'_A$ are the position vectors of the nucleons in the center-of-mass frame (we omitted the spin and isospin indices for simplicity). The function $\phi_{cm}(\vec{R}_{cm})$ is not, in some obvious way, an eigenstate of the center-of-mass harmonic-oscillator Hamiltonian, since this term is not included in the variational treatment. For what we know, it is simply a normalization constant, which can only depend on the c.m. coordinates. The projectors are the appropriate ones if the center of mass is in an S state. Let us assume for the sake of argument that we are using the J^2, J_z projector. If we are determining the states with high excitation energy, than the intrinsic wave function could have an intrinsic angular momentum different from the desired one. For the ground state, the above objection does not pose a problem, because the requirement of energy minimization will generate the lowest intrinsic energy. However, for excited states, it is necessary to evaluate the energy of the center of mass in order to rule out the possibility that we are determining a wave function with the lowest intrinsic state and an excited center-of-mass wave function. As discussed in the next section, for the excited states considered in this paper, we found that ϕ_{cm} has an harmonic-oscillator energy close to the value $3\hbar\Omega/2$ and hence it is almost in the $0S$ eigenstate. We ascribe the small discrepancy to an imperfect minimization, a not sufficiently large number of Slater determinants and to the truncation of the single-particle space. Therefore, the requirement that eq. (1) give the minimum of the intrinsic energy for a given total angular momentum will generate the correct intrinsic state provided the minimization is exact and provided we are not looking for highly excited eigenstates with low angular momemtum. For example, if we would attempt to determine a highly excited eigenstate with, say $J = 2$, we cannot exclude that we would determine a D state for the center of mass and a lowest $J = 0$ intrinsic state. Since we are interested in the first few low-energy intrinsic states, this problem does not appear. If we were interested in highly excited eigenstates, it is safer to consider $\hat{H}_{int} + \beta\hat{H}_{cm}$, with a reasonably large value of β (see also ref. [25]). Inaccuracies due to the finite size of the space should become smaller as we increase the number oscillator shells. We have used the intrinsic Hamiltonian, rather than $H_{int} + \beta\hat{H}_{cm}$, since as we increase the number of Slater determinants convergence is faster.

The standard method to exactly factorize the wave function in an intrinsic wave function and a center-of-mass wave function is by considering as a many-body basis all possible $N\hbar\Omega$ excitations up to some $N_{max}\hbar\Omega$, since the center-of-mass Hamiltonian preserves the number of oscillator quanta. This however poses a conceptual problem. The intrinsic Hamiltonian does not conserve the number of oscillator quanta and therefore it can generate states outside of the model space which violates the basic requirement that the renormalized Hamiltonian should not couple the model space with the excluded space. Consider for example the case of ^{4}He with all possible $4\hbar\Omega$ excitations. There are non-zero matrix elements of the type $\langle N = 2N = 1 | H_{int} | N = 1N = 0 \rangle$, for example the antisymmetrized coupled to $J = 0$, $T = 0$ matrix elements $\langle 1s1/2, 0p1/2 | H_{int} | 0s1/2, 0p1/2 \rangle$. Acting on a configuration containing one nucleon in the $N = 0$ shell and 3 nucleons in the $N = 3$ shell, of the type $|(N = 0)^1(N = 1)^3\rangle$, it generates a configuration of type $|(N = 1)^3(N = 2)^1\rangle$ which is a $5\hbar\Omega$ excitation. The same matrix elements acting on a configuration of the type $|(N = 0)^1(N = 1)^2(N = 2)^1\rangle$ will generate a $6\hbar\Omega$ excitation. As the number of $\hbar\Omega$ excitation is increased the terms which couple the model space and the excluded space will be less and less important. Similarly, in all approaches that use a specified number of major shells (as the one used in this work), the approximate treatment of the center of mass will become increasingly accurate as more oscillator shells are included in the model space.

In principle, the value of $\hbar\Omega$ can be arbitrary. We considered the value that minimizes approximately the

Table 1. Dimensionality of the Hilbert space d_H for for nuclei labeled by N and Z for several J_z and N_{lab} values. For $N_{lab} = 5$ only states with $l \leq 4$ were kept.

