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Influence of boundary conditions on the growth of condensate fraction in a finite Bose system*

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In a recent paper we carried out a rigorous, asymptotic analysis of the low-temperature behavior of a Bose gas confined to a finite cubic geometry and subjected to periodic boundary conditions. That analysis is now extended to Dirichlet, Neumann, and antiperiodic boundary conditions. As before, the thermogeometric parameter y and the condensate fraction N_0/N are studied as functions of temperature and are evaluated explicitly for cubes with $L/\bar{l} = 40$ and 100, where L is the edge length of the enclosure and $\bar{l}$ the mean interparticle distance in the system. The finite-size corrections to the condensate fraction under Dirichlet or Neumann boundary conditions turn out to be qualitatively different from those under periodic or antiperiodic boundary conditions. This difference becomes manifest when one tries to express these corrections in a form consistent with the standard scaling theory for finite-size effects.

I. INTRODUCTION

In a recent paper[1] (hereafter referred to as I) we carried out a rigorous asymptotic evaluation of the temperature dependence of the thermogeometric parameter y and of the condensate fraction N_0/N for an ideal Bose gas confined to a finite cubic geometry and subject to periodic boundary conditions. The enhancement in the condensate fraction, over the bulk value, was found to be

$$\left(\frac{N_0}{N}\right)_P^{\times} = \Theta\{T - T_c(\infty)\}\left[1 - \left(\frac{T}{T_c(\infty)}\right)^{3/2}\right] + \frac{\bar{l}}{L}[\zeta(\tfrac{3}{2})]^{-2/3}\frac{T}{T_c(\infty)} \times \left(-\frac{C_3}{\pi} + \frac{y^2}{\pi}\sum_{q_{1,2,3}=-\infty}^{\infty}{}' \frac{1}{q^2(y^2+\pi^2 q^2)}\right), \qquad (1)$$

where $\Theta\{x\}$ is the step function ($=0$ for $x<0$, 1 for $x>0$) while the other symbols have been defined in I.[1a] For a large temperature range below $T_c(\infty)$, where $y^2 \simeq 0$, the enhancement varies linearly with temperature and can be written in the standard scaled form, namely,

$$\left(\frac{N_0}{N}\right)_P^{\times}\left(\frac{L}{\bar{l}}\right) \simeq -\frac{C_3}{\pi}[\zeta(\tfrac{3}{2})]^{-2/3}\frac{T}{T_c(\infty)} \quad (C_3 = -8.913\,633), \qquad (2)$$

independently of the actual size of the system.

In this communication we present an extension of the foregoing analysis to systems under Dirichlet, Neumann, and antiperiodic boundary conditions.

II. DIRICHLET AND NEUMANN BOUNDARY CONDITIONS

Under these boundary conditions we encounter sums running over quantum numbers $1,2,3,\ldots$ and $0,1,2,3,\ldots$, respectively. For an application of the Poisson summation formula these sums can be expressed as[2]

$$\sum_{n_{1,2,3}=(1-\theta)/2}^{\infty} f(n_1,n_2,n_3) = \frac{1}{8}\left[\sum_{n_{1,2,3}=-\infty}^{\infty} f(n_1,n_2,n_3) + \theta\left(\sum_{n_{1,2}=-\infty}^{\infty} f(n_1,n_2,0) + \sum_{n_{1,3}=-\infty}^{\infty} f(n_1,0,n_3) + \sum_{n_{2,3}=-\infty}^{\infty} f(0,n_2,n_3)\right) + \left(\sum_{n_1=-\infty}^{\infty} f(n_1,0,0) + \sum_{n_2=-\infty}^{\infty} f(0,n_2,0) + \sum_{n_3=-\infty}^{\infty} f(0,0,n_3)\right) + \theta\right], \qquad (3)$$

where $f(n_1,n_2,n_3)$ is an even function of the quantum numbers n_1, n_2, and n_3, while $\theta = -1$ for Dirichlet boundary conditions and $+1$ for Neumann.

