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TRANSLATIONALLY-INVARIANT COUPLED CLUSTER THEORY APPLIED TO THE ^{4}He NUCLEUS

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Abstract

In this work we discuss a series of calculations for the ^4He nucleus which have been motivated by the coupled cluster method. For pedagogical reasons we restrict ourselves to the case of pure Wigner nucleon-nucleon interactions. All numerical work is done in the standard harmonic oscillator basis and with an exact treatment of the centre-of-mass motion. Particular emphasis is placed on elucidating the meaning of the coupled cluster wave function and its coordinate-space representation, as well as the relation with a variational-like use of the coupled cluster ansatz.

1. Introduction

Since the original proposal of Coester and Kümmel [1,2] a large amount of work has been carried out within the framework of exp(S) or coupled cluster (CC) theory. A full description of CC theory may be found in the article of Kümmel, Lührmann and Zabolitzky [3] that has become a classical reference in this field. On the other hand, in order to acquire a flavour of the wide domain of applications and the success of CC theory it is suggested that the reader consult the recent pedagogical review given in Ref. [4].

In spite of the many well-recognized successes of CC theory, it is still perhaps true that many of its underlying features remain obscure. As is often the case in many-body theories, the basic ansatz is rather simple. Its physical content is quite clearly established in its starting form for the wave function. However, when going to practical applications, simplicity is lost. The algebraic details of applying the underlying formalism tend to make the theory more and more obscure. Of course, this should be expected, given the richness and rather universal applicability of the CC ansatz. To quote a particular example, the $SUB(2)$ approximation, i.e., considering only $2p-2h$ excitations, in an infinite medium gives for the basic two-body amplitude a non-linear integral equation which contains not only

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Table 1. The ground-state energy of the ^4He nucleus using the MTV interaction, and as obtained by means of various theoretical methods.

Method	Reference	g.s. energy (MeV)
Green Function Monte Carlo	[10]	-31.3 ± 0.2
Coupled Cluster	[11]	-31.36
ATMS (Amalgamation of two-body corr...)	[12]	$-32.8 \leq E \leq -31.3$
Jastrow full Euler-Lagrange variational	[13]	-31.35
Jastrow variational second-order	[14]	-31.19 ± 0.05
Hyperspherical harmonics	[8]	$-31.22 \leq E \leq -30.48$
Yakubowsky equations	[15]	-29.6
Configuration interaction ($10\hbar\omega$) space	[16]	-18.31

such individual contributions as the RPA terms, with Pauli exchanges, the various ladder contributions (hh, pp and ph), the particle and hole potential insertions, among other terms, but also the self-consistent union of *all* such terms iterated simultaneously [5].

The aim of this work is to present with clarity the underlying structure of the CC wave function, as well as to study the characteristics of the energies obtained by solving the CC equations. In order to expose these essential features it is convenient to deal with a rather simplified problem. We found particularly adequate for this purpose the study of the ^4He nucleus where the nucleons interact by means of Wigner-type two-body potentials.

Ignoring the spin and isospin dependence of the two-body interaction undoubtedly means moving relatively far away from the real physical structure of ^4He. For example, we know that the physical nucleon-nucleon interaction has a very important tensor component. Nevertheless, the advantages of working in these simplified conditions are considerable. First of all, we may view the ^4He nucleus under these circunstances as a system of four bosons, with a fully space-symmetric ground-state wave function. This will permit the determination of exact reference or benchmark values, by means of Monte Carlo integration of the many-body equation [6]. In addition, all of the ensuing Fock algebra will deal with bosonic (i.e., obeying commutation relations) creation and anihilation operators.

The second reason is of a didactic character. Our four-nucleon system will be simple enough to permit its study in both Fock and coordinate space. In this manner we will be able to show explicitly the way CC theory describes the nuclear wave function in coordinate space. In turn, this will permit us to connect CC theory with such other theories as the Jastrow variational theory [7] or the hyperspherical harmonics integro-differential equation method [8], which are entirely described in coordinate space.

