

DEDICATED TO PROFESSOR IWO BIAŁYŃICKI-BIRULA ON HIS 90TH BIRTHDAY

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Fock State Sampling Method — Characteristic Temperature of Maximal Fluctuations for Interacting Bosons in Box Potentials

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We study the statistical properties of a gas of interacting bosons trapped in a box potential in two and three dimensions. Our primary focus is the characteristic temperature T_p , i.e., the temperature at which the fluctuations of the number of condensed atoms (or, in 2D, the number of motionless atoms) are maximal. Using the Fock state sampling method, we show that T_p increases due to interaction. In 3D, this temperature converges to the critical temperature in the thermodynamic limit. In 2D, we show the general applicability of the method by obtaining a generalized dependence of the characteristic temperature on the interaction strength. Finally, we discuss the experimental conditions necessary for the verification of our theoretical predictions.

topics: Bose–Einstein condensate, statistical ensembles, quantum gases

1. Introduction

The statistical properties of interacting ultracold gases of bosonic atoms and, in particular, of Bose–Einstein condensates (BEC) remain a considerable challenge of current interest. While the statistical properties of non-interacting gases are well described by a number of methods, a soluble model for interacting bosons exists only in one dimension. In two and three dimensions, reliable results are only available for weakly interacting gases at low temperatures within the Bogoliubov approximation. Hence, the dependence of the critical temperature on interaction remains a challenging issue.

Over the years, a large number of mutually exclusive predictions of the change of the critical temperature due to interactions were made [1–11]. Practically all of them dealt with a gas trapped in a three-dimensional cubic box potential. The conflicting results are summarized in Table I [2–14]. Note that even the sign of the correction was

uncertain initially. Later the consensus emerged that in the thermodynamic limit, the shift to the critical temperature is $\Delta T_c \approx 1.3 a \rho^{1/3}$, where ρ is the gas density, and a is the s -wave scattering length.

During the struggle to compute the shift of the critical temperature, a number of theoretical methods were used (see the review [11]). The correct result was eventually obtained by using the classical field approximation (CFA) [10]. The CFA method itself suffers from a cut-off problem, which was cleverly overcome in [10]. Recently, we proposed yet another method based on a direct quantum description of the system and the definitions of the statistical ensembles. The method, called the Fock state sampling (FSS) method [15], is presented in Sect. 2.

Most BEC experiments to date are performed with harmonic traps. However, recently Bose–Einstein condensates were created in nearly perfect box potentials [16]. Nonetheless, experimental verification of the theoretical prediction remains chal-

TABLE I

Coefficient c of the shift of the critical temperature $\Delta T_c/T_c = c a \rho^{1/3}$ obtained by various analytic and numerical methods. See also the review by J. Andersen [11]. In [14], four different many-body methods were used yielding results in the range $c \in [1, 6.7]$.

Authors	Ref.	Coefficient c
Grueter et al. (1997)	[2]	0.34 ± 0.06
Holzmann et al. (1999)	[3]	0.7
Holzmann et al. (1999)	[4]	2.3 ± 0.25
Baym et al. (1999)	[5]	2.9
Wilkens et al. (2000)	[6]	-0.93
Arnold et al. (2000)	[7]	1.71
Baym et al. (2000)	[8]	2.33
Souza Cruz et al. (2001)	[9]	3.059
Kashurnikov et al. (2001)	[10]	1.29 ± 0.05
Davis et al. (2003)	[12]	1.3 ± 0.4
Nho et al. (2004)	[13]	1.32 ± 0.14
Watabe et al. (2013)	[14]	1 to 6.7

lenging. One of the problems is due to the fact that experiments are performed with a finite number of atoms, and for such a system, there is no unique way of determining the critical temperature. Namely, for a finite-size system, the number of condensed atoms is an analytic function of temperature, and thus there is not a definite value of temperature beyond which the number of condensed atoms is strictly zero. The remedy for this difficulty, proposed in [17], is to study the temperature of maximal variance of the number of condensed atoms instead of the critical temperature. The temperature of the maximal variance tends to the critical temperature in the thermodynamic limit [17] and is well-defined for finite-size systems, which makes it applicable to gases exhibiting only quasi-condensation.

