Calculation of Bose-Einstein Condensation of Gases in a Harmonic Potential Trap Using A Macro Canonical Ensemble by Use of The Mathematical and Hermitian Functions

B. Adib*, A. Heidari and P. Zarshekan Zamanpour

Department of Chemistry, Islamic Azad University, Tehran North Branch P.O. Box 1913674711, Tehran, Iran Fax: (98)(21)22222512; E-mail: b_adibb@yahoo.com

In this work, a mathematical analysis of Bose-Einstein condensation (BEC) for a device of particles by zero spin which has no interaction on each other in one harmonic potential trap has been discussed. It is indicated that a trapped device, quantitatively and qualitatively, differs from non-trapped device of free boson gas. One of its most important differences is that in contrast to a free boson gas device, there is no critical temperature for phase transition in a harmonic oscillator trap. In this paper, BEC in a harmonic oscillator trap in numerical and analytical points of view by using macro canonical ensemble, Mathematica software and Hermitian functions have been investigated.

Key Words: Bose-Einstein condensation, Boson gas, Phase transition, Harmonic potential trap, Macro canonical ensemble, Hermitian functions.

INTRODUCTION

One of the most interesting properties of boson gases under special condition, is a possibility of a phase transition in a critical temperature, so that all boson gases condensate into ground state. This phenomenon is called Bose-Einstein condensation (BEC). In order to introduce the notion of BEC numerically, one can utilize the definition of One-Body density matrix:

$$\mathbf{n}^{(1)}(\mathbf{r},\mathbf{r}') = \left\langle \psi^{\dagger}(\mathbf{r})\psi(\mathbf{r}') \right\rangle \tag{1}$$

 $\psi(r)$ and $\psi^{\dagger}(r)$ are field operations which create and obliterate one particle in a point. Theses values are in complete correspond with Boson commutation relations:

$$\left(\psi(\mathbf{r}),\psi^{\dagger}(\mathbf{r}')\right) = \delta(\mathbf{r}-\mathbf{r}'), \left(\psi(\mathbf{r}), \psi(\mathbf{r}')\right) = 0$$
⁽²⁾

If the investigated system was in absolute state, it is described by the N-body density function of $\psi(r_1, r_2, r_3, ..., r_N)$. Thus, the average of equational in the standard rules of quantum mechanics is used. As a result of it we can write One-Body density matrix as follows:

$$n^{(1)}(\mathbf{r},\mathbf{r}') = N \int d\mathbf{r}_2,...,d\mathbf{r}_N \psi^*(\mathbf{r},\mathbf{r}_2,...,\mathbf{r}_N)$$
(3)

 $\psi(r', r_2, ..., r_N)$

which is consist of N-1 time integration from r_2 , ... r_N .

If we consider $n^{(1)}$ as a matrix function of r and r', then $n^{(1)}(r, r') = [n^{(1)}(r', r)]^*$.

Thus, according to the definition, the value of $n^{(1)}$ will be Hermitian. Then it is always possible to find a complete over to normal base from Eigen function of $\phi_i(r)$ in which density matrix is diagonal:

$$n^{(1)}(\mathbf{r},\mathbf{r}') = \sum_{i} n_{i} \phi_{i}^{*}(\mathbf{r}) \phi_{i}(\mathbf{r}')$$
(4)

The actual Eigen value of n_i will be under normalization state. $\sum_i n_i = N$ and it means the occupied spaces in single-body state of ϕ_i . When one of these numbers such as n_o became microscopic, the BEC phenomena will occur. It means that if $n_0 \equiv N_0$ was a number of N time, all other numbers will remain on one time. In this state, we can rewrite eqn. 4 as:

$$\mathbf{n}^{(1)}(\mathbf{r},\mathbf{r}') = \mathbf{N}_0 \phi_0^*(\mathbf{r}) \phi_0(\mathbf{r}') + \sum_{i \neq 0} \mathbf{n}_i \phi_i^*(\mathbf{r}) \phi_i(\mathbf{r}')$$
(5)

The delivered state by $\phi_0(\mathbf{r})$ is called Bose-Einstein condensation (BEC). Of course it is a general definition, because fit is used for each microscopy system (N>>1) of non distinguishable bosons. It should be noted that without considering mutual interactions and external fields, Bose-Einstein condensation (BEC) can be created easily for over cold atoms by changing and adjusting external potential. One-body density matrix consists of information about important quantities which are visible physically. By equalizing r and r' by each other, $\mathbf{r} = \mathbf{r}$ diagonal density of system is acquired.

$$\mathbf{n}(\mathbf{r}) \equiv \mathbf{n}^{(1)}(\mathbf{r}, \mathbf{r}) = \left(\psi^{\dagger}(\mathbf{r})\psi(\mathbf{r})\right) \tag{6}$$

Concerning to $N = \int n(r)dr$ for calculating distribution related to movement volume, we can use:

$$\mathbf{n}(\mathbf{p}) = \left(\boldsymbol{\psi}^{\dagger}(\mathbf{p}) \; \boldsymbol{\psi}(\mathbf{p}) \right) \tag{7}$$

In the above mentioned formula $\psi(p) = (2\pi h)^{-\frac{3}{2}} \int \psi(r) exp\left(\frac{-ip.r}{h}\right) dr$ is the operation of field in delivering angle operation. By entering this equation, instead of $\psi(p)$ in eqn. 7, the following equation will be acquired:

$$n(p) = \frac{1}{(2\pi h)^3} \int n^{(1)} \left(R + \frac{s}{2}, R - \frac{s}{2} \right) e^{-ip.s/h} dR ds$$
(8)

In the above formula s = r - r' and R = (r + r')/2

Asian J. Chem.

