# Bose-Einstein condensation in finite noninteracting systems: A relativistic gas with pair production

Surjit Singh and R. K. Pathria

Guelph-Waterloo Program for Graduate Work in Physics, Waterloo Campus, University of Waterloo,

Waterloo, Ontario, Canada N2L 3G1

(Received 6 February 1984)

Taking into account the possibility of particle-antiparticle pair production, we have investigated the onset of Bose-Einstein condensation in an ideal relativistic Bose gas confined to restricted geometries. Through an extensive use of the Poisson summation formula, we have carried out an explicit evaluation of the summations over states appearing in the problem, which enables us to make a rigorous analysis of the temperature dependence of the thermogeometric parameter  $y$  of the system in the case of a cubical enclosure under periodic boundary conditions. This, in turn, leads us to determine the growth of the condensate fraction  $\rho_0/\rho$  as a *smooth* function of temperature from  $T \geq T_c$  down to  $T=0$  K. Finite-size corrections to the standard bulk results are obtained in explicit terms and are shown to be in complete agreement with the Fisher-Barber scaling theory for such effects. In the end, special geometries, such as narrow channels and thin films, are also examined.

### I. INTRODUCTION

For one reason or another, the phenomenon of Bose-Einstein condensation has continued to be of abiding interest to theorists in different areas of condensed matter physics. Initially, the interest in this phenomenon arose from the role it plays in our understanding of the curious behavior of superfluid helium and, to a lesser extent, that of superconducting materials. Lately, it has caught the imagination of field theorists, who find it particularly relevant to problems such as pion condensation, gluon condensation, and quark confinement in the high-energy nuclear matter, and of theoretical astrophysicists who believe to have "encountered" it in the interior of the neutron stars. More recently, Kuzmin and Shaposhnikov' have discussed the cosmological consequences of the existence of a primordial massive photon gas, with Bose-Einstein condensation playing a vital role during the early epoch of the universe. The net result of these varied interests in this phenomenon is that the emphasis has gradually shifted from the study of nonrelativistic Bose systems to that of relativistic ones. Consequently, a number of authors<sup> $2-5$ </sup> have carried out detailed analyses of the ideal relativistic Bose gas in arbitrary dimensions and have examined the onset of Bose-Einstein condensation in a variety of limiting situations.

The foregoing studies seemed to have proceeded along a satisfactory path until about three years ago when Haber and Weldon<sup>6</sup> pointed out that in the analysis of a relativistic gas, composed of particles with nonzero rest mass m, at temperatures such that  $k_B T = O(mc^2)$  or greater, the possibility of particle-antiparticle pair production cannot be ignored. The inclusion of this possibility, they showed, had a profound influence on the phenomenon of Bose-Einstein condensation, both qualitatively and quantitatively; in particular, the dependence of the "charge density"  $\rho$ on T changed from the customary  $T^3$  to  $T^2$ , affecting drastically the dependence of the critical temperature  $T_c$ 

on  $\rho$ . The repercussion of this on other physical quantities is somewhat indirect but not insignificant. Following Haber and Weldon, Singh and Pandita<sup>7</sup> carried out a detailed examination of the critical behavior of the system in the vicinity of  $T_c$  and found that the onset of Bose-Einstein condensation depended on the dimensionality d of the system in very much the same way as in a nonrelativistic gas rather than in a conventional relativistic gas, viz. , the one without pair production. In particular, the critical indices governing the nature of the singularities in the various physical quantities pertaining to the system turned out to be the same as in the case of a nonrelativistic gas, though the critical amplitudes were different.

These investigations prompted us to carry out a theoretical analysis of the onset of Bose-Einstein condensation in a relativistic Bose gas confined to an enclosure of finite physical dimensions  $(L_1 \times L_2 \times L_3)$ , including at the same time the possibility of particle-antiparticle pair production. Such an analysis is markedly different in nature from the one customarily carried out for the bulk system in which the summations over states are replaced by integrations, using an asymptotic expression for the density of states in the given space (supposedly infinite in extent). This yields effects only due to the *normal fraction* of the particles, with the result that the effects due to the condensate, if any, have to be included additionally-and somewhat artificially. Not only does this procedure preclude the possibility of studying finite-size effects and the influence of boundary conditions on the various physical properties of the system but also drains away some of the very basic subtleties of the condensation process. Using techniques developed in a series of papers dealing with the nonrelativistic Bose gas confined to restricted geometries, $8-13$  we have now carried out a rigorous analysis of the present problem and have investigated in detail the joint influence of (i) the relativistic effects, (ii) the pair production, and (iii) the finiteness of the enclosure, on the nature of the phenomenon of Bose-Einstein condensation. Our procedure makes extensive use of the Poisson summation formula which obviates the necessity of using a density-of-states function  $D(\epsilon)$ ; it is, therefore, immune to errors that can, and are known to, creep into the analysis if one introduces approximations into the form of the function  $D(\epsilon)$ <sup>2,4</sup> It provides instead a rigorous means of studying the problem of Bose-Einstein condensation in an unambiguous manner, without having to resort to the unnatural act of extracting the condensate term from the original sum over states and approximating the remainder by a poor integral. We are thus able to unravel a number of important aspects of the smoothed-out transition in the ideal Bose gas which may, in the end, be converted into a sharp one (accompanied by a singularity in the thermodynamic behavior of the system) by letting the dimensions of the system tend to infinity, keeping the density constant.

During the course of this work we have derived an explicit expression for the growth of the condensate fraction,  $\rho_0/\rho$ , as a function of temperature which brings out clearly the deviations from the standard bulk result<sup>6,7</sup> and their dependence on the size of the container to which the system is confined. One remarkable result emerging here is that, for  $m > 0$ , while the inclusion of the possibility of particle-antiparticle pair production modifies the expression for  $T_c$  and also affects several properties associated with the transition, both qualitatively and quantitatively, the condensate itself consists almost entirely of particles alone; this contrasts sharply with the singular case of massless bosons for which the condensate contains as many antiparticles as particles.

