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Variational calculation of ground-state properties of a binary boson system: Properties of dilute mixtures of ^{3}He atoms in superfluid ^{4}He

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In the theory of Woo, Tan, and Massey the properties of ^{3}He atoms in superfluid ^{4}He are determined by ground-state properties of the corresponding binary boson system. Here, we present a variational calculation for these ground-state properties of the binary boson system as well as for the ^{3}He-^{4}He mixture. A correction to the long-wavelength effective interaction is calculated by a paired-phonon analysis using the ground-state wave function of pure liquid ^{4}He. The present results are consistent with other phenomenological theories. Particularly, the effective ^{3}He quasiparticle interaction above about 7.4 atm is qualitatively in agreement with that obtained by Landau, Tough, Brubaker, and Edwards from osmotic-pressure data.

I. INTRODUCTION

The properties of dilute solutions of ^{3}He atoms in superfluid ^{4}He have received considerable attention, theoretically[1-17] and experimentally,[18-25] over the past decade and a half. The theoretical treatments have been either "phenomenological" or "microscopic" in their approaches. In phenomenological approaches[1-9] a quasiparticle Hamiltonian is assumed at the outset and experimental data are used to fit certain undetermined parameters. Microscopic theories[10-17] usually begin with a consideration of the Hamiltonian describing "bare" helium atoms and attempt to develop a quasiparticle Hamiltonian containing no undetermined parameters. Pertinent physical parameters to be calculated in any theory include the chemical potential and the effective mass of a ^{3}He atom, and the effective interaction between a pair of ^{3}He quasiparticles. Woo, Tan, and Massey[10] (WTM) have developed a microscopic theory of dilute mixtures which expresses these physical parameters in terms of pair distribution functions appropriate to a binary boson system. These pair distribution functions, $g^{(\alpha,\beta)}(r)$'s, and their Fourier transformations, $F^{(\alpha,\beta)}(k)$'s,[10,13,15] are defined by

$$g^{(\alpha,\beta)}(r_{i_\alpha j_\beta})=\frac{N_\alpha(N_\beta-\delta_{\alpha\beta})}{n_\alpha n_\beta}\frac{\int|\psi_0^m|^2\,d(\vec{r}_{i_\alpha},\vec{r}_{j_\beta})}{\int|\psi_0^m|^2\,d\vec{r}_1\cdots d\vec{r}_N} \tag{1}$$

and

$$F^{(\alpha,\beta)}(k)=n\int[g^{(\alpha,\beta)}(r)-1]\,e^{i\vec{k}\cdot\vec{r}}\,d\vec{r}, \tag{2}$$

where ψ_0^m is the ground-state wave function for the binary boson system; $d(\vec{r}_{i_\alpha},\vec{r}_{j_\beta})$ denotes $d\vec{r}_1\cdots d\vec{r}_N$ with $d\vec{r}_{i_\alpha}d\vec{r}_{j_\beta}$ omitted; N_3 and N_4 are the number of mass-3 and mass-4 bosons, respectively; n_3 and n_4 are partial number densities of mass-3 and mass-4 bosons, respectively, α or β can be either 3 or 4, and

$$n=n_3+n_4\,. \tag{3}$$

Applications of the WTM theory[10] to the real ^{3}He-^{4}He mixture, therefore, depend on an accurate knowledge of $g^{(\alpha,\beta)}(r)$'s [or $F^{(\alpha,\beta)}(k)$'s]. In their original paper Massey, Woo and, Tan[13] (MWT) calculated the $g^{(\alpha,\beta)}(r)$'s for this system by a variational procedure which utilized a set of coupled integro-differential equations relating the ground-state wave function to pair distribution functions. Although this procedure yields numerical results which compare favorably with experiments, the formulation of the problem is not physically intuitive, and it suffers from the defects that $F^{(\alpha,\beta)}(k)$ does not satisfy the general conditions[15]

$$\lim_{k\to 0}F^{(4,3)}(k)\big|_{x=0}=-(1+\alpha_0)+z(n),$$

and at $k=0$

$$F^{(4,3)}(0)=0\,, \tag{4}$$

where α_0 and $z(n)$ are the volume-excess parameter at zero concentration $(x=N_3/N=0)$ and a positive-definite function less than α_0, respectively. These conditions are very different from the sum-rule requirements for stability of the binary boson system against phase separation.[14,15] Variational calculations, such as MWT,[13] which depends on the minimization of the total energy are not sufficiently sensitive to yield accurate information about distribution functions in the limit of small k. Hence, in such calculations the total ground-state energy is determined primarily by short- and intermediate-range correlations which extend over the order of two interparticle spacings (~7 Å).[26-28] In this paper we present an alternative method for the calculation of the ground-state properties of the binary boson system. This procedure utilizes a simplified cluster expansion of $g^{(\alpha,\beta)}(r)$,[15,29] which is amenable to numerical calculations, and which can be conveniently and accurately used to calculate the ground-state energy over a wide range of densities. Also, $F^{(4,3)}(k)$ satisfies the general condition, Eq. (4). A further correction[15,17] to the long-wavelength effective interaction is considered in a paired-phonon analysis using the ground-state wave function of pure liquid ^{4}He.[15]

II. THEORY: THE BINARY BOSON SYSTEM

The binary boson system is defined by the Hamiltonian[10]

$$H^m = -\frac{\hbar^2}{2m_4}\sum_{i=1}^{N_4}\nabla_i^2 + \left(-\frac{\hbar^2}{2m_3}\right)\sum_{j=N_4+1}^{N}\nabla_j^2 + \sum_{i<j=1}^{N} V(r_{ij}), \tag{5}$$

where m_4 and m_3 are, respectively, the masses of mass-4 and mass-3 bosons obeying Bose statistics; $V(r)$, the two-body potential, is taken to be the same for both types of particles, and for numerical calculations we use the usual Lennard-Jones 6-12 potential. The ground-state properties of pure liquid ^{4}He are known to be fairly accurately described by a Jastrow-type wave function,

$$\psi_0^B(\vec{r}_1, \ldots, \vec{r}_N) = \exp\left(\frac{1}{2}\sum_{i<j=1}^{N} u(r_{ij})\right) \tag{6}$$

where $u(r)$ measures the correlations between two ^{4}He atoms.