To see what is expected, we may initially employ a crude continuum approach whereby

$$N = N_0 + \int_0^{\infty} n(k)\, a(k)\, dk\,; \qquad (4)$$

here, $n(k)$ is the usual mean occupation number, while $a(k)$ is the density of states — modified, in a gross manner, by the boundary conditions imposed on the system. We have[3]

$$a(k)\,dk = \frac{Vk^2\,dk}{2\pi^2} + \theta\frac{Sk\,dk}{8\pi} + o(k\,dk), \qquad (5)$$

where V and S are the volume and the surface area of the enclosure. This leads to

$$N = N_0 + (L/\lambda)^3 g_{3/2}(\alpha) + \tfrac{3}{2}\theta(L/\lambda)^2 g_1(\alpha). \qquad (6)$$

For $\alpha \ll 1$, we obtain, after some rearrangement,

$$\frac{N_0}{N} \simeq \left[1 - \left(\frac{T}{T_c(\infty)}\right)^{3/2}\right] - \theta \frac{\bar{l}}{L} [\zeta(\tfrac{3}{2})]^{-2/3} \left(\frac{T}{T_c(\infty)}\right) \times \left[\tfrac{3}{2} \ln(4\pi) + \ln\left(\frac{N}{\zeta(\frac{3}{2})}\right) + \tfrac{3}{2} \ln\left(\frac{T}{T_c(\infty)}\right)\right] + \frac{\bar{l}}{L} [\zeta(\tfrac{3}{2})]^{-2/3} \frac{T}{T_c(\infty)} (y + \tfrac{3}{2}\theta \ln y^2), \quad (7)$$

where $y\ [= 2\pi^{1/2}\alpha^{1/2}(L/\lambda)]$ is the thermogeometric parameter appropriate to the boundary conditions in question. The first term here is the customary bulk result, the second term is a surface correction which leads to an enhancement ($\theta = -1$) or a suppression ($\theta = +1$) of the condensate fraction, while the third term requires special attention. Since, for Dirichlet boundary conditions, the ground-state energy is nonzero, the parameter y^2 ultimately assumes negative values — approaching the limiting value $-3\pi^2$ as $T \to 0$ °K. In view of this, the third term in Eq. (7) represents a nonanalytic contribution to the condensate fraction N_0/N. We hasten to remark that this unwelcome feature is due to the approximations inherent in the continuum approach and that this contribution disappears altogether if we treat our discrete sums appropriately.

For such a treatment we write

$$N = \sum_{\vec{k}} n(\vec{k}) = \sum_{j=1}^{\infty} e^{-j\alpha} \sum_{n_{1,2,3}=(1-\theta)/2}^{\infty} \exp\left[-j\frac{\pi}{4}\left(\frac{\lambda}{L}\right)^2 (n_1^2 + n_2^2 + n_3^2)\right], \quad (8)$$

use (3) to express the partial summations over $n_{1,2,3}$ in terms of complete summations in three, two, and one dimensions, and apply Poisson's summation formula to these summations. We get (for $L \gg \lambda$)

$$N = \left(\frac{L}{\lambda}\right)^3 \left(g_{3/2}(\alpha) + \frac{1}{2}\frac{\lambda}{L} \sum_{q_{1,2,3}=-\infty}^{\infty}{}' \frac{e^{-2yq}}{q}\right) + \tfrac{3}{2}\theta \left(\frac{L}{\lambda}\right)^2 \left(g_1(\alpha) + 2 \sum_{q_{1,2}=-\infty}^{\infty}{}' K_0(2yq')\right) + \frac{3}{4}\frac{L}{\lambda}[g_{1/2}(\alpha) + 2\pi^{1/2}\alpha^{-1/2} g_0(2y)] + \tfrac{1}{8}\theta\, g_0(\alpha), \quad (9)$$

where $q = (q_1^2 + q_2^2 + q_3^2)^{1/2}$ and $q' = (q_1^2 + q_2^2)^{1/2}$. Application of Eq. (7) of I and Eq. (14) of Ref. 4 now gives, for $\alpha \ll 1$,