Finally, wherever it has seemed desirable and feasible, we have sorted out special cases of our problem in respect of (i) the strength of the relativistic effects, i.e.,  $k_B T$  vs  $mc<sup>2</sup>$ , and (ii) the precise shape of the enclosure, i.e.,  $L_1$  vs  $L_2$  vs  $L_3$ .

# II. FORMULATION OF THE PROBLEM

We consider an ideal Bose gas composed of  $N_1$  particles and  $N_2$  antiparticles, each of mass m, confined to a cuboidal enclosure of sides  $L_1$ ,  $L_2$ , and  $L_3$ . Since particles and antiparticles are supposed to be created in pairs, the system is governed by the conservation of the number  $Q (=N_1-N_2)$ , rather than of the numbers  $N_1$  and  $N_2$ separately; the conserved quantity  $Q$  may be looked upon as a kind of generalized "charge." In equilibrium, the chemical potentials of the two species will be equal and opposite:  $\mu_1 = -\mu_2 = \mu$ , say, with the result that<sup>6</sup>

$$
N_1 = \sum_{\epsilon} (e^{\beta(\epsilon - \mu)} - 1)^{-1},
$$
  
\n
$$
N_2 = \sum_{\epsilon} (e^{\beta(\epsilon + \mu)} - 1)^{-1},
$$
\n(1)

where  $\beta=1/T$  and  $\epsilon=(\vec{k}^2+m^2)^{1/2}$ ; for simplicity, we shall use units such that  $\hbar = c = k_B = 1$ . Note that both  $\epsilon$ and  $\mu$  include the rest energy m of the particle (or the antiparticle) and, for the mean occupation numbers in the various states to be positive definite, we must have  $|\mu| \leq m$ . Assuming that, to begin with,  $\mu > 0$ , it readily follows that  $N_1 > N_2$  and hence  $Q > 0$ . In view of the conservation of  $Q$ ,  $\mu$  then stays positive under all circumstances. Without loss of generality, we shall assume that this indeed is the case.

Under periodic boundary conditions, the eigenvalues  $k_i$  $(i=1,2,3)$  of the wave vector k are given by

$$
k_i = (2\pi/L_i)n_i \quad (n_i = 0, \pm 1, \pm 2, \dots) \tag{2}
$$

the expression for  $N_1$  may, therefore, be written as

$$
N_1 = \sum_{j=1}^{\infty} e^{j\beta\mu} \sum_{n_1, n_2, n_3 = -\infty}^{\infty} \exp\left[-j\beta m \left[1 + \frac{4\pi^2}{m^2} \sum_{i=1}^3 \frac{n_i^2}{L_i^2}\right]^{1/2}\right].
$$
 (3)

The summation over  $n_i$  may be rendered into an expedient form by using the Poisson summation formula (PSF), name- $1v^{14}$ 

$$
\sum_{n_1,n_2,n_3=-\infty}^{\infty} f(n_1,n_2,n_3) = \sum_{q_1,q_2,q_3=-\infty}^{\infty} \mathcal{F}(q_1,q_2,q_3) ,
$$
 (4)

where

$$
\mathcal{F}(\vec{q}) = \int_{-\infty}^{\infty} f(\vec{n}) e^{2\pi i (\vec{q} \cdot \vec{n})} d^3 n \tag{5}
$$

It is obvious that the term with  $\vec{q} = 0$  on the right-hand side of (4) is precisely the result one would obtain by replacing the original summation over  $\vec{n}$  by an integration over  $d^3n$ . It follows that the term  $\mathcal{F}(0)$  would correspond to the bulk situation (exclusive of the condensate) and, hence, terms  $\mathcal{F}(\vec{q})$  with  $\vec{q} \neq 0$  would contain the condensate as well as the finite-size effects. An added benefit of using PSF is that, almost invariably, it converts a slowly convergent sum into a rapidly convergent one. Applying the Poisson transformation to (3), we obtain

$$
N_1 = \sum_{j=1}^{\infty} e^{j\beta\mu} \sum_{q_1, q_2, q_3 = -\infty}^{\infty} \left[ \frac{Vm^2}{2\pi^2 \beta} \right] \frac{j}{j^2 + \beta^{-2} \gamma^2(\vec{q})} K_2(\beta m[j^2 + \beta^{-2} \gamma^2(\vec{q})]^{1/2}), \tag{6}
$$

where  $V(= L_1L_2L_3)$  is the volume of the container,  $\gamma(\vec{q})=(q_1^2L_1^2+q_2^2L_2^2+q_3^2L_3^2)^{1/2}$  while  $K_2(z)$  is the modified Bessel function. Note that the  $\vec{q} = (0,0,0)$  term yields

$$
(N_1)_B = \frac{Vm^2}{2\pi^2 \beta} \sum_{j=1}^{\infty} j^{-1} e^{j\beta \mu} K_2(j\beta m) , \qquad (7)
$$

in agreement with the standard bulk result for  $N_1$ .<sup>3-5</sup> Equation (6) may now be written as

$$
N_1 = (N_1)_B + \frac{Vm^2}{2\pi^2\beta} \sum_{q_1, q_2, q_3 = -\infty}^{\infty} \sum_{j=1}^{\infty} \frac{je^{j\beta\mu}K_2(\beta m[j^2 + \beta^{-2}\gamma^2(\vec{q})]^{1/2})}{j^2 + \beta^{-2}\gamma^2(\vec{q})},
$$
\n(8)

where the primed summation over  $\vec{q}$  implies that the term with  $\vec{q} = (0,0,0)$  is excluded.

