

Fermion Monte Carlo calculations of liquid ^3He

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Methods and results for calculations of the ground state energy of the bulk system of ^3He atoms are discussed. Results are encouraging: we believe that they demonstrate that our methods offer a solution of the “fermion sign problem” and the possibility of direct computation of many-fermion systems with no uncontrolled approximations. Although the method is still rather inefficient compared to variational or fixed-node methods, we have been able to obtain useful answers.

PACS numbers: 67.55.-s, 02.70.Ss

1. INTRODUCTION

Powerful Monte Carlo methods ¹ can provide estimates of ground state properties of bosonic many-body systems that are not subject to uncontrolled approximations. But the mapping of the many-body quantum wavefunction to a probability distribution function faces severe challenges when considering the global antisymmetry that a fermionic wavefunction must satisfy. The methods that we have adopted to face this “fermion sign problem” ² are based on a population of pairs of positive and negative walkers which is generated using Diffusion Monte Carlo modified in the following ways:

- (1) Different guiding functions are used for walkers of different signs;
- (2) When walkers of different signs branch differently (as they must) new pairs are created;
- (3) The “diffusion” steps of the walkers in a pair are correlated;
- (4) Walkers in a pair that come close can be canceled in a way that guarantees that the future value of any projection with an antisymmetric

function is exactly preserved;

(5) We have been able to adapt the technique of “acceptance-rejection” to our method.

(6) We have experimented with “second-stage importance sampling” (SSIS), in which a function of the coordinates of both walkers of a pair is used to modify the distribution of the walkers.

2. THE METHOD

Let us consider a system of N atoms of which the coordinates of the i th particle are represented by a tridimensional vector \mathbf{r}_i . The atoms interact with one another via two- and three-body forces summarized by a potential $V(\mathbf{r}_1, \dots, \mathbf{r}_N)$. Our primary interest is in the ground state energy E_0 of the system, for which we need to solve the many-body Schrödinger equation. Diffusion Monte Carlo follows the evolution in imaginary time; using atomic units, this equation translates into

$$\left[-\frac{1}{2}\nabla^2 + V(\mathbf{R}) - E_T \right] \psi(\mathbf{R}, \tau) = -\frac{\partial \psi(\mathbf{R}, \tau)}{\partial \tau} \quad (1)$$

which is a diffusion and absorption equation, solved by iterating an appropriate Green’s function $G(\mathbf{R}, \mathbf{R}', \delta\tau)$ on the $3N$ -dimensional vector $\mathbf{R}'(x_1, \dots, x_{3N})$ that represents a whole configuration (“walker”) of the system,

$$\psi(\mathbf{R}, \tau + \delta\tau) = \int G(\mathbf{R}, \mathbf{R}', \delta\tau) \psi(\mathbf{R}', \tau) d\mathbf{R}' \quad (2)$$

At each step $\psi(\mathbf{R}, \tau)$ is represented by an ensemble of discrete points $\{\mathbf{R}_m\}$ that are then advanced and reproduced or removed according to $G(\mathbf{R}, \mathbf{R}', \delta\tau)$. In the limit of sufficiently long imaginary-time τ , only the term with the lowest energy survives

$$\psi(\mathbf{R}, \tau) = N_0 e^{-\tau(E_0 - E_T)} \phi_0(\mathbf{R}) \quad (3)$$

and, if $E_T = E_0$, the walkers $\{\mathbf{R}_m\}$ are sampled from a stationary probability density distribution that maps the symmetric ground state $\phi_0(\mathbf{R})$.

In order to improve the efficiency of this filtering of the solution, one introduces a known trial wavefunction $\psi_T(\mathbf{R})$ with the aim of changing the sampling process in a known way³ while preserving averages. In our FMC algorithm this concept is split into two separate auxiliary functions: a strictly positive guiding function $\psi_G(\mathbf{R})$ whose role is to modify the random walk, while an antisymmetric trial function $\psi_T(\mathbf{R})$ that should resemble the solution as closely as possible is used to project out quantities of interest, such

as the local energy E_T . Thus the density of walkers generated by the walk will be

$$f(\mathbf{R}, \tau) = \psi_G(\mathbf{R})\psi(\mathbf{R}, \tau) \xrightarrow{\tau \rightarrow \infty} \psi_G(\mathbf{R})\phi_0(\mathbf{R}) \quad (4)$$