Experimentally, it is more demanding to measure the fluctuations of the condensate atom number than the mean of this number. However, the experimental difficulties were recently overcome due to a stabilization technique of the evaporation process [18], allowing for a measurement of the fluctuations [19]. Furthermore, it was shown that the canonical ensemble fails to describe the experimental situation, and one must invoke the microcanonical one [20]. These experiments directly measure the temperature of the maximal fluctuations rather than the temperature at which the condensate vanishes.

It is the purpose of this paper to discuss the interaction-induced shifts of the temperature of maximal fluctuations, which is referred to as the characteristic temperature T_p . Based on the FSS method, we provide, to our knowledge for the first time, results for a bosonic gas in a box potential in the microcanonical ensemble.

The paper is organized as follows. In Sect. 2, we briefly review the FSS method. Section 3 applies the method to a gas trapped in the three-dimensional box potential in both the canonical and microcanonical ensembles. In Sect. 4, the case of the two-dimensional box potential is discussed. Note that there is no phase transition and no critical temperature in this case, and nonetheless, the characteristic temperature can be defined. Section 5 concludes the discussion and provides an outlook on future experiments.

2. Fock state sampling method

We consider N bosonic atoms trapped in a box potential with periodic boundary conditions and interacting via short-range interaction potential. The Hamiltonian of the system is

$$\hat{H} = -\frac{\hbar^2}{2m} \int d^d r \hat{\Psi}^\dagger(\mathbf{r}) \nabla^2 \hat{\Psi}(\mathbf{r}) + \frac{g_d}{2} \int d^d r \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \hat{\Psi}(\mathbf{r}), \quad (1)$$

where $\hat{\Psi}(\mathbf{r})$ is a bosonic annihilation operator, m is a mass, and $g_d > 0$ is a coupling constant related to short-range interactions. In Sect. 3, we consider three-dimensional systems, where the coupling constant is $g_{d=3} \equiv g_{3D} = 4\pi\hbar^2 a/m$ and a is the scattering length. In Sect. 4, devoted to two-dimensional systems, we use the notation $g_{d=2} \equiv g_{2D}$. In the case of a box potential with periodic boundary conditions, the macroscopically occupied orbital (the BEC wave function in 3D) is just a constant function, i.e., a plane wave with momentum 0.

In what follows, we focus on the fluctuations of the number of atoms in BEC at finite temperature. We use the canonical and the microcanonical ensembles, which were shown to be close to the experimental reality [19, 20].

There are several different ways to describe the statistical properties of ultra-cold Bose gases theoretically. In this paper, we sample many-body states to generate a set of copies that properly approximates the canonical ensemble of a gas. Given a sufficiently large set of copies, the expectation values are defined as the average over the set. By post-selecting the set, we obtain results in the microcanonical ensemble. To define the appropriate Metropolis algorithm [21], we need to define “the stage”, which is the set of available states, and the “Metropolis dynamics” or the specific algorithm defining the Markov chain generating the approximation to the canonical ensemble.

2.1. Setting “the stage”

All states of N particles belong to the suitable Hilbert space. A convenient parametrization is provided by the basis of single-particle states in the

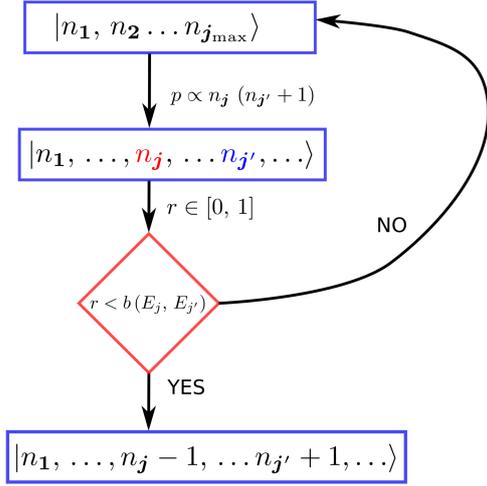


Fig. 1. Single step of the FSS method: one draws two states — one from which an atom might be taken (index j) and one in which the atom may land (index j') with probability distribution proportional to $n_j(n_{j'} + 1)$. The new state is accepted only if a random number r drawn from a uniform distribution in $[0, 1]$ is smaller than the Boltzmann factor b given in (5).