Our next task is to carry out the summation over  $j$ . For this we observe that, with  $\gamma(\vec{q})\neq 0$ , the sum in question is

$$
\sum_{j=1}^{\infty} f(j) = \sum_{j=0}^{\infty} f(j) = \sum_{j=-\infty}^{\infty} \int_0^{\infty} \delta(x-j) f(x) dx
$$

$$
= \sum_{l=-\infty}^{\infty} \int_0^{\infty} e^{2\pi i k} f(x) dx , \qquad (9)
$$

where the last step follows from the identity

$$
\sum_{l=-\infty}^{\infty} e^{2\pi i k} = \sum_{j=-\infty}^{\infty} \delta(x-j) , \qquad (10)
$$

which forms the backbone of the PSF. This converts the summation over  $j$  appearing in  $(8)$  into a summation over  $l$ , viz.,

$$
\sum_{l=-\infty}^{\infty} \int_0^{\infty} \frac{xe^{x(\beta\mu+2\pi il)}}{x^2+\beta^{-2}\gamma^2(\vec{q})} K_2(\beta m[x^2+\beta^{-2}\gamma^2(\vec{q})]^{1/2}) dx .
$$
\n(11)

For the modified Bessel function we employ the integral representation<sup>15</sup>

$$
K_{\nu}(z) = \frac{z^{\nu}}{2} \int_0^{\infty} \exp\left[-\frac{1}{2}\left[t + \frac{z^2}{t}\right]\right] t^{-\nu - 1} dt,
$$

whence (11) becomes

$$
\frac{\beta^2 m^2}{2} \sum_{l=-\infty}^{\infty} \int_0^{\infty} \left[ \int_0^{\infty} \exp \left[ \beta \mu' x - \frac{\beta^2 m^2}{2t} x^2 \right] x \, dx \right] \times \exp \left[ -\frac{1}{2} \left[ t + \frac{m^2 \gamma^2 (\vec{q})}{t} \right] \right] t^{-3} dt ,
$$

where

$$
\mu' = \mu + 2\pi i \beta^{-1} l \tag{12}
$$

The integration over  $x$  yields

$$
\frac{t}{\beta^2 m^2} \exp\left[\frac{\mu'^2}{4m^2} t\right] D_{-2} \left[-\frac{\mu'}{m} t^{1/2}\right]
$$

where  $D_p(z)$  denotes the parabolic cylinder function. Equation (8) now becomes

$$
N_1 = (N_1)_B + \frac{Vm^2}{4\pi^2 \beta} \sum_{q_1, q_2, q_3 = -\infty}^{\infty} \sum_{l=-\infty}^{\infty} \int_0^{\infty} D_{-2} \left[ -\frac{\mu'}{m} t^{1/2} \right] \exp \left\{ -\frac{1}{2} \left[ \left( 1 - \frac{\mu'^2}{2m^2} \right) t + \frac{m^2 \gamma^2 (\vec{q})}{t} \right] \right\} t^{-2} dt \; .
$$

The integration over t appearing here seems intractable. If, however, we include the antiparticles and make use of the relation<sup>16</sup>

$$
D_{-2}(z) - D_{-2}(-z) = -\sqrt{2\pi}z \exp(\tfrac{1}{4}z^2) ,
$$

we obtain

$$
Q = N_1 - N_2
$$
  
=  $Q_B + \frac{Vm}{(2\pi)^{3/2}\beta} \sum_{q_1, q_2, q_3 = -\infty}^{\infty} \sum_{l=-\infty}^{\infty} \mu' \int_0^{\infty} \exp \left\{-\frac{1}{2} \left[ \left(1 - \frac{\mu'^2}{m^2} \right) t + \frac{m^2 \gamma^2 (\vec{q})}{t} \right] \right\} t^{-3/2} dt$ 

where

$$
Q_B = (N_1)_B - (N_2)_B = \frac{Vm^3}{2\pi^2} W(\beta, \mu) \tag{13}
$$

with

$$
W(\beta,\mu) = 2\sum_{j=1}^{\infty} (j\beta m)^{-1} \sinh(j\beta\mu) K_2(j\beta m) \tag{14}
$$

The integration over t appearing here is a tabulated Laplace transform, yielding<sup>17</sup>

$$
\frac{(2\pi)^{1/2}}{m\gamma(\vec{q})}\exp[-(m^2-\mu'^2)^{1/2}\gamma(\vec{q})],
$$

444

whence

$$
Q = Q_B + \frac{V}{2\pi\beta} \sum_{q_1, q_2, q_3 = -\infty}^{\infty} \sum_{l=-\infty}^{\infty} \frac{\mu'}{\gamma(\vec{q})} \exp[-(m^2 - \mu'^2)^{1/2}\gamma(\vec{q})]. \tag{15}
$$

Equation (15) constitutes the most basic result of our analysis; in the derivation of this result, we have made no approximation whatsoever.

