Fermion Monte Carlo Algorithms and Liquid ^{3}He

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Variational Monte Carlo and several many-fermion Green's-function Monte Carlo (GFMC) algorithms are used to study the ground state of liquid ^{3}He. We report the first mirror-potential GFMC calculations in a many-fermion problem, comparing them with transient estimation and fixed-node studies to illustrate the strengths and weaknesses of each. GFMC results with the Aziz HFDHE2 interaction are in good agreement with experiment, yielding energies within approximately 0.1 K per particle. In addition, each of these calculations predicts a kinetic energy per particle of between 12 and 12.5 K.

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The structure and properties of bulk liquid ^{3}He at zero temperature have been subjects of intense theoretical and experimental interest in recent years.[1−8] In particular, accurate first-principles calculation of the macroscopic properties of ^{3}He from microscopic interactions has long been a goal of condensed-matter theorists. A simple state-independent interaction provides an accurate description of the Hamiltonian of bulk helium, yet this interaction is strong enough to produce large correlations between the atoms. Consequently, liquid ^{3}He provides an ideal testing ground for diverse many-body calculational schemes.

Monte Carlo methods are employed to study many-fermion systems in many areas of physics, from atomic and condensed matter to nuclear and high-energy physics. Difficulties associated with the antisymmetric nature of the fermion wave function are well known and widely discussed.[1,3,9,10] In straightforward Green's-function Monte Carlo (GFMC) calculations, the fermion problem manifests itself as an exponential increase in statistical error as the calculation proceeds. In this Letter, we present new results and a detailed comparison of methods designed to reduce or eliminate this difficulty.

For a nonrelativistic system of N helium atoms interacting via static two-body forces only, the Hamiltonian has the form

$$H=-\sum_{i=1}^{N}\frac{\hbar^2}{2m}\nabla_i^2+\sum_{1\le i<j\le N}v(r_{ij})\,. \tag{1}$$

The pair interaction $v(r_{ij})$ is taken to be the HFDHE2 interaction of Aziz *et al.*[11] which for ^{4}He yields excellent agreement with experiment.[12] Accurate variational calculations yielding a good ground-state trial function are an essential preliminary to practical and reliable GFMC calculation. Improved trial wave functions significantly reduce the statistical error by initiating the iterative calculation nearer the ground state; moreover, an improved importance function acts to suppress population fluctuations. A good trial wave function is especially crucial to a successful attack on the fermion problem.

We have used a trial wave function of the form

$$\Psi_T=\psi_3\det\left\{\exp\left[i\mathbf{k}_i\cdot\left(\mathbf{r}_j+\sum_{l\neq j}\eta(r_{lj})\mathbf{r}_{lj}\right)\right]\right\}, \tag{2}$$

where

$$\psi_3=\exp\left[-\tfrac{1}{2}\sum_{i<j}\tilde{u}(r_{ij})-\frac{\lambda_T}{4}\sum_l\sum_{i<j\neq l}\xi(r_{li})\xi(r_{lj})\mathbf{r}_{li}\cdot\mathbf{r}_{lj}\right] \tag{3}$$

and

$$\tilde{u}(r)=u(r)-\lambda_T\xi^2(r)r^2\,. \tag{4}$$

This *Ansatz* includes explicit two- and three-body correlations as well as state-dependent correlations which incorporate "backflow" effects.[4] The two-body correlation $u(r_{ij})$ is an appropriately scaled solution of an Euler-Lagrange equation obtained from Fermi-hypernetted chain methods[13] or the solution of a parametrized two-body Schrödinger-type equation.[14] The triplet correlations are parametrized as

$$\xi(r)=\exp\{-[(r-r_T)/w_T]^2\} \tag{5}$$

and the momentum-dependent correlations are introduced through

$$\eta(r)=\lambda_B\exp\{-[(r-r_B)/w_B]^2\}+\lambda_B'/r^3\,. \tag{6}$$

The wave function is required to be periodic, so that all correlations smoothly go to zero at a distance equal to half the side of the simulation volume, $r_{\max}$, according to the replacement

$$f(r)\to f(r)+f(2r_{\max}-r)-2f(r_{\max})\,. \tag{7}$$

Since the correlations which minimize the variational energy in our study are relatively short ranged, this finite-size adaptation has no real effect on the magnitude of the correlations.

