Low-temperature behavior of Bose systems confined to restricted geometries: Growth of the condensate fraction and spatial correlations*

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Through an extensive use of the Poisson summation formula, we have elucidated the description of the phenomenon of Bose-Einstein condensation in finite systems in terms of a "collapse in the thermogeometric space." In particular, we have carried out an explicit evaluation of the temperature dependence of the thermogeometric parameter y for a cubical enclosure under periodic boundary conditions, which in turn enables us to evaluate the temperature dependence of the condensate fraction N_0/N as well as the two-point correlation function $\rho(\vec{r}, \vec{r}')$ for cubes of arbitrary sizes. Numerical results are given for two specific sizes, $L/\bar{l} = 40$ and 100, where L is the edge length of the enclosure and $\bar{l}$ the mean interparticle distance in the system. In the appropriate limit, our results are in complete agreement with the Fisher-Barber scaling theory for finite-size effects. Application of the Poisson summation formula has also enabled us to extract information of direct physical interest about the growth of long-range order in general cuboidal geometries. The special case of the thin-film geometry has been studied in detail; the resulting formulas provide a considerable improvement over the ones obtained by previous workers.

I. INTRODUCTION

Interest in the study of finite Bose-Einstein systems arises principally for two reasons. Firstly, these systems possess the unique property that in the thermodynamic limit they undergo a phase transition even in the absence of interparticle interactions. The resulting phenomenon is purely a quantum-mechanical effect arising from the symmetrization of the wave functions. Being noninteracting, these systems are mathematically more tractable than the corresponding realistic ones; accordingly, they are more amenable to a rigorous theoretical analysis. One therefore hopes that a detailed study of these systems may lead to a better understanding of the general problem of finite-size effects in systems undergoing phase transitions.

Secondly, there exists a close connection between the phenomenon of Bose-Einstein condensation on one hand and that of superfluid transition in liquid ^{4}He on the other. Since the latter has been subjected to extensive experimental study in restricted geometries, such as thin films, narrow channels, and small pores, it becomes natural to make a corresponding theoretical study of Bose-Einstein systems confined to similar geometries, in the hope that this may elucidate the observed behavior of liquid ^{4}He under the aforementioned circumstances.

Since Osborne's[1] pioneering work of 1949, several authors have examined the problem of an ideal Bose gas confined to restricted geometries.[2] More recently, a rigorous asymptotic evaluation of the specific heat of a Bose gas confined to a thin-film geometry has been carried out by Pathria[3] and by Greenspoon and Pathria[4] under a variety of boundary conditions. The results of these evaluations turned out to be in excellent agreement with the corresponding numerical ones obtained earlier by Goble and Trainor[5] and with the corresponding theoretical ones obtained almost simultaneously by Barber and Fisher[6] using different mathematical techniques. In addition, the first-order results of Greenspoon and Pathria were shown to be consistent with the Fisher-Barber scaling theory for finite-size effects.[7]

Subsequently Greenspoon and Pathria[8] extended their analysis to a system confined to an arbitrary, finite *cuboidal* geometry under periodic boundary conditions. This analysis was based on the formalism of the grand canonical ensemble and depended on the use of the Poisson summation formula for evaluating the various summations over states that enter into the problem. One is thereby led to the construction of an abstract "thermogeometric lattice space" whose scale factors y_1, y_2, and y_3 are directly related to the chemical potential of the system as well as to the discrete level spacing which arises from the finiteness of the enclosure. In this picture, the phenomenon of Bose-Einstein condensation appears as a gradual "collapse" of the lattice points of the thermogeometric space onto its origin as the temperature of the system is lowered. In the thermodynamic limit, the collapse takes place abruptly at the bulk transition temperature $T_c(\infty)$, which corresponds to a transition accompanied by singularities in the thermodynamic functions of the system.

In this paper we apply the techniques developed by Greenspoon and Pathria[8] and by Chaba and Pathria[9] to examine two important aspects of the problem of Bose-Einstein condensation in finite geometries. First of all, we carry out an explicit evaluation of the temperature dependence of the thermogeometric parameter y ($=y_{1,2,3}$) of the cubic system under periodic boundary conditions. In view of the fact that this parameter plays a central role in the entire problem one is able to extract from these results considerable information of direct physical interest. For instance, in Sec. II we examine the growth of the condensate fraction and in Sec. III the growth of spatial correlations as a function of the temperature of the system. In Sec. IV some special cases are examined in depth. In each case we discuss the influence of the finite size of the system on the property studied and, wherever possible, a comparison is made with the results obtained by previous workers.