### III. ONSET OF THE PHASE TRANSITION

First of all we shall demonstrate that the set of terms other than  $Q_B$ , in Eq. (15), contains the condensate as well as the finite-size effects in the problem. To see this, the summation over  $\vec{q}$  may be replaced by an integration over  $d^3q$  plus a correction term of the form  $\mu' m \Delta(\mu'^2 / m^2, mL_i)$ . The former leads to the result

$$
\frac{2}{\beta}\sum_{l=-\infty}^{\infty}\frac{\mu'}{m^2-\mu'^2}\;,
$$

which may be written as, see (12),

$$
\frac{1}{\beta} \sum_{l=-\infty}^{\infty} \left[ \frac{1}{(m-\mu)-2\pi i \beta^{-1}l} - \frac{1}{(m+\mu)+2\pi i \beta^{-1}l} \right] = \frac{1}{2} \{ \coth[\frac{1}{2}\beta(m-\mu)] - \coth[\frac{1}{2}\beta(m+\mu)] \} \ . \tag{16}
$$

This is indeed identical with the expression for  $Q_0$  one obtains directly from the mean occupation numbers  $\langle n(k) \rangle$ , viz.,

$$
Q_0 = (N_0)_1 - (N_0)_2
$$
  
=  $(e^{\beta(m-\mu)} - 1)^{-1} - (e^{\beta(m+\mu)} - 1)^{-1}$ . (17)

It follows that Eq. (15) may be written as  
\n
$$
Q = Q_B + Q_0 + \frac{V \mu m}{\beta} F \left[ \frac{\mu^2}{m^2}, \beta^2 m^2, mL_i \right],
$$
\n(18)

the last term denoting exclusively the finite-size effects, a precise form for which will be derived in Sec. IV; see Eq.  $(44)$ .

According to Eq. (17), a macroscopically significant amount of condensate cannot arise unless  $\mu \rightarrow m$ .<sup>18</sup> In the bulk system, this limit defines the critical temperature,  $T_c$ , at which Bose-Einstein condensation sets in. A reference to Eqs. (13) and (14) shows that this requires the following condition to be satisfied:

$$
W(\beta_c, m) \equiv 2 \sum_{j=1}^{\infty} (j\beta_c m)^{-1} \sinh(j\beta_c m) K_2(j\beta_c m)
$$
  
= 
$$
\frac{2\pi^2 \rho}{m^3},
$$
 (19)

where  $\rho$  (=  $Q/V$ ) is the "charge density" in the system. At temperatures less than  $T_c$ , the density of the excited (or so-called normal) component is given by

$$
\rho_n = \frac{m^3}{2\pi^2} W(\beta, m) \quad (\beta > \beta_c)
$$
\n<sup>(20)</sup>

or, preferably, by the fraction

$$
\rho_n / \rho = W(\beta, m) / W(\beta_c, m) \quad (\beta > \beta_c) \tag{21}
$$

The condensate fraction is then given by

$$
\rho_0 / \rho = 1 - \rho_n / \rho
$$
  
= 1 - W(\beta, m) / W(\beta\_c, m) (\beta > \beta\_c). (22)

Note that the condensate part of the system can no longer be determined from Eq. (17) as such; actually, Eqs. (17) and (22) together now determine whatever little difference is still left between the chemical potential  $\mu$  and the rest mass energy  $m$ . The analysis of the bulk system does not care much about this "little difference"; for the analysis of the finite system, however, this is of central importance, as will be seen in the following.

At this stage it seems worthwhile to place on record two limiting cases of the problem.

(i) The nonrelativistic (NR) case ( $\rho \ll m^3$ ), which implies that  $\beta_c m \gg 1$ . Equation (19) then reduces to

$$
W(\beta_c, m) \simeq \left(\frac{\pi}{2\beta_c^3 m^3}\right)^{1/2} \zeta(\frac{3}{2}) = \frac{2\pi^2 \rho}{m^3} ,
$$

whence

$$
\beta_c = \frac{m}{2\pi} \left[ \zeta(\frac{3}{2}) / \rho \right]^{2/3};
$$
\n(23)

here,  $\zeta(s)$  denotes the Riemann zeta function. Equations

21) and (22) then take the well-known form<sup>19</sup>  

$$
\rho_n / \rho = (\beta_c / \beta)^{3/2}, \ \rho_0 / \rho = 1 - (\beta_c / \beta)^{3/2}
$$
. (24)

(ii) The extreme relativistic (ER) case<sup>20</sup> ( $\rho \gg m^3$ ), which implies that  $\beta_c m \ll 1$ . Equation (19) now reduces to

$$
W(\beta_c, m) \simeq \frac{2\pi^2}{3\beta_c^2 m^2} = \frac{2\pi^2 \rho}{m^3}
$$

whence

$$
\beta_c = (m/3\rho)^{1/2} \tag{25}
$$

Equations (21) and (22) now take the form<sup>6,7</sup>

$$
\rho_n / \rho = (\beta_c / \beta)^2
$$
,  $\rho_0 / \rho = 1 - (\beta_c / \beta)^2$ , (26a)

provided that  $\beta m$ , as well,  $\ll 1$ . The situation in this case changes significantly as the temperature of the system is lowered. For instance, at sufficiently low temperatures,  $\beta m$  would become much greater than unity; Eq. (21) would then give

$$
\frac{\rho_n}{\rho} = \frac{3^{3/4} \zeta(\frac{3}{2})}{(2\pi)^{3/2}} \left[\frac{m^3}{\rho}\right]^{1/4} \left[\frac{\beta_c}{\beta}\right]^{3/2},\tag{26b}
$$

with a temperature dependence similar to the one encountered in the nonrelativistic case. This crossover, from a typical extreme relativistic dependence on  $T$  to a typical nonrelativistic one, irrespective of the overall relativistic effects in the system, has already been noticed by Aragao de Carvalho and Rosa;<sup>4</sup> however, since in their analysis

the possibility of particle-antiparticle pair production was not included, their crossover took place from a  $T<sup>3</sup>$  dependence, rather than a  $T^2$  dependence, to the standard  $T^{3/2}$ dependence. In any case, the crossover phenomenon takes place when the parameter  $\beta m$  passes through values of order unity.

