Structure of the Ground State of a Fermion Fluid

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Variational many-body wave functions for the ground state of liquid ^{3}He which include triplet and backflow correlations are investigated with use of Monte Carlo integration. Our energy of $-1.9\,°$K removes half of the discrepancy between previous Jastrow–Slater calculations and experimental results. The first exact results for mass-three bosons are also presented. Triplet correlations in the variational wave function are equally effective in lowering the energy of both mass-three bosons and ^{3}He.

Variational Monte Carlo calculations are a straightforward way to obtain rigorous upper bounds to the ground-state energy of a quantum many-body system. In the case of Fermi liquids, the calculation is complicated by the necessity that the trial wave function be antisymmetric. The simplest useful trial wave function is given by

$$\psi_T(R) = \psi_J(R)D_0$$
$$= \exp\left[-\sum_{i<j}^{N} \tfrac{1}{2}u(r_{ij})\right] \det(e^{i\vec{K}_l \cdot \vec{r}_m}), \qquad (1)$$

where ψ_J is a Jastrow wave function, a symmetric product of two-body correlation factors; D_0 is the product of two Slater determinants of plane waves, one for each spin state. The Metropolis Monte Carlo procedure[1] may be employed to calculate the energy of this wave function.[2] The equilibrium energy and density so obtained ($-1.2\,°$K and $0.87\rho_0$) differ significantly from the experimental values[3] ($-2.47\,°$K and $\rho_0 = 0.277\sigma$, where $\sigma = 2.556\,$Å^{-3}). There are two possible sources for these discrepancies: The trial wave function of Eq. (1) is inadequate, and the Lennard–Jones pair potential used may be inaccurate. In this paper, we will investigate both improved wave functions and potentials. We compare our results to previous calculations.[4-9]

The improved wave functions considered here are similar to that of Eq. (1), being the product of a symmetric function of all particle coordinates with an antisymmetric function of orbitals. The improvement in the symmetric factor is suggested by recent work[4-8] in ^{3}He and ^{4}He. In particular, Ref. 8 demonstrates that a trial function much closer to the true boson many-body wave function may be obtained by the inclusion of three-body terms

$$\chi_{ijk} = \exp\left\{\xi(r_{ij})\xi(r_{ik})\vec{r}_{ij} \cdot \vec{r}_{ik}\right\}.$$

We thus define the new symmetric function

$$\psi_3^2(R) = \exp\left\{-\sum_{i<j} \tilde{u}_{ij} - \frac{\lambda_T}{2}\sum_l \vec{G}(l) \cdot \vec{G}(l)\right\}, \qquad (2)$$

where

$$\vec{G}(l) = \sum_{i \neq l} \xi(r_{li})\vec{r}_{li}$$

and $\tilde{u}$ is the usual Jastrow pseudopotential u, modified by the two-body terms introduced by $\vec{G}(l) \cdot \vec{G}(l)$, viz.

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

The parameter λ_T and the functions $u(r)$ and $\xi(r)$ are to be determined variationally.

An accurate fermion wave function should contain state dependent correlations.[4] This means that the correlation function between pairs of particles depends on the particular plane-wave states occupied by the pair. This effect can be incorporated into a variational wave function by modifying the orbitals of the Slater determinant. The specific replacement that we use,

$$\exp i\vec{k} \cdot \vec{r}_i \rightarrow \exp i\vec{k} \cdot \left[\vec{r}_i + \lambda_B \sum_{j \neq i} \eta(r_{ij})\vec{r}_{ij}\right], \qquad (3)$$

is analogous to including backflow effects in the spirit of Feynman and Cohen.[10]

Recent work by Kalos *et al.*[11] has compared several alternative helium potentials by using the exact Green's function Monte Carlo (GFMC) method for many-boson systems. The results show remarkable agreement between the experimental ^{4}He equation of state for fluids and crystals and the results obtained with use of the HFDHE2 po-

TABLE I. Comparison of results at the ^{3}He equilibrium density for mass-three bosons and ^{3}He using the Lennard-Jones (LJ) and HFDHE2 (Ref. 12) potentials. The values of the variational parameters for the wave functions were for ^{3}He: $\lambda_T = 12$, $S_T = 0.95$, $w_T = 0.6$, $\lambda_B = -1$, $S_B = 0.85$, $w_B = 0.5$, $R_T = R_B = 2.87$, with $b = 1.13$ for LJ, and $b = 1.15$ for HFDHE2; for bosons: $\lambda_T = -14$, $S_T = 0.82$, $w_T = 0.5$, $R_T = 3.0$, $b = 1.13$ for LJ, and $b = 1.17$ for HFDHE2. All distances are in units of σ.