MWT's generalization[13] of this ground-state wave function for the binary boson system is

$$\begin{aligned}\psi_0^{\mathrm{MWT}}(\vec{r}_1, \ldots, \vec{r}_{N_4}; \vec{r}_{N_4+1}, \ldots, \vec{r}_N) &= \exp\left(\frac{1}{2}\sum_{i<j=1}^{N_4} u^{(4,4)}(r_{ij})\right) \\ &\quad\times \exp\left(\frac{1}{2}\sum_{k=1}^{N_4}\sum_{l=N_4+1}^{N} u^{(4,3)}(r_{kl}) + \frac{1}{2}\sum_{n<m=N_4+1}^{N} u^{(3,3)}(r_{nm})\right),\end{aligned} \tag{7}$$

$u^{(\alpha,\beta)}(r)$ is a function describing the correlations between (α,β) particle pair, where α or β can be either 4 or 3. These correlation functions satisfy the usual boundary conditions

$$\lim_{r\to 0} u^{(\alpha,\beta)}(r) = -\infty\,,$$

and

$$\lim_{r\to\infty} u^{(\alpha,\beta)}(r) = 0\,, \qquad \alpha,\beta = 4, 3\,. \tag{8}$$

Pair distribution functions, $g^{(\alpha,\beta)}(r)$'s, are defined by Eq. (1), and $S^{(\alpha,\beta)}(k)$'s,[10,13] the liquid-structure functions, are defined as

$$S^{(\alpha,\beta)}(k) = 1 + (n_\alpha n_\beta)^{1/2} \times \int [g^{(\alpha,\beta)}(r) - 1]\, e^{i\vec{k}\cdot\vec{r}}\, d\vec{r}\,. \tag{9}$$

In principle the variational procedure can be carried out in the following steps: (a) The wave function, Eq. (7), is used as the trial wave function. (b) The ground-state expectation energy is expressed in terms of $u^{(\alpha,\beta)}(r)$'s and $g^{(\alpha,\beta)}(r)$'s. (c) The correlation functions, $u^{(\alpha,\beta)}(r)$'s, are expressed in terms of $g^{(\alpha,\beta)}(r)$'s using coupled integral equations. (d) The ground-state expectation energy is then represented only in terms of $g^{(\alpha,\beta)}(r)$'s, and the total ground-state energy is minimized with respect to the $g^{(\alpha,\beta)}(r)$'s. In practice it is very difficult to determine the ground state variationally as in step (d) because of small contributions of $O(x)$ and $O(x^2)$ to the total ground-state energy. MWT[13] introduced, therefore, a simpler variational procedure expected to give a negligible error to the ground-state energy. (We refer to their original paper for details.) This variational procedure is composed of three steps: (a) Consider a system of pure liquid ^{4}He and a trial wave function of the form in Eq. (6). Determine $g^{(4,4)}(r)$ and $u^{(4,4)}(r)$ variationally. (b) Replace a ^{4}He atom by a mass-3 boson and introduce the trial wave function

$$\psi_0^{\mathrm{MWT}}(\vec{r}_1, \ldots, \vec{r}_{N-1}; \vec{r}_N) = \exp\left(\frac{1}{2}\sum_{i<j=1}^{N-1} u^{(4,4)}(r_{ij}) + \frac{1}{2}\sum_{k=1}^{N-1} u^{(4,3)}(r_{kN})\right). \tag{10}$$

The energy expression then contains $g^{(4,4)}(r)$, $g^{(4,3)}(r)$, $u^{(4,4)}(r)$, and $u^{(4,3)}(r)$. Assuming that $g^{(4,3)}(r)$ has been optimally determined in step (a), $g^{(4,3)}(r)$ is determined variationally, solving in the process coupled equations for new $u^{(4,4)}(r)$ and $u^{(4,3)}(r)$. (c) Replace N_3 ^{4}He atoms by the same number of mass-3 bosons and introduce the trial wave function Eq. (7). Assuming that $g^{(4,4)}(r)$ and $g^{(4,3)}(r)$ have been fixed in step (b), $g^{(3,3)}(r)$ is finally determined and the upper bound to the ground-state energy of the binary boson system is also determined by solving in the process coupled equations for new $u^{(4,4)}(r)$, new $u^{(4,3)}(r)$, and $u^{(3,3)}(r)$. These procedures constitute the variational calculation of MWT.[13]

In the present calculation we choose *a slightly* *different trial ground-state wave function*, ψ_0^m, a simpler methodology requiring less computer time for numerical results, and which also explicitly shows the concentration dependences of the distribution functions; further, the general conditions, Eq. (4), are satisfied. ψ_0^m is defined as

$$\psi_0^m(\vec{r}_1,\ldots,\vec{r}_{N_4};\vec{r}_{N_4+1},\ldots,\vec{r}_N) = \psi_0^B(\vec{r}_1,\ldots,\vec{r}_N)\times\exp\left(\frac{1}{2}\sum_{i=1}^{N_4}\sum_{j=N_4+1}^{N} w(r_{ij}) + \frac{1}{2}\sum_{k<1=N_4+1}^{N} s(r_{kl})\right), \tag{11}$$

where $\psi_0^B(\vec{r}_1,\ldots,\vec{r}_N)$ is the ground state wave function for pure liquid ^{4}He at the same number density as the mixture. Instead of using coupled integral equations the $g^{(\alpha,\beta)}(r)$'s are expressed in terms of $g_0(r)$, $S_0(k)$, $w(r)$, and $s(r)$ by a cluster expansion,[15,29] where $g_0(r)$ and $S_0(k)$ are, respectively, the pair distribution and the liquid structure function of pure liquid ^{4}He. If ψ_0^B is considered to be of the Jastrow form [Eq. (6)], then $w(r)$ and $s(r)$ are a measure of the difference in correlations between (4,4) and (4,3) pairs and between (4,4) and (3,3) pairs, respectively. These differences are expected to be small over a large region of space. This should enhance the convergence of these cluster expansions.

