J. Phys. G: Nucl. Part. Phys. **16** (1990) L61–L66. Printed in the UK

LETTER TO THE EDITOR

On large-scale shell-model calculations in ^{4}He

R F Bishop†, M F Flynn†, M C Boscá‡, E Buendía‡
and R Guardiola‡
† Department of Mathematics, UMIST, PO Box 88, Manchester M60 1QD, UK
‡ Departamento de Física Moderna, Universidad de Granada, 18071 Granada, Spain

Received 1 December 1989

Abstract. Most shell-model calculations of ^{4}He require very large basis spaces for the energy spectrum to stabilise. Coupled cluster methods and an exact treatment of the centre-of-mass motion dramatically reduce the number of configurations. We thereby obtain almost exact results with small bases, but which include states of very high excitation energy.

Detailed analysis of the ground-state energy as well as the $T = 0$ spectrum of ^{4}He [1, 2] resulting from effective interactions like the B1 interaction of Brink and Boeker [3] and the V7 interaction of Volkov [4], or from quasirealistic interactions like the MTV potential of Malfliet and Tjon [5], have led to the conclusion that very large configuration spaces are necessary to obtain stabilised results. Even in a space including up to 10 $\hbar\omega$ harmonic oscillator excitation energies, which corresponds to a total of 2765 antisymmetrised states [2], the resulting ground-state energies are not very much different from the energies obtained by using a simple $(0s)^4$ wavefunction, and are still quite far from the values which may be obtained by means of well established many-body theories.

This is illustrated in table 1 for the V7 and B1 interactions. The first row corresponds to the energy obtained from a $(0s)^4$ harmonic oscillator wavefunction, optimised with respect to the single variational parameter $\alpha = (m\omega/\hbar)^{1/2}$. The second row corresponds to a correlated wavefunction of the simple Jastrow form

$$\Psi_J = \prod_{i<j} f(r_{ij})\Psi_0 \tag{1}$$

where Ψ_0 is again the $(0s)^4$ state, and the two-body correlation $f(r)$ has been taken to be of the simple form

$$f(r) = 1 + a \exp[-(r/c)^2] \tag{2}$$

where a controls the depth of the correlation and c its range. The energy values which appear in this second row of the table correspond to the variational minimum with regard to the three parameters $\{\alpha, a, c\}$ of the trial function. The gain in energy with respect to the uncorrelated case is impressive in the case of the B1 interaction, but, surprisingly, is quite small in the V7 case. Certainly the correlation operator $f(r)$ has not enough flexibility to adapt itself to the peculiarities of the V7 interaction.

0954-3899/90/030061 + 06 $03.50

Table 1. Ground-state energies in MeV of ^{4}He calculated with the V7 and B1 interactions. See the text for a full description of the table.

Method	V7	B1
$(0s)^4$	−27.33	−28.16
Jastrow	−27.53	−36.44
DFMC	-28.6 ± 0.1	-38.5 ± 0.1
Full CI ($10\hbar\omega$)	−28.0	−28.7
TICI2	−28.6	−37.80

The third row corresponds to the exact, within statistical errors, ground-state (GS) energies obtained by means of the diffusion Monte Carlo (DFMC) method. More details on the application of this method to the ^{4}He case may be found in [6, 7]. There is one characteristic regarding the DFMC calculation which should however be pointed out. For pure Wigner forces the eigenstates must have a definite spatial symmetry. On the other hand, both V7 and B1 interactions have a Majorana space-exchange component and the corresponding eigenstates may have a mixing of components with mixed spatial symmetry. Nevertheless we have consistently assumed a fully space-symmetric ^{4}He wavefunction, so that all our results are, strictly speaking, upper bounds to the GS energy. In other words, this is equivalent to consider only the Wigner part of the interactions. Thus, the third row of table 1 shows the best one can obtain for the GS energy in the subspace of fully spatially symmetric wavefunctions.