TABLE I. Variational parameters optimized for the ^{3}He wave function for 54 particles in a periodic box at $\rho\sigma^3=0.273$, where $\sigma=2.556$ Å.

λ_T	r_T	w_T	λ_B	r_B	w_B	λ'_B
-1.80	0.66σ	0.50σ	0.14	0.74σ	0.54σ	$0.15\sigma^3$

The optimum set of variational parameters obtained for a system of 54 particles at the experimental equilibrium density is given in Table I. Although the functional forms of the correlation functions are similar to those used in integral-equation studies,[5,15] there are significant differences between the optimum parameters obtained with the two methods. In the Monte Carlo calculations, no approximations are necessary in evaluating the variational upper bound, subject to the caveat that the calculation refers to a finite number of particles with periodic boundary conditions.

Employing the accurate variational wave function as an importance function, the Green's-function Monte Carlo[1,10,12,16–20] method is used to calculate ground-state properties of the system. The GFMC method is based upon the fact that the Schrödinger equation in imaginary time is equivalent to a diffusion equation in real time. The GFMC algorithm is implemented by choosing a set of points $\{R\}$ in configuration space and iterating the equation

$$\Psi^{n+1}(R)=E_T\int G(R,R')\Psi^n(R')dR'. \tag{8}$$

Although the Green's function is not known analytically, it can be sampled exactly through the use of an ancillary random walk. The GFMC method has been applied to macroscopic bosonic systems, such as liquid ^{4}He, with great success.[12,16,20]

Exact GFMC treatment of fermion systems, however, has proven to be very elusive. The antisymmetry requirement is a global property that is difficult to incorporate successfully into the diffusion algorithm, which is local in character. The fact that the wave function is not positive definite introduces a statistical error which grows exponentially as Eq. (8) is iterated. Fermion algorithms typically introduce two populations, the difference of which corresponds to the desired wave function:

$$\Psi^A=\Psi^+-\Psi^-. \tag{9}$$

The various fermion GFMC algorithms can be viewed in the framework of mirror potentials.[21] By introducing two coupled equations,

$$[H(R)+c(R)\Psi^+(R)]\Psi^-(R)=E\Psi^-(R), \tag{10a}$$

$$[H(R)+c(R)\Psi^-(R)]\Psi^+(R)=E\Psi^+(R), \tag{10b}$$

and making an appropriate choice of the mirror potentials $c(R)\Psi^{\pm}(R)$, it is possible, in principle, to retain two stable and distinct populations for Ψ^+ and Ψ^- such that the difference is a solution of the original Schrödinger equation. Two very useful methods that were introduced earlier—the fixed-node approximation[22,23] and transient estimation[3,22]—turn out to be limiting cases of Eqs. (10). The *fixed-node* approximation corresponds to the limit $c(R)\rightarrow\infty$ in Eqs. (10), whereby the diffusion of the two populations is restricted to two isolated regions in configuration space. This prescription yields an upper bound to the true ground-state energy, and leads to the lowest-energy wave function with the same nodes as the trial function. Alternatively, *transient estimation* corresponds to the limit $c(R)\rightarrow 0$ in Eqs. (10) and results in a series of decreasing upper bounds with exponentially increasing statistical error. Accurate trial functions are very important for this method, since the goal is to achieve convergence to the true ground state before the growing statistical error dominates.