Calculation of Bose-Einstein Condensation of Gases 2595

Now, we consider a harmonic system consists of N body in volume V. In which there is thermodynamic confines of N, $V \rightarrow \infty$ and density of N/V which is stable. Special function related to density matrix are the same flat waves and they are lower than the energy of ground state energy or the energy of zero point of movement volume equal to zero, p = 0 and they have the function of stable wave equal to $\phi_0(r) = V^{-1}/2$. Density matrix is only depending on s = r - r' and we can write is as the following form:

$$n^{(1)}(s) = \frac{N_0}{V} + \frac{1}{V} \sum_{p \neq 0} n_P e^{-ip.s/h}$$
(9)

It is observed that in the confines of $s \rightarrow \infty$, the total of (Σ) which is written on the right side of the above statement will equal to zero because of the destructive interactions between different flat waves. But, the first statement will remain as such. Thus, it is noted that by existence of BEC, one-body density matrix, in long and remarkable intervals tend to a stable and definite value. Instead p = 0 related to the space of movement volume will appear as the following:

$$n(p) = N_0 \delta(p) + \sum_{p' \neq 0} n_{p'} \delta(p - p')$$
(10)

The total of (Σ) which is written on the right side of the above statement indicates the number of non dense bodies of (N-N_o) and the value of N_o / N is called condensate fraction. But, if we have heterogeneous system, special function related to density matrix are not the same flat waves. But if N which was creates is big enough and the notion of BEC still remained, one microscopy occupation of the special one-body function, means $\phi_0(\mathbf{r})$ will be alongside density matrix. Therefore, dense bosons can be described as a function of $\psi(\mathbf{r}) = \sqrt{N_0 \phi_0(\mathbf{r})}$, which is actually a complex classic field which plays the role of order parameter. It should be mentioned that this case is exactly similar to classic confines in quantum thermodynamics in which electromagnetic field is replaced by the microscope photon definition. Function ψ may depend on the time variable (t). In this case, we can write it as the following:

$$\psi(\mathbf{r},\mathbf{t}) = |\psi(\mathbf{r},\mathbf{t})| e^{\mathbf{i}\mathbf{S}(\mathbf{r},\mathbf{t})}$$
(11)

This determines the absolute value of diagonal density condensate portion; where as phase S can properly indicate the phase factors and beyond fluidity of the system. Order parameter which is in eqn. 11 is called microscopy wave or function of condensate wave, is only described according to a stable phase factor. We always can multiply this function to numerical phase factor of $e^{i\alpha}$ without having any changes in physical properties or creating new physical state. In fact, this subject reflects gauge symmetry which is delivered by all physical equations. Therefore, a definite selection for the value of order parameter will be created and thus, one conventional fracture occurs in gauge symmetry for phase.

Asian J. Chem.

After Einstein had reviewed the paper of an Indian scientist, Bose, about photons' statistic and Planck's distribution, he stated this theory¹. But, it took 70 years till Cornell and Wicman could create BEC in laboratory in 1995. The fact is that in 1924, Indian scientist, Bose, introduced a new statistical method on black body radiation according to one gas from photo quantum (photon). His study alongside his contemporaneous scientist, de Broglie, about duality of wave-substance caused Einstein applied similar statistical method for the gas consist of N non-separatable body by the mass of m. One of the remarkable results was related to the anticipation of this fact that in the temperature below of some critical temperature, a definite fraction of all bodies condensate to the lowest state of body's energy and as pointed this phenomenon as Bose-Einstein condensation (BEC). For some years, this anticipation was not noticed till in 1938, London argued that BEC can be observed in the beyond fluidity properties of helium gas in the temperature below 2.17 K. Ultimately, in 1995 Cornell and Wicman observed BEC in the diluted gases which are locked in the magnetic traps and were refrigerated up to the multi nano Kelvin. As a result of it, a remarkable progress occurred in BEC. An important improvement which was occurred in recent years was observing BEC in very cold gases such as rubidium², lithium³ and sodium⁴. Theses gases are very dilute and by the approximate of first order it is expected that they have no interaction with a model of simple boson gas. These experimental studies caused excitement of theoretical studies in the field of finding physical principles which are dominate on this situation. For several aims, it is possible to estimate complex magnetic traps which are used in this experiment by the harmonic potential oscillator. Despite the situation in which one Boson gas is not under the external locker potential (free Boson), there is no critical temperature for Boson gas which is under the potential (device) which indicates phase transition. It was indicated that there is a temperature which is more in the special heat and can be considered as a temperature in which BEC occurs. It was proven that a gas of the Boson gases aside interactions, in the harmonic potential oscillator has no phase transition in critical temperatures. About a system of charged Boson gases in a homogeneous magnetic field, a similar situation will occur. A simple model was studied according to the Bosons with zero normal spin which is trapped by a harmonic potential oscillator. It is showed that in this case, BEC can not occur for a free Boson gas in free space and without trapping potential in a similar way which occurs for trapped Boson gases in harmonic potential oscillator is easily. By reducing temperature for a free Boson gas, chemical potential will increase from negative values to zero. It should be noted that the temperature in which chemical potential is equal to zero is described as a critical temperature (T_c) which was determined for body density. In the temperature below T_c the chemical potential will remain zero and the number of particles which are under the excitement situation is limited. If the total number of bodies exceeded from this level, BEC can only occur for the remained bodies which are on the ground state. Therefore, there is a quantitative and qualitative difference between free Boson gas and a system

