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Hypernetted-chain theory of the momentum distribution for Bose systems with mixture formalism

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The hypernetted-chain equations for the momentum distribution $n(k)$ of the N-particle Bose system are derived by relating its Fourier transform, the one-particle density matrix $n(r)$, to one of the three radial distribution functions, $g_{\beta\beta}(r)$, in a formally equivalent system of a two-component mixture of $N_\beta=2$ and $N_\alpha=N-1$ particles in the zero-concentration limit $\rho_\beta \approx 0$. The Bose-Einstein condensate fraction is shown to be proportional to the inverse of $g_{\beta\beta}(r)$ at the origin, $n_c=g_{\beta\beta}^{-1}(0)$. When the theory is used to calculate $n(k)$ in the ground state of liquid ^{4}He, it is found that the kinetic-energy sum rule required to be satisfied by $n(k)$ is strongly violated unless the elementary diagrams are taken into account. This is done using a scaling approximation for the lowest-order elementary diagrams by determining scaling factors so that different procedures for calculating the kinetic energy give the same result.

I. INTRODUCTION

Fantoni[1] derived a set of coupled hypernetted-chain-type (HNC) integral equations for the one-particle momentum distribution

$$n(k)=Nn(\infty)\delta(k)+\rho\int[n(r)-n(\infty)]e^{i\vec{k}\cdot\vec{r}}d^3r\ , \tag{1}$$

which is the Fourier transform of the one-particle density matrix

$$n(|\vec{r}_1-\vec{r}_1'|)=\frac{V\int d^3r_2\cdots d^3r_N\psi_0^*(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)\psi_0(\vec{r}_1',\vec{r}_2,\ldots,\vec{r}_N)}{\int d^3r_1d^3r_2\cdots d^3r_N\psi_0^2(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)}\ . \tag{2}$$

The procedure employed by Fantoni is essentially a generalization of the usual HNC approach for the radial distribution function $g(r)$ to sum up all nodal diagrams in the cluster expansion of $n(r)$. The calculation of the Bose-Einstein condensate fraction $n_c=n(\infty)$ is analogous to the calculation of the chemical potential in the HNC treatment of classical liquids by Morita and Hiroike.[1,2] The theory was subsequently generalized also for the temperature-dependent one-particle density matrices both in the cluster-expansion form[3] as well as within the HNC scheme of Fantoni.[4,5]

Numerical studies[6] of n_c with the HNC equations using Jastrow wave functions to describe the ground state of liquid ^{4}He lead to results in fairly good agreement with experiments and with Green's-function Monte Carlo calculations. However, at large k the distribution $n(k)$ is inaccurate and hence the kinetic energy is too large by a factor of 3. Also at low temperatures the temperature dependence of $n(k)$ and n_c is given correctly when $\rho\approx\rho_s$, where ρ_s is the superfluid density in the two-fluid model.[5] At higher temperatures the results based on the Jastrow ansatz together with the Penrose n-particle density matrix[7] are poor. In particular, one does not find any λ transition.[3,4] However, this is not due to inefficiency of the HNC approach in integrating $n(r)$ from the n-particle density matrix but follows from an inadequacy of the Penrose density matrix to correctly incorporate the depletion of the condensate.

In this paper we follow an approach where $n(k)$ can be expressed in terms of the radial distribution functions of a binary mixture, which was first proposed by Reatto and Chester.[8] A numerical implementation of this theory was done by Francis *et al.*[9] using extended Percus-Yevick equations for a fictitious classical two-component mixture with the interaction potentials

$$\beta V_{11}=-2\ln f,\ \ \beta V_{12}=-\ln f,\ \ \beta V_{22}=-\tfrac{1}{2}\ln f\ , \tag{3}$$

where f is the Jastrow correlation factor

$$\psi_0(1,\ldots,N)=\prod_{i<j}f(r_{ij})\ . \tag{4}$$

The best result obtained by these authors for n_c (about 13%) is not far from other calculations.

