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Structure of a model one-dimensional liquid ^{3}He–^{4}He mixture

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Abstract

We study the ground state properties of a one-dimensional liquid ^{3}He–^{4}He mixture interacting via a hard-core repulsive potential at zero temperature. We use the self-consistent field approach to calculate the ground state partial structure factors, the effective interactions between the species, and collective modes. Our results are in qualitative agreement with more sophisticated approaches. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

Ng and Singwi [1] in a series of papers have studied a model Fermi liquid interacting via a hard-core repulsive potential within the self-consistent field approach. This simple model remarkably reproduced some key features of both the normal and spin-polarized liquid ^{3}He providing insight into the nature of strongly coupled Fermi systems. These calculations along with some earlier reports [2] have shown that the self-consistent field method of Singwi, Tosi, Land, and Sjölander (STLS) [3] which was originally devised to treat the short-range correlation effects in Coulomb liquids is also capable of handling systems interacting via short-range potentials. We have recently extended the approach of Ng and Singwi [1] to study a boson–fermion mixture and found that our results are in good qualitative agreement with realistic ^{3}He–^{4}He mixtures [4].

In this work we apply the self-consistent field method of Ng and Singwi [1] to a boson–fermion mixture interacting via a repulsive hard-core potential in a one-dimensional (1D) system. Our main motivation is to study the 1D liquid ^{3}He–^{4}He mixture since a dilute solution of ^{3}He atoms in liquid ^{4}He form a fascinating quantum liquid as an example of interacting boson–fermion mixture [5]. There has been some experimental interest in 1D quantum liquids following the suggestion [6] and subsequent realization [7,8] of confining He in carbon nanotubes. On the theoretical side, the ground state properties of 1D liquid ^{4}He have recently been investigated by the variational hypernetted-chain calculations [9] and quantum Monte Carlo methods [10,11].

Our primary aim in this Letter is to see how well the ground state properties of a one-dimensional boson–fermion mixture, and in particular liquid ^{3}He–^{4}He mixtures are described within the STLS approximation scheme and a simple model interaction. For this

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purpose we employ a hard-core repulsive potential. Even though the model potential is far too simplistic our approach is microscopic in that the realistic helium potential can be incorporated. The self-consistent field method (or the STLS approximation) renormalizes the bare hard-core potentials to yield reasonable ground state structure factors. We find that the STLS method provides a reasonable qualitative description of liquid ^{3}He–^{4}He mixtures which may be useful in the analysis of static and dynamical properties. Static structure factors and collective modes can be qualitatively correctly described by a simple hard-core interaction model.

2. Model and theory

The two-component generalization of the STLS theory is based on the approximation that the fluctuations in the density (of a given component) within the linear response theory is written as $\delta n_\alpha(q,\omega) = \sum_\beta \chi_{\alpha\beta}(q,\omega) V_\beta^{\rm ext}$, where $\tilde{\chi}$ is the density–density response matrix, and $V_\alpha^{\rm ext}$ is the external perturbing field. In the self-consistent field approach of Singwi et al. [3] the response of the system to an external potential is expressed as

$$\delta n_\alpha = \chi_\alpha^0(q,\omega)\left[V_\alpha^{\rm ext} + \sum_\beta V_{\alpha\beta}^{\rm eff}(q)\delta n_\beta\right], \tag{1}$$

where $\chi_\alpha^0(q,\omega)$ is the response of the non-interacting αth component. Combining the above equations, we obtain the STLS expression for the density–density response function of the two-component system $\chi_{\alpha\beta}^{-1}(q,\omega) = [\chi_\alpha^0(q,\omega)]^{-1}\delta_{\alpha\beta} - V_{\alpha\beta}^{\rm eff}(q)$. The effective interparticle interactions within the STLS scheme are related to the pair-distribution functions $g_{\alpha\beta}(z)$ by [1,2]

$$V_{\alpha\beta}^{\rm eff}(z) = -\int_z^\infty dz'\, g_{\alpha\beta}(z')\frac{dV}{dz'}, \tag{2}$$