Going back to the finite system, which is governed by Eq. (15), we observe that, as  $\mu \rightarrow m$ , the term with  $l=0$ dominates heavily over terms with  $l\neq0$ . To see this, we write the summation over  $l$  in the form, see also Eq. (12),

$$
\frac{1}{\gamma(\vec{q})}\left[\mu \exp[-(m^2-\mu^2)^{1/2}\gamma(\vec{q})] + \sum_{l=-\infty}^{\infty} (\mu+2\pi i\beta^{-1}l)\exp\{-[(m^2-\mu^2)+4\pi^2\beta^{-2}l^2-4\pi i\mu\beta^{-1}l]^{1/2}\gamma(\vec{q})\}\right].
$$
 (27)

Now, as  $\mu \rightarrow m$ , so long as at least one of the three quantities  $(m^2 - \mu^2)^{1/2}L_i$  is of order unity or less, the main term in (27), summed over  $\vec{q}$ , would make a rather significant contribution to  $Q$ . The other terms, however, are at best of order exp[  $-(m/\beta)^{1/2}L_i$ ], i.e.,  $O(e^{-L_i/\lambda_T})$ , where  $\lambda_T$  $(=\sqrt{2\pi\beta/m})$  denotes the mean thermal wavelength of the particles. Assuming that, for all i,  $L_i \gg \lambda_T$ , these terms can be dropped with impunity. The important thing to note is that no errors of order  $(\lambda_T/L_i)^n$  are committed if we retain only the term with  $l=0$ . Introducing the thermogeometric parameters  $y_i$ <sup>21</sup>

$$
y_i = \frac{1}{2} (m^2 - \mu^2)^{1/2} L_i \quad (i = 1, 2, 3)
$$
 (28)

Eq. (15) may now be written as

$$
Q = \frac{Vm^3}{2\pi^2}W(\beta,\mu) + \frac{V\mu(m^2-\mu^2)^{1/2}}{4\pi\beta}S(y_i) ,
$$
 (29)

where

$$
S(y_i) = \sum_{\vec{q}}' \frac{1}{R(\vec{q})} \exp[-2R(\vec{q})], \qquad (30)
$$

with  $R(\vec{q}) = (q_1^2 y_1^2 + q_2^2 y_2^2 + q_3^2 y_3^2)^{1/2}$ .

For a study of the critical behavior of the finite system, we first of all consider the situation at  $\beta = \beta_c$ —the erstwhile critical temperature of the infinite system. Here, the function  $[W(\beta,\mu)]_{\mu=m}$  is finite, as seen in Eq. (19); its derivative  $\left(\frac{\partial W}{\partial \mu}\right)_{\mu=m}^{m}$ , however, diverges. Following Singh and Pandita, $'$  we can show that

$$
W(\beta,\mu) = W(\beta,m) - \frac{\pi}{\beta m^2} (m^2 - \mu^2)^{1/2} + O(m^2 - \mu^2)
$$
\n(31)

Substituting (19) and (31) into (29), we obtain the remarkable result that, to the desired order of magnitude,

$$
[S(y_i)]_{\beta=\beta_c} = 2.
$$

This shows that, at  $T = T_c$  (of the bulk system), the thermogeometric parameters of the problem, which determine the numerical value of the sum (30), are  $O(1)$ ; accordingly,

$$
[(m^2 - \mu^2)^{1/2}]_{\beta = \beta_c} = O(L^{-1}_<),
$$
\n(33)

where  $L<sub>5</sub>$  denotes the shortest side of the container. For  $T \simeq T_c$ , we obtain

 $\frac{T}{T_c} = 1 + A \frac{y_i}{L_i} [2 - S(y_i)],$ (34)

where

$$
A = \frac{\pi}{\beta_c^2 m^2} \left| \frac{\partial W(\beta, m)}{\partial \beta} \right|_{\beta = \beta_c}^{-1} = \left| \frac{\frac{2}{3} [\zeta(\frac{3}{2})]^{-2/3} \rho^{-1/3} \text{ (NR)}}{\frac{1}{4\pi} \left( \frac{3m}{\rho} \right)^{1/2} \text{ (ER)}} \right|
$$
 (35)

Equations (34) and (35) enable us to determine  $y_i$ 's as functions of T in the close neighborhood of  $T_c$ .

Specializing to a cubical geometry  $(L_1 = L_2 = L_3 = L,$ say) we have to deal with a single  $y$  common to all the indices *i*; see Eq. (28). Defining  $t = (T - T_c)/T_c$  and confining ourselves to the domain  $|t| \ll 1$ , we obtain three sets of results. First of all, we have the very "core" of the transition region where  $y = O(1)$ ; this requires  $|t|$  to be  $O(Q^{-1/3})$ . The precise value of y in this region can be determined only numerically. At  $t=0$ , y turns out to be about 0.97. Two other regions may now be demarcated.

(a) The region with  $y \gg 1$ ; this requires t to be positive but staying clear of the core region. Here,  $S(y) \ll 1$  and Eq. (34) yields

$$
y = D_{+} t \tag{36}
$$

where

$$
D_{+} = \frac{L}{2A} = \begin{cases} \frac{3}{4} [\zeta(\frac{3}{2})]^{2/3} Q^{1/3} & (NR) \\ \frac{2\pi}{\sqrt{3}} (\rho/m^3)^{1/6} Q^{1/3} & (ER) \end{cases}
$$
 (37)

(b) The region with  $y \ll 1$ ; this requires t to be negative and again staying clear of the core region. Here,  $S(y) \sim (\pi/y^3) \gg 1$  and we obtain

$$
y = D_{-} |t|^{-1/2}, \qquad (38)
$$

where

$$
D_{-} = \left[\frac{\pi A}{L}\right]^{1/2} = \begin{cases} \left[\frac{2\pi}{3}\right]^{1/2} [\zeta(\frac{3}{2})]^{-1/3} Q^{-1/6} & (NR) \\ \frac{3^{1/4}}{2} (\rho/m^3)^{-1/12} Q^{-1/6} & (ER) \end{cases}
$$
 (39)

446

Recalling that the amount of the condensate,  $Q_0$ , is given by the expression, see Eqs. (16) and (17),

$$
Q_0 \simeq \frac{2m}{\beta (m^2 - \mu^2)} = \frac{mL^2}{2\beta y^2} \propto \frac{Q^{2/3}}{y^2} , \qquad (40)
$$

the passage of y from values  $O(Q^{1/3})$  to values  $O(Q^{-1/6})$ is clearly vital for the growth of the condensate in the system. We shall now examine this question in some detail.