consists of trapped Boson gases in harmonic potential oscillator. Unfortunately, it is impossible to find a valid analytical approximate for special heat which allow us to find whether special heat is a more value or not and if it is, in which temperature it occurs. Atoms are trapped in a magnetic potential and it is possible to model this potential with harmonic potential oscillator. Many studies^{5,6} were conducted about BEC in trapped harmonic potential oscillator. In this paper, condensation of Boson gases in one harmonic potential oscillator is investigated by a method in which the approximate of states' density is not similar with previous reports^{5,6}. In the studies we come to this interesting conclusion that despite free Boson gases, in this state, there is no critical temperature which proves phase transition. Here, a temperature by analytical and numerical methods is acquired in which BEC will occur.

HERMITIAN FUNCTIONS

Generative function: Hermitian functions from the expansion of the function

$$g(x,t) = e^{2tx-t^2} = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!}$$
(12)

T = 0 will be acquired and then we have:

$$e^{2tx-t^{2}} = e^{-t^{2}}e^{2tx}$$

$$= \sum_{n=0}^{\infty} \frac{(-t^{2})^{n}}{n!} \sum_{n=0}^{\infty} \frac{(2tx)^{m}}{m!}$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{(-1)^{n}(2x)^{m}}{n!m!} t^{2n+m}$$
(13)

By changing denominator of 2n + m = 1 and omission of m,

$$e^{2tx-t^{2}} = \sum_{l=0}^{\infty} \sum_{n=0}^{\left(\frac{1}{2}\right)} \frac{(-1)^{n} (2x)^{l-2n}}{n! (l-2n)!}$$
(14)

[1/2] is a round portion of 1/2. The exponent of n is [1/2], because m = 1 - 2n should be remained a round and positive number. By comparison of (14) and (12) a series figure Hermit polynomial will be acquired:

$$H_{n}(x) = \sum_{m=0}^{\left(\frac{1}{2}\right)} \frac{(-1)^{n} n! 2n^{n-2m}}{m!(n-2m)!} x^{n-2m}$$
(15)

Some of these polynomials alongside their variation curves are shown in Fig. 1. $H_0(x) = 1$

Asian J. Chem.

$$H_{1}(x) = 2x$$

$$H_{2}(x) = 4x^{2} - 2$$

$$H_{3}(x) = 8x^{3} - 12x$$

$$H_{4}(x) = 16x^{4} - 48x^{2} + 12$$

$$H_{5}(x) = 32x^{5} - 160x^{3} + 120x$$

$$H_{6}(x) = 64x^{6} - 480x^{4} + 720x^{2} - 120$$

$$H_{1}(x)$$

$$H_{1}(x)$$

$$H_{1}(x)$$

$$H_{1}(x)$$

$$H_{2}(x)$$

$$H_{1}(x)$$

$$H_{2}(x)$$

$$H_{2}(x)$$

$$H_{2}(x)$$

$$H_{2}(x)$$

$$H_{2}(x)$$

$$H_{2}(x)$$

$$H_{2}(x)$$

$$H_{2}(x)$$

$$H_{2}(x)$$

Fig. 1. Hermit polynomials

Recessive relations of Hermitian functions: We derivate (12) with t:

$$(2x-2t)e^{-t^{2}+2tx} = \sum_{n=0}^{\infty} H_{n}(x)\frac{t^{n-1}}{(n-1)!}$$
(17)

Applying (12) in (17) and simplifying it:

$$\sum 2xH_{n}(x)\frac{t^{n}}{n!} - \sum 2H_{n}(x)\frac{t^{n+1}}{(n!)} - \sum H_{n}(x)\frac{t^{n-1}}{(n-1)!} = 0$$
(18)

By selecting coefficient of general term of t^n and equaling it to zero, the first recessive relations of Hermitian functions will acquire.

