

Variational theory of binary boson mixture at  $T = 0$  K

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We present a general formalism for the ground state of binary boson mixtures where the Jastrow-type ground-state wave function is optimized by solving the Euler-Lagrange equations in the hypernetted-chain scheme. This method is expected to provide more accurate information for the binary boson systems compared to the methods currently available. For the isotopic  $T\uparrow$ - $H\uparrow$  mixture, complete phase separation in its ground state is observed.

During the last few years, the study of the low-temperature properties of a stable bulk spin-oriented atomic hydrogen and its isotopes ( $H\uparrow$ ,  $D\uparrow$ , and  $T\uparrow$ ) has received much attention.<sup>1,2</sup> It has been predicted<sup>2</sup> that because of the small mass and weak interaction,  $H\uparrow$  system will be a Bose gas with a quantal behavior much more pronounced than that in <sup>4</sup>He.  $D\uparrow$  is expected to be a Fermi gas, while  $T\uparrow$  will be a self-bound liquid very much like <sup>4</sup>He. Should it be possible to make these systems available for a long period they could be utilized for several interesting experiments.

One of the possible experiments is the mixture of  $H\uparrow$  and its isotopes with <sup>4</sup>He or mixture of these species with each other. While the earlier works<sup>3</sup> on binary boson mixtures centered around the "isotopic mixture," Miller<sup>4</sup> has recently analyzed the ground-state properties of both isotopic and nonisotopic mixtures of  $H(H\uparrow$ -<sup>4</sup>He,  $H\uparrow$ - $T\uparrow$ ). In these calculations Miller used the "average correlation approximation" (ACA), which at given pressure and concentration restricts the correlation functions for different pairs of particles so that they are the same. Using this approximation and the Lennard-Jones form of interac-

tion, the energy equation for binary boson system was mapped onto an equivalent single-boson problem. Even if these approximations are quite successful in describing the ground-state properties of some binary boson systems, this simple choice of wave functions might not be appropriate in all cases. In fact, a more general approach would be to allow for different correlations for different pairs of particles and to use, whenever available, the exact form of interaction potentials. Some years ago, Campbell initiated such a study<sup>5</sup> formally in the "paired phonon analysis" scheme.

In this paper, we wish to develop such a general approach where the Jastrow-type ground-state wave function is optimized by solving the Euler-Lagrange equation in the hypernetted-chain (HNC) scheme. Our method is essentially a generalization of a prudent method, originally proposed<sup>6-8</sup> for the one-component Bose systems.

We assume that a system of homogeneous mixture of two types of bosons (type 1 and type 2), with the total number of particles  $N(N = N_1 + N_2)$  in a box of volume  $\Omega$  is described by the Hamiltonian

$$H = -\frac{\hbar^2}{2m_1} \sum_{i=1}^{N_1} \Delta_i - \frac{\hbar^2}{2m_2} \sum_{i=1}^{N_2} \Delta_i + \sum_{i < j}^{N_1} v_{11}(r_{ij}) + \sum_{i < j}^{N_2} v_{22}(r_{ij}) + \sum_{\substack{i=1, N_1 \\ j=1, N_2}} v_{12}(r_{ij}) ,$$

where  $v_{\alpha\beta}(r)$  represents the interactions between the three particle pairs (11), (22), and (12). For  $H\uparrow$  and its isotopes this is given very accurately by Kolos and Wolniewicz.<sup>9</sup> As a trial function we choose

$$\Psi(\bar{r}_{1,1} \cdots \bar{r}_{1,N_1}; \bar{r}_{2,1} \cdots \bar{r}_{2,N_2}) = \exp \frac{1}{2} \left[ \sum_{i < j}^{N_1} u_{11}(|\bar{r}_{1,i} - \bar{r}_{1,j}|) + \sum_{i < j}^{N_2} u_{22}(|\bar{r}_{2,i} - \bar{r}_{2,j}|) + \sum_{\substack{i=1, N_1 \\ j=1, N_2}} u_{12}(|\bar{r}_{1,i} - \bar{r}_{2,j}|) \right] , \quad (1)$$