where $V(z)$ is the bare potential which we take to be the same between all species. We consider a hard-core potential of the form $V(z) = V_0\,\theta(a_0 - z)$, where a_0 is the hard-core radius and V_0 is the strength of the potential (for purely hard-core potential, we let $V_0 \to \infty$). The Fourier transform of the effective potential is $V_{\alpha\beta}^{\rm eff}(q) = 2\,V_0 g_{\alpha\beta}(a_0)\sin(qa_0)/qa_0$. We determine the unknown quantities $g_{\alpha\beta}(a_0)$, using the pair-distribution functions

$$g_{\alpha\beta}(z) = 1 + \frac{1}{(n_\alpha n_\beta)^{1/2}} \times \int \frac{dq}{2\pi}\, e^{iqz}\left[S_{\alpha\beta}(q) - \delta_{\alpha\beta}\right], \tag{3}$$

in which the static partial structure factors are expressed in terms of the fluctuation–dissipation theorem

$$S_{\alpha\beta}(q) = -\frac{1}{\pi(n_\alpha n_\beta)^{1/2}}\int_0^\infty d\omega\, \chi_{\alpha\beta}(q,i\omega), \tag{4}$$

where $\chi_{\alpha\beta}(q,\omega)$ are the density–density response functions. Choosing $r = a_0$ in the above equations one obtains a set of non-linear equations for the unknown quantities $V_0 g_{\alpha\beta}(a_0)$ which are the multi-component generalization of the similar expressions considered by Ng and Singwi [1]. The self-consistent field method has the same general structure as the random-phase approximation (RPA) with bare interactions replaced by effective interactions.

3. Results and discussion

We now specialize to a 1D system of two-component (boson–fermion) mixture. The total number of particles in the sample with length L is given by $N = N_B + N_F$, in terms of the number of bosonic and fermionic particles, and the corresponding particle density is $N/L = n = n_B + n_F$. Denoting the fraction of fermions in the mixture by x, we have $n_F = xn$ and $n_B = (1-x)n$. We scale all lengths by the hard-core radius a_0, and the energies by the effective Rydberg $1/(2\mu a_0^2)$ (we take $\hbar = 1$) where $\mu = m_F m_B/(m_F + m_B)$ is the reduced mass. For convenience the density is expressed in terms of $n_0 = 1/(2a_0)$. For fermions in the mixture we also define the Fermi wave vector $k_F a_0 = (\pi/4)x(n/n_0)$.

We have solved the above set of equations for the unknown parameters $V_0 g_{\alpha\beta}(a_0)$ in the limit $V_0 \to \infty$ (purely hard-core potential) for various densities n/n_0, and fermion fraction x. We illustrate our results for $x = 0.05$ (dotted lines) and $x = 0.1$ (solid lines) in Fig. 1. The density dependence of $V_0 g_{\alpha\beta}(a_0)$ is smooth and shows a broad peak around $n/n_0 \sim 0.7$. Although at low density all coefficients $V_0 g_{\alpha\beta}(a_0)$

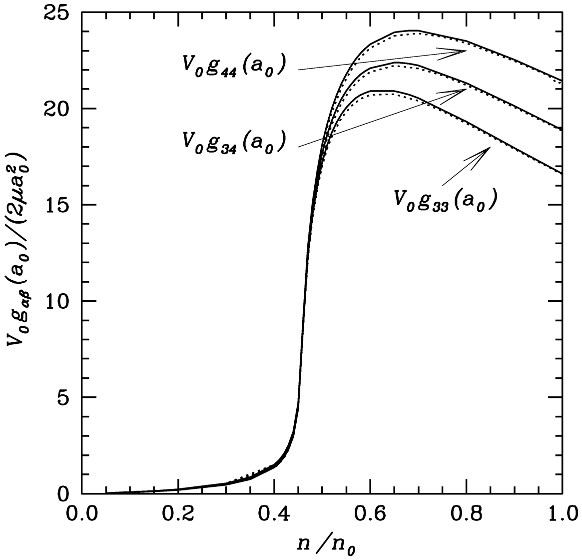

Fig. 1. The density dependence of the coefficients $V_0 g_{\alpha\beta}(a_0)$ for a strictly hard-core potential ($V_0 \to \infty$) at the ^{3}He mole fraction $x = 0.05$ (dotted lines) and $x = 0.1$ (solid lines).