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$$
(19)

This time we derivate (12) with variable x:

$$2te^{-t^{2}+2tx}\sum H_{n}(x)\frac{t^{n}}{n!}$$
(20)

and

$$\sum 2H_{n}(x)\frac{t^{n+1}}{n!} - \sum 2H_{n}'(x)\frac{t^{n}}{n!} = 0$$
(21)

At the end, by selecting coefficient of general term of tⁿ:

$$H'_{n}(x) = 2nH_{n-1}(x)$$
 (22)

Calculation of Bose-Einstein Condensation of Gases 2599

By putting x = 0 in (12):

$$e^{-t^{2}} = \sum_{n=0}^{\infty} H_{n}(0) \frac{t^{n}}{n!}$$
(23)

And extension of the (23) left side:

$$\sum_{n=0}^{\infty} (-1)^n \frac{t^{2n}}{n!} = \sum_{n=0}^{\infty} H_n(0) \frac{t^n}{n!}$$
(24)

By equaling equivalent terms, the following values will be acquired:

$$H_{2n+1}(0) = 0$$
, $H_{2n}(0) = (-1)^n \frac{(2n)!}{n!}$ (25)

On investigating the behaviour of Hermitian functions under the parity can be interesting and for its generative function, we have:

$$g(x,t) = g(-x,-t)$$
 (26)

$$\sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} = \sum_{n=0}^{\infty} H_n(-x) \frac{(-t)^n}{n!}$$
(27)

as a result:

$$H_{n}(x) = (-1)^{n} H_{n}(-x)$$
(28)

Hermitian functions by even fraction are even and by odd fraction are odd. **Hermitian differential equation:** By derivation of (19), we have:

$$\dot{H}_{n+1}(x) - 2H_{n}(x) - 2x\dot{H}_{n}(x) - 2n\dot{H}_{n-1}(x) = 0$$
 (29)

By applying (22) and its derivation:

$$H'_{n+1}(x) = 2(n+1)H_{n}(x)$$

$$H''_{n}(x) = 2xH'_{n-1}(x)$$
(30)

In equation (29) Hermitian differential equation will be acquired:

$$H'_{n}(x) - 2xH'_{n}(x) + 2nH_{n}(x) = 0$$
(31)

Integral figures of Hermitian functions: For acquiring integral figures of Hermitian functions, we multiply (12) to $t^{-m-1}dt$ and on the closed path, we integrate around the zero point (Fig. 1).

$$\int_{c}^{x} N \frac{e^{-t^{2}+2tx}}{t^{m+1}} dt = \sum_{n=0}^{\infty} \frac{H_{n}(x)}{n!} \int_{c}^{x} \frac{t^{n}}{t^{m+1}} dt = \sum_{n=0}^{\infty} \frac{H_{n}(x)}{n!} 2\pi i \delta_{m,n}$$
(32)

And by its simplification:

$$H_{n}(x) = \frac{n!}{2\pi i} \int_{c}^{x} N \frac{e^{-t^{2} + 2tx}}{t^{n+1}} dt$$
(33)

Asian J. Chem.



Fig. 2. Integral path of Hermitian functions

By changing the variable $t \rightarrow x - t$ in (33), we will have:

$$H_{n}(x) = \frac{(-1)^{n} n!}{2\pi i} \int_{c}^{x} N \frac{e^{-t^{2} + x^{2}}}{(t-x)^{n+1}} dt$$
(34)

The part of integration of c in (34) is a closed one around x point. From the comparison of (34) by the formula of nth derivation of hybrid functions, the differential figures of Hermitian functions will be acquired, it means:

$$H_{n}(x) = (-1)^{n} e^{x^{2}} \frac{d^{n}}{dx^{n}} e^{-x^{2}}$$
(35)

Intentional of Hermitian functions: The operation of Hermitian differential equation is not self-adjunct. For making itself-adjunct, we should multiply the equation by f(x) function:

$$f(x) = \frac{1}{P_0(x)} e^{\int_x^x x dt} = e^{-x^2}$$
(36)

Then,

$$e^{-x^2}H_n'(x) - 2xe^{-x^2}H_n(x) + 2ne^{-x^2}H_n(x) = 0$$
 (37)

On the other hand, the roots of equation $e^{-x^2} = 0$ are equal to $\pm \infty$, thus it can be written as:

$$\int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} dx = 0 \quad m \neq n$$
(38)

Due to calculate (38) for m = n we consider generative function of (12). Thus, by multiply to itself, we have:

$$e^{-t^2 - s^2 + 2tx + 2sx} = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} H_n(x) H_m(x) \frac{t^n s^m}{n! m!}$$
(39)

And by multiplying the current equation to e^{-x^2} and integration of it, we will have:

$$\int_{-\infty}^{\infty} e^{-t^2 - x^2 - s^2 + 2tx + 2sx} dx = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{t^n s^m}{n! m!}$$

$$\int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} dx$$
(40)

