Bose - Einstein Condensation and Thermodynamics of a Finite Number of Bosons Confined in a Harmonic Trap

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Abstract

We considered a system of N bosons confined in a three-dimensional isotropic harmonic trap. These particles undergo Bose- Einstein condensation under a critical temperature $T_c$. We calculated the condensate fraction as a function of Temperature. Furthermore, the energy of the system and the specific heat capacity are calculated for both normal and condensed phases. Finally, we calculated the entropy of the confined bosons.

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I. Introduction

The achievement of Bose-Einstein condensation of alkali atoms that are laser cooled and magnetically trapped has attracted much theoretical and experimental attention [$^1$-$^3$]. This experimental achievement which has been done more than twenty- five years
ago was a result of development in the experimental techniques of laser cooling and magnetic evaporation. Bose-Einstein condensation \(^4\) is the macroscopic occupation of the lowest momentum or ground state with a finite fraction of particles. It is a collective behavior and is a result of the Bose statistics that these atoms satisfy. Many approaches have been used to study atoms that undergo Bose-Einstein condensation. These approaches include numerical calculations like quantum Monte-Carlo techniques \(^5\), mean-field theories \(^6\) canonical and microcanonical ensemble approaches \(^7\) and variational approaches \(^8, 9\).

In this work, we will consider a finite number of non-interacting bosons confined in a three dimensional isotropic harmonic trap. We will replace the summation for the total number of bosons by integrations through the introduction of a suitable density of states.

We will not only calculate the condensate fraction and the energy, but also will calculate the specific heat capacity in both normal and condensed phases. Results will be obtained for different values of number of particles, namely, \(N=100\), \(N=1000\), \(N=10000\) as well as in the thermodynamic limit \(N \rightarrow \infty\).

The system which we consider here differs from the free Bose gas in two aspects: first the particles here are confined. Second, the number of particles is finite, so the thermodynamic limit is not well defined \(^{10-14}\).

Furthermore, the particles that are experimentally Bose condensed were actually weakly-interacting particles. However, in this work, the interaction between particles are neglected.

### II Condensate fraction

We consider a finite number of non-interacting bosons confined in a three dimensional isotropic harmonic trap. The energy of the trap is given by the well known relation;

\[
E_n = \left( n + \frac{3}{2} \right) \hbar \omega ,
\]

where, \((n = 0, 1, 2, \ldots etc)\). This energy is \(g_n\)-fold degenerate, where \(g_n\) is given by

\[
g_n = \frac{(n+1)(n+2)}{2} \tag{2}
\]

The starting point of our calculation is the evaluation of the partition function;
\[ Z = \sum_{n=0}^{\infty} e^{-\beta \left(n + \frac{3}{2}\right) \hbar \omega} \frac{(n+1)(n+2)}{2}, \]  

where \( \beta = \frac{1}{kT} \), and \( k \) is Boltzmann’s constant. 

This summation can be exactly evaluated with the result; 

\[ Z = e^{-\frac{3}{2} \beta \hbar \omega} \left[ 1 - e^{-\beta \hbar \omega} \right]^{-3}, \]  

For \( \beta \hbar \omega \ll 1 \) which is in consistent with the experimental values for both the trap frequency and temperature. Therefore, with the following approximation; 

\[ \left[ 1 - e^{-\beta \hbar \omega} \right]^{-3} \approx (\beta \hbar \omega)^{-3} + \frac{3}{2} (\beta \hbar \omega)^{-2} + (\beta \hbar \omega)^{-1}, \]  

Next, we calculate the density of states of the excited atoms from the definition[12]; 

\[ \rho(E) = \frac{1}{2\pi i} \int_{\beta-i\infty}^{\beta+i\infty} e^{\beta E} Z(\beta) d\beta, \]  

\[ \frac{1}{2\pi i} \int_{\beta-i\infty}^{\beta+i\infty} e^{\beta E} \left[ (\beta \hbar \omega)^{-3} + \frac{3}{2} (\beta \hbar \omega)^{-2} + (\beta \hbar \omega)^{-1} \right] d\beta, \]  

With the aid of the relation; 

\[ \frac{1}{2\pi i} \int_{s-i\infty}^{s+i\infty} e^{sx} \frac{e^{-sx}}{s^{n+1}} ds = \begin{cases} x^n, & x \geq 0 \\ n! \cdot \cdots \cdot x, & x \leq 0 \end{cases}, \]  

We get; 

\[ \rho(E) = \frac{E^2}{2(\hbar \omega)^3} + \frac{3}{2} \frac{E}{(h \omega)^2} + \frac{1}{\hbar \omega}, \]  

The total number of particles is given by 

\[ N = N_o + \int_{0}^{\infty} \frac{\rho(E) dE}{e^{\beta E} - 1}, \]  

