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Ground State of Liquid Helium-4 and Helium-3†

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A variational calculation of the ground-state energy of liquid helium-3 and liquid helium-4 is made using, respectively, Jastrow- and Slater-Jastrow-type trial wave functions. In the boson (He^4) case, the quantum average, analogous to a statistical average over a fictitious canonical ensemble, is computed by a molecular-dynamics method for a system of 864 atoms. The following quantities are obtained: ground-state energy: -5.95°K/atom (experiment: -7.14°K/atom); equilibrium density (0.020 ± 0.002) atoms/Å^3 (experiment: 0.022 atoms/Å^3); liquid-structure factor; fraction of particles condensed in the zero-momentum state: 0.105 ± 0.005. This is in good agreement with previous computations. In the fermion (He^3) case, the energy expectation value is calculated approximately by use, up to second order, of a cluster expansion of the effect of the antisymmetrization, developed by Wu and Feenberg. The ground-state energy obtained is -1.35°K/atom (experiment: -2.52°K/atom). The liquid-structure factor of liquid He^3, for which no experimental result is yet available, is calculated in this approximation.

I. INTRODUCTION

WE present in this paper a variational calculation of the ground-state energy of liquid helium-4 and liquid helium-3.

For the boson system (helium-3) we use a Bijl-Jastrow trial wave function

$$\Psi_B(\mathbf{r}_1,\cdots,\mathbf{r}_N)=\exp\{-\tfrac{1}{2}\sum_{i<j}u(|\mathbf{r}_i-\mathbf{r}_j|)\}, \qquad (1)$$

where $u(r)$ is a "short-range" function (decreasing faster than $1/r^3$ at infinity). The advantage of such a trial wave function is the formal analogy of its energy expectation value with the configuration-space integrals encountered in classical equilibrium statistical mechanics. This analogy has been used by several authors who evaluated the energy expectation value by different techniques borrowed from the theory of classical fluids: summation of chain diagrams, use of approximate integral equations,[1] and "exact" Monte Carlo computations.[2,3] In this work we have used the same molecular-dynamics method that has been used[4,5] for classical fluids.

In Sec. II the analogy of the Jastrow quantum variational problem with classical statistical mechanics is underlined, the principle of the molecular dynamics method is briefly recalled, and the numerical results concerning the ground-state energy of liquid helium-4 are given. These results are in good agreement with McMillan's[3] and with those obtained at Orsay[2]: the energy is -5.95 ± 0.2°K/atom (the experimental energy is -7.14°K/atm) and the equilibrium density is $(0.9\pm0.1)\rho_0$, where ρ_0 is the density of liquid He at zero pressure ($\rho_0=0.02185$ atoms/Å^3).

The energy is, in principle, the only quantity which is stationary with respect to small changes of the variational parameters. In Secs. III and IV we summarize the results concerning two other interesting quantities: the liquid-structure factor and the one-particle density matrix. The liquid-structure factor $S(k)$ seems to change very little when the variational parameters are varied slightly around their optimum value. It is in good agreement with the experimental data where they exist ($k>0.8$ Å^{-1}). However, a short-range trial function $u(r)$ cannot give rise to a structure factor $S(k)$ vanishing linearly for small magnitudes of the wave vector k (as it should, if the phonons are the only long-wavelength excitations of the liquid). Reatto and Chester[6] have recently suggested to include in $u(r)$ a long-range part

$$u_{\mathrm{LR}}(r)\propto[r^2+(1/k_c)^2]^{-1}. \qquad (2)$$

At the end of Sec. III we discuss the inclusion of such a term in the wave function, assuming that the cutoff $1/k_c$ is large so that the effect of (2) can be treated as a weak long-range perturbation.

The one-particle density matrix is discussed in Sec. IV: It seems to be somewhat more parameter-dependent than the energy and $S(k)$. The fraction of particles

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condensed in the zero-momentum state is

$$n_0/\rho = 0.105 \pm 0.005$$

in reasonable agreement with the estimates of Penrose and Onsager[7] and of McMillan.[3]

In Sec. V are given the results concerning liquid helium-3. For a fermion system a symmetrical wave function like (1) is inadequate. Several authors[8] have suggested to build an antisymmetrical wave function in the simplest way,

$$\Psi_F(\mathbf{r}_1, \cdots, \mathbf{r}_N) = \Psi_B \operatorname{Det}\{\exp(i\mathbf{k}_i\cdot \mathbf{r}_j)\chi_i(\sigma_j)\}, \quad (3)$$

where $\chi_i(\sigma_j)$ describes the spin state of particle number j. With a wave function like (3), the energy expectation value no longer has the same form as in classical statistical mechanics. However, Wu and Feenberg[8] have developed a useful cluster-expansion formalism for the effect of the antisymmetrization. Such an expansion is expected to be valid when the strongly repulsive short-range forces are such that the correlations due to the Pauli principle act as a small correction to the dynamical correlations described by Ψ_B. We have used the Wu–Feenberg expansion up to second order: the second-order correction is 10 times smaller than the first-order one and the ground-state energy found is −1.35°K/atom (the experimental[9] one is −2.52°K/atm). Finally, the structure factor of liquid helium-3 is obtained: Its Wu–Feenberg expansion seems to converge rather rapidly and it does not depend too much on the variational parameters. A comparison with experiment would be interesting (to our knowledge, no experimental data are available).

For solid helium, Nosanow[10] has suggested using a "localized Jastrow" trial wave function

$$\Psi = \Psi_B \prod_i \exp[-(\tfrac{1}{2}A) \mid \mathbf{r}_i - \mathbf{R}_i \mid^2],$$

where the $\mathbf{R}_i$ are the coordinates of the lattice sites and where A is a variational parameter. In Ref. 2 Monte Carlo calculations for 96 helium atoms with such a trial wave function were reported and reproduced fairly well the energy-density curve of solid helium-4; the density at which the optimum value of became zero was in rough agreement with the experimental liquid-solid transition. This question is now being investigated in further detail by Hansen and Levesque.

II. ENERGY EXPECTATION VALUE

We assume that the system of helium atoms (mass μ) is described by the Hamiltonian

$$H = \sum_{i=1}^{N} -(\hbar^2/2\mu)\Delta_i + \sum_{i<j} V(\mid \mathbf{r}_i - \mathbf{r}_j \mid), \quad (4)$$

and that the interatomic potential is of Lennard-Jones type

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

with[11] $\sigma = 2.556$ Å; $\epsilon = 10.22$°K. The energy expectation value per particle can be calculated, using (1) and (4), and cast into the following form:

$$\frac{\langle\Psi \mid H \mid \Psi\rangle}{N\langle\Psi \mid \Psi\rangle} = \tfrac{1}{2}\rho \int g(r)[V(r) + T(r)]d\mathbf{r},$$

where ρ is the particle density, $g(r)$ the pair function

$$g(r) = \frac{N(N-1)}{\rho^2}\left[\int d\mathbf{r}_3, \cdots, d\mathbf{r}_N \exp\{-\sum_{i<j} u(\mid \mathbf{r}_i - \mathbf{r}_j \mid)\}\right]\left[\int d\mathbf{r}_1, \cdots, d\mathbf{r}_N \exp\{-\sum_{i<j} u(\mid \mathbf{r}_i - \mathbf{r}_j \mid)\}\right]^{-1}, \quad (5)$$