And by applying (38):

$$e^{2ts} \int_{-\infty}^{\infty} e^{-(x-t-s)^2} dx = \sum_{n=0}^{\infty} \frac{(ts)^n}{(n!)^2}$$
$$\int_{-\infty}^{\infty} [H_n(x)]^2 e^{-x^2} dx$$
(41)

For calculating the integral of the left side of the eqn. (41):

$$\sqrt{\pi}e^{2ts} = \sum_{n=0}^{\infty} \frac{(ts)^n}{(n!)^2} \int_{-\infty}^{\infty} [H_n(x)]^2 e^{-x^2} dx$$
(42)

At the end by expansion of $\sqrt{\pi}e^{2ts}$ and setting equivalent terms and combining the result of (38) to it:

$$\int_{-\infty}^{\infty} H_{n}(x) H_{m}(x) e^{-x^{2}} dx = 2^{n} n! \sqrt{\pi} \delta_{m,n}$$
(43)

Expansion of f(x) function according to the Hermitian functions: Since Hermitian functions in $(-\infty,\infty)$ toward the weight function of e^{-x^2} , create a complete set, thus for optional function of f(x), it can be written:

$$f(\mathbf{x}) = \sum_{n=0}^{\infty} c_n H_n(\mathbf{x})$$
(44)

By multiplying (44) in $H_m(x)e^{-x^2}dx$ and integrating $(-\infty,\infty)$, we will have:

$$\int_{-\infty}^{\infty} f(x) H_{m}(x) e^{-x^{2}} dx = \sum_{n=0}^{\infty} c_{n} \int_{-\infty}^{\infty} H_{n}(x) H_{m}(x) e^{-x^{2}} dx$$
(45)

And by applying the result of (43):

$$c_{n} = \frac{1}{2^{n} n! \sqrt{\pi}} \int_{-\infty}^{\infty} f(x) H_{n}(x) e^{-x^{2}} dx$$
(46)

will be acquired.

Harmonic potential oscillator: Now in the first section of this discussion and before any other cases, we use Hermitian functions due to solve time-independent Schröndinger's equation for harmonic potential oscillator, $V(x) = \frac{1}{2}m\omega^2 x^2$. Time-independent Schröndinger's equation for the above mentioned potential is:

$$-\frac{h^2}{2m}u''(x) + \frac{1}{2}m\omega^2 x^2 u(x) = Eu(x)$$
(47)

Asian J. Chem.

The above equation will be as following by changing the variables of

$$y = \sqrt{\frac{m\omega}{h}}x$$
 and $\varepsilon = \frac{2E}{h\omega}$:
 $u''(y) + (\varepsilon - y^2)u(y) = 0$ (48)

By choosing $u(y) = e^{-\frac{y^2}{2}} f(y)$ and put it in the equation (48):

$$f''(y) - 2yf'(y) + (\varepsilon - 1)f(y) = 0$$
(49)

Will be acquired which is the same as Hermit differential equation. Of course it has one difference that the coefficient of f(y) and $u(y) = e^{-\frac{y^2}{2}}f(y)$ can has any value. But, since u(x) should be square integralable, means $u(\pm \infty) = 0$, it is necessary that $\varepsilon - 1$ should be round multiple of 2. Because the slope speed of f(y) should not be lower than $e^{-\frac{y^2}{2}}$. For $\varepsilon - 1 = 2n$, the answers of the equations of (49) should n=be the same of Hermit functions, it means:

$$f''(y) - 2yf'(y) + 2nf(y) = 0$$
(50)

and
$$f_n(y) = H_n(y)$$

Therefore, the special value or the levels of the oscillator's energy will be equal to:

$$\varepsilon - 1 = 2n \Longrightarrow E = \left(n + \frac{1}{2}\right)h\omega$$
 (51)

At the end, by using the definition of intentional of Hermitian functions, the special value of normalized functions of the harmonic oscillator will be equal to:

$$u_{n}(y) = \frac{1}{\sqrt{2^{n} n! \sqrt{\pi}}} e^{-\frac{y^{2}}{2}} H_{n}(y)$$
(52)

$$u_{n}(x) = (-1)^{n} \cdot \left\{ \frac{\left(\frac{h}{m\omega}\right)^{n}}{2n^{n}n!} \right\}^{\frac{1}{2}} \cdot \left(\frac{m\omega}{\pi h}\right)^{\frac{1}{4}} \cdot e^{\left(\frac{m\omega}{2h}\right)x^{2}} \cdot \frac{d^{n}}{dx^{n}} e^{-\left(\frac{m\omega}{h}\right)x^{2}}$$
(53)

or

It is assumed to describe this device by macro canonical ensemble. One ensemble is described as following:

$$q = -\sum_{N} \ln(1 - z \exp(-\beta E_{N}))$$
(54)

