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Ground states of polarized and unpolarized ^{3}He

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A variational computation of the ground-state energy of a Fermi fluid similar to ^{3}He is made using Slater-Jastrow-type wave functions. The calculation of the energy is performed by an exact Monte Carlo algorithm. The two cases of the polarized and unpolarized fluids are considered in the domain of densities corresponding to a stable thermodynamic state. For these densities the energy of the polarized fluid is shown to be lower than the energy of the unpolarized fluid. A comparison is made with the previous approximate computations of the ground state of unpolarized ^{3}He.

INTRODUCTION

Recently two articles[1,2] have discussed the existence of a metastable polarized phase of fluid ^{3}He. This phase, in which all the nuclear spins are parallel, is expected to have a lifetime large enough to be observed in a "quasithermodynamic" equilibrium. In Ref. 1, Lhuillier and Laloë have studied the effect of a total polarization on the equation of state and on the transport coefficients of the dilute gaseous phase. For the pressure and the viscosity these authors have found rather large differences between the polarized and the unpolarized gas. These results were obtained on the basis of the virial expansion for the pressure and of the collision integral expansion for the viscosity. For the liquid phase near zero temperature, these expansions are not valid, and the present work is an attempt at computing the equation of state of liquid ^{3}He both in a polarized and an unpolarized state at $T_0=0$ K.

The ground state of unpolarized ^{3}He has been studied by Schiff and Verlet,[3] who have used a variational method. In this method, the ground-state wave function was written as the product of a symmetrical function of the spatial coordinates of the ^{3}He atoms and of a Slater determinant. Then the ground-state energy was computed by use, up to second order, of a cluster expansion proposed by Wu and Feenberg.[4] In spite of a reasonable agreement with the experimental ground-state energy, the results of Ref. 3 were not an upper bound for the ground-state energy due to the truncation of the cluster expansion. Ceperley, Chester, and Kalos[5] have overcome this difficulty. They propose an exact Monte Carlo algorithm for the computation of the ground-state energy with the same kind of variational wave function as used in Ref. 3, and show that the estimation of the ground-state energy by Schiff and Verlet was almost exact for a density corresponding to zero pressure and that it was in error by ~1 K for a density near solidification.

Using the algorithm of Ref. 5, we extend the results of this article, and for $T_0=0$ K we give the equation of state of fluid ^{3}He in the range of densities from that at zero pressure to the solidification density. The computation is done both for the polarized and for the unpolarized phase.

Our paper is organized as follows. In Sec. I we give the expressions for our variational wave functions and results for the ground-state energy E. Section II is devoted to a detailed comparison of the polarized and unpolarized phases. In Sec. III we discuss the unexpected result that, for the variational wave functions used here, the polarized phase has an energy lower than the unpolarized phase. In the conclusion we summarize our results and sketch what we plan to do on the subject in the future.

I. COMPUTATION OF THE GROUND-STATE ENERGY

In this paper the interaction between the ^{3}He atoms is chosen to be a Lennard-Jones (LJ) potential $V(r)$:

$$V(r)=4\epsilon[(\sigma/r)^{12}-(\sigma/r)^{6}] \quad , \tag{1}$$

where $\sigma=2.556$ Å, $\epsilon=10.22$ K, σ is taken as the unit of length, and the density ρ is expressed in number of atoms by σ^3.

The trial wave function is assumed to have the following form for a system of N fermions:

$$\psi=\prod_{i=j=1}^{N}\exp[-\tfrac{1}{2}u(|\vec{r}_i-\vec{r}_j|)]D=\phi D \quad ,$$

where r_i are the coordinates of the ith atom, and D is the term which gives to ψ the desired antisymmetry. For the polarized fluid, D is a Slater determinant of plane waves, and for the unpolarized fluid, D is a product of two Slater determinants corresponding to the spin-up and spin-down particles.

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We have

$$u(r)=(b/r)^5 \ , \tag{2}$$

$$\psi_u=\phi \det \{d_{li}\} \det \{d'_{mj}\} (l,\ i,\ m, \text{ and } j=1,2,\ldots,\tfrac{1}{2}N) \tag{3}$$

for the unpolarized state, and

$$\psi_p=\phi \det \{d_{li}\} \quad (l,i=1,2,\ldots,N) \tag{4}$$

for the polarized state, where $d_{li}=(\exp(i\vec{k}_l\cdot\vec{r}_i))$ are the elements of the determinants.

