Monte Carlo method, classical fields and Bose statistics

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ABSTRACT

In this paper we combine the classical fields method with the Monte Carlo approach for description of statistical properties of a Bose–Einstein condensate. We show that the canonical ensemble of interacting classical fields can be generated using Metropolis algorithm. We obtain a probability distribution of the condensate occupation for the weakly interacting Bose gas at low temperatures and pay a particular attention to the two momenta of this distribution: mean and variance of the condensate occupation.

1. Introduction

Statistics of a multiparticle quantum state is at the heart of quantum physics. Fock, coherent, thermal or squeezed states of photons are all studied both theoretically and experimentally. With the advent of experiments with quantum degenerate atomic interactors the interest in the statistical properties of the Bose and Fermi gases has been revived. In this paper we concentrate our attention on the canonical ensemble of bosons confined by a trapping potential. It should be stressed from the very beginning that there are two major differences between photons and atoms. While photons are easily created and destroyed, the number of atoms is in the relevant ultra low temperatures strictly conserved. Besides, while photons are virtually noninteracting (except via host atoms, like in nonlinear optical processes) atoms do interact and their gross statistical features are modified by interactions.

Even the case of an ideal Bose gas was not fully understood when the atomic condensates were first created. A number of papers devoted to this problem demonstrated substantial differences between grand canonical (clearly not applicable to trapped atom experiments) canonical and microcanonical ensembles [1]. Exact results are available for the ideal Bose gas [2–4].

Understanding of equilibrium statistical properties of a weakly interacting Bose gas is still a challenge. Attention was mostly devoted to somewhat academic case of a finite number of atoms confined in a cubic volume with periodic boundary conditions for the multiparticle wave function. In 1D, and with the usual contact interaction, a lot is known about the eigenvalues and the eigenvectors of the N-particle Hamiltonian [5]. In more realistic 3D we have to apply approximations. Still, in the box confinement with periodic boundary conditions we know at least the condensate wave function. It is simply a zero momentum state. We also know analytically the dispersion relation and the wave functions of quasiparticle excitations – the Bogoliubov spectrum [6]. None of the two is analytically available for a realistic harmonic potential. In the box, for very low temperatures one can calculate analytically [7] the width of the probability distribution of the condensate occupation. The idea is rather simple: in the thermal state one assumes a free Bose statistics in every mode of the collective excitation. A generalization of the [7] approach, including the whole and not only the phonon branch of the spectrum, is presented in [8]. However, treating the quasiparticles in each mode as an ideal Bose gas one ignores their mutual interaction.

At higher temperatures the Bogoliubov spectrum gets modified – it goes to a form, known as Bogoliubov–Popov spectrum [9], which explicitly depends on the number of condensed atoms rather than their total number. One can still distribute the atoms among these quasiparticles according to the Bose statistics but the simplest approach [10], in which the occupation of the condensate, entering the spectrum, is kept at its mean value runs into a contradiction: the object of the study – the number of condensed atoms is a stochastic variable whose actual value depends on the number of excitations. In a recent paper [11] this shortcoming has been overcome and the treatment presented accounts for the fluctuating number of the condensed atoms and thus fluctuating spectrum of quasiparticles in a self-consistent way. Moreover, a secular term has been extracted from that in the full hamiltonian, which describes the interaction between the quasiparticles. Still, the interaction between quasiparticles was treated in a rather crude approximation.

In this paper we are going to present the first results for the fluctuating number of condensed atoms that fully account for the interaction between quasiparticles. Of course some other approximation will be made.
In our recent paper [13] we have shown that appropriate choice of the cut-off statistical properties of the condensate calculated with the help of the classical fields is nearly identical with the exact quantum one for the ideal Bose gas. In thermodynamic limit the optimal cut-off satisfies:
\[ \frac{\hbar^2 K_{\text{max}}}{2m k_B T} = \pi \left( \frac{(3/2)^2}{4} \right) , \]
where \( T \) is a temperature and \( k_B \) is the Boltzmann constant and \( \langle x \rangle \) is the Riemann zeta function. For finite system the correction to the formula (8) depends weakly on the temperature [13].

