Statistical properties of one-dimensional attractive Bose gas

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received 11 April 2011; accepted in final form 24 August 2011
published online 22 September 2011

PACS 03.75.Hh – Static properties of condensates; thermodynamical, statistical, and structural properties
PACS 67.85.-d – Ultracold gases, trapped gases

Abstract – Using the classical field approximation we present the first study of statistical properties of one-dimensional Bose gas with attractive interaction. The canonical probability distribution is generated with the help of a Monte Carlo method. This way we obtain not only the depletion of the condensate with growing temperature but also its fluctuations. The most important is our discovery of a reduced coherence length, the phenomenon observed earlier only for the repulsive gas, known as quasicondensation.

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Introduction. – Statistical properties of a finite number of bosons confined by a trapping potential have been intensively studied ever since the very first experiments on dilute gas Bose-Einstein condensates. Initially a full understanding has been reached of the statistics of the confined ideal Bose gas [1–6]. In this context criticism of the most widely used grand canonical ensemble has been raised. As is shown, it predicts unphysical fluctuations of the number of condensed atoms. Interactions, an essential aspect of Bose atoms physics, make the problem of statistics rather complicated. In the simplest, although still academic case, of the box with periodic boundary condition, at least we know a priori what is a condensate. It is the zero momentum component of the atomic field. In the box with periodic boundary conditions we know more. In addition we know analytically the spectrum and the expressions for the collective Bogoliubov excitations. So, one can look at the statistics of the gas as that of noninteracting bosonic quasiparticles. This determines the statistical properties of the gas at least at low temperatures [7]. The extension of the method to higher temperatures is already significantly more complicated. The Bogoliubov-Popov spectrum depends on the actual number of the condensed atoms rather than on their total number. Thus, this is itself a fluctuating variable. Several papers attempted to take this into account [8,9]. Another serious problem is the assumption that quasiparticles do not interact. In fact they do and they have a finite (temperature-dependent) lifetime. In a realistic harmonic trap we have no analytic formulae for the quasiparticles and also the condensate degree of freedom is known only a posteriori since it is a function of an interaction strength, a frequency of the harmonic trap, a number of atoms and a temperature of the sample.

In two recent papers [10,11] we have shown how to overcome most of these problems. To this end we proposed to use the classical field description of the system generating the proper thermal equilibrium distribution using a classical Metropolis algorithm [12]. Details of classical field approaches are presented in [13,14]. It is the purpose of this letter to report the first study of statistical properties of an attractive Bose gas. Confined to a box it is unstable. Hence, this simple model makes no sense for the attractive gas. The situation is different in a harmonic trap. Limited attractive condensates do exist in two and three dimensions. The lithium-7 condensate was among the first ones to be observed [15]. It then has led to the creation of bright solitons [16,17]. In strictly 1D systems the effective repulsion of the kinetic energy makes it stable for any number of particles. We therefore concentrate our attention on the one-dimensional, finite, attractive Bose gas trapped in a harmonic potential. Thus the Hamiltonian of the system
has the form

\[ H = \int \hat{\Psi}^\dagger(x) \left( \frac{\partial^2}{2m} + \frac{1}{2} m \omega_0^2 x^2 \right) \hat{\Psi}(x) dx + \frac{g_{1D}}{2} \int \hat{\Psi}^\dagger(x) \hat{\Psi}^\dagger(x) \hat{\Psi}(x) \hat{\Psi}(x), \]

where \( \hat{\Psi} \) is the atomic field operator, \( m \) is the mass of an atom, \( \omega_0 \) is the frequency of the harmonic trapping potential and we are particularly interested in \( g_{1D} < 0 \). The case of the positive coupling constant was studied in detail in [11].

**Model.** The classical fields approximation consists in the replacement of the quantized atomic field by a \( \alpha \)-number wave function. This wave function is then conveniently expanded as a sum over the harmonic-oscillator wave functions and expansion coefficients \( \alpha_n \) are classical stochastic complex variables,

\[ \Psi(x) = \sum_{n=0}^{n_{\text{max}}} \alpha_n \varphi_n(x), \]

where the oscillator eigenfunctions \( \varphi_n \) are chosen to correspond to a harmonic oscillator of the frequency \( \omega \). Note that \( \omega \) is not necessarily equal to \( \omega_0 \).