trapping potential. Since we consider box potentials with periodic boundary conditions, the basis states are just plane waves

$$f_{\mathbf{j}}(\mathbf{r}) := f_{j_x j_y j_z}(x, y, z) = \frac{1}{\sqrt{L_x L_y L_z}} e^{-i 2\pi(j_x x/L_x + j_y y/L_y + j_z z/L_z)}, \quad (2)$$

where L_x , L_y , and L_z are the lengths of the box potential and j_x , j_y , and j_z are positive and negative integers. It is worth stressing that due to translational invariance, these states remain eigenstates of the single-particle density matrix also for the interacting gas. Thus, the constant function $j_x = j_y = j_z = 0$ remains the condensate state also in the presence of interactions.

The space of all N -particle states is spanned by the Fock states

$$|\mathbf{n}\rangle := |n_1, n_2, \dots\rangle, \quad (3)$$

where n_j denotes the number of bosons in the single-particle state $f_{\mathbf{j}}(\mathbf{r})$. In the canonical ensemble, we fix the total number of atoms N and consider only the Fock states that contain N bosons

$$\sum_{\mathbf{j}} n_{\mathbf{j}} = N. \quad (4)$$

The whole Hilbert space contains all superpositions of all N -particle Fock states. The appropriate parameters are far too numerous for any efficient numerics. Instead, we restrict our set of available states just to the Fock states in (3), not accounting for their superpositions. This has two consequences. First, it neglects the phenomenon of quantum depletion. Thus, the method is expected to yield correct

results only for weak interactions. Second, it is not applicable to weakly interacting bosons confined in a harmonic trap, since, in this case, the condensate wave function is a superposition of many oscillator states.

2.2. Metropolis dynamics

The following algorithm defines our Markov chain used to generate the elements of our representation of the canonical ensemble. A single step of this algorithm is also shown in Fig. 1.

Each particle has the same probability of jumping out of a given single-particle state. The probability of jumping out is proportional to the number of particles in that state. The probability of landing in a given single-particle state is proportional to its occupation (stimulated process) plus one (to account for the spontaneous process). The acceptance criterion, usual for the Metropolis algorithm, is based on comparing a random number $0 < r < 1$ drawn from a uniform distribution versus the Boltzmann factor b of the initial and the final states

$$b(E_{\text{current}}, E_{\text{candidate}}) = e^{-\beta(E_{\text{current}} - E_{\text{candidate}})}, \quad (5)$$

where $\beta = 1/(k_B T)$, k_B is the Boltzmann constant and T is the temperature. The energy E_{current} is the expectation value of the Hamiltonian in the current Fock state. It is the sum of the kinetic energy and the interaction energy. The kinetic energy is simply

$$E_{\text{kin}} = \sum_{\mathbf{j}} n_{\mathbf{j}} e_{\mathbf{j}}, \quad (6)$$

where $e_{\mathbf{j}}$ is the energy of the \mathbf{j} -th level, i.e.,

$$e_{\mathbf{j}} := \frac{2\pi^2 \hbar^2}{m} \left[\left(\frac{j_x}{L_1} \right)^2 + \left(\frac{j_y}{L_2} \right)^2 + \left(\frac{j_z}{L_3} \right)^2 \right]. \quad (7)$$

The short-range interaction energy, which in the general case is a nontrivial quadratic form, reduces to a single sum in the case of a box potential and is averaged in a single Fock state

$$E_{\text{int}} = \left\langle \mathbf{n} \left| \frac{g_{3D}}{2} \int d^3r \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \right| \mathbf{n} \right\rangle = \frac{g_{3D}}{2} \left(2N(N-1) - \sum_{\mathbf{j}} n_{\mathbf{j}}^2 \right). \quad (8)$$

