Density matrices and momentum distributions in ^3He-^4He mixtures

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We report variational calculations, in the hypernetted-chain (HNC)−Fermi-HNC scheme, of one-body density matrices and one-particle momentum distributions for ^3He-^4He mixtures described by a Jastrow correlated wave function. The ^4He condensate fractions and the ^3He strength poles are examined and compared with the Monte Carlo available results. The agreement has been found to be very satisfactory. Their density dependence is also studied.

The ^3He-^4He mixtures have been, in the last years, the object of a large number of theoretical investigations,[1–4] mainly devoted to the study of the incomplete phase separation of the system. Besides these papers, in a recent publication, Lee and Goodman[5] (LG) have reported a Monte Carlo calculation of the one-body density matrices of the mixture using a Jastrow correlated wave function. To compare their results with those from other methods, we will extend, in this Brief Report, the hypernetted-chain (HNC)−Fermi-HNC methods[6,7(a),8] to calculate the one-body density matrices $\rho_\alpha(r)$, or equivalently the one-particle momentum distributions $n_\alpha(k)$, for a boson-fermion solution.

We present the results for the ^3He-^4He case, with special emphasis in the behavior of the ^4He condensate fraction and of the ^3He strength pole.

We will consider a system of N_4 ^4He atoms and N_3 ^3He atoms, in the volume Ω. The total density is $\rho=(N_4+N_3)/\Omega=\rho_4+\rho_3$ and the concentrations $x_\alpha=\rho_\alpha/\rho$. We will let N_4, N_3, and Ω go to infinity, but keep the densities constant.

The ground state of the solution is described by a Jastrow correlated wave function, a generalization of that used for the pure components

$$\psi(1,\ldots,N_3,N_3+1,\ldots,N_3+N_4)=\prod_{i<j}^{N_3} f_{ij}^{(3,3)} \prod_{\substack{m<n\\ m>N_3}}^{N_3+N_4} f_{mn}^{(4,4)} \prod_{p=1}^{N_3} \prod_{q>N_3}^{N_3+N_4} f_{pq}^{(3,4)} \phi(1,\ldots,N_3) \quad , \tag{1}$$

where $\phi(1,\ldots,N_3)$ is the Slater determinant of plane waves for the free ^3He atoms and $f_{ij}^{(\alpha,\beta)}$ is the dynamical correlation factor, induced by the mutual interactions, between the i particle of α type and the j particle of β type ($\alpha,\beta=3,4$). With the wave function (1), we will calculate the density matrices, $\rho_4(r)$ and $\rho_3(r)$, the one-particle momentum distributions,

$$n_\alpha(k)=\int d\vec{r}\exp(i\vec{k}\cdot\vec{r})[\rho_\alpha(r)-\rho_\alpha n_\alpha^0\delta_{\alpha 4}] \tag{2}$$

and the ^4He condensate fraction, $n_4^0=\rho_4(\infty)/\rho_4$.

Following Fantoni[6] we are able to write

$$\rho_4(r)=\rho_4 n_4^0\exp[G_{ww}^{(4)}(r)] \quad , \tag{3}$$

$$\rho_3(r)=\rho_3 n_3^0\exp[G_{ww}^{(3)}(r)][l(k_F r)/2-G_{c'c'}^{(3)}(r)] \quad . \tag{4}$$

Here $k_F^3=3\pi^2\rho_3$ and $l(x)=3[\sin(x)-x\cos(x)]/x^3$.

It must be pointed out that, here and henceforth, the approximation, where all the contributions coming from the "elementary" diagrams (HNC/0 and FHNC/0 approximations)[7(a)] are neglected, will be adopted.

