Correlation effects on the static structure factor of a Bose gas

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A theoretical treatment of the static structure factor $S(k)$ of a Bose gas is attempted. The low order expansion theory is implemented for the construction of the two body density distribution, while various trial functions for the radial distribution function $g(r)$ are used. $g(r)$ introduces the atomic correlations and describes the departure from the noninteracting gas. The Bose gas is studied as inhomogeneous one, trapped in harmonic oscillator well, as well as homogeneous. A suitable parametrization of the various trial functions $g(r)$ exists which leads to satisfactory reproduction of the experimental values of $S(k)$, both in inhomogeneous case as well as in homogeneous one. The phonon range behavior of the calculated $S(k)$ is also addressed and discussed both in finite and infinite Bose gas.

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I. INTRODUCTION

Spectroscopic studies have been used to assemble a complete understanding of the structure of atoms and simple molecules [1]. The static structure factor $S(k)$ is a fundamental quantity, which is connected with the atomic structure, and it is the Fourier transform of the radial distribution function $g(r)$. $S(k)$ gives the magnitude of the density fluctuation in the system (atomic, molecular, electronic or nuclear system) at wavelength $2\pi/k$, where $k$ is the momentum transfer. In recent papers, the Bragg spectroscopic method was used to measure $S(k)$ either in the phonon regime [1] or/and in the single-particle regime [2].

More specifically, the character of excitations in a weakly interacting Bose-Einstein condensed gas depends on the relation between the wave vector of the excitation $k$ and the inverse healing length $\xi^{-1} = \sqrt{2mc_s/\hbar} = \sqrt{8\pi a\rho}$, which is the wave vector related to the speed of Bogoliubov sound $c_s = \sqrt{\mu/m}$, where $\mu = 4\pi\hbar^2 a\rho/m$ is the chemical potential, $a$ is the scattering length, $\rho$ is the condensate density, and $m$ is the atomic mass [1,3]. There are two different regimes of excitation described by the Bogoliubov theory for the zero-temperature weakly interacting Bose-Einstein condensate: the phonon and the free-particle regimes. For small wave vectors ($k \ll \xi^{-1}$), the gas responds collectively and density perturbations propagate as phonons at the speed of Bogoliubov sound. For large wave vectors ($k \gg \xi^{-1}$) the excitations are particle-like with a quadratic dispersion relation [1,3].

In the present letter we focus on the theoretical calculation of $S(k)$ of a Bose gas. All the calculations are performed in the zero-temperature limit ($T = 0$). Various types of trial functions $g(r)$ are used and the entailed $S(k)$ are compared with the experimental data. The correlation parameters of $g(r)$ are determined by fit to the experimental data. The theoretical investigation is performed by applying two approaches. In the first approach, the Bose gas is treated as inhomogeneous gas, which is exactly the case of the experiments [2,1]. We consider that the Bose gas is trapped in a harmonic oscillator well with condensate radius $R$. In the second approach, the trapped bose gas is treated, in a rough approximation, as homogeneous gas in regard to its elementary excitations. This approximate treatment is reasonable in the sense that the coherence length $\xi$ satisfies the condition $\xi \ll R$ [4]. Actually in the experiments of Refs. [1,2] this condition is well satisfied.

As mentioned before, the key quantity of the above approaches, is the radial distribution function $g(r)$, which describes the relative probability for finding two particles at a distance $r$ apart and consequently it introduces the atomic correlations. In general, the function $g(r)$ can be calculated by the variational method [5]. However, in dilute Bose gas, in the framework of the lowest-order cluster expansion, trial expressions for $g(r)$ can be used [5-7] and the parameters can be fitted to reproduce the experimental data of $S(k)$. Up to now, $S(k)$ in a trapped Bose gas, is predicted successfully (compared to the experimental data) by the local density approximation [8,2].

