Ab-initio calculation of the $^6Li$ binding energy with the Hybrid Multideterminant scheme.

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Abstract

We perform an ab-initio calculation for the binding energy of $^6Li$ using the CD-Bonn 2000 NN potential renormalized with the Lee-Suzuki method. The many-body approach to the problem is the Hybrid Multideterminant method. The results indicate a binding energy of about 31$MeV$, within a few hundreds KeV uncertainty. The center of mass diagnostics are also discussed.

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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, either phenomenological or based on meson exchange theories, such as the Argonne V18 (ref.[1]) and the CD-Bonn 2000 (ref.[2]) or, based on chiral perturbation theory, the N3LO (ref.[3]) NN potential. Accurate predictions at the level of NN potentials are rather important in order to elucidate the role of the NNN interaction which are much more difficult to use in nuclear structure calculations.

Once the NN potential is selected, one is left with the many-body problem to evaluate nuclear properties. There are two main steps in order to achieve this goal. The first step is to renormalize the NN interaction in order to be able to use small model spaces, and the second one is the many-body problem itself. Although for very few nuclei (closed shells) sometimes the bare interaction is used, at the price of very large model spaces (ref. [4]), a popular prescription is the Lee-Suzuki method, (ref. [5]) whereby an effective interaction is constructed in a small model space, typically using an harmonic oscillator basis, or, as in the case of low momentum interactions, a momentum basis (ref. [6] and references in there). A limitation of this approach is that many-body interactions are introduced, and usually one keeps only the two-body part of the renormalized interaction (the 2-particle cluster approximation). As a consequence the independence of the results from the model space must be checked. To further complicate matters, the NN effective interaction derived in this way is not unique, especially because of the hermitization prescription. Although the freedom to hermitize the effective interaction is
large, two prescriptions are mostly used, the one of ref. [5] (known as the Okubo hermitization) and the one of ref.[7], mostly used with low momentum interactions. It is worthwhile to observe that, at least in principle, this freedom could be used to mimic three-body force effects, much in the same spirit it is done with the JISP interactions (ref.[8] and references in there). This could be very useful especially for low momentum interactions.

The second step is the solution of the Schroedinger equation for the nuclei under study. Several methods are available. For example the no core shell model (NCSM) (ref. [9],[10]), which diagonalizes the Hamiltonian renormalized up to a given number of \( \hbar \Omega \) excitations. Or the coupled cluster method (ref.[11] and references in there) whereby the wave function is written as an exponential of one-body+two-body+... operators acting on a reference Slater determinant. The first of these methods, although it is the most used in ab-initio studies of light nuclei, is limited by the large sizes of the Hilbert space. The second of these methods, namely the coupled cluster method, is usually applied at or around closed shells. A third type of methods are based on variational schemes, as the VAMPIR method and its variants (ref.[12]), the Quantum Monte Carlo method (ref.[13]) and the Hybrid Multideterminant method (HMD) (ref.[14]). In this work we shall use this last one which is based on the expansion of the nuclear wave function as a sum of a large number (as many as the accuracy demands) of symmetry unrestricted Slater determinants (SD) with the appropriate angular momentum and parity quantum numbers restored with projectors, the Slater determinants being determined solely by variational requirements. This method does not suffer from the limitation of the size of the Hilbert space, it approaches more and more the exact ground state wave function as the number of Slater determinants is increased,
and furthermore it is equally applicable to both closed and open shell nuclei. So far it has been applied in a no core fashion using the Argonne v8’ NN potential (ref.[14]) and to a phenomenological local potential in order to study shell effects using the bare interaction (ref.[15]). It has also been applied to nuclei in the fp region using phenomenological effective interactions (ref.[16]), however these systems are relatively easy since the bulk of the energies are of single-particle character.