Within this approximation, the classical probability distribution of finding the system in a given configuration of the mode amplitudes is:
\[ P(a_k) = \frac{1}{Z} \exp \left[ -E_\phi / k_B T \right] , \]
\( Z \) is the canonical partition function and the restriction to the fixed number of \( N \) atoms is a constraint on the amplitudes:
\[ \sum_{k \leq K_{\text{max}}} |a_k|^2 = N . \]
Our task now is to generate numerically the probability distribution of the condensate population (zero momentum component occupation). To this end we shall use the powerful Monte Carlo algorithm. Similar method has been used to determine a shift of the critical temperature induced by the presence of interactions [14].

2. The model

In this paper we consider \( N \) bosons confined in a cubic box of length \( L \) with periodic boundary conditions and interacting via a zero range potential characterized by the \( s \)-wave scattering length \( a \). Thus the full Hamiltonian in second quantization takes a form:
\[ H = \int d^3r \left( \frac{p^2}{2m} + V(r) + \frac{g}{2} \sum_{s} \int d^3r' |\Psi(r)|^2 |\Psi(r')|^2 \right) , \]
where the first term represents the kinetic energy of the gas and the second is the interaction energy of the contact binary collisions. The atomic field operators obey the standard equal time Bose commutation relations with the only nonzero one:
\[ [\Psi(r), \Psi'(r')] = \delta(r-r') , \]
and the coupling constant expressed in terms of the scattering length \( a \) and mass \( m \) is:
\[ g = \frac{4\pi \hbar^2 a}{m} . \]
It is convenient to expand the field operator in the plane wave basis:
\[ \Psi(r) = \sum_{k} \varphi_k \frac{1}{\sqrt{V}} e^{i k \cdot r} , \]
where \( \varphi_k \) is the bosonic annihilation operator of particle with momentum \( \hbar k \). The quantized plane waves are characterized by the wave vectors:
\[ k = \frac{2\pi}{L} (n_1, n_2, n_3) , \]
where \( n_1, n_2, n_3 \) are integers. The classical field approximation consists of: (1) replacement of the creation and annihilation operators of the plane waves by the complex amplitudes \( \varphi_k \), (2) restriction of the summation over modes to a finite number extended all the way to the momentum cut-off \( K_{\text{max}} \). This way the field operator \( \Psi(r) \) is replaced by the classical field of well defined number of momenta modes:
\[ \Phi(r) = \sum_{k \leq K_{\text{max}}} \varphi_k \frac{1}{\sqrt{V}} e^{i k \cdot r} , \]
and the energy given by:
\[ E_\phi = \int d^3r \left( \frac{p^2}{2m} \Phi(r) + \frac{g}{2} \sum_{s} \int d^3r' |\Phi(r)|^2 |\Phi(r')|^2 \right) . \]
In our recent publication [13] we have shown that with a proper choice of the cut-off the statistical properties of the condensate calculated with the help of the classical fields is nearly identical with the exact quantum one for the ideal Bose gas. In thermodynamic limit the optimal cut-off satisfies:
\[ \hbar^2 K_{\text{max}} = \pi \left( \frac{(3/2)^2}{4} \right) . \]

3. The method

The major problem in generating the canonical ensemble is to sample a phase space of all classical amplitudes \( \{a_k\} \). The uniform sampling of this many dimensional phase space is evidently inefficient. The question of how to sample only the relevant phase space regions has been answered in the middle of the last century [15]. The main idea of the suggested Monte Carlo method is to generate a Markovian process of a random walk in the phase space. All states of the system visited during this walk are becoming the members of the statistical ensemble and are used in the ensemble averages.

