

Bose Einstein Condensation and Thermodynamics Properties in Bose-Einstein Distribution

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Abstract

The calculation of the thermodynamic properties in the Bose-Einstein distribution is presented. The behaviour of the Bose-gas in the Bose-Einstein distribution is analysed based on high and low temperature dependence. At $T > T_B$ all particles are in the excited state and the ground state is essentially occupied. But at $T < T_B$ particles gradually falls to the ground state and eventually contains all the particles in the system as $T \rightarrow 0$. The analytical expressions for some important parameters such as Bose-Einstein condensation of an ideal Bose gas, the population density of the excited and ground state particles are also presented. Heat capacity of an ideal Bose gas and total internal energy are also calculated and the results presented graphically. The results obtained are consistent with those found in the literatures.

Keywords: Bose-Einstein condensation, thermodynamics properties, Bose-Einstein distribution, excited state particles

1.0 Introduction

Thermodynamic is a science that deals with the relations among heat, work and properties which are in equilibrium [1,2]. In Thermodynamic the physical properties of substance are often described as intensive or extensive depending on the size of the system. The distinction is based on the concept that smaller non-interacting identical subdivision of the system maybe identified so that property of interest does not change when the system is divided or combined [3,4]. For intensive properties; the physical property of a system does not depend on the system size or the amount of material in the system but an extensive property is additive for independent non interacting subsystems. The property is proportional to the amount of material in the system and depends on the size of the system [5,6].

The Bose-Einstein distribution describes the statistical behavior of integer spin particles (Bosons). At low temperature, an unlimited number of bosons can be occupied in the same state and this is known as Bose-Einstein condensation. However, the result and findings of this work is based on the population density of the Bose-Einstein gas. This population density depends on whether the temperature is high or low, at high temperature the particles generate an internal energy of which the heat capacity and other thermodynamic properties are also generated [7,8].

A theoretical aspect concerning the thermodynamic properties of an ideal bosonic gas trapped by harmonic potential was investigated and analyzed at the University of Saopaulo, Brazil [9]. This was done by properly working in the Grand canonical ensemble of which the extensive and intensive thermodynamics variables were properly identified. Hasan and Gain in 2013 calculated the heat capacity of a Bose-Einstein condensation with two different temperature regime which are $T > T_0$ and $T < T_0$. Heat capacity was obtained by differentiating total energy $E(T)$ with respect to temperature using the density of state approach [10]

The results are useful in determining how quick a substance will heat up or cool down, and it can also be used to estimate how much energy is needed to raise the temperature of a substance. The study can also be used in analyzing the distribution patterns in organelle for example, invertebrate smooth muscles filaments, microtubules in axons and micropirocytic vesicles in papillary endothelial cells [11]. This aimed at calculating the thermodynamics properties in the Bose-Einstein distribution and also deal with issues such as collection of indistinguishable boson which yield Bose-Einstein distribution, the Bose-Einstein condensation of an ideal Bose gas and the population density of an excited and ground state particles.

2.0 Indistinguishable Fermions and Bosons

In system consisting of collections of identical fermions or identical boson. The wave function of the system has to do with either antisymmetric (fermions) or symmetric (bosons) under the interchange of any two particles. With the allowed wave functions, it is no longer possible to identify a particular energy state. Instead, all the particles are shared between the occupied states and are said to be undistinguishable.

In the case of undistinguishable fermions, the wave function for an overall system must be antisymmetric under the interchange of any two particles. One consequence of this is the Pauli exclusive principle. For a system of two fermions, a possible wave function is [12, 13]

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}} = [\psi_A(x_1)\psi_B(x_2) - \psi_A(x_2)\psi_B(x_1)] \quad (3)$$

where x_1 and x_2 are the co-ordinate of the two particles and A and B are the two occupied state. If we try to put two particles in the same state, the wave function vanishes. Finding the distribution with the maximum number of microstate for system of identical fermions lead to the Fermi – Dirac distribution.

For undistinguishable Bosoms, the wave function for a system of identical bosoms must be symmetric with respect to the inter change of any two particles. For a system of two bosoms, a possible wave function is [14 15]

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}} [\psi_A(x_1)\psi_B(x_2) + \psi_A(x_2)\psi_B(x_1)] \quad (4)$$

If we put two particles in the same states, the wave function does not vanish, there is no limit in the number of particles we can put into any given state, and thus Pauli Exclusion Principle does not apply to bosons.

3.0 Bose- Einstein Distributions

The Bose-Einstein distribution describes the statistical behavior of integer spin particles (bosons). It is obeyed by identical indistinguishable particles of integral spin that have symmetric wave functions and is so named as it was devised by Bose for light quanta and generalized by Einstein [16]. Consider a system having n indistinguishable particles.

