Bose-Einstein Condensation in a One-Dimensional System at Constant Pressure*

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Using techniques developed by Greenspoon and Pathria and by Chaba and Pathria, a rigorous asymptotic analysis of the onset of Bose-Einstein condensation in a finite one-dimtnsional system at constant pressure, under Dirichlet boundary conditions and mixed boundary conditions, is cerried out. The role of the finite site corrections arising from a modification of the density of states of the system, as well as from the di,jcreteness of the single–particle energy levels is discussed. The heat capacity C_p passes through a srnooth maximum and the volume becomes subextensive at the critical temperature Tc. Somewhat below $T_c(\infty)$, the volume of the system, together with C_p, becomes $O(N^{1/3})$. We also discuss the behaviour of the system when it is cooled at constant volume below T_c and compare the results of the present study with those of the two–dimensional and the three–dimensional systems.

Usando técnicas desenvolvidas por Greenspoon e Pathria e por Chaba e Pathria, é levada a efeito uma rigorosa análise assintótica da ocorrência da condensação de Bose-Einstein em um sistema finito uni-dimensional à pressão constante, sob condições de contorno de Dirichlet e condições de contorno mistas. E discutido o papel das correções de dimensões finitas que surgem por causa da modificação da densidade de estados do sistema e por serem discretos os níveis de energia da partícula livre. A capacidade calorífica C_p passa através de um máximo suave e o volume torna-se subextensivo á temperatura crítica T_c. Um pouco abaixo de $T_c(\infty)$, o volume do sistema, junto com C_p, torna-se $O(N^{1/3})$. NÕS também discutimos o comportamento do sistema quando o mesmo é esfriado

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a volume constante abaixo de T_c e comparamos os resultados do presente estudo com os dos sistemas bi-dimensional e tri-dimensional.

1. INTRODUCTION

In a recent paper, Imry, Bergman and Gunther[1,2] considered the problem of Bose-Einstein condensation (B.E.C.) in a two-dimensional system at constant pressure and being subjected to Dirichlet boundary conditions ($\psi_s = 0$). They also gave some results for the one-dimensional system[2], for temperatures greater than the critical temperature $T_c(\infty)$

$$T_c(\infty) = (2\pi\hbar^2 P^2/m\xi^2(3/2))^{1/3}/k \ . \qquad (1.1)$$

Using techniques develop by Greenspoon and Pathria[3] and by Chaba and Pathria[4], the latter carried out a rigorous, asymptotic analysis of the onset of B.E.C. in a finite two-dimensional[5] system at constant pressure and later extended it to a three-dimensional[6] system, as well. Although ideal Bose systems of one and two dimensions[7] do not undergo B.E.C. at finite temperatures if the system is cooled at constant particle density which is finite[8] throughout the system, Imry et al[1,2] and Chaba and Pathria[5] showed that if the two-dimensional system is cooled at constant pressure instead, a phase transition characterized by a macroscopic condensation of particles in the lowest single-particle state ε_0 does take place at a finite temperature. This is understandable because in this case, the volume of the system becomes subextensive, so that, in the thermodynamic limit, the particle density no longer remains finite.

We have taken up a rigorous study of the B.E.C. in a one-dimensional system at constant pressure, using the techniques[3"+] referred to above, so as to be able to compare the results with those of the two-dimensional and three-dimensional systems and study the effects of dimensionality. The study has been carried out in the cases when the system is subjected to two different sets of boundary conditions: (i) Dirichlet boundary conditions (D.B.C.), at both ends ($\psi_s=0$); (ii) Mixed boundary conditions (M.B.C.), that is Dirichlet boundary condition at

one end and Neumann boundary condition $(\partial\psi_s/\partial n=0)$ at the other: in both these cases, the condensate can also make a contribution

$$P_0 = 2N_0\varepsilon_0/V \sim N_0 h^2/(mV^3) \qquad (V = L) \qquad (1.2)$$

towards the total pressure of the system and thus help in keeping it fixed at a given value of P even when the temperature of the system is less than the critical temperature T_c. It follows from Eqs. (1.1) and (1.2) that for N_0 to be a significant fraction of N and P_0 to be a significant fi-action of P, the volume of the system must be subextensive:

$$V \sim (h^2/mkT_c(\infty))^{1/2} N^{1/3} . \qquad (1.3)$$

In this paper, we wish to report the results of a rigorous, asymptotic analysis of the aforementioned problem. Finite size corrections, appearing in the expression for the total number of particles N can be regerded as arising partly from (i) a modification of the density of states of the system (which, if it exists, is more significant in the case of higher momentum states[9]) and partly from (ii) the discreteness of the single.particle energy levels (which is more significant in the' case of lower momentum states). These corrections crucially depend on the bouridary conditions to which the system is subjected. We discuss the probleni using D.B.C. in section 2 and M.B.C. in section 3. In both cases C_p passes through a smooth maximum and the volume becomes subextensive at $T = T_C$ (which is different in the two cases). Also the condensate pressure P_0 does not play an important role at T_c. Somewhat below $T_c(\infty)$, the volume of the system further reduces and becomes $O(N^{1/3})$. At this stage C_p too becomes $O(N^{1/3})$ and the role of P_0 becomes dominant.

As mentioned before, as $T \to T_c$ from above, the volume of the system V_c becomes subextensive; cf. Eqs. (2.23) and (3.14a). If the system is now cooled below T_c at constant volume $V=V_c$, the condensate fraction becomes macroscopic only when $T \to 0$, in the thermodynamic limit. This result differs from that in the two-dimensional[5] case, where it becomes so at a finite temperature.

2. DIRICHLET BOUNDARY CONDITIONS

2. 1. Formulation

We consider a one-dimensional system of non-interacting bosons subject to Dirichlet boundary conditions with mean occupation numbers $<n_i>$ for the single-particle states ε_i. The total number of particles N (throughout this paper, we shall assume N to be large but finite) and the total pressure P of the system are then given by

$$N = \sum_i <n_i> = \sum_i (e^{\alpha + \beta\varepsilon_i} - 1)^{-1} \qquad (2.1)$$

and

$$P = - \sum_i <n_i> \left(\frac{\partial\varepsilon_i}{\partial V}\right) \qquad (2.2)$$

where

$$\alpha = - (\mu/kT) \ ,$$

μ being the chemical potential of the system; the derivatives $(\partial\varepsilon_i/\partial V)$ appearing in Eq. (2.2) are determined by the energy spectrum of the single-particle states. For a one-dirnensional system of length L (and *volume* $V = L$ also), the energy spectrum under D.B.C. is given by

$$\varepsilon(n) = \frac{h^2}{8mL^2} n^2 \propto \frac{1}{V^2} \ . \qquad (n = 1,2,3,\ldots) \qquad (2.3)$$

It follows that $(\partial\varepsilon_i/\partial V) = - (2\varepsilon_i/V)$ and hence

$$P = 2 \sum_i <n_i> \frac{\varepsilon_i}{V} = \frac{2U}{V} \ , \qquad (2.4)$$

U being the total energy of the system.

Using the techniques developed in references, 3, 4, and 5, Eq. (2.1) becomes

$$N = \frac{L}{\lambda} \left[g_{1/2}(\alpha) - \frac{\lambda}{2L} g_0(\alpha) + 2\pi^{1/2} \ \alpha^{-1/2} g_0(2y)\right] \qquad (2.5)$$

where λ $(= h/(2\pi m k T)^{1/2})$ is the mean thermal wavelength of the particles (which is assumed to be much smaller than L), $g_n(\delta)$ are the familiar Bose-Einstein functions[10], while the thermogeometric parameter y is given by

$$y = 2\pi^{1/2} \alpha^{1/2}(L/\lambda) \ . \tag{2.6}$$

In (2.5), the first term represents the bulk behaviour of the system, the second term arises from the modification of the density of states of the system owing to its finite size (and depends crucially on the choice of the boundary conditions) while the last term arises explicitly from the discreteness of the single-particle states.

