LETTER TO THE EDITOR

Diffusion Monte Carlo determination of the binding energy of the ${}^4\text{He}$ nucleus for model Wigner potentials

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Received 24 October 1991

Abstract. The diffusion Monte Carlo method is used to integrate the four-body Schrödinger equation corresponding to the ${}^4\text{He}$ nucleus for several model potentials of Wigner type. Good importance sampling trial functions are used, and the sampling is large enough to obtain the ground-state energy with an error of only 0.01 to 0.02 MeV.

Recently there has been an increasing interest in the search for very precise methods for the description of light nuclear systems. Particular attention has been paid to the study of the ${}^4\text{He}$ nucleus based on nucleon–nucleon interactions of Wigner type, i.e. independent of spin and isospin, and with central radial potentials ranging from such smooth effective interactions as the B_1 form of Brink and Boeker [1] or the v_7 form of Volkov [2], up to the quasi-realistic interactions s_3 of Afnan and Tang [3] and mtv of Malfliet and Tjon [4]. The s_3 and mtv interactions originated from an attempt to explain both the s -wave nucleon–nucleon scattering data as well as the binding energy of light nuclear systems, particularly ${}^3\text{He}$ and ${}^4\text{He}$. In this sense they may be considered as quasi-realistic. Nevertheless, they do not include the very important tensor or spin–orbit components which are required for a detailed fit to the experimental data.

The calculations carried out with these interactions have reached a high degree of precision. Most of these calculations, but not all of them, are based on the variational principle and the basic difference between them lies in the way the two-body and, in general, many-body correlations are described.

Existing approaches are based on such methods as the Jastrow description of the wavefunction [5–7], the Faddeev–Yakubovsky techniques [8], hyperspherical harmonic approaches with independent pair correlations [9–13] or with Jastrow correlations [14, 15], large-basis shell-model techniques of the traditional configuration-interaction kind [16–18], the full coupled cluster theory [19], the ATMS method [20], the coupled rearrangement method [21] and the Green function Monte Carlo method [22]. We have ourselves also developed several closely related techniques based on the translationally-invariant coupled cluster theory [23–29].

The aim of the present work is to obtain with a very high precision the essentially exact estimates for the ground-state energy of ${}^4\text{He}$ with the four previously

mentioned interactions, v_7 , B_1 , s_3 and MTV . Because of the Wigner form of these potentials, we may consider our four nucleons to be four bosons, thus greatly simplifying the application of the DMC method. Our results are intended to serve as an accurate reference for other methods. The approach used is the so called diffusion Monte Carlo (DMC) method [30–33], incorporating importance sampling. We have been able to determine the ground-state energy with a total error, namely a combination of the statistical error and the extrapolation error, of 0.01 MeV for the smooth effective interactions (v_7 and B_1), and 0.02 MeV for the interactions with a strongly repulsive core at short distances (s_3 and MTV).

The DMC method solves stochastically the imaginary-time Schrödinger equation for a system of A particles

$$-\frac{\partial |\Psi(t)\rangle}{\partial t} = (H - E) |\Psi(t)\rangle. \quad (1)$$

In this equation an energy shift E , for the moment of arbitrary value, has been added to the Hamiltonian. The formal solution of equation (1) is

$$|\Psi(t)\rangle = \exp[-(H - E)t] |\Psi(0)\rangle, \quad (2)$$

so that, after a sufficiently long time t , and provided the starting state $|\Psi(0)\rangle$ has a non-null projection on the exact ground state $|\Phi\rangle$ of the system, the solution will tend to

$$|\Psi(t \rightarrow \infty)\rangle \rightarrow C \exp[-(E_{gs} - E)t] |\Phi\rangle, \quad (3)$$

where E_{gs} is the exact ground-state energy of the Hamiltonian and C is a constant, in general unknown, corresponding to the projection $\langle \Phi | \Psi(0) \rangle$. In equation (3) there also appear projections over all other eigenstates of the Hamiltonian, but their amplitudes will drop exponentially with t with respect to the dominant amplitude of the ground state. Equation (3) tells also how the eigenvalue is determined. The otherwise arbitrary energy shift E is adjusted so that the amplitude remains stable, i.e. does not change with time, after a sufficiently long time has elapsed. In this way one obtains both the ground-state wavefunction and its energy. In DMC terminology, this determination of E_{gs} is called the *population growth* estimator.

