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Microscopic and translationally-invariant calculations with tensor forces and tensor correlations

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Abstract. In this paper we discuss an approach to the *ab initio* study of ground states of light nuclei using realistic forces. The method constructs trial variational wavefunctions by superimposing state-dependent translationally-invariant pair correlations on a state-independent Jastrow-correlated wavefunction, with very promising results.

1. Introduction

When dealing with finite systems of mutually interacting particles, one of the important difficulties encountered is the proper treatment of the centre-of-mass (CM) motion. There are various techniques to deal with this problem, one of them being the translationally-invariant configuration-interaction (TICI) method [1]. This formalism is inspired by the coupled-cluster method (CCM), but in contrast to this method it is variational, and includes only a linearised correlation operator. It permits an unambiguous removal of the spurious CM motion. The method has mainly been used in a two-body implementation, called TICI2. In recent investigations [2, 3] this method has been extended to deal with saturated nuclei within the 0p shell, using state-dependent (SD) pair correlations between nucleons. Calculations have been performed for various nucleon–nucleon interactions.

In this work we report on an attempt to go beyond our previous TICI2 calculations. We study ^{4}He with tensor forces and tensor correlations. We find that in order to get a good description of the ^{4}He nucleus we need to mix the operatorial structure of the TICI2 wavefunction with a scalar Jastrow-like factor. We hope to use this method as a means of shedding some light on how to improve the prediction of the ground state energy of light and medium-mass nuclei.

2. Formalism

In the coordinate representation, the TICI2 wavefunction takes the form

$$\Psi(r_1, \ldots, r_N) = \sum_{i<j} f(r_{ij})\Phi(r_1, \ldots, r_N). \tag{1}$$

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We introduce state dependence into the pair correlation function f by expanding it in an appropriate operatorial basis, $f(r_{ij}) = \sum_p f_p(r_{ij})\Theta_p(ij)$. This basis is generally chosen to be consistent with that of the inter-nucleon potential. For interactions with the V6 structure, as studied here, the operators used are $\{\Theta_p\} = \{1, P_\sigma, P_\tau, P_\sigma P_\tau, S_{12}, S_{12}P_\tau\}$, where P_σ and P_τ are the spin- and isospin-exchange operators, and S_{12} is the tensor operator.

Results obtained with the ansatz described above show a strong dependence on the shape of the interaction [3], even when the binding energies are predicted to be similar. We find that the competition between the short-range repulsive core in the central force, and the longer range in the tensor force that contributes most of the binding energy, are not easily treated in the TICI2 reference state. This typically manifests itself in a relatively small value for the harmonic oscillator length parameter, which gets even smaller as the central repulsion increases. From this one can conclude that the method suffers a lack of correlations.

One could add additional correlations by employing the full TICC2 machinery, but we are not ready to do so yet. On the other hand, it is known that Jastrow correlations are very well suited to treat the effects of short-range repulsions. Thus we introduce a Jastrow factor into the operatorial TICI2 ansatz. Since we have most repulsion in the central channel, we shall incorporate a scalar Jastrow correlation only. This leads to the so-called J-TICI2 wavefunction

$$\Psi(r_1, \ldots, r_N) = \prod_{i<j} g(r_{ij}) \left(\sum_{k<l} f_p(r_{kl})\Theta_p(kl) \right) \Phi(r_1, \ldots, r_N). \tag{2}$$

To simplify our calculations, we have only used a single Gaussian to define the correlation part of the Jastrow function $g(r) = 1 + a\mathrm{e}^{-br^2}$. Our wavefunction now depends on three parameters, the harmonic oscillator scale factor α, and the amplitude and depth of the Jastrow function, a and b, in addition to the six functions $f_p(r)$. We have to optimize with respect to all these parameters to find the minimum of the energy expectation value $\langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle - E_{\mathrm{CM}}$. Here E_{CM} is the energy in the CM motion.