The system of N fermions of mass m is enclosed in a cubic box with periodic boundary conditions. These conditions determine the choice of the $\vec{k}_l$ vectors. These vectors have components equal to $2\pi n/L$, where n is some integer $(0,\ \pm 1,\ \pm 2,\ldots)$ and L is the side of the cubic box. The ground-state energy is obtained by taking the average of the Hamiltonian H:

$$\begin{aligned} E &= \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle \\ &= \int \psi^* \left(-\sum_{i=1}^{N} \frac{\hbar^2}{2m} \Delta_i \right) \psi \, d\vec{r}_1 \cdots d\vec{r}_N \Big/ \int \psi^* \psi \, d\vec{r}_1 \cdots d\vec{r}_N \\ &\quad + \tfrac{1}{2} \int \psi^* \sum_{i\neq j=1}^{N} V(|\vec{r}_i-\vec{r}_j|) \, d\vec{r}_1 \cdots d\vec{r}_N \Big/ \int \psi^* \psi \, d\vec{r}_1 \cdots d\vec{r}_N \\ &= T+U \ , \end{aligned} \tag{5}$$

where H is

$$H=-\sum_{i=1}^{N} \frac{\hbar^2}{2m}\Delta_i+\tfrac{1}{2}\sum_{i\neq j=1}^{N} V(|\vec{r}_i-\vec{r}_j|) \ . \tag{6}$$

The potential energy is easily expressed in terms of the two-body correlation function $g(r)$:

$$U=\frac{\rho}{2}\int V(r)g(r)\,d\vec{r} \tag{7}$$

with

$$g(r)=\frac{1}{N\rho}\sum_{i\neq j=1}^{N}\langle \delta(|\vec{r}_i-\vec{r}_j-\vec{r}|)\rangle \ . \tag{8}$$

The kinetic energy can be written in two different forms. We can write either

$$\begin{aligned} \Delta_i\psi &= \operatorname{div}_i[\vec{\nabla}_i(\phi D)] \\ &= \operatorname{div}_i \left[\left(-\tfrac{1}{2} \sum_{j\neq i=1}^{N} \vec{\nabla}_i u(r_{ij}) + \sum_{l=1}^{N} \bar{D}_{li} \vec{\nabla}_i d_{li} \right) \phi D \right] \\ &\equiv \operatorname{div}_i(\vec{F}_i\phi D) \ , \end{aligned} \tag{9}$$

where $\bar{D}_{li}$ is the cofactor of d_{li} divided by D, or

$$\begin{aligned} \Delta_i\psi = \Bigg[& -\tfrac{1}{2}\sum_{j\neq i=1}^{N}\Delta_i u(r_{ij})+\sum_{l=1}^{N}\bar{D}_{li}\Delta_i d_{li} \\ & -\left(\sum_{l}\bar{D}_{li}\vec{\nabla}_i d_{li}\right)^2+\vec{F}_i^2 \Bigg] \phi D \ . \end{aligned} \tag{10}$$

Using Green's theorem we obtain from Eq. (9)

$$T=\frac{\hbar^2}{2m}\sum_{i=1}^{N}\langle \vec{F}_i^2\rangle \tag{11}$$

and from formula Eq. (10)

$$\begin{aligned} T &= \frac{\hbar^2}{4m}\sum_{i=1}^{N}\left\langle \frac{1}{2}\sum_{j\neq i=1}^{N}\Delta u(r_{ij}) - \left(\sum_{l}\bar{D}_{li}\vec{\nabla} d_{li}\right)^2 - \sum_{l=1}^{N}\bar{D}_{li}\Delta_i d_{li} \right\rangle \\ &= \frac{\hbar^2}{8m}\rho\int \Delta u(r) g(r)\, d\vec{r} + T_F \\ &= T_u + T_F \ . \end{aligned} \tag{12}$$

The expressions of T are written in the case of the polarized fluid. For the unpolarized fluid, the sums over l go from 1 to $\frac{1}{2}N$ and d'_{li}, $\bar{D}'_{li}$ or d_{li}, $\bar{D}_{li}$ are used according to the determinant associated to the ith atom. On the average, both formulas for T give the same answer, as expected, but one formula is to be preferred, if its variance is smaller. In fact in the case of ^{3}He, we have not found large differences. The two terms T_u and T_F give the contributions to T due to the pseudopotential $u(r)$ and to the Slater determinant. According to the formulas (7) and (11) or (12), the computation of E is done as an average over configurations drawn from the probability distribution $\psi^*\psi/\int \psi^*\psi\, d\vec{r}_1 \cdots d\vec{r}_N$. The details of the Monte Carlo computation are given in Ref. 5, and we do not repeat them in this article.