E_{LJ}	E_{HF}	Wave function
Mass-three bosons		
-2.92 ± 0.03	-2.92 ± 0.03	Jastrow
-3.30 ± 0.03	-3.40 ± 0.02	Jastrow + triplets
-3.48 ± 0.03	-3.54 ± 0.01	GFMC
^{3}He		
-1.06 ± 0.03	-1.08 ± 0.03	Jastrow-Slater (JS)
-1.44 ± 0.03	-1.61 ± 0.03	JS + triplets
-1.50 ± 0.03	-1.55 ± 0.04	JS + backflow
-1.71 ± 0.02	-1.91 ± 0.03	JS + backflow and triplets
-2.47 ± 0.01		Experiment

tential suggested by Aziz $et\ al.$[12] We have therefore used both this potential and the traditional Lennard-Jones potential with the de Boer-Michels parameters ($\sigma = 2.556$ Å, $\epsilon = 10.22\,^\circ$K).

Our calculation proceeds by Monte Carlo sampling of the many-body probability density $\rho(R)$ $\propto \psi_T^2(R)$, where ψ_T contains particular choices of variational parameters. The energy is the average over the population of points $\{R\}$, drawn from $\rho(R)$, of the local energy $H\psi_T(R)/\psi_T(R)$.

$$\frac{H\psi_T(R)}{\psi_T(R)} = \sum_{i=1}^{N} (V_i + 2T_i - \vec{F}_i^{\ 2}),$$

where

$$T_i = (-\hbar^2/4m)\nabla_i^2 \ln\psi_T\,,$$

$$\vec{F}_i^{\ 2} = (\hbar^2/2m)[\nabla_i \ln\psi_T]^2\,,$$

and

$$V_i = \tfrac{1}{2} \sum_{j \neq i} v(r_{ij}).$$

Further reduction of the expressions is straightforward but too lengthy to be given here.

The parametrized forms of the variational func-

tions were taken to be

$$u(r) = \left(\frac{b\sigma}{r}\right)^5,$$

$$\xi(r) = \left(\frac{r - R_T}{R_T}\right)^3 \exp\left[-\left(\frac{r - S_T}{w_T}\right)^2\right],\quad r < R_T, \qquad (4)$$

$$\eta(r) = \left(\frac{r - R_B}{R_B}\right)^3 \exp\left[-\left(\frac{r - S_B}{w_B}\right)^2\right],\quad r < R_B,$$

where R_B and R_T are cutoff lengths, and S_T, S_B and w_T, w_B fix the location and width of the Gaussians. These parameters along with b, λ_B, and λ_T are varied to minimize the energy.

For purposes of comparison, we have calculated the energy of a mass-three boson fluid at the ^{3}He equilibrium density. The exact ground state of the boson fluid was obtained by using the GFMC method.[13] Variational calculations on this system were also performed with use of ψ_J and ψ_3 to determine the effect of triplet correlations.

Table I summarizes the results obtained at the experimental equilibrium density. Triplet correlations in ^{3}He and in the corresponding boson fluid are most effective in improving the many-body wave function. An additional important change in the energy of ^{3}He is observed with the inclusion of backflow. Several forms of the backflow function were used, and it was found that the results are very sensitive to the shape of the function in the region of $r = 1\sigma$ to 2σ. Several longer range forms were considered, including one designed to mimic a r^{-3} tail of the Feynman and Cohen type. Those functions which deviated from the rapidly decaying form of η in Eq. (3) gave much higher variational energies. We believe that these results demonstrate that the dominant effect to backflow occurs at intermediate distances. This is to be contrasted with the long-range hydrodynamic form suggested by Feynman and Cohen[10] for Bose bluids.