To our knowledge, the two superficially different approaches described above have not been compared analytically nor numerically using wave functions that were more refined than those accessible to Francis *et al.*[9] In this paper, we first show that, in fact, by using the HNC-mixture formalism that was recently applied successfully to several other problems,[10-12] we can quite easily derive the HNC equations of Fantoni[1] for the one-particle density matrix $n(r)$. Surprisingly, the two approaches give a different expression for the condensate fraction. In Sec. III we generalize the approach of Sec. II also for the temperature-dependent Penrose matrix. In Sec. IV we compare the two formalisms numerically for liquid ^{4}He in the pure HNC approach as well as including the elementary diagram contribution within the so-called scaling approximation.[13]

II. HNC EQUATIONS FOR $n(r)$ IN THE GROUND STATE

The one-particle density matrix can be written in a Jastrow approximation[1,6]

$$n(r_{11'})=VQ_N^{-1}\int d^3r_2\cdots d^3r_N\exp\left[\tfrac{1}{2}\sum_{2\le j}u(r_{1j})+\tfrac{1}{2}\sum_{2\le j}u(r_{1'j})+\sum_{2\le i<j}u(r_{ij})\right], \tag{5}$$

where Q_N is the normalization factor,

$$Q_N=\int d^3r_1\cdots d^3r_N\exp\left[\sum_{i<j}u(r_{ij})\right]. \tag{6}$$

Reatto and Chester[8] (also see an earlier paper of Penrose and Onsager[14]) noticed that the above integral is proportional to one of the three radial distribution functions of a binary mixture consisting of two particles $\{1,1'\}$ in the bath of $N-1$ particles $\{2,\ldots,N\}$.

The mixture wave function can be defined as[12,15]

$$\psi_M^2(1,2,\ldots,N)=\exp\left[\sum_{\substack{i,j=1\\ i<j}}^{N_\alpha}u_{\alpha\alpha}(r_i^\alpha-r_j^\alpha)+\sum_{\substack{i,j=1\\ i<j}}^{N_\beta}u_{\beta\beta}(r_i^\beta-r_j^\beta)+\sum_{j=1}^{N_\beta}\sum_{i=1}^{N_\alpha}u_{\alpha\beta}(r_j^\beta-r_i^\alpha)\right], \tag{7}$$

where $u_{\alpha\alpha}$, $u_{\alpha\beta}$, and $u_{\beta\beta}$ are correlations between three different particle pairs and $N_\alpha+N_\beta=N$. The three different radial distribution functions associated with these correlations can be defined in a compact form as follows:[12,15,16]

$$g_{\alpha\beta}(\vec{r}_i^{\,\alpha}-\vec{r}_j^{\,\beta})=\frac{N_\beta(N_\alpha-\delta_{\alpha\beta})}{\rho_\alpha\rho_\beta Q_N}\int\psi_M^2(1,\ldots,N)d^3r_1^\alpha\cdots d^3r_{i-1}^\alpha d^3r_{i+1}^\alpha\cdots d^3r_{j-1}^\beta d^3r_{j+1}^\beta\cdots d^3r_N^\beta, \tag{8}$$

where

$$Q_N=\int\psi_M^2(1,2,\ldots,N)d^3r_1\cdots d^3r_N, \tag{9}$$

and ρ_α or ρ_β are the partial densities of the α- or β-type particles.

The one-particle density $n(r)$ can be written in a form that is equivalent to $g_{\beta\beta}(r)$ apart from a constant factor A,

$$n(r_{11'})=Ag_{\beta\beta}(r_{11'}), \tag{10}$$

after the following identifications have been made:

$$u_{\alpha\alpha}(r)=u(r),\quad u_{\beta\beta}(r)=0,\quad u_{\alpha\beta}(r)=\tfrac{1}{2}u(r). \tag{11}$$

The constant A is easily calculated to be

$$\frac{1}{A}=\frac{N_\beta(N_{\beta-1})}{V\rho_\beta^2}\frac{\int d\vec{r}_{1'}d\vec{r}_1\cdots d\vec{r}_N\delta(\vec{r}_1-\vec{r}_{1'})\exp\left[\sum_{i<j}u(r_{ij})\right]}{\int d\vec{r}_{1'}d\vec{r}_1\cdots d\vec{r}_N\exp\left[u_{\beta\beta}(r_{11'})+\sum_{2\le j}[u_{\beta\alpha}(r_{1j})+u_{\beta\alpha}(r_{1'j})]+\sum_{2\le i<j}u_{\alpha\alpha}(r_{ij})\right]},\ =g_{\beta\beta}(0). \tag{12}$$

Then, the Bose-Einstein condensate fraction is

$$n_c=n(\infty)=g_{\beta\beta}^{-1}(0)g_{\beta\beta}(\infty)=g_{\beta\beta}^{-1}(0) \tag{13}$$

since $g_{\beta\beta}(\infty)=1$ in the ground state of liquid ^{4}He.