and

$$T(r) = (\hbar^2/4\mu)\Delta u(r). \quad (6)$$

The main problem is thus to calculate, for each trial function $u(r)$, the pair function $g(r)$. At this stage, the formal analogy of our quantum variational problem with the classical problem is obvious: Given a trial function $u(r)$, we may always choose some arbitrary nonzero number T and define an equivalent two-body potential through

$$\Phi(r) = kTu(r).$$

$g(r)$, calculated for a classical fluid of particles interacting through the potential $\Phi(r)$ at temperature T, is evidently equivalent to (5). In Refs. 2 and 3 the integration of (5) was made by a Monte Carlo method which applies in the canonical ensemble for the fictitious fluid at temperature T. Here, we use the equivalence of the canonical ensemble with the microcanonical one and, assuming ergodicity, we evaluate (5) by a time average on a fictitious system of particles interacting through the potential $\Phi(r)$. The "temperature" T of that system is given in terms of the average kinetic energy.

The computation was done in exactly the same way as in the case of the real Lennard-Jones fluid[5]: 864 particles, interacting by a potential $\Phi(r)$ cut at $r_v = 2.5\sigma$, were enclosed in a box with periodic boundary condi-

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TABLE I. Average values of $(\sigma/r)^6$, $(\sigma/r)^7$, $(\sigma/r)^{12}$ and potential and kinetic energy, for different values of the variational parameters m and b. Lengths are given in units σ and energies in °K/atom.

$m=4$ b	$\langle(\sigma/r)^6\rangle$	$\langle(\sigma/r)^{12}\rangle$	V	T	E
1.119	0.9031	0.7217	− 7.42	7.89	0.47
1.139	0.8772	0.6304	− 9.84	8.24	−1.60
1.160	0.8529	0.5708	−11.53	8.61	−2.92
1.181	0.8311	0.5164	−12.86	9.01	−3.83
1.201	0.8108	0.4691	−13.97	9.42	−4.54
1.222	0.7922	0.4265	−14.95	9.86	−5.09
1.243	0.7744	0.3891	−15.75	10.31	−5.44
1.264	0.7573	0.3576	−16.34	10.77	−5.57
1.284	0.7411	0.3280	−16.89	11.25	−5.64
1.305	0.7258	0.3011	−17.36	11.74	−5.61
1.326	0.7112	0.2782	−17.70	12.25	−5.45
1.346	0.6982	0.2572	−18.03	12.80	−5.23
1.367	0.6853	0.2382	−18.28	13.35	−4.92
1.388	0.6739	0.2211	−18.51	13.95	−4.56
1.409	0.6634	0.2060	−18.70	14.57	−4.13
1.429	0.6529	0.1922	−18.83	15.20	−3.63
1.450	0.6439	0.1804	−18.95	15.88	−3.07
1.471	0.6342	0.1686	−19.03	16.55	−2.48
1.491	0.6253	0.1581	−19.10	17.26	−1.84
1.512	0.6164	0.1489	−19.11	17.98	−1.13
1.533	0.6083	0.1404	−19.13	18.73	−0.39
1.554	0.6002	0.1325	−19.11	19.50	0.39
1.574	0.5921	0.1260	−19.05	20.29	1.23
1.595	0.5840	0.1194	−18.99	21.09	2.09
1.616	0.5759	0.1135	−18.90	21.89	2.99

$m=5$ b	$\langle(\sigma/r)^6\rangle$	$\langle(\sigma/r)^7\rangle$	$\langle(\sigma/r)^{12}\rangle$	V	T	E
0.988	1.0028	0.8753	0.9415	− 2.50	7.57	5.07
0.994	0.9914	0.8648	0.9828	− 3.62	7.71	4.08
1.015	0.9550	0.8076	0.7873	− 6.85	8.09	1.24
1.036	0.9210	0.7660	0.6876	− 9.54	8.50	−1.04
1.056	0.8910	0.7338	0.6062	−11.64	8.96	−2.68
1.077	0.8626	0.7006	0.5380	−13.27	9.44	−3.83
1.098	0.8367	0.6698	0.4763	−14.73	9.94	−4.79
1.119	0.8124	0.6418	0.4225	−15.94	10.43	−5.47
1.139	0.7897	0.6177	0.3766	−16.89	11.01	−5.88
1.160	0.769	0.5934	0.3385	−17.55	11.59	−5.96
1.181	0.7468	0.5701	0.3051	−18.06	12.18	−5.88
1.201	0.7274	0.5505	0.2769	−18.42	12.79	−5.62
1.222	0.7096	0.5312	0.2526	−18.68	13.46	−5.21
1.243	0.6934	0.5128	0.2296	−18.96	14.15	−4.81
1.264	0.6780	0.4956	0.2100	−19.13	14.87	−4.26
1.284	0.6642	0.4720	0.1935	−19.24	15.62	−3.61
1.297	0.6537	0.4717	0.1831	−19.24	16.10	−3.14
1.305	0.6512	0.4677	0.1771	−19.38	16.46	−2.92
1.326	0.6383	0.4544	0.1640	−19.39	17.33	−2.06
1.346	0.6269	0.440	0.1509	−19.46	18.24	−1.22
1.367	0.6164	0.4326	0.1378	−19.57	19.20	−0.36
1.388	0.6067	0.4221	0.1312	−19.44	20.22	0.78
1.409	0.5970	0.4123	0.1214	−19.44	21.29	1.85
1.429	0.5881	0.4039	0.1115	−19.48	22.38	2.90
1.450	0.5791	0.3950	0.1050	−19.38	23.54	4.15

tions and the equations of motion were integrated. 300 steps in time were used to reach "equilibrium" and then 1200 steps in time were made. Most computations were made on the CDC 6600 of the New York University where such a calculation took 30 min.

In a previous Monte Carlo calculation[2] we used as trial function a generalization of the one used by Wu and Feenberg,[12] namely,

$$u(r)=(b\sigma/r)^m[1+(ar/\sigma)e^{-r/\sigma}].$$

It was found that the best value of a was between 0 and −0.5. Moreover, as noticed by McMillan the form

$$u(r)=(b\sigma/r)^m \tag{7}$$

makes it possible, by a scaling procedure, to express results at different densities in terms of results at a given density. We have therefore used the trial form (7) with $m=4$ and 5 and $1\leq b\leq 1.5$. The computation averages of the form

$$\langle(\sigma/r)^n\rangle=\langle\Psi\mid\sum_{i<j}(\sigma/r_{ij})^n\mid\Psi\rangle(N\langle\Psi\mid\Psi\rangle)^{-1}$$

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[12] F. Y. Wu and E. Feenberg, Phys. Rev. 122, 739 (1961).