Finally, the fourth row corresponds to the full configuration-interaction calculation from [2] which includes all configurations up to $10\hbar\omega$ in excitation energy. The meaning of the fifth row will be discussed later on.

The configuration-interaction results shown in the fourth row are deceptively far from the essentially exact Monte Carlo eigenvalues and, moreover, they are scarcely better than the single-configuration calculation of the first row. Looking to figure 1 of [2] one is led to conclude that the configuration-interaction calculation has already converged. However, we believe that this not the case and that a wrong region of the harmonic oscillator parameter (their b is the inverse of our α) was considered, as discussed below. In order to get better results one should go beyond the $10\hbar\omega$ space, and probably a much higher value of the excitation energy is required. As a consequence, the size of the basis will grow to incredibly high values. Our alternative is to concentrate on a selected subset of configuration-interaction states in such a form that we can incorporate the very high harmonic oscillator excitations required, whereas the size of the basis remains quite small. Of course, we demonstrate that this is possible, while maintaining the translationally-invariant nature of the basis states.

Consider first the question of the centre-of-mass motion. The current point of view of most shell-model practitioners may be concisely but precisely stated by means of the statement due to McGrory and Wildenthal [8]. 'If one works in a harmonic oscillator representation, and if one allows all possible configurations for which the oscillator energy is within $N\hbar\omega$ of the lowest energy allowed configuration, then it is possible to construct a basis in which every basis state is an eigenstate of the centre-of-mass Hamiltonian'. Following this recipe one obtains several replicas of the intrinsic set of states, one on top of each possible centre-of-mass

state, and because of this the true basis set is much smaller than the real basis set in which actual calculations are carried out. Although the above statement is certainly correct, nevertheless the conditions are simply too strong. Actually, it is possible to construct fully factorisable basis states without considering all $N\hbar\omega$ possibilities, and with the centre-of-mass always in the 0s state.

We present a simple pedagogical argument. Let us start from the fully space-symmetric wavefunction Ψ_0 and classify the possible excited states as in coupled-cluster theory [9]. First we should consider $1p$–$1h$ excitations. The lowest energy excitation with the same orbital angular momentum and parity as Ψ_0 corresponds to promoting a particle from the 0s shell to the 1s shell. In the coordinate representation this 1p–1h state will be of the form

$$\Psi_1 = \left(\sum_i r_i^2 + C\right)\Psi_0 \tag{3}$$

and given that $\sum r_i^2 = \sum (\boldsymbol{r}_i - \boldsymbol{R})^2 + AR^2$, where $\boldsymbol{R}$ is the centre-of-mass coordinate and A the number of particles, it is clear that Ψ_1 is actually a combination of two states, one of them having a 0s centre-of-mass motion and the other a 1s motion. If we go on following coupled cluster theory we should include powers (up to four) of this 1p–1h excitation. It is well known that this full wavefunction including 1p–1h excitations and higher powers is fully equivalent to the Hartree–Fock ansatz [9]. However, for present purposes we will not consider these higher powers of the excitations.

The wavefunction Ψ_1 corresponds to a $2\hbar\omega$ excitation, and there is another state with the same energy which corresponds to a 2p–2h excitation where two particles are promoted to the next 0p shell. The corresponding coordinate representation of this state is

$$\Psi_2 = \left(\sum_{i<j} \boldsymbol{r}_i \cdot \boldsymbol{r}_j\right)\Psi_0 \tag{4}$$

and an obvious combination of Ψ_1 and Ψ_2 will produce a new state

$$\Psi_{1,2} = \left(\sum_{i<j} r_{ij}^2 + C\right)\Psi_0 \tag{5}$$

in which the centre-of-mass remains in the 0s state. This 2p–2h excitation would correspond to the first two-body cluster in coupled-cluster theory, and this simple example shows that an appropriate combination of one- and two-body clusters may produce states with the correct desired centre-of-mass properties.