seem to vanish, around the peak region we have $V_0 g_{44}(a_0) > V_0 g_{34}(a_0) > V_0 g_{33}(a_0)$. An interesting observation is that the behavior of $V_0 g_{\alpha\beta}(a_0)$ is largely independent of the ^{3}He mole fraction in the range $0.001 < x < 0.1$. In our previous calculations [4] for higher-dimensional systems, we had found noticeable x-dependence. To relate our dimensionless results to the physical situation, we take $a_0 \approx 2.2$ Å and obtain $n_0 \approx 0.23$ Å^{-1}. Using the recent Monte Carlo simulations [10,11] and hypernetted-chain [9] calculation results we take the equilibrium density to be $n = 0.036$ Å^{-1} which gives $n/n_0 = 0.16$ for the density of the liquid mixture. On the other hand, the crystallization density is not precisely defined. The peak region in Fig. 1 indicates the development of an ordered phase as we shall show in the following. Thus, we use $n/n_0 = 0.16$ and 0.7 to describe the liquid and more ordered phases, respectively.

In Fig. 2 we show our results for the static structure factors $S_{\alpha\beta}(q)$ for the ^{3}He–^{4}He mixture. The general behavior of the structure factors at $x = 0.05$ and at two different densities $n/n_0 = 0.16$ and 0.7 are depicted in Figs. 2(a) and (b), respectively. We observe that at the equilibrium density the mixture appears to be rather structureless, a behavior quite different than

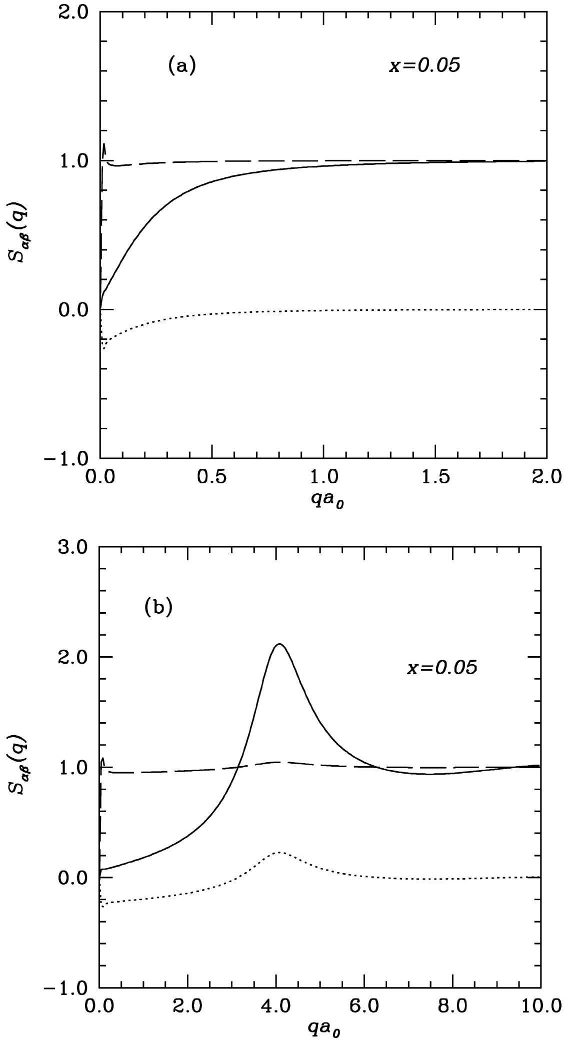

Fig. 2. (a) The partial static structure factors for liquid ^{3}He–^{4}He mixture at $x = 0.05$ and $n/n_0 = 0.16$. The solid, dashed, and dotted lines indicate $S_{44}(q)$, $S_{33}(q)$, and $S_{34}(q)$, respectively. (b) The same for $n/n_0 = 0.7$.

the situation in 3D. Structure builds up as the system moves towards a more ordered phase, a large peak in $S_{44}(q)$ develops around $qa_0 \approx 4$. When we compare our results for $S_{\alpha\beta}(q)$ with those of Krotscheck and Miller [9] we find reasonable qualitative agreement, which shows that the basic features of 1D helium mixtures may be qualitatively understood within a simple hard-core interaction model. We note, however, that the calculations of Krotscheck and Miller [9]