In this work we shall apply the HMD method to $^6Li$ starting from the accurate CD-Bonn 2000 interaction. This nucleus has been extensively studied within the NCSM approach, using both the CDBonn (ref. [17]), the CDBonn 2000 (ref.[18],[19]) and the N3LO interactions (ref. [19]). The motivation to perform a calculation for this nucleus using a different many-body method is the following. An ab-initio calculation requires the results to be independent on the size of the model space and also on the value of $\hbar\Omega$ of the harmonic oscillator single-particle basis, at least within some range of values. So far the calculations reported in the literature using the Lee-Suzuki renormalization prescription show a residual dependence on the value of $\hbar\Omega$. Such a dependence is not seen using soft potentials such as the low-momentum interaction or the JISP16 interaction (cf. ref. [20]). Eventually such a dependence should disappear using larger values of the maximum allowed number of $\hbar\Omega$ excitations ($N_{\text{max}}$). The HMD method does not use $\hbar\Omega$ excitations, but rather utilizes an Hamiltonian in a specified number of major harmonic oscillators shells, which contain a much larger (although not all possible) $N_{\text{max}}$ excitations. We do obtain a weaker dependence on $\hbar\Omega$, but the dependence does not disappear at large value $\hbar\Omega$. However we obtain a much lower value for the ground-state energy, closer to the experimental value.
The HMD method, in its ab-initio form, can be formulated in two different ways. One can construct the effective Hamiltonian directly in the lab frame for a specified number of harmonic oscillator major shells (up to $N_s$ total quantum number) using the standard Talmi-Moshinsky brackets (cf. for example ref.[21]) relating these matrix elements to the renormalized matrix elements in the center of mass frame (HMD-a version). In this case the renormalized matrix elements in the center of mass frame up to $N_{cm} = 2N_s$ total harmonic oscillator quantum number in the center of mass frame are needed. Differently one could first construct the matrix elements of the renormalized Hamiltonian using $N_{cm} + 1$ harmonic oscillator shells and then transform the Hamiltonian to the lab frame using the same number $N_{cm} + 1$ of harmonic oscillator shells (HMD-b version). The difference between the HMD-a and the HMD-b version consists in the fact that the HMD-a version truncates the Hamiltonian used in the HMD-b version. Conversely a large fraction of the matrix elements of the renormalized Hamiltonian used by HMD-b are set to 0, more precisely all matrix elements of the type $\langle ab|H_{\text{eff}}|cd \rangle$ for which the states $a, b$ or $c, d$ satisfy the relation $2n_a + l_a + 2n_b + l_b > N_{cm}$ ($n, l$ being the harmonic oscillator quantum numbers).

The HMD-b version for $A = 2$ is exact in the sense that reproduces to very high accuracy the eigenvalues of the bare Hamiltonian, while the HMD-a version converges to the exact values only in the limit of a large number of harmonic oscillator shells. As a consequence the HMD-a version needs to be validated. For $A = 2$ clearly HMD-b is superior, however we find that for $A = 3$, HMD-b overbinds and that the HMD-a version is superior even for a smaller number of major harmonic oscillator shells. This can be understood by recalling that both versions neglect 3-particle cluster contributions to the renormalized interaction.
and the implication is therefore that HMD-a has smaller 3-particle cluster effects. In other words, the truncation performed in the HMD-a version effectively takes into account at least some of the missing 3-body interaction induced by an exact renormalization, while in the HMD-b version this can be done only by increasing the number of major shells. This is of course a useful result, although empirical. For $^6\text{Li}$ we prefer to use the HMD-a version, since also for this nucleus HMD-b strongly overbinds even compared to the experimental binding energy.

The outline of this paper is the following. In section 2 we discuss the validation of the two versions and of the computer programs and in section 3 we discuss the case of $^6\text{Li}$ and also the center of mass diagnostic recently proposed in ref. [22]. We also discuss a calculation for the $3^+$ excited state.