In the region of interest (a << 1), we may write

$$g_{1/2}(\alpha) \simeq \pi^{1/2} \alpha^{-1/2} , g_0(\alpha) = (e^{\alpha} - 1)^{-1} \simeq \alpha^{-1} \tag{2.7}$$

Such an approximation is not permissible for a function of the parameter y because the latter varies drastically over the transition region. We, therefore, retain the relation

$$g_0(2y) = (e^{2y} - 1)^{-1} \tag{2.8}$$

and write

$$g_{1/2}(\alpha) + 2\pi^{1/2} \alpha^{-1/2} g_0(2y) \simeq \pi^{1/2} \alpha^{-1/2} \coth y \ . \tag{2.9}$$

Substituting (2.7) and (2.9) in (2.5), we finally obtain

$$N = 2\pi x^2 \left[\frac{\coth y}{y} - \frac{1}{y^2} \right] \tag{2.10}$$

where

$$x = L/\lambda \ . \tag{2.11}$$

Note that x is a measure of the *volume* of the system. For $y^2 < 0$, the Eq. (2.10) takes the form

$$N = 2\pi x^2 \left[-\frac{\cot y'}{y'} + \frac{1}{y'^2} \right] \qquad (2.10a)$$

where $y'^2 = -y^2$ and is positive. In the expressions for N in Eqs. (2.10) and (2.10a), the second term is due to the modification of the density of states (and depends crucially on the choice of the boundarycon- ditions[9,11]) whereas the firs't term includes the effect of discreteness of states in addition to the bulk term; see Eq. (2.9). At this point we wish to emphasize that our final expression for N passes smoothly from the region with $y^2 > 0$ to the region with $y^2 < 0$. This is important be- cause, under D.B.C., one must ultimately deal with the region of nega- tive y^2 — in particular, with the limiting situation $y^2 = -n^2$. In this connection, we observe that the zero-temperature limit of the chemical potential μ of the system is given by ε_0, which isequal to $\varepsilon(1) = h^2/8mL^2$; accordingly, the limiting value of a is $-h^2/(8mL^2 kT) = -\pi(\lambda/L)^2/4$ and, by Eq. (2.6), the corresponding value of y^2 is $-\pi^2$. The relevance of this limit is highlighted by the fact that the ground-state occupation number N_0 is given by

$$N_0 = \frac{1}{e^{\alpha + \beta \varepsilon_0} - 1} \simeq \frac{1}{\alpha + \beta \varepsilon_0} = \frac{4x}{y^2 + \pi^2} \qquad (2.12)$$

We notice from Eqs. (2.5) - (2.10a), that for $y^2 \gg 1$, the bulk term is the most important, the next in importance is the term due to the modi- fication of the density of states and the term due to the discreteness of states is negligible. For $y^2 > 0$ and of $O(1)$, all the three termsare comparable. For $y^2 < 0$ but not close to $-\pi^2$, the term due to the modi- fication of the density of states is comparable with thesumofthe other two but, for $y^2 = -n^2$, this term becomes negligible as compared to others.

Following a similar procedure, Eq. (2.2) becomes

$$P = \frac{kT}{\lambda} \left[\xi(3/2) - \frac{y \coth y}{x} \right]. \qquad (2.13)$$

Using Eq. (2.10), this takes the form

$$P = \left[\frac{2\pi m}{h^2}\right]^{1/2} (kT)^{3/2} \left[\xi(3/2) - \frac{1}{x} - \frac{y^2 N}{2\pi x^3}\right] \qquad (2.14)$$

The **pressure** P_0 exerted by the condensate can be extracted from the last term by letting $y^2 \to -\pi^2$; we obtain, as expected,

$$P_0 = \left[\frac{2\pi m}{h^2}\right]^{1/2} (kT)^{3/2} \frac{\pi}{2} \frac{N_0}{x^3} = N_0 \frac{h^2}{4mL^3} = \frac{2N_0 \epsilon_0}{V} . \qquad (2.15)$$

2.2. Heat Capacity, Critical Behaviour and Discussion

For studying the heat capacity and the **critical** behaviour of the system, we must **first** of **all** determine the manner in which the parameters z and y^2 vary as the system is **cooled** at constant N and P. From Eq. (2.10), we obtain

$$\left(\frac{\partial y^2}{\partial x}\right)_N = \frac{4uy^2}{x(u^2 y^2 + 3u - 1)} , \qquad (2.16)$$

where

$$u = \frac{N}{2\pi x^2} = \frac{\coth y}{y} - \frac{1}{y^2} . \qquad (2.17)$$

Eq. (2.14) now gives

$$\left(\frac{\partial P}{\partial T}\right)_N = \frac{3}{2} \cdot \frac{P}{T} + \frac{kT}{\lambda}\left[-\frac{N}{2\pi x^3} \cdot \left(\frac{\partial y^2}{\partial x}\right)_N + \frac{3y^2 N}{2\pi x^4} + \frac{1}{x^2}\right] \cdot \left(\frac{\partial x}{\partial T}\right)_N . (2.18)$$

The constancy of P, therefore, implies that

$$\left(\frac{\partial x}{\partial T}\right)_{N,P} = \frac{3}{4\pi} \frac{P\lambda}{kT^2} \frac{N}{u} \frac{u^2 y^2 + 3u - 1}{1 - 3u + 3uy^2 - 6u^2 y^2 - 3u^3 y^4} , \qquad (2.19)$$

where use has been made of Eq. (2.16). Now the heat capacity at constant pressure C_{13} is given by

$$C_p = \left[\frac{\partial}{\partial T}\,(U + PV)\right]_{N,P} = \frac{3}{2}\,P\!\left(\frac{\partial V}{\partial T}\right)_{N,P}$$

$$= \frac{3}{2}\,P\lambda \cdot \left[\left(\frac{\partial x}{\partial T}\right)_{N,P} - \frac{1}{2}\,\frac{x}{T}\right] \tag{2.20}$$

Using Eqs. (2.14), (2.17) and (2.19), Eq. (2.20) can be written as

$$\frac{C_p}{Nk} = \frac{9}{8\pi}\left[\xi(3/2) - \frac{(2\pi u)^{1/2}(1+uy^2)}{N^{1/2}}\right]^2 \cdot \left[\frac{u^2 y^2 + 3u - 1}{u - 3u^2 + 3u^2 y^2 - 6u^3 y^2 - 3u^4 y^4}\right.$$

$$\left. - \frac{(2\pi)^{1/2}}{3}\,\frac{11}{\xi(3/2)N^{1/2}u^{1/2} - (2\pi)^{1/2}u(1+uy^2)}\right] \cdot \tag{2.21}$$

We find that C_p considered as a function of temperature passes througha smooth maximum. We call the temperature (depending on N) 'corresponding to this maximum as the **critical** temperature T_c. Putting the derivative of C_p with respect to y equal to zero, we obtain the followingvalue of $y(= y_c)$ corresponding to the critical temperature:

$$y_c \simeq \left[\frac{6}{7} \cdot \frac{\xi(3/2)}{(2\pi)^{1/2}}\right]^{2/3} \cdot N^{1/3}, \tag{2.22}$$

and the corresponding $x(= x_c)$ is obtained from (2.17) and (2.22) as

$$x_c \simeq \left[\frac{y_c N}{2\pi}\right]^{1/2} = \left[\frac{6}{7}\,\xi(3/2)\right]^{1/3} \cdot \left(\frac{N}{2\pi}\right)^{2/3}. \tag{2.23}$$

For the amount of condensate at $T = T_c$, we have, from Eqs. (2.12), (2.22) and (2.23),

$$(N_0)_c \simeq \frac{4\pi x_c^2}{y_c^2} = \frac{2N}{y_c} = 2\left[\frac{6}{7}\,\frac{(3/2)}{(2\pi)^{1/2}}\right]^{-2/3} \cdot N^{2/3} = O(N^{2/3}), \tag{2.24}$$

and for C_p at $T = T_c$, we have, from Eqs. (2.17), (2.21) and (2.22)

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$$\frac{C_p}{Nk} \approx \frac{9}{8\pi} \cdot \left[\xi(3/2)\right]^2 \cdot \left[1 - 3 \left(\frac{6}{7} \frac{\xi(3/2)}{(2\pi)^{1/2}}\right)^{-2/3} N^{-1/3}\right]. \qquad (2.25)$$

In the thermodynamic limit, $C_p \rightarrow 9/8\pi \cdot \left[\xi(3/2)\right]^2$ and $T_c \rightarrow T_c(\infty)$. This is not in agreement with the results[12] of Imry et al. (see Eq. (25) of reference i!, where C_p/N diverges as $T \rightarrow T_c(\infty)^+$). Now Eq. (2.14) can be written as

$$T_c^{3/2}(\infty) = T^{3/2} \cdot \left[1 - \frac{1}{x\xi(3/2)} - \frac{y^2 N}{2\pi x^3 \xi(3/2)}\right] \qquad (2.26)$$

and from this, we get the following expression for T_c,

$$T_c = T_c(\infty) \cdot \left[1 + \frac{2}{3} \cdot \left(\frac{6}{7} \cdot \frac{2\pi}{\xi^2(3/2)}\right)^{1/3} \cdot N^{1/3}\right] \qquad (2.27)$$

where

$$T_c(\infty) = \frac{1}{k} \cdot \left[\frac{hP}{\xi(3/2)(2\pi m)^{1/2}}\right]^{2/3}$$

is the value of T_c in the thermodynamic limit. We notice from (2.23) that the *volume* of the system has become subextensive and the particle density n diverges, in the thermodynamic limit, in agreement with Imry et al[2] and from Eq. (2.24), it follows that the condensate is not macroscopic at $T = T_c$.