We report here results with an intermediate choice for $c(R)$,

$$c(R)\Psi^{\pm}=\frac{[E^*-H]\Psi_T^S}{\Psi_T^{\mp}}, \tag{11}$$

with

$$\Psi_T^{\pm}=\Psi_T^S\pm\Psi_T^A \tag{12}$$

and

$$\Psi_T^S=[(\Psi_T^A)^2+(\beta\Psi_T^B)^2]^{1/2}, \tag{13}$$

wherein Ψ_T^A is the antisymmetric trial wave function of Eq. (2). The "bosonic" wave function Ψ_T^B is taken as the product of the two- and three-body correlations ψ_3 of Eq. (3) only, and is therefore symmetric. The quantities E^* and β are parameters of the approximate mirror potential. Although the mirror potential itself is arbitrary, the use of Ψ_T rather than Ψ on the right-hand side of Eq. (11) gives only an approximate cancellation in Eqs. (10). In the limit that the antisymmetric trial function Ψ_T^A is exact, the mirror potential equations yield an exact solution independent of E^* and β.

Table II collects results obtained at the experimental equilibrium density. Mirror-potential results are presented along with results of variational, transient estimate, and fixed-node studies. The optimally determined trial function, as determined by the variational calculation, has been used in each of the GFMC studies. This wave function determines the antisymmetric part of the initial distribution in all cases, the antisymmetric part of the mirror potential, and the nodal surfaces in the fixed-node calculation. Calculations to date for the intermediate choice of mirror potential give energies between -2.24 ± 0.04 and -2.32 ± 0.07 K per particle, depending upon the parameters. This is significantly lower than the variational result, but not quite as low as the fixed-node result (-2.37 ± 0.01). However, the mirror potential procedure yields accurate energies *without the necessity of fixing the nodal surface of the wave function;* for this reason it should have greater applicability where the nodal surface is hard or even impossible to

TABLE II. Results of Monte Carlo calculations for 54 ^{3}He atoms in a periodic box at $\rho\sigma^3=0.273$, where $\sigma=2.556$ Å. All energies are in K per particle.

Method	E^*	β	Energy	$\langle T\rangle$	$\langle V\rangle$
Variational	···	···	-2.13 ± 0.02	12.22 ± 0.03	-14.35 ± 0.02
GFMC (mirror potential)	−2.30	60.0	-2.24 ± 0.04	12.33 ± 0.14	-14.57 ± 0.14
GFMC (mirror potential)	−2.35	70.0	-2.32 ± 0.07	12.22 ± 0.20	-14.54 ± 0.20
GFMC (mirror potential)	−2.40	70.0	-2.27 ± 0.03	12.42 ± 0.16	-14.69 ± 0.16
GFMC (mirror potential)	−2.35	80.0	-2.30 ± 0.04	12.34 ± 0.14	-14.64 ± 0.14
GFMC (fixed node)	···	···	-2.37 ± 0.01	12.28 ± 0.04	-14.65 ± 0.03
GFMC (transient estimation)	···	···	-2.44 ± 0.04	12.40 ± 0.10	-14.84 ± 0.10

specify. Moreover, mirror potentials allow for even more accurate higher-order treatments.[21] The rapid increase in the statistical error makes it hard to determine if the transient-estimate calculation has converged to the ground state; nevertheless, the upper bound of -2.44 ± 0.04 K/particle is the lowest obtained to date and is very close to the experimental equilibrium energy of -2.47 K/particle.

The kinetic energy $\langle T\rangle$ and potential energy $\langle V\rangle$ at equilibrium density are also given in Table II. In every case, the kinetic energy per particle is between 12 and 12.5 K, significantly larger than some previous interpretations of experimental data.[6,24] Details of the calculations, as well as results for the momentum distribution and other ground-state properties, will be presented elsewhere.

The various GFMC algorithms each require large amounts of supercomputer resources. More than 30 000 configurations were required in transient estimation, yet Eq. (8) was iterated only 50 times before the statistical error dominated. In contrast, the stable nature of the fixed-node calculation allowed more than 1000 iterations of Eq. (8) with only 500 configurations. The several mirror-potential calculations employed approximately 400 configurations iterated 500 times.