II. THERMOGEOMETRIC PARAMETERS AND THE CONDENSATE FRACTION

We start with the asymptotic expression[8]

$$N=\frac{L_1L_2L_3}{\lambda^3}[g_{3/2}(\alpha)+\pi^{1/2}\alpha^{1/2}S_1(y_1,y_2,y_3)], \qquad (1)$$

where N is the number of particles in the system, L_j are the dimensions of the cuboidal enclosure, $\lambda\ [=h/(2\pi mkT)^{1/2}\ll L_j]$ is the mean thermal wavelength of the particles, $\alpha=-\mu/kT$, μ being the chemical potential of the system, the $g_n(\alpha)$ are the familiar Bose-Einstein functions,[10] while

$$S_1(y_1,y_2,y_3)=\sum_{q_{1,2,3}=-\infty}^{\infty}{}' \frac{e^{-2R(\vec{q})}}{R(\vec{q})}, \qquad (2)$$

with

$$R(\vec{q})=(q_1^2y_1^2+q_2^2y_2^2+q_3^2y_3^2)^{1/2},$$
$$y_j=\pi^{1/2}\alpha^{1/2}L_j/\lambda, \quad j=1,2,3. \qquad (3)$$

It may be noted that the primed summation in Eq. (2) implies exclusion of the term with $\vec{q}=0$. Moreover, the system is assumed to be under periodic boundary conditions.

From Eq. (3) it follows that

$$y_j^2\sim\frac{|\mu|}{h^2/mL_j^2}; \qquad (4)$$

thus the y_j^2 represent the chemical potential of the system reduced in terms of its level spacings. In a more recent paper, Greenspoon and Pathria[11] have further pointed out that $y_j\sim L_j/\xi$, where ξ $[=\lambda/(2\pi^{1/2}\alpha^{1/2})]$ is the correlation length for the bulk system.

Insofar as the influence of finiteness on the growth of the condensate fraction N_0/N is concerned, we may restrict ourselves to the case of a cube ($L_j=L$, $y_j=y$). Introducing the reduced temperature $t=[T-T_c(\infty)]/T_c(\infty)$, where $T_c(\infty)$ is the bulk transition temperature, one finds that (i) for $t>0$ and $N^{-1/3}\ll t\ll 1$,

$$\alpha\sim1,\quad N_0\sim1,\quad y\sim N^{1/3}\gg1;$$

(ii) for $t<0$ and $N^{-1/3}\ll|t|\ll1$,

$$\alpha\sim N^{-1},\ N_0\sim N,\ y\sim N^{-1/6}\ll1;$$

while (iii) for $|t|\sim N^{-1/3}$,

$$\alpha\sim N^{-2/3},\ N_0\sim N^{2/3},\quad y\sim1.$$

Thus as the temperature of the system is lowered through the bulk transition temperature $T_c(\infty)$, the scale factor y goes from very large to very small values, the rapidity of the variation being governed by the size of the system. One clearly observes the abruptness of the transition as $N\to\infty$.

We now proceed to evaluate the parameter y explicitly as a function of temperature. In the case of the cube,

$$S_1(y)=\frac{1}{y}\sum_{q_{1,2,3}=-\infty}^{\infty}{}' \frac{e^{-2yq}}{q},\quad q=(q_1^2+q_2^2+q_3^2)^{1/2}. \qquad (5)$$

Recently, Chaba and Pathria[9] have established several identities for a class of multidimensional lattice sums, one of which is the following:

$$\sum_{q_{1,2,3}=-\infty}^{\infty}{}' \left(\frac{e^{-aq^2}}{q^2}+\frac{\pi^{1/2}}{q}\Gamma(\tfrac{1}{2},\pi^2q^2/a)\right)=\frac{2\pi^{3/2}}{a^{1/2}}+a+C_3, \qquad (6)$$

where

$$C_3=\lim_{a\to0}\left(\sum_{\vec{k}}{}'\frac{e^{-ak^2}}{k^2}-\int_{\text{all }\vec{k}}\frac{e^{-ak^2}}{k^2}d^3k\right)=-8.913\,633.$$