Values of E are given in Tables I and II; for each calculation, we give the number of particles in the system, the number of generated Monte Carlo configurations, and the estimated error. The values of E, U, and T_u contain a correction for the finite size of the system. These corrections are obtained by assuming $g(r)=1$ for r larger than $\frac{1}{2}L$; they are rather small (~1 K) because ρ is small, and they are identical for the two phases (polarized and unpolar-

TABLE I. Results for the unpolarized phase. ρ is the density, b is the parameter of the pseudopotential $u(r)$, N is the number of particles, n is the number of configurations ($\times 10^4$). E is the total energy, T is the kinetic energy, T_F is the Slater kinetic energy, U is the potential energy, and the error estimate is for E(in K).

ρ	b	N	n	E	T	T_F	U	Error
0.18	1.10	54	52	−1.14	6.80	1.83	−7.93	±0.15
0.20	1.08	54	52	−1.12	7.50	1.96	−8.62	±0.15
	1.10	54	52	−1.32	7.70	1.93	−9.03	±0.15
	1.12	54	52	−1.26	8.02	1.95	−9.27	±0.15
	1.145	54	52	−1.25	8.32	1.91	−9.66	±0.15
0.2189	1.10	54	60	−1.33	8.67	2.05	−10.00	±0.15
	1.12	54	52	−1.42	8.98	2.03	−10.40	±0.15
	1.145	54	52	−1.25	9.43	2.07	−10.67	±0.15
	1.17	54	52	−1.02	9.88	2.04	−10.90	±0.15
0.236	1.10	54	30	−1.18	9.63	2.16	−10.81	±0.20
	1.12	54	52	−1.33	9.95	2.12	−11.27	±0.15
	1.145	54	52	−1.29	10.40	2.09	−11.69	±0.15
	1.17	54	52	−0.94	10.98	2.12	−11.92	±0.15
0.2554	1.12	54	30	−1.20	11.11	2.22	−12.30	±0.20
0.2743	1.12	54	30	−0.90	12.37	2.40	−13.27	±0.20
0.3283	1.12	54	52	−0.34	15.84	2.58	−16.18	±0.15
0.3648	1.12	54	30	+0.99	18.57	2.74	−17.59	±0.20
0.414	1.10	54	52	+3.24	21.42	2.96	−18.17	±0.15
	1.12	54	82	+2.64	22.42	2.99	−19.78	±0.12
	1.145	54	82	+2.57	23.89	2.98	−21.32	±0.12
	1.17	54	52	+2.89	25.35	2.93	−22.46	±0.15

ized). For E, there is a cancellation between the correction for U and the correction for T. The influence of N on the value of E has been studied by Ceperley, Chester, and Kalos, who compared results for 38, 54, and 114 particles in the unpolarized state. They found a variation on E of the order of +0.15 K when N is increased. For the polarized state, we have performed computations with 33, 57, and 81 particles, and we have found a similar variation.

For unpolarized ^{3}He, we have made computations for a system of 54 atoms in the density range $0.18 < \rho < 0.414$. From these computations we have found that the density ρ_0 and the energy E_0 corresponding to zero pressure are equal to 0.22 and -1.42 K. These values of ρ_0 and E_0 should be compared with their experimental counterparts $\rho_0 = 0.274$ and $E_0 = -2.52$ K. The value of ρ_0 obtained variationally is thus erroneous by 25%. Schiff and Verlet[3] have found $\rho_0 = 0.237$ and $E_0 = -1.37$ K on the basis of the Wu and Feenberg expansion. As already pointed out by Ceperley, Chester, and Kalos, the result of Ref. 3 is in agreement with the exact Monte Carlo result for the density $\rho = 0.237$, but this agreement is in fact coincidental because Schiff and Verlet's results are above the exact variational results for $\rho \lesssim 0.24$ and below for $\rho > 0.24$.