We separate now the set $\{\mathbf{R}_m\}$ of walkers into two subsets of walkers $\{\mathbf{R}_m^+\}$, $\{\mathbf{R}_m^-\}$ that respectively add or subtract their contributions to statistical expectations such as the energy

$$E_0 = \frac{\sum_m^{N_p} \left[\frac{\hat{H}\psi_T(\mathbf{R}_m^+)}{\psi_G(\mathbf{R}_m^+)} - \frac{\hat{H}\psi_T(\mathbf{R}_m^-)}{\psi_G(\mathbf{R}_m^-)} \right]}{\sum_m^{N_p} \left[\frac{\psi_T(\mathbf{R}_m^+)}{\psi_G(\mathbf{R}_m^+)} - \frac{\psi_T(\mathbf{R}_m^-)}{\psi_G(\mathbf{R}_m^-)} \right]} \quad (5)$$

where N_p is the number of pairs of configurations that enter the averaging. If the signed walkers independently sample the configuration space according to the distribution (4) the result will be the decay of Monte Carlo signal to noise ratio characteristic of the “fermion sign problem.” In particular the denominator of Eq. (5) will be unstable since the $\{\mathbf{R}_m^+\}$ and the $\{\mathbf{R}_m^-\}$ will be symmetrically distributed, averaging their contributions around zero. The incorporation of a correlation between pairs of walkers in the random-walk process has been shown to be effective in avoiding this decay of the signal-to-noise ratio that regularly occurs in a fermionic DMC ^{4,5}. Before introducing correlation, we first start by distinguishing the signed walkers by means of different ψ_G 's which we call ψ_G^\pm respectively.

In FMC we introduce two functions ψ_G^\pm which bias differently the populations of plus and minus walkers and thus act as symmetry breaking fields. The ingredients of our guiding functions are Slater Determinants $D^{\uparrow(\downarrow)}$ of like-spin single particle wavefunctions, and two symmetric Jastrow products, $J^S(\mathbf{R})$ and $J^A(\mathbf{R})$ with different parameters. We now construct a function antisymmetric under permutation of atom labels

$$\psi_A(\mathbf{R}) = J^A(\mathbf{R})D^\uparrow(\mathbf{R})D^\downarrow(\mathbf{R}) \quad (6)$$

and a symmetric one

$$\psi_S(\mathbf{R}) = J^S(\mathbf{R}) \quad (7)$$

Finally, the guiding functions themselves are constructed by combining (6) and (7):

$$\psi_G^\pm(\mathbf{R}) = \sqrt{\psi_S^2(\mathbf{R}) + c^2\psi_A^2(\mathbf{R})} \pm c\psi_A(\mathbf{R}) \quad (8)$$

with c a small and adjustable parameter. The functions ψ_G^\pm are positive for any \mathbf{R} , as is necessary for an importance function. For an odd permutation of particles in a configuration one has that the biased distributions of the

two signed walkers map into each other.

The orbitals of our Slater determinants comprise the standard backflow function⁶, while the Jastrow products provide two-body correlations via a pseudopotential of the McMillan type and three-body correlations.

The diffusion process for the distribution (4), is generalized as follows: the two ψ_G^\pm are applied separately to drift the walkers of a pair from their old positions $\mathbf{R}_o^+, \mathbf{R}_o^-$:

$$\mathbf{R}_d^\pm = \mathbf{R}_o^\pm + 2\delta\tau \frac{\nabla \psi_G^\pm(\mathbf{R}_o^\pm)}{\psi_G^\pm(\mathbf{R}_o^\pm)}. \quad (9)$$

We make use of correlated dynamics in the pairs diffusion. The branching of the pairs is carried out taking into account the possibility of an overlap of the members of a pair, which leads to a partial cancellation of the contribution of the pair to the future statistics. Since the weights $\omega(\mathbf{R}^\pm)$ - which express the branching factor of the single walkers - in a pair can be different at each generation, a mechanism for repairing the lone walker must be introduced. Details of this algorithm can be found in Refs.^{7,8}

Quantities of interest, such as the total energy, are projected out by using a trial wave function. In our FMC method that role is played by the antisymmetric function ψ_A of Eq. (6). To account for the branching process, each pair may contribute once weighted with $\omega(\mathbf{R}_m^\pm)$ and Eq. (5) then becomes:

$$E_0 = \frac{\sum_m^{N_p} \left[\frac{\hat{H}\psi_A(\mathbf{R}_m^+)}{\psi_G(\mathbf{R}_m^+)} \omega(\mathbf{R}_m^+) - \frac{\hat{H}\psi_A(\mathbf{R}_m^-)}{\psi_G(\mathbf{R}_m^-)} \omega(\mathbf{R}_m^-) \right]}{\sum_m^{N_p} \left[\frac{\psi_A(\mathbf{R}_m^+)}{\psi_G(\mathbf{R}_m^+)} \omega(\mathbf{R}_m^+) - \frac{\psi_A(\mathbf{R}_m^-)}{\psi_G(\mathbf{R}_m^-)} \omega(\mathbf{R}_m^-) \right]}. \quad (10)$$

In order to improve the efficiency of our method we introduced and experimented with several classes of technical improvements.