The equations of state for liquid ^{3}He as obtained from the variational treatment and from fixed-node GFMC are compared with experimental results in Fig. 1, which we note has a very expanded energy scale. Differences between the fixed-node and experimental energies are typically of the order of 0.1 K/particle, similar in magnitude to the differences previously found for ^{4}He with the HFDHE2 potential.[12] The overall agreement with the experimental equation of state is very encouraging, in the sense that the differences are small and are similar in magnitude to a variety of uncertainties in the Hamiltonian and the calculation.

Several uncertainties remain in a comparison of these results and experiment. Finite-size effects play a role in the remaining difference, as these calculations were done for a system of 54 particles with periodic boundary conditions. In order to check the importance of this effect, variational calculations for up to 186 particles have been performed. This test indicates that energy differences of up to approximately 0.1 K/particle may be attributable to the finite size of the simulations.

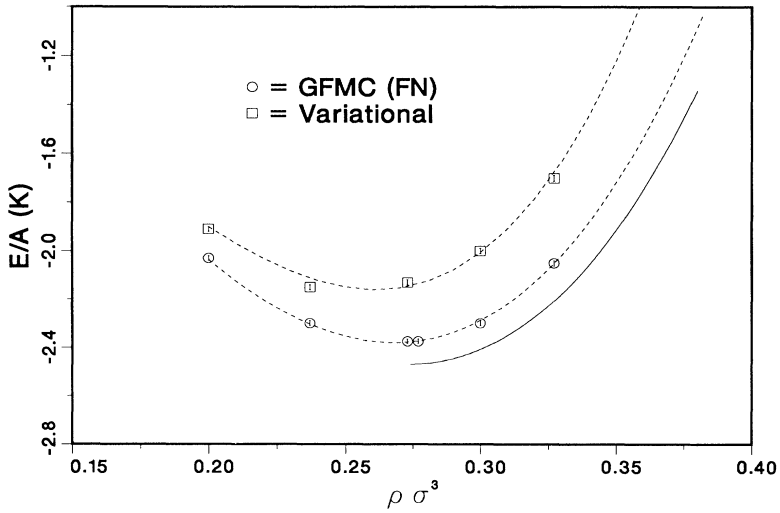

FIG. 1. Energy per particle vs density for liquid ^{3}He at zero temperature. The dashed lines are fits to the variational and fixed-node GFMC calculations, while the solid line gives the experimental equation of state.

In addition, there are theoretical uncertainties in the Hamiltonian used for ^{3}He. Recently, Aziz, McCourt, and Wong[25] have introduced another two-body interaction which has a somewhat deeper attractive well than the HFDHE2 potential. Perturbative estimates indicate that this interaction may provide an additional *attraction* of 0.2 K/particle at equilibrium density, thus giving an energy slightly lower than experiment.

On the other hand, three-body interactions may also be important at this level of precision. A straightforward evaluation of the Axilrod-Teller[26] three-body interaction yields a *repulsion* of 0.07 K/particle in first-order perturbation theory. Although this triple-dipole interaction is correct for large interatomic separations, its applicability at small distances in ^{3}He has not yet been shown.

Since each of the above effects is of about the same magnitude, it would be very difficult to determine the "correct" Hamiltonian of liquid ^{3}He from a calculation of its bulk ground-state properties. It may prove more fruitful to study the two- and three-body interactions by means of first-principles calculations of the atomic systems.

The overall agreement between theoretical and experimental results is excellent, similar to that obtained previously for ^{4}He. The kinetic energy obtained in each of the calculations is between 12 and 12.5 K per particle, indicating the importance of the high-momentum tails in the ^{3}He ground state and the value of further experimental and theoretical investigations of the momentum distribution. The development of exact fermion algorithms remains one of the outstanding problems in quantum Monte Carlo studies, and work in this area will be vigorously pursued.

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