The $G_{ww}^{(\alpha)}$ and $G_{c'c'}^{(\alpha)}$ are calculated from

$$G_{ww}^{(\alpha)}(r)=\sum_{\lambda=3,4}\rho_\lambda(X_{wd}^{(\alpha,\lambda)}|X_{dw}^{(\lambda,\alpha)}+G_{dw}^{(\lambda,\alpha)})+\rho_3(X_{wd}^{(\alpha,3)}|X_{ew}^{(3,\alpha)}+G_{ew}^{(3,\alpha)})+\rho_3(X_{we}^{(\alpha,3)}|X_{dw}^{(3,\alpha)}+G_{dw}^{(3,\alpha)}) \quad , \tag{5}$$

$$G_{c'c'}^{(3)}(r)=\rho_3(X_{c'c}^{(3,3)}|X_{cc'}^{(3,3)}+G_{cc'}^{(3,3)})+\rho_3(-l/2|X_{cc'}^{(3,3)}-2X_{cc'}^{(3,3)}) \tag{6}$$

where[7(b)] $G_{wd}^{(\alpha,\beta)}$, $G_{we}^{(\alpha,3)}$, $G_{c'c}^{(3,3)}$ and $X_{wd}^{(\alpha,\beta)}$, $X_{we}^{(\alpha,3)}$, $X_{c'c}^{(3,3)}$ are the solutions of this set of integral equations:

$$\begin{aligned}
G_{wd}^{(\alpha,\beta)}(r) &= \sum_{\lambda=3,4} \rho_\lambda (G_{wd}^{(\alpha,\lambda)} + X_{wd}^{(\alpha,\lambda)} | X_{dd}^{(\lambda,\beta)}) + \rho_3 (G_{wd}^{(\alpha,3)} + X_{wd}^{(\alpha,3)} | X_{ed}^{(3,\beta)}) + \rho_3 (X_{we}^{(\alpha,3)} + G_{we}^{(\alpha,3)} | X_{dd}^{(3,\beta)}) \ , \\
G_{we}^{(\alpha,3)}(r) &= \sum_{\lambda=3,4} \rho_\lambda (G_{wd}^{(\alpha,\lambda)} + X_{wd}^{(\alpha,\lambda)} | X_{de}^{(\lambda,3)}) + \rho_3 (G_{wd}^{(\alpha,3)} + X_{wd}^{(\alpha,3)} | X_{ee}^{(3,3)}) + \rho_3 (G_{we}^{(\alpha,3)} + X_{we}^{(\alpha,3)} | X_{de}^{(3,3)}) \ , \\
G_{c'c'}^{(3,3)}(r) &= \rho_3 (X_{c'c'}^{(3,3)} + G_{c'c'}^{(3,3)} | X_{cc}^{(3,3)}) + \rho_3 (X_{c'c}^{(3,3)} | -l/2) \ ,
\end{aligned} \tag{7}$$

with

$$\begin{aligned}
X_{wd}^{(\alpha,\beta)}(r) &= f^{(\alpha,\beta)}(r) \exp[G_{wd}^{(\alpha,\beta)}(r)] - 1 - G_{wd}^{(\alpha,\beta)}(r) \ , \\
X_{we}^{(\alpha,3)}(r) &= \{f^{(\alpha,3)}(r) \exp[G_{wd}^{(\alpha,3)}(r)] - 1\} G_{we}^{(\alpha,3)}(r) \ , \\
X_{c'c}^{(3,3)}(r) &= \{f^{(3,3)}(r) \exp[G_{wd}^{(3,3)}(r)] - 1\} [G_{c'c}^{(3,3)}(r) - l(k_F r)/2] \ .
\end{aligned} \tag{8}$$

The functions $X_{dd}^{(\alpha,\beta)}$, $X_{de}^{(\alpha,3)}$, $X_{ee}^{(3,3)}$, and $X_{cc}^{(3,3)}$ are the corresponding solutions of another set of integral equations given elsewhere.[4]

Finally, we have for n_α^0

$$n_\alpha^0 = \exp[2D^\alpha(w) - D^\alpha(d)] \tag{9}$$

where[6,7(c)]

$$D^{(\alpha)}(w) = \sum_{\lambda=3,4} x_\lambda \tilde{X}_{wd}^{(\alpha,\lambda)}(0) + x_3 \tilde{X}_{we}^{(\alpha,3)}(0) - \frac{1}{2\rho} \frac{1}{(2\pi)^3} \int d\bar{k} \left\{ \sum_{\lambda=3,4} x_\lambda [(\tilde{G}_{wd}^{(\alpha,\lambda)})^2 - (\tilde{X}_{wd}^{(\alpha,\lambda)})^2] + 2x_3 [\tilde{G}_{wd}^{(\alpha,3)} \tilde{G}_{ew}^{(3,\alpha)} - \tilde{X}_{wd}^{(\alpha,3)} \tilde{X}_{ew}^{(3,\alpha)}] + \tilde{G}_{ww}^{(\alpha)} \right\} \ . \tag{10}$$

The expression for $D^{(\alpha)}(d)$ is obtained from Eq. (14) by replacing the "w" subscripts by the "d" ones.