The three partial structure factors corresponding to the respective radial distribution functions are[12,15,16]

$$S_{\alpha\beta}(k)-\delta_{\alpha\beta}=(\rho_\alpha\rho_\beta)^{1/2}\int e^{i\vec{k}\cdot\vec{r}}[g_{\alpha\beta}(r)-1]d^3r. \tag{14}$$

The HNC equations relating $u_{\alpha\beta}$ and $g_{\alpha\beta}$,

$$g_{\alpha\beta}(r)=\exp[u_{\alpha\beta}(r)+N_{\alpha\beta}(r)+E_{\alpha\beta}(r)], \tag{15}$$

are then obtained by summing up all of the possible nodal graphs into $N_{\alpha\beta}$ (Ref. 12):

$$N_{\alpha\alpha}(r_{12})=\rho_\alpha\int dr_3c_{\alpha\alpha}(r_{13})h_{\alpha\alpha}(r_{23})+\rho_\beta\int dr_3c_{\alpha\beta}(r_{13})h_{\alpha\beta}(r_{23}), \tag{16a}$$

$$N_{\beta\beta}(r_{12})=\rho_\alpha\int dr_3c_{\alpha\beta}(r_{13})h_{\alpha\beta}(r_{23})+\rho_\beta\int dr_3c_{\beta\beta}(r_{13})h_{\beta\beta}(r_{23}), \tag{16b}$$

$$N_{\alpha\beta}(r_{12})=\rho_\alpha\int dr_3c_{\alpha\beta}(r_{13})h_{\alpha\alpha}(r_{23})+\rho_\beta\int dr_3c_{\beta\beta}(r_{13})h_{\alpha\beta}(r_{23}). \tag{16c}$$

Here, we have used an abbreviation

$$h_{\alpha}\beta(r)=g_{\alpha\beta}(r)-1 \tag{17}$$

and the direct correlation functions $c_{\alpha\beta}$ are defined as

$$c_{\alpha\beta}(r)=g_{\alpha\beta}(r)-1-N_{\alpha\beta}(r)\ . \tag{18}$$

When we take the zero-concentration limit $N_\beta=2$ or $\rho_\beta \ll \rho_\alpha$, the last terms in Eqs. (16) can be dropped. We now define new quantities that remain finite in the limit $\rho_\beta \approx 0$ as follows (we adapt the notation of Ristig and Lam[6] for the Fourier transforms of $N_{\alpha\beta}$, $N_{\beta\beta}$, and $c_{\alpha\beta}$):

$$N(k)=\frac{1}{(2\pi)^3\rho}\int N_{\alpha\alpha}(r)e^{-i\vec{k}\cdot\vec{r}}d^3r=N_{\alpha\alpha}(k)\ , \tag{19}$$

$$\begin{aligned}-Q(k)&=\frac{1}{(2\pi)^3\rho}\int N_{\beta\beta}(r)e^{-i\vec{k}\cdot\vec{r}}d^3r\\&=\frac{\rho_\alpha}{\rho_\beta}N_{\beta\beta}(k)\ ,\end{aligned} \tag{20}$$

$$\begin{aligned}Q_1(k)&=\frac{1}{(2\pi)^3\rho}\int c_{\alpha\beta}(r)e^{-i\vec{k}\cdot\vec{r}}d^3r\\&=\left[\frac{\rho_\alpha}{\rho_\beta}\right]^{1/2}c_{\alpha\beta}(k)\ ,\end{aligned} \tag{21}$$

$$\begin{aligned}Q_2(k)&=\frac{1}{(2\pi)^3\rho}\int N_{\alpha\beta}(r)e^{-i\vec{k}\cdot\vec{r}}d^3r\\&=\left[\frac{\rho_\alpha}{\rho_\beta}\right]^{1/2}N_{\alpha\beta}(k)\ ,\end{aligned} \tag{22}$$

where $N_{\alpha\beta}(k)$, etc., are defined according to the definitions of $S_{\alpha\beta}$, etc., in Eq. (14).