# IV. GROWTH OF THE CONDENSATE

In view of the above findings-especially Eqs.  $(36)$ - $(40)$ -we conclude that in region (a), where  $y = O(Q^{1/3})$ ,  $Q_0$  is of order unity and, hence, negligible. In the core region (which includes the erstwhile critical point  $t=0$ ,  $y=O(1)$  and  $Q_0$  is of order  $Q^{2/3}$ , which is still submacroscopic in magnitude. In region (b), where  $y = O(Q^{-1/6})$ ,  $Q_0$  is finally of order Q and is given by, see Eqs. (38)—(40),

$$
Q_0 = \begin{cases} \frac{3}{2} |t| Q & (\text{NR}) \\ 2 |t| Q & (\text{ER}) \end{cases}
$$
 (41)

note that in deriving these expressions for  $Q_0$  we have made use of Eqs. (23) and (25) as well. At this point it is indeed heartening to find that expressions (41), obtained here as a limiting case of our rigorous analysis of the  $fi$ nite system, are fully consistent with the bulk formulas (24) and (26a).

At this stage it seems worthwhile to point out that the three regions demarcated above are not as divisive as might appear at first sight; they can, in fact, be spanned in an essentially continuous manner. To see this, we note in an essentially continuous manner. To see this, we note that for  $t \ge 0$  we may set  $y = O(Q^{\zeta})$ , with  $0 \le \zeta \le \frac{1}{3}$ . In view of Eqs.  $(36)$ ,  $(37)$ , and  $(40)$ , we then have

$$
t = O(Q^{-1/3+\zeta}) = O(Q^{(-1/3,0)})
$$

and

$$
Q_0 = O(Q^{2/3-2\zeta}) = O(Q^{(2/3,0)})
$$

For  $t \le 0$  we may set  $y = O(Q^{\xi})$ , with  $-\frac{1}{6} \le \xi \le 0$ . view of Eqs. (38), (39), and (40), we now have

$$
|t| = O(Q^{-1/3-2\zeta}) = O(Q^{(-1/3,0)})
$$

and

$$
Q_0 = O(Q^{2/3-2\zeta}) = O(Q^{(2/3,1)})
$$

Thus all the regions of interest can be covered essentially continuously by letting  $\zeta$  vary between the limiting values  $-\frac{1}{6}$  and  $\frac{1}{3}$ .

For a fuller understanding of the problem, we need a more complete knowledge of the sum  $S(y)$  appearing in Eqs. (29) and (30). For this we make use of the identi-<br> $tw^{10,11}$ 

$$
\sum_{\vec{q}}'\left[\frac{e^{-2yq}}{q}+\frac{y^2}{\pi q^2(y^2+\pi^2 q^2)}\right]=\frac{\pi}{y^2}+\frac{C_3}{\pi}+2y,
$$
\n(42)

$$
C_3 = \pi \lim_{y \to 0} \left[ \sum_{\vec{q}}' \frac{e^{-2yq}}{q} - \int_{\text{all } \vec{q}} \frac{e^{-2yq}}{q} d^3q \right]
$$
  
= -8.913633.... (43)

It may be mentioned here that the constant  $C_3$  appearing in (42) is directly related to the Madelung constant of a simple cubic lattice.<sup>10,22</sup> Equations (28), (31), and (42) now enable us to write (29) as

$$
Q = \frac{Vm^3}{2\pi^2} W(\beta, m) + \frac{mL^2}{2\beta y^2} + \frac{mL^2}{2\pi^2 \beta} \left[ C_3 - y^2 \sum_{\vec{q}}' \frac{1}{q^2(y^2 + \pi^2 q^2)} \right],
$$
 (44)

which may be compared with the formal result embodied in Eq. (18). It will be noted that the singular term, containing  $(m^2-\mu^2)^{1/2}$ , in the bulk function  $W(\beta,\mu)$  is exactly cancelled by the term linear in  $y$  in the identity  $(42)$ for the sum  $S(y)$ . This is important because the thermodynamic functions pertaining to a finite system must be physically smooth and mathematically analytic, which is now guaranteed by the fact that our final expression for Q contains only  $y^2$ . The other thing to note is that the second term on the right-hand side of (44) is precisely the quantity  $Q_0$ , see Eq. (40), whose magnitude is determined by the combination  $(\beta y^2)$ . Clearly, the last term in (44), which is strictly  $O(Q^{2/3})$ , represents the finite-size effects in the problem.

