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Monte Carlo simulation of Bose-Einstein condensation in a harmonic potential trap

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M R Shipra[1], K M E Hasan[1], A Islam[2], K H Tuhin[1], M E Hoque[1*]

[1]Department of Physics, Shahjalal University of Science and Technology, Sylhet

[2]Department of Theoretical Physics, University of Dhaka

[*]Corresponding Author's Email: mjonyh-phy@sust.edu

Abstract

Bose-Einstein condensation has been attained using Monte Carlo simulation on non-interacting ideal bosons confined in a harmonic potential trap at near-zero temperature (~0K). A connection has been established between the cyclic paths originated by the interchange of identical bosons and condensation. At low temperatures, long cycles appear and condensation is obtained consequently. The simulated result is in perfect agreement with the corresponding theoretical findings.

Keywords: Bose-Einstein condensation; path integral Monte Carlo simulation; harmonic potential trap; diagonal density matrix.

1. Introduction

In 1924, Satyendranath Bose proposed a new statistic for indistinguishable particles of integral spin; subsequently, these particles became known as bosons [1]. His discovery paved the way to discovering a new state of matter at a temperature close to absolute zero (-273.16°C), namely Bose-Einstein condensate [2]. This state is formed by cooling a dilute gas of bosons to temperatures near absolute zero. At such a cool temperature, a large fraction of bosons occupies a singular state, i.e., the ground state, defying Pauli's exclusion principle. The observation of Bose-Einstein condensate was produced in a gas of rubidium atoms [3] using laser and magnetic traps that constitute a potential trap of harmonic nature [4].

The statistical mechanical properties of a system can be determined from its density matrix [5] $\rho(\chi, \chi', \beta)$. This density matrix is a function of coordinates x and x′ and inverse temperature β that can be thought of as an imaginary time. For N slices in β, the convolution property of the density matrices dictate that the density matrix can be broken into N density matrices in the domain. Each of them is a function of the coordinates of the intermediate steps and temperature N times greater and evaluated as a multiple integral over the intermediate coordinates [6]. These coordinates form the intermediate steps in the journey from x to x′ that constitute a path. Density matrices and partition functions are represented as multiple integrals over the paths.

Bosons are identical particles and for a system of N bosons, the density matrix is comprised of totally symmetric eigenfunctions [6]. Hence, an alternative way of the occurrence of an event, namely, the interchange of the particles must be considered as well. The interchange generates motion and its contribution decreases if the temperature is high or the particles are spread out [5].

Since, the partition function of a system only involves a diagonal density matrix, for a bosonic system, its path must close on any permutation of its starting position. All N! closures or cycles contribute to the partition function [7].

The cycles form a convoluted diagonal density matrix, which is comprised of many non-diagonal density matrices. The lengths of the cycles depend on temperature. The probability of finding longer cycles increases with lowering temperature. At zero temperature, the probability becomes independent of cycle length [8].

All N particles can be sampled in one cycle or the other. A closed path is constructed using the Lévy construction method [9]. This path represents the spatial distribution of the particles in the trap. The particles in a few long cycles at low temperatures populate the single-particle ground state [8].

In this article, the behavior of dilute Bose gas has been investigated numerically in the presence of a three-dimensional simple harmonic potential. Necessary theoretical formulations for the simulation are provided along with an appropriate discussion on this topic.

2. Theory

The theoretical framework is based on the density matrix formalism of identical Bose particles. Diagonal density matrices govern quantum statistical systems. The formulation of density matrices in a harmonic potential represents the statistical state of particles confined in a harmonic trap [5].