The generalisation is quite straightforward. Consider the operator

$$S = \sum_{i,j} S_{ij} a_i^\dagger a_j^\dagger a_0 a_0 \tag{6}$$

where the indices i and j stand for the set of quantum numbers $\{nlm\}$ necessary to label the single-particle harmonic oscillator states, with the subindex 0 corresponding to a 0s state, and the quantities S_{ij} are arbitrary amplitudes. We want S to be the Fock representation of a rotationally and translationally invariant two-body operator, which will be represented by $S(r_{12})$, so that the amplitudes S_{ij} correspond to the matrix element

$$S_{ij} = \langle \phi_i(r_1)\phi_j(r_2) \mid S(r_{12}) \mid \phi_0(r_1)\phi_0(r_2)\rangle. \tag{7}$$

Equation (7) may be simplified by appealing to the rotational and translational invariance of $S(r_{12})$ by using standard angular momentum coupling techniques as well as a Brody–Moshinsky transformation, with the result

$$S_{ij} = \sum_n \left(\int \phi_{n0}(r) S(r) \phi_{00}(r) \, \mathrm{d}\boldsymbol{r} \right) C(l_i l_j 0 \mid m_i m_j 0) \langle n0000 \mid n_i l_i n_j l_j 0 \rangle, \qquad (8)$$

One should note the implicit Kronecker deltas in both the Clebsch–Gordan and Brody–Moshinsky coefficients.

The integral over the relative coordinate r of the two particles is the only unknown (arbitrary) quantity of (8), and it depends only on n, the principal quantum number describing the relative motion of the two particles. We may call these integrals S_n, the unknown amplitudes, and express the operator which creates our basis states via the formula

$$S = \sum_{n>0} S_n \sum_{n_i n_j l} \langle n0000 \mid n_i l n_j l 0 \rangle [a^\dagger_{n_i l} \times a^\dagger_{n_j l}]^0 a_0 a_0 \qquad (9)$$

where the sum over $\{n_i n_j l\}$ has only the restriction implicit in the Brody-Moshinsky bracket, namely $n = n_i + n_j + l$. The operator multiplying S_n corresponds to a $2n\hbar\omega$ excitation. Note that the sum over $\{n_i n_j l\}$ *must* include the cases in which l is zero and one of n_i or n_j is zero, in order to preserve the translational invariance. This means that (9) includes 1p–1h excitations in addition to the obvious 2p–2h excitations.

The GS energy is now obtained by diagonalising in this (1p–1h plus) 2p–2h translationally invariant configuration-interaction (TICI2) approximation the Hamiltonian matrix in the basis generated by the uncorrelated $(0s)^4$ state, $|\Psi_0\rangle = (a_0^\dagger)^4 |0\rangle$, where $|0\rangle$ is the vacuum, and the further states obtained from it by allowing the operator S of (9) to act on it. In practice, a truncated basis is used by truncating the summation index n at some upper limit $n_{\max}$. The matrix elements are computed by means of the standard shell-model machinery. The results obtained for the GS energy are shown in the last row of table 1. The convergence of the GS energy with the number of basis states is shown in figure 1 as a function of the harmonic oscillator parameter α. We note that Ceuleneer *et al* [2] have chosen the value $\alpha = 0.5\mathrm{fm}^{-1}$ for the full CI calculations of ^{4}He using the V7 and B1 potentials, including all 2765 four-nucleon totally antisymmetric harmonic oscillator shell-model configurations of up to $10\hbar\omega$ excitation energy. It is these results which are shown for comparison purposes in the fourth row of table 1. It is on the basis of our figure 1 that we believe that their choice of $\alpha = 0.5\mathrm{fm}^{-1}$ is a very poor one for both the V7 and B1 potentials, and hence why their results are so close to the uncorrelated results shown in the first row of table 1. This belief is further reinforced by the results shown in the second row of table 1 which were obtained via the simple Jastrow variational ansatz of (1) and (2), and which also includes only two-body correlations. The fact that such dissimilar techniques of incorporating two-body correlations, as the TICI2 and the Jastrow variational methods, each yield about 95% of the binding energy, must inevitably cast strong doubt on the apparent convergence of the results of [2].