If the particle is divided into quantum groups or levels such that there are $n_1, n_2, \dots, n_i, \dots$ numbers of particles whose approximate constant energies are $E_1, E_2, \dots, E_i, \dots$ respectively. Assume g_i to be the number of eigen state (ie degeneracy or statistical weight) of the level. Then the Bose-Einstein distribution is given by [17, 18]

$$n_i = \frac{g_i}{B e^{\frac{E_i}{KT}} - 1} \quad (5)$$

where B is the normalization term, K is the Boltzmann's constant and T is the thermodynamic temperature.

4.0 Bose-Einstein Condensation

Let us consider a boson gas consisting of a large number of identical bosons in a box with rigid walls and fixed volume moving freely within the box but cannot move beyond its walls. Then the distribution is given in Eq.(5). Consider the behavior of the constant B that appears in the above equation. This quantity correspond to the partition function in the Boltzmann's distribution function and B can be determined by the constant.

$$\sum n_i = N, \quad (6)$$

where N is the total number of particles. But the density of state for spin zero particles moving freely in a box of volume V , mass of particle m and energy of the particle E is given as

$$g(E) = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{E}. \quad (7)$$

Replacing the summation in Eq.(6) over discrete energy levels by an integration over a continuum of energy levels, we have;

$$\sum n_i = \int_0^\infty n(E) dE = N \quad (8)$$

Substituting Eq. (5) and Eq. (7) into Eq.(8) gives

$$N = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \int_0^\infty \frac{\sqrt{E}}{B e^{\frac{E}{KT}} - 1} dE \quad (9)$$

defining a function $F(B)$ such that

$$F(B) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{E}}{B e^{\frac{E}{KT}} - 1} dE \quad (10)$$

Let $y = \frac{E}{KT}$ and the Eq. (9) and Eq. (10) becomes

$$N = \frac{V}{4\pi^2} \left(\frac{2mKT}{\hbar^2} \right)^{\frac{3}{2}} \int_0^\infty \frac{\sqrt{y}}{Be^y - 1} dy \quad (11)$$

$$F(B) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{y}}{Be^y - 1} dy \quad (12)$$

In terms of F(B) the total number of particles becomes

$$N = V \left(\frac{mKT}{2\pi\hbar^2} \right)^{\frac{3}{2}} F(B) \quad (13)$$

where $\int_0^\infty \frac{\sqrt{y}}{Be^y - 1} dy = \frac{\sqrt{\pi}}{2} F(B)$ (14)

Using Eq. (14) in Eq. (11) we have

$$N = \frac{\sqrt{\pi}}{2} F(B) \frac{V}{4\pi^2} \left(\frac{2mKT}{\hbar^2} \right)^{\frac{3}{2}} \quad (15)$$

From Eq. (12) we have noticed that for $B \gg 1$,

$$F(B) = \frac{1}{B}, \text{ then } Be^y - 1 = Be^y, \text{ and}$$

$$\frac{I}{B} = \frac{2}{\pi} \int_0^\infty \frac{\sqrt{y}}{Be^y} dy \quad (16)$$

The total number of particle for high temperature becomes:

$$N = V \left(\frac{2mKT}{2\pi\hbar^2} \right)^{\frac{3}{2}} \frac{1}{B} \quad (17)$$

and the Bose-Einstein gas B becomes

$$B = \frac{V}{N} \left(\frac{2mKT}{2\pi\hbar^2} \right)^{\frac{3}{2}} \quad (18)$$

Here, the Bose-Einstein condensation can be discussed. If $B < 1$, there is a possibility of an energy level E_i such that $n_i < 0$. Clearly we cannot have a negative number of particles in any level at so we expect $B \geq 1$. Since $F(B)$ takes a maximum value at $B = 1$, then the maximum value of $F(B)$ is given by

$$F(1) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{y}{e^y - 1} dy = \xi\left(\frac{3}{2}\right) \approx 2.612 \quad (19)$$

where $\xi(x)$ is the Riemann Zeta function defined as $\xi(x) = \sum_{n=1}^{\infty} \frac{1}{n^x}$

We expect that as temperature goes down, $F(B)$ has to go up. But $F(B)$ has a finite maximum below some temperature T_B at which the particle starts to disappear and is given by:

$$T_B = \frac{2\pi \hbar^2}{mk} \left(\frac{N}{\xi\left(\frac{3}{2}\right)V} \right)^{\frac{2}{3}} \quad (20)$$

T_B is known as the Bose-Einstein temperature or the critical temperature, for $T < T_B$ the particles disappear to the ground state.

Since the lower limit of the integral in Eq.(8) is zero, we assume that the ground state has a zero energy, the density of state and the population density is zero in the small energy range $0 \rightarrow dE$.