## 2 Validation of the method.

Both versions of the HMD method start, as in NCSM approach (refs.[9],[10]), from the Hamiltonian

$$\hat{H} = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j} V_{ij} = \hat{H}_{\text{int}} + \frac{P_{\text{cm}}^2}{2mA},$$  

(1)

$m$ being the average nucleon mass for the nucleus under consideration, $V$ the nucleon-nucleon potential, $P_{\text{cm}}$ is the total momentum and $\hat{H}_{\text{int}}$ is the intrinsic Hamiltonian. As in ref. [9], to this Hamiltonian an harmonic potential acting on the center of mass is added, that is

$$\hat{H}_{\Omega} = \hat{H}_{\text{int}} + \hat{H}_{\text{cm}} = \hat{H} + \frac{1}{2} m A \Omega^2 R_{\text{c.m.}}^2 = \sum_{i=1}^{A} \hbar_i + \sum_{i<j} V_{ij}^{(A)},$$  

(2)


with

\[ V_{ij}^{(A)} = V_{ij} - \frac{m\Omega^2}{2A} r_{ij}^2, \]

and

\[ h_i = \frac{P_i^2}{2m} + \frac{1}{2} m\Omega^2 r_i^2. \]

\( \hat{H}_{cm} \) in eq. (2) is the harmonic oscillator Hamiltonian of the center of mass

\[ \hat{H}_{cm} = \frac{P_{cm}^2}{2mA} + \frac{1}{2} mA\Omega^2 R_{c.m.}^2. \]

The Hamiltonian of eq. (2), in which \( A \) is considered as a parameter, is solved for the two-particle systems in an harmonic oscillator basis using a large number of major shells (typically 400 ÷ 500) in all possible angular momentum isospin and \( z \)-projection of the isospin channels \( jstt_z \) in the intrinsic frame of the two-particle system. The number of major shell is taken large enough so that the Hamiltonian can be considered in the "infinite" space (the P+Q space). All integrals are evaluated using typically 2000 integration points. After having done this, the Lee-Suzuki (with the Okubo hermitization) renormalization prescription is performed in which the model space is restricted to the first \( N_{cm} + 1 \) major harmonic oscillator shells (the P space) of the intrinsic frame (cf. also ref. [23] for a very compact derivation). \( N_{cm} \) is taken to be even, as it will clear in the following (\( N_{cm} = 2N_s \)). Once the renormalized \( A \)-dependent Hamiltonian for the two-particle system is obtained, the two-body matrix elements of the effective interaction are extracted and the matrix elements of the intrinsic Hamiltonian of the \( A \) particle system (the original nucleus) are evaluated.

The HMD method can now be branched into two. The two-body matrix elements for the nucleus under consideration can be transformed into the lab frame up to \( N_s + 1 \) major shells (HMD-a version), or can be transformed into the lab
frame up to $N_{cm} + 1$ major shells (HMD-b version). The situation is schematically illustrated in fig. 1. In the HMD-b version all matrix elements having one state in the upper right triangle are set to 0. One can optionally add to the lab frame Hamiltonian a term $\beta (H_{cm} - 3/2 \hbar \Omega)$ as commonly done. The effect of this term due to finite space sizes has been recently analyzed in ref. [22] in order to study unphysical couplings between intrinsic modes and center of mass excitations (cf. next section also). In both HMD-a and HMD-b versions the resulting Hamiltonian is the input for a variational calculation as done in ref. [14]. The variational method in the most recent computer programs is the one discussed in refs. [14],[24]. The wave function is a linear combination of Slater determinants (without symmetry restrictions) with good quantum numbers restored by projectors.