The solution of the HNC equations is then very easy and we obtain the following from Eqs. (10) and (15):

$$n(r)=\frac{g_{\beta\beta}(r)}{g_{\beta\beta}(0)}=n_c e^{-Q(r)}\ , \tag{23}$$

where

$$n_c=g_{\beta\beta}^{-1}(0)=e^{Q(0)}\ . \tag{24}$$

By keeping only the first terms in Eqs. (16), the function $Q(r)$ is calculated from the equations

$$\begin{aligned}Q(k)&=-Q_1(k)[Q_1(k)+Q_2(k)]\\&=-Q_1^2(k)S(k)=\xi^2(k)S^{-1}(k)\ ,\end{aligned} \tag{25}$$

$$Q_2(k)=Q_1(k)[S(k)-1]=\xi(k)\frac{S(k)-1}{S(k)}\ , \tag{26}$$

$$N(k)=\frac{[S(k)-1]^2}{S(k)}\ , \tag{27}$$

and

$$g_{\beta\beta}(r)=\exp[-Q(r)+E_{\beta\beta}(r)]\ , \tag{28a}$$

$$g_{\alpha\beta}(r)=\exp[\tfrac{1}{2}u(r)+Q_2(r)+E_{\alpha\beta}(r)]\ , \tag{28b}$$

$$g_{\alpha\alpha}(r)\approx g(r)=\exp[u(r)+N(r)+E_{\alpha\alpha}(r)]\ . \tag{28c}$$

Here, $E_{\alpha\alpha}$, $E_{\alpha\beta}$, and $E_{\beta\beta}$ are the elementary diagram contributions, and the function $\xi(k)$ is defined as

$$\xi(k)=\rho\int[g_{\alpha\beta}(r)-1]e^{i\vec{k}\cdot\vec{r}}d^3r=\left[\frac{\rho_\alpha}{\rho_\beta}\right]^{1/2}S_{\alpha\beta}(k)\ . \tag{29}$$

These equations are easy to solve by iteration; when $\xi(k)$ is solved from Eqs. (26) and (28b), the function $Q(r)$ is obtained as a single Fourier transform from Eq. (25). Thereafter, the one-particle momentum distribution can be calculated from

$$n(k)=Nn_c\delta(k)+n_c\rho\int\left[\frac{g_{\beta\beta}(r)}{g_{\beta\beta}(0)}-1\right]e^{i\vec{k}\cdot\vec{r}}d^3r\ . \tag{30}$$

The difference between our result and the approach of Fantoni[1] is that we calculate n_c from Eq. (24), whereas Fantoni uses the formulas analogous to the calculation of the chemical potential in a classical liquid[2] to obtain n_c. Fantoni's result is

$$n_c=\exp(2R[f-1]-R[f^2-1])\ , \tag{31}$$

where the function R is given by

$$R[f-1]=\rho\int[Q_1(r)-E_{\alpha\beta}(r)]-\frac{1}{(2\pi)^3\rho}\frac{1}{2}\int d^3k\,\xi(k)[Q_1(k)+2E_{\alpha\beta}(k)]+E_\beta\ , \tag{32a}$$

$$R[f^2-1]=\rho\int[g(r)-1-N(r)-E_{\alpha\alpha}(r)]-\frac{1}{(2\pi)^3\rho}\frac{1}{2}\int d^3k[S(k)-1][N(k)+2E_{\alpha\alpha}(k)]+E_\alpha\ , \tag{32b}$$

where E_α and E_β are one-particle elementary structures. These two approaches of calculating n_c can be used to check the accuracy of the approximations employed since the results should agree if all elementary diagrams are included.

III. HNC EQUATIONS FOR $n(r)$ AT FINITE TEMPERATURES

The theory described in Sec. II can easily be generalized also for finite temperatures using the Penrose density matrix[7,17] as an input:

$$\langle r_1',\ldots,r_N'|\hat{\rho}|r_1,\ldots,r_N\rangle=Q_N^{-1}\psi_0(r_1',\ldots,r_N')\psi_0(r_1,\ldots,r_N)\exp\left[\tfrac{1}{2}\sum_{i,j}[h_1(r_{ij})+h_1(r_{i'j'})+h_2(r_{i'j})+h_2(r_{ij'})]\right]\ . \tag{33}$$

Here, ψ_0 is the ground-state wave function defined in Eq. (4) and the functions h_1 and h_2 are obtained in terms of the Boltzmann factor for the thermal population of elementary excitations in liquid ^{4}He (Ref. 17):

$$h_1(r)=-\frac{1}{(2\pi)^3\rho}\int d^3k\frac{1}{S_0(k)}\frac{\kappa_k^2}{1-\kappa_k^2}e^{i\vec{k}\cdot\vec{r}}\,, \tag{34a}$$

$$h_2(r)=\frac{1}{(2\pi)^3\rho}\int d^3k\frac{1}{S_0(k)}\frac{\kappa_k}{1-\kappa_k^2}e^{i\vec{k}\cdot\vec{r}}\,. \tag{34b}$$

Here, $\kappa_k=\exp[-\beta\epsilon(k,T)]$, $\epsilon(k,T)$ is the temperature-dependent excitation spectrum for liquid ^{4}He, and $S_0(k)$ is the ground-state structure factor at $T=0$.