Taking the Laplace transform of (6), we obtain another identity, viz.,

$$\sum_{q_{1,2,3}=-\infty}^{\infty}{}' \left(\frac{y^2}{q^2(y^2+\pi^2q^2)}+\frac{\pi}{q}e^{-2yq}\right)=2\pi y+\frac{\pi^2}{y^2}+C_3. \qquad (7)$$

Since the second part of Eq. (7) is directly proportional to $S_1(y)$, we can rewrite (1) as

$$N=\left(\frac{L}{\lambda}\right)^3 g_{3/2}(\alpha)+\left(\frac{L}{\lambda}\right)^2\frac{\pi}{y^2}+\left(\frac{L}{\lambda}\right)^2\left(\frac{C_3}{\pi}+2y-\frac{y^2}{\pi}\sum_{q_{1,2,3}=-\infty}^{\infty}{}'\frac{1}{q^2(y^2+\pi^2q^2)}\right). \qquad (8)$$

Now, the ground-state occupation, under periodic boundary conditions, is given by

$$N_0=1/(e^\alpha-1)\simeq1/\alpha,\quad \text{for } \alpha\ll1. \qquad (9)$$

Note that for a macroscopic occupation of the ground state it is necessary to have $\alpha\ll1$. Recalling (3), we find that the second term on the right-hand side of Eq. (8) is precisely equal to N_0; the condensate therefore emerges rather naturally in this analysis and does not have to be extracted artificially, as is customarily done in the study of the bulk system.

Now, in view of the fact that for small α

$$g_{3/2}(\alpha) \simeq \zeta(\tfrac{3}{2}) - 2\pi^{1/2}\alpha^{1/2},$$

Eq. (8) is further simplified to

$$N = \left(\frac{L}{\lambda}\right)^3 \zeta(\tfrac{3}{2}) + N_0 + \left(\frac{L}{\lambda}\right)^2 \left(\frac{C_3}{\pi} - \frac{y^2}{\pi} \sum_{q_{1,2,3}=-\infty}^{\infty}{}' \frac{1}{q^2(y^2+\pi^2 q^2)}\right), \tag{10}$$

whence

$$N_0 = N\left[1 - \left(\frac{T}{T_c(\infty)}\right)^{3/2}\right] + \left(\frac{L}{\lambda}\right)^2 \left(-\frac{C_3}{\pi} + \frac{y^2}{\pi} \sum_{q_{1,2,3}=-\infty}^{\infty}{}' \frac{1}{q^2(y^2+\pi^2 q^2)}\right). \tag{11}$$

The first part in Eq. (11) is precisely the expression for N_0 in the bulk system; the second part therefore represents the finite-size correction. Since C_3 is negative, this correction is positive throughout and, except very close to $T_c(\infty)$, varies linearly with temperature (see Figs. 2 and 3). 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. In this case the ground-state energy in both the bulk and the finite systems is zero; however, as we go from the bulk to the finite case, the excited states become discrete and are shifted upwards, thereby shrinking the mean occupation numbers for these states and, consequently, enhancing the fraction of particles in the ground state. The situation may very well vary from one set of boundary conditions to another, but this requires the extension of the present analysis to other boundary conditions, such as Dirichlet, Neumann, etc.

Expanding the summand in Eq. (11) in powers of y^2 we can write for $y<\pi$

$$1 = b_1\left(\frac{y^2}{\pi^2}\right)^1 + b_2\left(\frac{y^2}{\pi^2}\right)^2 + b_3\left(\frac{y^2}{\pi^2}\right)^3 + \cdots, \tag{12}$$

where

$$b_1 = -C_3 + \pi N\left(\frac{\lambda}{L}\right)^2 \left[1 - \left(\frac{T}{T_c(\infty)}\right)^{3/2}\right], \tag{13}$$

$$b_k(k \geq 2) = (-1)^k \sum_{q_{1,2,3}=-\infty}^{\infty}{}' \frac{1}{q^{2k}}. \tag{14}$$

We note that in the series (12) the coefficient b_1 alone is temperature dependent; all other coefficients are pure numbers, as defined by (14). These numbers can be evaluated by expressing the sum over $\vec{q}$ in terms of other, strongly convergent sums by using a method developed by Van der Hoff and Benson[12] (see Appendix A). The resulting values are given in the second column of Table I.