We adopt the Metropolis scheme [15] to the system of the classical fields as described above. In order to obtain a statistical average of any observable \( A \)
\[ A = \frac{1}{V} \sum_{i=1}^{N} \langle \Phi_i | A | \Phi_i \rangle , \]
one should generate \( V \) copies of classical fields \( \Phi_i \). The canonical average is obtained in the limit of \( V \rightarrow \infty \) provided that a number of members of the ensemble with energy \( E_\phi \) is proportional to the Boltzmann factor \( e^{-E_\phi / k_B T} \). This goal can be achieved in a random walk where a single step of the Markov process is defined as follows:

1. A set of amplitudes \( \{a_k\} \) determines a state selected to be a member of the canonical ensemble at the s-th step of the random walk. The corresponding energy \( E_\phi \) of the classical field is calculated according to (7). As the initial condition \( s = 1 \) any state satisfied the condition (10) may be chosen as a member of the ensemble.
2. A trial set of amplitudes \( \{a_k\}^\prime \) is generated by a random disturbance of \( \{a_k\} \rightarrow \{a_k + \delta_k\} \) followed by the normalization to account for the condition (10). This way a trial classical field \( \Phi_\phi \) is obtained. The corresponding energy \( E_\phi^\prime \), the energy difference \( \Delta E = E_\phi^\prime - E_\phi \), as well as the Boltzmann factor \( p = e^{-E_\phi^\prime / k_B T} \) are then calculated.
3. A new member of the Markov chain \( \{ x^{(k+1)} \} \) is selected according to the following prescription:

- if \( A_s < 0 \) then the trial state becomes a new member of the ensemble, \( \{ x^{(k+1)} \} = \{ x^{(k)} \} \);
- if \( A_s > 0 \) then a random number \( 0 < u < 1 \) is generated. If \( u < p_s \), then the trial state becomes a new member of the ensemble, \( \{ x^{(k+1)} \} = \{ x^{(k)} \} \) and \( \{ x^{(k+1)} \} \) is once more included in the ensemble, \( \{ x^{(k+1)} \} = \{ x^{(k)} \} \).

In the limit of infinite Markov chain the selected states form the canonical ensemble.

A convergence of the procedure is the fastest if approximately every second trial state becomes a member of the ensemble. This factor depends on the assumed maximal value of the displacements \( \delta_{\text{max}} \) which can be modified during the walk. Let us add that some number of the initial members of the ensemble should be ignored in order to avoid an influence of the arbitrarily selected initial state of the system.

As a test of the numerical convergence of the algorithm we use the Bogoliubov method which is applicable at low temperatures, where excitations are of the form of independent quasiparticles of energy:

\[
u_k = \sqrt{(E_k + gn)^2 - (gn)^2}, \quad (12)
\]

where \( E_k = \hbar^2 k^2 / 2m \) and \( n = N/V \) is a particle density. In the limit of macroscopic occupation of quasiparticle modes the thermal part of the classical fields, \( \Phi_f(r) = \Phi_f - \Phi_0 \), can be expressed as:

\[
\Phi_f(r) = \sum_{k \neq 0} \left( U_k b_k \frac{1}{\sqrt{V}} e^{\omega r} + V_k b_k^* \frac{1}{\sqrt{V}} e^{-\omega r} \right), \quad (13)
\]

where \( U_k + V_k = 1 \) and

\[
U_k = \frac{E_k}{E_k + 2gn} \quad \text{and} \quad V_k = \frac{1}{E_k + 2gn}^{1/4}. \quad (14)
\]

In Eq. (13) the summation is limited by the cut-off momentum because we restrict the field \( \Phi_f(r) \) to the classical modes. \( b_k \) are amplitudes of the quasiparticles' excitations which at a state of the thermal equilibrium are distributed according to the classical statistics [16]:

\[
P(b_k^2) = \frac{\delta_{\text{max}}}{\pi k_B T} e^{-\omega k^2 / k_B T}. \quad (15)
\]

Our strategy is the following: (i) for a given temperature and the cut-off momentum we generate the amplitudes of the quasiparticles \( b_k \) according to (15), (ii) next we determine the plane wave amplitudes \( \omega_k = U_k b_k + V_k b_k^* \) and a number of thermal particles \( N_T = \sum_{k \neq 0} |\omega_k|^2 \), (iii) the occupation of the condensate is computed as \( N_0 = N - N_T \) and the data are collected to get the histogram corresponding to a condensate occupation probability distribution.