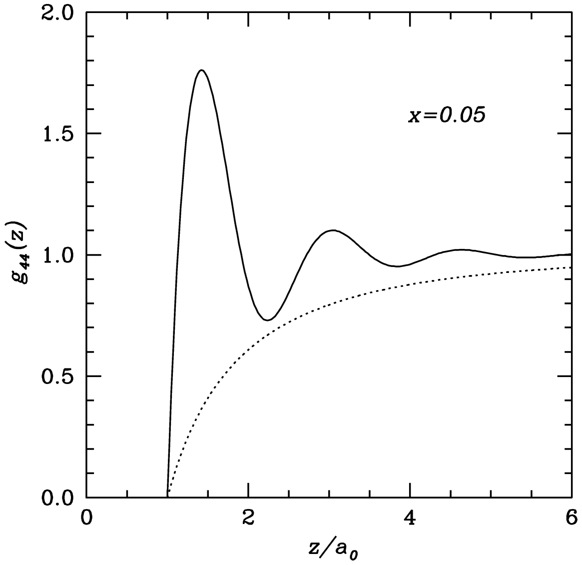

Fig. 3. The partial pair-distribution function $g_{44}(z)$ in a 1D liquid ^{3}He–^{4}He mixture at $x = 0.05$. The solid and dotted lines indicate $n/n_0 = 0.7$ and 0.16, respectively.

pertain to a single ^{3}He impurity in a fluid of ^{4}He particles. Furthermore, the weak x-dependence of the coefficients $V_0 g_{\alpha\beta}(a_0)$ suggests that the structure factors in 1D helium mixtures will not depend strongly on the ^{3}He concentration, again a situation rather different than in 3D.

Fig. 3 displays the pair-distribution function $g_{44}(z)$ at two different densities. At the equilibrium density ($n/n_0 = 0.16$) the $g_{44}(z)$ is a monotone function without any oscillatory character. As the density is increased, oscillations in the pair-distribution function set in. The overall behavior of $g_{44}(z)$ is similar to the case in pure ^{4}He as calculated by Krotscheck and Miller [9] and Boninsegni and Moroni [10].

The collective excitations are determined by solving for the roots of the determinant of the dynamic response matrix

$$
\begin{aligned}
1 &- V_{33}^{\mathrm{eff}}(q)\chi_3^0(q,\omega) - V_{44}^{\mathrm{eff}}(q)\chi_4^0(q,\omega) \\
&+ \left[V_{33}^{\mathrm{eff}}(q)V_{44}^{\mathrm{eff}}(q) - \left(V_{34}^{\mathrm{eff}}(q)\right)^2\right] \\
&\times \chi_3^0(q,\omega)\chi_4^0(q,\omega) = 0. \qquad (5)
\end{aligned}
$$

We analyze the collective excitations of the liquid ^{3}He–^{4}He mixture within the mean-spherical approximation [5] (MSA) for the ^{3}He component, which is known to yield reliable results in 3D. In the MSA, the particle–hole continuum and the collective mode of a Fermi system (described by the usual Lindhard function) is replaced by a single effective collective mode excitation. More specifically, the non-interacting response of ^{3}He atoms is given by

$$
\chi_{3,\mathrm{MSA}}^0(q,\omega) = \frac{2n_3\epsilon_q^{(3)}}{(\omega + i\eta)^2 - [\epsilon_q^{(3)}/S_0(q)]^2}, \qquad (6)
$$

where $\epsilon_q^{(3)} = q^2/2m_3$ and $S_0(q)$ is the Hartree–Fock static structure factor. Using the response function of the non-interacting Bose systems given by

$$
\chi_4^0(q,\omega) = \frac{2n_4\epsilon_q^{(4)}}{(\omega + i\eta)^2 - [\epsilon_q^{(4)}]^2}, \qquad (7)
$$

in Eq. (5), we obtain the collective mode energies

$$
\begin{aligned}
\omega_{1,2}(q) = \Bigg[&\frac{1}{2}(\psi_{33} + \psi_{44}) \\
&\pm \frac{1}{2}\left[(\psi_{33} - \psi_{44})^2 + 4\psi_{34}\right]^{1/2}\Bigg]^{1/2}, \qquad (8)
\end{aligned}
$$