The motivation of the present work is the theoretical study of $S(k)$, considering the Bose gas as a many-body system. It is well known that the ideal Bose gas model (noninteracting model) fails to reproduce the experimental values of $S(k)$. We focus our treatment on the effect of interatomic interaction on the properties of $S(k)$, both in small and large values of the momentum transfer $k$. It is fundamental to investigate how these effects modify the picture of $S(k)$ of an ideal gas and to predict values consistent with the experimental data. The possibility of linear behavior of $S(k)$ for small $k$, both in inhomogeneous and homogeneous Bose gas has also been examined. In section 2 we treat the inhomogeneous Bose gas while the case of homogeneous Bose gas is investigated in section 3.
II. INHOMOGENEOUS BOSE GAS

A dilute inhomogeneous Bose gas can be studied using the low-order approximation (LOA) [5–7]. In the LOA the two-body density distribution (TBDD) has the form

\[ \rho(r_1, r_2) = C \rho(r_1) \rho(r_2) f^2(r_{12}) = C \rho(r_1) \rho(r_2) g(r_{12}), \]  

where \( f(r_{12}) \) (\( r_{12} = r = |r_1 - r_2| \)) is the Jastrow correlation function [6], \( g(r_{12}) \) is the radial distribution function, \( C \) is the normalization factor which ensures that \( \int \rho(r_1, r_2) d\mathbf{r}_1 d\mathbf{r}_2 = N(N-1) \) (\( N \) is the number of the atoms of the Bose condensate) and \( \rho(r) \) is the density distribution (DD) of the system. The TBDD is proportional to the probability of simultaneously finding an atom at \( r_1 \) and another at \( r_2 \). In the uncorrelated case (noninteracting gas) the TBDD takes the simple form

\[ \rho(r_1, r_2) = \frac{N-1}{N} \rho(r_1) \rho(r_2). \]  

In the present work we consider that the atoms are confined in a harmonic oscillator trap where the ground state single-particle wave function \( \psi_0(r) \) has the form

\[ \psi_0(r) = \frac{N^{1/2}}{\pi^{3/4} b^{3/2}} \exp[-r^2/(2b^2)], \quad b = [\hbar/(m\omega)]^{1/2}. \]

The normalization of the DD is \( \int |\rho(r)|^2 d\mathbf{r} = \int |\psi_0(r)|^2 d\mathbf{r} = N \).

The static structure factor \( S(k) \), in a finite system, is defined as [8]

\[ S(k) = 1 + \frac{1}{N} \int e^{i \mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}_2)} [\rho(\mathbf{r}_1, \mathbf{r}_2) - \rho(\mathbf{r}_1) \rho(\mathbf{r}_2)] d\mathbf{r}_1 d\mathbf{r}_2 \]  

(3)

or using Eq. (1)

\[ S(k) = 1 + \frac{1}{N} \int e^{i \mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}_2)} \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) [C g(r_{12}) - 1] d\mathbf{r}_1 d\mathbf{r}_2 \]  

(4)

The integration in Eq. (4) can be performed if the function \( g(r) \) is known. \( g(r) \) must obey the rules \( g(r = 0) = 0 \) and \( \lim_{r \to \infty} g(r) \to 1 \). The first rule introduces the repulsive correlations between the atoms and the second the absence of such correlations in long distances. In general the form of \( S(k) \) is affected appreciably from the form of \( g(r) \). More specifically, the long range behavior of \( g(r) \) affects \( S(k) \) for small values of \( k \) while the short range behaviour of it affects \( S(k) \) for large values of \( k \) as a direct consequence of the Fourier transform theory.

In the present work, we choose two trial forms for \( g(r) \). The first one is a gaussian type which has been extensively and successfully used for the study of similar problems in atomic physics (Bose gas, liquid helium) as well in nuclear physics. The relevant \( g(r) \) and the entailed \( S(k) \) are

Case 1

\[ g(r) = 1 - \exp[-\beta r^2] \]

\[ S(k) = 1 + N(C_1 - 1) \exp[-k_b^2/2] - \frac{NC_1}{(1 + 2y)^{3/2}} \exp[-k_b^2/(1 + 2y)], \]  

(5)

where \( k_b = k b, y = \beta b^2, \beta \) is the correlation parameter and \( C_1 \) is the normalization factor.