At higher densities $\rho \simeq 0.4$, we find $E \simeq +2.6$ K, in good agreement with the value of Ref. 5. This value is higher by ~ 1 K than Schiff and Verlet's estimate and by 3 K than the experimental value for ^{3}He (~ -0.5 K).

The optimal value of b increases slightly with density from 1.11 at $\rho \sim 0.2$ to 1.13 at $\rho \sim 0.4$. The value $b = 1.12$ is a reasonable choice for all the intermediate densities ($0.2 < \rho < 0.4$).

For the unpolarized ^{3}He, the variational wave function ψ_u is not very satisfactory; especially if the results are compared with those obtained for ^{4}He with a variational Jastrow wave function. For ^{4}He, the minimum density calculated by a variational method is only 10% smaller than the experimental minimum density, and the value of E is ~ 1 K above the experimental energy in the fluid.[3,6]

In Table II, the values of E, U, and T are given for the polarized phase. For all the densities $\rho > 0.22$, E for the polarized phase is lower than the value of the

TABLE II. Results for the polarized phase. Same notation as in Table I.

ρ	b	N	n	E	T	T_F	U	Error
0.2189	1.00	33	15	−0.37	7.68	3.13	−8.05	±0.25
	1.05	33	20	−1.27	8.29	3.09	−9.57	±0.20
	1.10	33	20	−1.35	9.02	3.04	−10.37	±0.20
	1.13	33	20	−1.31	9.40	2.98	−10.71	±0.20
	1.16	33	15	−0.98	9.89	2.96	−10.87	±0.25
0.236	1.05	33	20	−1.07	9.16	3.23	−10.23	±0.20
	1.10	33	20	−1.50	9.87	3.15	−11.37	±0.20
	1.13	33	20	−1.26	10.48	3.16	−11.74	±0.20
0.2554	1.05	33	20	−1.11	10.03	3.34	−11.14	±0.20
	1.10	33	20	−1.62	10.90	3.24	−12.52	±0.20
	1.10	57	36	−1.40	11.10	3.27	−12.50	±0.20
	1.12	57	36	−1.36	11.47	3.30	−12.83	±0.20
	1.13	33	20	−1.36	11.60	3.21	−12.97	±0.20
	1.16	33	20	−1.14	12.11	3.16	−13.29	±0.20
0.2743	1.05	33	20	−1.01	11.08	3.57	−12.11	±0.20
	1.10	33	20	−1.46	12.08	3.41	−13.54	±0.20
	1.12	57	36	−1.28	12.66	3.46	−13.94	±0.20
	1.13	33	20	−1.44	12.64	3.34	−14.08	±0.20
	1.16	33	20	−1.07	13.43	3.28	−14.50	±0.20
0.3283	1.05	33	20	−0.23	13.91	3.81	−14.14	±0.20
	1.10	33	20	−0.81	15.44	3.72	−16.24	±0.20
	1.13	33	20	−1.04	16.37	3.67	−17.43	±0.20
0.3648	1.10	33	20	−0.21	17.98	3.98	−18.19	±0.20
	1.13	33	40	−0.22	19.10	3.87	−19.32	±0.15
	1.16	33	20	+0.13	20.44	3.86	−20.32	±0.20
0.414	1.10	33	30	+1.81	21.72	4.21	−19.91	±0.18
	1.12	57	37	+1.57	22.83	4.28	−21.25	±0.20
	1.13	33	50	+1.19	23.17	4.20	−21.98	±0.13
	1.145	81	227	+0.95	22.90	3.93	−21.95	±0.10
	1.16	33	30	+1.85	24.93	4.09	−23.08	±0.15

energy for the unpolarized phase. We find a density ρ_0 equal to 0.25 and an energy E_0 equal to 1.6 K. If the size effect and the estimated error on E are taken into account, the difference between the variational results for the unpolarized and the polarized phase is not larger than 0.1 K for the densities $0.2 < \rho < 0.29$, but the difference is 1 K, at least, for densities of the order of 0.4.

The fact that the energy computed with ψ_p is lower than the energy computed with ψ_u is in contradiction with experiment, and this is a failure of the variational method. However, if the results for ψ_p are considered as an upper bound for the ground-state energy, they are not bad and are comparable to those obtained for liquid ^{4}He with a Jastrow function.