Equation  $(44)$  is now supposed to be solved for y as a function of  $\beta$ , whereupon  $Q_0$  will follow from (40). The formal procedure for carrying out this calculation numerically has been laid down in Ref. 11 and need not be repeated here. Remarkably enough, a complete solution to the problem, from  $T=0$  K right up to  $T \leq T_c$ , can be written down explicitly by observing that, throughout this ange of temperatures,  $y^2 \ll 1$ . Equation (44) then gives, to an excellent degree of approximation,

$$
\frac{Q_0}{Q} = \left(\frac{Q_0}{Q}\right)_B + \frac{|C_3|}{2\pi^2} \frac{m}{\rho \beta L} , \qquad (45)
$$

where

$$
\left(\frac{Q_0}{Q}\right)_B = 1 - \frac{m^3}{2\pi^2 \rho} W(\beta, m) , \qquad (46)
$$

as we already have in Eq. (22). We thus find that, irrespective of the actual magnitude of the relativistic effects, the finite-size correction term in (45) is positive and is directly proportional to (i) the temperature of the system and (ii) the surface-to-volume ratio of the container. The fact that we obtain an enhancement of the condensate fraction over the bulk value is not surprising in the case of periodic boundary conditions. Here, the ground-state energy in both the bulk and the finite systems is the same; however, as we go from the bulk to the finite case, the excited states become discrete and are shifted upwards, thereby reducing the mean occupation numbers for these states and, consequently, enhancing the fraction of the particles in the ground state. It is indeed expected that

where

the situation will vary significantly from one set of boundary conditions to another. The fact that the correction term is directly proportional to the surface-to-volume ratio of the container, and hence to  $L^{-1}$ , is consistent with the scaling theory for finite-size effects, as formulated by Fisher et al.<sup>23-25</sup> As regards the linear dependence on  $T$ , one can understand it heuristically by noting that, since it is closely related to being a "surface effect," the finite-size correction must possess qualitative features similar to the ones characteristic of a two-dimensional bulk system.

Finally, we shall address ourselves to the question of the relative importance of the particles and antiparticles in the total condensate  $Q_0$ . Assuming that both the species are present in significant numbers, we have from Eq. (17)

 $(N_0)_{1\leq}[\beta(m-\mu)]^{-1}$ ,  $(N_0)_{2\leq}[\beta(m+\mu)]^{-1}$ ,

with

$$
Q_0 \simeq 2\mu [\beta(m^2-\mu^2)]^{-1} \simeq [\beta(m-\mu)]^{-1}
$$

Apparently,  $(N_0)_2$  is negligible in comparison with  $(N_0)_1$ . To be sure, we consider the ratio

$$
\frac{(N_0)_2}{(N_0)_1} \simeq \frac{m - \mu}{m + \mu} = \frac{m^2 - \mu^2}{(m + \mu)^2} \simeq \frac{y^2}{m^2 L^2}
$$

In the whole region of interest, this ratio is at best  $O(\lambda_c^2/L^2)$ , where  $\lambda_c$  denotes the Compton wavelength of the particles, and hence it is negligible. We, therefore, conclude that while the inclusion of the possibility of particle-antiparticle pair production modifies the very expression for  $T_c(\rho)$  and affects several important aspects of the phenomenon of Bose-Einstein condensation, the condensate itself consists almost entirely of particles alone. This contrasts sharply with the singular case of massless bosons for which the condensate contains as many particles as antiparticles<sup>6</sup>—essentially because the two species in that case are indistinguishable. This situation may be 'compared with the one arising in the Gibbs paradox<sup>3, 15</sup> where one encounters an "entropy of mixing" which is positive definite when the diffusing molecules are dissimilar but is zero when they are similar.

# V. CONDENSATION IN PARTIALLY INFINITE ASSEMBLIES

In the preceding section we examined the growth of the condensate, as a function of temperature, in a cubical assembly. Generally speaking, the results thus obtained, especially Eq. (45), would be valid for noncubical assemblies as well, except for the fact that numerical factors, such as  $C_3$ , would now be shape dependent. The situation, however, changes qualitatively if, in one or two of its dimensions, the system becomes infinite. In such cases we obtain the following results.

(i) Narrow-channel geometry  $(L_1 \gg L_{2,3})$ . Here, the sum  $S(y_i)$  essentially reduces to a two-dimensional sum which, for  $y_{2,3} \ll 1$ , turns out to be  $\pi/(y_2y_3)$ . Equation (29) then takes the form

$$
Q = Q_B + \frac{mL_1}{\beta (m^2 - \mu^2)^{1/2}} \ . \tag{47}
$$

One can now show that the second term in (47), which is supposed to contain the condensate, will be  $O(Q)$  only if the temperature of the system is sufficiently low, so that

$$
\beta \ge c_1 \frac{mL_1}{\rho L_2 L_3}, \quad c_1 = O(1) \ . \tag{48}
$$

If  $L_1 \rightarrow \infty$ , no condensate appears unless  $T \rightarrow 0$  K. Thus, irrespective of the actual values of  $L_2$  and  $L_3$ , so long as  $(L_{2,3}/L_1) \rightarrow 0$ , the system behaves essentially as a onedimensional bulk system.

(ii) Thin-film geometry  $(L_{1,2} \gg L_3)$ . Here, the sum  $S(y_i)$  essentially reduces to a one-dimensional sum which, for  $y_3 \ll 1$ , turns out to be  $-2y_3^{-1} \ln(2y_3)$ . Equation (29) then becomes

$$
Q = Q_B + \frac{mL_1L_2}{\pi\beta} \ln \left( \frac{1}{(m^2 - \mu^2)^{1/2}L_3} \right).
$$
 (49)

Now one requires that

$$
\beta \ge c_2 \frac{m}{\rho L_3} \ln \left[ \frac{L_1 L_2}{L_3^2} \right], \quad c_2 = O(1) \ . \tag{50}
$$

Again, if  $L_{1,2} \rightarrow \infty$ , no condensate appears unless  $T \rightarrow 0$ K. Thus, irrespective of the actual value of  $L_3$ , so long as  $(L_3/L_{1,2})\rightarrow 0$ , the system behaves essentially as a twodimensional bulk system; see also Ref. 25.

We, therefore, conclude that in partially infinite geometries Bose-Einstein condensation does not set in at any finite temperature; for this to happen, the system in three dimensions must be either completely infinite or else completely finite.