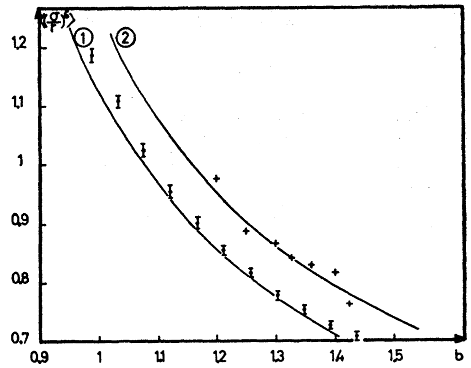

FIG. 1. Average value of $(\sigma/r)^6$, for liquid He^4 at $\rho=\rho_0$, as function of variational parameter b, for $m=5$ [curve (1)] and $m=4$ [curve (2)]: ——, present calculation; •, McMillan; +, previous Orsay (Ref. 2) results.

with Ψ given by (1) can be done, assuming equivalence of the canonical and microcanonical ensembles, by use of the molecular-dynamics technique. For each set of parameters (b, m) we have calculated the averages

$$\langle(\sigma/r)^6\rangle_{\mathrm{MD}}, \qquad \langle(\sigma/r)^{12}\rangle_{\mathrm{MD}}, \qquad \langle(\sigma/r)^{m+2}\rangle_{\mathrm{MD}}$$

and the pair function $g_{\mathrm{MD}}(r)$ at the equilibrium density of liquid helium-4 $\rho_0=0.3648$ atoms/σ^3.

The consistency of the use of a "potential" $\Phi(r)$ cutoff at r_v was checked in the same way as in Ref. 5: firstly, the effect of the tail $r>r_v$ of the potential, neglected in the dynamics, was taken into account in the calculation of the averages by assuming $g(r)=1$ for $r>r_v$, e.g.,

$$\langle(\sigma/r)^6\rangle=\langle(\sigma/r)^6\rangle_{\mathrm{MD}}+(2\pi\rho/3)(\sigma^6/r_v^3).$$

Secondly, the effect on the dynamics of the cutoff tail of $\Phi(r)$ was estimated, following a suggestion by Lebowitz, by treating the cutoff tail as a long-range perturbation [formulas (8) and (9) of Ref. 5, part II]. As in the classical case, this effect is negligibly small:

$$\delta g(r)\leq 0.002, \qquad \delta T=+0.01°\mathrm{K/atom},$$

$$\delta V=+0.03°\mathrm{K/atom}.$$

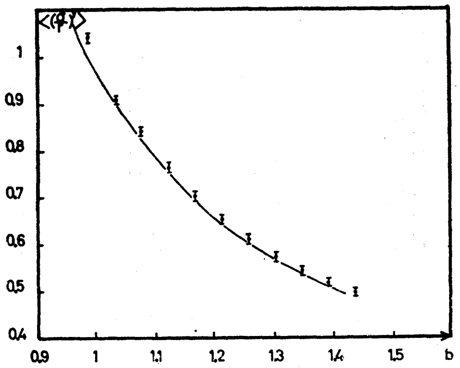

FIG. 2. Average value of $(\sigma/r)^7$ ($m=5$): ——, present calculation; •, McMillan.

TABLE II. Ground-state energy of liquid helium (in °K/atom) as a function of density.

ρ/ρ_0	T	V	E
0.65	6.84	−11.99	−5.15
0.7	7.57	−12.96	−5.39
0.75	8.82	−14.39	−5.57
0.8	9.68	−15.46	−5.78
0.85	10.60	−16.55	−5.95
0.9	11.59	−17.55	−5.96
0.95	12.63	−18.53	−5.9
1.	13.73	−19.46	−5.73
1.05	15.68	−21.19	−5.51
1.10	17.	−22.25	−5.25
1.15	17.51	−22.37	−4.86
1.2	19.94	−24.44	−4.5

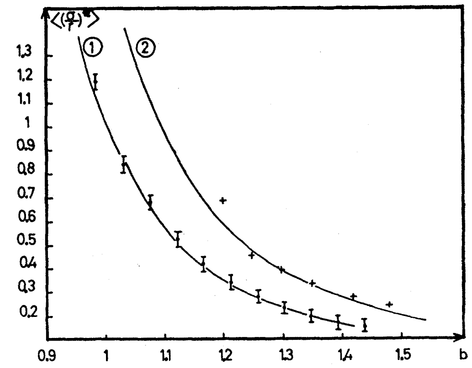

FIG. 3. Average value of $(\sigma/r)^{12}$ for $m=5$ [curve (1)] and $m=4$ [curve (2)]: ——, previous calculation; •, McMillan; +, previous Orsay results.

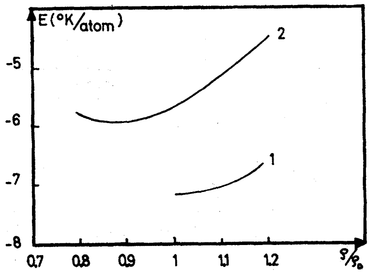

FIG. 4. Energy-density curve of liquid He^4 at 0°K. (1) Experiment; (2) present calculation.

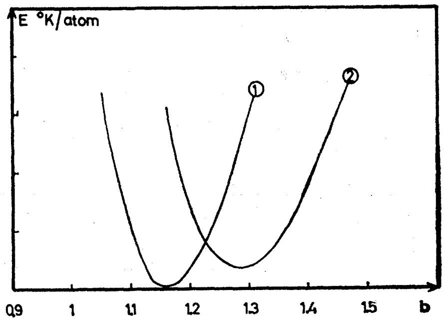

FIG. 5. Dependence of the energy on the variational parameter b for $m=5$ [curve (1)] and $m=4$ [curve (2)].

TABLE III. Comparison of the present results with McMillan's (Ref. 3), the ones obtained previously at Orsay (Ref. 2), and experiment (Ref. 9).

	m	b	$\rho_{\text{equil.}}/\rho_0$	V (°K/atom)	T (°K/atom)	E (°K/atom)
McMillan	5	1.17	0.89 ± 0.01	-17.6	11.7	-5.9 ± 0.1
Orsay	4	1.3	1 ± 0.1	-19.6	13.8	-5.8 ± 0.3
Present calculation	5	1.16	0.9 ± 0.1	-17.55	11.6	-5.95 ± 0.2
Experiment			1			-7.14

The values of $\langle(\sigma/r)^6\rangle$, $\langle(\sigma/r)^7\rangle$, and $\langle(\sigma/r)^{12}\rangle$ are plotted on Figs. 1, 2, 3. The expectation value of the energy for a set of parameters (b', m) at a density ρ' can be deduced from those results according to

$$E(\rho', b', m)=4\epsilon\{-S^6\langle(\sigma/r)^6\rangle+S^{12}\langle(\sigma/r)^{12}\rangle\}$$
$$+(\hbar^2/4\mu\sigma^2)m(m-1)b^mS^2\langle(\sigma/r)^{m+2}\rangle,$$

where $S=(\rho/\rho_0)^{1/3}$ and $b'=b/S$. Table I summarizes the results obtained at $\rho_{\text{eq}}=0.9\rho_0$.

The over-all error is believed to be 0.005 on $\langle(\sigma/r)^{12}\rangle$, 0.002 on $\langle(\sigma/r)^6\rangle$ and $\langle(\sigma/r)^7\rangle$, and 0.2°K/atom on the energy. Table II and Fig. 4 show the dependence of the energy on the density. The equilibrium density is $\rho_{\text{eq}}=(0.9\pm0.1)\rho_0$. The dependence of E on b and m at $\rho=\rho_{\text{eq}}$ is shown on Fig. 5. The dependence of the lowest energy obtained on the parameter m, though very weak, seems to lead to an optimum value $m=5$, in agreement with the findings of McMillan.

