Condensate fraction and momentum distribution in the ground state of liquid ^{4}He

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In an earlier paper we calculated the condensate fraction and momentum distribution of atoms in liquid ^{4}He, using a variational wave function which takes into account Jastrow and three-body correlations. In the present paper we point out an error in the expression used to compute the condensate fraction when three-body correlations were included. We report the corrected numerical results for both condensate fraction and momentum distributions for three densities. In addition, we calculate the condensate fraction and momentum distribution with and without the $l=0$ part of the three-body correlations in the wave function. Even though the $l=0$ part gives a small contribution to the ground-state energy, we find that the $l=0$ and $l=1$ terms have opposite and almost canceling effects on the condensate fraction and momentum distribution; each term separately alters the results obtained with pure Jastrow correlations by about 15–20%, while when considered together they give only a small contribution.

In our calculation of the condensate fraction and momentum distribution of liquid ^{4}He, we used[1] a variational wave function which included optimized Jastrow (J) pair correlations and three-body correlations [Jastrow plus triplet ($J+T$)]. The wave function is given by

$$\psi_0 = \prod_{1 \le i < j \le N} f(r_{ij}) \prod_{1 \le i < j < k \le N} f_3(r_{ij}, r_{jk}, r_{ik}) . \quad (1)$$

The Jastrow correlation factor $f(r_{ij})$ takes into account the short- and long-ranged correlations between the atoms, and it is optimized by solving the Euler-Lagrange equations with the asymptotic behavior

$$f(r \to \infty) = 1 - \frac{mc}{2\pi^2 \hbar \rho} \frac{1}{r^2} ,$$

which is a consequence of the long-wavelength phonons. Here c is the velocity of sound and ρ is the particle density. The three-body correlation is written as

$$f_3(r_{ij}, r_{jk}, r_{ik})$$
$$= \exp \left[\frac{1}{2} \sum_{\text{cyc}} \sum_{l=0,1,2} \xi_l(r_{ij}) \xi_l(r_{ik}) P_l(\hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{r}}_{ik}) \right] . \quad (2)$$

Here $\sum_{\text{cyc}}$ represents a sum of the three terms obtained by replacing ijk with jki and kij. P_l represents Legendre polynomials of lth order, and $\hat{\mathbf{r}}_{ij}$ are unit vectors. The ξ_l's are functions of the distance between the pairs of particles in the triplet and are determined variationally. The $l=1$ term describes Feynman-Cohen back-flow correla-

tions in the ground state and gives the dominant contribution to the energy; the $l=0$ term gives a small contribution to the energy, and the $l=2$ has a negligible effect in the calculation of the ground-state energy.

The expression (3.7) of Ref. 1, however, which is used to calculate the condensate fraction, when the effect of three-body correlations is taken into account, is incorrect. The correct expression is given by

$$R_x = \rho \int d^3 r [g_{xd}(r) - 1 - N_{xd}(r)]$$
$$- \tfrac{1}{2} \rho \int d^3 r [g_{xd}(r) - 1] N_{xd}(r)$$
$$- \rho \int d^3 r \, g_{xd}(r) [E_{xd}(r) + C_{xd}(r)] + E_x + C_x ,$$
$$\quad (3)$$

with $x = w, d$, and the condensate fraction n_0 is given by $n_0 = \exp(2R_w - R_d)$. Here the functions g_{xd}, N_{xd}, E_{xd}, and C_{xd} are regular ($x = d$) and auxiliary ($x = w$) distribution functions, the sum of nodal and elementary diagrams, and the dressed triplet, respectively, which are obtained by solving the HNC/S equations with the inclusion of triplet correlations.[1,2] E_w (E_d) are elementary diagrams with one external point which is the extremity of an $f_{ij} - 1$ ($f_{ij}^2 - 1$) correlation line. Such diagrams include both E^g- or E^t-type elementary diagrams which, respectively, do not or do involve explicit triplets joining the points of the diagram. C_x is the dressed triplet with one external point. Equation (3) can be simply obtained from Eq. (2.10) of Ref. 1 (which is the form for the pure Jastrow case) by simply substituting everywhere E by