The one-particle density is then obtained as usual by integrating over all coordinates except for r_1 and r_1':

$$n_T(r_{11'})=VQ_N^{-1}(T)\int d^3r_2\cdots d^Nr_N\exp\left[\tfrac{1}{2}\sum_{2\le j}u_T(r_{1j})+\tfrac{1}{2}\sum_{2\le j}u_T(r_{1'j})+\sum_{2\le i<j}u_T(r_{ij})-y_T(r_{11'})\right], \tag{35}$$

where $Q_N(T)$ is the normalization factor

$$Q_N(T)=\int d^3r_1\cdots d^3r_N\exp\left[\sum_{i<j}u_T(r_{ij})\right]. \tag{36}$$

The temperature-dependent correlation function $u_T(r)$ is now defined as

$$\begin{aligned}u_T(r)&=u_0(r)+2h_1(r)+2h_2(r)\\&=u_0(r)-\frac{2}{(2\pi)^3\rho}\int d^3k\frac{1}{S_0(k)}\frac{\kappa_k}{1+\kappa_k}e^{i\vec{k}\cdot\vec{r}}\,,\end{aligned} \tag{37}$$

which reduces to the ground-state correlation function $u_0(r)$ when $T=0$. $y_T(r)$ is the temperature-dependent correlation between particles at r_1 and r_1' (Refs. 5 and 7),

$$\begin{aligned}y_T(r)&=h_2(0)-h_2(r)\\&=\frac{1}{(2\pi)^3\rho}\int_0^\infty\left[1-\frac{\sin(kr)}{kr}\right]\\&\quad\times\frac{1}{S_0(k)\sinh[\beta\epsilon(k,T)]}k^2dk\,,\end{aligned} \tag{38}$$

which vanishes at $T=0$, $y_0(r)=0$.

The analysis for $n_T(r)$ proceeds in the same manner as in Sec. III for the ground-state density matrix except that now the following identifications for the mixture correlation functions must be made:

$$\begin{aligned}u_{\alpha\alpha}(r)&=u_T(r)\,,\\u_{\beta\beta}(r)&=-y_T(r)=h_2(r)-h_2(0)\,,\\u_{\alpha\beta}(r)&=\tfrac{1}{2}u_T(r)\,.\end{aligned} \tag{39}$$

The final equation is the same as in Sec. II but the Bose-Einstein condensate fraction is calculated from

$$n_c=n(\infty)=g_{\beta\beta}^{-1}(0)g_{\beta\beta}(\infty)\,, \tag{40}$$

where $g_{\beta\beta}(\infty)$ is now given by

$$\begin{aligned}g_{\beta\beta}(\infty)&=\exp[-\tfrac{1}{8}(T/T_0)^2]\,,\\T_0&=\rho(\hbar c)^3(mc^2k)^{-1}\,,\end{aligned} \tag{41}$$

where c is the speed of the sound. This result is in complete agreement with that of Schulz and Ristig.[5]

IV. APPLICATION TO THE GROUND STATE OF LIQUID ^{4}He

As an application of the mixture formalism, we calculate the Bose-Einstein condensate fraction n_c and the one-particle momentum distribution $n(k)$ for liquid ^{4}He in the ground state including the elementary diagrams. For the interaction of the two He atoms we use the standard Lennard-Jones 6-12 potential. The ground-state correlation function $u(r)$ is obtained by optimizing the ground-state energy as in Ref. 18. We have used the parametrized radial distribution functions of Smith *et al.*[18] as an input to our calculations. The HNC equations (16) and (28) are solved by using the iterative procedure of Ng,[19] which converges quite rapidly, requiring only about 20 iterations to obtain the root-mean-square difference beween the radial distribution functions from the two successive iterations to be less than 10^{-6}. The results for n_c are given in Table I using both Eq. (24) to calculate n_c and Fantoni's equation (31). We have also calculated the normalization of $n(k)$, which should satisfy

TABLE I. HNC/0 result for n_c, for $\sum_k n(k)$ and for the kinetic energy calculated from $n(k)$ as well as from the Jackson-Feenberg formula. The condensate fraction n_c is calculated from both Eq. (24) (mixture) and Eq. (31) (Fantoni).