The first was an adaptation to the correlated diffusion of pairs of walkers of the ‘‘Acceptance/Rejection’’ (A/R) method widely used in fixed-node computations^{9,10}.

The second was a class of refinements that we refer to collectively as ‘‘second-stage importance sampling.’’ Here we took note of the general character of importance sampling for random walks, namely that the stochastic dynamics should be biased by a function proportional to the chance that a walker contributes to the asymptotic distribution, namely the steady state of the population. That steady state can be measured by the denominator of the energy quotient. Quite clearly, the needed function depends on the positions of both of our walkers, a fact not accounted for in the method described above.

We tried several forms of second-stage importance functions with and without A/R, and found significant but not decisive improvements. Nev-

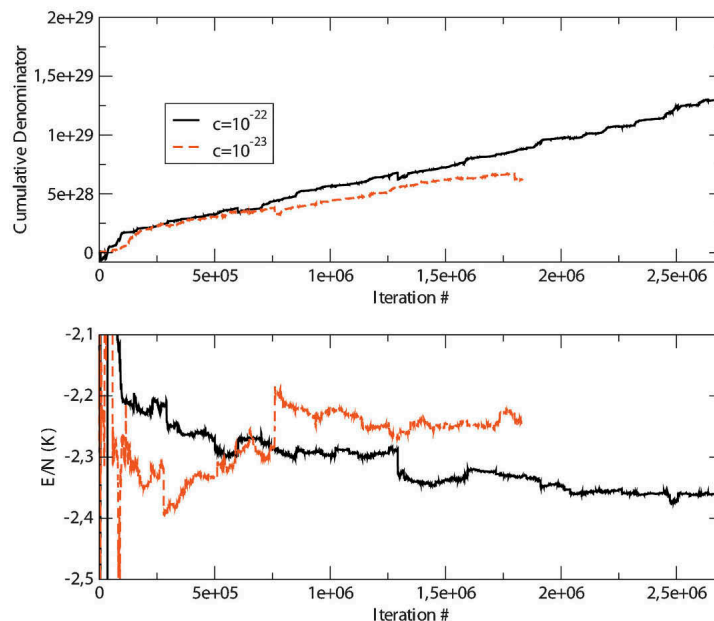


Fig. 1. Effect of the amount of antisymmetry (measured by c in Eq. (8)) in the guiding function. Top: cumulative denominator; Bottom: cumulative energy. These runs have been obtained with A/R, SSIS and $\delta\tau = 6 \times 10^{-5}$.

ertheless, we believe that the path to much better efficiency lies in better importance sampling of the dynamics and are actively pursuing new ideas.

3. RESULTS

Table 1 shows average results for the various runs. In particular it is shown that even with a small population of 192 pairs, a long FMC run with SSIS and A/R gives results that are comparable with the fixed node ones. Figure 1 shows the behavior of a typical run for 54 ${}^3\text{He}$ atoms. Top panel shows the behavior of the cumulative denominator. The growth is an indication of the stability of the run. In the bottom panel the cumulative value of the projected energy is shown. As can be seen, fluctuations are rather large but a clear converging behavior emerges.

Table 1. FMC results with respect to parameters used; “denom” refers to a S-shaped SSIS function of the denominator; “eucl” to a SSIS linear function of the euclidean distance between the walkers). τ_{rel} denotes the relaxation time. Note that no extrapolation to zero time step has been calculated. Bottom line: fixed node result.

N_p	c	$\delta\tau$ in K^{-1}	A/R	$SSIS$	length in τ_{rel}	$E(\Delta E)$ in K
192	10^{-23}	6×10^{-5}	yes	denom	16	-2.24(3)
192	10^{-23}	6×10^{-5}	yes	no	20	-2.26(13)
192	10^{-22}	6×10^{-5}	yes	eucl	11	-2.215(12)
192	10^{-22}	6×10^{-5}	no	denom	25	-2.24(14)
192	10^{-22}	6×10^{-5}	yes	denom	25	-2.38(3)
192	FXN	6×10^{-5}	yes	denom	10	-2.369(2)

ACKNOWLEDGMENTS

We gratefully thank David Ceperley, Geoffrey Chester, Berni Alder, Joseph Carlson, Kevin Schmidt, and Randolph Hood for stimulating comments. We are also indebted to David Hardin for a critical review of the manuscript. This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under contract No. W-7405-Eng-4, and funded by the Laboratory Directed Research and Development (LDRD) Program at Lawrence Livermore National Laboratory (LLNL) under project 01-LW-040.

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