It may be interesting to study the values of y^2, N_0 and x at certain special temperatures, in addition to the temperature T_c at which the values of these quantities have already been given. We shall consider the temperatures (i) $T_0(N)$ corresponding to $y^2 = 0$ and (ii) $T_c(\infty)$.

(i) $T = T_0$.

Putting $y^2 = 0$ in Eq. (2.10), we get $x_0 = (3/2)^{1/2}$ and then it readily follows from Eq. (2.26) that

$$T_0(N) = T_c(\infty) \cdot \left[1 + (2/3)^{3/2} \cdot \frac{1}{\xi(3/2)} \cdot (\pi/N)^{1/2} \right]. \quad (2.28)$$

Putting $y^2 = 0$ and the value of x_0 in Eq. (2.12), we obtain $(N_0)_0 = 6N/\pi^2$, that is, at temperature $T_0(N)$ which is less than T_c and greater than $T_c(\infty)$, the condensate is macroscopic.

(ii) $T = T_c(\infty)$.

Putting $T = T_c(\infty)$ in Eq. (2.26), we get $y^2 N = - 2rx^2$ and then solving this with Eq. (2.10a), we get $y^2 \simeq - (\pi^2/4)$ and $x = (\pi N/8)^{1/2}$. Using these values in Eq. (2.12), we get $N (T=T_c(\infty)) = (2N/3)$.

For temperatures below $T_c(\infty)$ (but not very close to it), $y^2 < - (\pi^2/4)$ and from Eq. (2.26), it follows that $x = O(N^{1/3})$. Further, as in this range $N_0 = O(N)$, it follows from Eq. (2.12) that $y^2 = - \pi^2 + + O(N^{-1/3})$. Then, in Eq. (2.26), the second term which is due to the modification of the density of states becomes negligible and one readily obtains the dependence of x on T,

$$x = \left[\frac{\pi}{2 \xi(3/2)} \right]^{1/3} \frac{T^{1/2}}{(T_c^{3/2}(\infty) - T^{3/2})^{1/3}} N^{1/3} \quad (2.29)$$

and

$$V = (\hbar^2 N/4mP)^{1/3} T_c^{1/2}(\infty) / \left[T_c^{3/2}(\infty) - T^{3/2} \right]^{1/3} \quad (2.30)$$

and as $T \to 0$, $V \to V_0 = (\hbar^2 N/4mP)^{1/3}$ which is precisely the volume required, in this limit, to maintain the system at constant pressure; see Eq. (2.15). To calculate y^2 in this region of temperature, we put $y^2 = - r^2 + + \varepsilon(T)$, $(\varepsilon(T) = O(N^{-1/3}))$ in Eq. (2.10) and obtain

$$\varepsilon(T) = \frac{4\pi x^2}{N} + \frac{12x^4}{N^2} , \quad (2.31)$$

and from (2.12)

$$N_0 = 4\pi x^2/\varepsilon(T) \simeq N - \frac{3}{\pi} x^2$$

which can be written as

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$$N_0 = N - N_e \quad , \qquad\qquad (2.32)$$

N_e being the number of particles in the excited states and is given by

$$N_e = \frac{3}{\pi} \cdot 2 = \frac{3}{\pi}\left[\frac{\pi}{2\xi(3/2)}\right]^{2/3} \cdot \frac{T}{(T_c^{3/2}(\infty) - T^{3/2})^{2/3}} N^{2/3}, \quad (2.33)$$

so that in the thermodynamic limit $N_e/N \to 0$ and $N_0/N \to 1$ at temperatures below $T_c(\infty)$ but not very close to it. Further, putting $y^2 \simeq -\pi^2$ and using Eq. (2.29) for x in Eq. (2.21), C_p is, then, given by

$$\frac{C_p}{k} = \frac{3}{4} \cdot (\pi\xi^2(3/2)/2)^{1/3} \cdot T^{1/2} \, T_c^{3/2}(\infty) \cdot \left[T_c^{3/2}(\infty) - T^{3/2}\right]^{-4/3} \cdot N^{1/3} \, ,$$

$$(2.34)$$

so that in this region, C_p has also become subextensive. For comparison, we tabulate below the values of y^2, x and N_0 at the special temperatures:

Temp.	y^2	x	N_0
T_c	$O(N^{2/3})$	$O(N^{2/3})$	$O(N^{2/3})$
T_0	0	$(3N/2\pi)^{1/2}$	$6N/\pi^2$
$T_c(\infty)$	$-\pi^2/4$	$(\pi N/8)^{1/2}$	$2N/3$
$T \to 0$	$y^2 \simeq -\pi^2$	$x \to 0$	$N_0 \to N$

From the comments after Eq. (2.12) and the discussion of the last paragraphs, it follows that in the critical region, the effects due to the modification of the density of states and the discreteness of states are of comparable importance and they together determine the precise nature of the physical behaviour of the system in this region. Further, for $T < T_c(\infty)$ (but not very close to it), the effect due to the modification of the density of states becomes negligible and the Eqs. (2.29) - (2.34) are valid in this range. Also in this range, the condensate pressure P_0 plays a dominant role. It can be casily shown that the temperature T_c', where the macroscopic condensation starts, is slightly greater than T_0 and is given by

$$T_c' = T_c(\infty) \cdot \left[1 + O(N^{-1/2})\right] \qquad (2.35)$$

It is possible to study, numerically, the dependence of $y^2, N_0/N$ and C_p/Nk on the temperature for given values of N. From Eqs.(2.10) and (2.26), we can find the dependence of r and y^2 on $T/T_c(\infty)$ for a given value of N and then using Eqs. (2.12) and (2.21), the values of N_0/N and C_p/Nk for different temperatures can be found out.

In Fig.1, we have plotted the thermogeometric parameter y^2 vs. $(T/T_c(\infty))$ for three different values of N. We find that as the tempera-
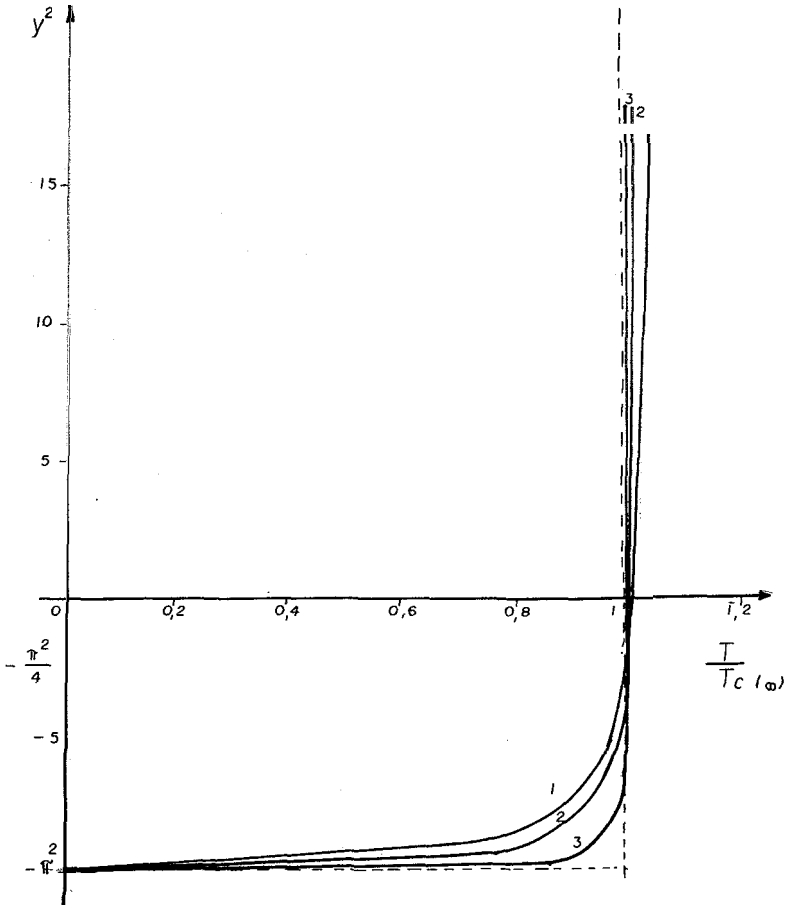
Fig.1 - Thermogeometric parameter y^2 as a function of scaled temperature $T/T_c(\infty)$, under Dirichlet boundary conditions (D.B.C.). Curves, 1, 2 and 3 correspond to $N = 10^3$, 10^4 and 10^6 respectively. Dotted line depicts the corresponding bulk behaviour.