The DMC method consists in a special procedure for solving equation (1) or its equivalent equation (2). It has three basic ingredients. First, the Green function appearing in equation (2) is approximated by a version valid for small time steps. Large times are reached by repeated application of this small-time Green function, on the starting state. The second ingredient is the way the wavefunction $|\Psi(t)\rangle$ at a given time is represented. In coordinate space, the wavefunction corresponding to the ground state of a bosonic system $\Psi(\mathbf{R}, t) = \langle \mathbf{R} | \Psi(t) \rangle$, where $\mathbf{R} \equiv \{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A\}$, is a positive function which may be interpreted as a multivariate probability distribution function. Then $\Psi(\mathbf{R}, t)$ is represented by a collection of *walkers*, $\{\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_N\}$, which are a collection of $3A$ -dimensional random vectors corresponding to the instantaneous probability distribution function $\Psi(\mathbf{R}, t)$. Finally, an important component of the DMC method is the use of an *importance sampling* driving trial function. This means that instead of solving equation (1), one solves the equation corresponding to a function $f(\mathbf{R}, t)$ defined in terms of the trial function $\Psi_T(\mathbf{R})$ as

$$f(\mathbf{R}, t) \equiv \Psi_T(\mathbf{R}) \Psi(\mathbf{R}, t). \quad (4)$$

The imaginary-time differential equation satisfied by $f(\mathbf{R}, t)$ is

$$-\frac{\partial f(\mathbf{R}, t)}{\partial t} = -D\nabla^2 f(\mathbf{R}, t) + D\nabla \cdot (\mathbf{F}(\mathbf{R})f(\mathbf{R}, t)) + (E_L(\mathbf{R}) - E)f(\mathbf{R}, t), \quad (5)$$

where ∇ is the $3A$ -dimensional coordinate-space gradient operator and $D = \hbar^2/2m$ is called the *diffusion constant*. The quantities which depend on the trial function are the *local energy* $E_L(\mathbf{R}) \equiv (1/\Psi_T(\mathbf{R}))H\Psi_T(\mathbf{R})$, and the *drift force* or, better, *drift velocity* $\mathbf{F}(\mathbf{R}) = 2\nabla \ln \Psi_T(\mathbf{R})$.

Among the various approximations for the small-time Green function [34] appropriate to equation (5) we have considered the $O(\tau^2)$ form

$$G(\mathbf{R}', \mathbf{R}, \tau) = (4\pi D\tau)^{-3A/2} \exp[-(\mathbf{R}' - \mathbf{R} - D\tau\mathbf{F}(\mathbf{R}))^2/4D\tau] \\ \times \exp\{[E - (E_L(\mathbf{R}) + E_L(\mathbf{R}'))/2]\tau\} + O(\tau^2). \quad (6)$$

Using the stochastic terminology, this Green function contains an isotropic diffusion combined with a drift (the Gaussian-like term) and a rate term (the second exponential). So, a given walker is first drifted and isotropically diffused, and afterwards the rate term may cause it to multiply or even to disappear.

Once the time has reached a sufficiently large value by the repeated operation of the small-time Green function, so that we are in the asymptotic regime of equation (3), the ground-state energy may be obtained by requiring stability of the number of walkers, as we have already commented, or by using the *mixed* estimator

$$E \approx \lim_{t \rightarrow \infty} \frac{\int E_L(\mathbf{R})f(\mathbf{R}, t) d\mathbf{R}}{\int f(\mathbf{R}, t) d\mathbf{R}} \quad (7)$$

which corresponds to the average $\langle E_L \rangle$ over the set of walkers.

With the $O(\tau^2)$ form of equation (6) for the Green function, the energy is obtained with an error proportional to τ . In practice one carries out several calculations for various values of the time step and afterwards extrapolates to $\tau \rightarrow 0$ to obtain the ground-state energy. In this way the only errors generated in this calculation, apart from the error related to the extrapolation, are of statistical nature. These latter errors may be made small by choosing a good trial function and/or by increasing the number of samples.

