Model boson fluid with disorder in the self-consistent field approximation

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Abstract

We study the ground-state properties of a model neutral boson fluid in the presence of disorder effects. The effective interaction between the bosons is obtained through the self-consistent field method which renormalizes the bare interaction consisting of a hard-core repulsive potential with an attractive tail at zero temperature. We introduce disorder effects within a number-conserving approximation by modifying the density–density response function. Our results for the static structure factor and the collective mode dispersion reflect the effect of disorder in qualitative agreement with other calculational approaches. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

Boson systems at low temperature in the presence of disorder effects is a subject of continuing interest [1]. The physical systems studied range from liquid ^{4}He in Vycor and aerogel [2], flux lines in superconductors in the presence of impurities [3], Josephson junction arrays [4] to granular films [5]. Recent experiments [6, 7] on liquid ^{4}He in porous media have focused on the collective excitations presenting a wealth of information on the static and dynamic properties of disordered Bose systems. Theoretical efforts to understand the effects of disorder on neutral Bose systems employed Monte Carlo simulations [8–10] and perturbation theory methods [11–14]. In these calculations, the phase diagram and elementary excitations are studied for lattice and continuum systems.

To understand the ground-state properties of Bose and Fermi liquids with hard-core interactions, simple models were introduced and studied within the self-consistent field approach [15,16]. The model calculations remarkably reproduced some key features of both the normal and spin-polarized liquid ^{3}He and superfluid liquid ^{4}He providing insight into the nature of strongly coupled quantum liquids. These calculations have shown that the self-consistent field method of Singwi, Tosi, Land, and Sjölander [17] (STLS) which was originally developed to treat the short-range correlation effects in Coulomb liquids (interacting via the long-range $1/r$ potential) is also capable of handling systems interacting via short-range potentials. A qualitative agreement was found between the calculated and the experimental results. Recently, Nafari and Doroudi [18] have used the realistic inter-atomic potential to study the ground state properties of liquid

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[3]He (in three and two dimensions) within the STLS scheme, improving the level of agreement with experiments.

In this work we apply the self-consistent field method of Lobo [15] and Ng and Singwi [16] to a boson liquid interacting via a repulsive hard-core and an attractive tail potential at zero temperature. We also include the effects of disorder in a phenomenological way within a number conserving approximation [19]. Our main motivation is to qualitatively understand the interplay between the interaction and weak disorder effects in neutral Bose fluids. More specifically, our aim is to see how well the ground-state properties of a hard-core boson fluid with weak disorder are described within the STLS approximation scheme. For this purpose we employ a hard-core repulsive potential with an attractive tail and treat the disorder effects in a number-conserving approximation. In the numerical calculations we specialize to disordered liquid [4]He. Even though the model potential is far too simplistic our approach is microscopic in that the realistic helium potential can be incorporated as was done in the previous works [18]. The self-consistent field method (or the STLS approximation) renormalizes the bare hard-core potential to yield reasonable ground state structure factor. We also study the effect disorder on the collective excitation modes. We find that the self-consistent field method provides a reasonable qualitative description of disordered liquid [4]He which may be useful in the analysis of static and dynamical properties.

The rest of this Letter is organized as follows. In the next section we outline the formulation of the self-consistent field method in application to a disordered boson fluid. In Section 3 we specialize to the liquid [4]He and present our results for the static structure factor and collective excitation mode. We discuss our results in relation to other theoretical works and experiments in the same section, and conclude with a brief summary.

2. Model and theory

The dynamic susceptibility in the generalized random-phase approximation is given by

$$\chi(q, \omega) = \frac{\chi_0(q, \omega)}{1 - V_{\text{eff}}(q)\chi_0(q, \omega)}, \tag{1}$$

where $\chi_0(q, \omega)$ describes the response of the noninteracting system and $V_{\text{eff}}(q)$ is the effective interaction, yet to be determined. When disorder is introduced to the system, the density fluctuations described by $\chi_0(q, \omega)$ are modified. We use the particle number conserving approximation developed by Mermin [19] to replace $\chi_0(q, \omega)$ by $\chi_0(q, \omega; \gamma)$, given by

$$\chi_0(q, \omega; \gamma) = \frac{(\omega + i\gamma)\chi_0(q, \omega + i\gamma)}{\omega + i\gamma \chi_0(q, \omega; \gamma)/\chi_0(q, 0)}, \tag{2}$$

where γ is a phenomenological disorder parameter. It may be interpreted as the broadening or damping arising from impurity scattering.

