Statistical properties of one-dimensional Bose gas

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The Monte Carlo method within the so-called classical field approximation is applied to one-dimensional, weakly interacting, repulsive Bose gas trapped in a harmonic potential. Equilibrium statistical properties of the condensate are calculated within a canonical ensemble. We also calculate experimentally relevant, low-order correlation functions of the whole gas.

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I. INTRODUCTION

Statistical properties of multiparticle quantum systems are at the heart of statistical physics. The best developments are found both in experiments and in the theory of statistical properties of photons. In the quickly developing physics of quantum degenerate dilute gases, there are two aspects that make the statistical properties of thermal equilibrium atoms notably different than that of photons. First, atoms collide and their interaction is necessary for the thermalization process, i.e., their approach to thermal equilibrium. Second, the total number of atoms is strictly conserved and the experiments on Bose-Einstein condensation are performed with almost perfect isolation of the system from an exchange of particles with the outside world. Moreover, the system often consists of as few as hundreds of atoms, thus it is far from a thermodynamic limit. Until now, only the statistics of an ideal Bose gas have been fully understood [1,2]. In a series of papers, it was found that the three commonly used statistical ensembles (grand canonical, canonical, and microcanonical), while giving an identical prediction for the extinction of the condensate with increasing temperature, differ in regard to the predicted fluctuations of the number of condensed atoms. In particular these fluctuations calculated via the grand canonical ensemble are absurdly large, the number of condensed atoms. In particular these fluctuations differ in regard to the predicted fluctuations of the number of condensed atoms. Moreover, the system often consists of as few as hundreds of atoms, thus it is far from a thermodynamic limit. Until now, only the statistics of an ideal Bose gas have been fully understood [1,2]. In a series of papers, it was found that the three commonly used statistical ensembles (grand canonical, canonical, and microcanonical), while giving an identical prediction for the extinction of the condensate with increasing temperature, differ in regard to the predicted fluctuations of the number of condensed atoms. In particular these fluctuations calculated via the grand canonical ensemble are absurdly large, as previously observed by Schrödinger [2]. The statistics of a weakly interacting Bose gas are still a challenge.

Nearly all papers in this area of research deal with the academic problem of a system of $N$ atoms confined in a rectangular box with periodic boundary conditions. There are two important simplifying aspects of such a confinement. First, even in the presence of a (repulsive) interaction, the condensate wave function is still the zero-momentum component of the atomic field, just as for the ideal gas. Second is a simplification of the Bogoliubov quasi-particle-excitation spectrum and an analytic relation between the annihilation and creation operators of quasi-particles and the corresponding operators for atoms [3]. Thus, in the Bogoliubov approximation, the total Hamiltonian may be written as

\[ H_B = E_0 + \sum_k \epsilon(k) b_k^\dagger b_k, \]

or the sum of the energy of the condensate $E_0$ and the sum of the independent energies of quasi-particles (created and annihilated by $b_k^\dagger$ and $b_k$, respectively), which in this approximation are treated as independent bosons with simple and well-understood equilibrium thermodynamic properties. Thus ignoring the changing number of background condensed atoms, one can compute the statistics of the excited thermal atoms just from the statistics of the independent quasi-particles [4]. In this way, one gets reliable results for low temperatures only. At higher temperatures, the Bogoliubov spectrum gets modified and it takes a Bogoliubov-Popov form [5]. In this approximation, the spectrum depends on the number of condensed atoms rather than on their total number. Moreover, $E_0$ depends on $N_0$. Both parameters depend on the random variable, which presents a serious technical difficulty [6] that has been overcome in a self-consistent way [7].