In principle, the temperature dependence of y can now be determined by inverting the series in (12). However, since the coefficients b_k approach their asymptotic value $6(-1)^k$ at about $k=10$, it is in practice simpler to replace coefficients higher than a suitable value of k by their asymptotic value and collect all these higher-order terms into a closed form. Thus we may write with negligible error

$$b_1\left(\frac{N\lambda^2}{L^2}, \frac{T}{T_c(\infty)}\right) = \frac{\pi^2}{y^2} - \sum_{j=2}^{K} b_j\left(\frac{y^2}{\pi^2}\right)^{j-1} + 6(-1)^K \left(\frac{y^2}{\pi^2}\right)^K \left(1 + \frac{y^2}{\pi^2}\right)^{-1}. \tag{15}$$

Another advantage of the foregoing expression is that now one need not restrict oneself to $y<\pi$, although this restriction was never a severe one

TABLE I. β coefficients.

k	$\beta_k(0,0,0) \equiv (-1)^k b_k$	$\beta_k(0,0,\frac{1}{2})$	$\beta_k(0,\frac{1}{2},\frac{1}{2})$	$\beta_k(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
1	...	−0.301 38	−1.830 05	−2.519 36
2	16.532 32	0.689 22	−2.156 89	−3.863 16
3	8.401 92	1.341 11	−2.195 52	−4.788 44
4	6.945 81	1.683 75	−2.144 81	−5.345 57
5	6.426 12	1.849 81	−2.089 56	−5.656 67
6	6.202 15	1.928 38	−2.050 71	−5.823 03
7	6.098 18	1.965 54	−2.027 35	−5.909 76
8	6.048 26	1.983 26	−2.014 34	−5.954 30
9	6.023 88	1.991 80	−2.007 39	−5.976 95
10	6.011 86	1.995 96	−2.003 76	−5.988 40
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∞	6.000 00	2.000 00	−2.000 00	−6.000 00

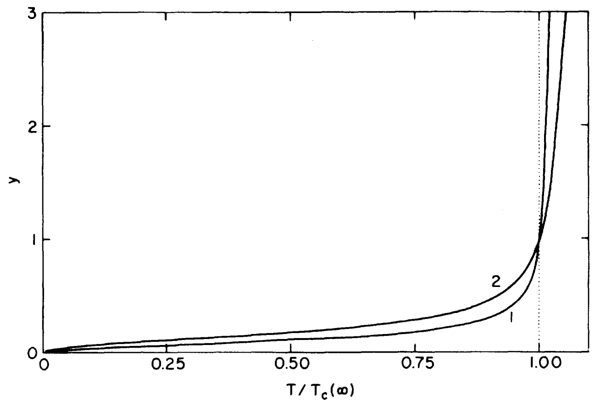

FIG. 1. Thermogeometric parameter y for a cubical enclosure as a function of the scaled temperature $T/T_c(\infty)$. Curve 1 is for a cube containing 10^6 particles, curve 2 for a cube containing 6.4×10^4 particles. Dotted line depicts the corresponding bulk behavior.

anyway.[13]

Equation (15) can be used to determine $y(T)$ for cubical enclosures of different sizes. In Fig. 1 we have plotted results for two specific sizes, viz., $L/\bar{l}=40$ and 100, where $\bar{l}$ is the mean interparticle distance in the system; these values correspond to $N=6.4\times10^4$ and 10^6, respectively. As expected, the rise is steeper in the case of the system containing a larger number of particles and is closer in behavior to the limiting bulk case for which y undergoes an infinite step at $T_c(\infty)$. We also note that as predicted by Greenspoon and Pathria[8] these curves pass through a common point $y\simeq 0.973$ at the bulk transition temperature $T_c(\infty)$, irrespective of the actual size of the system.