The effective inter-particle interactions within the STLS scheme are related to the pair-distribution functions $g(r)$ through [15,16]

$$V^{\text{eff}}(r) = -\int_r^\infty dr' \, g(r') \frac{dV}{dr'}, \tag{3}$$

where $V(r)$ is the bare potential which we take to be

$$V(r) = \begin{cases} V_0, & r < a_0, \\ -\epsilon, & a_0 < r < a_1, \\ 0, & a_1 < r, \end{cases} \tag{4}$$

consisting of a hard-core and an attractive tail. Here V_0 is the strength of the potential (which will be taken as $V_0 \to \infty$ for purely hard-core), a_0 is the hard-core radius, ϵ and a_1 are the depth and width of the attractive potential well, respectively. Adding an attractive well to the model potential is important to obtain the salient features of helium liquids. The Fourier transform of the effective potential is given by

$$\begin{aligned} V^{\text{eff}}(q) &= \frac{4\pi}{q^3}(V_0 + \epsilon)g(a_0) \\ &\quad \times \left[\sin(qa_0) - qa_0\cos(qa_0)\right] \\ &\quad - \frac{4\pi}{q^3}\epsilon g(a_1)\left[\sin(qa_1) - qa_1\cos(qa_1)\right]. \end{aligned} \tag{5}$$

We determine the unknown quantities $g(a_0)$ and $g(a_1)$, using first the fluctuation–dissipation theorem

$$S(q) = -\frac{1}{\pi n}\int_0^\infty d\omega \, \chi(q, i\omega; \gamma), \tag{6}$$

in which $\chi(q, \omega; \gamma)$ is the density–density response function including the disorder effects evaluated at

imaginary frequencies and then the Fourier transform relation

$$g(r) = 1 + \frac{1}{n} \int \frac{d\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} [S(q) - 1]. \qquad (7)$$

Choosing $r = a_0$ and $r = a_1$ in the above equations we obtain two coupled nonlinear equations for the unknown quantities $(V_0 + \epsilon)g(a_0)$ and $\epsilon g(a_1)$. The self-consistent field method has the same general structure as the random-phase approximation (RPA) with bare interactions replaced by effective interactions. Because the effective interactions are purely static, and self-energy effects are not inserted in the response functions, the model does not include multi-particle effects.

3. Results and discussion

We now specialize to the system of liquid ^{4}He with disorder effects. Although the model we use may appear to be simple it is expected give give us insight into the ground-state properties of neutral Bose fluids in the presence of weak disorder. We scale all lengths by the hard-core radius a_0, and the energies by the energy unit $E_0 = 1/(2ma_0^2)$ (we take $\hbar = 1$ throughout the Letter). In the attractive tail of the pair-potential we take $\epsilon = 5$ K and $a_1/a_0 = 2$. For convenience the density is expressed in terms of $n_0 = 3/(4\pi a_0^3)$.

We have solved the above set of equations for the unknown parameters $(V_0 + \epsilon)g(a_0)$ and $\epsilon g(a_1)$ in the limit $V_0 \to \infty$ (purely hard-core potential) for various densities and and values of the disorder parameter γ. We illustrate our results for $\gamma = 0$, 5, and 10 in Fig. 1. The density dependence of $(V_0 + \epsilon)g(a_0)$ is smooth and shows a broad peak around $n/n_0 \sim 0.8$. We also observe that $(V_0 + \epsilon)g(a_0)$ rapidly decreases as the density is lowered. The disorder dependence, on the other hand, appears to be nonuniform. The parameter $\epsilon g(a_1)$ shown in Fig. 1(b) displays a stronger dependence on disorder. We relate our dimensionless results to the physical situation of disordered liquid ^{4}He by taking $a_0 \approx 2.2$ Å and obtain $n_0 \approx 0.0224$ Å^{-3} which is close to the equilibrium density. Thus, physical quantities calculated for the densities $n/n_0 \sim 0.8$–1.1 should be reasonable when comparison with experiments is made. Furthermore, a typical value of

$\gamma = 10 E_0$ yields $\gamma \approx 1.3$ meV for the strength of disorder, close in magnitude in experimental situations.

In Fig. 2 we show our results for the static structure factor $S(q)$ for the clean and disordered liquid. We note that an overall reduction in $S(q)$ occurs when disorder is introduced. The disorder effects are most visible in the peak region around $qa_0 \approx 5.5$. Such behavior should be observable in neutron scattering experiments. Qualitatively similar results in the static structure factor were also found in the path-integral Monte Carlo simulations by Boninsegni and Glyde [10]. We have also checked that the peak height in $S(q)$ increases with increasing density but the position of the peak remains unchanged. The reduction in $S(q)$ remains for other values of density.