In which $\beta = (kT)^{-1}$ and E_N are the energy of levels. $z = e^{\beta\mu}$ is described as a fugicity of the device which is a factor according to the chemical potential of μ . By expansion of logarithm in the equation 54, we can acquire the following equation:

$$q = \sum_{n=1}^{\infty} \frac{z^n}{n} \sum_{n} \exp(-n\beta E_N)$$
(55)

For a harmonic oscillator by the angle frequency of ω , the levels' energy are given by the relation of $E_{n_1n_2n_3} = h\omega\left(n_1 + n_2 + n_3 + \frac{3}{2}\right)$. If we put $n_1 + n_2 + n_3 = K$ and (K \in N) in it, the levels' energy is arranged with pluralism of $\frac{(K+1)(K+2)}{2}$ by the manner of $E_{\kappa} - \left(K + \frac{3}{2}\right)h\omega$. By execution of addition on the eqn. 55, the following equation is obtained:

$$q = \sum_{n=1}^{\infty} \frac{e^{n\beta\left(\mu - \frac{3}{2}h\omega\right)}}{n(1 - e^{-nx})^3}$$
(56)

In this equation, we enter non dimension variable of $x = \frac{h\omega}{kT}$. Number of particles will be acquired from the following equation:

$$\mathbf{n} = \beta^{-1} \left(\frac{\partial \mathbf{q}}{\partial \mu} \right) \mathbf{T}, \boldsymbol{\omega}$$
(57)

By using eqn. 56, we have:

$$N = \sum \frac{e^{n\beta\left(\mu - \frac{3}{2}h\omega\right)}}{(1 - e^{-nx})^3}$$
(58)

For keeping the number of particles positive and limited, it is necessary to have $\mu \leq \frac{3}{2}h\omega$ in which $h \equiv \frac{h}{2\pi}$ is a Dirac constant. Generally, it is necessary that $\mu \leq E_0$ in which E_0 is ground state energy or zero point or the lowest state. Commonly, the critical temperature for BEC is a temperature in which $\mu = E_0$. For harmonic oscillator $\mu = \frac{3}{2}h\omega$. Now, it is easy to indicate that BEC can not occur in Boson gases in free space in a way which is occurring for trapped Boson gases in harmonic oscillator. About Boson gases in free space without any limitative potential, besides the reduction of temperature, the chemical potential will arise from negative values to zero and it is completely compatible with the general result of $\mu = E_0$ which was mentioned above (the lowest energy level or ground state energy or energy level of

Asian J. Chem.

2604 Adib et al.

zero point for free Boson gas is equal to zero). It should be mentioned that the temperature in which $\mu = 0$ is called the critical temperature of T_c. This temperature is determined according to the density of bodies and particles. For free Boson gas in the temperature lower than T_c, μ will remain in zero value and since the number of particles is limited in excited state, therefore, when the number of particles exceed from the maximum number of the excited state, only possibility for remained particle is remaining in ground state. This case will result BEC and its full details are given in any book of statistical mechanics or thermodynamics^{7,8}. The root of differences in the behaviours of free Boson gas and trapped Boson gas is related to the number

of particles of the ground state with the energy of $\frac{3}{2}h\omega$. Here, besides the quantity of x non-dimension, the quantity of $\left\{\mu = h\omega\left(\frac{3}{2} - \varepsilon\right)\right\}$ is introduced. Level of $\varepsilon \to s$ is correspondent with the chemical potential which reaches critical values. The number of particles in the ground state according to x and ε are:

$$N_{Ca} = \frac{1}{e^{\varepsilon x} - 1}$$
(59)

For $\varepsilon \to 0$, the ground state N will tend to infinite. For a definite value of x and N (the total number of particles in the ground state and in the excited state) from the equation 59, it is observed that $\varepsilon > \left(\frac{1}{x}\right) \ln\left(\frac{(N+1)}{N}\right)$ and ε will be zero if $T \to 0$ or $N \to \infty$. As it is indicated in equation 59, for one constant N once ε become small sufficiently, necessarily only the ground state will be occupied. The temperature in which the ground state starts to increase number of particles remarkably, is very important and essential. This remarkable increase will occur by the smooth and gradual changes of temperature, so that despite the behaviour of free Boson gas, no phase transition will be observed. In other word, although quantities will change fast, but any transition will occur gradually and no discontinuity will be seen. Special

heat will be in the level of high temperature, when $x = \frac{h\omega}{kT} = 1$, as following:

$$\frac{C}{k} = \frac{12\xi_{R}(4)}{x^{3}} + \frac{q\xi_{R}(3)}{x^{2}} + \frac{2\xi_{R}(2)}{x} - \frac{12\xi_{R}(3)}{x^{2}} - \frac{18\epsilon^{2}\xi_{R}(2)\xi_{R}(3)}{x^{3}} - \frac{9\epsilon^{2}\xi_{R}(3)^{2}}{x^{4}} + \frac{9\epsilon^{2}\xi_{R}(2)\xi_{R}(3)^{2}}{x^{6}} + O\left(\ln x, \frac{\epsilon}{x}\right)$$
(60)