The second trial function \( g(r) \) and the relevant \( S(k) \) are of the form

Case 2

\[ g(r) = 1 - \frac{\sin^4 \alpha r}{(\alpha r)^4} \]

\[ S(k) = 1 + N(C_2 - 1) \exp[-k_b^2/2] \]

\[ - \frac{NC_2}{2^{15/2} a b \pi k_b} \sum_{i=1}^{5} \alpha_i \left[ \beta_i \exp[-\beta_i^2/4] + \sqrt{\pi}(1 + \frac{\beta_i^2}{2}) \text{erf}(\frac{\beta_i}{2}) \right] \]  

(6)

where \( \alpha \) is the correlation parameter, \( \alpha_i \) are known coefficients, \( \beta_i = \beta_i(k b, a, b), \text{erf}(z) = 2/\sqrt{\pi} \int_0^z e^{-t^2} dt \) and \( C_2 \) is the normalization factor.
Trial functions $g(r)$ of hard-sphere form ($g(r) = 1-a/r$) and soft repulsive form ($g(r) = 1-\sin{ar/ar}$) are also used. Both of them, lead either to the ideal Bose gas results (negligible correlations) or to abnormal fluctuating negative and positive values for $S(k)$ (strong correlations) and consequently in complete disagreement with the experimental data [9]. Therefore, it should be emphasized that the choice of a trial function $g(r)$ should be made under certain restrictions in order to get reasonable values for $S(k)$.

The behavior of $S(k)$, in case 1, for different values of the correlation parameter $\beta$ is shown in Fig. 1(a). It is obvious that the effect of correlations, induced by the function $g(r)$, becomes large when the parameter $\beta$ becomes small and vice versa. The case where $\beta \to \infty$, corresponds to the uncorrelated case (HO). For the values of $k$ employed in the experiment of Ref. [2] (hereafter EXP-1) the prediction of the HO model is always close to 1 for $S(k)$. When the correlation parameter $\beta$ decreases considerably (strong correlations) the theoretical prediction of $S(k)$ is in good agreement with the experimental data. The value $\beta = 5.3 \mu m^{-2}$ gives the best least squares fit in that case. In general the gaussian form of $g(r)$, in spite of its simplicity, reproduces fairly well the experimental data of EXP-1, both in low and high values of the momentum $k$. It reproduces also the experimental data of Ref. [1] (hereafter EXP-2) as can been seen from Fig. 1(c). Within our theoretical model, the gaussian type of $g(r)$ is flexible enough to obtain values for $S(k)$ in agreement with the experimental data.

Fig. 1(b) displays the results in case 2, which are compared with those of the data of EXP-1. The model reproduces well the experimental data in the range $1.5 - 3 \mu m^{-1}$ (with best least squares fit value $a = 1.34 \mu m^{-1}$), but fails in the range $k > 3 \mu m^{-1}$. The main drawback of this model is the predicted negative values of $S(k)$ in the range close to $k = 0$ when the correlation parameter $a$ decreases considerably (strong correlation case).

The correlation function $g(r)$ corresponding to cases 1 and 2 for the correlation parameters $\beta = 5.3 \mu m^{-2}$ and $a = 1.34 \mu m^{-1}$ respectively is sketched in Fig. 2(a). Those values of the parameters $\beta$ and $a$ give the best $x^2$ value in the fit of the theoretical expressions of $S(k)$ to the data of EXP-1. The most striking feature in case 2 is the existence of strong correlations, introduced by $g(r)$, in order to reproduce the experimental data of $S(k)$. It is worthwhile to point out that $g(r)$, in case 2, exhibits fluctuations in the range $r > 2 \mu m$ but this is not visible in Fig. 2(a).

The possibility of a linear dependence of $S(k)$ on $k$ for small values of $k$, as predicted from other works [8], is prohibitive, on the basis of Eq. (3) at least in the case where the trap is an harmonic oscillator one. That can be seen considering the ground state wave function to be the harmonic oscillator one and transforming $r_1$ and $r_2$ in Eq. (3) into the coordinates of the relative motion ($r = r_1 - r_2$) and the center of mass motion ($R = (r_1 + r_2)/2$). After some algebra $S(k)$ takes the form

$$S(k) \sim \int e^{ikr}e^{-r^2}[Cg(r) - 1]dr \quad (7)$$

For finite systems, as is a trapped Bose gas, we can expand the exponential $e^{ikr}$, since $r$ is bounded. So that:

$$e^{ikr} = 1 + ikr + \frac{(ikr)^2}{2!} + \frac{(ikr)^3}{3!} + \cdots \quad (8)$$

Substituting Eq. (8) into Eq. (7) and considering that the terms with odd powers of $k$ do not contribute on the integral, $S(k)$ takes the form

$$S(k) \sim a_1k^2 + a_2k^4 + \cdots \quad (9)$$

Thus, for small values of $k$, $S(k)$ depends linearly on $k^2$. The gaussian factor $e^{-r^2}$, originating from the harmonic oscillator wave function of the trapped Bose gas, ensures the convergence of the integrals $a_i$ corresponding to the even powers of the expansion.