N	Z	J_z	N_{lab}	d_H	N	Z	J_z	N_{lab}	d_H
8	8	0	4	5.01889×10^{18}	8	8	0	5	3.36507×10^{20}
8	8	1	4	4.96969×10^{18}	8	8	1	5	3.33242×10^{20}
8	8	2	4	4.82493×10^{18}	8	8	2	5	3.23633×10^{20}
6	6	0	4	1.09991×10^{15}	6	6	0	5	2.47508×10^{16}
6	6	1	4	1.08602×10^{15}	6	6	1	5	2.44395×10^{16}
6	6	2	4	1.04538×10^{15}	6	6	2	5	2.35285×10^{16}
3	3	0	4	264, 638, 868	3	3	0	5	1.22122×10^{9}
3	3	1	4	258, 315, 270	3	3	1	5	1.19202×10^{9}
3	3	2	4	240, 224, 412	3	3	2	5	1.10847×10^{9}

Hartree-Fock energy, as a function of $\hbar\Omega$. The value obtained for a given N_{lab} was used also for the other choices of N_{lab}. For ^{6}Li, $\hbar\Omega = 10\,\mathrm{MeV}$, for ^{12}C, $\hbar\Omega = 11\,\mathrm{MeV}$, and for ^{16}O, $\hbar\Omega = 12\,\mathrm{MeV}$.

3 Results

In this section we shall discuss the results. For $N_{lab} = 3$ we have 80 nucleon states, for $N_{lab} = 4$, 140 nucleon states and for $N_{lab} = 5$, excluding $l > 4$, we have 180 nucleon states. The dimensionality of the Hilbert space (for a specified J_z) is shown in table 1, for the nuclei under study. We omitted the single-particle states with $l > 4$ since these single-particle states are never appreciably populated for the nuclei and levels considered in this work.

We focused on heavy systems in the *sp* region because of the large dimensionality of the Hilbert space, especially for ^{16}O.

Before discussing the results, we briefly recall how the calculation has been performed, a more detailed discussion can be found in ref. [15]. We use a partial projector to good z-component of the angular momentum J_z and parity. The number of Slater determinants needed to minimize the intrinsic energy strongly depends on the type of projector. With the aforementioned projector we need few hundred J^π_Z Slater determinants. A full three-dimensional angular-momentum projector would give more detailed information by changing the angular momentum and parity. With the partial projector we obtain the lowest state with a specified J^π_z. The initial start is the Hartree-Fock solution. We progressively increase the set of Slater determinants (addition step) by adding a trial Slater determinant initially a $0\hbar\Omega$ with a random component (about 20%), we optimize this added trial state with energy gradient methods and with the Broyden-Fletcher-Goldfabr-Shanno (BFGS) method (ref. [26]) as done in ref. [19]. Once the energy has been minimized we vary anew all the Slater determinants in the set several times using only the BFGS method (recycling step). Once the energy no longer decreases, we increase the set of Slater determinants again by adding one more state (typically this added state is always the same) and we repeat the procedure by varying again all members of the set. We alternate the addition steps with the recycling steps. Since the recycling steps can be time consuming (we have used personal computers), we apply it fully only if the set contains few members, otherwise we apply it once the set contains several new members. For sets with more than one hundred states this recycling step is omitted and we apply only the addition steps. The ansatz of eq. (1) is capable anyway to reach the exact ground state (with the specified J^π_z) in the limit of large number of Slater determinants. The final number of Slater determinants strongly depends on whether this recycling step is applied. Since, as we increase the set (even for large sets the energy still decreases, although by small amounts), we performed a final calculation with the final set using the full three-dimensional angular momentum and parity projector, in order to get rid of the small components in the wave function having angular momentum different from the desired one. In other words, the addition and recycling steps are of the type Variation After (partial) Projection (VAP) and at the end we re-evaluate the energies Projecting without Variation (PAV) (these terms are not used here with the meaning usually given, since they both will give the correct wave function without model assumptions). This last PAV step decreases the necessary number of Slater determinants by about a factor of 2–3. If excited states with specified quantum numbers are desired, only full angular-momentum projectors can be used (and this PAV re-evaluation is not necessary), and orthogonalization against the previously determined eigenstates must be performed (as in the EXCITED VAMPIR method of ref. [19]). The convergence of the energies as a function of the number of Slater determinants is smooth for the VAP calculation and less so, but faster, for the PAV phase.

We considered first ^{6}Li. In fig. 1a we show the convergence of the energies for the 1^+ ground state and in fig. 1b we show the corresponding PAV energies.