The probability of finding a particle in a position x in the ground state of a harmonic trap [10],

$$\pi(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} exp\left(-\frac{m\omega}{\hbar}x^2\right) \qquad 1$$

The diagonal density matrix for such a system appears as a Gaussian [6],

$$\rho(x,x,\beta) = A\, exp\left[-\frac{x^2}{2\,\sigma^2}\right] \qquad 2$$

Where,

$$\sigma^2 = \frac{\hbar}{2m\omega tanh\left(\frac{\hbar\omega}{2}\beta\right)}$$

and

$$A = \sqrt{\frac{m\omega}{2\pi\hbar\, sinh(\hbar\omega\beta)}}$$

The trace of the diagonal matrix $\rho(x,x,\beta)$ creates the partition function of this system [8],

$$Z(\beta) = \int dx\, \rho(x,x,\beta) = \frac{1}{2sinh\left(\frac{\hbar\omega}{2}\beta\right)} \qquad 3$$

Bosons are identical particles and their wave functions are symmetric, hence, permutations among the particles must be considered. The density matrix can be symmetrized for bosons by summing over permutations P[11],

$$\rho(x,x',\beta) = \frac{1}{N!}\sum_{p}\rho(x,x'_p,\beta)$$

A motion of a particle from one position to a permuted position is reckoned in this case. This motion continues until the particle comes back to its original position and a cycle is complete. This motion creates a closed path which can be generated by Lévy construction [9].

The Lévy construction yields a Gaussian by the probability of x_k [8],

$$\pi(x_k|x',x'') \propto exp\left[-\frac{1}{2\sigma^2}(x_k - \langle x_k\rangle)^2\right] \qquad 4$$

where,

$$\langle x_k\rangle = \frac{\Upsilon_2}{\Upsilon_1}$$

$$\sigma = \frac{1}{\sqrt{\Upsilon_1}}$$

$$\Upsilon_1 = coth(\beta_k - \beta') + coth(\beta'' - \beta_k)$$

and,

$$\Upsilon_2 = \frac{x'}{sinh(\beta_k - \beta')} + \frac{x''}{sinh(\beta'' - \beta)}$$

The Monte Carlo analysis was performed in a system of N bosons whose density matrices were evaluated in time slices β using Lévy path integral [8]. The system was defined by randomly selecting a set of positions for bosons using the gaussian variation in Eq. (2) at first. Then a boson from this set was swapped with another boson selected randomly from that set of positions. This process was repeated until the boson returned to its initial position. A path for the boson was thus created with cycle length k using Eq. (4). The switching of two bosons was confirmed by running a metropolis algorithm.

For a cycle of length k in range N, the partition function is given by [12]

$$Z_N = \frac{1}{N}\int_{k=1}^{N} z_k\, Z_{N-k} \qquad 5$$

Here, Z_k (β) is the single-particle partition function for cycle length k and is given by $\left(\frac{1}{1-e^{-k\beta}}\right)^3$ and the component Z_{N-k} is related to the previous partition functions by the above relation.

In a system of N particles,

$$N = \sum_k kN_k$$

if there are n_k cycles of length k [13].

The probability of having a particle in a cycle of length k is

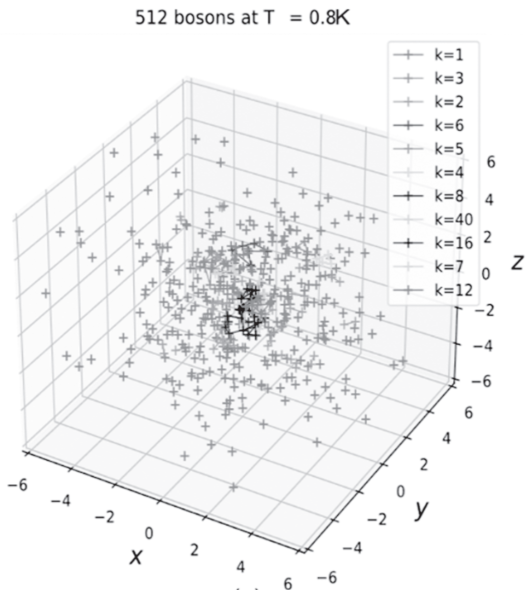
$$\pi_k = \frac{z_k\, Z_{N-k}}{NZ_N} \qquad 6$$

The probability of a particle being in longer cycles varies with temperature. The probability of finding a cycle of length, say k, was shown in a scatter plot obtained from the system of bosons along with a theoretical plotting of Eq. (6). In high temperatures, the contribution from permutations other than the identity permutation contributes negligibly [5]. It is quite different in low temperatures, where longer cycle lengths are more visible.