The ground-state expectation energy of the binary boson system can be expressed in terms of $g^{(\alpha,\beta)}(r)$'s, $u(r)$, $w(r)$, and $s(r)$ as

$$E_0^m = \frac{\langle\psi_0^m|H^m|\psi_0^m\rangle}{\langle\psi_0^m|\psi_0^m\rangle} = \langle T^m\rangle + \langle V^m\rangle, \tag{12}$$

where

$$\begin{aligned}\langle T^m\rangle = &-\frac{N_4\hbar^2}{8m_4}\left(n_4\int g^{(4,4)}(r)\,\nabla^2 u(r)\,d\vec{r} + n_3\int g^{(4,3)}(r)\,\nabla^2[u(r)+w(r)]\,d\vec{r}\right)\\ &-\frac{N_3\hbar^2}{8m_3}\left(n_4\int g^{(4,3)}(r)\,\nabla^2[u(r)+w(r)]\,d\vec{r} + n_3\int g^{(3,3)}(r)\,\nabla^2[u(r)+s(r)]\,d\vec{r}\right)\end{aligned} \tag{13}$$

and

$$\begin{aligned}\langle V^m\rangle = N_4\binom{n_4}{2}&\int V(r)g^{(4,4)}(r)\,d\vec{r}\\ &+ N_3 n_4\int V(r)g^{(4,3)}(r)\,d\vec{r}\\ &+ N_3\binom{n_3}{2}\int V(r)g^{(3,3)}(r)\,d\vec{r}\,.\end{aligned} \tag{14}$$

Using a cluster expansion the pair distribution functions, $g^{(\alpha,\beta)}(r)$'s, can be expressed in terms of $g_0(r)$, $S_0(k)$, $w(r)$ and $s(r)$ in the form[15]

$$g^{(4,4)}(r) = g_0(r) + xg_1^{(4,4)}(r) + x^2 g_2^{(4,4)}(r)\,, \tag{15}$$

$$g^{(4,3)}(r) = g_0^{(4,3)}(r) + xg_1^{(4,3)}(r) + \cdots\,, \tag{16}$$

and

$$g^{(3,3)}(r) = g_0^{(3,3)}(r) + xg_1^{(3,3)}(r) + \cdots\,, \tag{17}$$

where $x = (N_3/N)$, and

$$g_1^{(4,4)}(r) = \frac{g_0(r)}{(2\pi)^3 n}\left(\int d\vec{k}\,e^{-i\vec{k}\cdot\vec{r}}\{2[S_0(k)-1]K_{\vec{k}} + K_{\vec{k}}^2\} + \Delta g_1^{(4,4)}(r)\right), \tag{18}$$

$$g_0^{(4,3)}(r)=g_0(r)\,e^{w(r)}\left(1+\frac{1}{(2\pi)^3 n}\int d\vec{k}\;e^{-i\vec{k}\cdot\vec{r}}[S_0(k)-1]K_{\vec{k}}+\Delta g_0^{(4,3)}(r)\right), \tag{19}$$

$$g_1^{(4,3)}(r)=\frac{g_0(r)\,e^{w(r)}}{(2\pi)^3 n}\left(\int d\vec{k}\,e^{-i\vec{k}\cdot\vec{r}}\{L_{\vec{k}}[S_0(k)-1]+L_{\vec{k}}K_{\vec{k}}\}+\Delta g_1^{(4,3)}(r)\right), \tag{20}$$

$$g_0^{(3,3)}(r)=g_0(r)\,e^{s(r)}\left(1+\frac{1}{(2\pi)^3 n}\int d\vec{k}\,e^{-i\vec{k}\cdot\vec{r}}\{2[S_0(k)-1]K_{\vec{k}}+K_{\vec{k}}^2\}+\Delta g_0^{(3,3)}(r)\right), \tag{21}$$

$$g_1^{(3,3)}(r)=\frac{g_0(r)\,e^{s(r)}}{(2\pi)^3 n}\left(2\int d\vec{k}\,e^{-i\vec{k}\cdot\vec{r}}[S_0(k)-1](L_{\vec{k}}-K_{\vec{k}})+\int d\vec{k}\,e^{-i\vec{k}\cdot\vec{r}}(L_{\vec{k}}^2-K_{\vec{k}}^2)+\Delta g_1^{(3,3)}(r)\right), \tag{22}$$

where the $\Delta g_i^{(\alpha,\beta)}(r)$'s are complicated expressions involving the n-particle distribution function ($n \geq 4$). $K_{\vec{k}}$ and $L_{\vec{k}}$ are given by

$$K_{\vec{k}}=n\int d\vec{r}\,e^{i\vec{k}\cdot\vec{r}}g_0(r)\,(e^{w(r)}-1),$$

and

$$L_{\vec{k}}=n\int d\vec{r}\,e^{i\vec{k}\cdot\vec{r}}g_0(r)\,(e^{s(r)}-1). \tag{23}$$