Needless to say HMD-a is computationally cheaper than HMD-b. A 5 major shells calculation with HMD-a translates into a 9 major shells calculation with HMD-b, for example. The details of the optimization techniques will discussed in the next section, since they are the same utilized for the validation. The validation of the whole set of the computer codes is performed first on Deuterium. Actually in this (and only in this case) a numerical cancellation in the renormalization step prevents the exact reproduction of the “bare” eigenvalues. For all other nuclei, the renormalization step reproduces the “bare” eigenvalues belonging to the model space to very high accuracy. For $\hbar \Omega = 16 \, MeV$ with $N_{cm} = 8$ we obtained the renormalized binding energy of deuterium with an error of $0.26 \, eV$ using 15 Slater determinants (projected to $J^{\pi}_z = 1^+$) using the version HMD-b. The situation is different for the HMD-a version since not all matrix elements in the intrinsic frame are used. We therefore expect that the variational calculation will reproduce the renormalized binding energy only in the limit of large $N_s$. We performed some
Figure 1: Schematic representation of the model spaces used in the HMD-a and HMD-b for $N_s = 4$. In the HMD-b all matrix elements in the upper triangle are to 0.
tests for $\hbar \Omega = 12 \text{MeV}$. For $N_s = 4$ the difference between the binding energy obtained by the variational calculation and the exact value is $\delta = 0.041 \text{MeV}$, for $N_s = 5$, we obtained $\delta = 0.026 \text{MeV}$ and for $N_s = 7$ (excluding all states with $l = 7$) we obtained $\delta = 0.012 \text{MeV}$. This test validates both versions of the methods.

We performed also some tests for $^3H$ and $^4He$. For $^3H$ the binding energy obtained with the Faddeev equation method (ref. [25]) using the CD-Bonn 2000 interaction, is $-7.998 \text{MeV}$. In this case both versions can reach the exact value only in the limit of large $N_s$ (or $N_{cm} = 2N_s$). For the HMD-a version and $\hbar \Omega = 16 \text{MeV}$, we obtained a ground state energy (in MeV) of $-8.29$, $-8.30$, $-8.14$, $-8.03$ for $N_s = 3$, $N_s = 4$, $N_s = 5$ and $N_s = 6$ respectively. For low $N_s$, about $35 \div 50$ Slater determinants (with the $J^z$ projector) are needed to converge. For large $N_s$ the number of Slater determinants is larger. For $\hbar \Omega = 18 \text{MeV}$, the ground-state energy in MeV is $-8.183$, $-8.176$, $-8.125$ and $-7.961$ for $N_s = 3$, $N_s = 4$, $N_s = 5$ and $N_s = 6$ respectively. As before, the calculations for large model space are more involved and a large number of Slater determinants is necessary. We estimate a possible further decrease in the energy of few tens of KeV. For larger values of $\hbar \Omega$ the calculation becomes increasingly more difficult for large model space. For $\hbar \Omega = 20 \text{MeV}$ we obtained for the ground-state energy (in MeV) $-8.023$, $-8.044$, $-7.914$ for $N_s = 3$, $N_s = 4$, $N_s = 5$ respectively. The wave functions obtained with the HMD-a version can serve as a variational input for the HMD-b version with $N_{cm} = 2N_s$. For this version we performed only few calculations since the model spaces are very large and the omission of large $l$ values of the single-particle orbits is necessary. As an example for $\hbar \Omega = 16 \text{MeV}$ and $N_{cm} = 6$ omitting all single-particle states having $l$ values larger than $4$ and using
only 15 Slater determinants we obtained a ground-state energy of $-8.843\, MeV$. The inclusion of larger $l$-values and the increase of the number of Slater determinants will necessarily lower the energy. This value should be compared with the value obtained with the HMD-a version which is much closer to the exact Faddeev result.

The only source of discrepancy between the Faddeev result and the HMD-b result comes from the missing 3-particle cluster contributions. The conclusion that we can draw is that the missing 3-particle cluster contributions are strongly repulsive. The effect of such contributions is much smaller in the HMD-a version. One expects that in order to suppress such contributions in the HMD-b implementation one has to increase the number of major shells. For $\hbar\Omega = 18\, MeV$ and $N_{cm} = 8$ we obtained a ground-state energy of $-8.574\, MeV$, in this case we excluded from the calculation all $l > 6$ values. The inclusion of these states will necessarily decrease the energy. The conclusion we can draw form these calculations is that the HMD-b version, although in principle more rigorous, strongly overbinds since it misses 3-particle cluster contributions, which seem less relevant in the HMD-a version. We performed a calculation also for $^6Li$ using the HMD-b version, but even without full convergence to a large number of Slater determinants we obtained strong overbinding. As done in all past calculations with the HMD method, we therefore use only the HMD-a implementation. It is inaccurate only for the 2-particle system, but that is hardly relevant for many-body problems.