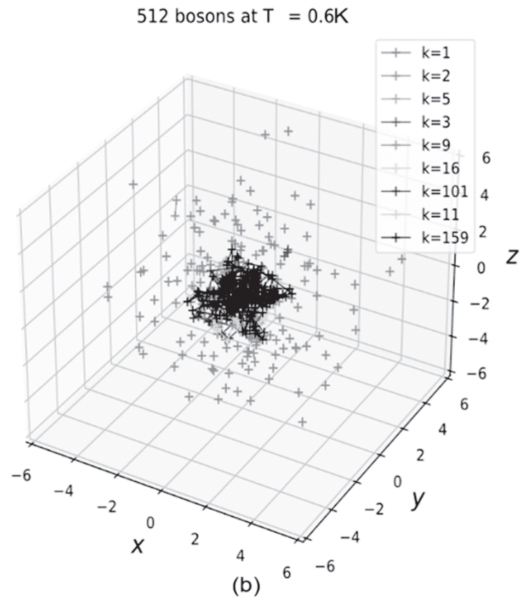
3. Results

The path integral Monte Carlo theory was utilized in a Monte Carlo algorithm written in python [14]. The system under consideration has non-interacting ideal bosons. These identical particles are kept at temperature 1K, which is then reduced gradually to 0.1K at 0.1K intervals. The constants of the system such as m, ω, π, ℏ have been taken to be unity.

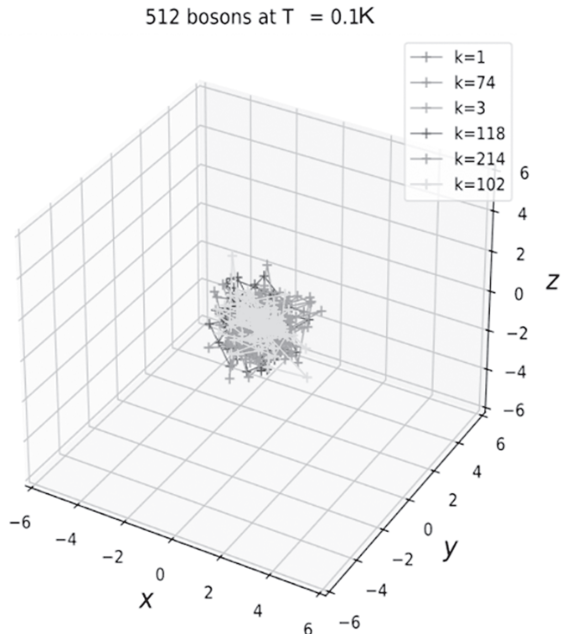
Particles are found to cluster around the center of the potential, and condensation occurs at near-zero temperature (Fig. 3). The tendency to pursue a central position is perceived in Fig.1 in a three-dimensional spatial frame as well as the probability of the particles to be in a position in two-dimensional space in Fig.2. The comparison of all bosons and bosons in cycles longer than 10 with the ground state probability of harmonic trap has been performed in Fig.3.



(a)

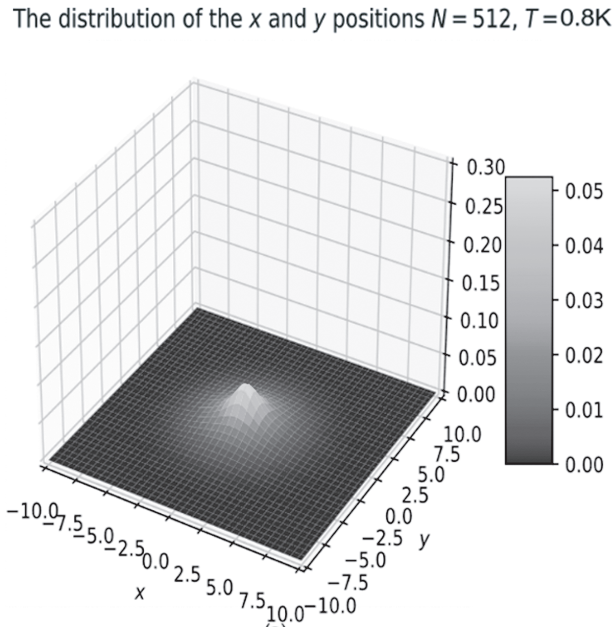


(b)