Whenever the 3-particle distribution function enters in these cluster expansions, the Kirkwood Superposition approximation[30] (KSA) is used. These cluster expansions[15] are double expansions in powers of the concentration x and expansion parameters related to $K_{\vec{k}}$ and $L_{\vec{k}}$. $\langle T^m\rangle$ and $\langle V^m\rangle$ in Eqs. (13) and (14) can be expressed in terms of $u(r)$, $g_0(r)$, $w(r)$, and $s(r)$ by using the $g^{(\alpha,\beta)}(r)$'s expressions from Eq. (15) to Eq. (17). In computing $\langle T^m\rangle$ and $\langle V^m\rangle$ it is assumed that $u(r)$ and $g_0(r)$ are known. We then parametrize analytic forms for $w(r)$ and $s(r)$ and minimize the total energy with respect to the variation of these parameters. In order to obtain the energy to $O(x^2)$ we need $g^{(4,4)}(r)$ to $O(x^2)$, $g^{(4,3)}(r)$ to $O(x)$ and $g^{(3,3)}(r)$ to $O(x^0)$. The contribution of the x^2 term of $g^{(4,4)}(r)$ [and therefore, $\Delta g_i^{(\alpha,\beta)}(r)$'s] to the energy is known to be small. [See the Appendix of Ref. 15.] It is, therefore, enough to know $g^{(4,4)}(r)$ to $O(x)$ and $\Delta g_i^{(\alpha,\beta)}(r)$ can be neglected. The total ground-state energy is expected to be determined primarily by the short- and intermediate-range correlations which extend over the order of two interparticle spacings (~7 Å) as in pure liquid ^{4}He.[26-28] Thus we may choose $w(r)$ and $s(r)$ to be short-range functions similar to $u(r)$ in pure ^{4}He. If we substitute the $g^{(\alpha,\beta)}(r)$'s from the cluster expressions into Eqs. (15) to (17), the ground-state energy is expressed as follows:

$$E_0^m(n,x)=N_4\,e_0(n)+N_3\,e_1(n)+(N_3^2/N)\,e_2(n)+O(N_3^3/N^2), \tag{24}$$

where

$$e_0(n)=-\frac{\hbar^2 n}{8m_4}\int g_0(r)\,\nabla^2u(r)\,d\vec{r}+\frac{1}{2}n\int g_0(r)\,V(r)\,d\vec{r}, \tag{25}$$

$$\begin{aligned}e_1(n)=&-\frac{7}{3}\frac{\hbar^2 n}{8m_4}\int g_0^{(4,3)}(r)\,\nabla^2[u(r)+w(r)]\,d\vec{r}+n\int g_0^{(4,3)}(r)\,V(r)\,d\vec{r}\\&-\frac{\hbar^2 n}{8m_4}\int g_1^{(4,4)}(r)\,\nabla^2u(r)\,d\vec{r}+\frac{1}{2}n\int g_1^{(4,4)}(r)V(r)\,d\vec{r}-e_0(n),\end{aligned} \tag{26}$$

and

$$e_2(n) = -\frac{4}{3}\frac{\hbar^2 n}{8m_4}\int g_0^{(3,3)}(r)\,\nabla^2[u(r)+s(r)]\,d\vec{r} + \frac{1}{2}n\int g_0^{(3,3)}(r)\,V(r)\,d\vec{r} + \frac{\hbar^2 n}{8m_4}\int g_1^{(4,4)}(r)\nabla^2 u(r)\,d\vec{r}$$
$$-\frac{1}{2}n\int g_1^{(4,4)}(r)\,V(r)\,d\vec{r} - \frac{7}{3}\frac{\hbar^2 n}{8m_4}\int g_1^{(4,3)}(r)\,\nabla^2[u(r)+w(r)]\,d\vec{r} + n\int g_1^{(4,3)}(r)\,V(r)\,d\vec{r}$$
$$-\frac{\hbar^2 n}{8m_4}\int g_2^{(4,4)}(r)\,\nabla^2 u(r)\,d\vec{r} + \frac{1}{2}n\int g_2^{(4,4)}(r)\,V(r)\,d\vec{r} - e_1(n)\,; \qquad (27)$$

$e_0(n)$ is the ground-state energy per particle of pure liquid ^{4}He at density n. At zero concentration and zero pressure $e_1(n)$ becomes the chemical potential of a single ^{3}He atom in the mixture, and the fourth term, $O(N_3^3/N^2)$, is shown to be unimportant in Ref. 15. The variational calculation is carried out in three steps: (a) The correlation function, $u(r)$, for pure liquid ^{4}He is assumed to be known; (b) we consider the problem of one mass-3 boson in liquid ^{4}He. The trial wave function then reduces to

$$\psi_0^m(\vec{r}_1,\ldots,\vec{r}_{N-1};\vec{r}_N) = \psi_0^B(\vec{r}_1,\ldots,\vec{r}_N)\exp\left(\frac{1}{2}\sum_{i=1}^{N-1} w(r_{iN})\right). \qquad (28)$$

$w(r)$, $g_0^{(4,3)}(r)$, and $g_1^{(4,4)}(r)$ are then determined by minimizing $e_1(n)$; (c) Assuming that $w(r)$ has been fixed in step (b) we finally determine $s(r)$, $g_0^{(3,3)}(r)$, $g_1^{(4,3)}(r)$, and $g_2^{(4,4)}(r)$ by minimizing $e_2(n)$.

III. NUMERICAL RESULTS

A. Ground-state energy

The correlation functions of (4,3) particle pairs and (3,3) particle pairs can be expected to have the same form as $u(r)$. Therefore, for numerical calculations we choose the correlation difference functions, $w(r)$ and $s(r)$, as follows:

$$w(r) = -(a\sigma/r)^5 \qquad (29)$$

and

$$s(r) = -(c\sigma/r)^5\,, \qquad (30)$$

where a and c are variational parameters. We perform calculations of $e_1(n)$ and $e_2(n)$ by using $u(r)$, $S_0(k)$, $g_0(r)$, and $e_0(n)$ as determined by Schiff and Verlet[28] at number densities of $n = 0.0196$, 0.0207, and 0.0218 Å^{-3}. For $V(r)$ we use $\epsilon_0 = 10.22$ °K and $\sigma = 2.556$ Å,[31] where

$$V(r) = 4\epsilon_0[(\sigma/r)^{12} - (\sigma/r)^6]\,. \qquad (31)$$

The pressures corresponding to the three densities are calculated from the virial theorem.[15,32] The optimum values of the parameters (a, c), $e_1(n)$, and $e_2(n)$ are given in Table I.