Moreover, for comparison of the Boltzmann factors, only the difference of the energies of the final and initial state enters (see (5))

$$E_{\text{current}} - E_{\text{candidate}} = e_{\mathbf{j}} - e_{\mathbf{j}'} + g_{3D}(n_{\mathbf{j}'} - n_{\mathbf{j}}), \quad (9)$$

where \mathbf{j} and \mathbf{j}' are the indices of the single-particle states from which the atom escaped and in which it lands, respectively. A single step of this algorithm is presented in Fig. 1.

The algorithm satisfies the detailed balance principle and guarantees access to all important N particle states. When the number of steps goes to infinity, the expectation value of any physical quantity

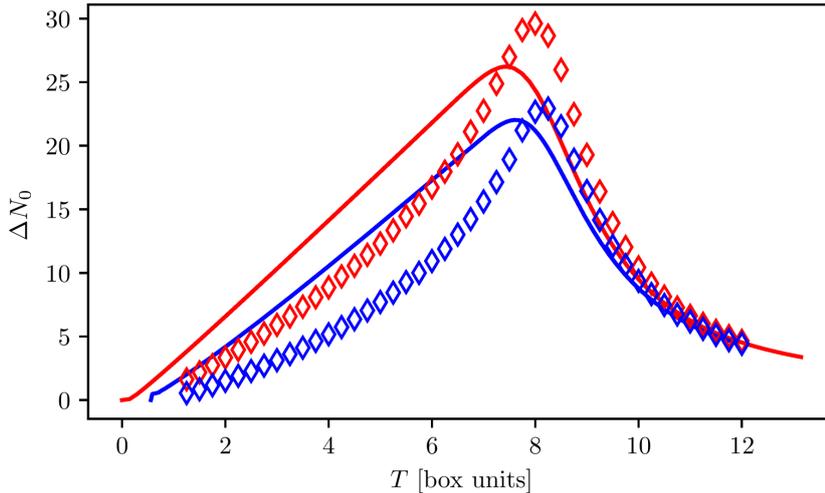


Fig. 2. Standard deviation of the number of condensed atoms confined in a 3D box potential with periodic boundary conditions for $N = 300$ atoms for a non-interacting (solid lines) and an interacting gas with a gas parameter $a\rho^{1/3} = 0.05$ (empty diamonds). Red symbols indicate canonical and blue microcanonical results. The solid lines are exact, obtained with the help of recurrence relations. The empty diamonds represent canonical and microcanonical results obtained with the help of the Fock state sampling method. Note similar shifts of the characteristic temperature in both statistical ensembles. Also, note that the maximal fluctuations are increased by interactions.

does not depend on the state used to initiate the algorithm. In practice, we perform only a finite number of steps and discard approximately $10N$ initial steps during which the quantities of interest are not only fluctuating but also drifting.

Importantly, the Fock state sampling method also offers access to the microcanonical ensemble. This is accomplished simply by reducing the number of states to those with energy in the small interval around the most probable one.

In the following, we present the results obtained with Fock state sampling method (FSSM) for a gas in a 3D (Sect. 3) and 2D (Sect. 4) box potential, including interactions between the atoms.

3. Characteristic temperature for gas in 3D box potential

We illustrate the results of our method for ultracold gases of bosonic atoms in a 3D box potential in Fig. 2. The figure shows the temperature dependence of the standard deviation of the number of atoms in a Bose–Einstein condensate ΔN_0 for both canonical and microcanonical ensembles. The results for the non-interacting gas are exact and obtained with the recurrence relations [6], while the results for the interacting gas are obtained with the FSS method described in the previous section. Note that the microcanonical ensemble yields significantly lower fluctuations. Moreover, interactions increase the peak fluctuations in both ensembles, and similarly, the temperature of the maximal fluctuations is increased.