Our new variational results for E modify the previous estimates[7] concerning the densities and the volume variation of the liquid-solid phase transition of ^{3}He. It is clear that, if the values of E in the solid phase are kept the same as in Ref. 7, the volume variation will be too large if E is computed by using ψ_u and will be better than in Ref. 7 if E is computed by using ψ_p. This is due to the fact that the energy for the fluid phase used in Ref. 7 is the energy calculated by Schiff and Verlet. Near solidification this energy is intermediate between the energies calculated from ψ_u and from ψ_p, but a precise determination of the transition is not very interesting because the best results correspond to the ψ_p wave function. Since Schiff and Verlet's article, various variational methods, the so-called hypernetted chain (HNC) and Fermi hypernetted chain (FHNC) methods, have been used for the study of the fermion system at $T_0 = 0$ K. All these methods, reviewed in Ref. 8, contain an approximation which has as a consequence that the calculated ground-state energy is not a true upper bound. However, these methods are rather accurate. For instance, for the fluid, unpolarized

^{3}He, the work of Pandharipande and Bethe[9] and of Zabolitzky[10] give a minimum density $\rho \simeq 0.24-0.25$ with an energy $E \simeq -1.3$ K. In these papers, for the densities $\rho < 0.3$, the values of the energy are very close to the values found by Schiff and Verlet. The preceding discussion remains valid for the results of Refs. 9 and 10, and it shows the limitation of the HNC or FHNC methods in the domain of density $\rho < 0.3$.

The errors quoted in Table I and II are estimated from independent Monte Carlo computations at fixed b and ρ. For instance in the case of $\rho = 0.414$, $b = 1.145$ for the polarized state, we have done five different calculations of $\sim 4.5 \times 10^5$ configurations for $N = 81$. The values of E are 0.92, 1.21, 1.10, 0.75, and 0.75 K; those of U are -21.95, -21.82, -21.86, -22.07, and -22.07 K; and those of T are 22.88, 23.02, 22.95, 22.82, and 22.82 K. In spite of a very good precision for U and T (better than 1%), the error on E is rather large due to the cancellation between U and T. This is a familiar result for the variational computations on helium.

II. COMPARISON OF THE EQUATIONS OF STATE OF THE POLARIZED AND UNPOLARIZED PHASES

In this section we attempt to explain why the best ground-state energy is associated with ψ_p for $\rho > 0.22$. A rough estimate of the effect of a total polarization on the ground-state energy consists in considering firstly that U is the same for both the polarized and unpolarized states, and secondly that T increases as in a perfect Fermi gas. With these hypotheses, the energy of the polarized state should be larger by $\sim +1.5$ K than the energy of the unpolarized state.

Obviously these hypotheses do not seem to hold when the functions ψ_u and ψ_p are used as trial functions in a variational calculation. From Tables I and II, where we compare the results for a given value of b and for fixed ρ, we see that, as expected, T_F is larger by ~ 1 K in the polarized phase. But the total increases of T is not 1 K but is only $+0.2$ or $+0.3$ K. The potential energy U varies also by $\sim 1-2$ K and, in absolute value, U is larger in the polarized phase. The origin of these different variations for U and T is easily traced in the behavior of the two-body correlation function $g(r)$, which pictures the relative localization of the atoms in the system.

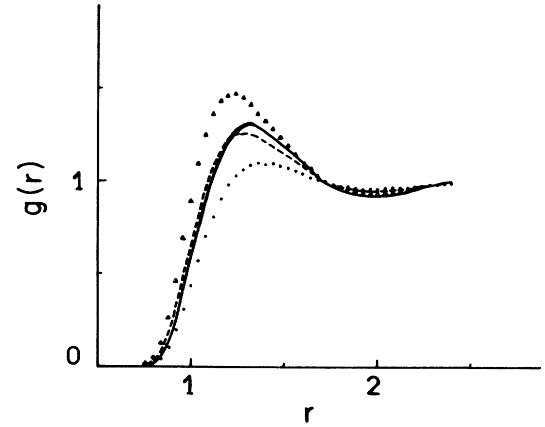

FIG. 1. Two-body correlation functions at $\rho = 0.414$ and $b = 1.12$. $g_p(r)$: ——, $g_u(r)$: – – –, $g_L(r)$· · · ·, $g_v(r)$: ▲ ▲ ▲.