Thus, the energy functional

\[ E[\Psi] = \int \Psi^\dagger(x) \left( \frac{\partial^2}{2m} + \frac{1}{2} m \omega_0^2 x^2 \right) \Psi(x) dx + \frac{g_{1D}}{2} \int |\Psi(x)|^4, \]

takes the form

\[ E(\{\alpha_i\}) = \sum_{n=0}^{n_{\text{max}}} \hbar \omega_n |\alpha_n|^2 + E_{\text{int}}(\{\alpha_i\}) \]

\[ + \sum_{n,n'=0}^{n_{\text{max}}} \frac{1}{2} m (\omega_0^2 - \omega^2) \langle n|x|^2|n'\rangle \alpha_n^* \alpha_{n'}, \]

with the interaction energy \( E_{\text{int}} \) being a quartic form in the variables \( \alpha_n \) and \( \langle n|x|^2|n'\rangle \) is the matrix element in the oscillator basis.

We are going to look at the statistics of a sample composed of \( N \) atoms, so the amplitudes are subject to a constraint:

\[ \sum_{n=0}^{n_{\text{max}}} |\alpha_n|^2 = N. \]

Having converted a quantum-statistical physics problem into a classical one, we then define a canonical equilibrium distribution of the amplitudes \( \alpha_n \) as

\[ P(\{\alpha_i\}) \propto \exp \left[ -\frac{E(\{\alpha_i\})}{k_B T} \right]. \]

An efficient algorithm generating this probability distribution has been invented by Metropolis [12].

It is easy to check with the help of the imaginary-time Gross-Pitaevskii equation that the zero-temperature attractive 1D Bose gas has a wave function which is very close to a Gaussian. Its width shrinks with a growing number of condensed atoms and with the growing absolute value of the negative coupling constant \( g_{1D} \). This is our guide to the optimal choice of the frequency \( \omega \) defining the actual oscillator base in the expansion of the atomic classical field (2). Thus, this frequency becomes a function of the coupling and of the temperature as they both determine the width of the condensate wave function. More precisely: as we have shown in [10] the classical fields reproduce faithfully the available analytically exact probability distribution (see also fig. 1) of the the condensate in a harmonically confined ideal Bose gas for the cut-off parameter \( n_{\text{max}} \) satisfying

\[ n_{\text{max}} \hbar \omega_0 = k_B T, \]

where \( T \) is the temperature of the gas.

To further illustrate the accuracy of the classical fields approximation applied to the statistics of the 1D harmonically confined ideal Bose gas we present in fig. 1 the temperature dependence of the variance of the condensate occupation. We see that the discrepancy is small in the whole range of relevant temperatures and that it decreases with a growing number of atoms. We add that the expectation values of a number of condensate atoms for both classical fields and full quantum model are indistinguishable for more than 100 atoms. A natural generalization of the above cut-off condition for a weakly attractive 1D Bose gas is

\[ n_{\text{max}} \hbar \omega(N, T) = k_B T, \]

where the frequency \( \omega(N, T) \) is chosen such that the corresponding Gaussian function describes the ground state of the Gross-Pitaevskii equation for \( N_0 \) interacting atoms. Strictly speaking \( N_0 \) should be chosen self-consistently.
In this letter, however, we are satisfied with \( N_0 \) being a number of condensed ideal gas atoms at a given temperature. The general rule for the determination of the condensate wave function follows from the Onsager-Penrose [18] definition calling for the diagonalization of the one-particle density matrix,

\[
\rho_{i,j} = \langle \alpha_i^* \alpha_j \rangle = \sum_n \lambda_n \beta_i^*(n) \beta_j(n),
\]

and identification of the condensate wave function with the eigenvector corresponding to the leading eigenvalue. As a cross-check we verified that our identification of the base indeed yields the condensate wave function very close to the \( n = 0 \) state.

It is clear that our choice of the frequency \( \omega(N,T) \) makes it monotonically decrease with the temperature and tend to that of the empty trap: \( \omega_0 \). In fig. 2 we illustrate this for several values of the coupling \( g \). In the inset we also confirm the consistency of our choice of the base by comparing the width of the ground state of the Gross-Pitaevskii equation with the width of the actual condensate wave function computed via diagonalization of the one-particle density matrix. Small steps visible in the inset result from taking the solution of (8) for the cut-off as the nearest integer.

The multiparticle Hamiltonian with interactions dependent on the mutual distances has the form

\[
H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} m \omega_0^2 \sum_{i=1}^{N} x_i^2 + \sum_{i \neq j}^{N} V_{int}(x_i - x_j),
\]

where \( V_{int}(x_i - x_j) \) is an interaction energy between atoms placed in positions \( x_i \) and \( x_j \) and \( N \) is the total number of atoms. Therefore the center of mass of the system \( x_{CM} = \frac{x_1 + x_2 + \ldots + x_N}{N} \) is decoupled from all other degrees of freedom [19]. Thus, this variable is entirely missing from any mean-field approximation in which a nonlinear Gross-Pitaevskii equation describes the system. This does not have important consequences for the repulsive gas. In this case, the condensate is broader than the ground state of the harmonic potential, so the uncertainty over the position of the center is just a correction. The situation for the attractive gas is different. Now, the condensate is spatially squeezed and the shot-to-shot variation of the position of the center of mass is at least as broad as the ground state of the empty harmonic potential [20,21].