$$N_0 = N\left[1 - \left(\frac{T}{T_c(\infty)}\right)^{3/2}\right] - 3\theta \left(\frac{L}{\lambda}\right)^2 \ln\left(\frac{L}{\lambda}\right) + D_\theta \left(\frac{L}{\lambda}\right)^2 + \frac{4y^2}{\pi}\left(\frac{L}{\lambda}\right)^2 \sum_{q_{1,2,3}=(1-\theta)/2}^{\infty}{}' \frac{1}{q^2(y^2 + \pi^2 q^2)}, \quad (10)$$

where

$$D_\theta = \theta\left[3 \ln\left(\frac{[\Gamma(\frac{1}{4})]^2}{4\pi}\right) - 3\gamma\right] - \frac{C_3}{2\pi} - \frac{\pi}{2} + (1-\theta)\frac{2}{3\pi}; \quad (11)$$

note that the primed summation in (10) excludes the term corresponding to the ground state, viz., (1, 1, 1) for $\theta = -1$, (0, 0, 0) for $\theta = +1$.

For comparison with the continuum approximation (7), we write (10) as

$$\frac{N_0}{N} = \left[1 - \left(\frac{T}{T_c(\infty)}\right)^{3/2}\right] - \theta \frac{\bar{l}}{L}[\zeta(\tfrac{3}{2})]^{-2/3} \frac{T}{T_c(\infty)} \times \left\{\tfrac{3}{2} \ln\left(\frac{T}{T_c(\infty)}\right) + \left[\ln\left(\frac{N}{\zeta(\frac{3}{2})}\right) - \theta D_\theta\right]\right\} + \frac{4y^2}{\pi}\frac{\bar{l}}{L}[\zeta(\tfrac{3}{2})]^{-2/3}\frac{T}{T_c(\infty)} \sum_{q_{1,2,3}=(1-\theta)/2}^{\infty}{}' \frac{1}{q^2(y^2 + \pi^2 q^2)}. \quad (12)$$

First of all, we note that the terms involving $T \ln T$ and $T \ln N$ are given correctly by the continuum approximation, whereas the terms linear in T are somewhat different. More importantly, however, the nonanalytic terms appearing in the continuum approximation cancel out exactly in the more accurate analysis. This last fact has a specially important bearing on the case of Dirichlet boundary conditions. Here, y^2 passes from positive to negative values whereas many of the mathematical steps leading to (12) are strictly defined only for $y^2 > 0$. The attitude to take is that we initially carry out our calculation in the regime $y^2 > 0$; then in the end, when all nonanalytic terms disappear, the solution is analytically continued into the regime $y^2 < 0$. This procedure also has to be invoked in the case of antiperiodic boundary conditions because, there too, we have a nonzero ground-state energy and hence a negative limiting value of y^2.

Equation (12), coupled with the relation

$$N_0 \simeq \frac{1}{\alpha + \beta\epsilon_0} = \begin{cases} \dfrac{4\pi}{y^2 + 3\pi^2}\left(\dfrac{L}{\lambda}\right)^2 & \text{(Dirichlet)}, \\ \dfrac{4\pi}{y^2}\left(\dfrac{L}{\lambda}\right)^2 & \text{(Neumann)}, \end{cases} \quad (13)$$

can be solved numerically to obtain $y(T)$ which in turn can be used to determine the low-temperature behavior of the condensate fraction N_0/N for either boundary condition. Results for cubes of two different sizes are shown in Figs. 1–3.

According to Figs. 1 and 2 there exists a broad range of temperatures in which $(y^2)_D \simeq -3\pi^2$ and $(y^2)_N \simeq 0$. In this region the finite-size corrections to the condensate fraction can be approximated as

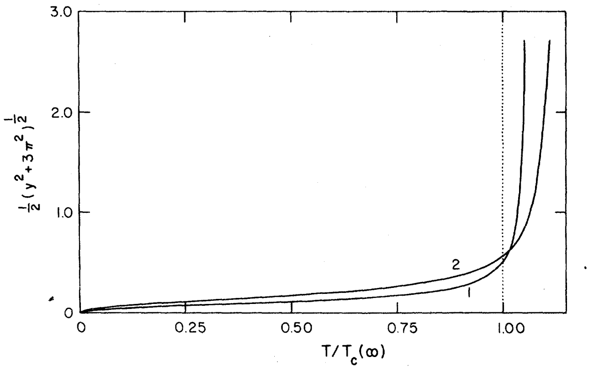

FIG. 1. Quantity $\frac{1}{2}(y^2+3\pi^2)^{1/2}$, for a cubical enclosure with Dirichlet boundary conditions, as a function of the scaled temperature $T/T_c(\infty)$. Curve 1 is for a cube containing 10^6 particles, curve 2 for a cube containing 6.4×10^4 particles. Dotted line depicts the corresponding bulk behavior.