In Figs. 1 and 2 the functions $g(r)$ for the densities $\rho = 0.414$ and 0.2189 are plotted both for the polarized phase $[g_p(r)]$ and for the unpolarized phase $[g_u(r)]$. In the case of the unpolarized phase, $g_u(r)$ can be divided into a function for the atoms with like spins $g_L(r)$ and another function for the atoms with unlike spins $g_v(r)$ [all $g(r)$ functions are normalized in such a way that they go to unity for $r \rightarrow \infty$]. For the unpolarized phase our results are in perfect agreement with those of Ref. 5. For $\rho = 0.2189$ $g_L(r)$ has no structure and $g_v(r)$ has a pronounced peak at $r \simeq 1.35$. For $\rho = 0.414$, the two functions have a peak; this peak is located at $r = 1.23$ in $g_v(r)$ and at $r = 1.4$ in $g_L(r)$. As discussed in Ref. 5, the antisymmetrization of ψ_u is responsible for the differences between $g_v(r)$ and $g_L(r)$. The atoms with like spins tend to stay away as far as possible. On the contrary, the atoms with unlike spins are near neighbors, and this fact compensates the reduction of the potential energy due to the larger distances between the atoms with like spins.

The functions $g_p(r)$ and $g_u(r)$ differ by the positions and the heights of the peaks. In Fig. 1, the positions of the peaks are $r = 1.26$ for $g_u(r)$ and $r = 1.32$ for $g_p(r)$. The heights are 1.25 and 1.30, respectively. For all the fluid densities, there are similar differences, as shown in Fig. 2 for $\rho = 0.2189$.

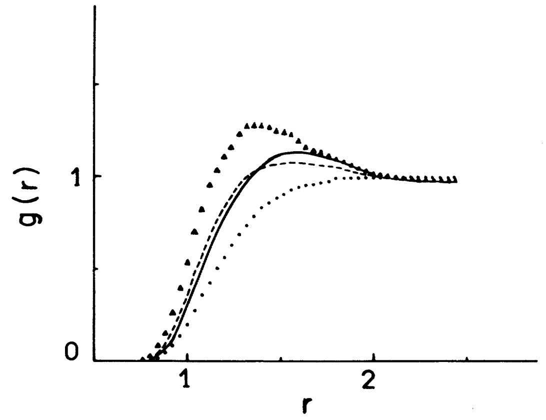

FIG. 2. Two-body correlation functions at $\rho = 0.21892$ and $b = 1.10$. $g_p(r)$: ——, $g_u(r)$: – – –, $g_L(r)$· · · ·, $g_v(r)$: ▲ ▲ ▲.

The displacement of the peak to large r in the polarized phase reduces the value of T_u because $\Delta u(r)$ is a monotonic function of r proportional to $(b/r)^7$. For the potential energy U, the contribution of the positive part of $V(r)(r<1)$ is reduced in the polarized phase because, in the domain $r<1$, $g_p(r)$ is smaller than $g_u(r)$. The contribution of the negative part of $V(r)(r>1)$ is more difficult to guess: $g_p(r)$ is smaller than $g_u(r)$ for $1<r\lesssim 1.2$, but the opposite is true for $r \gtrsim 1.2$. In fact, in the two phases, the negative part of $V(r)$ gives an almost equal contribution to U. For instance, at $\rho=0.414$ and $b=1.12$ (Fig. 1), the contributions to U coming from the domain $r>1$ are -25.7 (unpolarized phase) and -25.9 K (polarized phase). The difference on U between the two phases is due to the contributions for $r<1$ which are equal to $+6.0$ (unpolarized phase) and $+4.7$ K (polarized phase). A similar analysis is valid for the other values of ρ and b. Briefly, if the unpolarized state is transformed into a polarized state, T increases and U gets more negative. For all the densities $\rho>0.22$, the negative variation of U exceeds the positive change of T if ψ_u and ψ_p are used as trial wave functions. This fact implies that our variational computation gives a polarized ground state for ^{3}He.