#### VI. CONCLUDING REMARKS

Ideal Bose gas is one of the few models in the theory of phase transitions that can be solved exactly but gives results different from the ones obtained in the usual meanfield approximation. In this paper we have carried out a rigorous analysis of the relativistic version of this model, inluding the effects of particle-antiparticle pair production, in a finite cuboidal geometry  $(L_1 \times L_2 \times L_3)$  under periodic boundary conditions. We have shown that, as the temperature of the system is lowered, phase transition sets in smoothly and is marked by the growth of the condensate  $Q_0$ , from  $O(1)$  to  $O(Q)$ , over a temperature range  $\Delta T$  $[=\tilde{O(Q}^{-1/3})]$  in the vicinity of the erstwhile critical temperature  $T_c$  of the bulk system. We have obtained explicit expressions for the condensate fraction,  $Q_0/Q$ , for a cubical geometry  $(L \times L \times L)$ , which are valid throughout the critical region down to 0 K. Further, in this study, we have examined the manner in which the singularity, so manifestly present in the bulk limit  $(L \rightarrow \infty)$ , disappears when the dimension  $L$  of the container is kept finite.

Finally, we have examined the question of the onset of phase transition in partially infinite geometries, such as those of a narrow channel and a thin film. In both these cases, we find that there is no buildup at all of the condensate  $Q_0$  near  $T = T_c$ . Even at lower temperatures, the condensate remains of an order lower than Q, so that  $Q_0/Q\rightarrow 0$  as  $Q\rightarrow \infty$ . However, when T becomes sufficiently small to satisfy the inequality (48) or (50), as the case may be,  $Q_0/Q$  does become  $O(1)$  and ultimately, as T approaches 0 K,  $Q_0/Q$  approaches unity.

#### ACKNOWLEDGMENT

Financial support from the Natural Sciences and Engineering Research Council of Canada is gratefully acknowledged.

- V. A. Kuzmin and M. E. Shaposhnikov, Phys. Lett. 69A, 462 (1979).
- 2P. T. Landsberg and J. Dunning-Davies, Phys. Rev. 138, A1049 (1965); see also J. Dunning-Davies, J. Phys. A 14, 3005 (1981).
- <sup>3</sup>R. Beckmann, F. Karsch, and D. E. Miller, Phys. Rev. Lett. 43, 1277 (1979); Phys. Rev. A 25, 561 (1982); see also F. Karsch and D. E. Miller, ibid. 22, 1210 (1980).
- ~C. Aragao de Carvalho and S. Goulart Rosa, Jr., J. Phys. A 13, 3233 (1980); see also H. O. da Frota and S. Goulart Rosa, Jr., ibid. 15, 2221 (1982).
- 5P. T. Landsberg, in Statistical Mechanics of Quarks and Hadrons, edited by H. Satz (North-Holland, Amsterdam, 1981), p. 355.
- <sup>6</sup>H. E. Haber and H. A. Weldon, Phys. Rev. Lett. 46, 1497 (1981);Phys. Rev. D 25, 502 (1982).
- 7S. Singh and P. N. Pandita, Phys. Rev. A 28, 1752 (1983).
- R. K. Pathria, Phys. Rev. A 5, 1451 (1972).
- <sup>9</sup>S. Greenspoon and R. K. Pathria, Phys. Rev. A 9, 2103 (1974).
- <sup>10</sup>A. N. Chaba and R. K. Pathria, J. Math. Phys. 16, 1457 (1975).
- <sup>11</sup>C. S. Zasada and R. K. Pathria, Phys. Rev. A 14, 1269 (1976).
- $^{12}$ H. R. Pajkowski and R. K. Pathria, J. Phys. A 10, 561 (1977).
- <sup>13</sup>R. K. Pathria, Can. J. Phys. 61, 228 (1983).
- <sup>14</sup>L. Schwartz, Mathematics for the Physical Sciences (Addison-Wesley, Reading, Mass., 1966), Chap. V.
- <sup>15</sup>G. N. Watson, Theory of Bessel Functions (Cambridge Univer-

sity Press, Cambridge, 1944), Sec. 6.22.

- <sup>16</sup>I. S. Gradshteyn and I. M. Ryzhik, Table of Integrals, Series and Products (Academic, New York, 1980).
- <sup>17</sup>M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions (Dover, New York, 1970).
- <sup>18</sup>The other possibility, that  $\mu \rightarrow -m$ , would produce a condensate dominated by the antiparticles. That possibility, however, is ruled out by our initial assumption that  $\mu > 0$ .
- <sup>19</sup>R. K. Pathria, Statistical Mechanics (Pergamon, Oxford, 1972).
- <sup>20</sup>We prefer to use the older term "extreme relativistic," rather than the term "ultrarelativistic," for the main reason that, in line with the commonly used terms such as "ultrasonics," "uline with the commonly used terms such as "ultrasonics," "ultraviolet," etc., the term "ultrarelativistic" tends to give the impression that the case under consideration is "beyond relativistic" —which clearly is not the intention.
- The inclusion of the factor  $\frac{1}{2}$  in the definition of  $y_i$  might seem artificial here; it is, however, essential for ensuring consistency with the nonrelativistic  $y_i$  already in use (Refs.  $8 - 13$ .
- <sup>22</sup>F. E. Harris and H. J. Monkhorst, Phys. Rev. B 2, 4400 (1970).
- M. E. Fisher and A. E. Ferdinand, Phys. Rev. Lett. 19, 169 (1967); Phys. Rev. 185, 832 (1969).
- M. E. Fisher and M. N. Barber, Phys. Rev. Lett. 28, 1516 (1972).
- 25M. E. Fisher, J. Vac. Sci. Technol. 10, 665 (1973).