The ground-state energy we find is -5.95 ± 0.2°K/atom, at $\rho=(0.9\pm0.1)\rho_0$. Table III shows a comparison of these results with (a) the ones previously obtained at Orsay (by a Monte Carlo calculation on a system of 96 particles), (b) the results of McMillan, (c) experiment. When comparing with the experimental[12] values -7.14°K/atom $\rho=\rho_0$, one must take into account the uncertainties on the interatomic potential: If instead of the Lennard-Jones (LJ) 6–12, a Lennard-Jones (6–8)[13] or an "exponential-6"[14] potential is used, differences of the order of 1 or 2°K appear in the ground-state energy. This is illustrated in Table IV, where the expectation value of the potential energies of these three potentials, with a wave function of the form (1) with $m=5$, are listed at $\rho=\rho_0$.

With the LJ (6–8) potential of Haberlandt:

$$V=\tfrac{256}{27}\epsilon[(\sigma'/r)^8-(\sigma'/r)^6],$$

where $\epsilon=6.34$°K/atom, and $\sigma'=2.84$ Å, the optimum parameters are $b=1.09$, $m=5$, the equilibrium density is $0.8\rho_0$ but the ground-state energy is -7.9°K/atom, 0.75°K *below* the experimental energy, which seems to indicate that the Haberlandt potential is not consistent with the experimental energy of liquid helium-4 at 0°K.

III. LIQUID-STRUCTURE FACTOR

To evaluate the liquid-structure factor

$$S(k)=1+\rho\int\exp(-i\mathbf{k}\cdot\mathbf{r})[g(r)-1]d\mathbf{r},$$

one has to extend carefully the function $g_{\text{MD}}(r)$, in order to avoid truncation errors in the Fourier transform. We have used[15] the same prolongation procedure as in Ref. 5:

$$g(r)=g_{\text{MD}}(r), \qquad r<r_c,$$
$$c(r)=-g(r)\,(e^{u(r)}-1)\,, \qquad r>r_c, \quad (\text{PY}),$$
$$g(r)-1=c(r)+\rho\int c(r-r')[g(r')-1]d\mathbf{r}' \quad (\text{OZ}). \qquad (8)$$

The consistency of this prolongation procedure was checked in the following way: we made one particular molecular-dynamics calculation with a "potential" $\Phi(r)$ cutoff at 3.2σ. We then solved (8) successively for $r_c=3.2\sigma$ and $r_c=2.4\sigma$: the resulting $S(k)$ nowhere differed by more than 0.002.

The dependence of $S(k)$ on the values of the variational parameters is small, as illustrated by Figs. 6. The agreement with experiment is very good wherever unambiguous results exist. The experimental situation about the height of the first peak (around $k=2$ Å^{-1})

TABLE IV. Average values of potential energy (in °K/atom) with wave function (1) ($m=5$, $\rho=\rho_0$) obtained by using three different forms for the interatomic potential. LJ = Lennard-Jones.

b	LJ(6–12)	LJ(6–8)	exp-6
0.95	5.2	7.6	11.5
1.00	− 4.4	− 1.4	2.7
1.05	−11.3	− 8.7	− 4.6
1.10	−16.2	−14.7	−10.8
1.12	−17.5	−16.4	−12.6
1.15	−18.7	−18.3	−14.5
1.17	−19.7	−20.1	−16.3
1.18	−20	−20.5	−16.8
1.23	−21.2	−22.9	−19.3
1.25	−21.5	−23.8	−20.3
1.30	−22	−25.3	−21.8
1.34	−22.2	−26.5	−22.2

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[13] R. Haberlandt, Phys. Letters **14,** 197 (1965).

[14] J. E. Kilpatrick, W. E. Keller, and E. F. Hammel, Phys. Rev. **97,** 9 (1955).

[15] The second equation is the Percus-Yevick approximation to the direct correlation function $c(r)$, dedfined by the last equation (Ornstein-Zernike relation).

is not quite clear: Firstly, it seems to depend sensitively on the temperature and no results very near 0°K are available; secondly, different x-ray[16] and neutron[17] diffraction experiments give different results, varying between 1.28 and 1.49. Numerical values of $g(r)$ and $S(k)$ are given in Tables V and VI.

For small k, where experimental data do not exist yet, the phonon theory of liquid He requires[18] that $S(k)\simeq(\hbar k/2\mu c)$, where c is the sound velocity. For our equivalent fictitious fluid we have on the other hand

$$S(0)=kT(\partial\rho/\partial p).$$

This can vanish only if the classical fluid is incompressible, which is not realizable for any of the short-range $u(r)$ usually assumed in classical fluids. A possible way to improve (1) so that $S(k)$ has the right behavior at small k is the introduction of a long-range (decreasing more slowly than $1/r^3$) part in $u(r)$, suggested recently by Reatto and Chester. These authors suggested to add to the short-range trial function $u_{\mathrm{SR}}(r)$ a long-range part

$$u_{\mathrm{LR}}(r)=(\mu c/\rho\pi^2\hbar)[r^2+(1/k_c)^2]^{-1} \tag{9}$$

chosen so as to give the right behavior of $S(k)$ for $k\rightarrow0$.

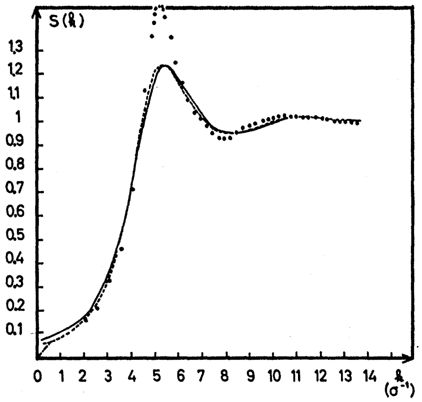

FIG. 6. Liquid-structure factor of liquid He^4 ($\rho=\rho_0$) •, neutron diffraction experiment (Ref. 16) at 1.06°K; ——, present calculation, $m=5$, $b=1.17$, $E=-5.7$; – – – –, present calculation, $m=4$, $b=1.3$, $E=-5.5$ •–•–, theoretical, A. Miller, P. Nozieres, and D. Pines, Phys. Rev. **127**, 1452 (1962). Extrapolation of $S(k)$ for small k.

Since our molecular-dynamics calculation is not adapted to such a long-range potential, we have only been able to evaluate approximately its effects, by the same long-range perturbation technique that we used already to evaluate the effect of the tail of the potential.