The main conclusion of the previous discussion is that, for a Fermi system of particles interacting by a potential of the LJ type, there is a very delicate balance between the positive and negative contributions to E. Then it is very difficult to predict correctly the value of E and the polarization state at $T_0=0$ K. It is worthwhile to notice that this conclusion is probably not valid for a fermion one-component plasma,[11] where $V(r)$ is positive for all values of r and where there is no cancellation between U and T.

III. POSSIBLE IMPROVEMENTS OF THE VARIATIONAL RESULTS

The present calculation fails to give the true polarization of the ground state of fluid ^{3}He. The origin of this failure can be the form of the variational functions or the potential $V(r)$.

We have considered the first possibility by doing calculations for the unpolarized state with a wave function which is different from ψ. In this function, the b parameter of the pseudopotential $u(r)$, has two different values b_1 and b_2, b_1 for the pairs of atoms with parallel spins and b_2 for the pairs of atoms with antiparallel spins. The choice $b_2>b_1$ seems appropriate in order to decrease the contribution of the positive part of $V(r)$ or equivalently, in order to reduce the value of $g_L(r)$ for $r<1$. However, the domain of reasonable values for b_1 and b_2 is rather small, because from Table I we see that the optimal value of b is around 1.12 with a variation of a few percent in the whole domain of densities and that, for a fixed density, it is not possible to vary b strongly without increasing E. With these limitations on the values of b_1 and b_2, the condition $b_1 \neq b_2$ involves rather weak variations on E. For instance, for $\rho=0.414$ if b_1 and b_2 are equal to 1.13 and 1.145, we find $E=+2.53$ K, and if they are equal to 1.10 and 1.12, we obtain $E=+2.70$ K. These values of E must be compared to the best value found with $b_1=b_2$ which is $+2.57$ K and to the value $+1.1$ K corresponding to the polarized phase.

Obviously there is a very large choice of pseudopotentials $u(r)$. But, from the numerous variational calculations[12,13] on ^{4}He, it is possible to conclude that a maximum decrease of only ~ 0.2 K can be obtained from a modification of $u(r)$. This decrease is too weak to bring the energy computed with ψ_u below the energy computed with ψ_p.

Recently Schmidt and Pandharipande[14] using a FHNC method have shown that the inclusion of three-body correlations in ψ decreases the minimum energy by ~ 0.8 K. The order of magnitude of the variation on E seems to be sufficient to correct our results for the densities $\rho<0.3$. For the densities $\rho\sim 0.4$ it is very difficult to guess whether the three-body correlations are able to eliminate the discrepancy of ~ 3 K on the energy derived from ψ_u.

For the LJ-boson system, Whitlock *et al.*[15] have made an exact calculation of the ground-state energy. This computation has proved that the ground-state energy of this potential is slightly above the energy of ^{4}He at $T_0=0$ K. The difference is about 0.5 K in the fluid phase, if the contribution of the three-body interaction is subtracted from the energy of ^{4}He. With the hypothesis of an identical interatomic interaction in ^{3}He and ^{4}He, a difference of ~ 0.5 K is probable in the computation of the energy of ^{3}He due to the inadequacy of the LJ potential. However, the discussion of the second section has shown the important role of the positive part of $V(r)$ in the determination of the values of E and of the polarization of the ground state. Then a weak modification of $V(r)$ around $r=1$ can involve a variation on E, maybe, larger than 0.5 K. But with our hypothesis of an identical $V(r)$ in ^{3}He and ^{4}He, we must be careful in the choice of a new potential for ^{3}He in order to obtain also a correct value of the ground-state energy of ^{4}He.

Finally, the most significant improvement to the present variational calculation seems to include three-body correlation in ψ.

IV. CONCLUSION

The energy calculated here with the function ψ_p is a true upper bound for the ground-state energy of a polarized fermion fluid interacting by a LJ potential.

If the three-body correlation effects (about ~ -0.7 K) and the inadequacy of the LJ potential (about ~ -0.5 K) are taken into account, we conclude that the difference between the energies of the polarized and unpolarized ^{3}He is probably not larger than 0.2–0.3 K. This result follows from the fact that our upper bound for the polarized LJ fermion system exceeds the energy of fluid ^{3}He at most by $+1.5$ K.

We plan further work on the subject in order to find a variational function giving the true polarization of the ground state of ^{3}He and the best way seems to include three-body correlations in the trial wave function. We also plan computations with partial polarization.

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