The energy convergence is very satisfactory. The final VAP energies in MeV of fig. 1a are -28.06, -28.942 and -29.008 for $N_{lab} = 3$, 4, 5, respectively. The final energies of the PAV calculation are -28.258, -29.002 and -29.183 for $N_{lab} = 3$, 4, 5, respectively. The near overlap of the $N_{lab} = 4$ and $N_{lab} = 5$ curves in fig. 1a and in fig. 1b shows

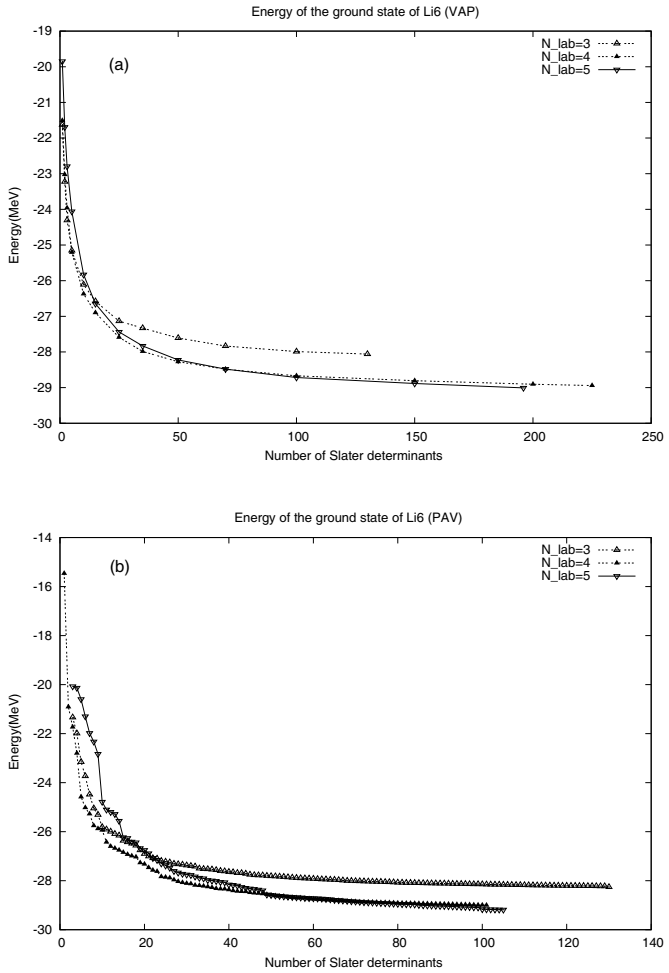

Fig. 1.

nicely that the Lee-Suzuki renormalization prescription converges rather rapidly already with 5 major oscillator shells ($N_{lab} = 4$).

In principle the Lee-Suzuki method, if carried out exactly, is as difficult as the full many-body problem. From a two-body Hamiltonian, it generates two-body, three-body, etc. forces. We include in our calculation only the two-body part of the renormalized Hamiltonian. This is an approximation (the 2-particle cluster). As the model space is increased ($N_{lab} \to \infty$) we recover the original bare Hamiltonian, that is, these many-body forces become more and more irrelevant and the calculation becomes increasingly exact. The fact that already with $N_{lab} = 4$ and $N_{lab} = 5$ we obtain nearly the same values points out that already with 5 and 6 major shells these many-body forces have a negligible effect. Even with 4 major shells the effect of these effective many-body forces is less than 1 MeV. The exact limiting values for the energies are never exactly reached (we would need a very large number of Slater determinants). From the variation of the energies in the end part of the curves, we estimate about one hundred KeV of possible further decrease. This should be regarded as a rough order of magnitude estimate. Interestingly, the PAV calculation shows that not the all set of Slater determinants obtained in the VAP phase, are necessary.

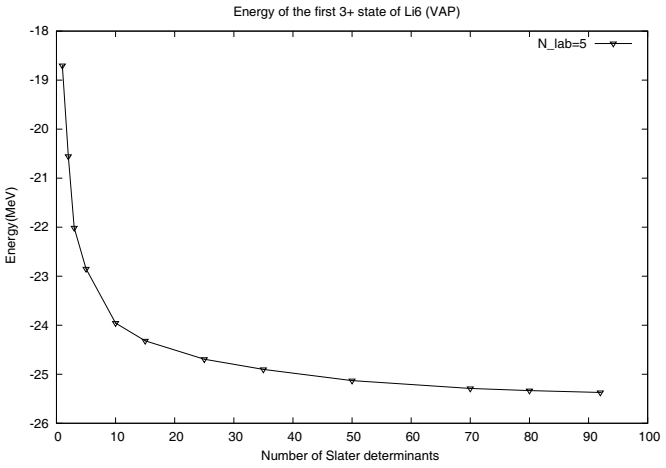

Fig. 2.