$$\left(\frac{N_0}{N}\right)_D^{\times} \simeq \frac{\bar{l}}{L}[\zeta(\tfrac{3}{2})]^{-2/3}\frac{T}{T_c(\infty)} \times\left[\tfrac{3}{2}\ln\left(\frac{T}{T_c(\infty)}\right)-1.5723\right] +3\frac{\bar{l}}{L}\ln\left(\frac{L}{\bar{l}}\right)[\zeta(\tfrac{3}{2})]^{-2/3}\frac{T}{T_c(\infty)} \tag{14}$$

and

$$\left(\frac{N_0}{N}\right)_N^{\times} \simeq -\frac{\bar{l}}{L}[\zeta(\tfrac{3}{2})]^{-2/3}\frac{T}{T_c(\infty)} \times\left[\tfrac{3}{2}\ln\left(\frac{T}{T_c(\infty)}\right)+0.7885\right] -3\frac{\bar{l}}{L}\ln\left(\frac{L}{\bar{l}}\right)[\zeta(\tfrac{3}{2})]^{-2/3}\frac{T}{T_c(\infty)}. \tag{15}$$

These results are plotted in Figs. 4 and 5 which also include the more accurate results obtained from the full expression (12). Clearly, the approximation provided by (14) and (15) is very good for a considerable range of temperatures.

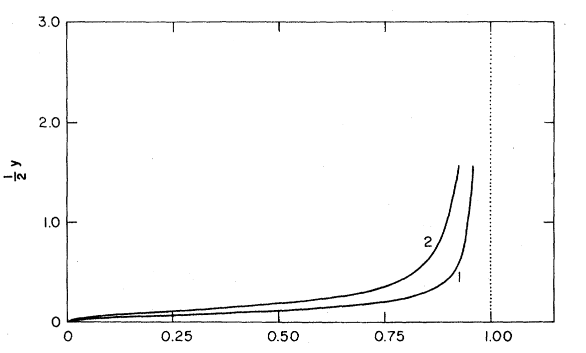

FIG. 2. Quantity $\frac{1}{2}y$, for a cubical enclosure with Neumann boundary conditions, as a function of the scaled temperature $T/T_c(\infty)$. Rest as in Fig. 1.

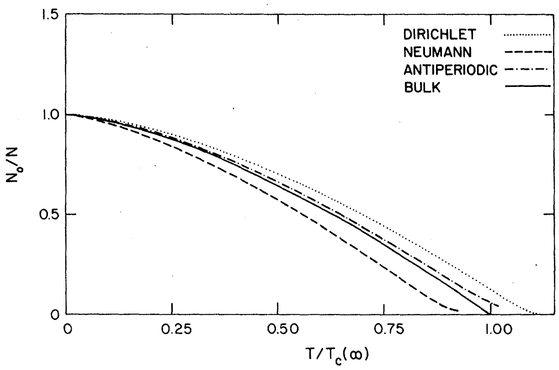

FIG. 3. Temperature dependence of the condensate fraction (N_0/N) for a cube containing 6.4×10^4 particles. Dotted curve is for Dirichlet boundary conditions, dashed for Neumann boundary conditions, and dash-dotted for antiperiodic boundary conditions. Bulk behavior is depicted by the solid line.