	Mixture HNC			Fantoni HNC					Lam and Ristig (Ref. 6)
ρ (Å^{-3})	n_c	$\sum_{k(\neq 0)} n(k)$	$\langle T\rangle$	n_c	$\sum_{k(\neq 0)} n(k)$	$\langle T\rangle$	$\langle T\rangle_{\rm JF}$	Input function	n_c
0.02185	0.066	0.93	24.9	0.120	1.70	45.5	14.99	$u_{\rm HNC}$	0.120
0.02460	0.040	0.96	31.7	0.083	2.01	66.5	18.53	$u_{\rm HNC}$	$\approx$0.08
0.02185	0.080	0.92	23.6	0.141	1.60	41.1	14.45	$u_{\rm HNCE}$	
0.02280	0.064	0.93	25.6	0.126	1.69	46.6	15.50	$u_{\rm HNCE}$	
0.02460	0.052	0.95	29.8	0.102	1.87	58.9	17.69	$u_{\rm HNCE}$	

the sum rule

$$n_c=1-\frac{1}{N}\sum_{k(\neq 0)} n(k)\ . \tag{42}$$

Also the kinetic energy is obtained from $n(k)$ via the integral

$$\frac{\langle T\rangle}{N}=\frac{\hbar^2}{2m}\sum_k k^2 n(k)\ . \tag{43}$$

The kinetic energy in the Jackson-Feenberg form can be calculated in the Jastrow approximation from[18]

$$\frac{\langle T\rangle}{N}=-\frac{\hbar^2}{8m}\rho\int \nabla^2 u(r)g(r)d^3r\ . \tag{44}$$

It is seen from Table I that our formalism satisfies the sum rule (42) but that Fantoni's equation does not. In both approaches the kinetic energies are too large and especially Fantoni's equation gives 3 times the expected value for $\langle T\rangle$.

To remedy the failures of these two theories we must include the elementary diagrams in both calculations. This can be done most easily by using the so-called scaling approximation which was recently found to give rather good results for the ground energy of liquid ^{4}He in Jastrow approximations.[13,18]

In this HNCE (hypernetted-chain, elementary) theory, the elementary diagram functions $E_{\alpha\beta}$ are approximated by multiplying the lowest-order contributions $E_{\alpha\beta}^{(4)}$ by appropriate scaling factors $\kappa_{\alpha\beta}$:

$$E_{\alpha\beta}(r)=\kappa_{\alpha\beta}E_{\alpha\beta}^{(4)}(r)\ . \tag{45}$$

The nonvanishing lowest-order elementary diagrams $E_{\alpha\beta}^{(4)}$ in the zero-concentration limit $\rho_\beta\approx 0$ are given in Fig. 1(a). The scaling factor $K_{\alpha\alpha}$ is determined so that the Jackson-Feenberg (JF) energy functional (44) gives the same result as the Pandharipande-Bethe (PB) functional[13]

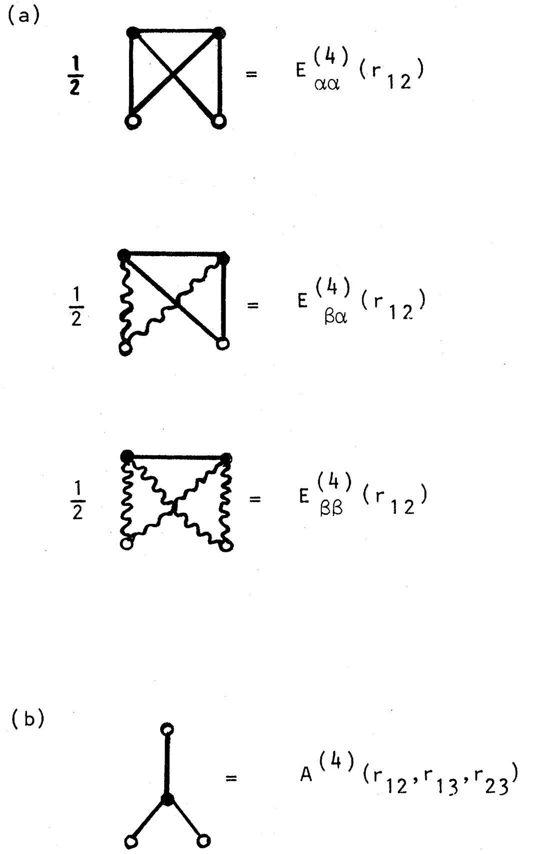

FIG. 1. (a) Lowest-order elementary diagrams $E_{\alpha\alpha}^{(4)}$, $E_{\alpha\beta}^{(4)}$, and $E_{\beta\beta}^{(4)}$. (b) Lowest-order Abe correction for g_3. Solid circles carry a factor ρ_α, solid lines are $g_{\alpha\alpha}-1$ links, and wavy lines are $g_{\alpha\beta}-1$ links.