A step which needs to be performed first, prior to the DMC calculation, is the determination of a good trial function. We have chosen a Jastrow form

$$\Psi(\mathbf{R}) = \prod_{i < j=1}^4 g(r_{ij}) \exp[-\frac{1}{2}\alpha^2(r_1^2 + r_2^2 + r_3^2 + r_4^2)] \quad (8)$$

with the parametrization

$$g(r) = 1 + a_1 \exp[-(r/b_1)^2] + a_2 \exp[-(r/b_2)^2]. \quad (9)$$

The results obtained with a trial function of this kind are shown in table 1. In this table we have also included some simpler calculations related to our trial wavefunction. The first row in table 1 corresponds to the energy obtained from the simplest $(0s)^4$ harmonic oscillator shell-model (HOSM) wavefunction, optimized with respect to the single variational parameter α . It corresponds to the totally

Table 1. The ground-state energy (in MeV) of the ^4He nucleus for the four interactions described in the text, and with the MTV potential with the parametrization of [19]. The present diffusion Monte Carlo (DMC) results are compared with those from the variational calculations HOSM, Jastrow-1 and Jastrow-2. These latter minimize the energy expectation value with trial wavefunctions of the Jastrow kind given in equation (8) and (9), except that $a_1 = a_2 \equiv 0$ (HOSM) and $a_2 \equiv 0$ (Jastrow-1).

Method	Interaction			
	V7	B1	S3	MTV
HOSM	-27.3326	-28.1580	-5.8936	-6.3904
Jastrow-1	-27.5546	-36.6865	-24.3515	-29.0071
Jastrow-2	-28.7206	-38.2733	-27.1525	-30.8259
DMC	-28.76 ± 0.01	-38.32 ± 0.01	-27.35 ± 0.02	-31.32 ± 0.02

uncorrelated case where $g(r) \rightarrow 1$. The second row, labelled Jastrow-1, corresponds to constraining the Jastrow correlation function $g(r)$ of equation (9) with $a_2 \equiv 0$, and minimizing the expectation value of the Hamiltonian with respect to the remaining parameters $\{\alpha, a_1, b_1\}$. Finally, the row labelled Jastrow-2 gives the results of the energy minimization using the full five-parameter trial function of equation (9). The corresponding optimum values of these parameters are shown in table 2 for each of the four interactions considered.

The ground-state energies obtained with the five-parameter trial function are actually very close to our DMC results, listed in the last row of table 1, for the case of the smooth effective interactions V7 and B1, but they still differ by some few tenths of 1 MeV for the quasi-realistic interactions S3 and MTV. We should mention that even these are not the *lowest* values for the ground-state energy that one may obtain by using a Jastrow wavefunction, as has been incorrectly assumed in some other works [35]. Actually, other more elaborate calculations based on the Jastrow ansatz have been reported for the case of the MTV interaction, with the respective results of -31.19 ± 0.05 MeV [7] and -31.35 MeV [5]. In both cases, rather than parametrizing the function $g(r)$ with some predetermined form as in equation (9), the functional form was evaluated by doing a full Euler-Lagrange variational calculation with respect to the correlation function $g(r)$. In the former case [7], the energy functional was approximated by truncation to the second-order term in the cluster expansion. Although the latter result [5] used the exact functional, we should mention that it required the use of quasi-random number techniques to evaluate the

Table 2. The values of the five (Jastrow-2) variational parameters of the two-body correlation function $g(r)$ given by equation (9), which minimize the energy expectation value of the ^4He nucleus with a trial Jastrow wavefunction of the form of equation (8), for the four interactions described in the text.

Parameter	Interaction			
	V7	B1	S3	MTV
α (fm^{-1})	0.5110	0.5651	0.6055	0.5094
a_1	-0.3518	-1.2149	-1.4912	-1.9029
b_1 (fm)	0.9430	0.9048	0.7977	0.5394
a_2	1.1202	1.2382	0.9900	1.4056
b_2 (fm)	2.7732	2.3901	1.9520	2.6198

multidimensional integrals needed for the energy expectation value, and the authors do not quote any value for the associated statistical errors in the stochastic part of their calculations.