ture $T_c(\infty)$ is approached from above, y^2 falls from large values to the value $-\pi^2/4$. As the temperature further falls from $T_c(\infty)$ to very low temperaturss tending to zero, y^2 falls from $-\pi^2/4$ to $-\pi^2$. For finite N, the curves are smooth. As N increases, the fall in the value of y^2 becomes more rapid. In the case of thermogeometric limit, the fall would be abrupt. This shows the effect of the size being finite.

Fig. 2 shows graphs between condensate fraction N_0/N and $T/T_c(\infty)$ for three different values of N. again we notice that the condensate grows smoothly for finite N, the growth being large in the neighbourhood of $T_c(\infty)$. As N increases, the growth. becomes more rapid and finally, in the thermodynamic limit, the condensate will build up abruptly at $T_c(\infty)$. Further, for any N at $T = T_c(\infty)$, $N_0/N = 2/3$ and as $T \to 0, N_0 \to N$.

In Fig.3, we have shown the variation of C_p/Nk with $T/T_c(\infty)$ for three different values of N. The curves pass through smooth maxima. The
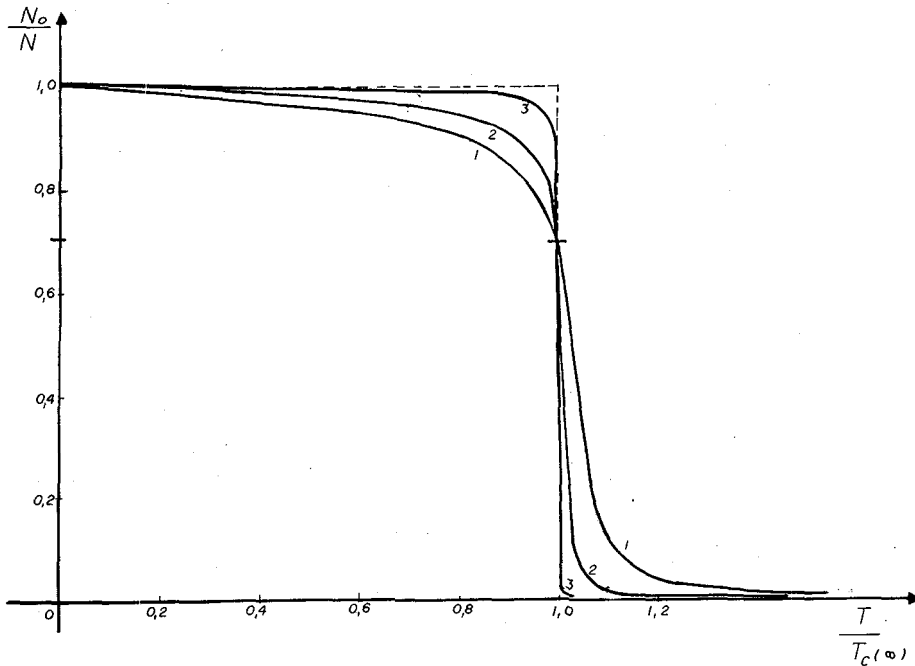

Fig.2 - Temperature dependence of the condensate fraction N_0/N, under D.B.C.. Curves 1, 2 and 3 correspond to N = 103, 10^4 and 10^6 respectively. The bulk behaviour is shown by the dotted curve.
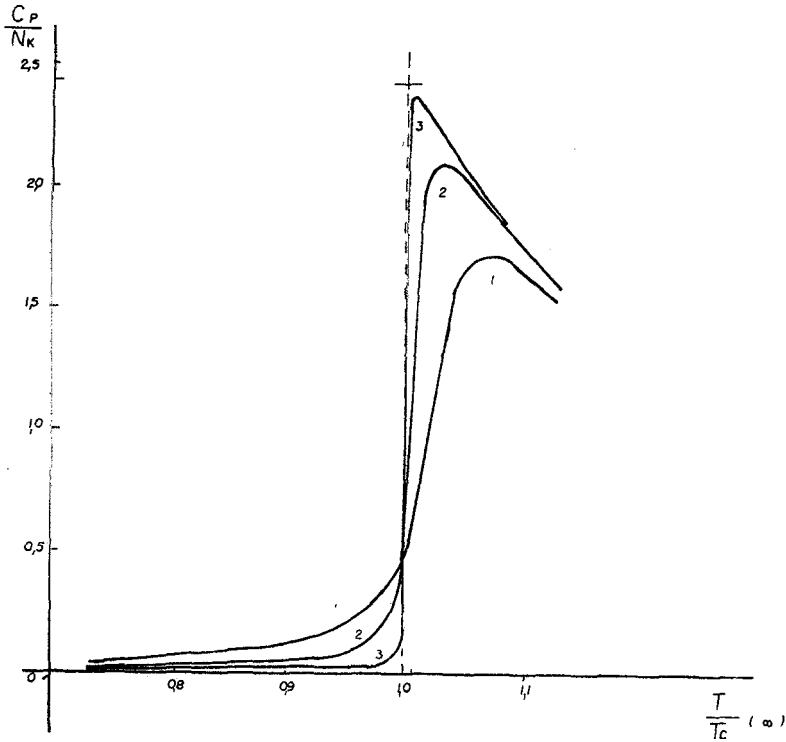
Fig.3 - The specific heat C_p/Nk as function of temperature, under 0.8 C.. Curves 1, 2 and 3 correspond to $N = 10^3$, 10^4 and 10^6 respectively.

temperature corresponding to these maxima, T_c, decreases as N increases and approaches $T_c(\infty)$ for $N \to \infty$. The value of C_p/Nk at T_c increases with increasing N and approaches $\frac{9}{8\pi} \xi^2(3/2) \simeq 2.44$ for $N \to \infty$. For high temperatures $T \gg T_c(\infty)$, it should tend to the classical value 1.5 but our expressions are not valid at these temperatures. As the temperature falls below $T_c(\infty)$, C_p quickly falls to subextensive values $O(N^{1/3})$. The fall becomes more rapid as N increases and would be abrupt in the case of thermodynamic limit. Further, for any N, as $T \to 0$, $C_p \to 0$.

At this point, it may be worthwhile to compare these results with those for the corresponding two-dimensional and three-dimensional problems. Though most of the features in the present case are similar to the ones in the previous cases, the results are different in the region close to the critical temperature. The problem in two dimensions was solved in such a way that there were to regions having different solutions

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for x, y^2, N_0/N and C_p/Nk and the awkward feature of the results was that these regioiis somewhat overlapped. In the case of the problem in three dimensions also, this awkward feature existed but assuming the continuity of C_p, this feature was removed (a similar procedure could for adopted for the two-dimensional case as well) but then x, y^2, N_0/N and the slope of C_p became discontinuous at T_c. In the present case, we find that x, y^2 and N_0/N all vary smoothly, even at the critical temperature and C_p passes through a smooth maximum and no discontinuities such as those in the other cases appear.

