

Boson-boson mixtures and triplet correlations

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(Received 12 January 1984)

The hypernetted-chain formalism for boson-boson mixtures described by an extended Jastrow correlated wave function is derived, taking into account elementary diagrams and triplet correlations. The energy of an ideal boson ^3He - ^4He mixture is computed for low values of the ^3He concentration. The zero- ^3He -concentration limit provides a ^3He chemical potential in good agreement with the experimental value, when a McMillan two-body correlation factor and the Lennard-Jones potential are adopted. If the Euler equations for the two-body correlation factors are solved in presence of triplet correlations, the agreement is again improved. At the experimental ^4He equilibrium density, the ^3He chemical potential turns out to be -2.58 K, to be compared with the experimental value, -2.79 K.

I. INTRODUCTION

Boson-boson^{1,2} and boson-fermion^{3,4} mixtures are largely theoretically analyzed systems. The ^3He - ^4He solutions are the most deeply studied among them, because of their known experimental properties.⁵ At zero temperature and zero pressure, ^3He is miscible up to a concentration of $\sim 6\%$. The characteristics of one ^3He atom in ^4He can be derived by the ^3He zero-concentration limit. ^3He - ^4He is a fermion-boson mixture and the ^3He antisymmetry plays an essential role in its miscibility property. A well-established result is that if one considers a model boson ^3He - ^4He solution, no ^3He miscibility is obtained. However, the zero-concentration limit is not affected by the statistics. Thus the boson-boson model can provide correct results in that case.

In the last few years, the variational calculations of the ground-state properties of quantum fluids have achieved a high degree of accuracy. Starting from a microscopic two-body interaction between the particles, the wave function has been taken as a product of n -body ($n=2,3$) Jastrow factors times a Slater determinant of plane waves, if the fluid follows the Fermi statistics. In these theories, the approximated sum of the hypernetted-chain^{6,7} (HNC) diagrams has shown to give results comparable to those provided by the exact Monte Carlo methods.^{8,9} Both of these results are in good agreement with the Green-function Monte Carlo¹⁰ (GFMC) estimates and with the experimental results.

The aim of this paper is to extend the recent variational

techniques [HNC scaling approximation (HNC/S) and triplet correlations^{6,7}] to the boson-boson mixtures in order to improve the preceding results obtained by HNC/0 (to assume as zero the elementary diagram contribution), Born-Bogoliubov-Green-Kirkwood-Yvon (to use this relation between the two- and the three-body distribution functions to evaluate the first one), and Monte Carlo calculations. The paper is divided into four sections. After the Introduction, we present the general formalism for evaluating the energy and the radial distribution functions of a boson-boson solution described by a Jastrow-extended correlated wave function, with two- and three-body correlation factors. The low-concentration limit is also derived.

The beginning of Sec. III gives the results, with the Lennard-Jones potential, for a boson ^3He - ^4He mixture in the average correlation approximation. A McMillan¹¹ two-body correlation factor is adopted. The three-body correlation factor is that of Ref. 8. Different approximations are compared.

The excess volume parameter α_0 of one ^3He in ^4He and the ^3He zero-concentration chemical potential μ_3 are evaluated. Noticeable agreement with the experimental results is found. The final part of Sec. III presents the formalism for deriving, in the zero-concentration limit, the optimal two-body correlation factors when the triplet functions are fixed. This approach again improves the results of the first part of the section. Finally, brief conclusions are given in Sec. IV.

II. BOSON-BOSON MIXTURES AND THE ZERO-CONCENTRATION LIMIT

An extended Jastrow correlated wave function, containing two- and three-body correlation factors, of the type

$$\Psi(1, \dots, N_\alpha, N_\alpha + 1, \dots, N_\alpha + N_\beta) = \prod f^{(2)}(i_\alpha, j_\alpha) \prod f^{(3)}(i_\alpha, j_\alpha, l_\alpha) \prod f^{(2)}(i_\beta, j_\beta) \\ \times \prod f^{(3)}(i_\beta, j_\beta, l_\beta) \prod f^{(2)}(i_\alpha, i_\beta) \prod f^{(3)}(i_\alpha, j_\alpha, l_\beta) \prod f^{(3)}(i_\beta, j_\beta, l_\alpha), \quad (1)$$

represents a realistic wave function for the ground state of a binary boson solution constituted by N_α α particles and N_β β particles. In Eq. (1) i_γ ($\gamma = \alpha, \beta$) runs over the coordinates of the γ -type particles and $i_\gamma < j_\gamma$ and $i_\gamma < j_\gamma < l_\gamma$. The $f^{(n)}(i_\gamma, i_\lambda, \dots, i_\mu)$ is the n -body dynamical correlation factor involving n bosons of types $\gamma, \lambda, \dots, \mu$, respectively.