Also, in this level, we have:

$$N = N_{Ca} + \frac{\xi_{R}(3)}{x^{3}} + \frac{\left(\frac{3}{2} - \varepsilon\right)\xi_{R}(2)}{x^{2}} + O\left(\frac{\ln x}{x}\right)$$
(61)

The above results deliver a general description on the total range of the considered temperature for the tests which were executed in this field. For instance, we choose the parameters which were used for rubidium atoms. In this case, N = 3000 and $\frac{\omega}{2\pi}$ = 60 Hz. It is aimed to calculate the chemical potential which is given by ε (it

 $\frac{1}{2\pi}$ = 00 HZ. It is aimed to calculate the chemical potential which is given by ε (it

should be remark that $\left\{ \mu = h\omega \left(\frac{3}{2} - \varepsilon \right) \right\}$). This calculation can be executed by solving

equation 58 for ε as a function of x. The numerical result of this calculation is indicated as bold lines in the Fig. 3 by the Mathematica software. As it can be observed in this diagram, ε drops from the value of the unique order to the value of 10^{-2} order on very small range of x. After this fast reduction, ε will reduce by the increase of x (or reduction of T) to zero. This result is inconsistent with the actual phase transmission such as those which occur in free Boson gas, because in free Boson gas, ε will be equal to zero in non-zero temperature which is called critical temperature. From N-base from harmonic oscillator it is observed that the immediate reduction of ε is depend on the immediate increase of occupy number of ground state. Therefore, this phenomenon will result Bose-Einstein condensation (BEC). Although, chemical potential has an immediate change, but this changing occurs evenly. By this way, it is impossible to identify special critical temperature. One approximate which is used in the device by the finite volume is the calculation of special maximum heat. The temperature in which the maximum temperature occurs is called the critical temperature. In Fig. 4, we precisely indicate the results of the special heat's calculation by the Mathematica software by using harmonic oscillator sets as a bold curve. As it is indicated in this diagram, special maximum heat in x_m $\approx 0/0921$ is observed which is according to T $\approx 3/127 \times 10^{-8}$. In this figure, phase transition is not observed. For comparison of the above results by the results of different researches which were done in this case, Fig. 5 is indicated in the potential of oscillator according to the temperature which was concluded from reference⁹. As it is observed in the figure, special heat for different values of particles, N, has no transition. On the other word, as Fig. 4, identification of critical temperature is not possible. In Fig. 6, the changes of the special heat according to the temperature for different number of particles, are shown alongside the exact numerical results¹⁰. Despite Figs. 4 and 5, the above diagram shows phase transition in the point of $F = T_0$. Also, the executed calculation by the semi classical approximate and by using threedimensional heterogeneous harmonic oscillator, phase transition will be acquired again¹¹. By all these, in the reference¹⁰ it is declared that whenever modification executed on the calculation, this discontinuity will be eliminated in the curve of special heat which results actual phase transition. In this order, it may be concluded that in the devices by the limited number of particles, there is no phase transition.

On the other hand, in these kinds of devices there is a semi condense area in which the main part of particles in the temperature is depend on N, will drop to the lowest level or zero level. It should be mentioned that the real tests show these semi-transition^{12,13}.



Fig. 3. Changes of $\boldsymbol{\epsilon}$ as a function of \boldsymbol{x} for harmonic oscillator





Fig. 5. Changes of C_V according to the temperature for harmonic oscillator⁹

Calculation of Bose-Einstein Condensation of Gases 2607



Fig. 6. Changes of C_V according to the temperature for harmonic oscillator¹⁰

Now we will discuss about the analytical calculation of the subject. Since in the applied approximate the assumption is that x and ε should be very small, results for $x \le x_m \approx 0/0921$ will face trouble, because the Fig. 3 shows that ε for this definite value of x is very large. If we describe f as a fraction of bodies in ground state, we have:

$$N_{Ca} = f N \tag{62}$$

In this case, by considering equation 59, we will have:

$$\varepsilon \mathbf{x} = \ln \left(1 + \frac{1}{\mathrm{f N}} \right) \tag{63}$$

$$(1-f)N \approx \xi_{R}(3)x^{-3} + \left(\frac{3}{2} - \varepsilon\right)\xi_{R}(2)x^{-2}$$
 (64)

 ε can be omitted from the equations 63 and 64. Executing this operation results homogeneous linear third rate by the constant coefficients as a general form of $x^3 + a_1x^2 + a_2x + a_3 = 0$ which is solved as the following in this case:

$$Q = \frac{3a_2 - a_1^2}{9}$$
(65)

$$R = \frac{9a_1a_2 - 27a_3 - 2a_1^3}{54} \tag{66}$$

$$S = \sqrt{R + \sqrt{Q^3 + R^2}} \tag{67}$$

$$T = \sqrt{R - \sqrt{Q^3 + R^2}} \tag{68}$$

Asian J. Chem.