None of these papers, however, fully take into account the higher-order terms in the interaction Hamiltonian. Physically, these terms describe the interaction between quasi-particles that leads to their instability. In a recent paper [8], we have shown how to calculate the statistical properties of the weakly interacting Bose gas, retaining full value of the interaction energy. To this end, we have proposed to use the so-called classical field approximation [9]. In this approximation, all long wavelength degrees of freedom of the atomic field are stripped off of their operator character and are described by complex amplitudes. The procedure requires macroscopic occupation of the considered modes. Thus this approximation may be applied below the degeneracy temperature $T_d \approx N_0 \hbar \omega$. The question of whether practically all atoms may be accounted for within the classical field approximation has been answered in the affirmative. In a recent paper [10], we have shown that, with a proper choice of the short wavelength cutoff, all statistical properties of an ideal Bose gas may be reproduced using the classical field approximation. There are several classical field approaches that generally lead to similar results. The comparisons between our method and other classical field methods are presented in detail in [11,12].
In [8] we have applied the classical field approach to describe the statistical properties of weakly interacting bosons, again confined in a box with the periodic boundary conditions. In this paper we extend the Monte Carlo method to an experimentally relevant, one-dimensional, weakly interacting Bose gas trapped in a harmonic potential. The results are obtained with the help of the classical field approach, but fully account for the interaction energy. In this case, there are both theoretical [13] and experimental results [14] for the limited phase coherence of a very cold atomic sample, known as a quasicondensate, as well as recent measurements of the local density fluctuations [15].

While the choice between the canonical and the microcanonical statistical ensemble makes a difference for the ideal Bose gas, these ensembles are expected to be closer for the weakly interacting gas. However, even in the interacting regime, some differences can still exist [16]. The important advantage of the canonical ensemble is that the temperature rather than the energy is a control parameter, making it an ensemble of choice for experimenters. Moreover, the canonical approach is also a frequent choice of theorists because calculations in the microcanonical ensemble are always more complicated. We too choose this approach in this paper.

In Sec. II we formulate the problem and describe the proposed scheme based on the classic Metropolis algorithm. In Sec. III we present statistical properties of the condensate. In Sec. IV we present the results for low-order correlation functions of the whole gas.

II. THE METHOD

We study a one-dimensional (1D), repulsive, weakly interacting Bose gas confined in a harmonic trap. Excellent realizations of such a system are available [15]. Thus, our Hamiltonian of the one-dimensional Bose gas has the form

\[ H = \int \Psi^\dagger(x) \left( \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 \right) \Psi(x) \, dx + \frac{g}{2} \int \Psi^\dagger(x) \Psi^\dagger(x) \Psi(x) \Psi(x). \]  

(2)

The Hamiltonian is a sum of the single-particle oscillator energy with mass \( m \) and angular frequency \( \omega \), and a conventional contact interaction with the coupling constant \( g \). A convenient basis is provided by the eigenstates of the harmonic oscillators \( \phi_n(x) \),

\[ \Psi(x) = \sum_n \phi_n(x) \hat{a}_n, \]  

(3)

where \( \hat{a}_n \) annihilates an atom in the \( n \)th harmonic-oscillator state. The classical field approximation consists of replacing the creation and annihilation operators with classical complex amplitudes,

\[ \hat{a}_n, \hat{a}_n^\dagger \mapsto \alpha_n, \alpha_n^\dagger. \]  

(4)

In [10] we have shown that probabilistic properties of the condensate for one-dimensional ideal Bose gas in a harmonic trap are perfectly reproduced by the classical field approximation, provided the number of degrees of freedom is kept finite with the last retained state chosen as

\[ K = \frac{k_B T}{\hbar \omega}, \]  

where \( T \) is the absolute temperature and \( k_B \) is the Boltzmann constant. This suggests the classical field approach may be used also for the weakly interacting gas [8]. In this approximation, the energy of a given configuration of the field is given as

\[ E (\{\alpha_n\}) = \hbar \omega \sum_{n=0}^K n|\alpha_n|^2 + E_{\text{int}} (\{\alpha_n\}), \]  

(6)

where \( E_{\text{int}} (\{\alpha_n\}) \) is the quartic polynomial in the amplitudes \( \alpha \). Hence, the probability distribution of a given configuration of the classical field according to the canonical ensemble is

\[ P (\{\alpha_n\}) = \frac{1}{Z(N,T)} \exp \left( -\frac{E (\{\alpha_n\})}{k_B T} \right). \]  

(7)

where \( Z(N,T) \) is the classical partition function for \( N \) atoms at temperature \( T \). We need to generate this probability distribution with a set of the amplitudes subject to the constraint given by the fixed number of particles

\[ \sum_{n=0}^K |\alpha_n|^2 = N. \]  