TABLE V. Pair function $g(r)$ of liquid helium at $\rho=\rho_0$.

r/σ	$g(r)$	r/σ	$g(r)$
≤0.72	0	1.92	0.955
0.76	0.002	1.96	0.953
0.8	0.010	2	0.950
0.84	0.037	2.04	0.948
0.88	0.099	2.08	0.950
0.92	0.209	2.12	0.952
0.96	0.347	2.16	0.953
1.	0.512	2.2	0.961
1.04	0.680	2.24	0.976
1.08	0.841	2.28	0.985
1.12	0.976	2.32	0.986
1.16	1.095	2.36	0.987
1.2	1.174	2.4	0.992
1.24	1.232	2.44	1.003
1.28	1.255	2.48	1.008
1.32	1.268	2.52	1.009
1.36	1.264	2.56	1.010
1.4	1.251	2.6	1.012
1.44	1.233	2.64	1.012
1.48	1.206	2.68	1.013
1.52	1.162	2.72	1.012
1.56	1.129	2.76	1.011
1.6	1.099	2.8	1.010
1.64	1.069	2.84	1.010
1.68	1.041	2.88	1.007
1.72	1.020	2.92	1.006
1.76	1.004	2.96	1.004
1.8	0.986	3.	1.003
1.84	0.975	3.04	1.001
1.88	0.966	3.08	1.

The effect of $u_{\mathrm{LR}}(r)$ is firstly to add a term

$$\delta T^{(1)}=(\hbar^2/4\mu)\langle\Delta u_{\mathrm{LR}}\rangle$$

to the kinetic energy, secondly to modify the pair correlation function $g_0(r)$ corresponding to the "unperturbed" short-range $u(r)$ by

$$\delta g(r)=-g_0(r)\,\frac{1}{(2\pi)^3}\int\exp(i\mathbf{k}\cdot\mathbf{r})\,\frac{u_{\mathrm{LR}}(k)}{1+\rho S_0(k)\,u_{\mathrm{LR}}(k)}\,d\mathbf{k},$$

with $u_{\mathrm{LR}}(k)=(\mu c/\rho\hbar)2\pi^2\,[\exp(-k/k_c)/k]$. This gives

TABLE VI. Liquid-structure factor $S(k)$ of helium-4 at $\rho=\rho_0$.

$k\sigma$	$S(k)$	$k\sigma$	$S(k)$
0.3	0.085	7.2	1.001
0.6	0.094	7.5	0.975
0.9	0.105	7.8	0.956
1.2	0.12	8.1	0.948
1.5	0.135	8.4	0.946
1.8	0.157	8.7	0.95
2.1	0.186	9.	0.958
2.4	0.224	9.3	0.968
2.7	0.275	9.6	0.978
3.	0.345	9.9	0.988
3.3	0.43	10.2	1.
3.6	0.54	10.5	1.008
3.9	0.68	10.8	1.012
4.2	0.84	11.1	1.014
4.5	0.98	11.4	1.013
4.8	1.115	11.7	1.012
5.1	1.201	12.	1.011
5.4	1.236	12.3	1.008
5.7	1.219	12.6	1.006
6.	1.174	12.9	1.003
6.3	1.122	13.2	1.001
6.6	1.075	13.5	1.
6.9	1.031		

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[16] W. Gordon, C. S. Shaw, and J. Daunt, J. Phys. Chem. Solids **5**, 117 (1958).

[17] D. G. Henshaw, Phys. Rev. **119**, 9 (1960).

[18] R. P. Feynman, Phys. Rev. **94**, 262 (1954).

TABLE VII. Effect of the Reatto-Chester (9) factor on the ground-state energy (estimated by perturbation theory), in °K/atom.

k_c	b	T	V	E	$\delta T^{(2)}$	$\delta T^{(1)}$	$\delta V^{(1)}$	δE
0.167	1.12	12.4	−17.7	− 5.3	−0.21	0.17	0.28	0.24
	1.15	13.4	−19.1	− 5.7	−0.23	0.17	0.31	0.25
0.25	1.12	12.4	−17.7	− 5.3	−0.49	0.11	0.6	0.27
	1.15	13.4	−19.1	− 5.7	−0.53	0.11	0.67	0.25
	1.17	14	−19.7	− 5.7	−0.56	0.11	0.72	0.27
	1.18	14.4	−20.1	− 5.7	−0.58	0.11	0.73	0.26
	1.23	16.4	−21.3	− 4.9	−0.69	0.11	0.83	0.25
0.33	0.95	8.12	8.05	16.2	−0.5	+0.08	−0.7	−1.12
	1	9.12	− 3.64	5.5	−0.59	0.08	−0.04	−0.55
	1.12	12.4	−17.7	− 5.3	−0.85	0.08	+0.1	−0.67
	1.15	13.4	−19.1	− 5.7	−0.91	0.08	+1.09	+0.26
	1.17	14	−19.7	− 5.7	−0.96	0.08	+1.18	+0.30
0.4	0.95	8.12	8.05	16.2	−0.69	0.09	−0.12	−0.74
	1	9.12	− 3.64	5.5	−0.81	0.08	−0.17	−0.9
	1.12	12.4	−17.7	− 5.3	−1.16	0.08	+1.26	+0.18
	1.15	13.4	−19.1	− 5.7	−1.26	0.08	+1.43	+0.31
	1.17	14	−19.7	− 5.7	−1.32	0.08	+1.55	+0.31
0.5	0.95	8.12	+ 8.05	16.2	−1	0.09	−1.93	−2.84
	1.	9.12	− 3.64	5.5	−1.18	0.1	−0.49	−2.57
	1.12	12.4	−17.7	− 5.3	−1.66	0.1	+1.65	+0.11
	1.15	13.4	−19.1	− 5.7	−1.79	0.1	+1.90	+0.21
	1.17	14	−19.7	− 5.7	−1.87	0.1	+2.09	+0.32
1.	0.95	8.12	8.05	16.2	−2.35	0.48	−7.44	−9.31
	1.	9.12	− 3.64	5.5	−2.71	0.5	−3.41	−5.62
	1.12	12.4	−17.7	− 5.3	−3.65	0.53	+2.42	−0.7
	1.15	13.4	−19.1	− 5.7	−3.9	0.54	+3.07	−0.09
	1.17	14	−19.7	− 5.7	−4.06	0.54	+3.57	+0.05

rise to modifications of both kinetic and potential energy:

$$\delta T^{(2)}=\tfrac{1}{2}\rho\int\delta g(r)\,T(r)\,d\mathbf{r},$$

$$\delta V^{(2)}=\tfrac{1}{2}\rho\int\delta g(r)\,V(r)\,d\mathbf{r}.$$

The results corresponding to $m=5$ and several values of b and k_c, at $\rho=\rho_0$, are summarized in Table VII. As is often the case when an approximate method is used simultaneously with a variational principle, the results are not very meaningful: As the cutoff value k_c increases, the energy seems to decrease but so does the validity of the perturbation calculation.

Thus this approximate method does not give a definite answer to the question of whether the modification of the wave function (1) proposed by Reatto and Chester lowers the energy; it seems, however, to indicate that their modification leads to a reasonable $S(k)$ without spoiling the results for the energy. The "perturbed" $S(k)$

$$S(k)=S_0(k)/[1+\rho u_{\mathrm{LR}}(k)S_0(k)]$$

is shown on Fig. 7 for $b=1.17$, $\rho=\rho_0$, $m=5$, and several values of k_c.