TABLE I. Results for $kn(k)$ with the $J+T$ wave function at various densities.

k (Å^{-1})	$\rho=0.365\sigma^{-3}$	$\rho=0.401\sigma^{-3}$	$\rho=0.438\sigma^{-3}$
0.05	0.0167	0.0138	0.0106
0.15	0.0247	0.0205	0.0160
0.25	0.0317	0.0264	0.0208
0.35	0.0374	0.0312	0.0248
0.45	0.0415	0.0349	0.0279
0.55	0.0442	0.0375	0.0302
0.65	0.0457	0.0391	0.0318
0.75	0.0460	0.0398	0.0327
0.85	0.0454	0.0398	0.0331
0.95	0.0439	0.0390	0.0330
1.05	0.0416	0.0377	0.0325
1.15	0.0386	0.0357	0.0314
1.25	0.0349	0.0332	0.0298
1.35	0.0308	0.0301	0.0278
1.45	0.0264	0.0266	0.0253
1.55	0.0218	0.0228	0.0225
1.65	0.0175	0.0190	0.0196
1.75	0.0138	0.0156	0.0168
1.85	0.0112	0.0129	0.0144
1.95	0.0097	0.0113	0.0127
2.05	0.0091	0.0104	0.0117
2.15	0.0088	0.0101	0.0112
2.25	0.0083	0.0097	0.0109
2.35	0.0076	0.0090	0.0103
2.45	0.0066	0.0080	0.0094
2.55	0.0055	0.0069	0.0083
2.65	0.0045	0.0058	0.0072
2.75	0.0037	0.0049	0.0063
2.85	0.0029	0.0041	0.0054
2.95	0.0023	0.0033	0.0046
3.05	0.0018	0.0027	0.0039
3.15	0.0015	0.0022	0.0033
3.25	0.0011	0.0018	0.0027
3.35	0.0009	0.0014	0.0023

$E+C$ with the corresponding subscript. Equation (2.14) of Ref. 1 should also be corrected to

$$E_x \simeq (1+\tfrac{9}{8}S_{xd})E_{x,4} , \qquad (4)$$

with $x=w,d$. However, as was noted in Ref. 1, because $2E_w-E_d \sim 0.03$, their contribution is negligible.

The calculation is performed with exactly the same approximations used in Ref. 1. The results with the full wave function are summarized in Tables I (replacing Table II of Ref. 1), II, and III (replacing Table III of Ref. 1), and Fig. 1 (replacing Fig. 9 of Ref. 1) and Fig. 2. The results have also been normalized according to Eq. (4.6) of Ref. 1. Note that the results for the normalized
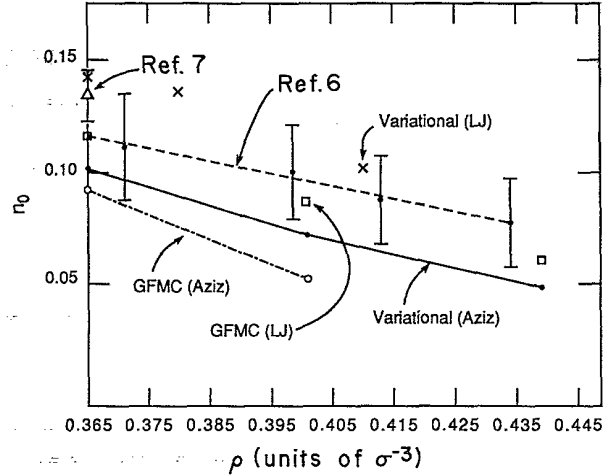