The Hamiltonian of the system is given by

$$H = -\frac{\hbar^2}{2m_\alpha} \sum_{i_\alpha=1, N_\alpha} \nabla_{i_\alpha}^2 - \frac{\hbar^2}{2m_\beta} \sum_{i_\beta=1, N_\beta} \nabla_{i_\beta}^2 + \sum_{i_\alpha < j_\alpha} V(i_\alpha, j_\alpha) + \sum_{i_\beta < j_\beta} V(i_\beta, j_\beta) + \sum_{i_\alpha, i_\beta} V(i_\alpha, i_\beta). \quad (2)$$

$\rho_\gamma = N_\gamma / \Omega$ ($\gamma = \alpha, \beta$) are the partial densities of the solution and Ω is the volume of the box where the particles are embedded. The total density is given by $\rho = \rho_\alpha + \rho_\beta$ and the concentration of the γ component by $x_\gamma = \rho_\gamma / \rho = N_\gamma / (N_\alpha + N_\beta)$. If not otherwise specified, any greek index, different from α and β , may assume the α and β values. We operate in the limit $N_\gamma \rightarrow \infty$, $\Omega \rightarrow \infty$, and $\rho_\gamma = \text{const}$.

The expectation value of the Hamiltonian is better expressed by

$$\langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle = \mathcal{E}(N_\alpha, N_\beta) = \mathcal{E}^{(2)}(N_\alpha, N_\beta) + \mathcal{E}^{(3)}(N_\alpha, N_\beta), \quad (3)$$

with

$$\mathcal{E}^{(2)}(N_\alpha, N_\beta) = N_\alpha \mathcal{E}_{\alpha\alpha}^{(2)}(\rho_\alpha, \rho_\beta) + N_\beta \mathcal{E}_{\beta\beta}^{(2)}(\rho_\alpha, \rho_\beta) + 2(N_\alpha N_\beta)^{1/2} \mathcal{E}_{\alpha\beta}^{(2)}(\rho_\alpha, \rho_\beta) \quad (4)$$

and

$$\mathcal{E}^{(3)}(N_\alpha, N_\beta) = N_\alpha \mathcal{E}_{\alpha\alpha\alpha}^{(3)}(\rho_\alpha, \rho_\beta) + N_\beta \mathcal{E}_{\beta\beta\beta}^{(3)}(\rho_\alpha, \rho_\beta) + 3[(N_\alpha^2 N_\beta)^{1/3} \mathcal{E}_{\alpha\alpha\beta}^{(3)}(\rho_\alpha, \rho_\beta) + (N_\beta^2 N_\alpha)^{1/3} \mathcal{E}_{\beta\beta\alpha}^{(3)}(\rho_\alpha, \rho_\beta)]. \quad (5)$$

The two- and three-body energies are given by

$$\mathcal{E}_{\gamma\lambda}^{(2)}(\rho_\alpha, \rho_\beta) = (\rho_\gamma \rho_\lambda)^{1/2} / (2\Omega) \times \int d\vec{r}_\gamma d\vec{r}_\lambda g^{(2)}(r_{\gamma\lambda}) \times [V(r_{\gamma\lambda}) - (\hbar/4)(\nabla_\gamma^2/m_\gamma + \nabla_\lambda^2/m_\lambda) \times \ln f^{(2)}(r_{\gamma\lambda})], \quad (6)$$

$$\mathcal{E}_{\gamma\lambda\mu}^{(3)}(\rho_\alpha, \rho_\beta) = -(\rho_\gamma \rho_\lambda \rho_\mu)^{2/3} (\hbar^2/4) / (6\Omega) \times \int d\vec{r}_\gamma d\vec{r}_\lambda d\vec{r}_\mu g^{(3)}(\vec{r}_\gamma, \vec{r}_\lambda, \vec{r}_\mu) \times [\nabla_\gamma^2/m_\gamma + \nabla_\lambda^2/m_\lambda + \nabla_\mu^2/m_\mu] \times \ln f^{(3)}(\vec{r}_\gamma, \vec{r}_\lambda, \vec{r}_\mu). \quad (7)$$