The correlation factors between the particles are chosen to be the same for all the values of α and β

$$f^{(\alpha,\beta)}(r) = f(r) = \exp[-(b\sigma/r)^5/2] \ . \tag{11}$$

The parameter b is determined by minimizing the energy per particle of the mixture at a given density with the interaction potential taken to be the Lennard-Jones potential

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

with $\epsilon = 10.22$ K and $\sigma = 2.556$ Å.

As starting point, we have considered, in our scheme, two of the cases presented in LG. The results are summarized in Table I. The quantities labeled HF (HNC-Fermi HNC) come from our calculations; those labeled MC from LG.

It must be said that the discrepancies in the energies per particle are of the same order as in the pure phases[9,10]; the relative difference increases with the ^{3}He concentration. This is according with the fact that the error in the energy is percentually smaller for pure ^{4}He than for pure ^{3}He.

A good agreement for the condensate fraction has been found. We note, as in LG, an increase of n_4^0 when the total density decreases. We realize that the percent difference between $n_{4\mathrm{MC}}^0$ and $n_{4\mathrm{HF}}^0$ increases with ρ. This may be ascribed to the influence of the disregarded elementary diagrams.

In the last column of Table I, the values of the discontinuity at n_3 ($k = k_F$) (Z_F) are reported. Unfortunately, we cannot compare them with other results, but, for $x_3 = 0.4375$, the upper bound established in LG ($Z_F < 0.2$) is respected. Going from

TABLE I. Results for n_4^0, Z_F, and E/N from this paper (HF) and from LG (MC). The densities are in σ^{-3} and the energies in K.

x_3	ρ	b	E/N_{HF}	E/N_{MC}	$n_{4\mathrm{HF}}^0$	$n_{4\mathrm{MC}}^0$	Z_F
0.1228	0.351	1.160	−4.02	−5.25	0.131	0.137	0.139
0.4375	0.323	1.145	−2.60	−3.68	0.174	0.180	0.189

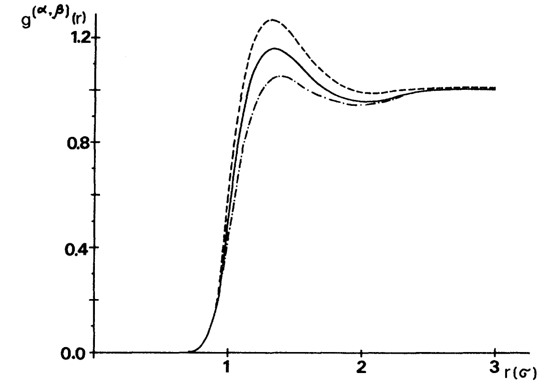

FIG. 1. Radial distribution functions for $\rho = 0.323\sigma^{-3}$ and $x_3 = 0.4375$. Solid line, $g^{(4,4)}$; dashed line, $g^{(3,4)}$; and dot-dashed lines $g^{(3,3)}$.

$x_3 = 0.1228$ to 0.4375 we have an increase of ρ_3 from $0.042\sigma^{-3}$ to $0.139\sigma^{-3}$, so we should expect a reduction of Z_F. This does not happen because, even if Z_F is a typical fermionic quantity, its value is modulated by ρ.

We want to add also that our $g^{(\alpha,\beta)}(r)$'s (the radial distribution functions) are in good agreement with those reported in LG. The locations and the relative altitudes of the first maxima of the $g^{(\alpha,\beta)}$'s are practically the same. In Fig. 1 we present the HF $g^{(\alpha,\beta)}$'s for $\rho = 0.323\sigma^{-3}$ and $x_3 = 0.4375$.

It may be interesting to see how n_4^0 and Z_F vary with x_3 along the $P = 0$ isobar (P is the pressure of the system, $P = \rho\partial E/\partial\rho$, and the condition $P = 0$ fixes the equilibrium density at each concentration). The results are presented in Table II.