where $\psi_{33} = [\epsilon_q^{(3)}/S_0(q)]^2 + 2n_3\epsilon_q^{(3)}V_{33}^{\mathrm{eff}}$, $\psi_{44} = [\epsilon_q^{(4)}]^2 + 2n_4\epsilon_q^{(4)}V_{44}^{\mathrm{eff}}$, and $\psi_{34} = 2n_3\epsilon_q^{(3)}2n_4\epsilon_q^{(4)} \times [V_{34}^{\mathrm{eff}}]^2$. We note that free-particle energies $\epsilon_q^{(4)} = q^2/2m_4$ for the ^{4}He component are used in the non-interacting Bose response function, unlike the Feynman spectrum which contains the structure factor in the single-particle dispersion relation. The MSA is similar to the binary-boson approximation [12] in which the ^{3}He response function $\chi_3^0(q,\omega)$ is approximated by the Bogoliubov form as for ^{4}He component. In Fig. 4 we show the collective modes within the MSA for liquid ^{3}He–^{4}He mixture at $x = 0.05$, and three different densities. We find two discrete modes which may be associated with the ^{3}He and ^{4}He components. At equilibrium density, the collective modes have free-particle like character. This is mainly because at $n/n_0 = 0.16$, the effective interactions are very small. Such a behavior for 1D liquid ^{4}He was also noted by Krotscheck and Miller [9]. As the density increases a phonon–roton (pr) branch corresponding to ^{4}He atoms (upper curves), and a second branch corresponding to ^{3}He atoms (lower curves) develop. These modes in the small q region can be identified as zeroth and second sound modes associated with the collective ^{3}He and ^{4}He excitations, respectively [5]. The ^{3}He excitations at higher density show a dip similar to the

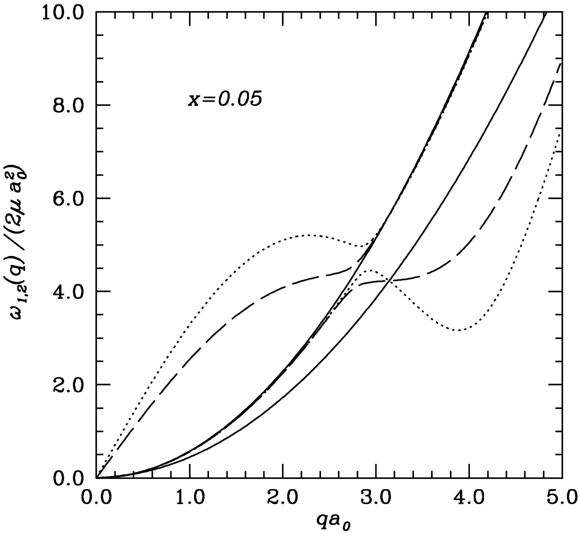

Fig. 4. The collective modes of a 1D liquid ^{3}He–^{4}He mixture at $x = 0.05$ and $n/n_0 = 0.16$ (solid lines), $n/n_0 = 0.5$ (dashed lines), and $n/n_0 = 0.7$ (dotted lines).

roton minimum which can be regarded as a mode coupling effect. It is expected that relaxing the MSA and using the 1D Lindhard function for $\chi_3^0(q,\omega)$ in solving the collective mode equation, will not affect our results for small q.

It is important to note that a weak attactive interaction can lead to a dimerized phase of ^{3}He atoms as first pointed out by Bashkin [13]. Our purely repulsive interaction model does not consider this possibility. A more elaborate approach using HNC approximation by Krotscheck and Miller [9] shows the formation of bound state of two ^{3}He atoms in the liquid mixture.

4. Summary

We have extended the model Fermi liquid interacting with hard-core repulsive potential problem of Ng and Singwi [1] to a mixture of boson–fermion system in 1D. The self-consistent field method with this model interaction is capable of describing qualitatively the main static and dynamic properties of 1D liquid ^{3}He–^{4}He mixtures. We have found that the overall properties of the mixture are reasonably well accounted for in the range of densities describing a liquid phase in equilibrium and a high density ordered phase. Interestingly, the structure factors show very little dependence on the ^{3}He concentration. The collective modes of the mixture show rather different behavior depending on the density which would be interesting to explore experimentally.

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