Using the HMD-a approach we performed a calculation for the binding energy of $^4He$. We considered a reasonable value of the harmonic oscillator frequency, $\hbar\Omega = 20\, MeV$, rather than a full set of frequencies, and took $N_s = 3, 4, 5, 6, 7$. The ground-state energies are (in MeV) $E = -29.259, -28.504, -27.603, -26.938$
and \(-26.354\) for \(N_s = 3, 4, 5, 6, 7\) respectively. The calculations become increasingly time consuming for large values of \(N_s\). In the case of \(N_s = 6\) we built 150 Slater determinants using the partial \(J^\pi_z = 0^+\) projector and later reprojecting the energies using the full angular momentum projector. For \(N_s = 7\) we took only 100 Slater determinants. The uncertainty in the calculation are about 100\(KeV\) or less and 140\(KeV\) for \(N_s = 7\). The ncsm result from ref. [27] is \(-26.16MeV\), indicating that for \(\hbar \Omega = 20MeV\) a larger number of major shells are necessary for good accuracy.

\[ 3 \quad ^6Li. \]

The nucleus \(^6Li\) with the CDBonn-2000 interaction has been studied in the past in the framework of the NCSM method (ref. [18],[19]). The ground-state energy obtained with this method is \(-29.07MeV\) (the experimental value from ref. [26] is \(-31.994MeV\)). The ab-initio approach imposes at least for some \(\hbar \Omega\) interval constancy of the energies as the model space sizes are increased, and as \(\hbar \Omega\) is varied. We performed several calculations for this nucleus. The most relevant ones are the ones concerning the intrinsic energy. Most often a center of mass term of the type \(\beta(\hat{H}_{cm} - 3\hbar \Omega/2)\), where \(\hat{H}_{cm}\) is the center of mass harmonic oscillator Hamiltonian, is added to the intrinsic Hamiltonian. The effects of the addition of such a term has been recently scrutinized in ref.[22] and the unphysical coupling between intrinsic and center of mass Hamiltonian caused by the finite size of the model space, has been assessed. It was found in ref.[22] that this unphysical coupling using model space defined by a specified number of major shells can
decrease the binding energy in an appreciable way. Here the calculations with the HMD-a method are performed using the intrinsic Hamiltonian. The effect of the addition of the center of mass Hamiltonian will be analyzed at the end of the section. The HMD-a calculations proceed in two phases. In the first phase a large number of Slater determinants, typically $100 \div 400$ is generated using only a partial angular momentum and parity projector to good $J_{z}^{\pi} = 1^{+}$. In the second phase this set is reprojected using the full angular momentum and parity projector $J_{z}^{\pi} = 1^{+}$. At least for this nucleus and for this interaction, we find this optimization technique computationally more efficient than performing from the beginning the variational calculations with the full angular momentum and parity projector.

The first phase is a combination of two steps. We first increase the number of Slater determinants (SD) $N_{D}$ and optimize the last added SD using the steepest descent method, much in the same way it has been done in ref. [14]. In the second step we vary anew all SD’s one at a time using the quasi-newtonian rank-3 update of ref. [24]. This second step is repeated several times until the energy decrease is less than a specified amount. Afterwards, the addition step is repeated. We test the accuracy of the final wave function by plotting the energy vs $1/N_{D}$. As it will be shown, for large $N_{D}$ in many cases the energy is linear in $1/N_{D}$.