It is convenient to express the ground state in terms of n_4 and n_3 (MWT's expression[13]) instead of n and n_3 in order to compare these results to the WTM theory.[10] The expression for the ground-state energy, Eq. (24), can be written in terms of n_4 and n_3 as

$$E_0^m(n_4,n_3) = N_4\,e_0(n_4) + N_3[e_1(n_4) + n_4\,e_0'(n_4)] + (N_3^2/N_4)\,[e_2(n_4) + n_4\,e_1'(n_4) + \tfrac{1}{2}n_4^2\,e_0''(n_4)] + O(N_3^3/N_4^2)\,, \qquad (32)$$

where

$$e_0'(n_4) = \frac{\partial e_0(n_4)}{\partial n_4}\,,$$

$$e_0''(n_4) = \frac{\partial^2 e_0(n_4)}{\partial n_4^2}\,,$$

and

$$e_1'(n_4) = \frac{\partial e_1(n_4)}{\partial n_4}\,. \qquad (33)$$

If we compare the ground-state energy expression, Eq. (32), with the MWT's expression[13], E_0^{MWT}, where

TABLE I. e_1 and e_2 by the present variational calculation. The optimum variational parameters, a and c, are calculated at three densities. The pressures corresponding to three densities are calculated by the virial theorem (Refs. 15 and 32).

Pressure (atm)	Variational parameters a	c	e_1 (°K)	e_2 (°K)
0	0.784	0.788	−2.59	0.62
4.6	0.784	0.788	−2.32	0.653
7.4	0.784	0.788	−2.04	0.95

$$E_0^{\mathrm{MWT}}(n_4,n_3)=N_4\,\varepsilon_0^{\mathrm{MWT}}(n_4)+N_3\,\varepsilon_1^{\mathrm{MWT}}(n_4)+(N_3^2/N_4)\,\varepsilon_2^{\mathrm{MWT}}(n_4,n_3)\,, \qquad (34)$$

the relations between $\varepsilon_i^{\mathrm{MWT}}$'s and e_i's, where $i=0$, 1, and 2, are given as [comparing Eq. (34) with Eq. (32)]

$$\varepsilon_0^{\mathrm{MWT}}(n_4)=e_0(n_4)\,,$$

$$\varepsilon_1^{\mathrm{MWT}}(n_4)=e_1(n_4)+n_4\,e_0'(n_4)\,,$$

and

$$\varepsilon_2^{\mathrm{MWT}}(n_4,n_3)=e_2(n_4)+n_4\,e_1'(n_4)+\frac{1}{2}n_4^2\,e_0''(n_4)+O(N_3/N_4)\,, \qquad (35)$$

where $\varepsilon_0^{\mathrm{MWT}}(n_4)$ is the binding energy of a ^{4}He atom in pure liquid ^{4}He, $\varepsilon_1^{\mathrm{MWT}}(n_4)$ is the chemical potential of a ^{3}He atom in the ^{3}He-^{4}He mixture at zero concentration, and $2\,\varepsilon_2^{\mathrm{MWT}}(n_4,n_3)|_{n_3=0}$ is the direct part of the long-wavelength effective interaction, V_0, between two ^{3}He quasi-particles,[15] as the concentration goes to zero. The pressure of pure liquid ^{4}He is given by

$$P_0=n_{40}^2\,\frac{\partial e_0(n_{40})}{\partial n_{40}} \qquad (36)$$

and it[15] can be shown that

$$m_4 s^2=\frac{\partial P_0}{\partial n_{40}}=n_{40}^2\,\frac{\partial^2 e_0(n_{40})}{\partial n_{40}^2}+2n_{40}\,\frac{\partial e_0(n_{40})}{\partial n_{40}}\,, \qquad (37)$$

and

$$\frac{\partial[e_1(n_{40})+n_{40}e_0'(n_{40})]}{\partial n_{40}}=(1+\alpha_0)\frac{m_4 s^2}{n_{40}}\,, \qquad (38)$$

where n_{40} and s are the number density and the sound velocity of pure liquid ^{4}He at pressure P_0, respectively. From Eqs. (36)-(38), we have

$$\varepsilon_1^{\mathrm{MWT}}(n_{40})=e_1(n_{40})+(P_0/n_{40})\,, \qquad (39)$$

and

$$\varepsilon_2^{\mathrm{MWT}}(n_{40})=e_2(n_{40})+(\tfrac{1}{2}+\alpha_0)m_4 s^2\,, \qquad (40)$$

where

$$\alpha_0=\frac{n_{40}}{m_4 s^2}\,\frac{\partial \varepsilon_1^{MWT}}{\partial n_{40}}-1\,. \qquad (41)$$

In Table II the results of the chemical potential at zero concentration, $\varepsilon_1^{\mathrm{MWT}}(n_{40})$, in the present calculation are shown and also compared with the results of $\varepsilon_1^{\mathrm{MWT}}(n_{40})$ by Ebner and Edwards[6] obtained from integrating Eq. (41) using experimental measurements[20-24] of α_0's, n_{40}, and s. The results for $\varepsilon_1^{\mathrm{MWT}}(n_{40})$ in the present calculation are in reasonable agreement with the results obtained by Ebner and Edwards[6] at the same pressures.