Where we have approximated the sum \( N = \sum_{n=0}^{\infty} \frac{g_n}{e^{\beta (e_n - \mu)} - 1} \) by an integral and introduced \( Z = e^{\beta \mu} \) as the fugacity. Using Eq (6) of the density of states and evaluate the integrals we get;
\[ N = N_o + \left( \frac{kT}{\hbar \omega} \right)^3 g_3(z) + \frac{3}{2} \left( \frac{kT}{\hbar \omega} \right)^2 g_2(z) + \left( \frac{kT}{\hbar \omega} \right) g_1(z), \] \tag{11}

Where, \( g_n(z) \) is the Bose function which is defined by:
\[ g_n(z) = \frac{1}{\Gamma(n)} \int_0^\infty \frac{x^{n-1}}{z^e x - 1} dx, \] \tag{12}

At the onset of condensation, \( N_s \approx 0 \) and, \( z \approx 1 \) we get:
\[ N = \left( \frac{kT}{\hbar \omega} \right)^3 \zeta(3) \left[ 1 + \frac{3 \hbar \omega \zeta(2)}{2 kT \zeta(3)} \right], \] \tag{13}

Where, \( g_n(1) = \zeta(n) \). So we get for the transition temperature:
\[ T_c = T_o \left[ 1 - \frac{\zeta(2)}{2(\zeta(3))^{2/3}} \frac{1}{N^{1/3}} \right], \] \tag{14}

Where,
\[ T_o = \frac{\hbar \omega}{k \left( \frac{N}{\zeta(3)} \right)^{1/3}}. \] \tag{15}

The second term of Eq.(14) vanishes in the thermodynamic limit (\( N \to \infty, V \to \infty \) and \( \frac{N}{V} = \text{cons.} \) ) and by substituting the value of \( \zeta(2) = 1.64 \) and the value of \( \zeta(3) = 1.20 \) we get:
\[ \frac{T_c - T_o}{T_o} \approx -0.73 N^{-1/3}, \] \tag{16}

Therefore, for \( N = 100 \), there is a reduction 15.7\% reduction in the value of the critical temperature. Moreover, for \( N = 1000 \) and \( N = 10,000 \), the reduction will be around 7.3\% and 3.4\% respectively.

Upon substituting Eq (14) and Eq (15) in Eq (11) we will get for the condensate fraction:
\[ \frac{N_o}{N} = 1 - \left( \frac{T}{T_o} \right)^3 - \frac{3}{2} \frac{\zeta(2)}{(\zeta(3))^{2/3}} \frac{1}{N^{1/3}} \left( \frac{T}{T_o} \right)^2, \] \tag{17}

This in turn will become;
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\[ \frac{N_o}{N} = 1 - \left( \frac{T}{T_o} \right)^3 - 2.18N^{-1/3} \left( \frac{T}{T_o} \right)^2, \quad (18) \]

Figure (1) shows the plot of \( \frac{N_o}{N} \) Vs. \( \frac{T}{T_o} \) for the values of \( N=100, N=1000, N=10,000, \) and \( N \to \infty \).

**III Energy and Specific heat**

The average energy of the N-Particle system is given by;

\[ U = \frac{3}{2} N \hbar \omega + \int_0^\infty E \rho(E) dE \]

\[ \frac{E}{\hbar \omega} - 1, \quad (19) \]

And upon substituting for \( \rho(E) \) from Eq(9), we obtain;

\[ U = \frac{3}{2} N \hbar \omega + \frac{3(kT)^4}{(\hbar \omega)^3} \zeta(4) + 3 \frac{(kT)^3}{(\hbar \omega)^2} \zeta(3) + \frac{(kT)^2}{\hbar \omega} \zeta(2), \quad (20) \]

In the condensed phase (i.e \( z = 1 \)), we will get;

\[ U = \frac{3}{2} N \hbar \omega + \frac{3(kT)^4}{(\hbar \omega)^3} \zeta(4) + 3 \frac{(kT)^3}{(\hbar \omega)^2} \zeta(3) + \frac{(kT)^2}{\hbar \omega} \zeta(2), \quad (21) \]

Therefore, the specific heat at constant volume in the condensed phase is given by;

\[ C_V = \left( \frac{\partial U}{\partial T} \right)_V = 12 \left( \frac{kT}{\hbar \omega} \right)^3 \zeta(4) + 9 \left( \frac{kT}{\hbar \omega} \right)^2 \zeta(3) + 2 \left( \frac{kT}{\hbar \omega} \right) \zeta(2), \quad (22) \]

Upon writing down the heat capacity \( (C_V) \) in terms of \( \frac{T}{T_o} \), we will get;

\[ \frac{C_V}{Nk} = 12 \zeta(4) \left( \frac{T}{T_o} \right)^3 + 9 \left( \zeta(3) \right)^{1/3} N^{-1/3} \left( \frac{T}{T_o} \right)^2 + 2 \left( \frac{\zeta(2)}{\zeta(3)^{1/3}} \right) N^{-2/3} \left( \frac{T}{T_o} \right) \]

\[ (23) \]

After introducing the values of \( \zeta_n(z) \), \( \frac{C_V}{Nk} \) will become:

\[ \frac{C_V}{Nk} = 10.8 \left( \frac{T}{T_o} \right)^3 + 9.56N^{-1/3} \left( \frac{T}{T_o} \right)^2 + 3.09N^{-2/3} \left( \frac{T}{T_o} \right), \quad (24) \]
This equation gives the specific heat capacity of the system in the condensed Phase. In the thermodynamic limit i.e. \( (N \rightarrow \infty) \), the second and third terms vanish and the maximum specific heat would be \( C_V = 10.8 N k \). For a finite number of particles, the maximum heat capacity occurs when \( T = T_c \) which is somehow lower than \( T_o \) as explained earlier. These results are shown in Fig(2).