For ^{6}Li and with this potential, a GFMC calculation was performed in ref. [27] giving a ground-state energy of $-28.15(3)$ MeV slightly higher than our result. It should be stressed that in ref. [27] the bare nucleon-nucleon potential has been used. In ref. [28] the NCSM was used for this nucleus with a basis space up to $6\hbar\Omega$ excitations and the obtained value is -28.406 MeV.

We also evaluated the energy of the first 3^+ state. In fig. 2 we show the convergence of the energy for $N_{lab} = 5$. In this case we have used the projector to good $J^\pi_z = 3^+$. The reprojection to good $J^\pi = 3^+$ was not carried out in this case since the gain in energy is not as pronounced as in the cases with lower J values. Again we estimate about one hundred KeV of possible further decrease. The value of the energy for this state is $E = -25.371$ MeV. This should be compared with the GFMC calculation of ref. [5] which gives for the first 3^+ state an energy of $-25.33(3)$ MeV and with the NCSM calculation with up to $6\hbar\Omega$ excitations of ref. [28] which gives an energy of -25.42 MeV.

As the next case we considered the ground state of ^{12}C.

The PAV curves for the convergence of the energy for $N_{lab} = 3$ and $N_{lab} = 5$ are shown in fig. 3. The $N_{lab} = 3$

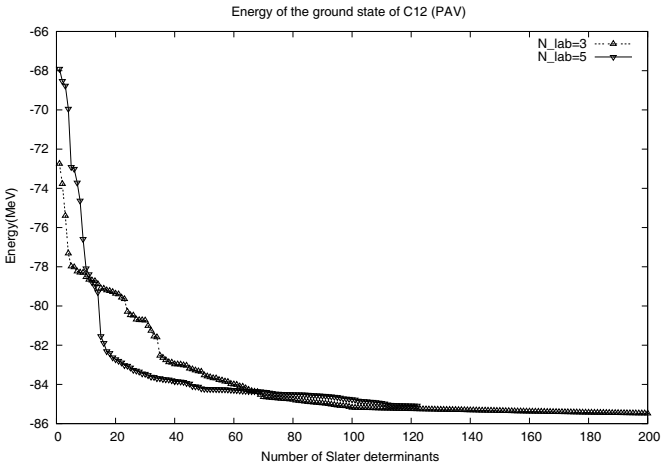

Fig. 3.

Table 2. Fractional number of neutrons (protons) f_n (f_p) for the ground state of ^{16}O and $N_{lab} = 5$ obtained with the first 98 Slater determinants.

n	l	j	f_n	f_p	n	l	j	f_n	f_p
0	0	1/2	1.676911	1.671120	0	2	5/2	0.000524	0.000589
1	0	1/2	0.274256	0.277568	0	2	3/2	0.000269	0.000310
2	0	1/2	0.048696	0.051129	1	2	5/2	0.000295	0.000321
0	1	3/2	2.991101	2.983189	1	2	3/2	0.000159	0.000197
0	1	1/2	1.715886	1.706746	0	3	7/2	0.000077	0.000072
1	1	3/2	0.733862	0.739194	0	3	5/2	0.000061	0.000099
1	1	1/2	0.231867	0.239353	1	3	7/2	0.000068	0.000059
2	1	3/2	0.274324	0.276870	1	3	5/2	0.000055	0.000085
2	1	1/2	0.051536	0.053045	0	4	9/2	0.000017	0.000021
					0	4	7/2	0.000025	0.000022

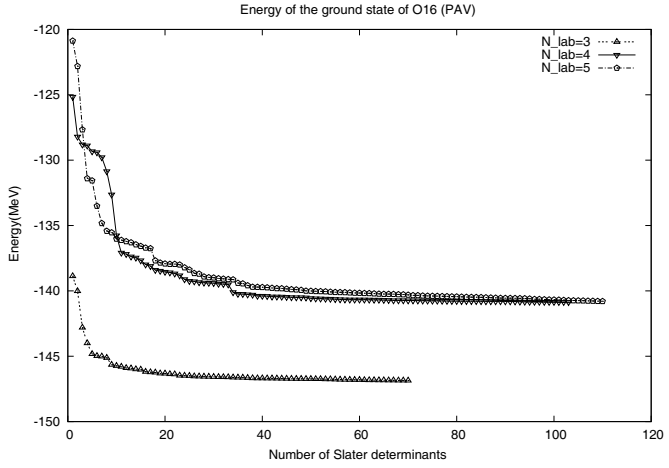

Fig. 4.