TABLE II. ε_1. EE are the result of Ebner and Edwards (Ref. 6). MWT is the result by Massey, Woo, and Tan (Ref. 13). YM are the results by the present variational calculation.

Pressure (atm)	ε_1 (°K) EE	MWT	YM
0	−2.785	−2.79	−2.59
4	−1.13	⋯	⋯
4.6	⋯	⋯	−0.69
6	−0.34	⋯	⋯
7.4	⋯	⋯	0.45
8	0.42	⋯	⋯

B. Pair distribution functions, $g^{(\alpha,\beta)}(r)$'s, and their Fourier transformations, $F^{(\alpha,\beta)}(k)$'s

The pair distribution functions, $g^{(\alpha,\beta)}(r)$'s, are obtained by using parameters, a and c, determined in steps (b) and (c). The pair distribution functions, $g^{(\alpha,\beta)}(r)$'s, and their Fourier transformations, $F^{(\alpha,\beta)}(k)$'s, at number density $n=0.0218$ Å^{-3} are shown in Figs. 1 and 2, respectively. These results [in particular, $F^{(4,3)}(k)$'s] are different from MWT's[13] and sum rule results of Woo, Tan and Wu,[14] i.e.,

$$\lim_{k\to 0} F_{\mathrm{MWT}}^{(4,3)}(k)|_{x=0}=F_{\mathrm{MWT}}^{(4,3)}(0)|_{x=0}=0 \qquad (42)$$

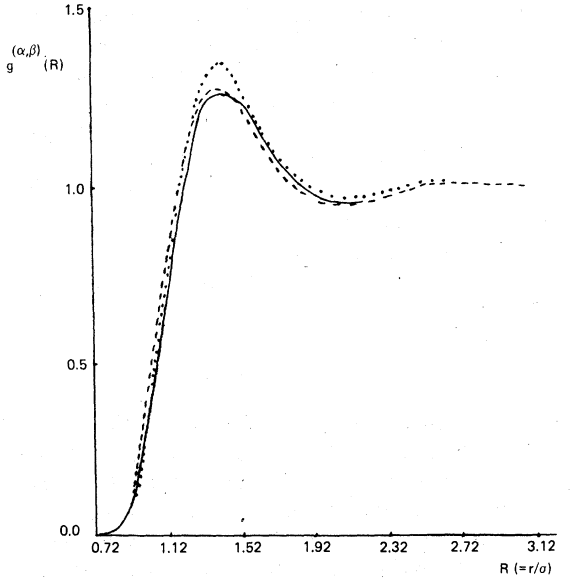

FIG. 1. ----, ——, and ...... are $g^{(4,4)}(R)$, $g^{(4,3)}(R)$, and $g^{(3,3)}(R)$, respectively, at zero concentration and $n=0.0218$ Å^{-3}.

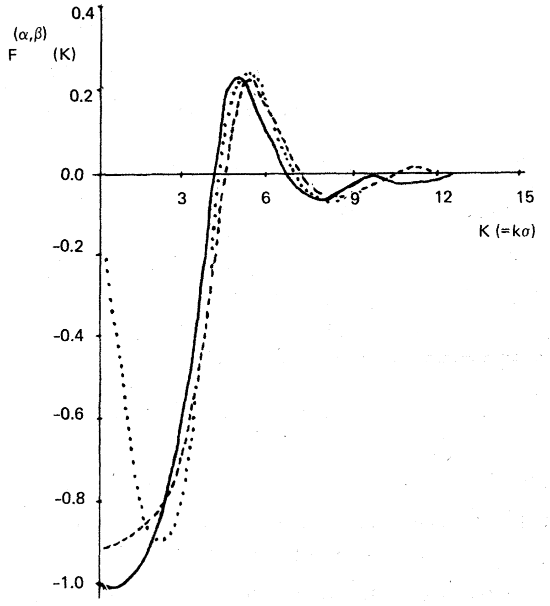

FIG. 2. ----, ——, and ...... are $F^{(4,4)}(K)$, $F^{(4,3)}(K)$, and $F^{(3,3)}(K)$, respectively, at zero concentration and $n = 0.0218$ Å^{-3}.

and

$$\lim_{k\to 0} F^{(4,3)}_{\mathrm{YM}}(k)\big|_{x=0} \neq F^{(4,3)}_{\mathrm{YM}}(0)\big|_{x=0} = 0\,, \tag{43}$$

where MWT and YM are the results of MWT[13] and the present variational calculation, respectively. Although figures are shown for $g^{(\alpha,\beta)}(r)$ and $F^{(\alpha,\beta)}(k)$ only at $n = 0.0218$ Å^{-3} (which corresponds to $P_0 = 7.4$ atm), we also obtained $g^{(\alpha,\beta)}(r)$'s and $F^{(\alpha,\beta)}(k)$'s at $n = 0.0196$ and 0.0207 Å^{-3} (which correspond to $P_0 = 0$ and 4.6 atm, respectively). From the Saam's result[4] and the WTM theory[10] it can be shown that

$$\lim_{k\to 0} F^{(4,3)}(k)\big|_{x=0} = -(1+\alpha_0) + z(n)\,,$$

and at $k = 0$

$$F^{(4,3)}(0) = 0 \tag{44}$$

for *a dilute-gas model of fermions in a Bose gas* [refer to Ref. 15 for the derivation of Eq. (44) and this relation may also hold for the ^{3}He-^{4}He mixture], where α_0 and $z(n)$ are the volume-excess parameter and a positive-definite function less than α_0, respectively. In the present variational calculation

$$\lim_{k\to 0} F^{(4,3)}(k)\big|_{x=0} = -1.00$$

at

$$n = 0.0218 \text{ Å}^{-3} \quad (P_0 = 7.4 \text{ atm}), \tag{45}$$

where the exact value of $F^{(4,3)}(k)\big|_{x=0}$, as k goes to zero, is *little larger than* -1.22 *at* $P_0 = 7.4$ *atm*. [See also Eq. (50) below.] This discrepancy probably comes from the neglect of long-range correlations in pure ^{4}He and the binary boson system.