The total number of SD necessary to obtain a reasonable convergence varies depending on the model space (typically $N_{D}$ increases as $N_{s}$ is increased and the variational problem becomes harder as $\hbar \Omega$ is increased). It does not seem that $N_{D}$ depends in any obvious way from the sizes of the Hilbert space which can become very large as $N_{s}$ is increased. Actually one the main reasons for using methods such as the HMD, is that the calculations can be performed even
Figure 2: Ground-state energy of $^{12}$C as a function of the inverse of the number of Slater determinants for $\hbar \Omega = 15 \text{MeV}$, $N_s = 3$ and $\beta = 0.5$.

for very large size of the Hilbert space. However feasibility does not necessarily imply accuracy, as the value of $N_D$ necessary to reach a given accuracy could depend on the size of the Hilbert space. We performed a test using a set of 400 SD, for the same interaction, obtained as a part of another calculation for $^{12}$C with $N_s = 3$ (not discussed in this work), $\hbar \Omega = 15 \text{MeV}$ and $\beta = 0.5$. A reprojection was performed as explained above. For $^6\text{Li}$ typical size of the Hilbert space range from about $10^5$ for $N_s = 2$ to about $10^8$ for $N_s = 4$, while for $^{12}$C at $N_s = 3$ the size of the Hilbert space is about $10^{12}$. The calculated value for the ground-state energy of $^{12}$C is $-91.91 \text{MeV}$ (to be compared with the experimental value of $-92.162 \text{MeV}$). In fig. 2 we show the behaviour of $E(1/N_D)$ for large $N_D$. A linear extrapolation shows that a plausible final energy
Figure 3: Ground-state energy of $^6Li$ as a function of the inverse of the number of Slater determinants for $\hbar \Omega = 15\, MeV$, $N_s = 4$ and $\beta = 0$. A similar behavior is also seen for $^6Li$. For comparison in fig. 3 we show the behavior of $E(1/N_D)$ for $^6Li$ at $\hbar \Omega = 15\, MeV$ and $N_s = 4$ with $\beta = 0$. Since there is increase of several orders of magnitude in the size of the Hilbert space from $^6Li$ to $^{12}C$ it is reasonable to conclude that if there a dependence of $N_D$ on the size of the Hilbert space, such a dependence is very mild. The behavior of the energy as a function of $1/N_D$ can change for different $N_s$ in the vicinity of the origin. Sometimes the energy behaves as a higher power of $1/N_D$ especially for small $N_s$. We performed calculations for $^6Li$ for $\hbar \Omega = 10\, MeV,\ 12.5\, MeV,\ 15\, MeV,\ 17.5\, MeV,\ 20\, MeV$. The results are presented in the table. The results for $N_s = 2$ and $N_s = 3$ are well converged. For $N_s = 2$ good convergence is reached using 150 SD’s (however for $\hbar \Omega = 20\, MeV$
Table 1: Ground-state energies for $^6\text{Li}$ for different values of $\hbar\Omega(\text{MeV})$ and different model spaces $N_s$. Energies are in MeV. * Result not fully converged. ** Only 300 SD were used. For $N_s = 4$, 400 SD were employed.

| $\hbar\Omega(\text{MeV})$ | $N_s = 2$  | $N_s = 3$  | $N_s = 4$  | $N_s = 5$  |
|---------------------------|------------|------------|------------|------------|
| 10.0                      | -28.712    | -28.940    | -30.14     | -30.65 **  |
| 12.5                      | -30.707    | -30.558    | -31.18     | -30.99 **  |
| 15.0                      | -31.525    | -31.140    | -31.22     | -          |
| 17.5                      | -31.381    | -30.843    | -30.57     | -          |
| 20.0                      | -30.455    | -30.097    | -29.55*    | -          |

we had to use 180 SD’s. For $N_s = 3$ we used 400 SD’s (450 for $\hbar\Omega = 20\text{MeV}$) and also for $N_s = 4$. The results for $N_s = 5$ should be considered as partial ones (we used a set of 300 or less Slater determinants). In fact the computational cost of the variational calculation depends mostly on the size of the single-particle space. The dependence on the particle number is rather mild.