(8)

The best-known Monte Carlo realization of this distribution is given by the Metropolis algorithm [17]. Before we turn to the results, there are two important remarks to be made. First, for interacting atoms, the condensate wave function is no longer the empty harmonic-potential ground state, thus its occupation is not \( |\alpha|^2 \). Instead, following [18], the identification of the condensate requires a diagonalization of the single-particle density matrix, which in our harmonic-oscillator representation is

\[ \rho_{ij} = \langle \alpha^* \alpha \rangle = \sum_n \lambda_n \beta^*_n(n) \beta(n), \]  

(9)

where the mean value is taken with the probability distribution (7) and the eigenvector corresponding to the dominant eigenvalue is the condensate. The second remark concerns the cutoff condition (5). For the interacting gas, we need a higher cutoff. We know that the repulsive gas at zero temperature is broader than the ground state of the harmonic potential, thus its wave function needs higher energy terms. Remembering that in the Bogoliubov approximation the quasiparticle excitations have energies counted not from zero but from the chemical potential \( \mu \), we postulate the modification of the cutoff condition in the form

\[ \hbar \omega = \mu + k_B T, \]  

(10)

which will be independently verified in the next section.

III. STATISTICAL PROPERTIES OF 1D CONDENSATE

Equipped with the numerical scheme described in some detail in the preceding section, we turn now to the discussion of results. We begin with statistical properties of the condensate. All previous results were obtained either with the help of the time-dependent methods [19,20] or in the frame of the local
density approximation [21–23]. In this paper we present the results obtained with the methods of equilibrium statistical mechanics. In our classical field approximation, however, effects of quantum fluctuations, such as quantum depletion, are missing. With our method, we describe weakly interacting gas in the degenerate regime.

Throughout this paper, we use the oscillator units of position, energy, and temperature: $\sqrt{\frac{\hbar}{m\omega}}$, $\hbar\omega$, and $\frac{\hbar\omega}{k_B}$, respectively. In all figures, the temperature is presented in units of the transition temperature for the finite trapped system $T_C$, which obeys the relation

$$N = T_C \ln(2T_C),$$

where $N$ is the total number of atoms. All calculations are performed for 500 atoms. Our main parameter is just the coupling constant $g$; all simulations are done for $g = 0.02$ (which corresponds with the experimental data from [14]) and $g = 1$. For these parameters and for most considered temperatures, the gas could not be described by the local-density-approximation method. As a reference point, we always have the ideal-gas case. For the ideal-gas case, we have an exact probability distribution of the number of uncondensed atoms $N_{ex}$ (thus with remaining $N_0 = N - N_{ex}$ in the condensate),

$$P(N_{ex}, T) = \frac{1}{\xi N_{ex}} \prod_{i=N_{ex}+1}^{N} (1 - \xi^i),$$

(11)

where $\xi = \exp(-\hbar\omega/k_BT)$. We also have its best classical field approximation

$$P_{cl}(N_{ex}, T) = \frac{\xi^{N_{ex}}}{1 - \xi^N} \left( \frac{1 - \xi N_{ex}}{1 - \xi^N} \right)^{K-1},$$

(12)

with the cutoff parameter $K$ chosen according to (5) and the Monte Carlo representation of the classical distribution. The detailed derivation of (12) is given in the Appendix.

From these coinciding reference points, we are departing to the largely unchartered territory of the interacting gas. In Fig. 1 we plot the zero-temperature spatial distribution of the condensate for several values of the coupling. Note the standard broadening of the condensate wave function. At this point our method merely seeks the minimum of the classical energy functional (7), satisfying the constraint (8). In fact this is nearly the same as the ground state of the Gross-Pitaevskii equation, conveniently computed by the imaginary-time propagation. Next we look at the mean number of condensed atoms as a function of temperature in Fig 2. In the 1D case, this number decreases gradually, even in the $N \to \infty$ limit. As it should be, the exact ideal-gas result (solid red line) is reproduced very well by the corresponding classical-field Monte Carlo results (green crosses). Note that for a stronger coupling, the depletion of the condensate with growing temperature becomes very rapid. This plot provides a direct test of our proposed modification of the cutoff condition for the interacting gas. The shift of the cutoff energy by the chemical potential is the smallest increase that guarantees $\frac{N_0}{N} \to 1$ and, at the same time, gives the correct zero-temperature condensate wave function.