2.3. Cooling the System at Constant Volume L_c

In the problem of two dimensions, we noticed that when the system is cooled at constant pressure P to temperature T_c from above, the volume becomes somewhat subextensive and the amount of condensate in the single-particle ground state ε_0 does not become macroscopic at T_c. If now we cool the system at constant volume, the macroscopic occupation of the ground state does take place at finite temperatures. Let us now see what happens in the case of the one-dimensional system, when treated in the same way.

We have seen that when this system is cooled at constant pressure P to the temperature T_c from above, the value of L becomes subextensive,

$$L \to L_c = \lambda_c \, x_c = \lambda_c . O(N^{2/3}) \ .$$

At this stage, the amount of condensate in the single-particle ground state ε_0 is $O(N^{2/3})$ which is not macroscopic. Now let us cool the system at constant volume L_c. Under this constraint, we would have

$$x = L_c/\lambda = x_c (T/T_c)^{1/2} . \tag{2.36}$$

With the help of Eq. (2.36), Eq. (2.10) can be written as

$$N = 2\pi \, x_c^2 (T/T_c) \left[\frac{\coth y}{y} - \frac{1}{y^2} \right] \tag{2.37}$$

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and Eq. (2.12) can be written as

$$N_0 = \frac{4\pi \, x_c}{y^2 + \pi^2} \cdot (\frac{T}{T_c}) \quad .$$

We rewrite this equation'with the help of Eq. (2.23) as

$$(N_0/N) = (\frac{T}{T_c}) \cdot \frac{1}{y^2 + \pi^2} \cdot O(N^{1/3}) \quad . \qquad (2.38)$$

For (N_0/N) to be of $O(1)$ and for very large N, y must be of $O(N^{1/6})$ and then Eq. (2.37) gives the corresponding temperature

$$T/T_c = (N/2\pi x_c^2) \, y = O(N^{-1/6})$$

which goes to zero for $N \to \infty$. Thus macroscopic condensation in the ground state ε_0 will take place only at $T \to 0$ in the thermodynamic limit and not at finite temperatures unlike the case of the two-dimensional system.

3. MIXED BOUNDARY CONDITIONS

3.1. Formulation

We again consider a onerdimensional system of non-interacting bosons but subject to mixed boundary conditions (M.B.C.) i.e. $\psi_s = 0$ at one end and $\partial \psi_s / \partial n = 0$ at the other. Let $<n_t>$ be the mean occupation number for the single-particle states ε_i. The Eqs. (2.1) and (2.2) for the total number of particles and the total pressure P of the system are valid in this case also. The energy spectrum in this case is given by

$$\varepsilon(n) = \frac{h^2}{8mL^2} (n + \frac{1}{2})^2 \propto \frac{1}{V^2} \quad . \quad (n = 0,1,2,3,\dots) \qquad (3.1)$$

(instead of Eq. (2.3)). We further notice that Eq. (2.4) is also valid in the present case. Using techniques[4] referred to earlier, we get from Eq. (2.1)

$$N = \frac{L}{\lambda} \left[g_{1/2}(\alpha) - 2\pi^{1/2} \cdot \alpha^{-1/2} \cdot \sum_{q=0}^{\infty} (-1)^q \cdot e^{-2(q+1)y} \right] \quad , \qquad (3.2)$$

and noting that

$$\sum_{q=0}^{\infty} (-1)^q \cdot e^{-2(q+1)y} = \frac{1}{2} \cdot (1 - \tanh y) ,$$

this can be written as

$$N = \frac{L}{\lambda} \cdot \left[g_{1/2}(\alpha) - \pi^{1/2} \cdot \alpha^{-1/2} \cdot (1 - \tanh y) \right] \qquad (3.3)$$

where A, y, $g_n(\delta)$ occuring here were defined in section 2. In Eq. (3.2), the first term represents the bulk behaviour of the system while the second term arises explicitly from the discreteness of the single-particle states. As there is no modification in the density of states, no term arising from this effect occurs in Eq. (3.2) ..

In the region of interest (a << 1), the above equation with the help of Eq. (2.7) becomes

$$N = 2\pi x^2 \cdot (\tanh y/y) \qquad (3.4)$$

where again $x = (L/\lambda)$ is the measure of the *volume* of the system. For $y^2 < 0$, the Eq. (3.4) takes the form

$$N = 2\pi x^2 \cdot (\tan y'/y') \qquad (3.4a)$$

where $y'^2 = - y^2$ and is positive. We see from Eqs. (3.4) and (3.4a) that our final expression for N, in this case also, passes smoothly from the region with $y^2 > 0$ the region with $y^2 < 0$. This is quite satisfying because, one must ultimately deal with the region of negative y^2, in particular, with the limiting situation $y^2 = - \pi^2/4$. Here the zero-temperature limit of chemical potential μ of the system is given by ε_0, which, in this case, is equal to $\varepsilon(0) = h^2/(32mL^2)$; accordingly, the limiting value of a is $-h^2/(32mL^2kT) = - \pi(\lambda/L)^2/16$ and, by Eq. (2.6), the corresponding value of $y^2 = - \pi^2/4$. The relevance of this limit is again highlighted by the fact that the ground-state occupation number N_0 is given by

$$N_0 = \frac{1}{e^{a + \beta\epsilon_0} - 1} \quad \frac{1}{\alpha + \beta\epsilon_0} \quad \frac{4\pi \; x^2}{y^2 + (\pi^2/4)} \qquad (3.5)$$

We notice from Eq. (3.3), that for $y^2 \gg 1$, the term due to the discreteness of states is negligible whereas for smaller values of y^2 (including negative ones), it is quite important.

Following a similar procedure, Eq. (2.2) now becomes

$$P = \frac{kT}{\lambda} \cdot \left[\xi(3/2) - \frac{y}{x} \cdot \tanh y \right] . \qquad (3.6)$$

Using Eq. (3.4), this takes the form

$$P = \left(\frac{2\pi m}{h^2}\right)^{1/2} \cdot (kT)^{3/2} \cdot \left[\xi(3/2) - \frac{Ny^2}{2\pi \; x^3} \right] . \qquad (3.7)$$

In this case, the pressure P_0 exerted by the condensate can also be extracted from the last term by letting $y^2 \rightarrow {}^- \pi^2/4$, we obtain, as expected,

$$P_0 = \left(\frac{2\pi m}{h^2}\right)^{1/2} \cdot (kT)^{3/2} \cdot \frac{\pi}{x^8} \cdot \frac{N_0}{x^3} = N_0 \cdot \frac{h^2}{16mL^3} = 2\, N_0 \cdot \frac{E_0}{V} . \qquad (3.8)$$

3.2. Heat capacity, Critical Behaviour and Discussion

For studying the heat capacity and the critical behaviour, we again calculate $(\partial y^2/\partial x)_N$ and $(\partial x/\partial T)_{N,P}$. From Eq. (3.4), we obtain,

$$\left(\frac{\partial y^2}{\partial x}\right)_N = \frac{4uy^2}{x(u^2y^2 + u - 1)} , \qquad (3.9)$$

where

$$u = \frac{N}{2\pi x^2} = \frac{\tanh y}{y} . \qquad (3.10)$$

Using Eqs. (3.7) and (3.9), we get

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$$\left(\frac{\partial x}{\partial T}\right)_{N,P} = \frac{3}{4\pi} \frac{P\lambda}{kT^2} \frac{N}{u^2y^2} \frac{u^2y^2 + u - 1}{3 + u - 3u^2y^2} . \tag{3.11}$$

Eq. (2.20) for the heat capacity C_p is valid in this case also. Using Eqs. (3.7), (3.10) and (3.11), we obtain

$$\frac{C_p}{Nk} = \frac{9}{8} \cdot \xi^2(3/2) \cdot \left[1 - \left(\frac{2\pi}{N}\right)^{1/2} \frac{y^2u^{3/2}}{\xi(3/2)}\right]^2 \cdot \left[\frac{u^2y^2 + - 1}{u^2y^2(3+u-3u^2y^2)} - \frac{1}{3}\left(\frac{2\pi}{Nu}\right)^{1/2}\right.$$

$$\left. \cdot \frac{1}{\xi(3/2)} \cdot \frac{1}{1 - \left(\frac{2\pi}{N}\right)^{1/2}\frac{y^2u^{3/2}}{\xi(3/2)}}\right] . \tag{3.12}$$