The equation of state obtained from each type of wave function is shown in Fig. 1. Similar, but slightly higher energies were obtained with use of a Lennard-Jones potential. The difference due to the different potentials is about 0.1 $^\circ$K, and is principally manifested by the need for a larger Jastrow parameter (b) in the case of the HFDHE2 potential.

The experimental energy of ^{3}He is 1.4 $^\circ$K below that obtained from variational calculations with the Jastrow-Slater wave function. Most previous investigations which attempt to explain this difference have employed integral equation tech-
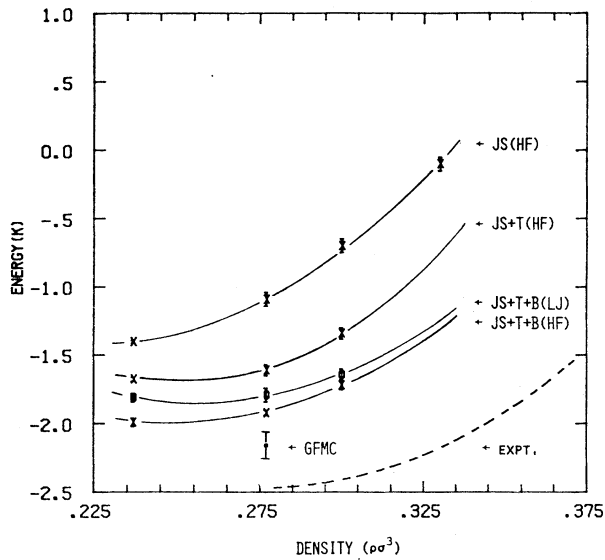
FIG. 1. Ground-state energy vs density for wave functions with and without backflow and triplet correlations. JS indicates the simple Jastrow-Slater wave function, $+T$ indicates triplets added, and $+B$ indicates that backflow correlations have been added. HF and LJ indicate results for the HFDHE2 potential (Ref. 12) and Lennard-Jones potential, respectively. Lines are drawn for clarity only. The result of Ref. 14 is labeled GFMC. The experimental curve is obtained from Refs. 13 and 15.

niques or perturbation theory or both. These methods, unlike Monte Carlo integration, require that approximations be made to avoid doing many-body integrals.

Triplet correlations in ^{4}He have been considered by Chang and Campbell[5] and by Pandharipande.[6] These calculations have been compared to our Monte Carlo results[8] with satisfactory agreement. The lower density of the mass-three bosons should make integral-equation methods more reliable in this system, and we expect even better agreement. The extension of triplet correlations to ^{3}He has been investigated by Schmidt and Pandharipande[4] using integral-equation methods, and by Lhuillier and Levesque[7] using the Monte Carlo method. The decrease in energy obtained, $0.3°$K and $0.4°$K, respectively, for the Lennard-Jones fluid is comparable to our observation of $0.4°$K.

Only Schmidt and Pandharipande have made attempts to include explicitly backflow correlations. They obtain results in qualitative agreement with ours concerning the short-range nature of the correlation, and a decrease of $0.7°$K, by

including backflow and triplet correlations. Clark et al.,[9] using the method of correlated basis functions, found that second-order perturbation theory predicted a decrease of $0.6°$K. Elsewhere[14] we have shown that it is possible to apply the GFMC method to this problem, in a way which gives a further improved upper bound of $-2.2°$K for the ground state of ^{3}He.

The discrepancy with experiment as seen in Fig. 1 is much reduced by the improved wave function and a more accurate potential. We do see an improvement in the equilibrium energy and density ($-2.0°$K and $0.95\rho_0$), but the need for a better wave function remains. Numerous possibilities exist for constructing increasingly complicated wave functions. Determinants with particle-hole states, spin-dependent correlation factors, state-dependent backflow, and four-body correlations offer themselves as candidates. The difficulties of these investigations, however, require that they await clearer motivation.

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