It is evident from Eqs. (14) and (15) that, unlike the case of periodic boundary conditions, no uniform scaling factor can be applied to the finite-size correction for either Dirichlet or Neumann boundary conditions. Here, we encounter a rather *anomalous* scaling behavior in which the finite-size correction to the condensate fraction consists of two parts, each of which requires a different scaling factor. Thus, in general, one may write

$$\left(\frac{N_0}{N}\right)^{\times}=\left(\frac{N_0}{N}\right)_1^{\times}+\left(\frac{N_0}{N}\right)_2^{\times}, \tag{16}$$

such that

$$\left(\frac{N_0}{N}\right)_1^{\times}\left(\frac{L}{\bar{l}}\right) \text{ and } \left(\frac{N_0}{N}\right)_2^{\times}\left(\frac{L}{\bar{l}}\right)\Big/\ln\left(\frac{L}{\bar{l}}\right)$$

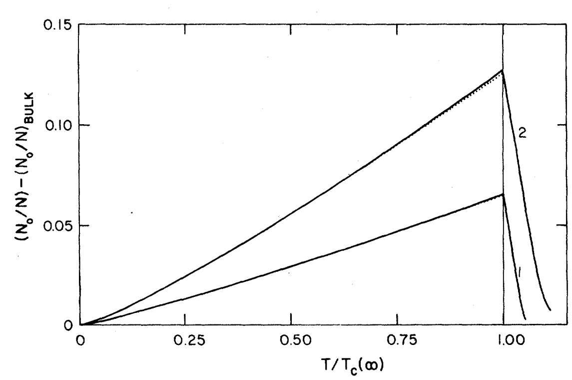

FIG. 4. Enhancement of the condensate fraction (N_0/N) for Dirichlet boundary conditions. Curve 1 is for a cube containing 10^6 particles, curve 2 for a cube containing 6.4×10^4 particles. Dotted curves represent the approximation expressed by Eq. (14).

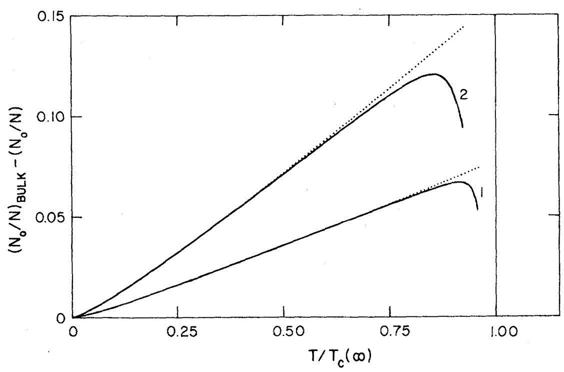

FIG. 5. Depression of the condensate fraction (N_0/N) for Neumann boundary conditions. Curve 1 is for a cube containing 10^6 particles, curve 2 for a cube containing 6.4×10^4 particles. Dotted curves represent the approximation expressed by Eq. (15).

are *each* independent of the actual size of the system. Such a generalization of the scaling theory for finite-size effects may be necessary in some other problems as well.

III. ANTIPERIODIC BOUNDARY CONDITIONS

This model possesses features common to both Dirichlet and periodic boundary conditions. On one hand, since the quantization condition in this case is

$$k_i=(2\pi/L)(n_i+\tfrac{1}{2})\quad (n_i=0,\pm1,\pm2,\ldots),$$

the ground-state energy is nonzero, and hence y^2 has a negative limiting value, viz., $-\frac{3}{4}\pi^2$. On the other hand, since the sum over states now runs over the entire $\vec{k}$ space, the analysis closely parallels that in the periodic case.

Going through the same formal steps as in the periodic case,[5] we obtain

$$N=(L/\lambda)^3[\,g_{3/2}(\alpha)+\pi^{1/2}\alpha^{1/2}\mathcal{R}(y)]\,, \tag{17}$$

where

$$\mathcal{R}(y)=\frac{1}{y}\sum_{q_{1,2,3}=-\infty}^{\infty}{}' (-1)^{q_1+q_2+q_3}\frac{e^{-2yq}}{q}$$

$$[q=(q_1^2+q_2^2+q_3^2)^{1/2}]\,; \tag{18}$$

here, $y=\pi^{1/2}\alpha^{1/2}(L/\lambda)$, as in the periodic case. Starting from the generalized Poisson identity for theta functions,

$$\sum_{n=-\infty}^{\infty} e^{-t(n+a)^2}=\left(\frac{\pi}{t}\right)^{1/2}\sum_{q=-\infty}^{\infty} e^{-\pi^2q^2/t}\cos(2\pi aq), \tag{19}$$