II. HOMOGENEOUS BOSE GAS

The condensate of an inhomogeneous (finite) Bose gas, can be treated as homogeneous in regard to its elementary excitations considering that the coherence length $\xi$ satisfies $\xi \ll R$ [4]. Actually, this is a rough approximation, but can effectively describe fairly well the excitation properties of a trapped Bose gas.

In infinite systems $\rho(r_1)$ is constant ($\rho(r_1) = \rho$) and thus the TBDD is given by $\rho(r_1, r_2) = \rho^2 g(r_{12})$. Thus, the structure factor of homogeneous gas (or quantum fluid in general) is given by the relation [10]

$$S(k) = 1 + \rho \int e^{ikr}[g(r) - 1]dr, \quad (10)$$

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or after performing the angular integration

\[ S(k) = 1 + 4\pi \int_0^\infty \frac{\sin kr}{kr} r^2 [g(r) - 1] dr. \] (11)

The necessary conditions which must be obeyed by \( g(r) \) and \( S(k) \), when a given \( g(r) \) is not generated directly and explicitly by a wave function, include [10]

\[ g(r) \geq 0, \quad S(k) \geq 0, \quad \lim_{k \to 0} S(k) = \frac{\hbar k}{2mc}, \]

\[ S(0) = 0 \Rightarrow 4\pi \rho \int_0^\infty r^2 [g(r) - 1] dr = -1 \] (12)

The third condition of (12) imposes the condition for the phonon like excitation on the Bose gas and is satisfied if and only if [10]

\[ \lim_{r \to \infty} r^4 [g(r) - 1] = \frac{-\hbar}{2\pi^2 m \rho c}. \] (13)

where the bar denotes an average over a range \( \delta r \) somewhat larger than \( \rho^{-1/3} \) [10].

We have used three different trial expressions for \( g(r) \) to study \( S(k) \) in a uniform Bose gas. The first two were used already in the study of the inhomogeneous Bose gas. However, the relevant structure factor, as expected, has different forms compared to inhomogenous case. The used forms of \( g(r) \) and the entailed \( S(k) \) are

**Case 3**

\[ g(r) = 1 - \exp[-\beta r^2] \]

\[ S(k) = 1 - \exp[-\frac{k^2}{4\beta}] \] (14)

**Case 4**

\[ g(r) = 1 - \frac{\sin^2 \alpha r}{(ar)^2} \]

\[ S(k) = \begin{cases} 
\frac{3\hbar}{2\pi}, & k < 2a \\
2 - \frac{3\alpha^2}{8\pi}, & 2a < k < 4a \\
\frac{k^2}{3\pi^2}, & 4a < k 
\end{cases} \] (15)

**Case 5** is a combination, in a way, of cases 3 and 4 and takes the form

**Case 5**

\[ g(r) = 1 - \frac{\sin \alpha r}{ar} \exp[-cr] \]

\[ S(k) = \frac{k^2(k^2 + 2c^2 - 2a^2)}{(a^2 + c^2)^2 + k^2(k^2 + 2c^2 - 2a^2)} \] (16)

It is worth noticing that in homogeneous cases, due to the fourth condition of Eq. (12), the correlation parameters of \( g(r) \), in all the cases, depend directly on the density \( \rho \). Thus, the fourth condition of Eq. (12), leads to the relations \( \rho = \beta^{3/2} / \pi^{3/2} \) (case 3), \( \rho = a^3 / \pi^2 \) (case 4) and \( \rho = (a^2 + c^2)^2 / 8\pi \) (case 5).

In the present work we compare also our results for \( S(k) \) with those of the hard-sphere interaction in uniform dilute gas, which was predicted long ago by Lee et al. [11] and has the form

\[ S(k) = \frac{k}{\sqrt{k^2 + 16\pi \alpha \rho}} \] (17)

where \( \alpha \) is the hard-sphere diameter (see also Refs. [12,13]).