(c)

Fig. 1: The position of 512 particles in a three-dimensional spatial frame for three different temperatures: (a) 0.8K, (b) 0.6K and (c) 0.1K



(a)

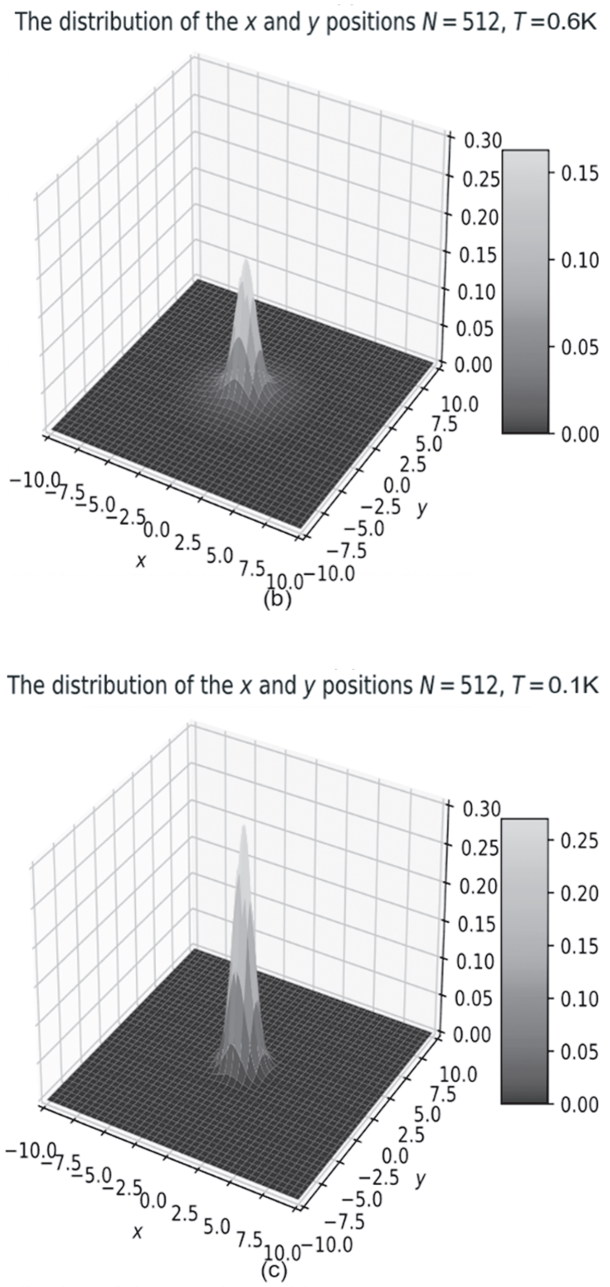


Fig. 2: The probability distribution of 512 particles in two spatial dimensions for temperatures (a) 0.8K, (b) 0.6K and (c) 0.1K