with  $u_{\alpha\beta}(r)$  as the correlation functions between the three particle pairs. In terms of  $\Psi$ , three types of pair-distribution functions can be defined as

$$g_{\alpha\beta}(r) = \frac{N_\alpha(N_\beta - \delta_{\alpha\beta})}{\rho_\alpha\rho_\beta} \frac{\int \Psi^2 d\vec{r}(i_\alpha, i_\beta)}{\int \Psi^2 d\vec{r}_1 \cdots d\vec{r}_N}, \quad (2)$$

where  $d\vec{r}(i_\alpha, i_\beta)$  denotes  $d\vec{r}_1 \cdots d\vec{r}_N$  with  $d\vec{r}_{i_\alpha}$  and  $d\vec{r}_{i_\beta}$  omitted, and  $\rho_\alpha$  is the partial density of the species  $\alpha$  ( $\rho_\alpha = N_\alpha/\Omega$ ). Defining the concentration of the species  $\alpha$  as  $x_\alpha = \rho_\alpha/\rho$ ,  $\rho$  is the total density of the system and the energy per particle is

$$E = x_1^2 E_{11} + x_2^2 E_{22} + 2x_1 x_2 E_{12}, \quad (3)$$

where

$$E_{\alpha\beta} = \frac{1}{2} \rho \int g_{\alpha\beta}(r) \tilde{v}_{\alpha\beta}(r) d\vec{r}, \quad (4)$$

$$E_{\alpha\beta} = \frac{\hbar^2 \rho}{8m_{\alpha\beta}} \int \frac{1}{g_{\alpha\beta}(r)} [\nabla g_{\alpha\beta}(r)]^2 d\vec{r} + \frac{1}{2} \rho \int g_{\alpha\beta}(r) v_{\alpha\beta}(r) d\vec{r} - \frac{\hbar^2 \rho}{8m_{\alpha\beta}} \frac{\delta_{\alpha\beta}}{(2\pi)^3 \rho_\alpha \rho_\beta} \int \left[ S_{\alpha\beta}(k) [S_{\alpha\beta}(k) - 3] - \frac{S_{\gamma\gamma}}{D(k)} + S_{\alpha\gamma}^2(k) + 3 \right] k^2 d\vec{k}. \quad (8)$$

It is, however, to be noted that, due to the insertion of the coupled equation (6) in (3),  $E_{\alpha\beta}$  in (8) are not  $E_{\alpha\beta}[g_{\alpha\beta}]$ , as they are in Eq. (4). In Eq. (8),  $\alpha \neq \gamma$ ,  $D(k) = S_{11}(k) \cdot S_{22}(k) - S_{12}^2(k)$ , and  $S_{\alpha\beta}(k)$  are the Fourier transforms of  $g_{\alpha\beta}(r)$ . Then the condition for Eqs. (3) and (8) to be minimum with respect to arbitrary variations of  $g_{\alpha\beta}(r)$  is

$$\left[ -\frac{\hbar^2}{m_{\alpha\beta}} \Delta + v_{\alpha\beta}(r) + W_{\alpha\beta}(r) \right] g_{\alpha\beta}^{1/2}(r) = 0, \quad (9)$$

with the "induced potentials"  $W_{\alpha\beta}(r)$  given in the momentum space by

$$W_{\alpha\alpha}(k) = -\frac{\hbar^2 k^2}{4\rho_\alpha} \left[ \frac{1}{m_\alpha} \left[ 2S_{\alpha\alpha}(k) - 3 \right] + \frac{S_{\beta\beta}^2(k)}{D^2(k)} + \frac{1}{m_\beta} \frac{S_{\alpha\beta}^2(k)}{D^2(k)} \right],$$

$$W_{\alpha\beta}(k) = -\frac{\hbar^2 k^2}{4\sqrt{\rho_\alpha \rho_\beta}} \left[ 2m_{\alpha\beta}^{-1} S_{\alpha\beta}(k) - \frac{S_{\alpha\beta}(k)}{D^2(k)} \times \left( \frac{S_{\beta\beta}(k)}{m_\alpha} + \frac{S_{\alpha\alpha}(k)}{m_\beta} \right) \right]. \quad (10)$$

In Eq. (10),  $W_{\alpha\beta}(k) = W_{\beta\alpha}(k)$ ,  $\alpha \neq \beta$ . From Eqs. (3) and (8) the pressure equation in the HNC scheme can readily be obtained<sup>6,8</sup> by  $p = \rho^2 (\partial E / \partial \rho)_{x_1}$ .