For a Bose Einstein gas, there is no limit to the number of particles that can fall to the ground state. At $T > T_B$ all particles are in excited state and the ground state is essentially occupied. But at $T < T_B$ particles gradually fall to the ground state and eventually contains all the particle in the system as $T \rightarrow 0$.

5.0 The Population Density of an excited state particles in the Bose-Einstein Gas

Let the population density of an excited state be given by:

$$n_{ex}(E) = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \frac{\sqrt{E}}{Be^{\frac{E}{KT}} - 1} dE \quad (21)$$

Let the function $B(T)$ be the Bose-Einstein distribution, then for Bose-gas $B(T)$ is given by

$$B(T) = \begin{cases} 1, & T < T_B \\ F^{-1} \left[\zeta \left(\frac{3}{2} \right) \left(\frac{T_B}{T} \right)^{\frac{3}{2}} \right], & T \geq T_B \end{cases} \quad (22)$$

where F^{-1} is the inverse of F given by Eq. (11) and for $T \gg T_B$ we have

$$B = \frac{1}{\zeta \left(\frac{3}{2} \right) \left(\frac{T}{T_B} \right)^{\frac{3}{2}}}, \quad (23)$$

where B is the Bose-Einstein gas of the population density in an excited state. Then the total population density of an excited and ground state particles of Bose-gas is given by

$$N_{ex} = \frac{V}{4\pi^2} \left(\frac{2mKT}{\hbar^2} \right)^{\frac{3}{2}} \int_0^\infty \frac{\sqrt{y}}{e^y - 1} dy = N \left(\frac{T}{T_B} \right)^{\frac{3}{2}} \quad (24)$$

This leaves the remaining population in the ground state as

$$N_o = N \left[1 - \left(\frac{T}{T_B} \right)^{\frac{3}{2}} \right], \quad \text{for } T < T_B \quad (25)$$

6.0 Total Energy of the Bose-Einstein Gas and Thermodynamics Properties

If we assume that the ground state is a state of zero energy, then particles in the Bose-Einstein condensation makes no contribution to the total energy (u) and it's written as

$$u = \int_0^\infty E n_{ex}(E) dE = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \int_0^\infty \frac{E^{\frac{3}{2}}}{Be^{\frac{E}{KT}} - 1} dE \quad (26)$$

where we have used Eq. (24) for the density of particle in an excited state, and the total energy expressed as

$$u = \frac{2}{\sqrt{\pi} \zeta \left(\frac{3}{2} \right)} NKT \left(\frac{T}{T_B} \right)^{\frac{3}{2}} \int_0^\infty \frac{y^{\frac{3}{2}}}{Be^y - 1} dy \quad (27)$$

At low temperature ($T < T_B$) we can take $B = 1$, and

$$u = \frac{3\xi\left(\frac{5}{2}\right)}{2\xi\left(\frac{3}{2}\right)} NKT \left(\frac{T}{T_B}\right)^{\frac{3}{2}} \approx 0.0770 NKT \left(\frac{T}{T_B}\right)^{\frac{3}{2}} \quad (28)$$

We see that at $T < T_B$, $u \propto T^{\frac{5}{2}}$, but at $T \geq T_B$, $B \gg 1$ so we make the approximation $Be^y - 1 \approx Be^y$ from Eq. (27) we have that

$$u = \frac{3}{2\xi\left(\frac{3}{2}\right)} NKT \left(\frac{T}{T_B}\right)^{\frac{3}{2}} \frac{1}{B} \quad (29)$$

Substituting Eq. (23) into Eq. (29), we have

$$u = \frac{3}{2} NKT \quad (30)$$

The behavior this internal energy with temperature is presented in Fig.1.