Once the parameters $(V_0 + \epsilon)g(a_0)$ and $\epsilon g(a_1)$ are known we obtain the resulting effective interaction $V^{\text{eff}}(q)$ within our model. The interesting feature is that the bare hard-core potential $(V_0 \to \infty)$ is renormalized within the self-consistent field approximation to yield a soft-core and an attractive part. The self-consistent treatment of the disorder effects further change the overall magnitude of the effective interaction. Our calculations show that the concentration dependence of V^{eff} is not very strong.

The collective excitation mode is determined by solving for the root of the denominator of the dynamic response function

$$1 - V^{\text{eff}}(q)\chi_0(q, \omega; \gamma) = 0, \qquad (8)$$

which yields

$$\omega_q = \left(\epsilon_q^2 + 2n\epsilon_q V^{\text{eff}}(q) - \gamma^2/4\right)^{1/2} - i\gamma/2, \qquad (9)$$

where $\epsilon_q = q^2/2m$ is the free-particle energy. The most notable feature of the collective mode dispersion given above is the fact that disorder gives rise to damping. That is, ω_q acquires an imaginary part for any finite value of γ. The collective mode becomes overdamped below a critical value of wave vector q_c, which may be determined by the solution of $\epsilon_q^2 + 2n\epsilon_q V^{\text{eff}}(q) - \gamma^2/4 = 0$. For a clean system $(\gamma = 0)$ the collective mode dispersion coincides with the Feynman excitation spectrum $\omega_q = \epsilon_q/S(q)$. When disorder is introduced, the situation changes and Feynman spectrum notion does not apply. In Fig. 3 we show the collective mode dispersion at the equilibrium density $n/n_0 = 1$, for $\gamma = 0$ and 10.
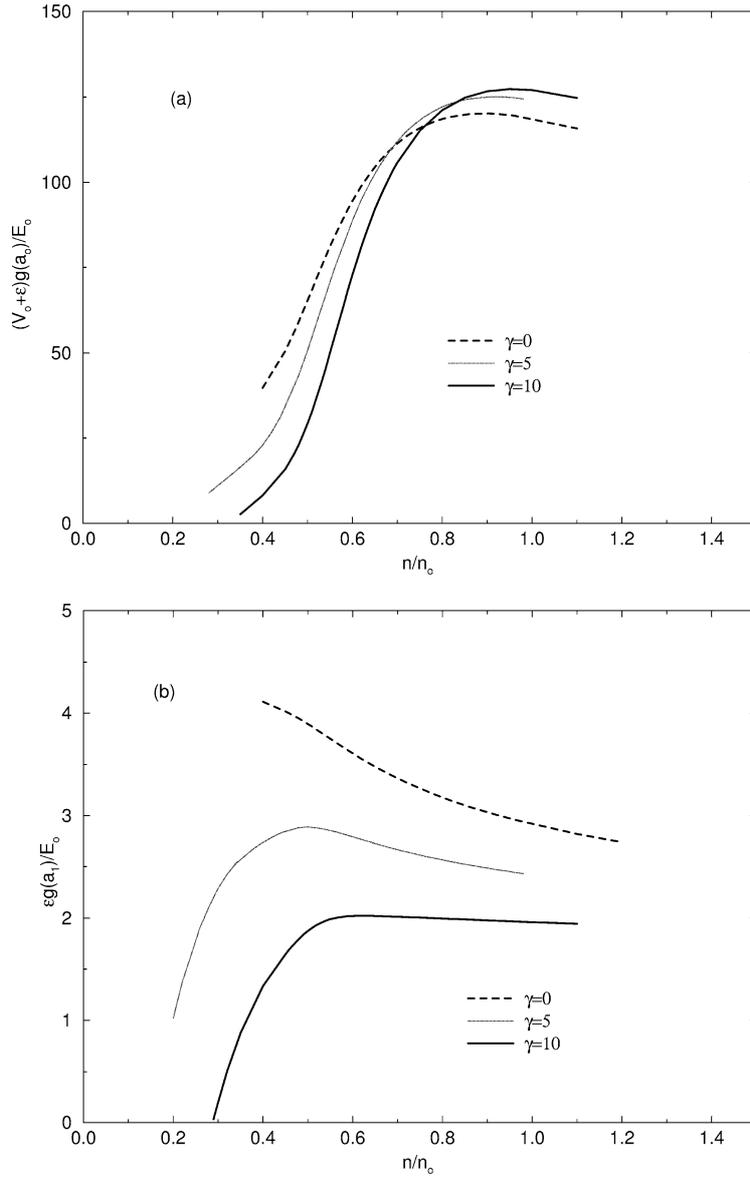
Fig. 1. The density dependence of the coefficients (a) $(V_0 + \epsilon)g(a_0)$ and (b) $\epsilon g(a_1)$ for a hard-core potential with attractive tail ($V_0 \to \infty$) at different levels of disorder.