IV. ONE-PARTICLE DENSITY MATRIX

The one-particle reduced density matrix is defined by

$$\rho^{(1)}(\mathbf{r}_1-\mathbf{r}_1')=N\left[\int\Psi(\mathbf{r}_1',\mathbf{r}_2,\cdots,\mathbf{r}_N)\Psi(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_N)d\mathbf{r}_2,\cdots,d\mathbf{r}_N\right]\left[\int|\Psi(\mathbf{r}_1,\cdots,\mathbf{r}_N)|^2d\mathbf{r}_1,\cdots,d\mathbf{r}_N\right]^{-1}.$$

For large values of r, $\rho^{(1)}(r)$ approaches n_0, the density of particles condensed in the zero-momentum state. Penrose and Onsager[7] have shown that the superfluid phase of the boson system is characterized by the fact that n_0 is some finite fraction of the particle density ρ and they have given the estimate $n_0\simeq0.08\rho$. McMillan,[3] using the Monte-Carlo method, has computed $\rho^{(1)}(r)$ and has found the asymptotic value $n_0=0.11\rho$. $\rho^{(1)}(r)$ can be cast, following McMillan, in the following form:

$$\rho^{(1)}(r)=\rho\,\frac{\displaystyle\int|\Psi(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_N)|^2\sum_k\exp\{-\tfrac{1}{2}\sum_{j>k}[u(|\mathbf{r}_k+\mathbf{r}-\mathbf{r}_j|)-u(|\mathbf{r}_k-\mathbf{r}_j|)]\}d\mathbf{r}_1,d\mathbf{r}_2,\cdots,d\mathbf{r}_N}{\displaystyle\int|\Psi(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_N)|^2d\mathbf{r}_1,d\mathbf{r}_2,\cdots,d\mathbf{r}_N}.\quad(10)$$

TABLE VIII. Helium-3 ground-state energy (in °K/atom); results in columns 2, 5, and 8 correspond to zeroth, first, and second order in the WF expansion.

b	$E^{(0)}$	$\epsilon_b{}^{(1)}$	$\epsilon_a{}^{(1)}$	$E^{(1)}$	$\epsilon_b{}^{(2)}$	$\epsilon_a{}^{(2)}$	$E^{(2)}$
$\rho=0.65$	$m=5$						
1.10	−2.78	2.24	+0.61	−1.15	−0.06	−0.12	−1.33
1.11	−2.82	2.24	+0.5	−1.08	−0.06	−0.11	−1.25
1.13	−2.92	2.24	+0.5	−1.18	−0.06	−0.11	−1.35
1.15	−2.87	2.24	+0.48	−1.11	−0.06	−0.10	−1.27
1.18	−2.64	2.24	+0.45	+0.85	−0.06	−0.08	−0.99
1.2	−2.28	2.24	+0.44	+0.48	−0.06	−0.06	+0.60
$\rho=0.7$	$m=4$						
1.15	−1.2	2.4	+0.84	+0.36	−0.06	−0.11	+0.19
1.2	−2.6	2.38	+0.54	+0.76	−0.06	−0.13	−0.95
1.26	−2.7	2.36	+0.41	+0.75	−0.06	−0.13	−0.94
1.375	−1.25	2.34	+0.31	+0.78	−0.06	−0.05	0.67
1.46	−1.02	2.32	+0.37	+0.96	−0.06	+0.03	0.93
1.48	+1.5	2.31	+0.47	+3.36	−0.06	+0.06	3.36

Again, when Ψ is given by (1), use can be made of the equivalence of the canonical and microcanonical ensembles to compute the average indicated in (10) by the same molecular dynamics method that was used in Sec. II. $\rho^{(1)}(r)$ was calculated for several values of the variational parameters for $r\leq 2$ and in a few cases for $r\leq 4$. The difference between $\rho^{(1)}(2)$ and $\rho^{(1)}(4)$ is of the order of 0.005. Figure 8 shows $\rho^{(1)}(r)/\rho$: it seems to depend slightly more than $S(k)$ on the parameters. The asymptotic value is

$$n_0=(0.105\pm 0.005)\rho$$

in good agreement with the result of McMillan. Figure 9 shows the dependence of n_0 on the density. When the solid region ($\rho=1.3\rho_0$) is reached, n_0 is not exactly equal to zero but of the order of 0.03; most probably the wave function (1) describes the metastable states of the liquid.

V. GROUND-STATE ENERGY AND LIQUID-STRUCTURE FACTOR OF LIQUID HELIUM-3

A symmetrical wave function like (1) is no longer suitable in the case of a fermion system. Following [8] we take as trial wave function

$$\Psi_F(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)=\Psi_B(\mathbf{r}_1, \cdots, \mathbf{r}_N)\cdot\Phi_F(\mathbf{r}_1, \cdots, \mathbf{r}_N), \tag{11}$$

product of Ψ_B, still of the form (1) and of a Slater determinant

$$\Phi_F(\mathbf{r}_1, \cdots, \mathbf{r}_N)=\mathrm{Det}\{\exp(i\mathbf{k}_i\cdot\mathbf{r}_j)\chi_i(\boldsymbol{\sigma}_j)\}$$

of plane waves of wave vector $\mathbf{k}_i$ in the spin state χ_i, filling up two Fermi spheres of equal radius

$$k_F=(3\pi^2\rho)^{1/3}.$$

Equation (11) is not a product of pair functions and the analogy with classical statistical mechanics is no longer true. Wu and Feenberg[8] (WF) have developed a very useful set of approximations to deal with such a case: their method amounts to treating exactly the "dynamical" part of the wave function, Ψ_B, and to treating approximately, by a suitable cluster expansion, the effect of the Pauli principle contained in Φ_F. A physical justification of this procedure is that the hard core of the interatomic potential prevents atoms from overlapping, so that the exclusion principle might be expected to act only as a correction to the "dynamical" correlations. A more quantitative argument is that, as we shall see, the successive approximants seem to converge rather rapidly.

WF express, at each order of their cluster expansion, the quantities relative to the fermion wave function Ψ_F in terms of quantities relative to the boson wave function Ψ_B and of suitable corrections. We shall use their results and refer the reader to their paper for detailed derivation. The following quantities are useful:

$$g_B(\mathbf{r}_1, \mathbf{r}_2)=\frac{N(N-1)}{\rho^2}\int d\mathbf{r}_3, \cdots, d\mathbf{r}_N\,|\Psi_B|^2\left(\int d\mathbf{r}_1, \cdots, d\mathbf{r}_N\,|\Psi_B|^2\right)^{-1},$$

$$g_F(\mathbf{r}_1, \mathbf{r}_2)=\frac{N(N-1)}{\rho^2}\int d\tau_3, \cdots, d\tau_N\,|\Psi_F|^2\left(\int d\tau \cdots, d\tau_N\,|\Psi_F|^2\right)^{-1},$$

where $\int d\tau$ includes summation over spin coordinates;

$$f_B(r)=g_B(r)-1,$$

$$S_B(k)=1+\rho\int \exp(i\mathbf{k}\cdot\mathbf{r})f_B(r)\,d\mathbf{r},$$

$$u_B(k)=S_B(k)-1.$$

For the fermion system, the functions $f_F(r)$, $S_F(k)$ and $u_F(k)$ are related in the same way to the fermion pair-distribution function $g_F(r)$.