The related shift of the critical temperature due to collisions in weakly interacting Bose gas in a 3D box potential has been the subject of a longstanding debate, as outlined in the introduction. The final result for the correction was obtained with a sophisticated numerical method [10], based on techniques developed over the past 20 years. Our method, on the contrary, although approximate, is simple to implement for as many as 10 000 atoms.

Here, we study the temperature of the maximal fluctuations T_p instead of looking at the critical temperature T_c . This characteristic temperature is well-defined for systems with a finite number of atoms. Moreover, it has been recently shown that it can be measured for a Bose gas in a harmonic trap [19, 20].

Thus, the main quantity of interest is the interaction-induced relative shift to the characteristic temperature T_p

$$\delta T_p(N, a) := \frac{T_p(N, a) - T_p(N, 0)}{T_p(N, 0)}, \quad (10)$$

where $T_p(N, a)$ is the characteristic temperature for a gas with N atoms interacting with the s -wave scattering length a . To find the dependence of δT_p on N and a , we study the system with atom numbers ranging from 100 to 10000 and interaction strengths g corresponding to gas parameters $a\rho^{1/3}$ from 0.005 to 0.02. All temperatures are given in units of $2\pi^2\hbar^2/(mk_B L^2)$.

The results are illustrated in Fig. 3, which shows the relative standard deviation of the number of condensed atoms as a function of temperature for different total numbers of atoms and various interaction strengths g . Since the main focus is the shift

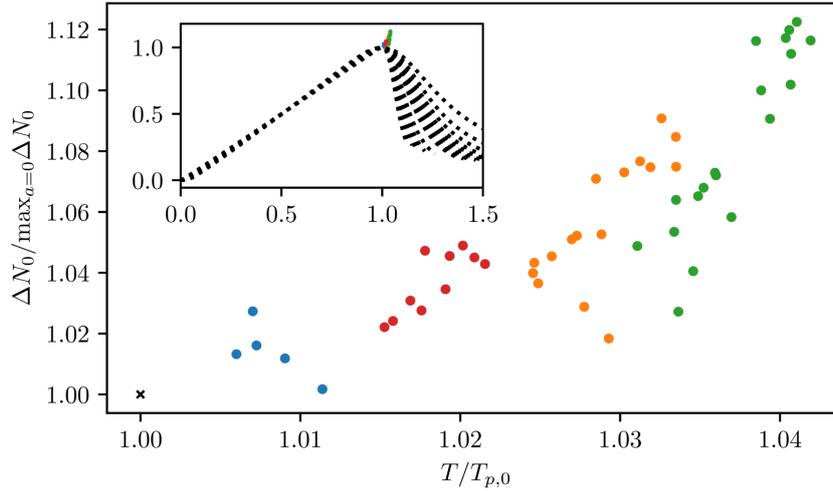


Fig. 3. Relative standard deviation of the BEC atom number for an interacting gas (colored points) for various total numbers of atoms, and interaction strengths. All points are rescaled by the maximal value of the fluctuations in the non-interacting case. Results for systems with the same gas parameter are marked with the same color, i.e., $a\rho^{1/3}$ corresponds to 0.005 (blue), 0.01 (red), 0.015 (orange), 0.02 (green). The quantity $T_{p,0}$ is the temperature of maximal fluctuations of the non-interacting gas and the symbol “x” marks the reference point — the maximal BEC fluctuations of the non-interacting gas. The atom number is in the range $N = 100, 200, \dots, 1000, 2000, \dots, 10000$. The inset shows an overview of the entire temperature range with the results for the non-interacting gas (dashed lines).

of the characteristic temperature T_p , all results for the non-interacting gas are normalized in terms of both the maximal value and its temperature. The same scaling factors are used for the results for the interacting gas, i.e., the temperature (relative standard deviation) is divided by the temperature $T_{p,0}$ (maximal relative standard deviation) of the non-interacting gas with the same number of atoms. After rescaling, one can easily follow the interaction-induced shifts. The points of a given color show the maximal variance at the characteristic temperature for various atom numbers N and scattering lengths a , but a common gas parameter $a\rho^{1/3}$.