4. The results

The probability distribution of the condensate occupation of the ideal Bose gas (IBG) trapped in a periodic box can be found analytically within the full quantum treatment in one spatial dimension only [13]. These results are the best benchmarks for the classical fields Monte Carlo algorithm described in the previous section. In Fig. 1 we compare results of the Monte Carlo calculations with the exact quantum formula, and with the analytic expression based on the classical fields method [13]. For the classical fields treatments i.e. the Monte Carlo and the analytic one, we chose the optimal cut-off of high momenta states [13]. The probability distributions of the occupation of excited modes (thermal cloud) for various temperatures are shown in Fig. 1. The agreement between these three results is remarkable.

After gaining a confidence that the Monte Carlo algorithm for the classical fields was very efficient in reproducing statistical properties of the ideal Bose gas we may study a weakly interacting case. In Fig. 2 we present results for the 3D periodic box potential. We compare a probability of the thermal cloud occupation \( P(N_{ex}) \) of the ideal Bose gas with the corresponding probabilities of the interacting system. Each curve corresponds to a different interaction strength parameter \( a^{1/3} \) but the same temperature. The results for the ideal Bose gas are obtained in two ways: using the asymptotic quantum formula given in [10] (full line) and according
results of the Monte Carlo simulations while dashed lines are results obtained with the help of Bogoliubov method. Parameters of the simulations are: \( \epsilon = 3 \times 10^7 \) Monte Carlo steps and \( \epsilon = 3 \times 10^6 \) realizations of the field in the Bogoliubov method. Number of bosons is \( N = 10,000 \) and the cut-off was chosen according to \( \beta \hbar^2 K_{\text{max}}^2 / 2m = 2.68 \). Two sets of data correspond to two different temperature: \( T/T_c = 0.057 \) (number of momenta modes \( \epsilon = 4^3 \)) – full circles, and \( T/T_c = 0.129 \), (number of momenta modes \( \epsilon = 6^3 \)) – full squares. The leading term of condensate fluctuation in the large \( N \) limit \( [10] \) is \( dN_0 / N \approx 0.00129 \) at \( T/T_c = 0.057 \) and \( dN_0 / N \approx 0.0029 \) at \( T/T_c = 0.129 \) what is comparable with ours results.

\[
\int dN_0 / N \approx 0.00129 \quad \text{at} \quad T/T_c = 0.057 \\
\int dN_0 / N \approx 0.0029 \quad \text{at} \quad T/T_c = 0.129
\]

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\]

Condensate fraction (left) and condensate fluctuations (right) versus \( T/T_c \). Points are the results of the Monte Carlo simulations (with \( 3 \times 10^7 \) steps) for the ideal gas (full circle) and for the interacting system \( \epsilon = 0 \) (3D box potential). Points correspond to finite system (with \( 3 \times 10^7 \) steps) and \( \epsilon = 3 \times 10^6 \) realizations of the field in the Bogoliubov method. Number of bosons is \( N = 10,000 \) and the cut-off was chosen according to \( \beta \hbar^2 K_{\text{max}}^2 / 2m = 2.68 \). The number of different momenta modes varies with the temperature from \( \epsilon = 2^3 \) for the lowest one to \( \epsilon = 20^3 \) for the highest temperature.

5. Conclusions

In this paper we have presented a promising method of studying statistical properties of the weakly interacting Bose gas. It is based on the classical fields approximation. Combined with the Metropolis algorithm it offers an efficient scheme for generating numerically the canonical ensemble of the Bose system. A very similar method has already been used to calculate the shift of the critical temperature induced by interactions \( [14] \). This notoriously difficult problem was studied by many authors and let them to vastly different predictions. The result of \( [14] \) is considered to be one of the most accurate. However, calculated there is the ratio of the shift to the critical temperature. This ratio is independent of the cut-off provided the cut-off is sufficiently large. Equipped with our earlier study of the optimal cut-off, we are now able to calculate the statistical properties of the interacting Bose gas as a function of temperature. Practically all results obtained to date for the statistics of the weakly interacting Bose gas (including the present paper) are obtained for the box confinement with the periodic boundary conditions. Our method may be extended to more realistic situations, such as the binding by the harmonic potential. The work in this direction is in progress.

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