The last motivation for dealing with this simplified problem is the existence of a large amount of work for the ^4He using the MTV potential of Malfliet and Tjon [9] , and employing both many-body and few-body methods, with which we may compare. A selected set of results concerning the ^4He nucleus with MTV forces is shown in Table 1.

2. Nucleon-nucleon interactions

We have considered four different forms for the two-body nucleon-nucleon interaction which between them cover a wide range of *complexity*. We use this word in the common many-body sense, i.e., interactions with a strong repulsion at short distances are considered *complex*, whereas interactions without core or a quite small one are said to be *simple*. Our aim is then to show the performance of CC theory over as wide a range of problems as our simple model permits.

The simplest potential we use was introduced by Malvin Kalos [17] in a pioneering paper on the application of stochastic methods to quantum systems. It is a fully attractive interaction given by

$$V_K = -72.2 \exp\{-(r/1.191555)^2)\}, \tag{1}$$

and it is included here largely for historical reasons.

Our second potential in order of increasing complexity is the Wigner part of the Brink and Boeker $B1$ interaction [18],

$$V_B = 389.5 \exp\{-(r/0.7)^2\} - 140.6 \exp\{-(r/1.4)^2\}, \tag{2}$$

which has received very much attention in nuclear structure calculations.

The above two interactions are *effective* interactions, which have no direct relation with two-body nucleon-nucleon scattering data. We have also considered two other *realistic* interactions, namely the Wigner part of the $S3$ interaction of Afnan and Tang [19],

$$V_S = 1000\, e^{-3r^2} - 163.35\, e^{-1.05r^2} - 83\, e^{-0.8r^2} - 21.5\, e^{-0.6r^2} - 11.5\, e^{-0.4r^2} \tag{3}$$

and the already-mentioned MTV interaction [9],

$$V_{MTV} = 1458.27 \exp(-3.11r)/r - 578.18 \exp(-1.55r)/r. \tag{4}$$

These last two potentials correspond to the Wigner part of interactions fitted to the $\ell = 0$ two-body phase shifts and to the deuteron binding energy. In each of equations (1-4) the potential is measured in MeV and the internucleon distance r is measured in fm. In order to fix all details of our calculations, we also note that our value for the nucleon mass m has been chosen so that $\hbar^2/m = 41.5\ MeV\ fm^2$.

With the exception of the MTV potential, all of the other interactions are combinations of gaussians. Given that we will work exclusively in the harmonic oscillator basis, all calculations regarding these gaussian interactions can be carried out by means of semi-numerical algorithms. In addition to speeding up the computations, our corresponding calculations will be free of most numerical approximation errors.

3. An irritating question: the centre-of-mass spuriosity

In a light system, like ^4He, the quantum mechanical description may be explicitly written down in terms of a set of intrinsic, translationally-invariant coordinates, such as the Jacobi set of coordinates. The price that has to be paid is that to impose the Bose or the Fermi statistics one has to translate simple nucleon exchange permutations into some much

more complicated transformations among the intrinsic coordinates. On the other hand, in CC theory, as well as in shell-model theory, all states are most readily expressed in terms of the individual nucleon coordinates, referred to some external origin, and because of this the wave function is not translationally-invariant. It is possible to insert by hand some constraint to remove the spurious centre-of-mass coordinate [20], or even to try to remove it optimally [21]. Nevertheless, both of these two approaches will result in tying all of the nucleon coordinates together, thereby converting the calculation of matrix elements of one- or two-body operators into a calculation which involves all of the nucleon coordinates.

There is, however, a special case where the effects of the spurious centre-of-mass coordinate may be removed without paying the heavy price of an intrinsically A-body description. It corresponds to wave functions constructed in a shell model with single particle wave functions from within a harmonic oscillator potential. It is well-known that such a suitably (anti)symmetrized non-interacting many-body harmonic oscillator wave functions ($HOWF$) in which the single particle levels are filled up in order of increasing energy, so that a new major shell is only started when all lower energy shells are completely filled, factorizes into the product of two terms, one depending only on the centre-of-mass (CM) coordinate $\mathbf{R} = \sum_i \mathbf{r}_i/A$, and the other depending only on internucleon distances

$$\Psi_{HOWF}(\mathbf{r}_1, ..., \mathbf{r}_A) = \Psi_{CM}(\mathbf{R}) \prod_{i=1}^{A} \Psi(\mathbf{r}_i - \mathbf{R}), \tag{5}$$

with the centre of mass being in the $0s$ state of a scaled harmonic oscillator. This factorization property permits us to work directly with Ψ_{HOWF}, and all spurious contributions due to Ψ_{CM} may be removed quite easily at the end of the calculations. In this way one can still work with the individual nucleon coordinates, rather than with the much more complicated and less symmetric (under permutations) intrinsic coordinates.