Resolution:

$$\begin{cases}
x_1 = S + -\frac{1}{3}a_1 \\
x_2 = -\frac{1}{2}(S+T) - \frac{1}{3}a_1 + \frac{1}{2}i\sqrt{3}(S-T) \\
x_3 = -\frac{1}{2}(S+T) - \frac{1}{3}a_1 - \frac{1}{2}i\sqrt{3}(S-T)
\end{cases}$$
(69)

From this equation we can assume x for N and f. Additionally, in the batch of the equations 63, $i \equiv \sqrt{-1}$, is a delusive number. After determining x by this method, ε can be acquired by the equation 63. The results of this approximate calculation ε , was indicated in the Fig. 3 as a rhombus by the Mathematica software. It is expected, whenever x reaches to the lower level x_m ; 0/0921, compatibility between approximate result and exact result will be violated. In the area in which the maximum special heat occurs, these two results will be compatible by each other completely. By increasing x (so that the temperature be lower than the critical temperature) the compatibility between approximate value for ε and the real value will improve. Increase of the x value is correspondent by the increase of the particles' fraction in the ground state. Now we will investigate the details of special heat. In second diagram, the rhombus of the approximate special heat is done in the level of x = 1, $\varepsilon = 1$ is done as a similar way of the done method in the first figure. The bold curve indicates the exact results. As if is shown in figure, two results which is acquired in the area of $x < x_m$ are compatible. Thus, for the value of $x < x_m$, this compatibility will violated. Because in this area ε for different value of x, is large remarkably. Of course our calculation is done according to the small ε . In the above figure, the maximum special heat correspond to x_m; 0/0921. This maximum special heat which is according to the temperature of this temperature is accumulated remarkably. This temperature is called transition temperature.

Conclusion

In this paper, the authors execute an analysis from several dynamic variables for the device consists on interactive bodies by zero spin in the harmonic potential oscillator and we compare the acquired results from different searches which were done in this field. Although despite what was observed about free Boson gas, there is no phase transition, but by observing maximum special heat, it is possible to identify the temperature in which BEC occurs. It is shown that this temperature is remarkably equal to the temperature in which the occupied number of ground state starts to increase. It should be mentioned that this kind of phase transition, differs from the real phase transition which occurs in an ideal gas. Because due to acquiring a real phase transition, the number of particles and the occupied volume by them should be very large. However, the density of particles should be kept constant. It is clear that no real device is able to possess these properties. Of course in many heterogeneous microscopy devices, the thermodynamic level in which boundary

conditions play unimportant role, is a good approximate for this experimental situation. On the other hand, the harmonic potential oscillator in which harmony Bose-Einstein condensation (BEC) not only the number of particles are very limited in comparision with the ordinary devices, but, also the boundary condition which is identifies by the potential well, are spread in the device. Due to provide thermodynamic level in these kinds of devices, it is necessary to reduce potential so that by increasing of the number of the particles, the mean of the density be constant. In this case, it may be assumed that the energy level in the harmonic oscillator continuous as a microscopy device and acquire phase transition as an ideal gas^{12,13}.

REFERENCES

- 1. A. Einstein and S.B. Preus, Akad. Wiss, 22, 261 (1924).
- 2. M.H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman and E.A. Cornell, *Science*, **269**, 198 (1995).
- 3. C.C. Bradley, C.A. Sackett, J.J. Tollet and R.G. Hulet, *Phys. Rev. Lett.*, **75**, 1687 (1995).
- 4. K.B. Davis, M.O. Mewes, M.R. Andrews, N.J. van Druten, D.S. Durfee, D.M. Kurn and W. Ketterle, *Phys. Rev. Lett.*, **75**, 3969 (1995).
- 5. V. Bagnato, D.E. Pritchard and D. Kleppner, Phys. Rev. A, 35, 4354 (1987).
- 6. S. Grossmann and M. Holthaus, Phys. Lett. A, 208, 188 (1995).
- 7. K. Huang, Statistical Mechanics Wiley, New York (1987).
- 8. R.K. Pathria, Statistical Mechanics Pergampn, Oxford (1972).
- 9. H.J. Schmidt and J. Batke, *Physica A*, **335**, 143 (2004).
- 10. H. Haugerud, T. Haugset and F. Ravndal, Phys. Lett. A, 225, 18 (1997).
- 11. H. Haugerud and F. Ravndal, Phys. Rev. D, 43, 2736 (1991).
- 12. W.J. Mullin, R. Krotkov and F. Latoe, Phys. Rev. A, 74, 23610 (2006).
- 13. S. Grossmann and M. Holthaus, Z. Phys. B, 97, 319 (1995).

(Received: 7 February 2008; Accepted: 7 January 2009) AJC-7096

FARADAY DISCUSSION 143: SOFT NANOTECHNOLOGY

15-17 JUNE 2009

LONDON, U.K.

Contact:

RSC Conferences Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge CB4 0WF, U.K. Tel:+44-(0)1223-432254, Fax:+44-(0)1223-423623