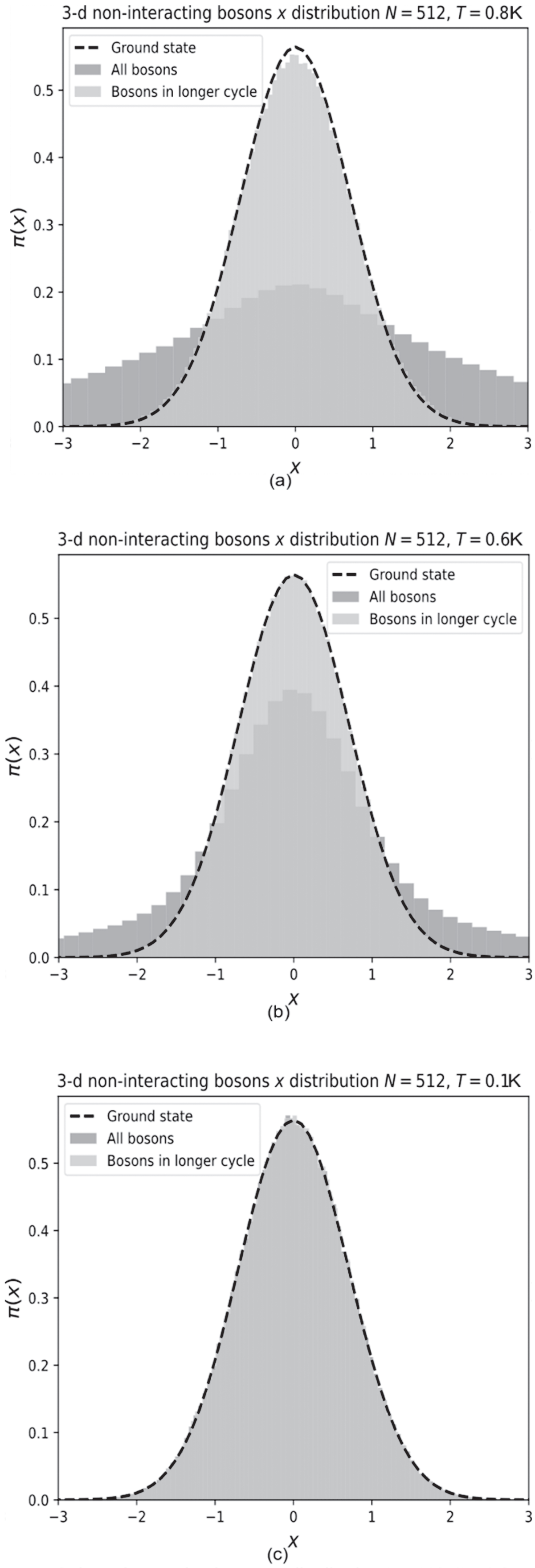


Fig. 3: A visual comparison between the probability distribution in one dimension of all 512 bosons (blue) and bosons in a cycle length greater than 10 (green) with the analytical curve of ground state (black dotted line) obtained from Eq (1) for three different temperatures:(a) 0.8K, (b) 0.6K and (c) 0.1K

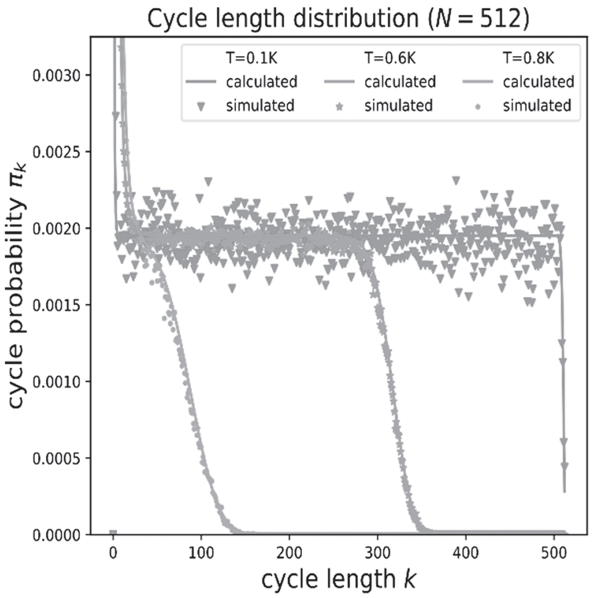


Fig. 4: Comparison between the probability of appearances of cycles regarding their lengths at temperatures 0.1K (blue triangle), 0.6K (orange star), and 0.8K (green circle) for 512 bosons obtained by Monte Carlo simulation (scatter) and theoretical analysis (solid lines) obtained from Eq. (7).

The distribution of particles in 0.8K temperature is spread out in space and end up in cycles of short length with the highest cycle length being 40 in Fig.1 (a). As the temperature is decreased, the particles get closer and fall into longer cycles with the highest one being 159 for 0.6K [Fig.1 (b)] and 214 for 0.1K [Fig.1 (c)].