We have solved Eqs. (9) and (10) for the isotopic T $\uparrow$ -H $\uparrow$  mixture. The prime reason for our choice of

and the effective interaction

$$\tilde{v}_{\alpha\beta}(r) = v_{\alpha\beta}(r) - \frac{\hbar^2}{4m_{\alpha\beta}} \Delta u_{\alpha\beta}(r), \quad (5)$$

$$m_{\alpha\beta}^{-1} = 0.5(m_\alpha^{-1} + m_\beta^{-1}).$$

Introducing the HNC equation for binary boson mixture<sup>6</sup>

$$u_{\alpha\beta}(r) = \ln g_{\alpha\beta}(r) - [g_{\alpha\beta}(r) - 1] + c_{\alpha\beta}(r), \quad (6)$$

with  $C_{\alpha\beta}(r)$  given in the momentum space as

$$S_{\alpha\beta}(k) - \delta_{\alpha\beta} = C_{\alpha\beta}(k) + \sum_{\gamma=1,2} [S_{\alpha\gamma}(k) - \delta_{\alpha\gamma}] C_{\gamma\beta}(k), \quad (7)$$

Eq. (3) can be rewritten as

this system is that, in the density range needed for this mixture, our method is presumably very accurate. Besides, the interaction potential is very accurately known. The numerical procedure is the linearization method discussed at length in Ref. 8, modified properly for the present case. The computational maneuver is quite intricate though not formidable. In Fig. 1, we show the enthalpy as a function of H $\uparrow$

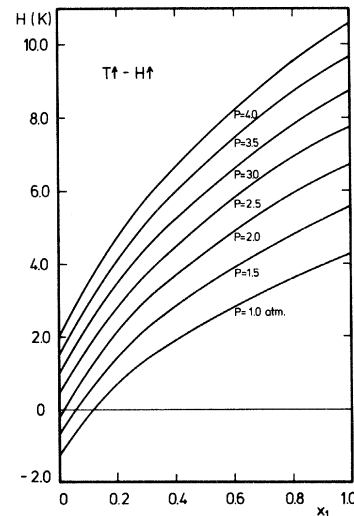


FIG. 1. Enthalpy (K) as a function of H $\uparrow$  concentration for the isotopic T $\uparrow$ -H $\uparrow$  mixture.

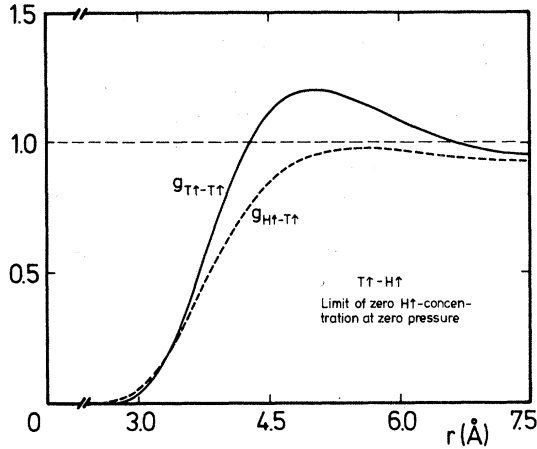


FIG. 2. Radial distribution functions  $g_{\alpha\beta}(r)$  for  $T\uparrow$ - $H\uparrow$  mixture in the zero- $H\uparrow$ -concentration limit.

concentration for various pressures. In all cases, the curvature is negative implying complete separation of the system in its ground state. In the ACA scheme, Miller<sup>4</sup> also observed complete phase separation for various Lennard-Jones binary boson mixtures. However, because of more flexibility of the correlation functions and correct asymptotic behavior of the distribution functions due to optimization, the present method might prove to be very useful for a detailed study of the ground state of binary boson mixture.