The calculations for $^6\text{Li}$ were performed without the center of mass Hamiltonian $\hat{H}' = \beta(\hat{H}_{cm} - 3/2\hbar\Omega)$, i.e. $\beta = 0$. In ref. [22], The problem of the effect of the addition of $\hat{H}'$ was studied. The main point in ref. [22] was that the addition of this term can significantly change the evaluation of the intrinsic energies. To be more precise, In a finite space, the eigenstates $|\psi(\beta)\rangle$ of $\hat{H}_{\text{int}} + \hat{H}'$ are not a product of intrinsic eigenstates and center of mass eigenstates. Thus the intrinsic energies, defined as $E(\beta) = \langle \psi(\beta) | \hat{H}_{\text{int}} | \psi(\beta) \rangle$ acquire a $\beta$ dependence. These considerations do not apply to the calculations for $^6\text{Li}$ discussed in this work for the following reason. Our wave-functions are obtained by minimizing the energy expectation value of $\hat{H}_{\text{int}}$. Therefore, since the wave-functions contain 3A space variables, it must factorize into a product of the intrinsic eigenstate and a function (not necessarily an eigenstate) of the center of mass coordinates. The only requirement is that good convergence must be reached.

One can verify, however, the amount of contamination caused by $\hat{H}'$ to the intrin-
sic energies by first minimizing the expectation values of $\hat{H}_{\text{int}} + \hat{H}'$ in order to obtain the wave functions $|\psi(\beta)\rangle$, by evaluating the expectation values of $\hat{H}_{\text{int}}$ with $|\psi(\beta)\rangle$ and then by comparing the energies obtained in this way with the real intrinsic energies. Actually, it is easy to do slightly better than this because of the structure of the HMD ansatz for the wave-functions which are a linear combination of Slater determinants (intrinsic states). The coefficients of this linear combination can easily be determined anew in such a way to minimize the intrinsic energy without a re-variation of the intrinsic states. As an example we consider $N_s = 2$ and $\hbar\Omega = 15\text{MeV}$ and $\beta = 1$. The ground-state energy of $\hat{H}_{\text{int}} + \hat{H}'$ is $-30.354\text{MeV}$ (obtained with 150 SD’s), while the intrinsic energy obtained using this eigenstate of $\hat{H}_{\text{int}} + \hat{H}'$ is $-31.066\text{MeV}$ (the coefficients of each SD was redetermined). This value should be compared with the value given in the table of $-31.525\text{MeV}$. The discrepancy, almost 500 KeV, is appreciable. For this case, i.e. $N_s = 2$ $\hbar\Omega = 15\text{MeV}$ we show in fig. 4 the behavior of $E(\beta)$ as a function of $\beta$.

We also performed a calculation for the excitation energy of the first $3^+$ state, by re-evaluating the $J_z^x = 1^+$ and $J_z^x = 3^+$ states using exactly the same numerical steps (this is necessary since both states contain some error compared to the values for $N_d = \infty$ and these errors cancel out provided the same numerical steps are taken for both states). Only the $J_z^x$ projector has been used. In fig. 5 we show the excitation energy for the $3^+$ state as a function of the number of Slater determinants for $N_s = 4, 5, 6$. The value obtained for $N_s = 6$ is $2.9\text{MeV}$ higher than the experimental value of $2.18\text{MeV}$, but consistent with the ncsim value of $2.86\text{MeV}$.

In conclusion, we have performed an ab-initio calculation of the binding en-
Figure 4: $E_{\text{int}}$ for $^6Li$ for several $\beta$ values with $N_s = 2$ and for $\hbar\Omega = 15\text{MeV}$
Figure 5: $E(3^+)$ for $^6Li$ for $N_s = 4, 5, 6$ and for $\hbar\Omega = 12.5\,MeV$
ergy of $^6Li$ with the Hybrid Multideterminant method in a form that has small 3-particle cluster contributions. The evaluated binding energy is about $31\, MeV$ with an uncertainty of few hundreds KeV. This estimate for the CD-Bonn 2000 interaction is closer to the experimental value than previously thought.
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