FIG. 1. Comparison of the theoretical and experimental condensate fraction. The solid curve shows the results of this work with the Aziz potential. The open circles, joined by a dot-dashed line, are the results of a GFMC calculation (Ref. 3) with the Aziz potential. GFMC results with Lennard-Jones (LJ) potential are shown with open squares (Ref. 4). The crosses represent the results of the variational calculation using the LJ potential (Ref. 5). The solid circles with the error bars show data taken from Ref. 6. The dashed line is a guide to the eye. The triangle gives the experimental results of Ref. 7 at equilibrium density.

momentum distribution are not significantly affected by the error. Thus we do not redraw Fig. 8, in which we compared the results obtained with the J and $J+T$ wave function, with the Green's function Monte Carlo (GFMC) and the experimental results, because the new and the momentum distributions of Ref. 1 are identical within the resolution of this figure. The error on the condensate fraction is larger; for example, at the equilibrium density with the $J+T$ wave function, we find $n_0=0.103$ a value which is very close to that with pure J wave function.

In Ref. 1, n_0 was calculated including both the $l=0$ and 1 terms in Eq. (2). Here we have calculated the condensate fraction with and without the $l=0$ term in f_3: Including only the $l=1$ term, we find that the condensate fraction at the equilibrium density is reduced from $n_0=0.098$ obtained with the J wave function to $n_0=0.082$ with the $J+T$ wave function. However, if we include both the $l=1$ and 0 terms, the calculated condensate fraction at the equilibrium density is $n_0=0.103$, which is close to the value obtained with the J wave function.

Figure 1 replaces Fig. 9 of Ref. 1, where we compare

TABLE II. Results for the condensate fraction with optimized J and $J+T$ wave functions.

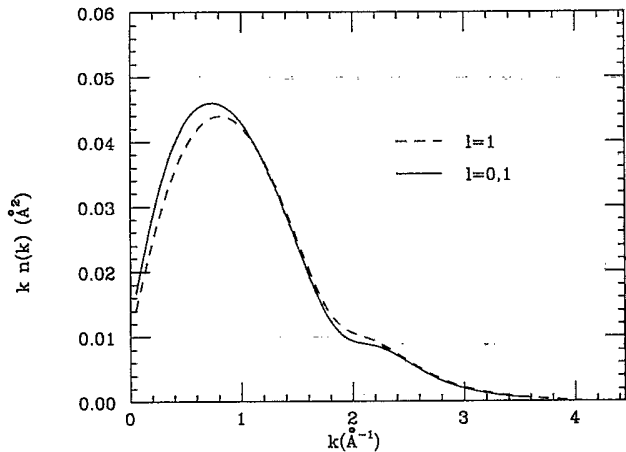| $\rho(\sigma^{-3})$	s_{dd}	s_{wd}	s_{ww}	J	$J+T(l=1)$	$J+T(l=0,1)$	GFMC
0.365	2.44	2.24	2.404	0.098	0.082	0.103	0.092
0.401	2.78	2.78	2.916	0.071	0.056	0.073	0.052
0.438	3.12	3.12	3.28	0.048	0.037	0.048	

FIG. 2. $kn(k)$ calculated with the $J+T$ wave function with and without the inclusion of the $l=0$ part of the triplet correlation.

TABLE III. Kinetic energy calculated from the normalized momentum distribution using $J+T$ wave function $(l=0,1)$ is compared with T_{JF} at three densities.

$\rho(\sigma^{-3})$	T_{MD}	T_{JF}
0.365	15.20	14.72
0.401	18.40	17.45
0.438	22.95	20.53

our results obtained with the wave function which includes both the $l=0$ and 1 terms with other available results. In Fig. 2 we compare the momentum distribution obtained with and without the $l=0$ part in the wave function. We note that the effect of either term on $n(k)$ is larger than the effect of both. In addition, the presence

of the $l=0$ part of the three-body correlation puts back particles removed from the $k=0$ state and its neighborhood by the $l=1$ part of the correlations.

Because of the fact that the contribution to the ground-state energy of the $l=0$ is small, this part of the correlation function cannot be accurately optimized. Thus the contribution of this term to the condensate fraction and momentum distribution, which is rather significant, is crudely estimated by our approach.

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