![FIG. 1. (Color online) Zero-temperature spatial distribution of the ground state for various values of the parameter $g$. Comparison between the classical field approximation (data from Metropolis algorithm) and Gross-Pitaevskii equation (from imaginary-time evolution). The solid red line corresponds to the exact result for noninteracting gas.](image1)

![FIG. 2. (Color online) Relative average number of atoms in the ground state as a function of temperature $T$. The solid red line corresponds to the exact result for noninteracting gas; points correspond to the results of the classical field approximation.](image2)

![FIG. 3. (Color online) Relative fluctuation of number of atoms in the ground state. The solid red line corresponds to the exact result for noninteracting gas; points correspond to the results of the classical field approximation.](image3)
Next let us look at fluctuations. It is the fluctuations that were ensemble dependent for the ideal gas. In Fig. 3 we plot the variance of the condensate-occupation probability distribution for the interacting gas, again compared to the ideal-gas canonical result (solid red line). We see the shift of the curve toward lower temperatures. As for all finite systems, it is not easy to define a characteristic crossover temperature based on the depletion plots as in Fig. 2. It is natural to define such a crossover characteristic temperature as the one corresponding to the maximum variance [24]. Of course our Monte Carlo method also gives access to the full probability distribution of the occupation of the condensate state. For $T = 0.2 T_c$, this is shown in Fig. 4.

IV. LOW-ORDER CORRELATION FUNCTIONS OF 1D BOSE GAS

Despite all the theoretical effort, there are currently no experimental measurements of the temperature-dependent statistical properties of the condensate. The relative fluctuations are significant only for small samples of several hundred atoms. A sufficiently precise determination of the condensate fraction with nearly perfect control of the total number of trapped atoms remains a challenge. However, the temperature-dependent coherence properties of nearly 1D Bose gas have been measured indirectly [25] and so have the local density fluctuations of such a gas [15]. Those are, of course, also accessible to us. There are two remarks in order here. First, our cutoff was optimized to reproduce statistics of the condensate. This way it is not optimized for the thermal atoms. In fact, as was shown in [10], it overestimates the population of thermal modes. This must be so since, in the classical field approximation, all atoms are distributed over a finite number of low-lying states instead of over the infinite number of them. Thus, particularly at high temperatures when most atoms are thermal, we expect a deteriorating accuracy of the method. Second is the problem of ordering. Of course, within the classical field approximation, fields do commute. Thus, there is no difference between the density-density correlation function and the fourth-order, normally ordered correlation function

$$\langle \hat{\Psi}^\dagger(\pm x)\hat{\Psi}(x) \rangle = \langle \hat{\Psi}^\dagger(\pm x)\hat{\Psi}(x) \rangle + \langle \hat{\Psi}^\dagger \hat{\Psi} \rangle.$$ 

But at very high temperatures, the last term, missing for the classical field approach, becomes dominant and gives rise to what experimenters call the shot noise. The classical field approximation cannot possibly reproduce this contribution unless it is introduced by hand. The most interesting property of the lowest-order correlation function for the 1D Bose gas was first noted in [13]. Unlike in three dimensions, the coherence length in 1D gas may be shorter than the length of the condensate. This phenomenon is called a quasicondensate. In the experiment [14], it has been observed indirectly: Upon expansion, the quasicondensate phase fluctuations turn into density fluctuations that can be directly observed in standard absorptive imaging. In Fig. 5 we show the comparison of the condensate wave function and the lowest-order correlation function

$$g_1(-x,x) = \frac{\langle \Psi^*(x)\Psi(x) \rangle}{\langle |\Psi(x)|^2 \rangle}$$

in the quasicondensate regime. More quantitative analysis is shown in Fig. 6. Here we vary the temperature, comparing the length of the condensate with the correlation length. We define the correlation length $L_{coh}$ as a full width at half maximum. Note the crossing of the two curves at the temperature $T_\phi \approx 40$, defining the onset of the quasicondensate. We add that the 1D ideal gas has no quasicondensate.