Some confidence in the present $F^{(4,3)}(k)$'s comes from the following reason: In the WTM theory[10] the effective interaction induced by the phonon coupling at constant number density, $\overline{V}^{\mathrm{ph}}_k$, is given by

$$\overline{V}^{\mathrm{ph}}_k\Big|_{x=0} = \frac{\omega(k)\,[\varepsilon_0(k) + \omega_0(k)]^2\,[F^{(4,3)}(k)]^2}{2n\,s^{(4,4)}(k)\,[\varepsilon(k)^2 - \omega(k)^2]}\Bigg|_{x=0}\,, \tag{46}$$

where $\varepsilon_0(k)$, $\omega_0(k)$, $\varepsilon(k)$, and $\omega(k)$ are the excitation energies of a bare ^{3}He atom, a free phonon, a renormalized ^{3}He atom, and a renormalized phonon, respectively, which are given by

$$\varepsilon_0(k) = \hbar^2k^2/2m_3$$

and

$$\varepsilon(k) = \hbar^2k^2/2m + O(k^4)\,, \tag{47}$$

where m is the effective mass of a ^{3}He atom at zero concentration. The denominator of Eq. (46) at zero pressure becomes zero at $k = 1.68$ Å^{-1} and therefore it diverges at $k = 1.68$ Å^{-1}. But the first zero of $F^{(4,3)}(k)\big|_{x=0}$ at zero pressure is at $k = 1.68$ Å^{-1} and it makes the $\overline{V}^{\mathrm{ph}}_k\big|_{x=0}$ finite.

C. Volume excess parameters α_0's

The volume-excess parameter α_0 is defined by

$$v_m = v_p(1 + x\alpha_0), \tag{48}$$

where v_m and v_p are specific volumes of the mixture and pure liquid ^{4}He, respectively. We can estimate the ratio of effective volumes occupied by a ^{3}He atom and a ^{4}He atom by a method due to MWT.[13] α_0 is approximately given by

$$1 + \alpha_0 = [(2r_m^{(4,3)} - r_m^{(4,4)})/r_m^{(4,4)}]^3, \tag{49}$$

where $r_m^{(\alpha,\beta)}$ is the position of the first maximum in $g^{(\alpha,\beta)}(r)$. [Refer to Ref. 13 for the detail derivation.] α_0's obtained from Eq. (49) are very sensitive to the first maximums of pair distribution functions, $g_0(r)$ and $g_0^{(4,3)}(r)$, and are only expected to give approximate results as was pointed by MWT. Equation (41) yields a more accurate determination of α_0's, α_0's obtained from Eqs. (49) ($\equiv\alpha_{01}$) and (41) ($\equiv\alpha_{02}$) are shown in Table III along with MWT's[13] and experimental results.[22-24] Since in this calculation the long-range correlations were not included, Eq. (44) may be redeter-

TABLE III. Volume excess parameter α_0. Expt. are the experimental results (Refs. 22–24). MWT is the result by Massey, Woo, and Tan (Ref. 13). YM are the results obtained from the present variational calculation.

			α_0		
Pressure				YM	
(atm)	Expt.	MTW	α_{01}	α_{02}	α_{03}
0	0.284	0.33	0.193	0.237	0.236
4.6	0.24	...	0.191	...	0.171
7.4	0.22	...	0.192	...	0.194

TABLE IV. Effective mass. Expt. is the experimental result by Anderson *et al.* (Ref. 19). WTM is the theoretical result by Woo, Tan, and Massey (Ref. 10). YM are the present results by neglecting phonon renormalization.

Pressure		m/m_3		
(atm)	Expt.	WTM	DF	YM
0	2.34	1.85[a] 2.37[b]	1.99	1.65
4.6	...	...	...	1.84
7.4	...	...	...	1.89

[a] Result by neglecting phonon renormalization.
[b] Result by including phonon renormalization.

mined by

$$\lim_{k\to 0} F^{(4,3)}(k)/F_0(k)^2\,\big|_{x=0} \approx -(1+\alpha_0) \ , \qquad (50)$$

where

$$F_0(k) = n \int [g_0(r) - 1]\, e^{i\vec{k}\cdot\vec{r}}\, d\vec{r}$$

and we take $\lim_{k\to 0} F_0(k) = -0.9237$, -0.9647, and -0.915 at $n = 0.0196$, 0.0207, and 0.0218 Å^{-3}, respectively.[28] α_0's by Eq. (50) ($\equiv \alpha_{03}$) are shown in the same table.

D. Effective mass of one ^{3}He atom at zero concentration

The effective mass of a ^{3}He quasiparticle at zero concentration is calculated by neglecting the phonon renormalization process in WTM's results.[10] The approximate expression is then

$$\frac{m}{m_3} = \left[1 - \frac{n_4}{6\pi^2} \int dk\, k^2 \frac{[F^{(4,3)}(k)]^2}{n^2[S^{(4,4)}(k) + m_3/m_4]}\right]^{-1} \qquad (51)$$

where m is the effective mass of ^{3}He atom at zero concentration. Present results are shown in Table IV. These results are comparable to those of Woo, Tan, and Massey,[10] and Davison and Feenberg.[12] The present results also have the correct pressure dependence. (The effective mass of a ^{3}He atom increases as the pressure increases.[23])

E. Long-wavelength effective interaction V_0 at constant pressure

V_0, the long-wavelength effective interaction of two ^{3}He quasiparticles, at constant pressure and zero concentration is given by

$$V_0 = \frac{2\varepsilon_2^{\mathrm{MWT}}(n_{40})}{n_{40}} - (1+\alpha_0)^2 \frac{m_4 s^2}{n_{40}} \ .$$