We therefore stress that our approach disregards this uncertainty, so the statistical properties derived here pertain to the reference frame of the center of mass of the system. Measurements in the center-of-mass system can meet some difficulties due to the uncertainty of position of the center of mass. However, a single-shot simultaneous detection of many particles resolves this problem [21].

In our classical field approximation effects of quantum fluctuations and quantum depletion are missing. The method is suitable for weakly interacting Bose gas in the quantum degenerate regime.

**Results.** Throughout this paper we use the oscillator units of position, energy and temperature, \( \sqrt{\hbar/(m \omega_0)} \), \( \hbar \omega_0 \) and \( \hbar \omega_0 / k_B \), respectively. Hence a dimensionless coupling \( g \) is in units of \( \sqrt{\hbar \omega_0 / m} \). All presented results are for \( N = 500 \) atoms and the temperature is in units of the characteristic temperature indicating a transition to the quantum degenerate regime of a finite sample of an ideal Bose gas \( N = T_C \ln(2T_C) \), where \( N \) is the total number of atoms [22]. In fig. 3 we plotted a number of condensed...
atoms as a function of the coupling constant $g$ for negative and also positive values (using the method explained in detail in [11]) for two temperatures, one very low ($T/T_C = 0.26$) and the other $T/T_C = 0.63$. Since the condensation depends on the local density of particles, the effects of repulsive and attractive interactions are opposite. The first one swells the condensate reducing the local density with respect to the ideal gas, while the other shrinks it enhancing the condensation process. Thus, the number of condensed atoms is a monotonically decreasing function of the interaction parameter $g$ as we go from the negative to the positive values.

In fig. 4 we present the relative fluctuations also as a function of changing sign $g$ and for the same temperatures as in fig. 3. A general observation is that fluctuations of the condensed-atoms number grow with the strength of the interaction in both negative and positive directions. An unexpected feature, however, is that the minimal fluctuations are observed not for $g = 0$ but for tiny attractive interaction of $-0.0025$.

Perhaps the most interesting aspect of a 1D repulsive Bose gas predicted [23] and then observed experimentally [24,25] is the phenomenon of a quasicondensation. It is a reduction of the coherence length to values smaller than the length of the condensate above a certain characteristic temperature. In the recent letter [26] the correlation length has been related to the gray solitons formed during a rapid cooling process [27]. We have computed the temperature-dependent correlation length for the attractive case and found that the quasicondensation occurs also in this case. This is probably the most important result of this letter. We note that one does not expect gray solitons to appear in rapidly cooled attractive Bose gas, so the above-mentioned connection to solitons certainly does not hold in this case. The first-order correlation function is defined as

$$g_1(x,-x) = \frac{\langle \Psi(-x)^\dagger \Psi(x) \rangle}{\langle |\Psi(x)|^2 \rangle}. \quad (11)$$

In fig. 5 we plot its full width at half-maximum as a function of temperature and compare it with the width of the condensate. The effect of quasicondensation is visible. It occurs at the temperature $T \approx 0.6T_C$. In fig. 6 we present the dependence of the temperature above which the system exhibits the quasicondensation as a function of the dimensionless coupling constant $g$. We see a nearly linear dependence. Remembe that dimensionless $g$ depends on the experimental coupling strength and the trap frequency $\omega_0$ via $g_{1D} = g\sqrt{\frac{\hbar}{m\omega_0}}$. Thus, if we attribute changes of $g$ to the changes of $\omega_0$, then for

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1For $T > 0.75$ the fluctuations start to decrease, see fig. 3 in [11].
As \( \omega_0 \to 0 \) the quasicondensation temperature tends to 0. This last property is probably related to the instability of the system in a homogeneous case.

Summarizing: we have presented the first study of equilibrium thermodynamics of the attractive 1D Bose gas trapped in a harmonic potential. Our results are for the canonical statistical ensemble, thus the temperature is a control parameter. The classical field approximation is used. The appropriate probability distribution is obtained numerically using a Monte Carlo technique. We found a reduced coherence length above some characteristic temperature. This phenomenon was previously known only for a repulsive gas.

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This work was supported by Polish Government Funds for the years 2010–2012. Two of us (KP and KR) acknowledge financial support of the project “Decoherence in long-range interacting quantum systems and devices” sponsored by the Baden-Württemberg Stiftung.

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