Note that the maximal relative standard deviations are grouped into small regions for a common gas parameter. For larger gas parameters corresponding to larger interactions, the maximal relative standard deviations are larger and are reached at higher temperatures as compared to the non-interacting gas.

We fit the average shift for each characteristic temperature with a linear dependence on the gas parameter and obtain

$$\delta T_p \approx (2.039 \pm 0.014) a\rho^{\frac{1}{3}} \quad (11)$$

in the range of the number of atoms N between 4000 and 10000. Thus the scaling is similar to the one obtained for the critical temperature of an infinitely large system, while the prefactor is larger.

Note that the maximal relative standard deviations for a common gas parameter form elongated regions, indicating that the maximal variance and the characteristic temperature may have a further

dependence on the scattering length and density. The remaining spread of the points indicates the precision of our method.

Also note that interactions increase the maximal fluctuations in this case. This point has also been the subject of a long-standing controversy (see, for instance, the inset in Fig. 4 in [19]). It was recently addressed using the FSS method [15], showing that the size of the fluctuations depends on all system parameters, and thus it is not possible to generalize the effect of interactions on the magnitude of condensate fluctuations.

Importantly, the characteristic temperature discussed in this section is also well-defined for systems that do not exhibit a phase transition in a thermodynamic limit. An example of such a system is a gas in a 2D box potential, discussed in the next section.

4. Characteristic temperature in 2D box potential

It is well known that Bose–Einstein condensation appears as a phase transition for sufficiently high dimensions. In a box potential, the phase transition occurs only in three dimensions, while it is absent in lower dimensionality. Despite the fact that there is no phase transition and, therefore, no critical temperature in the case of two dimensions, the notion of the characteristic temperature T_p , marking the temperature of maximal fluctuations, is still applicable. Of course, in the absence of the phase transition, interactions still affect the fluctuations.

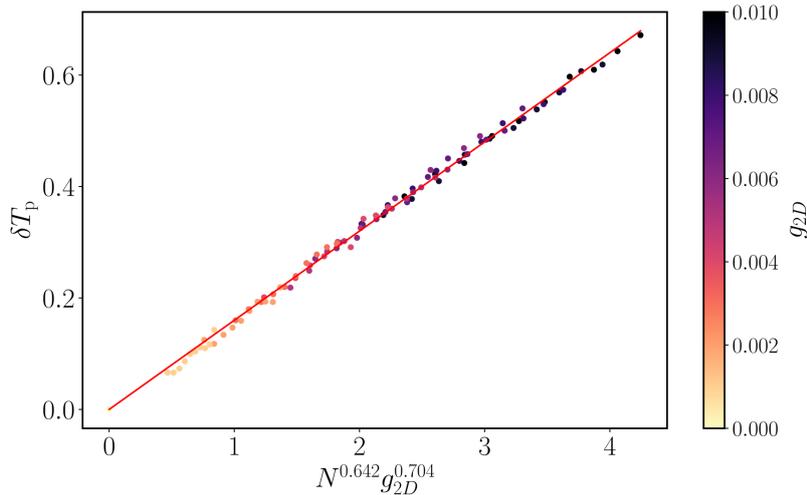


Fig. 4. Relative shift of the characteristic temperature for Bose gases in a 2D box potential with periodic boundary conditions due to interactions. The coupling constant g_{2D} was varied from 0 to 0.01 and the number of atoms was adjusted from 600 to 1500.

We illustrate this by investigating a two-dimensional box potential with periodic boundary conditions. The calculation is analogous to the 3D box potential, and the condensate wave function is still a constant one, regardless of interaction. The algorithm, after omitting all Z -dependent variables, is identical to the one introduced in the previous section. The relative shift of the characteristic temperature due to interactions was calculated for various atom numbers N and interaction strengths g_{2D} , as defined in the Hamiltonian (1). In this section, we do not refer to the gas parameter, which would be more complicated than in the 3D case.