The specific heat capacity above the transition temperature is obtained from Eq (20)

\[
C_V = \left( \frac{\partial U}{\partial T} \right)_V = 12k \left( \frac{kT}{\hbar \omega} \right)^3 g_4(z) + 9k \left( \frac{kT}{\hbar \omega} \right)^2 g_3(z) + 2k \left( \frac{kT}{\hbar \omega} \right) g_2(z) + 3 \frac{\partial g_4(z)}{\partial z} \frac{dz}{dT} + 3 \frac{\partial g_3(z)}{\partial z} \frac{dz}{dT}, \tag{25}
\]

\[
C_V = \frac{12 g_4(z) T^3}{\zeta(3)} N^{-1/3} \left( \frac{T}{T_o} \right) + 9 \frac{g_3(z)}{(\zeta(3))^{2/3}} N^{-1/3} \left( \frac{T}{T_o} \right)^2 + 2 \frac{g_2(z)}{(\zeta(3))^{1/3}} N^{-2/3} \left( \frac{T}{T_o} \right)^3 - 3 \ln z \frac{g_3(z)}{\zeta(3)} \left( \frac{T}{T_o} \right)^3, \tag{26}
\]

The specific heat in both normal and condensed phases for \( N = 10000 \) is shown in Fig(3). We note that the maximum specific heat occurs at \( T/T_0 = 0.97 \) which is the transition temperature in this case.

**IV Free energy and entropy**

The Helmholtz free energy of \( N \)-atoms confined in the harmonic trap is given by;

\[
F = -N k T \ln Z, \tag{27}
\]

\[
F = -N k T \left[ -\frac{3 \hbar \omega}{2 k T} - 3 \ln \left( 1 - e^{-\frac{\hbar \omega}{k T}} \right) \right], \tag{28}
\]
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\[ F = \frac{3}{2} N \hbar \omega + 3NkT \ln \left(1 - e^{\frac{\hbar \omega}{kT}}\right), \]  

(29)

The entropy \( S \) is given by;

\[ S = -\left(\frac{\partial F}{\partial T}\right)_V, \]  

(30)

\[ S = 3Nk \left[ \frac{\hbar \omega}{kT} \frac{1}{e^{\frac{\hbar \omega}{kT}} - 1} - \ln \left(1 - e^{\frac{\hbar \omega}{kT}}\right)\right], \]  

(31)

Or by using \( T_o = \frac{\hbar \omega}{k} \left(\frac{N}{\zeta(3)}\right)^{1/3} \) the entropy \( S \) becomes;

\[ S = 3Nk \left[ \left(\frac{\zeta(3)}{N}\right)^{1/3} \left(\frac{T_o}{T}\right) \frac{1}{e^{\left(\frac{\zeta(3)}{N}\right)^{1/3} T_o/T} - 1} - \ln \left(1 - e^{\left(\frac{\zeta(3)}{N}\right)^{1/3} T_o/T}\right)\right]\],  

(32)

We note that as \( T \to 0, S \to 0 \) which is consistent with the third law of thermodynamics.

Figure (4) represents the variation of \( S/3Nk \) with respect to \( T_o/T \).

V. Conclusion

In this work, we have considered a system of a finite number of Bose particles confined in a three dimensional isotropic harmonic trap. The discrete sum of the Bose distribution is replaced by integrals through the introduction of a suitable density of states. The finite number of particles results in a reduction of the critical temperature from that of the infinite system. We have calculated the condensate fraction as a function of temperature. The average energy of the system and the specific heat capacity were obtained both in the normal and condensed phases for different values of particle number, namely \( N=100, 1000, 10000 \) as well as \( N \to \infty \). Finally we have calculated the Helmholtz free energy and the entropy of the system. Results for entropy are consistent with the third law of thermodynamics. In general, our results in this work are in a good agreement with other works.

Furthermore, in the experiments on Bose condensation for alkali atoms, the particles are weakly interacting. However, although we have neglected this weak interaction in this study, the general feature of the system is almost the same.
Figure 1: Condensate variations vs. $T/T_0$

Figure 2: Specific heat variations with respect to $T/T_0$ in the condensed phase
Figure 3: Specific heat variations with respect to $T/T_0$ in the condensed and normal phases

Figure 4: Entropy variations with respect to $T/T_0$
References


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