Use of the trial wave function (11) and of the Hamiltonian (4) leads, after some integrations by parts, to the still exact expression

$$E=\frac{\langle\Psi_F\mid H\mid\Psi_F\rangle}{N\langle\Psi_F\mid\Psi_F\rangle}=\tfrac{1}{2}\rho\int g_F(r)[V(r)+T(r)]dr$$
$$+\frac{\hbar^2}{\mu}\left\{\frac{3}{5}\frac{k_F^2}{2}+\frac{1}{2}\sum_i\left[\int\Phi_F^*\nabla_i(\Phi_F\Psi_B)\nabla_i\Psi_B d\tau_1,\cdots,d\tau_N\right]\left[\int|\Psi_F|^2 d\tau_1,\cdots,d\tau_N\right]^{-1}\right\}\quad(12)$$

with $T(r)$ still given by (6).[19]

The WF zeroth order is obtained by neglecting completely the effect of the Pauli principle:

$$E_{\mathrm{WF}}^{(0)}=\tfrac{1}{2}\rho\int g_B(r)[V(r)+T(r)]d\mathbf{r}.\quad(13)$$

The WF first order is obtained by keeping only those terms of the cluster expansion in which the Pauli principle acts on pairs of particles:

$$E_{\mathrm{WF}}^{(1)}=E_{\mathrm{WF}}^{(0)}-\epsilon_a^{(1)}+\epsilon_b^{(1)},\quad(14)$$

with

$$\epsilon_a^{(1)}=\tfrac{1}{4}\rho\int g_B(r)h^2(k_Fr)[T(r)+V(r)]d\mathbf{r},$$

$$\epsilon_b^{(1)}=\tfrac{3}{5}(\hbar^2k_F^2/2\mu)\left[1+20\int_0^1 u_B(2k_Fy)(1-\tfrac{3}{2}y+\tfrac{1}{2}y^3)y^4dy\right],$$

where $h(x)=3\ (\sin x-x\cos x)/x^3$.

The ϵ_a and ϵ_b in (14) correspond, respectively, to the first and second term in (12).

To second order, WF assume the Kirkwood superposition form, for the boson three-particle distribution function, so that the corrections are still expressible in terms of $g_B(r)$ only:

$$E_{\mathrm{WF}}^{(2)}=E_{\mathrm{WF}}^{(1)}+\epsilon_a^{(2)}+\epsilon_b^{(2)},\quad(15)$$

with

$$\epsilon_a^{(2)}=\frac{\rho^2}{2}\int g_B(r_{12})\,(V(r_{12})+T(r_{12}))\left[-\int g_B(r_{23})f_B(r_{13})h^2(k_Fr_{23})d\mathbf{r}_3+\frac{h(k_Fr_{12})}{2}\int g_B(r_{23})f_B(r_{13})h(k_Fr_{13})h(k_Fr_{23})d\mathbf{r}_3\right]d\mathbf{r}_{12},$$

$$\epsilon_b^{(2)}=\frac{3}{5}\frac{\hbar^2k_F^2}{2\mu}\left(\frac{3}{8\pi}\right)^3\frac{1}{2}\iiint_{|x_1|,\,|x_2|,\,|x_3|<1}x_{12}^2S(k_Fx_{12})u(k_Fx_{23})u(k_Fx_{13})\,d\mathbf{x}_1d\mathbf{x}_2d\mathbf{x}_3.$$

Our calculation was done in the following way:

(a) We determined the radial distribution function $g_B(r)$ corresponding to a boson (mass 3) system with wave function Ψ_B by a molecular-dynamics calculation (in fact, because of McMillan's scaling trick, no new calculation was necessary). This was done for several values of the variational parameters b and m. The resulting $E_{\mathrm{WF}}^{(0)}$ is shown in the second column of Table VIII.

(b) For each value of these parameters we then calculated $E_{\mathrm{WF}}^{(1)}$ and $E_{\mathrm{WF}}^{(2)}$ according to Eqs. (14) and (15). $\epsilon_a^{(2)}$ was calculated by Fourier transforming the convolution product, and the 9-dimensional integral appearing in $\epsilon_b^{(2)}$ was computed by a Monte-Carlo method. The results are shown in Table VIII. It is seen that the convergence seems to be rather rapid. The "best" wave function is obtained for $b=1.13$ and $m=5$. Table IX gives the values of the energy as a function of the density. The equilibrium density is $0.65\rho_0$ and the ground-state energy is -1.35°K/atom (the experimental[9] values are $0.752\rho_0$ and -2.52°K/atom, respectively).

TABLE IX. Ground-state energy of liquid helium-3 as a function of density.

ρ/ρ_0	E
0.6	−1.23
0.65	−1.35
0.7	−1.32
0.8	−1.13
0.9	+0.77

---

[19] The last term in (12) differs by a factor $\frac{1}{2}$ from the corresponding term in WF [their Eq. (9)] because WF assumed for Ψ_B the exact ground-state wave function of H, whereas we perform the variation on the total wave function Ψ_F, so that Ψ_B is no longer solution of the Schrödinger equation for the mass-3 boson problem.

TABLE X. Comparison of the present results for boson and fermion mass-3 systems with the ones obtained by Massey (Ref. 21) and Woo (Ref. 20).

		ρ_{eq}/ρ_0	T (°K/atom)	V (°K/atom)	E (°K/atom)
Boson (mass 3)	Massey-Woo	0.675	11.76	−14.64	−2.87
	Here	0.65	8.68	−11.60	−2.92
Fermion	Woo	0.675			−1.35
	Here	0.65	9.87	−11.22	−1.35
	Experiment	0.75			−2.52

A calculation of the ground-state properties of liquid helium-3 has been made by Woo,[20] this author assumed a trial wave function of the form (11) and applied the WF cluster expansion up to second order. The difference with our calculation is that Woo used for the boson mass-3 wave function Ψ_B the wave function derived by Massey[21] through use of the Kirkwood superposition approximation. Table X gives the results of both methods and shows that they lead to kinetic and potential energies of the boson mass-3 system differing by 30%.

TABLE XI. Pair function $g_F^{(2)}(r)$ of liquid helium-3 at $\rho=0.752\rho_0$.

r/σ	$g_F^{(2)}(r)$	r/σ	$g_F^{(2)}(r)$
≤0.76	0	1.72	1.08
0.8	0.025	1.76	1.07
0.84	0.07	1.8	1.061
0.88	0.13	1.84	1.054
0.92	0.21	1.88	1.047
0.96	0.325	1.92	1.039
1	0.435	1.96	1.03
1.04	0.545	2	1.02
1.08	0.655	2.04	1.011
1.12	0.755	2.08	1.002
1.16	0.845	2.12	0.995
1.2	0.917	2.16	0.99
1.24	0.977	2.2	0.988
1.28	1.025	2.24	0.987
1.32	1.058	2.28	0.988
1.26	1.082	2.32	0.989
1.4	1.102	2.36	0.99
1.44	1.12	2.4	0.99
1.48	1.128	2.44	0.99
1.52	1.127	2.48	0.991
1.56	1.12	2.52	0.992
1.6	1.112	2.56	0.994
1.64	1.103	2.6	0.998
1.68	1.092		

The liquid-structure factor $S(k)$ can be calculated, in the WF approximation, by Fourier-transforming the successive approximants to $g_F(r)$ [WF, formula (44)]:

$$g_F^{(0)}(r)=g_B(r),$$

$$g_F^{(1)}(r)=g_B(r)[1-h^2(k_Fr)/2],$$

$$g_F^{(2)}(r_{12})=g_F^{(1)}(r_{12})+g_B(r_{12}) \times\left[-\rho\int g_B(r_{23})u_B(r_{13})h^2(k_Fr_{23})\,d\mathbf{r}_3 +(\tfrac{1}{2}\rho)h(k_Fr_{12})\int g_B(r_{23})u_B(r_{13})h(k_Fr_{13})h(k_Fr_{23})\,d\mathbf{r}_3\right].$$

Figure 10 shows $g_F^{(0)}(r)$, $g_F^{(1)}(r)$, and $g_F^{(2)}(r)$ corre-

TABLE XII. Liquid-structure factor $S_F^{(2)}(r)$ of helium-3 at $\rho=0.752\rho_0$.