3. Results and discussion

We have calculated the ground state of the ^{4}He nucleus using several interactions. We have used the V6 parts of the Reid soft-core (REID) [4], the Gogny–Pires–de Tourreil (GPDT) [5], the de Tourreil–Sprung super-soft-core (SSC) [6], and the Argonne v_{14} (AV14) [7] and v_{18} (AV18) [8] potentials. The results for the binding energy of ^{4}He are summarized in table 1. In addition to the TICI2 and J-TICI2 descriptions, we also include calculations with a V6 state-dependent Jastrow correlation computed with the variational Monte Carlo (VMC) method, and also the V6 contribution to the energy computed with the Green function Monte Carlo (GFMC) method. In the VMC method we have used a Jastrow correlation obtained by solving Schrödinger-like equations for each operatorial channel, as in [9].

Table 1. Comparison between different results for the ^{4}He binding energy (in MeV) using several V6 potentials. We have taken from [10] the sum of the kinetic energy and the $\langle V_6\rangle$ part of the potential.

	TICI2	J-TICI2	VMC	GFMC
REID	5.67	22.70	27.82 ± 0.12	28.30 ± 0.12 [10]
GPDT	27.37	27.58	27.71 ± 0.06	
SSC	24.12	26.74	29.20 ± 0.12	
AV14	14.77	20.37	23.24 ± 0.08	24.79 ± 0.20 [11]
AV18	15.40	21.08	24.80 ± 0.09	

We note first that, as already shown in a previous publication [3], the TICI2 results are not very good for strongly repulsive realistic potentials. This was one of the main motivations for the inclusion of Jastrow correlations. Their effect is impressive in some cases, like the Reid one, in which the gain in binding energy is about 17 MeV. With the exception of the very soft potentials such as GPDT, we are still rather far from the VMC and GFMC results [3]. Nevertheless, this hybrid treatment seems to be a promising method to describe these situations.

The optimal values of the HO parameter α in the J-TICI2 wavefunction do not change very much between the various interactions, ranging between 0.71 and 0.78 fm^{-1} and thus giving similar overall sizes for the system. By contrast, the values of the Jastrow parameters show a wider range of variation, reflecting the different short-range behaviour of the potentials.

In conclusion, the results of the Jastrow-correlated TICI2 appear to indicate that this might be a rather good way of describing light systems with realistic interactions. Our results still give several MeV less binding than the much more precise VMC and GFMC calculations. Our belief is that the central part of the correlation used here is too simple, and conclusions about the limitations of our approach must be delayed until we have included a more complex central Jastrow correlation.

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References

[1] Bishop R F, Buendía E, Flynn M F and Guardiola R 1993 *J. Phys. G: Nucl. Part. Phys.* **19** 1163 and references therein
[2] Guardiola R, Moliner P I, Navarro J, Bishop R F, Puente A and Walet N R 1996 *Nucl. Phys.* A **609** 218
[3] Moliner P I, Guardiola R, Navarro J, Bishop R F, Walet N R and Puente A 1998 *Condensed Matter Theories* vol 13, ed J da Providencia and R F Bishop (New York: Nova Science) in press
[4] Reid R V 1968 *Ann. Phys., NY* **50** 411
[5] Gogny D, Pires P and de Tourreil R 1970 *Phys. Lett.* B **32** 591
[6] de Tourreil R and Sprung D W L 1973 *Nucl. Phys.* A **201** 193
[7] Wiringa R B, Smith R A and Ainsworth T L 1984 *Phys. Rev.* C **29** 1207
[8] Wiringa R B, Stoks V G J and Schiavilla R *Phys. Rev.* C **51** 38
[9] Carlson J A and Wiringa R B 1991 *Computational Nuclear Physics* vol 1, ed K Langanke, J A Maruhn and S E Koonin (Berlin: Springer)
[10] Carlson J 1988 *Phys. Rev.* C **38** 1879
[11] Carlson J 1987 *Phys. Rev.* C **36** 2026