Lastly, we have also studied the zero-concentration limit to calculate the value of the initial slope  $\eta$  of the ground-state energy  $\eta = 2(E_{12} - E_{22})$  and the separation energy  $\epsilon_0$  of a single  $H\uparrow$  atom in  $T\uparrow$ . In the limit  $x_1 \rightarrow 0$ , Eq. (9) decouples and the various  $g_{\alpha\beta}(r)$  can be calculated consecutively. For a single impurity atom,<sup>4</sup>  $x_1 \rightarrow 0$ ,

$$W_{22}(k) = -\frac{\hbar^2 k^2 (S_{22} - 1)^2 (2S_{22} + 1)}{4m_2 \rho_2 S_{22}^2},$$

$$W_{12}(k) = -\frac{\hbar^2 k^2 S_{12} (S_{22} - 1)}{4m_2 \rho_2 S_{22}^2} (2m_1^{-1} m_2 S_{22} + 1). \quad (11)$$

The results for  $T\uparrow$ - $H\uparrow$  mixture in the zero- $H\uparrow$ -concentration limit are given in Fig. 2, while  $\eta$  and  $\epsilon_0$  are given in Table I. The latter value can be compared with that obtained from Baym's equation (Ref. 10),  $\epsilon_0^B = E + T(m_2/m_1 - 1)$ ;  $E$ ,  $T$ , and  $m_2$  being respectively total energy, kinetic energy, and mass of  $T\uparrow$  and  $m_1$  is the  $H\uparrow$  mass. In Table I we also give the results for  ${}^3\text{He}(\text{Bose})$ - ${}^4\text{He}$  mixture in the zero-

TABLE I. Separation energy of an impurity atom in the bulk medium  $\epsilon_0$ ;  $\epsilon_0^B$  obtained from Baym's equation (Ref. 10) and the initial slope of the ground-state energy  $\eta$  at zero pressure.

System	$\rho$ ( $\text{\AA}^{-3}$ )	$\epsilon_0^B$ (K)	$\epsilon_0$ (K)	$\eta$ (K)
${}^3\text{He}$ - ${}^4\text{He}$ <sup>a</sup> $x_{{}^3\text{He}} \rightarrow 0$	0.0176	-1.82	-2.25	3.0
$T\uparrow$ - $H\uparrow$ $x_{H\uparrow} \rightarrow 0$	0.0056	8.42	5.78	8.26
$T\uparrow$ - $H\uparrow$ <sup>b</sup> $x_{H\uparrow} \rightarrow 0$	0.0058	9.69	7.40	10.68
$H\uparrow$ - ${}^4\text{He}$ <sup>c</sup> $x_{H\uparrow} \rightarrow 0$	0.0172	-	37.0	42.0

<sup>a</sup>Experimental results,  $\epsilon_0 = -2.78$  K,  $\eta = -0.312$  K.

<sup>b</sup>Results for Lennard-Jones interaction.

<sup>c</sup>Reference 4.

${}^3\text{He}$ -concentration limit. The third row is the result for the Lennard-Jones fit<sup>2</sup> of  $T\uparrow$ - $H\uparrow$  interaction. In the last row, we give the results<sup>4</sup> for  $H\uparrow$ - ${}^4\text{He}$  for comparison.

The radial distribution functions in the zero-concentration limit has found use in an interesting study of the binding<sup>11</sup> of  $H\uparrow$  and its isotopes to the free surface of  ${}^4\text{He}$ . This study has a direct effect on the future measurements on these new quantum systems. However, in the face of large difference between the experimental result<sup>12</sup> and the theoretical estimates, attempts should be made to develop a general formalism, much in the same way as we present here for the bulk medium.

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