Unfortunately, this property is in general lost when considering the $1p-1h$, $2p-2h$, ... states which are necessary to describe the physical correlations induced in the system by the interparticle forces. There is still a way of removing the spurious CM effect but which is very costly in terms of computational effort [22]. It necessarily involves considering the full space corresponding to a given number of excitation quanta in top of the model non-interacting $HOWF$. In other words, it corresponds to considering all $np-nh$ states with a total harmonic oscillator energy less than or equal to a given energy $N_{max}\hbar\omega$. The disadvantage of this approach is that many of the states which result after the diagonalization of the hamiltonian matrix are not physical, because they correspond to excitations of the centre-of-mass. Moreover, the dimension of the space grows very rapidly with N_{max} [16,23].

We have found a method which produces factorizable wave functions, i.e. which maintains the centre of mass in the $0s$ state. For simplicity of presentation we concentrate on the present ^4He case to discuss the technicalities. The starting state is the non-interacting $HOWF$ in a $(0s)^4$ configuration,

$$\Psi_0 = (4!)^{-1/2} (a_0^\dagger)^4 |0\rangle \tag{6}$$

where the subindex 0 represents the $0s$ orbital. Excitations with respect to Ψ_0 which maintain the basic factorization and preserve the symmetry of the wave function must correspond,

in coordinate space, to at least two-body operators depending only on relative coordinates, i.e., something like $\mathrm{S} = \sum_{i<j} S(r_{ij})$. We note furthermore that $S(r_{ij})$ depends only on the distance between particles i and j in order to maintain the zero angular momentum of the starting wave function. The Fock representation of this operator will be of the type $\mathrm{S} = \frac{1}{2}\sum_{ijkl} S_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$, where each of the indices represents the three quantum numbers necessary to label the single particle wave functions, namely $\{n\ell m\}$. The symmetrized amplitudes S_{ijkl} correspond formally to the matrix element

$$S_{ijkl} = \langle \phi_i(r_1)\phi_j(r_2) + \phi_j(r_1)\phi_i(r_2)|S(r_{12})|\phi_k(r_1)\phi_l(r_2)\rangle/2.$$

The important point here is the strong simplifications which arise in our specific ^4He problem: thus k and l must correspond to $0s$ states, and i and j must couple to zero angular momentum. Finally, when transforming $\phi_i(r_1)\phi_j(r_2)$ to centre-of-mass and relative coordinates, the centre of mass *must* remain in the $0s$ state. Putting all of these constraints together, there results for the operator S the form

$$\mathrm{S} = \sum_{n>0} S_n \sum_{n_i n_j \ell} \langle n\,0\,0\,0\,0|n_i\,\ell\,n_j\,\ell\,0\rangle [a^\dagger_{n_i\ell} \times a^\dagger_{n_j\ell}]^0\, a_0\, a_0, \tag{7}$$

where the amplitudes $\{S_n\}$ are arbitrary. For a given value of n one has to consider *all* possible sets of indices $\{n_i\, n_j\, \ell\}$ which are compatible with the restriction implied in the Brody-Moshinsky bracket $n = n_i + n_j + \ell$. A given value of n thus corresponds to $2n\hbar\omega$ excitation energy and there is hence only *one* $2p-2h$ state with this energy which respects the restriction of zero angular momentum, while maintaining the $0s$ centre-of-mass motion.