We have explicitly assumed that the two-body γ - λ potentials, correlation factors, and distribution functions $g^{(2)}(r_{\gamma\lambda})$ depend only on the interparticle distances. The three-body γ - λ - μ distribution functions, $g^{(3)}(\vec{r}_\gamma, \vec{r}_\lambda, \vec{r}_\mu)$,

have also been introduced. It is clear that $\mathcal{E}_\gamma = \mathcal{E}_{\gamma\gamma}^{(2)} + \mathcal{E}_{\gamma\gamma\gamma}^{(3)}$ is the energy per particle of the pure phases, when evaluated at $x_\gamma = 1$.

The HNC techniques, providing the radial distribution functions $g^{(2)}(r)$ of a one-component fluid, can be generalized to obtain

$$g^{(2)}(r_{\gamma\lambda}) = [f^{(2)}(r_{\gamma\lambda})]^2 \exp[G(r_{\gamma\lambda}) + C(r_{\gamma\lambda}) + E(r_{\gamma\lambda})]. \quad (8)$$

$G(r_{\gamma\lambda})$ is the γ - λ nodal function, solution of

$$G(r_{\gamma\lambda}) = \sum_\mu \rho_\mu \int d\vec{r}_\mu [g^{(2)}(r_{\gamma\mu}) - 1 - G(r_{\gamma\mu})] \times [g^{(2)}(r_{\mu\lambda}) - 1], \quad (9)$$

$C(r_{\gamma\lambda})$ is the integral of the dressed triplet function

$$C(r_{\gamma\lambda}) = \sum_\mu \rho_\mu \int d\vec{r}_\mu g^{(2)}(r_{\gamma\mu}) g^{(2)}(r_{\mu\lambda}) \times \{ [f^{(3)}(\vec{r}_\gamma, \vec{r}_\mu, \vec{r}_\lambda)]^2 - 1 \}, \quad (10)$$

and $E(r_{\gamma\lambda})$ represents the sum of all the "elementary" diagrams of the γ - λ type.

The three-body distribution functions are written as

$$g^{(3)}(\vec{r}_\gamma, \vec{r}_\lambda, \vec{r}_\mu) = g^{(2)}(r_{\gamma\lambda}) g^{(2)}(r_{\gamma\mu}) g^{(2)}(r_{\lambda\mu}) \times [f^{(3)}(\vec{r}_\gamma, \vec{r}_\lambda, \vec{r}_\mu)]^2 e^{A(\vec{r}_\gamma, \vec{r}_\lambda, \vec{r}_\mu)}, \quad (11)$$

where $A(\vec{r}_\gamma, \vec{r}_\lambda, \vec{r}_\mu)$ is the sum of the contributions of all the Abe¹² terms of the γ - λ - μ type.

The main difficulty in the exact evaluation of the g functions lies in computing the elementary and Abe contributions. The simplest choice, $E = 0$ and $A = 0$, gives the well-known HNC/0 approximation. Further improvements are obtained by summing certain classes of diagrams with a few interval points (HNC/4, HNC/5, ..., HNC/ n when the n -point elementary diagrams are evaluated). Monte Carlo techniques provide exact results, but they require large computing efforts. Approximated methods to fully evaluate these contributions have recently shown to be very powerful in the pure fluids [HNC/S (Ref. 6) and the interpolating equations method¹³]. In this paper, the HNC/S approximation will be adopted. It consists in approximating $E(r_{\gamma\lambda})$ by $s[E^J(r_{\gamma\lambda})/4] + E^T(r_{\gamma\lambda})/4$, $E^J/4$, and $E^T/4$ being the four-point elementary diagrams with (T) or without (J) triplet correlations. The constant factor s is derived by imposing the consistency between the Pandharipande-Bethe and the Jackson-Feenberg (JF) forms of the kinetic energy when the triplet function is set to be 1. The JF kinetic energy is the one adopted here. For the Abe terms, we follow Ref. 6, approximating

$$e^{A(\vec{r}_\gamma, \vec{r}_\lambda, \vec{r}_\mu)} = 1 + (1+s/2)[A^J(\vec{r}_\gamma, \vec{r}_\lambda, \vec{r}_\mu)/4] + A^T(\vec{r}_\gamma, \vec{r}_\lambda, \vec{r}_\mu)/4. \quad (12)$$