we can generate the three-dimensional identity

$$\sum_{q_{1,2,3}=-\infty}^{\infty}{}' \left[\frac{e^{-tQ^2}}{Q^2}+\frac{\pi(-1)^{q_1+q_2+q_3}}{q}\,\mathrm{erfc}\left(\frac{\pi q}{t^{1/2}}\right)\right]$$

$$=\frac{2\pi^{3/2}}{t^{1/2}}-\tfrac{4}{3}e^{-3t/4}+\chi_3\,, \tag{20}$$

where

$$Q=[(q_1+\tfrac{1}{2})^2+(q_2+\tfrac{1}{2})^2+(q_3+\tfrac{1}{2})^2]^{1/2}$$

and

$$\chi_3=\pi\sum_{q_{1,2,3}=-\infty}^{\infty}{}' \frac{(-1)^{q_1+q_2+q_3}}{(q_1^2+q_2^2+q_3^2)^{1/2}}=-5.490\,136\,.$$

Taking the Laplace transform of (20), we obtain another identity:

$$\sum_{q_{1,2,3}=-\infty}^{\infty}{}' \left(\frac{y^2}{\pi Q^2(y^2+\pi^2Q^2)}+(-1)^{q_1+q_2+q_3}\frac{e^{-2yq}}{q}\right)$$

$$=2y-\frac{4y^2}{3\pi(y^2+\frac{3}{4}\pi^2)}+\frac{\chi_3}{\pi}. \tag{21}$$

The second sum here is directly proportional to $\mathcal{R}(y)$, which enables us to express Eq. (17) in the form

$$N=\left(\frac{L}{\lambda}\right)^3\zeta(\tfrac{3}{2})+\frac{1}{\pi}\left(\chi_3-\frac{32}{3}\right)\left(\frac{L}{\lambda}\right)^2$$

$$-\frac{y^2}{\pi}\left(\frac{L}{\lambda}\right)^2\sum_{q_{1,2,3}=-\infty}^{\infty}{}^{*}\frac{1}{Q^2(y^2+\pi^2Q^2)}+\frac{8\pi}{y^2+\frac{3}{4}\pi^2}\left(\frac{L}{\lambda}\right)^2, \tag{22}$$

where the summation $\sum^*$ excludes the set of terms for which $Q^2=\frac{3}{4}$, viz., the terms with $q_{1,2,3}=0$ or -1.

Identifying the ground-state occupation as

$$N_0\simeq\frac{g(\epsilon_0)}{\alpha+\beta\epsilon_0}=\frac{8\pi}{y^2+\frac{3}{4}\pi^2}\left(\frac{L}{\lambda}\right)^2, \tag{23}$$

since the single-particle ground state is now eightfold degenerate (each of the three quantum numbers n_i being 0 or -1), we obtain

$$\frac{N_0}{N}=\left[1-\left(\frac{T}{T_c(\infty)}\right)^{3/2}\right]-\frac{1}{\pi N}\left(\chi_3-\frac{32}{3}\right)\left(\frac{L}{\lambda}\right)^2$$

$$+\frac{y^2}{\pi N}\left(\frac{L}{\lambda}\right)^2\sum_{q_{1,2,3}=-\infty}^{\infty}{}^{*}\frac{1}{Q^2(y^2+\pi^2Q^2)}. \tag{24}$$

Equation (22) can now be solved for $y(T)$ for any given value of L. In Fig. 6 we show these results for $L/\bar{l}=40$ and 100. As in the case of periodic boundary conditions, these curves pass through a common point at the bulk critical temperature. The temperature dependence of the condensate fraction can now be calculated from (23); a typical result for this is included in Fig. 3. As for the finite-size correction to N_0/N, we find that, in the temperature range where $y^2\simeq-\frac{3}{4}\pi^2$,