We also note that in eq. (7) there appear also terms where $n_i = n$, $n_j = 0$ and $\ell = 0$, as well as $n_i = 0$, $n_j = n$ and $\ell = 0$, which effectively correspond to $1p-1h$ excitations. So, even if we started from a (formally) two-body operator, we have ended up with a mixture of $1p-1h$ and $2p-2h$ operators. Finally, this discussion could also be extended in principle to consider $3p-3h$ and $4p-4h$ excitations from Ψ_0, but for present purposes we restrict ourselves to the $1p-1h$ and $2p-2h$ excitations considered above.

4. Translationally-invariant coupled cluster theory (TICC)

Standard coupled cluster theory assumes for the ground-state wave function the general form

$$\Psi = \exp\{\mathcal{S}_1 + \mathcal{S}_2 + \mathcal{S}_3 + \ldots\}\Psi_0, \tag{8}$$

where each $\mathcal{S}_n$ corresponds to $np-nh$ excitations with respect to some suitable model or reference state Ψ_0. We have shown in the previous section that this ansatz will spoil the centre-of-mass factorizability property and that at least operators $\mathcal{S}_1$ and $\mathcal{S}_2$ must appear in a special combination. Restricting ourselves to $SUB(2)$ approximation, i.e. only up to $2p-2h$ operators, our $TICC$ ansatz will be

$$\Psi = \exp\{\mathrm{S}\}\Psi_0, \tag{9}$$

with S given by eq. (7). Given that ^4He has only four particles, eq. (9) is equivalent to

$$\Psi = (1 + \mathrm{S} + \mathrm{S}^2/2)\Psi_0, \tag{10}$$

and the question now arises as to wether the quadratic terms will also respect the factorization property. The answer is that *they do not*, and that the $TICC$ ansatz must be correspondingly modified by adding a normal-ordering prescription to the exponential of the operator, namely

$$\Psi_{TICC} =: \exp\{S\} : \Psi_0. \tag{11}$$

A particular way of checking this statement is to examine the coordinate representation of Ψ_{TICC}, as will be described in detail elsewere [24]. One has to project over the Fock space field operators [25], and after various Brody-Moshinsky transformations there results the expression

$$\Psi_{TICC}(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4) = \frac{\alpha^6}{\pi^3}\{1+2\sum_n S_n \sum_{i<j} \mathcal{F}_n(r_{ij})+2\sum_{nm} S_n S_m \sum_{i<j} \mathcal{F}_n(r_{ij})\mathcal{F}_m(r_{kl})\}e^{-\alpha^2\sum_{p=1}^4 r_p^2/2} \tag{12}$$

where

$$\mathcal{F}_n(r) = \{\frac{2^n n!}{(2n+1)!!}\}^{1/2} L_n^{(1/2)}(\alpha^2 r^2/2), \tag{13}$$

and where $L_n^{1/2}(x)$ is the usual associated Laguerre polynomial. The last term in the curly bracket of eq. (12) has to be understood in a special way, namely the pair $\{kl\}$ represents the remaining two particles once the pair $\{ij\}$ has been selected. This wave function is not normalized althoug it does obey the so-called intermediate normalization condition, $\langle\Psi_0|\Psi_{TICC}\rangle = 1$. Finally, in these equations we have assumed a harmonic oscillator parameter $\alpha = (m\omega/\hbar)^{1/2}$. We note in addition that the quantities $\mathcal{F}(r)$ represent a relative n, s-wave motion for the pair of particles.

The equation equivalent to (12) but in terms of Fock operators is

$$\Psi_{TICC} = (4!)^{-1/2}\{(a_0^\dagger)^4 + 12\sum_n S_n\Omega_n\, a_0^\dagger a_0^\dagger + 12\sum_{nm} S_n S_m \Omega_n\Omega_m\}|0\rangle, \tag{14}$$

with

$$\Omega_n = \sum_{n_i n_j \ell} \langle n\,0\,0\,0\,0|n_i\,\ell\,n_j\,\ell\,0\rangle [a_{n_i\ell}^\dagger \times a_{n_j\ell}^\dagger]^0. \tag{15}$$

In conclusion, the $SUB(2)$ ansatz for a translationally-invariant coupled cluster theory of ^4He has three kinds of terms. The first is the non-interacting harmonic oscillator ground state corresponding to the first term inside the curly brackets in eq. (12). Then we have terms with only one function $\mathcal{F}_n$ corresponding to the excitation of a pair of particles in all possible ways to a state with relative n and $\ell = 0$ motion, and finally there are other terms in which one pair is excited to $n, \ell = 0$ and the other to $m, \ell = 0$. The unknowns of the problem are the c-number coefficients $\{S_n\}$ which have to be determined by solving the Schrödinger equation.