We should warn the reader that although our TICI2 calculations involve only relatively few many-body basis states, and hence an extremely simple diagonalisation, the calculations with values of $n_{\max} \approx 30$ are far from being trivial. This is because we still have to calculate the matrix elements of the Hamiltonian in the basis. As observed from (9), this involves the calculation of a very large number of

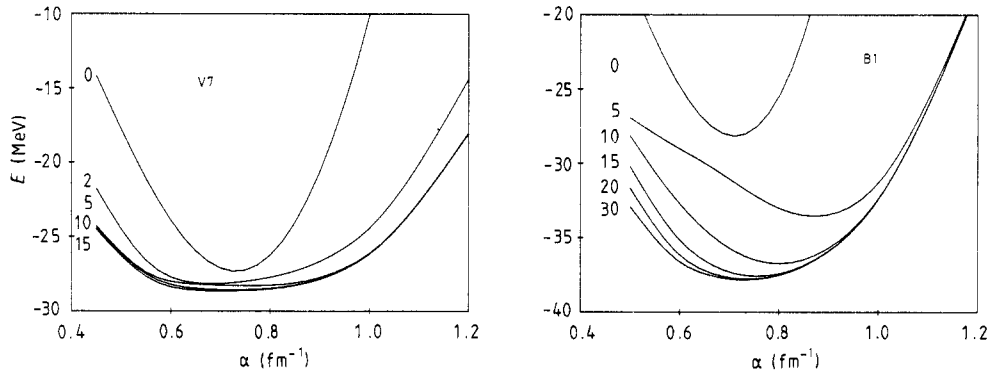

Figure 1. The ground-state energy (MeV) as a function of the harmonic oscillator parameter $\alpha(\mathrm{fm}^{-1})$ for the V7 (left) and the B1 (right) interactions. The numbers close to the curves correspond to the number of basis states $n_{\max}$ given by truncating the sum over the index n in (9).

Brody–Moshinsky transformation coefficients. The computational effect involved in their evaluation is considerable. For potentials like the V7 and B1 interactions considered here, whose analytic form is given purely in terms of Gaussian factors, the resulting equations can also be very conveniently handled in coordinate space, since all of the needed integrals can be performed exactly by suitable recursion formulae.

The results in the last row of table 1 are both stimulating and pleasing: we obtain almost the full binding energy in the two cases considered, and the maximum deviation from the DFMC calculation is just 0.7 MeV for the B1 interaction case. The results plotted in figure 1 also speak for themselves: to reach stability in the GS energy it is necessary to go up to quite high values of $n_{\max}$, at least 10 for the V7 force (this corresponds to a $20\hbar\omega$ space) and up to 20, i.e. a $40\hbar\omega$ space, for the B1 force. The various curves become flatter near the minimum when $n_{\max}$ is high. Nevertheless, there is still a residual dependence upon the harmonic oscillator parameter. Presumably this dependence will disappear when other excitations, i.e. 3p–3h and 4p–4h, are included in the construction of the basis.

Our results are not wholly unexpected. Shell-model calculations in three-body systems have also shown that stability of the results requires a very large basis [10]. However, our most interesting finding is that by choosing specific configurations one can obtain almost all of the binding energy with very few basis states, even when they correspond to high-energy excitation. Unfortunately we do not have any qualitative explanation of why we have *so* good a representation of the GS wavefunction, at least for calculations of the energy, by using only our translationally invariant 2p–2h amplitudes.