It is clear that the collective mode ceases to exist below the critical wave vector q_c. The situation here is similar to the occurrence of damping in electron systems when disorder effects are treated within the same number-conserving approximation [20]. Path integral Monte Carlo simulations [10] did not explore

the long-wavelength region to observe the vanishing of ω_q. In the remaining parts of the collective mode dispersion, the disorder appears to lower the roton minimum considerably, but leaves the maxon region largely unaffected. We point out that the attractive tail in the bare interaction modifies the dispersion relation
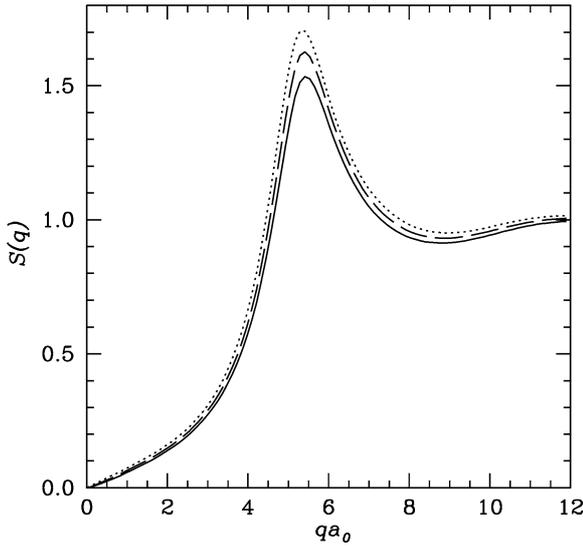
Fig. 2. The static structure factor for liquid ^{4}He at $n/n_0 = 1$. The solid, dashed, and dotted lines indicate the disorder parameter $\gamma/E_0 = 10,\ 5$, and 0, respectively.

Fig. 3. The collective mode dispersion for a clean and disordered liquid ^{4}He at $n/n_0 = 1.0$. The dotted and solid lines indicate $\gamma/E_0 = 0$ and 10, respectively.

slightly, around the roton minimum in the upper curve and beyond the dip structure in the lower curve. The roton effective mass calculated from the curvature of the dispersion relation around the roton minimum is $m^*/m \sim 0.2$ for a clean system [16] and we find a similar value for the disordered system ($\gamma = 10$) at $n/n_0 = 1$. In the experiments of Dimeo et al. [6] roton effective mass was measured to be very close to that in bulk helium. We also calculate the density of states of the collective mode using $D(\omega) = \sum_q \delta(\omega - \omega_q)$. A straightforward calculation yields

$$D(\omega) = \frac{1}{n(2\pi)^3} \sum_i \frac{q_i^2}{|df(q_i)/dq|}, \qquad (10)$$

where $f(q) = \omega - \omega_q$, and q_i are the roots of $f(q) = 0$. Fig. 4 shows $D(\omega)$ as a function of frequency for a clean and a disordered system. The two peaks in $D(\omega)$ correspond to the maxon and roton regions where the dispersion relation ω_q change its curvature. The location of the maxon peak appearing at higher energies is not affected by disorder. The roton peak, on the other hand, moves toward the low energy side, when disorder is introduced.

To see the effect of interactions and disorder on the condensate within our model, we employ the Bogoliubov theory. The condensate fraction is given
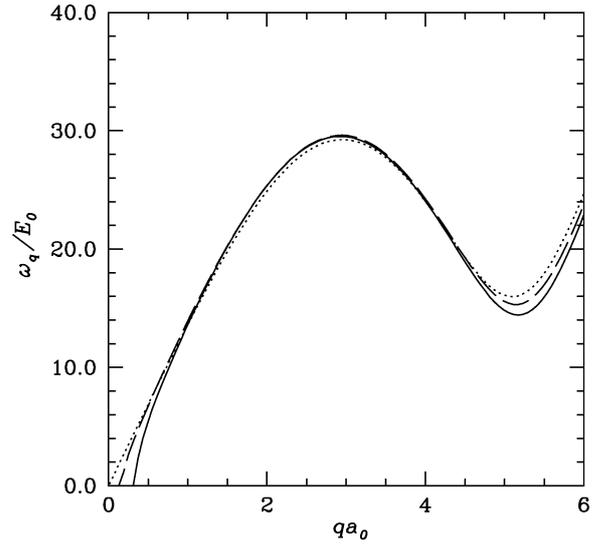
by the expression