The problem is thus reduced to solving a set of non-linear algebraic equations for the coefficients $\{S_n\}$ and the energy eigenvalue. There is however another way of viewing eq. (12) which consists of introducing a two-body *correlation function*

$$g(r_{ij}) = \sum_n S_n \mathcal{F}_n(r_{ij}), \tag{16}$$

in terms of which we may rewrite the wave function as

$$\Psi_{TICC} = \frac{\alpha^6}{\pi^3}\{1 + 2\sum_{i<j} g(r_{ij}) + 2\sum_{i<j} g(r_{ij})g(r_{kl})\}\exp\{-\alpha^2\sum_p r_p^2/2\}. \qquad (17)$$

In this form we have only an unknown function $g(r_{ij})$ to be determined. For this function it is possible to write down an integro-differential equation following the CC evaluation method [26] or by means of an Euler-Lagrange variational approach, as in the case of Jastrow correlations [13], or, finally, by following a method similar to the hyperspherical harmonics method of describing nuclei [8]. Actually, if the quadratic terms were omitted from eq. (17) we would have a form for the trial wave function very similar to the one used in the hyperspherical harmonics theory (e.g., see eq. (5) of ref. [27]). For present purposes we have decided to work in the harmonic oscillator basis, by using directly eqs. (12) or (14). In the first case the calculation were carried out by using specific properties of the generating function of the associated Laguerre polynomials. In the second option, eq. (14), we have simply used standard shell-model machinery. Details of the calculations will be published elsewhere [24].

There are several ways of actually using the parametrization given by eqs. (12, 14) which we briefly mention. The first is to consider the linear approximation in which the terms quadratic in the coefficients $\{S_n\}$ are neglected. By minimization of the resulting expectation value $\langle\Psi_{TICC}|H|\Psi_{TICC}\rangle/\langle\Psi_{TICC}|\Psi_{TICC}\rangle$ with respect to the set of coefficients $\{S_n\}$ we will end up with a matrix eigenvalue problem. This is equivalent to a configuration-interaction calculation using a selected set of basis states. The calculations performed in this way will be referred as $LTICC$, L standing for *linear*.

Secondly, we may determine the amplitudes $\{S_n\}$ in the standard coupled cluster way, i.e. by projecting the Schrödinger equation for the full wave function eq. (14) onto the uncorrelated state $(a_0^\dagger)^4|0\rangle$ and onto our special $2p-2h$ states $\Omega_n\, a_0^\dagger a_0^\dagger|0\rangle$. Once a maximum value for $n = n_{max}$ has been assumed, we will thereby end up with $n_{max}+1$ non-linear equations involving the ground-state energy E and the unknown amplitudes $\{S_n\}$. This method will be referred to as $TICC$, namely the standard, translationally-invariant coupled cluster approach.

Thirdly, once the amplitudes $\{S_n\}$ have been determined as above, we can compute the expectation value of the hamiltonian with the already known approximate wave function. This method will be referred to as $\langle TICC\rangle$. The difference between this way of determining the energy and the $TICC$ form gives a measure of the goodness of the coupled cluster approximation.

Fourthly and lastly, one may generalize eqs.(12, 14) by the formal replacement of $S_nS_m \rightarrow C_{nm}$, so that the amplitudes of the quadratic terms are no longer tied to the amplitudes of the linear terms. This is again a configuration-interaction calculation with a larger basis space than in the $LTICC$ approach. This kind of calculation will be referred to as the $QTICC$ method, with Q standing for *quadratic*.