Figure 4 shows this shift as a function of $g_{2D}^\alpha N^\beta$ with optimally chosen exponents α and β obtained from a fit to the data, yielding

$$\delta T_p^{(2D)}(N, g_{2D}) := (0.16 \pm 0.03) N^{0.642 \pm 0.015} g_{2D}^{0.704 \pm 0.006}. \quad (12)$$

The stated errors may be reduced at the expense of the numerical effort. The convergence is very slow, and errors scale with the square root of the number of Metropolis steps.

The results presented in this section illustrate the power and generality of the FSS method. The method is conceptually very simple, and its successful application merely requires a numerical effort.

5. Conclusions

In conclusion, we have investigated the fluctuations of the ideal and weakly interacting Bose-Einstein condensates trapped in box potentials with periodic boundary conditions. The temperature of maximal BEC atom number fluctuations T_p was analyzed under various conditions. The advantage of

T_p over T_c lies in the fact that it is unambiguously defined also for a finite system, and it can be studied also in systems that do not exhibit phase transition.

In our study, we used the Fock state sampling method, which turns out to be easy to use, exact for the non-interacting system (see [15]), and applicable to a wide range of problems. With this method, we found the shift of the characteristic temperature in the 3D box potential to be $\approx 2.03 a \rho^{1/3}$, where a is the scattering length, and ρ is the gas density. This is reasonably close to the expected shift of the critical temperature in this system $\approx 1.3 a \rho^{1/3}$.

We also applied our method to a two-dimensional system and obtained a generalized dependence of the characteristic temperature on the interaction strength and atom number $\approx 0.16 N^{0.642} g_{2D}^{0.704}$, showing the applicability in a system that does not exhibit a phase transition.

Experimentally, the recent realization of box potentials provides an opportunity to address the predictions presented above. In particular, combining box potentials with atomic species that allow for tunability of the interaction strength will provide access to a wide variation of gas parameters.

Box potentials are typically created using blue-detuned light to form the walls of a box, such as, e.g., a hollow beam with two narrow light sheets as end caps [22]. To flatten the bottom of the potential, gravity must be compensated using a magnetic field gradient. Alternatively, a light field with a linearly varying intensity produced by an acousto-optic deflector can be used [23]. The necessary beam shapes for box potentials can be generated using spatial light modulators, digital micromirror devices, or specialized optical elements such as axicons.

Tunability of the scattering length would be highly beneficial to isolate the effect of interactions on the characteristic temperature and the

magnitude of atom number fluctuations. This can be achieved by adjusting the magnetic field near a Feshbach resonance [24]. Since a magnetic field gradient is the most common way to cancel gravity within a box potential, this will typically necessitate independent control of the magnetic field gradient and its mean value. The field gradient will thus introduce a spatial dependence of the scattering length, and hence atomic species with broad resonances such as, e.g., the bosonic isotopes of potassium should be used.

Furthermore, it is important to distinguish between BEC and the thermal part of partially condensed atomic clouds to measure the atom number fluctuations. Thus, the bimodality of the momentum distribution is crucial for determining the BEC number and the number of thermal atoms. Fortunately, both the bimodality and an appropriate fitting function for the thermal cloud have been confirmed [16] experimentally.

The most significant outstanding challenge towards the measurement of fluctuations proposed here is the combination of box potentials with atom number stabilization. There are two primary technical sources of variations in the total number of atoms. The first one is due to the statistical nature of evaporative cooling, which relates the atom number to the temperature. This is predictable and can be accounted for in the evaluation of atom number fluctuations. The second source of atom number variation is typically due to various technical noise sources in the experiment and should be minimized since it can distort the measured atom number fluctuation when different mean values of the BEC atom number are probed. Thus, to conduct the experiment, it will be necessary to combine the box potential with atom number stabilization. However, it is not yet clear whether it is sufficient to stabilize the atom number before loading the cloud into the box potential or if methods for stabilization within the box potential must be developed.

The combination of the Fock state sampling method and current experimental developments will allow for further experiments in the near future. Especially since the FSSM can provide precise predictions for experimentally relevant atom numbers in a variety of potentials, the time has now come for a new generation of experiments on these fundamental questions.

Acknowledgments

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