(Refer to Ref. 15.) Numerical results by the present variational calculation and the further corrections by the paired-phonon analysis[15] are shown and compared with other results in Table V. The present result at $P_0 = 0$ agrees well with Emery's result.[2] V_0's have the same pressure dependences as in other theories.[1,5] (V_0 increases as the pressure increases.) V_0 in the present calculation should be a lower bound to the actual V_0. The proof for this is as follows: $\varepsilon_2^{\mathrm{MWT}}(n_{40})$ in Eq. (40) becomes larger (or smaller) as $\varepsilon_1^{\mathrm{MWT}}(n_{40})$ in Eq. (39) becomes smaller (or larger).[15] Therefore, $V_0(n_{40})$'s in the present calculation are lower bounds since $\varepsilon_1^{\mathrm{MWT}}(n_{40})$'s in the present calculation are upper bounds. Furthermore, the k dependences of this effective interaction V_k near 7.4

TABLE V. Long-wavelength effective interaction V_0. The result by Emery is from Ref. 2. BE is the result by Baym and Ebner (Ref. 3). KE is the result by Kuenhold and Ebner (Ref. 9). Corr. is the correction by the paired-phonon analysis (Ref. 15); we use the same values at three pressures as at $P_0 = 7.4$ atm. YM are the results of the present calculation using experimental values of $\alpha_0^2 m_4 s^2$ (Ref. 7).

Pressure			$n_{40}V_0$ (°K)		
(atm)	Emery	BE	KE	Corr.	YM
0	−1.2	−1.75	−1.94	−0.11	−0.96[a] −1.07[b]
4.6	...	...	...	−0.11	−0.694[a] −0.804[b]
7.4	...	...	...	−0.11	−0.1[a] −0.21[b]

[a] Present variational calculation.
[b] Lower bound, sum of a and Corr.

atm are qualitatively in agreements with those of Landau *et al.*[23] obtained from fitting the osmotic-pressure data. From results of Landau *et al.*[23] V_k should be a concave function for small k above about 7.4 atm instead of a monotonic increasing function as in the theory of Bardeen, Baym, and Pines[1] and a monotonic increasing function for small k below about 7.4 atm, where

$$V_k=\left(\frac{2\varepsilon_2^{\mathrm{MWT}}(n_{40})}{n_{40}}-(1+\alpha_0)^2\frac{m_4s^2}{n_{40}}+\frac{\omega(k)[\varepsilon_0(k)+\omega_0(k)]^2[F^{(4,3)}(k)]^2}{2n_{40}S^{(4,4)}(k)[\varepsilon(k)^2-\omega(k)^2]}\right.$$
$$\left.+(1+\alpha_0)^2\frac{m_4s^2}{n_{40}}(1-\delta_{\vec{k},0})-\frac{1}{2}\frac{\varepsilon_0(k)F^{(3,3)}(k)}{n_{40}}\right)\Bigg|_{x=0}\,. \qquad (52)$$

In order to render the effective interaction induced by the phonon coupling at constant pressure, V_k^{ph}, continuous at $k=0$, $\overline{V}_k^{\mathrm{ph}}$ should be

$$\lim_{k\to 0}\overline{V}_k^{\mathrm{ph}}\big|_{x=0}=-(1+\alpha_0)^2m_4s^2/n_{40}. \qquad (53)$$

(Refer to Ref. 15.) This effective interaction by the present calculation can be used to interpret the solubility as a function of pressure measured by Watson *et al.*[22] and Landau *et al.*[23] Here, we give only a qualitative interpretation: The maximum solubilities can be determined by

$$\mu_{3p}=\left[\varepsilon_1^{\mathrm{MWT}}+\varepsilon(k_F)+n_3V_0\right.$$
$$\left.-\frac{1}{4\pi^2}\int_0^{2k_F}\left(1-\frac{k}{2k_F}\right)k^2V_k\,dk\right]\Bigg|_{x=x_m}, \qquad (54)$$

where k_F is the Fermi wave vector, and μ_{3p} and x_m are, respectively, the chemical potential of a ^{3}He atom in pure liquid ^{3}He and the maximum solubility of ^{3}He atoms in the liquid ^{4}He at $P=P_0$. In this calculation V_k as for small k is a negatively decreasing function for $P_0=7.4$ atm. This qualitatively explains the solubility curves by Watson *et al.*[22] and Landau *et al.*[23]

IV. CONCLUSION

The results of the present calculation agree well with those of other phenomenological theories[2,6] except for the volume-excess parameters α_0's. To obtain accurate results for the α_0's the chemical potentials of a ^{3}He quasiparticle at zero concentration, $\varepsilon_1^{\mathrm{MWT}}$'s, have to be determined more accurately along with ^{4}He-atom densities. The wave function, Eq. (11), is not, of course, the exact boson-type ground-state wave function of the Hamiltonian H^m Eq. (5). Therefore, in order to use the present variational calculation as the input information of the WTM theory[10] the WTM theory[10] has to be slightly modified. Instead of the procedure outlined above for V_0 we consider corrections induced by the paired-phonon analysis.[15] From Eq. (53) of the argument the difference between this system at constant pressure and at constant number density comes from $F^{(4,3)}(k)$, i.e.,

$$\lim_{k\to 0}F^{(4,3)}(k)\big|_{P_0,x=0}=F^{(4,3)}(0)\big|_{P_0,x=0}$$

and

$$\lim_{k\to 0}F^{(4,3)}(k)\big|_{n,x=0}\neq F^{(4,3)}(0)\big|_{n,x=0}=0. \qquad (55)$$

where P_0 and n denote the results at constant pressure and at constant number density, respectively.

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