The four approaches have been mentioned in order of computational complexity. For example, at $n_{max} = 29$, which corresponds to $58\hbar\omega$ excitation, the first method requires the computation of $30X30$ matrix elements, whereas the $QTICC$ requires the calculation of

Table 2. The ground-state energy in MeV of ^4He for the four interactions considered. The results shown correspond respectively to a variational calculation with respect to the oscillator parameter α in an uncorrelated wave function given by eq. (6) ($HOWF$), linear CC theory ($LTICC$), standard coupled cluster theory ($TICC$), diffusion Monte Carlo (DMC) and the Jastrow variational method ($JASTROW$). The asterisks indicate results not fully converged.

	METHOD				
POTENTIAL	HOWF	LTICC	TICC	DMC	JASTROW
Kalos	−23.15	−28.74	−28.79	-29.25 ± 0.05	−29.11
B1	−28.16	−37.80	−37.85	-38.5 ± 0.10	−36.44
S3	−5.89	−25.29*	−25.47*	-26.9 ± 0.20	−24.29
MTV	−6.40	−26.77*	−27.06*	-31.5 ± 0.20	−29.48

465 × 465 matrix elements. In any case, these numbers are still very much smaller than the dimensions corresponding to a full configuration interaction calculation [23] in the complete $n_{max}\hbar\omega$ space.

5. Results and discussion

The results of our calculations are shown in Tables 2 and 3, and in Figures 1 and 2. The two figures analyze the convergence of the $LTICC$ calculation in terms of the number of basis states and also in terms of the harmonic oscillator parameter α. We were very surprised by the results displayed in these two figures, as well as the equivalent plots for Fig. 1 in the case of the other three interactions. In order to get convergence it is necessary to go up to $n_{max} \simeq 15$ for the mild interactions (K and $B1$), but even $n_{max} = 30$ is not high enough to get a stabilized result for either the $S3$ or the MTV potentials. Naive (and unjustified) extrapolations to $n \to \infty$ suggest that the ground-state energy will reach values around $-26\,MeV$ for $S3$ and around $-28\,MeV$ for MTV. Unfortunately we could not go even further in our calculations, because it was already necessary at an appreciably lower level to move to quartic precision (128 bits) in order to avoid rounding errors associated with the Laguerre polynomials of correspondingly high orders. In other words, it is clearly not appropriate to work in the harmonic oscillator basis for these model problems. Instead it would have been more convenient to work directly in the coordinate representation. The second property to be stressed is the dependence of the energy on the harmonic oscillator parameter α. We have shown only the case of the $S3$ interaction (see Fig. 1) where there is only a small region around the minimum which can be considered flat. The same happens in the case of the MTV interaction, and also in the case of the smooth interactions K and $B1$, even if in these two cases the flat region is wider. The usual received wisdom in such generalized shell-model calculations is that one expects the results to be independent of the basis, once convergence is reached, but this is clearly not the case for our results. In other words, the $3p-3h$ and $4p-4h$ states which are lacking in our calculation must be responsible for making the comparable plots to those of Fig. 1 flat. Formulated in yet a different way, it is dangerous to extract conclusions about the relative importance of various clusters unless the

Table 3. The ground-state energy in MeV of ^4He for the three interactions of gaussian shape. The calculations correspond to the quadratic configuration-interaction method ($QTICC$), coupled cluster theory ($TICC$), and the expectation value of the energy for the coupled cluster wave function ($\langle TICC \rangle$). In these calculations $n_{max} = 12$ so the $S3$ results are very far from convergence.

	METHOD		
POTENTIAL	QTICC	TICC	⟨TICC⟩
Kalos	−28.873	−28.791	−28.802
B1	−37.193	−37.178	−37.182
S3	−20.216	−20.186	−20.193

proper harmonic oscillator parameter is used. We note that the two main conclusions coming from the analysis of Figs. 1 and 2, namely the need for very large bases, and the residual dependence on the harmonic oscillator parameter, are by no means exclusive to our coupled cluster approach. They also apply to more general configuration-interaction calculations.