There are only a few results beyond the local density approximation for ultracold gas trapped in the harmonic potential. The author of [20] used the stochastic Langevin approach and compared results with mean-field theories (see [26]). He observed the following relation:

$$L_{coh}(T) = 2 R_{TF} e^{-T/T_\phi},$$

where $R_{TF}$ is a Thomas-Fermi radius at zero temperature and $T_\phi$ is a temperature of the onset of quasicondensation. We compared the formula (13), applying $T_\phi$ and replacing $R_{TF}$ with the full width at full maximum (both from our

FIG. 4. (Color online) Probability distribution of ground-state occupation at the temperature $T = 0.2 T_c$. The solid red line corresponds to the exact results for noninteracting gas; symbols correspond to the results of the classical field approximation.

FIG. 5. (Color online) The first-order correlation function and the density of the ground state. For easier comparison, the quasicondensate density profile has been rescaled by the values at the center of the trap.
FIG. 6. (Color online) The correlation length and the size of the ground-state wave function. Both lengths defined as full width at half maximum. The solid line is the formula for correlation length from [20]. The dashed line is the estimation from [13].

The appropriate comparison is presented in Fig. 6 (solid line). One of the first estimations for correlation length was given in [13] as

\[ L_{\text{coh}} = \frac{3NH^2 \omega^2 R_{\text{TF}}}{4\mu T} \ln(2) \]

where \( \mu \) is a chemical potential. The latter expression does not fit to our results (see Fig. 6, dashed line).

Finally, we present results for the local density fluctuations. They were measured recently by groups in Hanover [25] and Orsay [15]. In Fig. 7 we present the temperature dependence of the second-order correlation function at the center of the trap defined as

\[ g^2(0) = \frac{\langle |\Psi(0)^{4}| \rangle}{\langle |\Psi(0)^2| \rangle^2} \]

For low temperatures, the gas is in a coherent regime so the correlation function is close to 1. As shown in Fig. 6, the system for small (but non-zero) temperatures is in the quasicondensate regime. The main features of the system in this region correspond to the so-called Gross-Pitaevski regime [21,27], defined within the local density approximation. Although our system does not satisfy the inequalities for this approximation, the result of [21] derived for low temperatures,

\[ g^2(0) = 1 + \frac{4\sqrt{2}}{3} \frac{T}{T_d} \]

correctly estimates the behavior of \( g^2 \), as in our case.

For higher temperatures, the interaction energy becomes less important in comparison to thermal energy. Thus the system enters the nearly ideal-gas regime that is manifested by a bunching effect (\( g^2 \approx 2 \)). In the literature, the latter regime is also called the quantum decoherent regime (see [21,27]).

Unlike in the statistical properties of the condensate itself, even for the ideal gas there is a certain difference between the exact (solid red line in Fig. 7) and the Monte Carlo classical field approximation. As mentioned above, it is a result of the distorted occupation of the thermal modes in the classical field approach. The interaction reduces the density fluctuations, as predicted in [27]. In Ref. [15] the density fluctuations were measured in situ across a nearly one-dimensional sample versus the local density. The comparison of the ideal gas and the interacting gas of the same dependence is presented in Fig. 8. It has the main qualitative properties just like in the experiment, again showing the reduction of the local fluctuations due to the interactions. The quantitative comparison is difficult since experimental parameters of the number of particles or the temperature are known with large error bars. The authors of [15] also explored a very-high-temperature regime with the density fluctuations dominated by the shot noise. This regime is not accessible to the classical field approach for two related reasons: (1) in this regime, all states have a very small, fractional occupation and (2) classical field approximations are missing the quadratic term resulting from the commutator of the Bose fields, which is an essential term in the high-temperature regime.

FIG. 7. (Color online) Second-order correlation function at the center of the trap as a function of the temperature. The solid red line corresponds to the exact result for noninteracting gas; points correspond to the results of the classical field approximation. The solid black line corresponds to the estimation from [21] corresponding to \( g = 0.02 \) and low temperatures. Note the imperfect agreement of the classical field approximation for an ideal gas.