The probability of the particles to be in any position on a plane peaks at the center of that two-dimensional domain with the reduction of temperature as shown in Fig.2. The peak is around 0.07 at 0.8K, 0.17 at 0.6K, and 0.27 at 0.1K.

The comparison in Fig.3 shows that bosons in longer cycles tend to show a similar trend with the analytical probability of the ground state indicating those particles all occupying that state. As the temperature is reduced, the histogram generated by Monte Carlo fits the analytical ground state probability perfectly [Fig.3 (c)].

The probability of having a particle in cycle length k is displayed both analytically and using Monte Carlo in Fig.4. The result obtained by Monte Carlo simulation is consistent with the analytical curve. Fig.4 shows that the probability of being in longer cycle length increases with reducing the temperature. At temperature 0.1K, the probable length of the cycles goes as far as 512, while at a higher temperature, a cycle this long has zero probability of appearing. The probability goes to zero at above 130 and 350 at 0.8K and 0.6K respectively.

4. Discussion

The crux of this article is to analyze the response of a system of bosons with lowering temperature confined in a three-dimensional isotropic harmonic trap. The results exhibit a relation between cycle lengths and condensation.

The Monte Carlo analysis of the probability of cycles with respect to their lengths is in excellent agreement with the analytical curve obtained from Eq. (6) (Fig.4). Longer cycles have become prominent with the reduction in temperature. In all temperatures, short cycles are the most probable ones and the longest are the least. The central values have probabilities that cluster around a particular value regardless of the temperature.

A cycle is merely a path closing on itself. A long cycle indicates that the density matrices have a tendency to become off-diagonal. This is a consequence of the uncertainty principle. The diagonal density matrix provides the probability of finding a particle at its coordinate. At high temperature with increased uncertainty in momentum, the position of a particle remains fairly certain, which accounts for the diagonality of density matrices in coordinate space in most slices rendering small cycles. On the contrary, reduction in uncertainty in momentum at low temperatures results in longer chains of non-diagonal density matrices resulting in long cycles.

The analytical ground state probability curve obtained from Eq. (1) is closely followed by the particles in cycles of length greater than 10 (Fig.3). As temperature reduces, the correspondence of the bosonic probability with the analytical curve is improved. Concurrently, all the bosons in the system, irrespective of their cycle lengths, have probability outside the ground state. These too, fit into the ground state with lowering temperature which suggests that all the bosons in the system occupy the ground state simultaneously.

It is also observed in Fig.2 that the probability of finding the particles peaks around the center of the trap. This is in accordance with the property of a harmonic potential.

To sum up, the reduction in temperature triggers non-diagonality in density matrices which consequently increases cycle lengths. The particles in long cycles tend to cluster around the center and fall into the single-particle ground state.

5. Conclusion

The experimental discovery of Bose-Einstein condensation in trapped potential has opened up new possibilities for the exploration of quantum phenomena in a qualitatively new regime. Bosons in a harmonic trap have provided the setting for groundbreaking experiments in atomic physics, where Bose-Einstein condensation has actually been achieved and extended to study interacting quantum systems from superfluid gases, to interacting fermions and bosons in condensed matter physics, and atomic gases. This article is focused on the modeling of non-interacting ideal bosons in near-zero temperatures. Monte Carlo method has successfully been used to simulate the condensation of bosons in temperature comparable to absolute zero and shows that all the bosons condensate to ground state defying Pauli's exclusion principle.

It can be concluded from the simulation that as identical particles, the permutation among the bosons plays a key role in condensation. The motion created by switching two bosons in space forms closed paths or cycles in imaginary time. These cycles appear in various lengths depending on the temperature. Reduction in temperature results in prolonged cycles and the particles residing on these cycles fall into the single-particle ground state attaining condensation.

This study can be extended to examine the case using different potential traps. The effect of interaction between particles at low temperatures can also be explored. Besides, the effect of temperature reduction on the particles that obey Pauli's exclusion principle, namely, fermions might also be studied in order to perceive the nature of their condensation.

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