Now that y is known as a function of T it is straightforward to study the temperature dependence of the condensate fraction N_0/N for systems of different sizes. This is given by the expression

$$\frac{N_0}{N}=\frac{\pi}{y^2}\;\frac{L^2}{N\lambda^2}=\pi N^{-1/3}[\zeta(\tfrac{3}{2})]^{-2/3}\left[\frac{1}{y^2}\left(\frac{T}{T_c(\infty)}\right)\right]. \qquad (16)$$

Figure 2 shows the growth of the condensate fraction with temperature for the case $L/\bar{l}=40$; the corresponding bulk behavior is also displayed for comparison. As expected, the singularity in N_0/N, which is characteristic of the bulk system, is smoothed out in the case of the finite system. A detailed analysis of this result, especially its relevance to the onset of superfluidity, will be reported separately by Pajkowski and Pathria.[14]

From the point of view of the scaling theory for finite-size effects, it seems more instructive to consider the difference between the condensate fraction for a finite system and that for the bulk system. This is shown in Fig. 3, for both $L/\bar{l}=40$

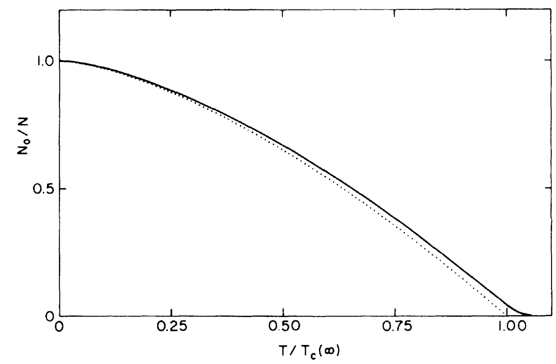

FIG. 2. Temperature dependence of the condensate fraction N_0/N for a cube containing 6.4×10^4 particles. The bulk behavior is shown by the dotted curve.

and 100. The appearance of a cusp in these curves is a reflection of the singularity in the bulk behavior of N_0/N. For small values of y^2

$$\frac{1}{y^2}\simeq\frac{b_1}{\pi}=-\frac{C_3}{\pi}+\frac{N}{\pi}\left(\frac{\lambda}{L}\right)^2\left[1-\left(\frac{T}{T_c(\infty)}\right)^{3/2}\right]; \qquad (17)$$

the condensate fraction in the finite system is then given by

$$\frac{N_0}{N}=\left(\frac{N_0}{N}\right)_{\text{bulk}}-\frac{C_3}{\pi}[\zeta(\tfrac{3}{2})]^{-2/3}\left(\frac{\bar{l}}{L}\right)\frac{T}{T_c(\infty)}. \qquad (18)$$

The "excess" in N_0/N, being directly proportional to the surface-to-volume ratio of the enclosure, is in complete agreement with the scaling theory for finite-size effects.[15]

III. SPATIAL CORRELATIONS

After studying the temperature dependence of the condensate fraction N_0/N, which is directly related to the diagonal elements of the density matrix, we now examine the two-point correlation function

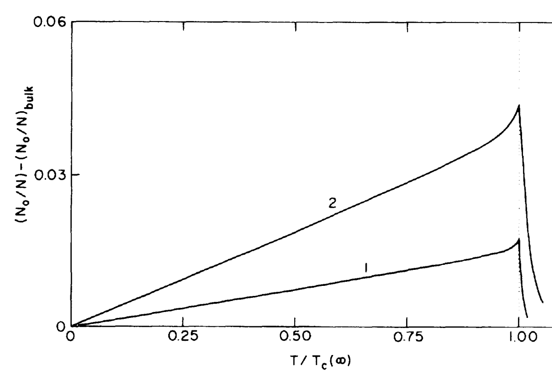

FIG. 3. Condensate fraction in excess of the bulk value. Curve 1 is for a cube containing 10^6 particles, curve 2 for a cube containing 6.4×10^4 particles.

$\rho_1(\vec{r},\vec{r}')$, which is related to the off-diagonal elements of the same matrix. By definition, $\rho_1(\vec{r},\vec{r}')$ is a measure of the overlap between a given wave function of the system and the one obtained by transferring one of the particles in the system from a point $\vec{r}$ to another point $\vec{r}'$. This quantity evokes considerable interest in the study of Bose-Einstein condensation, for the main reason that it can be regarded as a measure of the degree of long-range order prevailing in the system. We have

$$\rho_1(\vec{r},\vec{r}')=\langle\hat{\psi}(\vec{r})\hat{\psi}^\dagger(\vec{r}')\rangle, \tag{19}$$

where $\langle\cdots\rangle$ denotes a grand canonical average. Expanding the field operators $\hat{\psi}(\vec{r})$ as