The resulting optimal wavefunctions from our Jastrow-2 calculations were then used to carry out the DMC calculation in the usual manner [32, 33]. The incremental time step τ was varied between 0.00005 MeV^{-1} and 0.0002 MeV^{-1} (with a larger range considered in the case of the MTV potential), and after reaching the asymptotic regime a total of 18 000 further steps were carried out to increase the statistics, with a population of 1000 walkers on the average. Figure 1 shows the dependence on the time step of the mixed estimator for the energy from equation (7), as well as the linear fit used for the $\tau \rightarrow 0$ extrapolation. The error bars of the individual points are much smaller than the size of the dots used to plot them. Our final values for the energy, which are the main results of this work, are shown in the last row of table 1, as we have already mentioned.

There is not a great deal more to be said concerning our actual results, except to report that they now provide an extremely accurate set of reference numbers against which other approximate techniques for solving the many-body Schrödinger equation may be tested and refined. To the best of our knowledge, our results for each of the four interactions considered represent the most accurate ones available. By and large, where other (less accurate) results exist from methods which also purport to solve *exactly* the four-body equation by stochastic simulation, they are also in broad agreement with ours. For example, Zabolitzky and Kalos [22], using a Green function Monte Carlo (GFMC) method, quote the result $E = -31.3 \pm 0.2 \text{ MeV}$ for the ground-state energy of the ^4He nucleus using the MTV potential.

We close with some remarks concerning the overall quality of our results, i.e. the smallness of the errors that we have obtained. Even though we have used trial functions with expectation values of the energy very close to the final DMC result, it was necessary to carry out a very long random walk to reach such small errors. Of course, if we had used the *exact* wavefunction as the importance trial function, any short random walk would have produced results with null variance, as can be seen from equation (7). The inescapable conclusion is therefore that our trial functions are not as good as the values of the energy might suggest. This statement is particularly

Figure 1. Plot of the diffusion Monte Carlo (DMC) results for the ground-state energy E of the ^4He nucleus, using the four interactions described in the text, as a function of the time step τ . The lines are the linear fits used for the extrapolated value at $\tau \rightarrow 0$.

clarified by using the Monte Carlo terminology. Thus, whereas the variational upper bound is the average of the values of the local energy $E_L(\mathbf{R})$ corresponding to a probability distribution which is the square of the trial wavefunction, our DMC method does something similar but uses as the probability distribution the function $f(\mathbf{R}, t \rightarrow \infty)$. If the local energy has strong fluctuations, the variance will be large and a large number of samples will be required to have a small final error, with the error decreasing as the square root of the number of samples. We have been using as many as 18×10^6 samples per point as reported above, so we may infer from the inverse of this observation that the Jastrow trial function cannot be as good as the expectation value of the energy might suggest. Furthermore, the trial Jastrow function is much better for the smooth effective interactions v_7 and b_1 than for the quasi-realistic interactions s_3 and MTV , as one naively expects.

It is clear from the above discussion that the usefulness, in both the present and other contexts, of a variationally determined trial wavefunction $|\Psi_T\rangle$ would be very much enhanced if, as well as quoting the associated upper bound for the ground-state energy, one always also quoted some other measure of its *goodness*. An obvious candidate in this regard is the variance, in the usual quantum-mechanical uncertainty sense,

$$(\Delta E)^2 = \langle \Psi_T | H^2 | \Psi_T \rangle - \langle \Psi_T | H | \Psi_T \rangle^2 \quad (10)$$

with $|\Psi_T\rangle$ normalized to 1. Certainly, other, possibly better, measures may also exist.

EB and RG are supported by the Comisión Interministerial de Ciencia y Tecnología, Spain. MFF acknowledges support via a fellowship from the Ministerio de Educación y Ciencia, Spain, under the program Estancias Temporales de Científicos y Tecólogos Extranjeros. RFB acknowledges the support of a research grant from the Science and Engineering Research Council (SERC) of Great Britain.

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