To complete this section, we notice that the problem of one β -type impurity in the α -particle fluid can be studied by considering the low- x_β limit of the α - β mixture. If Eq. (3) is expanded in powers of N_β , at the leading order one obtains

$$\mathcal{E}(N_\alpha, N_\beta) = N_\alpha \mathcal{E}_\alpha + N_\beta \mu_\beta + O(N_\beta^2). \quad (13)$$

The μ_β chemical potential of one β particle in the α -particle fluid is explicitly given by

$$\begin{aligned} \mu_\beta = & \{ 2(\rho_\alpha/\rho_\beta)^{1/2} \mathcal{E}_{\alpha\beta}^{(2)}(\rho_\alpha, \rho_\beta) \\ & + 3(\rho_\alpha/\rho_\beta)^{2/3} \mathcal{E}_{\alpha\alpha\beta}^{(3)}(\rho_\alpha, \rho_\beta) \\ & + \rho_\alpha \frac{\partial}{\partial \rho_\beta} [\mathcal{E}_{\alpha\alpha}^{(2)}(\rho_\alpha, \rho_\beta) + \mathcal{E}_{\alpha\alpha\alpha}^{(3)}(\rho_\alpha, \rho_\beta)] \}_{\rho_\beta=0}. \quad (14) \end{aligned}$$

III. CORRELATION FACTORS AND RESULTS

In this section, the method presented in Sec. II is applied to an ideal boson ${}^3\text{He}$ - ${}^4\text{He}$ mixture ($\alpha=3$ and $\beta=4$) at 0 K. The incorrect treatment of the ${}^3\text{He}$ statistics is unimportant in the $x_3=0$ limit. The interaction potential is the Lennard-Jones one for every pair of particles:

$$V(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6], \quad (15)$$

with $\sigma=2.556 \text{ \AA}$ and $\epsilon=10.22 \text{ K}$. Different types of correlation factors will be examined.

A. Average correlation approximation

A very popular approach in the variational theories of quantum mixtures is to use some analytical and parametrized form of $f^{(2,3)}$ and to minimize the total energy respect on the parameters. In principle, one could have different parameters for different pairs and triplets but, in a recent paper,³ we have shown that this degree of freedom gives no substantial improvement, at least for simple two-body correlations, respect on the average correlation approximation (ACA), consisting in setting $f^{(2)}(r_{\gamma\lambda}) = f^{(2)}(r)$ for every γ - λ pair. Therefore, as a first step, ACA has been adopted here and it has been extended to $f^{(3)}$. A very practical aspect of ACA is that all the $g^{(2)}(r_{\gamma\lambda})$'s are identical to the radial distribution function of a single-component system, at $\rho = \rho_\alpha + \rho_\beta$. The same property holds for $g^{(3)}(\vec{r}_\gamma, \vec{r}_\lambda, \vec{r}_\mu)$. $f^{(2)}$ has the McMillan¹¹ form

$$f^{(2)}(r) = e^{-(b\sigma/r)^5/2}, \quad b = 1.17 \quad (16)$$

and the three-body correlation factor is

$$f^{(3)}(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \exp \left[\sum_{\text{cycl}} \lambda \xi(r_{ij}) \xi(r_{ik}) \vec{r}_{ij} \cdot \vec{r}_{ik} \right] \quad (17)$$

with

$$\begin{aligned} \xi(r) &= F(r) e^{[(r-r_t)/\omega]^2}, \\ F(r \leq r_b) &= [(r-r_b)/r_b]^3 \quad \text{and} \quad F(r > r_b) = 0. \end{aligned} \quad (18)$$

This $f^{(3)}$ is the one adopted in Ref. 8, with $\lambda=8\sigma^{-2}$, $r_t=0.82\sigma$, $\omega=0.5\sigma$, and r_b is half the size of the Monte Carlo simulation cube, $r_b=(108/\rho)^{1/3}/2$.