We find thet C_p passes through a **smooth maximum** at an N-dependent **temperature** T_c, the **critical** temperature. Putting the derivative of C_p with respect to y equal to zero, we find that the value of $y(= y_c)$ **corresponding** to T_c satisfies the following equation approximately,

$$y_c - \frac{1}{4} \ln\left[y_c(4y_c - 3)^2\right] \cong \frac{1}{4} \ln N - \frac{1}{2} \ln\left[\frac{7}{48} \frac{(2\pi)^{1/2}}{(3/2)}\right]. \tag{3.13}$$

We note thet y_c is of $O(\ln N)$. for a given **value** of N, we can find y_c **numerically from** Eq. (3.13). In the thermdynamic limit, y_c is given by

$$y_c = \frac{1}{4} \ln N . \tag{3.13a}$$

From Eqs. (3.4) and (3.13), we obtain for x_c

$$x_c = \left[\frac{Y, N}{2 \tanh y_c}\right]^{1/2} = O(N \ln N)^{1/2} \tag{3.14}$$

which, in the **thermodynamic** limit, is

$$x_c = \frac{1}{2} \left[\frac{N \ln N}{2\pi}\right]^{1/2} \tag{3.14a}$$

Using Eqs. (3.5) and (3.14), we obtain for the amount of condensate at T $= T_c$,

$$(N_0)_c = \frac{2y_c N}{(y_c^2 + \frac{\pi^2}{4}) \tanh y_c} = O(N/\ln N) \quad (3.15)$$

which, in the thermodynamic limit, is

$$(N_0)_c = 8N/\ln N. \quad (3.15a)$$

For C_p at $T = T_c$, we have, from Eqs. (3.12) and (3.14),

$$C_p/Nk = \frac{9}{8\pi} \xi^2(3/2) \left[1 - \frac{7}{3\xi(3/2)} \cdot \left(\frac{2\pi y_c}{N} \right)^{1/2} + (4 - 16y_c) \cdot e^{-2y_c} \right]$$

$$(3.16)$$

which, in the thermodynamic limit, is

$$(C_p/Nk) = \frac{9}{8} \xi^2(3/2) \cdot \left[1 - O\left(\frac{\ln N}{N^{1/2}} \right) \right] \simeq \frac{9}{8\pi} \xi^2(3/2) . \quad (3.16a)$$

Now Eq. (3.7) can be written as

$$T_c^{3/2}(\infty) = T^{3/2} \cdot \left[1 - \frac{Ny^2}{2\pi\xi(3/2)x^3} \right] \quad (3.17)$$

and from this, we get the following expression for T_c,

$$T_c = T_c(\infty) \cdot \left[1 + \frac{Ny_c^2}{3\pi\xi(3/2)x_c^3} \right] = T_c(\infty) \cdot \left[1 + O(\frac{\ln N}{N})^{1/2} \right] \quad (3.18)$$

From Eq. (3.14), it follows that the volume of the system has become sub-extensive and from Eq. (3.15), we find that the condensate is not yet macroscopic at $T = T_c$. Further, comparing Eqs. (2.27) and (3.18), we notice that the critical temperature in the case of M.B.C. is lower than that for D.B.C. and comparing Eqs. (2.25) and (3.16), we observe that the maximum of C_p/Nk for M.B.C. is higher than that for D.B.C., for the same

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value of N. Further, it may be worthwhile to compare Eqs. (3.13), (3.14) and (3.15) for the M.B.C. with Eqs. (2.22), (2.23) and (2.24) for D.B.C. respectively.

We may now study the values of y^2, x and N_0 at another special temperature $T_c(\infty)$ $(= T_0)$. From Eq. (3.17), it follows that at this temperature, $y^2 = 0$ and then from Eq. (3.4), we get $x_0 = (N/2\pi)^{1/2}$. Using these values in Eq. (3.5), we get $(N_0)_0 = (16x_0^2/\pi) = 8N/\pi^2$.

For temperatures below $T_c(\infty)$ but not very close to it, $-\pi^2/4 < y^2 < 0$ and then from Eq.(3.17), it follows that $x = O(N^{1/3})$. Further, as in this range $N_0 = O(N)$, we find from Eq. (3.5) that $y^2 = -(\pi^2/4) + O(N^{-1/3})$, and then from Eq. (3.17), we get the following (x, T) relationship,

$$x = (\pi/8\xi(3/2))^{1/3} \ \frac{T^{1/2}}{(T_c^{3/2}(\infty) - T^{3/2})^{1/3}} \ N^{1/3} \qquad (3.19)$$

and

$$V = (h^2 N/16mP)^{1/3} \ \frac{T_c^{1/2}(\infty)}{(T_c^{3/2}(\infty) - T^{3/2})^{1/3}} \qquad (3.20)$$

and as $T \to 0$, $V \to V_0 = (h^2 N/16mP)^{1/3}$ which is the volume required, in this limit, to maintain the system at constant pressure; see Eq. (3.8). To calculate y^2 in this range of temperature, we put $y^2 = -\pi^2/4 + \epsilon(T)$, $(\epsilon(T) = O(N^{-1/3}))$ in Eq. (3.4) and obtain

$$\epsilon(T) = \frac{4\pi x^2}{N} + \frac{16x^4}{N^2} \qquad (3.21)$$

and from Eq. (3.5)

$$N_0 = 4\pi x^2/\epsilon(T) \simeq N - 4x^2/\pi = N - N_e , \qquad (3.22)$$

where N_e, the number of particles in the excited states, is given by

$$N_e = (4/\pi)(\pi/8\xi(3/2))^{2/3} \cdot \frac{T}{(T_c^{3/2}(\infty) - T^{3/2})^{2/3}} \ N^{2/3} \qquad (3.23)$$

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Further, putting $y^2 = -(\pi^2/4)$ and using Eq. (3.19) for x in Eq. (3.12), C_p is then given by

$$\frac{C_p}{k} = \frac{3}{4} \left(\pi \xi^2 (3/2)/8\right)^{1/3} \cdot \frac{T^{1/2} \, T_c^{3/2} (\infty)}{(T_c^{3/2} (\infty) - T^{3/2})^{4/3}} \, N^{1/3} \, , \qquad (3.24)$$

so that in this region C_p has also become subextensive. For comparison, we tabulate below the values of y^2, x and N_0 at the special temperatures:

Temperature	y^2		N_0
T_c	$O(\ln N)^2$	$O(N \ln N)^{1/2}$	$O(N \ln N)$
$T_c(\infty) = T_0$	0	$(N/2\pi)^{1/2}$	$8N/\pi^2$
$T \to 0$	$y^2 \approx -\pi^2/4$	$x \to 0$	$N_0 \to N$

combining the comments after Eq. (3.5) and the discussion above, we observe that for temperatures around and above T_c, the effect due to the discreteness of states is negligible whereas for temperatures around and below $T_c(\infty)$, it is quite important and further, for temperatures below $T_c(\infty)$, P_0 plays a dominant role.

From Eqs. (3.4) and (3.17), we can find numerically the variations of s and y^2 with $T/T_c(\infty)$, for given values of N. Then from Eqs. (3.5) and (3.12), we can determine N_0/N and C_p/Nk as functions of temperature.