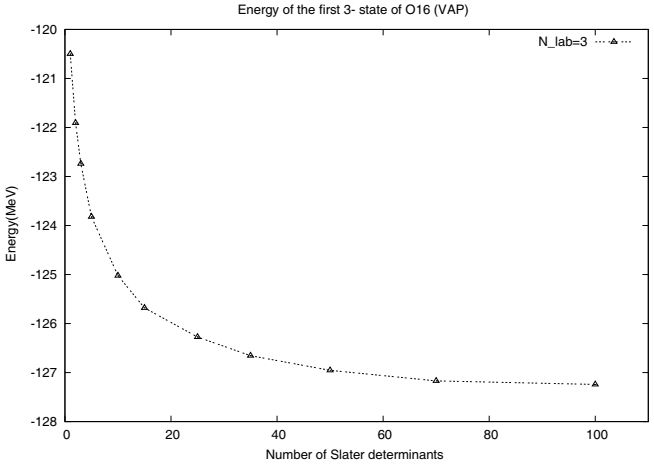

Fig. 5.

case is computationally less demanding and we considered 200 Slater determinants in this case, because of slower convergence. The final energies are in MeV, −85.479 and −85.086 for $N_{lab} = 3$ and $N_{lab} = 5$, respectively. Again $N_{lab} = 5$ (6 oscillator shells) seems to be a sufficiently large space for the convergence of the renormalization prescription. The ground-state energy for this nucleus obtained in ref. [28] with No-Core Shell model method is −85.945 MeV including up to $4\hbar\Omega$ excitations. As mentioned in the introduction, the Hamiltonian matrices in the NCSM and in our method are not completely equivalent, but the agreement is rather good. Both results are about 6 MeV above the experimental value, pointing out to the need of genuine three-nucleon potentials.

As a last case we considered ^{16}O. In fig. 4 we show again the energy convergence for this nucleus.

As it can be seen, $N_{lab} = 3$ is inadequate for this nucleus, the energy obtained is −146.86 MeV, while for $N_{lab} = 4$ and $N_{lab} = 5$ we obtained −140.864 MeV and −140.791, respectively. The experimental value is −127.619 MeV. The AV8' potential overestimates the energy in this case, while in the previous one the binding energy is underestimated. We attempted also to evaluate the location of the first 3^- state (see fig. 5), but the VAP energy, obtained for $N_{lab} = 3$ using 100 Slater determinants is −127.242 MeV giving an excitation of about 19 MeV, too large compared with the experimental value of 6.13 MeV.

Similar difficulties for this state were encountered in the coupled-cluster calculation of ref. [6], using a different two-body potential. Because of such a strong discrepancy with the experimental value the $N_{lab} = 4$, 5 calculations were not carried out.

As mentioned in the previous section, we must test the expectation values of the center-of-mass harmonic-oscillator Hamiltonian in order to make sure that we are evaluating the energy of an excited intrinsic state. For the 3^+ state of ^{6}Li, the expectation value of the center-of-mass Hamiltonian is $\langle \hat{H}_{cm} \rangle - 3\hbar\Omega/2 = 1.34$ MeV. For the first 3^- state of ^{16}O we obtained, for the appropriate value of $\hbar\Omega$ for this nucleus, $\langle \hat{H}_{cm} \rangle - 3\hbar\Omega/2 = 1.75$ MeV. To the extent that our wave functions of eq. (11) are eigenstates, we conclude that $\phi_{cm}(\vec{R}_{cm})$ is an S state. The above expectation values were evaluated using the projectors to $J^\pi_z = 3^+$ and $J^\pi_z = 3^-$ for ^{6}Li and ^{16}O, respectively.

As mentioned at the beginning of this section we omitted all single-particle states having $l > 4$. In table 2 we show the fractional number of particles occupying the single particle orbits n, l, j. As can be seen, the assumption is well satisfied.

The small differences of the fractional number of neutrons and protons are a remnant of the fact the starting Slater determinants for neutrons and protons are different. As it can be seen, the population of high-l orbitals is negligible. From the table one can also notice that the shell closure of $N = 0$ and $N = 1$ oscillator shells is broken.

In conclusion, we have presented in this work *ab initio* calculations of energies using the Hybrid Multideterminant method. The method can in principle be applied also to heavier nuclei, still preserving its *ab initio* features. Moreover, the method can easily be applied to open-shell nuclei. Actually in the *fp* region, this method can naturally describe collective phenomena induced by deformation, if present. So far, collective phenomena have been described using phenomenologically adjusted effective potentials, rather than bare nucleon-nucleon potentials. Other *ab initio* methods, except the coupled-cluster method, cannot easily be used beyond the *sp* region, while the computational effort in our method has a polynomial dependence on the number of particles. In the future we plan to extend the use of our method to other nucleon-nucleon potentials and to other nuclei.

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