It must be considered that our approximation gives equilibrium densities smaller than the real ones. For instance, the experimental $\rho_{\text{eq}}(x_3 = 0)$ is $0.365\sigma^{-3}$, while our calculated value is $0.289\sigma^{-3}$. This difference affects the value of n_4^0 and Z_F, but we think that the qualitative behavior is still realistic.

The densities of the mixture decrease along the isobar when x_3 increases, as a consequence of the

TABLE II. Results for n_4^0 and Z_F along the $P = 0$ isobar. Unities as in Table I.

x_3	ρ	n_4^0	Z_F
0.0	0.289	0.200	
0.0625	0.284	0.206	0.209
0.1250	0.278	0.214	0.218
0.1875	0.272	0.223	0.229
1.0	0.189		0.509

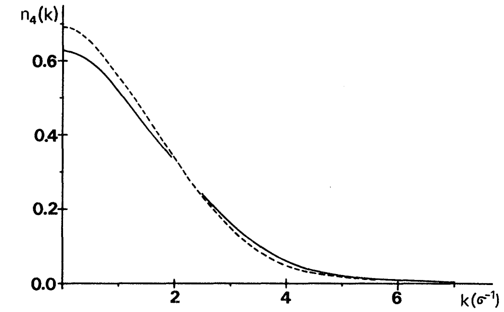

FIG. 2. $n_4(k)$ for mixture at $\rho = 0.278\sigma^{-3}$ and $x_3 = 0.125$ (solid line) and for pure ^{4}He at $\rho_4 = 0.243\sigma^{-3}$ (dashed line).

Pauli repulsion; this fact essentially explains the behavior of n_4^0 and Z_F. We want to say that the increasing values of these quantities are well understood in terms of the smaller or larger density of the solution respect to the pure ^{4}He or ^{3}He.

The n_4^0 values do not depend too much on the ^{3}He Fermi statistics; to see this effect, we have calculated them putting $\phi(1, \ldots, N_3) = 1$ in Eq. (1). This statement is equivalent to consider a boson-mass-3—boson-mass-4 mixture. The results are practically the same as in Table II.

Finally, we shortly examine the influence of one component of the solution on the other one by comparing n_4^0 and Z_F in the solution at the equilibrium density for $x_3 = 0.125$ with those for the corresponding pure phases ($\rho = \rho_3$, ρ_4). The n_4^0 value increase from 0.214 to 0.267 and the Z_F one from 0.218 to 0.904. A similar comparison is made for $n_4(k)$ in Fig. 2 and for $n_3(k)$ in Fig. 3.

The decrease of the number of the interactions, when one of the components is suppressed, leads to expected increasing values of n_4^0 and Z_F. This is dramatically true for Z_F because of the small density of the fermionic component.

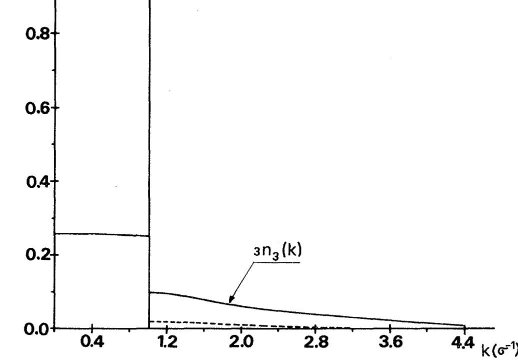

FIG. 3. $n_3(k)$ for mixture as Fig. 2 (solid line) and for pure ^{3}He at $\rho_3 = 0.035\sigma^{-3}$ (dashed line).

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[7](a) *Many Body Problems,* edited by S. Rosati and S. Fantoni, Lecture Notes in Physics, Vol. 138 (Springer-Verlag, New York, 1981), p. 1; (b) the convolution integral is given by

$$(A|B)=\int d\vec{r}_3 A(r_{13})B(r_{32}) \ ,$$

(c) the Fourier transform of $f(r)$ is defined as

$$\tilde{f}(k)=\rho\int d\vec{r}\exp(i\vec{k}\cdot\vec{r})f(r) \ .$$

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