In figs. 4, 5 and 6, we have shown graphs, y^2 vs. $T/T_c(\infty)$, N_0/N vs. $T/T_c(\infty)$ and C_p/Nk vs. $T/T_c(\infty)$ respectively. From Fig.4, it is clear that as the temperature $T_c(\infty)$ is approached from above, y^2 falls from large values to zero. As the temperature further falls from $T_c(\infty)$ to very low temperatures tending to zero, y^2 falls from zero to $-\pi^2/4$. Further, in Fig. 5, for any N, $N_0/N = 8/\pi^2$ at $T = T_c(\infty)$. The other comments concerning Figs. 1, 2, and 3 apply to Figs. 4, 5 and 6 respectively. In Figs. 7, 8 and 9, 10 and 11, we compare variations of y^2 vs. $T/T_c(\infty)$, N_0/N vs. $T/T_c(\infty)$ and C_p/Nk vs. $T/T_c(\infty)$ in the case of D.B.C. with those in the case of M.B.C.. We observe that at higher temperatures,
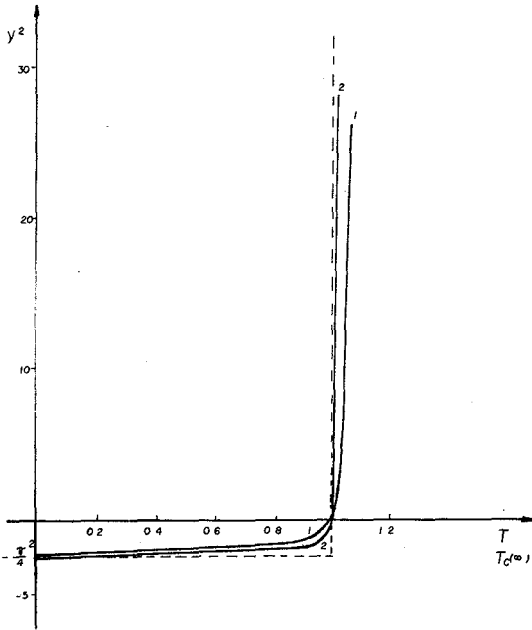
Fig.4 - Thermogemetric parameter y^2 as a function of temperature, under mixed boundary conditions (M.B.C.). Curves 1 and 2 correspond to $N = 10^3$ and 10^4 respectively. The dotted curve shows the bulk behaviour.
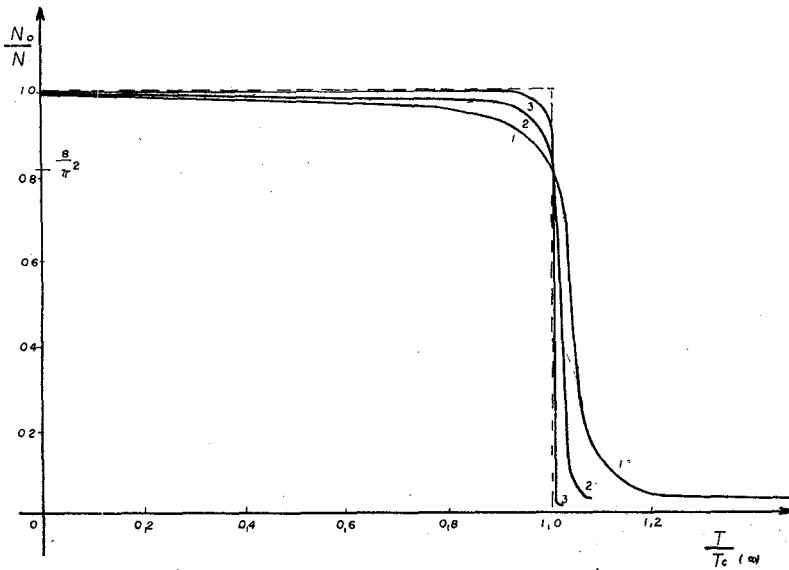

Fig.5 - The temperature dependence of the condensate fraction N_0/N, under M.B.C.. Curves 1, 2 and 3 correspond to $N = 103$, 10^4 and 10^6 respectively. The bulk behaviour is shown by the dotted curve.
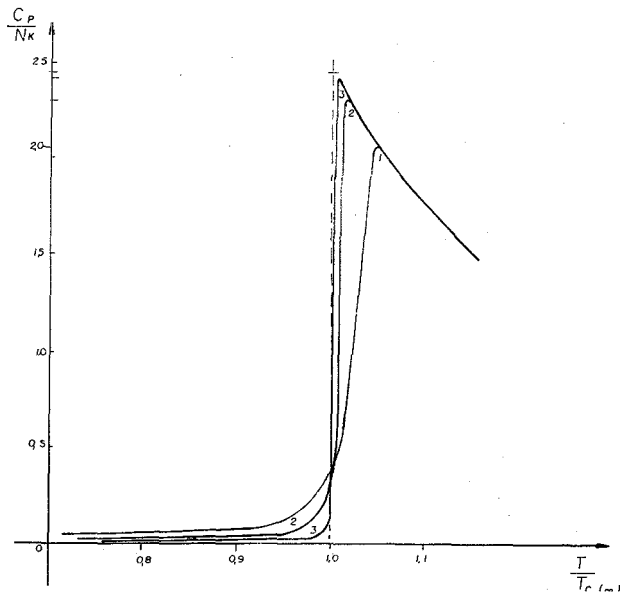
Fig.6 - The specific heat C_P/Nk as a function of temperature, under M. B.C.. Curves 1, 2 and 3 correspond to $N = 10^3$, 10^4 and 106 respectively.
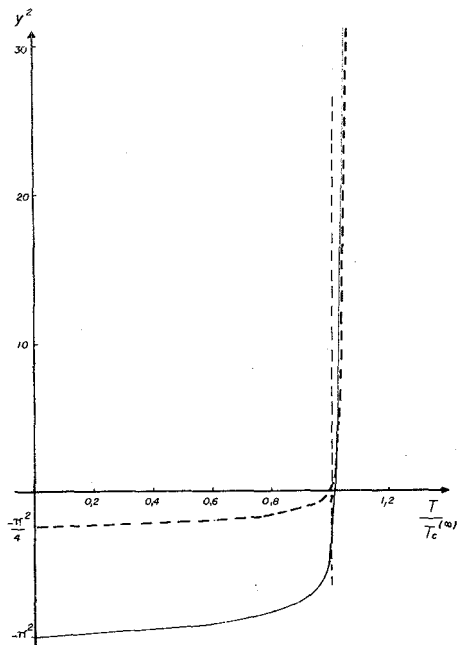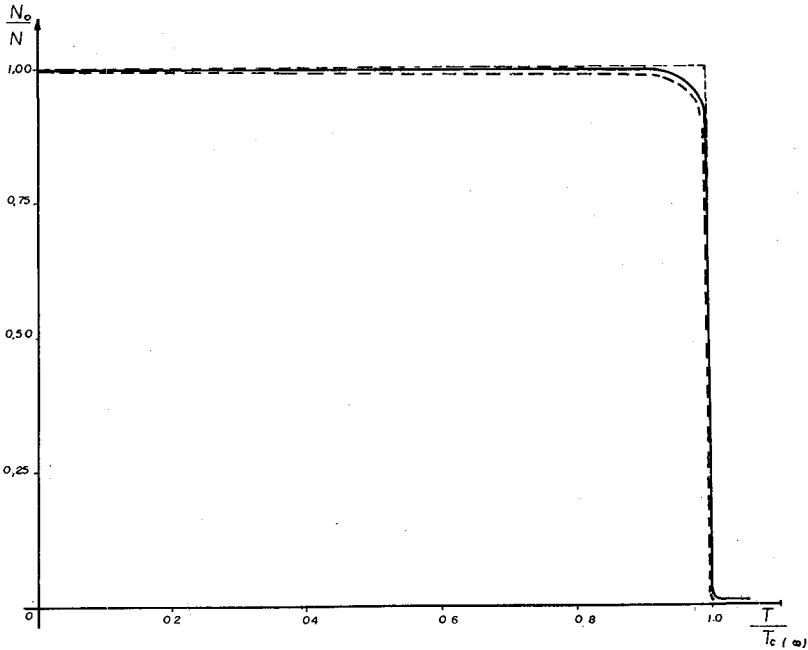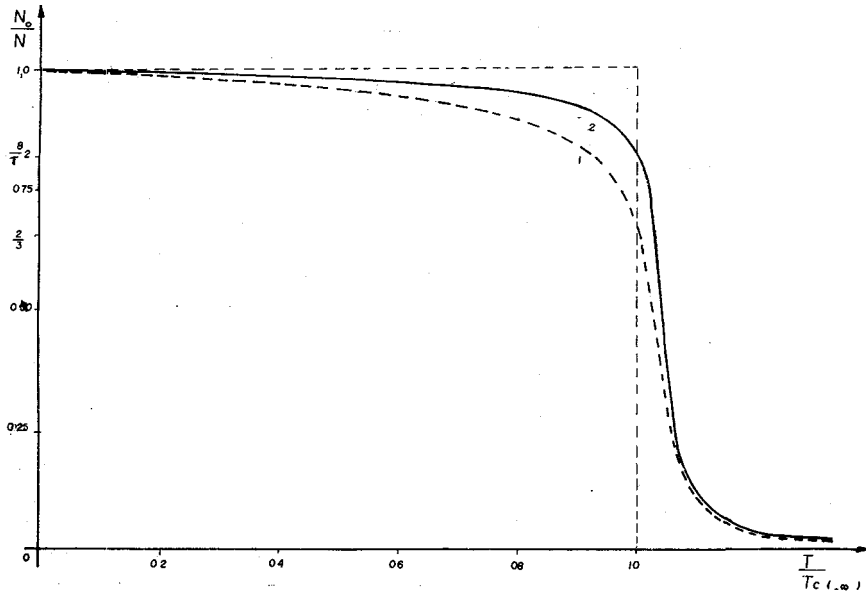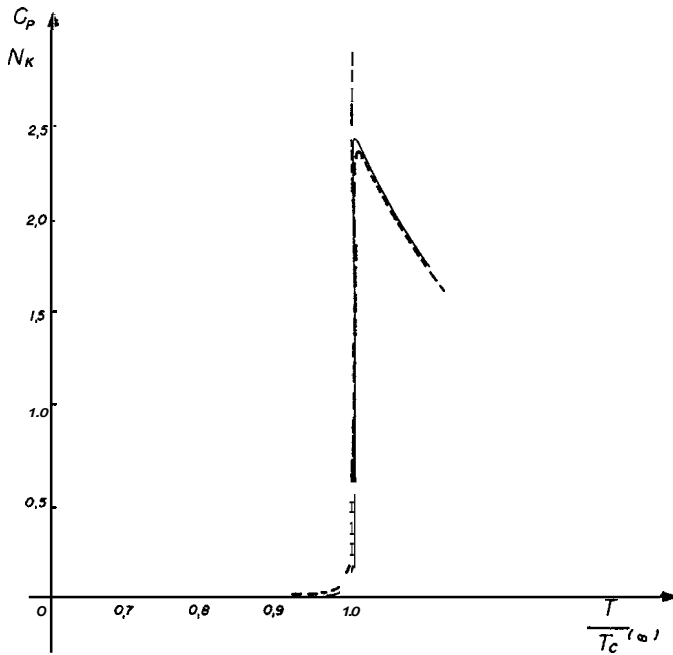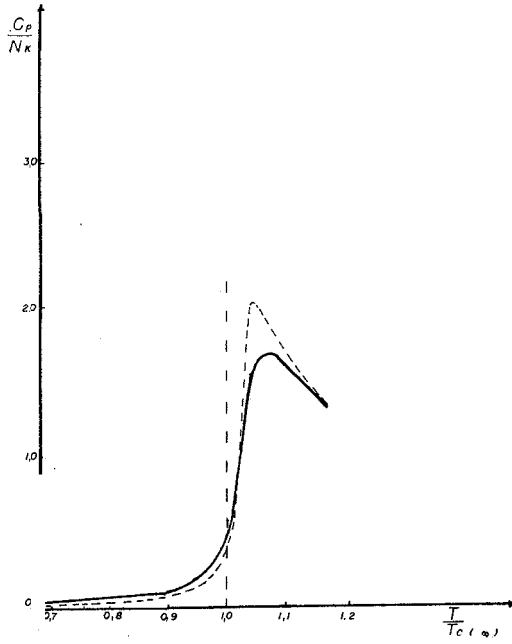