The numerical results of our calculations are also shown in Table 2. The column labelled $HOWF$ corresponds to the optimal value for a $(0s)^4$ configuration, and the $LTICC$ and $TICC$ columns correspond respectively to the linear and to the general translationally-invariant coupled cluster calculation. The results are compared with the exact (within statistical errors) results of a diffusion Monte Carlo calculation (column DMC) [24,28] and with the results of a variational calculation for a simple trial Jastrow function depending on three parameters [28]. We see from this Table that the dominant contribution to the energy comes from the linear part of the coupled cluster wave function, the contribution of quadratic terms being a rather small fraction of $1\,MeV$. Focussing attention on our fully converged results, we observe that we are less than $1\,MeV$ from the exact results, thus indicating that $2p-2h$ excitations are by far the most important contribution to the correlated wave function.

Finally, Table 3 is concerned with the goodness of the coupled cluster form of solving the Schrödinger equation. In this Table we show in the column labelled $QTICC$ the results computed as discussed at the end of the preceeding Section, i.e., by decoupling the quadratic terms from the linear terms, and diagonalizing the hamiltonian in our special $2p-2h$ and $4p-4h$ basis with pairs of particles coupled to zero angular momentum. In addition, the third column labelled $\langle TICC \rangle$ corresponds to first performing the standard coupled cluster theory (with translation invariance incorporated, as in column $TICC$) and then taking the expectation value of the energy for the wave function so determined. These three columns should in principle be the same in the case of an exact calculation in which no truncations in the coupled cluster basis are made. Actually they are very close, the difference being less than $0.1\,MeV$, and this clearly implies that the $SUB(n)$ truncation scheme is a very appropriate one. We note that the calculations needed to compute this Table are much more time-consuming than the corresponding calculations shown in Table 2. For this reason, we could not compute with such a very large value of n_{max}, being only able to reach the value of 12. However, the same behaviour was observed at smaller values of n_{max} so that one should

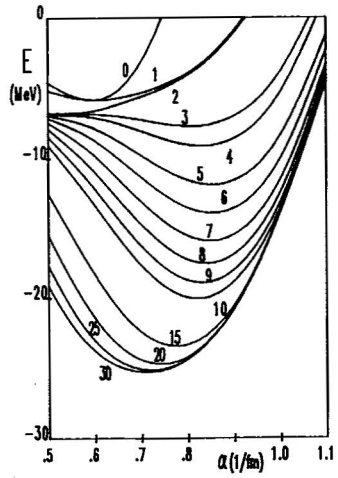

Figure 1: The convergence of the *LTICC* method for the *S3* interaction as a function of the harmonic oscillator parameter α for different values of n_{max}. The curves are labelled by the value of n_{max}.

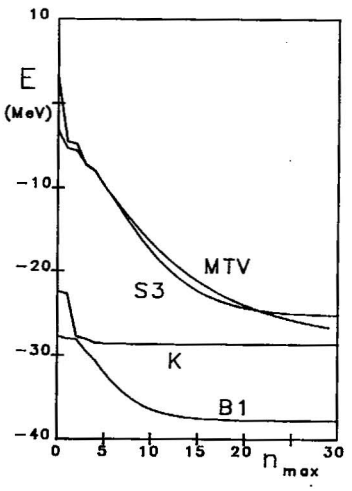

Figure 2: The convergence of the *LTICC* calculations in terms of n_{max} for the four interactions considered. The harmonic oscillator parameter is the optimal value (for $n_{max} \simeq 30$) in each case.

not expect singnificant changes at the higher values of n_{max} needed to attain fully converged results.

The main conclusion of our work is that for this light system the most important part of the wave function may be written in the form $\{\sum_{i<j} f(r_{ij})\}|(0s)^4\rangle$. This form is very similar to that used in the hyperspherical harmonics approximation. Furthermore it corresponds to a configuration-interaction calculation in a special basis and it is also equivalent to a small-correlation expansion of the Jastrow form. Thus, we see rather clearly that all of these theories are very efficient to describe light systems like ^4He. Conversely, the very slow an rather non-uniform approach to convergence of all of our calculations in the harmonic oscillator basis, even when carried out to such virtually unprecedently high levels of excitation energy as the $60\hbar\omega$ reported here must cause grave concern about the efficacy of the standard implementations of the nuclear shell model which aim to go beyond an effective-interaction level of approximation.

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