$$\frac{T_{\rm PB}}{N}=\frac{-\hbar^2}{4m}\rho\int g(r_{12})\{-\nabla_1^2u(r_{12})+\tfrac{1}{2}[\nabla_1 u(r_{12})]^2\}d^3r_{12}-\frac{\hbar^2}{8m}\rho\int g_3(r_{12},r_{13},r_{23})\vec{\nabla}_1u(r_{12})\cdot\vec{\nabla}_1u(r_{13})d^3r_{12}d^3r_{13}\ . \tag{46}$$

As described recently by Usmani *et al.*,[13] the three-particle distribution function can be approximated by

$$g_3(r_{12},r_{13},r_{23})=g(r_{12})g(r_{13})g(r_{23})[1+\tfrac{1}{2}(1+\kappa_{\alpha\alpha})A^{(4)}(r_{12},r_{13},r_{23})]\ , \tag{47}$$

TABLE II. Results in the HNCE-scaling approximation for n_c, for $\sum_k n(k)$ and for the kinetic energies. $\kappa_{\alpha\alpha}$, $\kappa_{\alpha\beta}$, and $\kappa_{\beta\beta}$ are the scaling factors.

		Mixture HNCE scaling			Fantoni HNCE scaling				
ρ (Å^{-3})	n_c	$\sum_{k(\neq 0)} n(k)$	$\langle T\rangle$	n_c	$\sum_{k(\neq 0)} n(k)$	$\langle T\rangle$	$\langle T\rangle_{\rm JF}$	$\kappa_{\alpha\alpha}=\kappa_{\alpha\beta}=\kappa_{\beta\beta}$	Input function
0.02185	0.139	0.86	13.9	0.140	0.87	14.0	13.99	3.36	$u_{\rm HNCE}$
0.02280	0.124	0.88	15.0	0.125	0.88	15.1	14.99	3.50	$u_{\rm HNCE}$
0.02460	0.102	0.90	17.2	0.101	0.89	16.9	17.07	3.83	$u_{\rm HNCE}$
0.02185	0.117	0.88	14.4	0.118	0.89	14.6	14.53	3.50	$u_{\rm HNC}$
0.02460	0.0824	0.92	18.0	0.081	0.90	17.8	17.91	4.05	$u_{\rm HNC}$

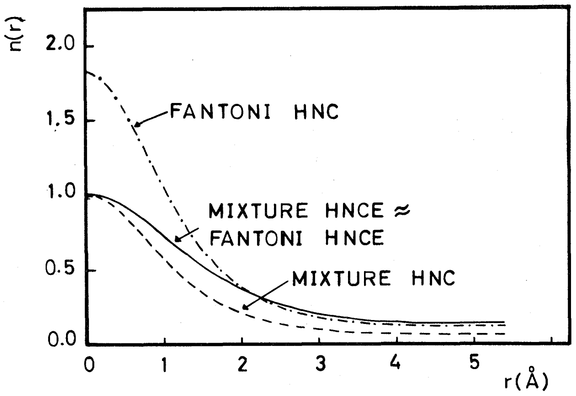

FIG. 2. One-particle density matrix $n(r)$. Solid line is the HNCE-scaling approximation, dashed line is the HNC/0 approximation with mixture formalism, and dashed-dotted line is the HNC/0 approximation with Fantoni's formula. Both the mixture formalism and Fantoni's formula with the HNCE-scaling approximation give results that are indistinguishable in this scale.