Fig.7 - Comparison of the variation of y^2 as a function of $T/T_c(\infty)$ under D.B.C. with that under M.B.C.. Solid curve is for D.B.C. and dotted curve for M.B.C.. Here $N = 10^3$.

Figs. 8 and 9 - Comparison of variation of N_0/N as a function tempera-
ture under D.B.C. with those under M.B.C.. Solid curves are for D.B.C.
and dotted curves for M.B.C.. In Fig. 8, $N = 10^3$ and in Fig. 9, N = 106.

Figs. 10 and 11 – Comparison of the variation of C_p/Nk as functions of temperature under D.B.C. with those under M.B.C.. Solid curves are for D.B.C. and dotted for M.B.C.. In fig. 10, $N = 10^3$ and in Fig. 11, $N = 10^6$.

these quantities tend to agree in the two cases whereas for the critical region, there are significant deviations. This would be expected, because at high temperatures, the higher single-particle energy states are more important and comparing Eqs. (2.3) and (3.1), we find that the energy spectra for these states tend to be similar, whereas for lower temperatures, the lower single-particle energy states are more important and these are clearly different in the two cases.

3. 3. Cooling the System at Constant Volume L_c

When the system is cooled at constant pressure P to the temperature T_c from above, the value of L, as we have seen, becomes subextensive,

$$L \to L_c = x_c \lambda_c = \lambda_c O(N \ln N)^{1/2} \ .$$

At this temperature, the amount of condensate in the singla-particle ground state ε_0 is $O(N/\ln N)$ which is not yet macroscopic. Now let us cool the system at constant volume L_c. Under this constraint, we would have

$$x = L_c/\lambda = x_c (T/T_c)^{1/2} \tag{3.25}$$

Using Eq. (3.25), Eq. (3.4) can be written as

$$N = 2\pi x_c^2 (T/T_c) \quad (\tanh y/y) \tag{3.26}$$

and Eq. (3.5) can be written as

$$N_0 = \frac{4\pi x_c^2}{y^2 + (\pi^2/4)} \cdot (T/T_c) \ . \tag{3.27}$$

We rewrite this equation with the help of Eq. (3.14), as

$$(N_0/N) = (T/T_c) \frac{1}{y^2 + (\pi^2/4)} \cdot O(\ln N) \ . \tag{3.28}$$

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For $(N_0/N$ to be of the $O(1)$ and for very large N, y must be of $O(\ln N)^{1/2}$ and then Eq. (3.26) gives the corresponding temperature

$$(T/T_c) \simeq (N/2\pi x_c^2)y = O(\ln N)^{-1/2}$$

which goes to zero for N → ∞. Thus macroscopic condensation in the ground state ε_0 will take place only at T → 0, in the thermodynamic limit, in this case, as well.

4. FURTHER DISCUSSION

We have discussed the onset of Bose-Einstein condensation in a finite one-dimensional system of free bosons, under Dirichlet boundary conditions and mixed boundary conditions. In both these cases, $\varepsilon_0 \neq 0$ and so the quantum-mechanical zero-point pressure P_0 is also non-zero and it is possible to keep the pressure of the system constant even for temperatures below the critical temperature. If the system is subjected to periodic or Neumann boundary conditions, ε_0 is equal to zero the condensate does not contribute to the pressure. In these cases, it is not possible to keep the pressure constant below the critical temperature and system collapses to a point. Under these 'conditions, one can, therefore, study the behaviour of the system under constant pressure for $T>T_c$ only. Details of this will be reported elsewhere[13].

We have earlier pointed out that B.E.C. in a one-dimensional system, under constant pressure, is possible because the particle density n diverges in the thermodynamic limit. In the presence of interactions (e.q. short-range repulsive potential which may be replaced by a hard core), the particle density cannot become infinite and so B.E.C. will not take place in the case of real bosons.

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REFERENCES

1. Y. Imry, D.J. Bergman and L. Gunther, in *Proceedings of the 13th International Conference on Low Temperature Physics, Boulder, Colorado, 1972.* (Plenum, New York, 1974), Vol.I, p.80.

2. L. Gunther, Y. Imry and D.J. Bergman, J.Stat.Phys. 10, 299 (1974).

3. S. Greenspoon and R.K. Pathria, Phys. Rev. $A9$, 2103 (1974).

4. A.N. Chaba and R.K. Pathria, J.Math.Phys. 16, 1457 (1975).

5. A.N. Chaba and R.K. Pathria, Phys. Rev. $B12$, 3697 (1975).

6. A.N. Chaba and R.K. Pathria, to be published in Phys. Rev. A.

7. P.C. Hohenberg, Phys. Rev. 158, 383 (1967).

8. J.J. Rehr and N.D. Mermin, Phys. Rev. B 1, 3160 (1970).

9. R.K. Pathria, Nuovo Cimento Suppl. 4, 276 (1966).

10. R.K. Pathria, Statistical Mechanics (Pergamon, New York, 1972).

11. R.K. F'athria, Phys. Lett. A35, 351 (1971).

12. The expressions for the particle density n and the specific heat C_p given in Eq. (25) of reference 2 appear to be in error.

13. A.M. Ferreira, Master's Thesis, UFPb., João Pessoa, in preparation.