We have evaluated the energies of the ${}^3\text{He}$ - ${}^4\text{He}$ boson-boson mixtures at zero pressure for different values of x_3 . The scaling factors are taken from Ref. 7.

The results, in different approximations [HNC/O, HNC/S with (T) and without (J) triplet correlations], are shown in Fig. 1. Table I contains the estimated zero-

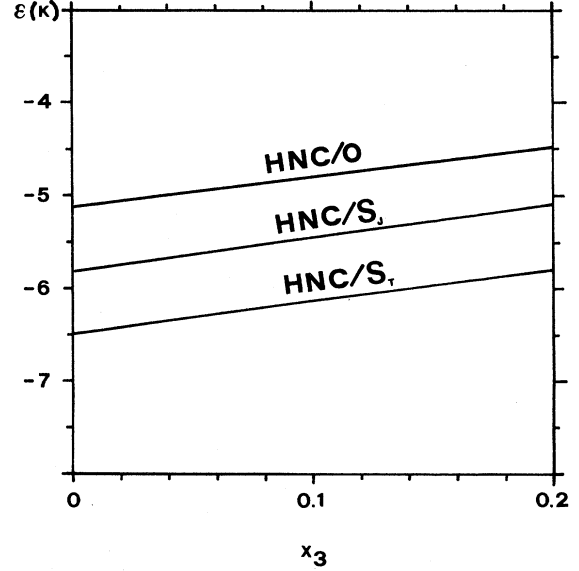


FIG. 1. Low- ${}^3\text{He}$ -concentration behavior of the energy per particle of a boson ${}^3\text{He}$ - ${}^4\text{He}$ solution, at zero pressure, with the McMillan correlation factor in ACA, in different approximations.

concentration ${}^3\text{He}$ chemical potential, evaluated at the equilibrium densities provided by the approximations. The ${}^4\text{He}$ chemical potential $\mu_4 = \mathcal{E}_4 + \rho_4 \partial \mathcal{E}_4 / \partial \rho_4$, the experimental values, and those obtained by the Green-function Monte Carlo results in Ref. 10 are also given. α_0 can be obtained as

$$\lim_{x_3 \rightarrow 0} [\rho(x_3) - \rho(0)] / [x_3 \rho(0)]$$

and its value at the computed equilibrium density is 0.25, to be compared with the experimental 0.28.

Table II presents results at the ${}^4\text{He}$ experimental equilibrium density $\rho_{\text{expt.}} = 0.365\sigma^{-3}$. The difference between μ_4 and \mathcal{E}_4 is a measure of the quality of the approximations in reproducing the equilibrium density. The large discrepancies between μ_3 and its experimental value at $\rho_{\text{expt.}}$ must be ascribed mainly to this incorrect density behavior. This behavior is analogous to that of the velocity of the sound in ${}^4\text{He}$, $c(\rho) = [(1/m_4) \partial P / \partial \rho]^{1/2}$; the computed value of $c(\rho_{\text{expt.}})$ in HNC/O is 367.2 m/sec, to

TABLE I. One- ${}^3\text{He}$ and ${}^4\text{He}$ chemical potentials in ${}^4\text{He}$ with the McMillan two-body correlation factor and the ACA, at the equilibrium densities provided by the HNC/O, HNC/S_J (without triplets), and HNC/S_T (with triplets) approximations. The last two rows give the experimental values and the GFMC results of Ref. 10.

	$\rho_{\text{eq}} (\sigma^{-3})$	μ_4 (K)	μ_3 (K)
HNC/O	0.292	-5.13	-1.80
HNC/S _J	0.327	-5.83	-1.97
HNC/S _T	0.360	-6.49	-2.82
Expt.	0.365	-7.14	-2.79
GFMC	0.365	-6.85	

TABLE II. Chemical potentials of one ^3He and ^4He in ^4He , computed pressures and energy per particle of ^4He at $\rho_{\text{expt.}} = 0.365\sigma^{-3}$ with the McMillan function in ACA. All energies are in K.