$$\begin{aligned} 1 - \frac{n_C}{n} \\ = \frac{1}{n} \sum_{k \neq 0} \left\{ \frac{n_C V^{\text{eff}}(k) + k^2/2m}{(n_C k^2 V^{\text{eff}}(k)/m + (k^2/2m)^2)^{1/2}} - 1 \right\}, \end{aligned} \qquad (11)$$

where n_C is the number of condensed atoms. We solve the above expression for n_C/n for various values of n and disorder parameter γ, and our results are tabulated in Table 1. We find that about 23% of the atoms are in the condensate when $\gamma = 0$. If we compare this with the experimental results in liquid ^{4}He, given the crudeness of our model, we conclude that there is a reasonable agreement. As the degree of disorder is increased, n_C/n slightly decreases. In various other calculations such as disordered Bose–Hubbard model [13,14] similar trends for the condensate fraction has been observed.

In this work we have extended the model Bose liquid interacting with hard-core repulsive potential and an attractive tail problem to include disorder effects. The self-consistent field method for this model interaction and disorder effects taken into account within a number conserving scheme describes qualitatively the main static and dynamic properties of liquid ^{4}He
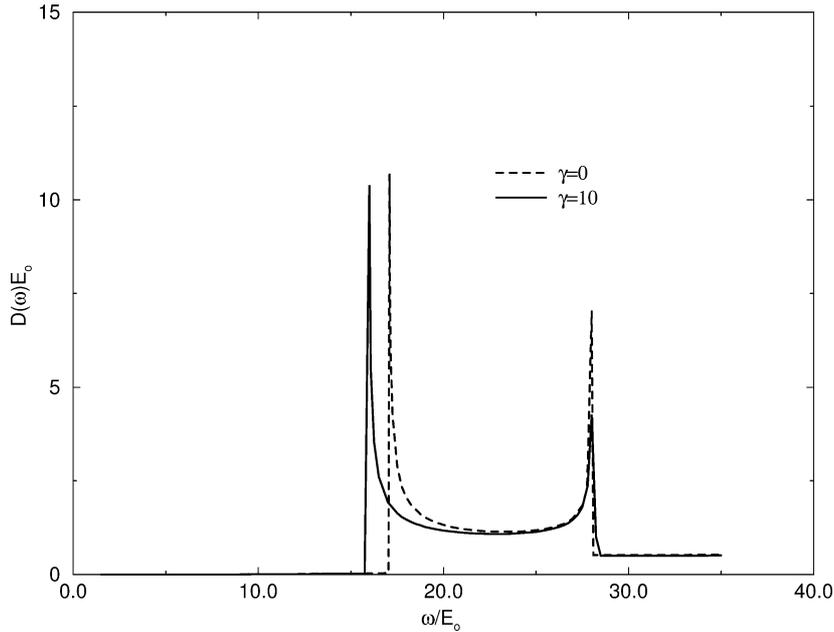
Fig. 4. The density of states for the collective mode $D(\omega)$ as a function of energy, for a clean and disordered system. The dashed and solid lines indicate $\gamma/E_0 = 0$ and 10, respectively.

Table 1
The condensate fraction n_C/n for clean and disordered systems at various densities n/n_0

n/n_0	0.8	1.0	1.1
$(n_C/n)_{\gamma=0}$	0.225	0.227	0.233
$(n_C/n)_{\gamma=5}$	0.218	0.218	0.230
$(n_C/n)_{\gamma=10}$	0.217	0.213	0.218

in disordered media. We have found that the quantities such as the static structure factor and collective mode dispersion are significantly affected by the presence of disorder. Some of our results are in qualitative agreement with other theoretical calculations and experimental results. Our calculations of the ground state properties of disordered liquid ^{4}He can be extended into several directions. The multi-particle effects are not taken into account within the present approach. Although the static properties are little affected, the dynamic properties such as $S(q, \omega)$ are not fully represented. Using the self-energy insertions in the response functions, it should be possible to extend the present approach to include multi-particle effects. Finally, as our calculations demonstrate that even a hard-core potential can be treated within the STLS scheme, it would be interesting to use the realistic two-body interaction potentials between the helium atoms to make better contact with the experimental results. We expect the model calculations provided in this Letter will find interesting applications in other disordered Bose liquids.

Acknowledgements

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