The values of \( S(k) \) in case 3 (gaussian \( g(r) \)) for various values of the constant density \( \rho \) (or of the correlation parameter \( \beta \)) are displayed in Fig. 3(a). As in the corresponding case of the inhomogeneous Bose gas that type of \( g(r) \) reproduces the data of both experiments, see also Fig. 1(c), when the density of the gas is approximately \( \approx 1 \mu m^{-3} = \ldots \)
Increasing the density, lower values of $S$ in phonon regime (best fit value of the correlation parameter $a$ corresponds, as in the previous case, to density $\rho \sim 1 \mu m^{-3} = 10^{12} cm^{-3}$.)

The behavior of $S(k)$, in case 4, is illustrated in Fig. 3(b). A striking feature in this case is the linear behavior of $S(k)$ ($\lim_{k \to 0} S(k) \sim k$), in the phonon regime, as a consequence of the proper long range behavior of the function $g(r)$. The best fit value of the correlation parameter $a$ corresponds, as in the previous case, to density $\rho \sim 1 \mu m^{-3} = 10^{12} cm^{-3}$. Increasing the density, lower values of $S(k)$ appear for the same range of the momentum $k$.

$S(k)$ in case 5, is plotted in Fig. 3(c). In this case $g(r)$, combines in a way cases 3 and 4. $S(k)$ behaves quadratically in phonon regime ($S(k \to 0) \sim k^2$) but reproduces quite well the experimental data, especially in the range $0 \sim 4 \mu m^{-1}$. $S(k)$, derived by Lee et al. [11], is also plotted in Fig. 3(c). In that case, the phonon behavior is ensured, while the prediction is in good agreement with the experimental data.

The theoretical results of $S(k)$ in cases 1,3,4 and 5 using the best fit values of the parameters are compared with the experimental data of Exp-2 in Fig. 1(c). It is seen that in all cases there is a good agreement between the theoretical values and the experimental data.

The behavior of the correlation function $g(r)$, for cases 3,4 and 5, is sketched in Fig. 2(b). The most striking feature is that though the behavior of $g(r)$ is almost the same in cases 3 and 4, the corresponding $S(k)$, display different behavior, especially for the lower values of the momentum $k$. It is concluded that $S(k)$ is very sensitive to the form of $g(r)$ and specifically, the long range behavior of $g(r)$ affects considerably the behavior of $S(k)$ in the phonon regime (small values of $k$). This is a well known property of the Fourier transform.

It is worth remarking that a correlation function of the hard-sphere form, $g(r) = 1 - a/r$, thought it is as realistic one, mainly for low values of the interatomic distance $r$, leads to $S(k) = 1 - 4\pi \rho a/k^2$ which diverges when $k \to 0$.

In conclusion, we report a theoretical calculation of the static structure factor $S(k)$ both for inhomogeneous and homogeneous Bose gas, in the framework of the low order expansion theory, by applying various trial forms for the radial distribution function $g(r)$. We compared our results with recent experimental data concerning trapped Bose gas. The correlation parameters of $g(r)$ are adjusted in order to reproduce the experimental data. By applying suitable parametrization the experimental data are reproduced quite well. The low $k$ behavior of the calculated $S(k)$ is also addressed and discussed both in inhomogeneous and homogeneous Bose gas.

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FIG. 1. The static structure factor $S(k)$ of the inhomogeneous and homogeneous Bose gas in various cases versus the momentum $k$. (a) in Case 1 for various values of the correlation parameter $\beta$ as well as for the uncorrelated case (harmonic oscillator), (b) in Case 2 for the least squares best fit value of the parameter $a$, (c) in Cases 1, 3, 4 and 5 for the best fit values of the correlation parameters. The experimental points EXP-1 and EXP-2 are from references [2] and [1] respectively. For the various cases see text.

FIG. 2. The radial distribution function $g(r)$ for Case 1 and 2 (a) (corresponding to inhomogeneous Bose gas), and Cases 3, 4 and 5 (b) (corresponding to homogeneous Bose gas) with the best fit values of the correlation parameters.
FIG. 3. The static structure factor $S(k)$ for Case 3 (a) and Case 4 (b), for various values of the density $\rho$. The Case 5 (c) for the best fit value of the density and also for the hard-sphere interaction of Lee et.al. [11] (indicated LHY). The experimental data are from Ref. [2]