	μ_4	μ_3	\mathcal{E}_4	$P/\rho_{\text{expt.}}$
HNC/0	4.95	9.75	-4.44	9.39
HNC/ S_J	-3.20	1.40	-5.70	2.49
HNC/ S_T	-6.15	-2.39	-6.49	0.34

be compared with the experimental 238.2 m/sec. It must be noticed that, at the HNC/0 equilibrium density $\rho_0 = 0.292\sigma^{-3}$, the value of c is 248.5 m/sec. The HNC/0 results are partially improved by the introduction of the elementary diagrams, but both μ_3 and the equilibrium density become very close to the experimental values when triplet correlations are considered.

B. $x_3 = 0$ Euler equations

An alternative procedure consists in employing the $f^{(2,3)}$ giving the minimum of the energy in the class of the extended Jastrow correlated wave functions. To this extent, the functional variation of $\mathcal{E}(N_\alpha, N_\beta)$ with respect to $f^{(2,3)}$ must be performed and the Euler equations originated by $\delta\mathcal{E}/\delta f^{(2)}(r_{\gamma\lambda}) = 0$ and $\delta\mathcal{E}/\delta f^{(3)}(\vec{r}_\gamma, \vec{r}_\lambda, \vec{r}_\mu) = 0$ must be solved. This has been made in HNC/0 and in the absence of triplet correlations.⁽²⁾ The presence of these correlations would lead to very complicated expressions. In this paper we use a simpler method. Firstly, we examine only the $x_3 = 0$ limit, then we choose an analytical and parametrized form of $f^{(3)}$ and solve the corresponding Euler equations for $f^{(2)}$. Finally, we look for the lowest

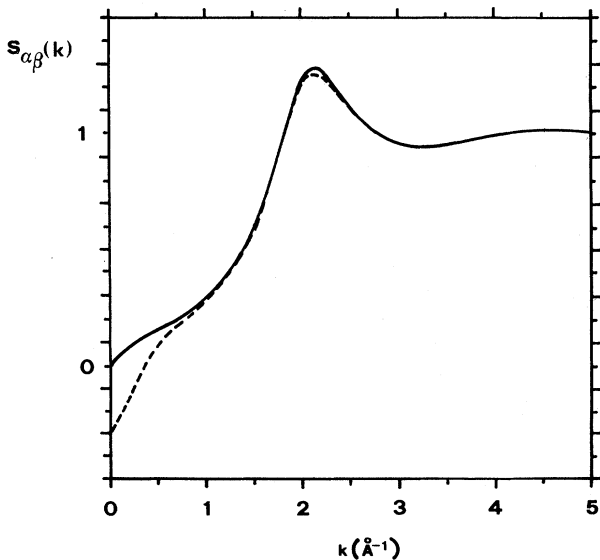


FIG. 2. $S_{44}(k)$ (solid line) and $S_{43}(k)$ (dashed line) in the zero- ^3He -concentration limit in the ^3He - ^4He solution, as provided by the Euler equations with triplet correlations at $\rho_{\text{expt.}}$.

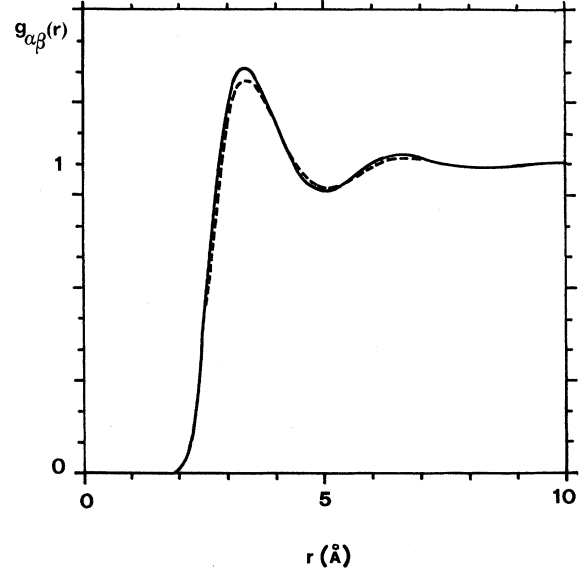


FIG. 3. Optimal radial distribution functions $g^{(2)}(r_{44})$ (solid line) and $g^{(2)}(r_{43})$ (dashed line) with triplet correlations, in the zero- ^3He -concentration limit in the ^3He - ^4He solution at $\rho_{\text{expt.}}$.