FIG. 8. (Color online) Fluctuations of number of atoms found in each bin vs number of atoms in each bin at the temperature \( T = 0.27T_c \). As the strength of interaction increases, the bosonic gas enters the quasicondensate regime.
V. CONCLUSIONS

In this paper we have demonstrated the power of the alternative computational tool to tackle the equilibrium thermodynamics of weakly interacting gas consisting of Bose particles. The method, based on classical field approximation to the full quantum theory, exploits the classical Monte Carlo technique to explore the phase space of the underlying finite-dimensional classical system for which the set of canonical variables replaces the annihilation and creation operators.

We have applied the method to the 1D repulsive gas trapped in a harmonic potential, calculating not only the statistical properties of the condensate, but also the low-order correlation functions of the whole gas that may be directly compared with the measurements.

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APPENDIX: PARTITION FUNCTION FOR THE IDEAL BOSE GAS IN A HARMONIC TRAP: CLASSICAL FIELD APPROXIMATION

The quantum partition function in the canonical ensemble may be written as follows:

\[ Z(N,\beta) = \sum_{n_0=0}^{\infty} \sum_{n_1=0}^{\infty} \ldots e^{-\beta \hbar \omega} \sum_{m_1=0}^{n_1} \delta(n_1-m_1) \cdot N, \]  
(A1)

where \( \beta = 1/k_B T \) and \( \omega \) is a frequency of the harmonic trap. The Kronecker \( \delta \) in Eq. (A1) enforces the conservation of the total number of particles. In the classical version, the sums have to be replaced with integrals, \( \sum_{n_1=0}^{\infty} \rightarrow \frac{1}{2 \pi} \int d^2\alpha_k \), and the Kronecker \( \delta \) turns into the Dirac \( \delta(\sum_{n_1=0}^{\infty} |\alpha_n|^2 - N) \). Thus the classical counterpart of the above formula reads

\[ Z(N,\beta) = \int \frac{d^2\alpha_0}{\pi} \ldots \int \frac{d^2\alpha_K}{\pi} e^{-\beta \hbar \omega \sum_{x=0}^{K} |\alpha_x|^2} \delta(\sum_{x=0}^{K} |\alpha_x|^2 - N) \]

\[ = \frac{1}{K!} \left( \frac{1 + \xi N}{\beta \hbar \omega} \right)^K. \]  
(A2)

where \( \xi = e^{-\beta \hbar \omega}. \)

Note that the expression \( \sum_{k=0}^{K} \frac{1}{\beta \hbar \omega} \) is just equal to \( \frac{1}{\beta \hbar \omega} \left( \frac{K+1}{K} \right) \), and the whole sum of products can be rewritten in the simpler form

\[ Z(N,\beta) = \frac{1}{K!} \left( \frac{1 + \xi N}{\beta \hbar \omega} \right)^K. \]  
(A3)

Finally, using the Newton formula, we can further simplify the partition function as

\[ Z(N,\beta) = \frac{1}{K!} \left( 1 - \frac{1}{1 - \frac{\xi N}{(K+1)}} \right)^K. \]  
(A4)

In the same manner, we can compute the partition function for excited atoms as

\[ Z_{\text{ex}}(N_{\text{ex}},T) = \frac{\xi^{N_{\text{ex}}}}{(K-1)!} \left( \frac{1 - \frac{\xi N_{\text{ex}}}{(K+1)}}{\beta \hbar \omega} \right)^{K-1}, \]

where \( N_{\text{ex}} \) is the number of atoms in all excited states. Thus the probability of finding exactly \( N_{\text{ex}} \) excited atoms in the sample of \( N \) atoms at the temperature \( T = \frac{\hbar \omega}{k_B} \) is

\[ P_\text{ex}(N_{\text{ex}},T) = \frac{Z_{\text{ex}}(N_{\text{ex}},T)}{Z(N,\beta)} = \frac{\xi^{N_{\text{ex}}}}{1 - \xi N} \left( 1 - \xi^{N_{\text{ex}}} \right)^{K-1}. \]  
(A5)