$k\sigma$	$S_F^{(2)}(k)$	$k\sigma$	$S_F^{(2)}(k)$
1.2	0.12	7.5	0.971
1.5	0.135	7.8	0.967
1.8	0.166	8.1	0.968
2.1	0.215	8.4	0.969
2.4	0.28	8.7	0.971
2.7	0.357	9.	0.976
3.	0.495	9.3	0.983
3.3	0.655	9.6	0.99
3.6	0.795	9.9	0.997
3.9	0.925	10.2	1.001
4.2	1.025	10.5	1.006
4.5	1.095	10.8	1.008
4.8	1.135	11.1	1.009
5.1	1.146	11.4	1.010
5.4	1.134	11.7	1.011
5.7	1.111	12.	1.011
6.	1.078	12.3	1.010
6.3	1.045	12.6	1.008
6.6	1.018	12.9	1.007
6.9	0.996	13.2	1.003
7.2	0.98	13.5	1.

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[20] C. W. Woo, Phys. Rev. **151**, 138 (1966).

[21] W. E. Massey, Phys. Rev. **151**, 153 (1966).

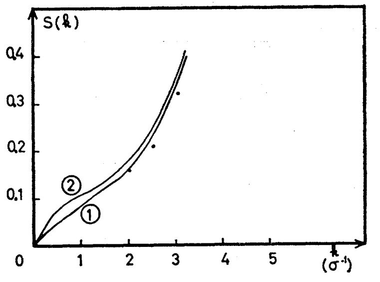

FIG. 7. Low k behavior of $S(k)$. •, experiment; ——, theory with Reatto–Chester wave function for two values of the cutoff $k_c=1$ [curve (1)] and $k_c=0.25$ [curve (2)].

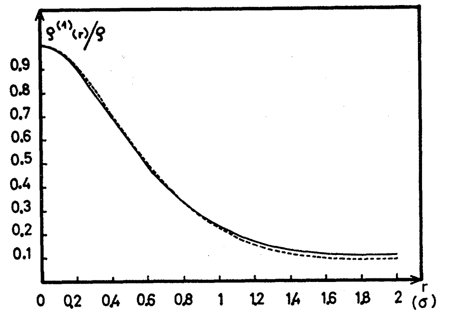

FIG. 8. One-particle reduced density matrix of liquid He^4 ($\rho=\rho_0$) for two sets of values of the variational parameters: ——, $m=5$; $b=1.17$. ----, $m=4$; $b=1.3$.

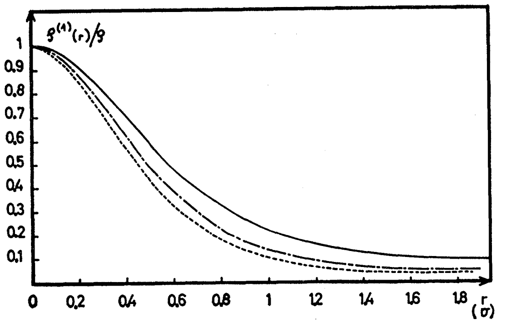

FIG. 9. One-particle reduced density matrix of liquid He^4 at several densities. ——, $\rho=\rho_0$; —•—•, $\rho=1.2\rho_0$; ----, $\rho=1.27\rho_0$.

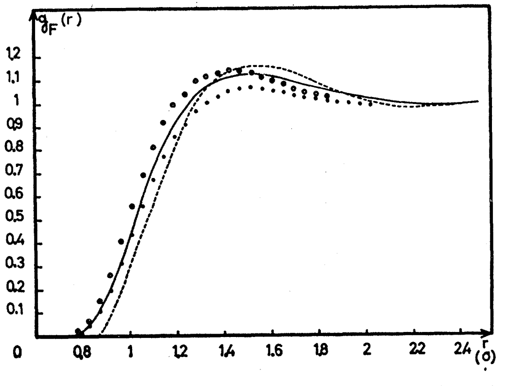

FIG. 10. Radial distribution function of liquid He^3 ($\rho=0.752\rho_0$) obtained by WF expansion up to zeroth (...), first (•••), and second (——) order. ---- is the curve obtained by Woo.

sponding to the optimum values of the parameters $m=5$, $b=1.13$. Also shown on Fig. 10 is the $g_F(r)$ derived by Woo. The corresponding $S_F^{(0)}(k)$, $S_F^{(1)}(k)$, and $S_F^{(2)}(k)$ are shown on Fig. 11. The convergence of the WF approximants seems to be rather rapid and a comparison with experiment would be interesting. Numerical values of $g_F^{(2)}(r)$ and $S_F^{(2)}(k)$ are given in Tables XI and XII.

VI. CONCLUSION

The calculations performed confirm that a Jastrow wave function like (1) adequately describes liquid helium-4 at zero temperature. The discrepancy between the theoretical and experimental values of the energy and equilibrium density are of the order of those due to the uncertainties in the two-body potential. The liquid-structure factor $S(k)$ is in good agreement with experiment except, maybe, at the peak $k\simeq 2$ Å^{-1}. With a "short-range" trial $u(r)$ the low k behavior of $S(k)$ is not correct, as expected: whether the inclusion of a "long-range" term in $u(r)$ would lower the energy is an open question.

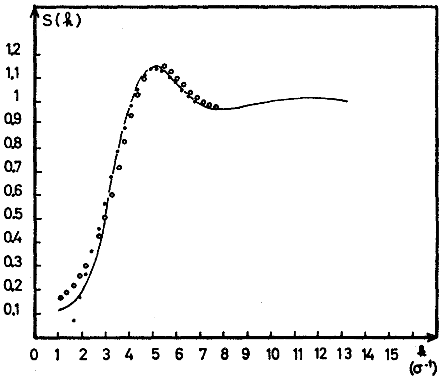

FIG. 11. Liquid-structure factor of liquid He^3 obtained by WF expansion up to zeroth (...), first (•••), and second order (——).

A Jastrow-Slater trial wave function like (11) seems to give reasonable results for the ground-state energy and equilibrium-density liquid helium-3. The discrepancy between experimental and theoretical energy is the same as in the case of helium-4. Experiment should decide whether the liquid-structure factor predicted for He^3 is reasonable.

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