energy respect on variations of the triplet parameters. If we fix $f^{(3)}$ identical for all the triplets and we minimize Eq. (13), the following set of Schrödinger-type equations results:

$$0 = -\frac{\hbar^2}{2}(1/m_4 + 1/m_\gamma)\nabla^2[g^{(2)}(r_{4\gamma})]^{1/2} + [g^{(2)}(r_{4\gamma})]^{1/2}[V(r) + w^0(r_{4\gamma}) + w^E(r_{4\gamma}) + w^C(r_{4\gamma}) + w^T(r_{4\gamma})], \quad (19)$$

with $\gamma = 3, 4$.

The induced potentials w^x are defined as

$$\rho_4 \bar{w}_{4\gamma}^0(k) = \frac{-\hbar^2 k^2}{4} [S_{4\gamma}(k) - 1][S_{44}(k) - 1] \times (S_{44}(k) \{1/m_4 [1 + 1/S_{44}(k)] + 1/m_\gamma\})^{-1}, \quad (20a)$$

$$w^E(r_{4\gamma}) = \frac{\hbar^2}{8}(1/m_4 + 1/m_\gamma)\nabla^2 E(r_{4\gamma}) + \Delta w^E(r_{4\gamma}), \quad (20b)$$

$$w^C(r_{4\gamma}) = \frac{\hbar^2}{8}(1/m_4 + 1/m_\gamma)\nabla^2 C(r_{4\gamma}) + \Delta w^C(r_{4\gamma}). \quad (20c)$$

In the above equations, $\bar{w}_{4\gamma}^0(k)$ is the Fourier transform of $w^0(r_{4\gamma})$, $S_{4\gamma}(k) = 1 + \rho_4$ [the Fourier transform of

TABLE III. Same quantities of Table II with the optimal $f^{(2)}_{\text{s}}$. All energies in K.

	μ_4	μ_3	\mathcal{E}_4	$P/\rho_{\text{expt.}}$
HNC/0	2.06	6.78	-4.66	6.72
HNC/ S_J	-4.10	0.26	-5.85	1.74
HNC/ S_T	-6.53	-2.58	-6.58	0.05

$g^2(r_{4\gamma}) - 1]$ are the structure factors and Δw^x are terms involving $\delta C/\delta g^{(2)}$ and $\delta E/\delta g^{(2)}$. Equation (20a) is the well-known HNC/O induced potentials¹⁴ and Eqs. (20b) and (20c) are contributions arising from the elementary and triplet terms in the energy. The $w^T(r_{4\gamma})$ is the induced potential coming from $\delta \mathcal{E}_{44\gamma}^{(3)}/\delta g^{(2)}(r_{4\gamma})$. In solving Eq. (19), the Δw^x and w^T terms have been dropped. We have also approximated $E(r_{43})$ by $E(r_{44})$. These approximations have shown to be very accurate in the HNC/4 case.

If the Lennard-Jones potential is adopted, the resulting structure factors have a linear behavior at low- k values. S_{44} tends to zero and the slope, $S'_{44}(0)$, is related to the sound velocity in pure ${}^4\text{He}$. $S_{43}(k)$ tends to a finite value, namely minus the excess volume parameter of ${}^3\text{He}$ in solution.

In Figs. 2 and 3 we present $S_{44}(k)$, $S_{43}(k)$ and $g^{(2)}(r_{44})$, $g^{(2)}(r_{43})$ at $\rho_{\text{expt.}}$ in HNC/ S_T , as obtained by Eq. (19). The $f^{(3)}$ parameters are $\lambda = -7\sigma^{-2}$, $r_t = 0.82\sigma$, and $\omega = 0.50\sigma$. The value of $S_{43}(0)$ is -0.29 . In HNC/O and HNC/S without triplets the values are -0.32 and -0.30 , respectively.