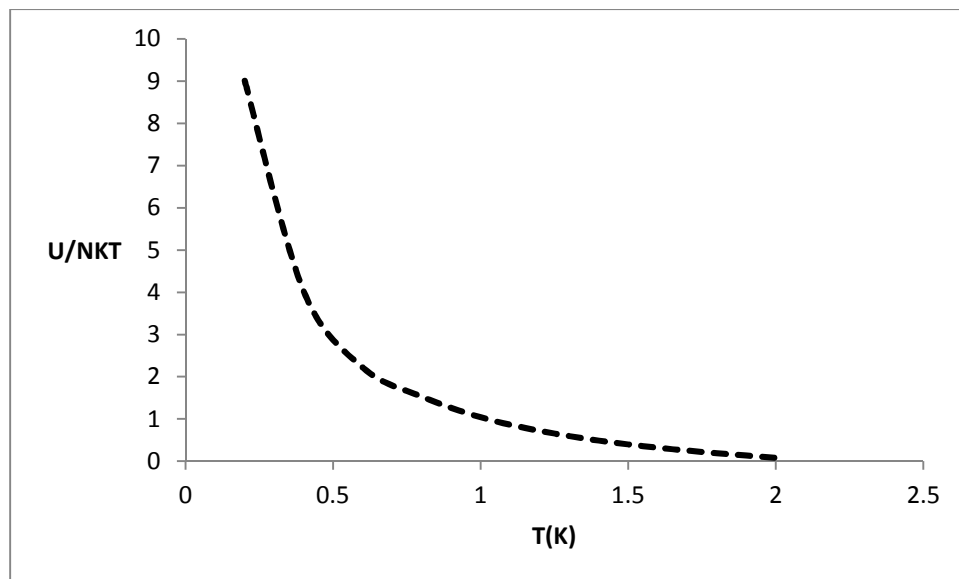


Fig. 1: Internal energy versus temperature

By the implication of Eq. (30) the thermodynamics properties such as heat capacity and grand potential for this system can be obtained. Heat capacity for this system can be obtained by differentiating the total energy in Eq. (30) with respect to temperature at constant volume as

$$C_v = \left(\frac{\partial u}{\partial T} \right)_v \quad (31)$$

for an ideal gas, kinetic Energy E_k is the same as potential energy E_p so $u = 2E_k$ and $Nk = R$ where R is the molar gas constant, $N =$ Avogadro's constant so from Eq. (31)

$$C_v = 3R \quad (32)$$

Equation (32) is known as Dulong-Petit law [19].

The variation of heat capacity with temperature is presented in Fig. 2 below.

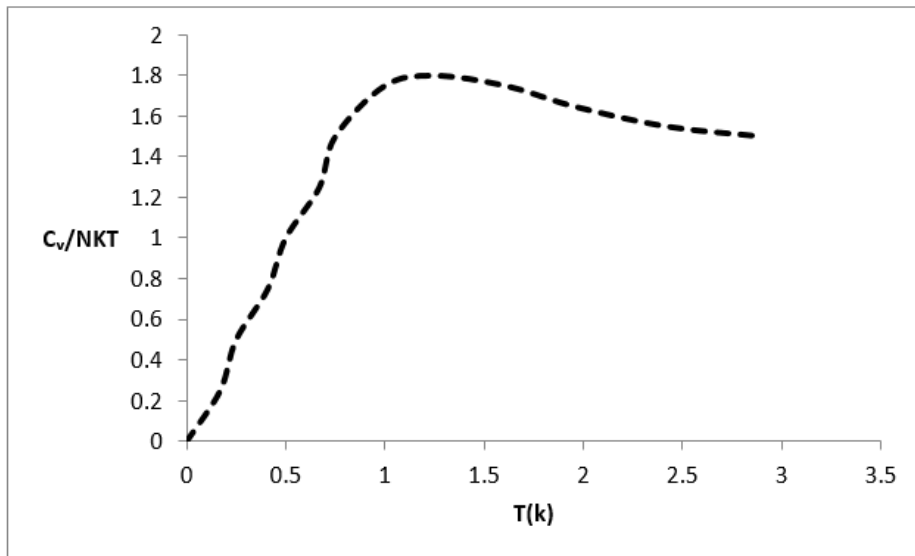


Fig. 2: Heat capacity versus temperature

Another thermodynamics property to be evaluated is the grand potential, the Grand potential is a thermodynamics potential denoted by $\Omega(T, \mu)$. This potential is a function of temperature T and chemical potential μ [20]

$$d\Omega = -sdT - Nd\mu \quad (33)$$

Obtaining N at constant temperature (T)

$$N = -\left(\frac{\partial\Omega}{\partial\mu}\right)_T \quad (34)$$

Also obtaining S at constant μ

$$S = -\left(\frac{\partial\Omega}{\partial T}\right)_\mu \quad (35)$$

7.0 Conclusion

A Bose-Einstein condensation is a rare state of matter in which a large percentage of boson collapse into their lowest quantum state, allowing quantum effect to be observed on a macroscopic scale. We used an accurate semi-classical approach to calculate the thermodynamics properties of a Bose-Einstein gas. An expression for the critical temperature T_B , the Bose-Einstein condensation and the population density of particles in an excited state and ground state was properly identified. The calculated results shows that for $T < T_B$, the particles of boson disappears to the ground state and this constitute Bose-Einstein condensation and at this point the internal energy is zero. But for $T > T_B$ the particle of bosons are in excited state and an internal energy is said to occur. Consequently, the heat capacity is obtained from the derivative of total internal energy with respect to temperature. The variation of these properties; internal energy and heat capacity with temperature are discussed in Figs. 1 and 2 respectively.

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