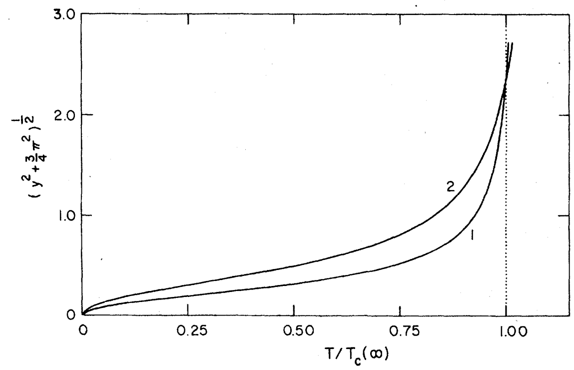

FIG. 6. Quantity $(y^2+\frac{3}{4}\pi^2)^{1/2}$, for a cubical enclosure with antiperiodic boundary conditions, as a function of the scaled temperature $T/T_c(\infty)$. Rest as in Fig. 1.

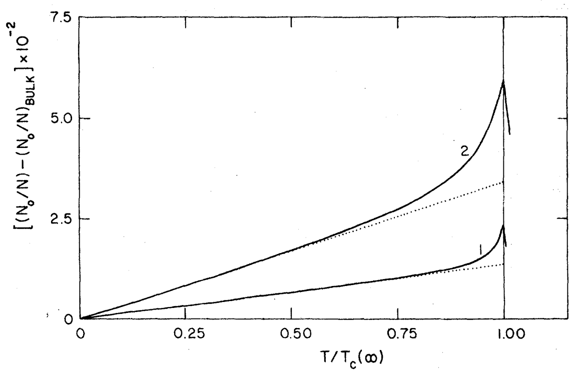

FIG. 7. Enhancement of the condensate fraction (N_0/N) for antiperiodic boundary conditions. Curve 1 is for a cube containing 10^6 particles, curve 2 for a cube containing 6.4×10^4 particles. Dotted curves represent the approximation expressed by Eq. (25).

$$\left(\frac{N_0}{N}\right)^{\times}_{\mathrm{AP}}\frac{L}{\bar{l}}\simeq-\frac{C_3^*}{\pi}[\zeta(\tfrac{3}{2})]^{-2/3}\frac{T}{T_c(\infty)},\qquad(25)$$

where

$$C_3^*=\chi_3-\frac{32}{3}+\frac{3}{4}\sum_{q_{1,2,3}=-\infty}^{\infty}{}^{*}\frac{1}{Q(Q^2-\frac{3}{4})}=-7.81085\,.$$

Comparing this with the corresponding expression for the periodic case, Eq. (2), we find that the enhancement of the condensate fraction in the two cases is comparable in magnitude. From (25) it is clear that the finite-size correction in the antiperiodic case is in conformity with the standard scaling theory. In Fig. 7 we plot the finite-size correction $(N_0/N)^{\times}$ for $L/\bar{l}=40$ and 100, as given by the full expression (24) as well as by the approximate expression (25). The two results agree very well over a considerable range of temperatures.

IV. CONCLUDING REMARKS

Although the foregoing analysis enables us to make explicit calculations of the finite-size corrections, and demonstrates the scaling behavior, in the case of an ideal Bose gas confined to restricted geometries, it is not clear what results would obtain for a more realistic interacting system. To this end it seems desirable to examine the properties of a weakly interacting Bose gas in restricted geometries by studying the statistical mechanics of the quasiparticle excitations. The application of Poisson's summation technique to an excitation spectrum, such as of Bogoliubov or of Brueckner and Sawada, would be quite complicated because of the complex mathematical nature of the spectrum; however, it is possible to study the problem at very low temperatures where only the linear phonon part of the spectrum is operative. One expects that the above technique, when applied to a system of phonons, will again lead to a decomposition of the thermodynamic properties into a bulk term and a finite-size correction conforming to the scaling theory for finite-size effects; the numerical coefficients will, of course, be different from the ones resulting from a quadratic energy spectrum.

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[1]C. S. Zasada and R. K. Pathria, Phys. Rev. A 14, 1269 (1976), hereafter referred to as I.

[1a]The superscript "×" denotes the difference between a quantity f for a finite system and the same quantity for a bulk system: $f^{\times}\equiv f_N-f_{\infty}$.

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[5]S. Greenspoon and R. K. Pathria, Phys. Rev. A 9, 2103 (1974).