Table III is analogous to Table II, but the Euler equations solutions are employed in computing the energies. Adopting the Euler equations solutions makes the equilibrium density closer to the experimental value than the McMillan choice. This explains the larger improvement in μ_4 than in \mathcal{E}_4 . μ_3 also is affected by the better choice of the correlation factors passing from -2.39 to -2.58 K at $\rho_{\text{expt.}}$.

IV. CONCLUSIONS

The main result of this paper is that large improvements are found in the description of the properties of a

boson-boson mixture, at low concentrations if elementary diagrams and triplet correlations are considered. When this approach is applied to an ideal boson ${}^3\text{He}$ - ${}^4\text{He}$ solution at zero temperature and zero pressure, the ${}^3\text{He}$ chemical potential and its excess volume parameter are well described by an extended-Jastrow correlated wave function. At the experimental equilibrium density of the ${}^4\text{He}$, μ_3 is closer to the experimental value if the Euler equations are solved with triplet and elementary contributions. The error in the evaluated equilibrium density, which is crucial in estimating μ_3 at $\rho_{\text{expt.}}$, is lowered by the introduction of $f^{(3)}$.

It will be very interesting to use more realistic potentials. The very satisfactory results provided in the pure phases by the HFDEHE2 potential of Aziz *et al.*¹⁵ allow us to think that a similar accuracy can be obtained in the mixtures problem also. Then, wider classes of triplet functions could be examined.

In conclusion, it must be noticed that if the zero-concentration limit of ${}^3\text{He}$ - ${}^4\text{He}$ mixtures can be studied in the boson-boson model, the correct behavior of the phases is not predicted by it. The ${}^3\text{He}$ maximum solubility and the spinoidal point cannot be evaluated because of the absence of a proper ${}^3\text{He}$ antisymmetrization. To this extent, the fermion-boson mixture formalism³ must be generalized to deal with triplet correlations. Work is in progress along this direction.

ACKNOWLEDGMENTS

The authors are much indebted to Professor S. Fantoni for helpful discussions and a critical reading of this paper. Also acknowledged is the Spanish Comisión Asesora Científica y Técnica for partial financial support.

¹M. D. Miller, Ann. Phys. (N.Y.) **127**, 367 (1980); W. E. Massey, C. W. Woo, and M. T. Tan, Phys. Rev. A **1**, 519 (1970); M. B. Yim and W. Massey, Phys. Rev. B **19**, 3529 (1979).

²C. E. Campbell, Ann. Phys. (N.Y.) **74**, 43 (1972); T. Chakraborty, Phys. Rev. B **25**, 3177 (1982).

³A. Fabrocini and A. Polls, Phys. Rev. B **25**, 4533 (1982).

⁴R. A. Guyer and M. D. Miller, Phys. Rev. B **22**, 142 (1980).

⁵C. Ebner and D. O. Edwards, Phys. Rep. **22**, 77 (1970).

⁶Q. N. Usmani, B. Friedman, and V. R. Pandharipande, Phys. Rev. B **25**, 4502 (1982).

⁷Q. N. Usmani, S. Fantoni, and V. R. Pandharipande, Phys. Rev. B **26**, 6123 (1982).

⁸K. Schmidt, M. H. Kalos, M. A. Lee, and G. V. Chester, Phys.

Rev. Lett. **45**, 573 (1980).

⁹D. M. Ceperley and M. H. Kalos, in *Monte Carlo Methods in Statistical Physics*, edited by K. Binder (Springer, Berlin, 1979).

¹⁰P. A. Whitlock, D. M. Ceperley, G. V. Chester, and M. H. Kalos, Phys. Rev. B **19**, 5598 (1979).

¹¹W. L. McMillan, Phys. Rev. **138**, 442 (1965).

¹²R. Abe, Prog. Theor. Phys. **21**, 421 (1959).

¹³A. Fabrocini and S. Rosati, Nuovo Cimento D **1**, 615 (1982).

¹⁴J. C. Owen, Phys. Rev. Lett. **47**, 586 (1981); K. E. Kürten and M. L. Ristig, Phys. Rev. B **27**, 5479 (1983).

¹⁵R. A. Aziz, V. P. S. Nain, J. S. Carley, W. L. Taylor, and G. T. McConville, J. Chem. Phys. **70**, 4430 (1979).