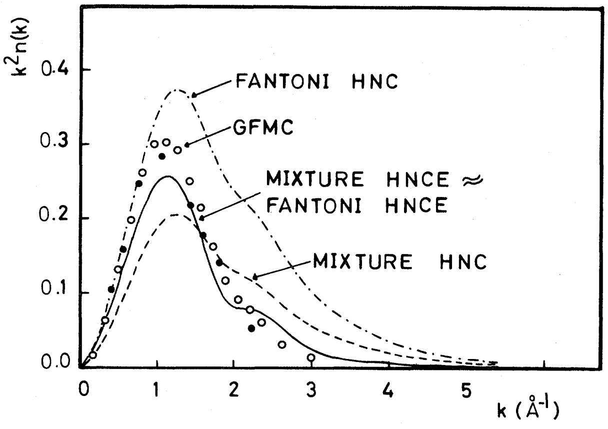

FIG. 3. One-particle momentum distribution $k^2n(k)$. Notation is the same as in Fig. 2. Open circles are Green's-function Monte Carlo (GFMC) results and the solid circles are neutron scattering results from Ref. 21.

where the lowest-order correction to the superposition approximation $A^{(4)}$ is given in Fig. 1(b). The other two scaling factors $\kappa_{\alpha\beta}$ and $\kappa_{\beta\beta}$ are determined so that the kinetic energies calculated from the momentum distribution via Eq. (43) agree with the JF and PB results both when n_c is calculated with our formalism and with Fantoni's formalism. In conclusion, the three different scaling factors $\kappa_{\alpha\alpha}$, $\kappa_{\alpha\beta}$, and $\kappa_{\beta\beta}$ are nearly the same. For example, at $\rho=0.021\,85$ Å^{-3} we obtain the following results: $\kappa_{\alpha\alpha}=3.36$, $\kappa_{\beta\beta}=3.34$, and $\kappa_{\alpha\beta}=3.37$. Thus we can use only one common scaling factor for all three different elementary diagrams $E_{\alpha\alpha}$, $E_{\alpha\beta}$, and $E_{\beta\beta}$. The results from the HNCE calculations within the scaling approximation are given in Table II. In calculations of the R functions from Eq. (32) we have omitted the one-particle elementary diagrams E_α and E_β. From the HNCE equations we obtain very good agreement between the two formalisms in calculating n_c. Also for the normalization of $n(k)$ and for the kinetic energy we now obtain the correct values. The one-particle density matrix $n(r)$ and the momentum distribution $n(k)$ are shown in Figs. 2 and 3, respectively. It is seen that Fantoni's equation violates the normalization of $n(r)$, $n(r=0)=1$, quite severely in the HNC/0 approximation, whereas in our approach $n(r)$ starts from 1. The reason is that our way of calculating n_c is in fact equivalent to this normalization condition. It is also seen from Tables I and II as well as from Fig. 2 that Fantoni's formalism for calculating n_c is already very accurate at the HNC/0 level. The reason is obviously because the two elementary diagram contributions $E_{\alpha\beta}$ and $E_{\alpha\alpha}$ in Eq. (31) cancel each other very effectively. Also in the first terms of Eqs. (32a) and (32b) there is a cancellation since both $Q_1(k=0)$ and $N(k=0)$ diverge. Therefore, the value of n_c is mostly determined by integrals of ξQ_1 and $(S-1)N$ in momentum space. Despite this success in the calculation of n_c the kinetic energy is much too large in that HNC/0 approximation since it is very sensitive to the tail of $n(k)$ due to the weight factor k^4 in the integral (43).

V. DISCUSSION AND CONCLUSIONS

We have shown that the HNC integral equation for the momentum distribution $n(k)$ can be derived very easily using the HNC mixture formalism. In our mixture equation at $T=0$ there are no direct correlations between impurity particles $u_{\beta\beta}(r_{11'})=0$, but only indirect correlations mediated by the α-type host particles. The formula obtained in this way for the Bose-Einstein condensate fraction n_c is different from Fantoni's results.[1] For liquid ^{4}He, n_c calculated from the mixture formalism is about 30% smaller than the result from Fantoni's equation, but the one-particle density matrix is correctly normalized, $n(r=0)=1$, leading to the somewhat better result for the kinetic energy when calculated in the pure HNC approximation. Both formalisms can be made to agree by including elementary diagrams within the scaling approximation. Our final results for n_c, $n(r)$, and $n(k)$ are in fairly good agreement with experiment[20,21] as well as with Monte Carlo calculations.[22,23] The Green's-function Monte Carlo result for n_c is 11%, whereas the most recent experiment[21] gives $n_c \cong 13\%$ which is close to our result, which gives $n_c=14\%$. The elementary diagram contribution improves the behavior of $n(r)$ especially near the origin or equivalently the behavior of the tail of $n(k)$, which leads to a much better agreement with experiment in these regions than earlier HNC calculations do.[6]

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