We may also determine the excited states of the system. Specifically, the set of eigenvalues resulting from the diagonalisation will correspond to the class of $J^+ = 0^+$ states with fully space symmetric structure. In other words, we should not expect to obtain the experimentally first 0^+ excited state, which may have mixed symmetry, from this calculation. The obvious candidates to be assigned to our excited levels are breathing modes (i.e. monopole resonances) which have the same spatial structure as the ground state. The excitation energies that we obtain for the first monopole resonance are $\Delta E = 26.6$ MeV for the V7 interaction, and $\Delta E = 35.8$ MeV for the

B1 interaction. This last value is not far from the excitation energy of $\Delta E = 33.1$ MeV [11] obtained by means of the generator coordinate method applied to a Jastrow wavefunction. Both of these B1 values are significantly higher than the shell-model value of $\Delta E = 26.6$ MeV [12, 13].

To conclude we would like to make a general point regarding the use of effective interactions in nuclear physics. As we have already mentioned the V7 and B1 potentials are effective interactions, and a calculation involving this class of interactions without any restriction of the basis space cannot be expected to reproduce experimental results. However, it is a common practice, and certainly a perfectly valid approximate procedure, to use an *effective* interaction fitted to a number of nuclear properties, in a *fixed* and highly restricted shell-model space. The well known Skyrme Hartree–Fock calculations or Gogny force calculations are precisely of this type. What is quite clear, however, is that there is no justification to use these same effective interactions in an enlarged space of shell-model configurations without simultaneously readjusting the parameters of the effective interactions. The logical endpoint of such a procedure is clearly to use the bare microscopic internucleon force and no curtailment of the many-body configuration space other than what is permitted by a numerical investigation of the convergence properties. We have also performed similar calculations for more realistic, *microscopic* nucleon–nucleon forces, with the same general observation that convergence is reached only for very high values of n_{max}. What we observe from these results is that the convergence is then so disappointingly slow as to bring into severe doubt the practical implementation of the aim of using realistic microscopic potentials in shell-model calculations of the heavier nuclei.

This work was developed under an Acciones Integradas program between Spain and the United Kingdom. The authors acknowledge the financial support from the corresponding joint committee. MCB, EB and RG are also supported by the *Comisión Interministerial de Ciencia y Tecnología, Spain* under contract 969/87. RFB also acknowledges the support of a research grant from the SERC of Great Britain.

References

[1] Ceuleneer R and Vandepeutte R 1985 *Phys. Rev.* C **31** 1528
[2] Ceuleneer R, Vandepeutte P and Semay C 1987 *Phys. Lett.* **196B** 303
[3] Brink D M and Boeker E 1967 *Nucl. Phys.* A **91** 1
[4] Volkov A B 1965 *Nucl. Phys.* A **74** 33
[5] Malfliet R A and Tjon J A 1969 *Nucl. Phys.* A **127** 161
[6] Bishop R F, Flynn M F, Boscá M C, Buendía E and Guardiola R 1990 *Proc. NATO School, The Nuclear Equation of State* ed W Greiner (New York: Plenum) to be published
[7] Bishop R F, Flynn M F, Boscá M C, Buendía E and Guardiola R 1990 UMIST preprint
[8] McGrory J B and Wildenthal B H 1975 *Phys. Lett.* **60B** 5
[9] Kümmel H, Lührmann K H and Zabolitzky J G 1978 *Phys. Rep.* **36** C 1
[10] Ciofi degli Atti C 1986 *Proc. Primo Convegno su Problemi di Fisica Nucleare Teorica* ed L Bracci, P Christillin, A Fabrocini, S Fantoni, G Fiorentini, M Rosa-Clot, S Rosati, S Servadio and M Viviani (Pisa: ETS, e) p 1
[11] Dehesa J S, Guardiola R, Polls A and Ros J 1982 *Phys. Lett.* **118B** 13
[12] Caurier E, Bourotte-Bilwes B and Abgrall Y 1973 *Phys. Lett.* **44B** 411
[13] Navarro J 1975 *Phys. Lett.* **59B** 15