$$\hat{\psi}(\vec{r})=\frac{1}{\sqrt{V}}\sum_{\vec{k}}\hat{a}_{\vec{k}}e^{i\vec{k}\cdot\vec{r}}, \tag{20}$$

we obtain for free particles in a box, under periodic boundary conditions,

$$\rho_1(\vec{r},\vec{r}')=\rho_1(|\vec{r}-\vec{r}'|)=\frac{1}{V}\sum_{\vec{k}}\langle n_{\vec{k}}\rangle e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}, \tag{21}$$

where

$$\begin{aligned}&\langle n_{\vec{k}}\rangle=(e^{\alpha+\beta\epsilon(\vec{k})}-1)^{-1},\\ &\epsilon(\vec{k})=\hbar^2k^2/2m=(\hbar^2/2m)(k_1^2+k_2^2+k_3^2),\\ &k_i=2\pi n_i/L_i,\quad n_i=0,\pm1,\pm2,\ldots.\end{aligned} \tag{22}$$

Writing (22) as a geometric progression,

$$\langle n_{\vec{k}}\rangle=\sum_{j=1}^{\infty}e^{-j\alpha}e^{-j\beta\epsilon}, \tag{23}$$

and interchanging the order of summations over j and $\vec{k}$, which is legitimate in the case of a finite system, we obtain[16]

$$\rho_1(|\vec{r}-\vec{r}'|)=\frac{1}{V}\sum_{j=1}^{\infty}e^{-j\alpha}\sum_{k_1}e^{-ik_1(x_1'-x_1)}e^{-j\lambda^2k_1^2/4\pi}\sum_{k_2}e^{-ik_2(x_2'-x_2)}e^{-j\lambda^2k_2^2/4\pi}\sum_{k_3}e^{-ik_3(x_3'-x_3)}e^{-j\lambda^2k_3^2/4\pi}. \tag{24}$$

Noting that the summations over k_i are really summations over n_i, viz.,

$$\sum_{k_i}=\sum_{n_i=-\infty}^{\infty}\exp\left[-\frac{2\pi in_i(x_i'-x_i)}{L_i}-j\pi n_i^2\left(\frac{\lambda}{L_i}\right)^2\right], \tag{25}$$

we apply Poisson's summation formula,[17] with the result

$$\sum_{n_i=-\infty}^{\infty}=\frac{L_i}{j^{1/2}\lambda}\sum_{q_i=-\infty}^{\infty}\exp\left[-\pi\left(\frac{L_i}{\lambda}\right)^2\frac{(q_i+\tilde{x}_i/L_i)^2}{j}\right],\qquad \tilde{x}_i=x_i'-x_i. \tag{26}$$

Equation (24) now takes the form

$$\rho_1(|\vec{r}-\vec{r}'|)=\frac{1}{\lambda^3}\sum_{j=1}^{\infty}j^{-3/2}e^{-j\alpha}\sum_{q_{1,2,3}=-\infty}^{\infty}e^{-\gamma(\vec{q})/j}, \tag{27}$$

where

$$\gamma(\vec{q})=\pi\left[\left(\frac{L_1}{\lambda}\right)^2(q_1+a_1)^2+\left(\frac{L_2}{\lambda}\right)^2(q_2+a_2)^2+\left(\frac{L_3}{\lambda}\right)^2(q_3+a_3)^2\right],\quad a_i=\frac{\tilde{x}_i}{L_i}. \tag{28}$$

We again interchange the order of summations over j and $\vec{q}$ and apply Poisson's summation formula to the sum over j. Assuming that $|\vec{a}|\neq0$, we get[18]

$$\sum_{j=1}^{\infty}j^{-3/2}e^{-j\alpha}e^{-\gamma(\vec{q})/j}\equiv\sum_{j=0}^{\infty}j^{-3/2}e^{-j\alpha}e^{-\gamma(\vec{q})/j}=\sum_{j=-\infty}^{\infty}\int_0^{\infty}\delta(x-j)x^{-3/2}e^{-\alpha x}e^{-\gamma(\vec{q})/x}dx=\sum_{l=-\infty}^{\infty}\int_0^{\infty}x^{-3/2}e^{-(\alpha+2\pi il)x}e^{-\gamma(\vec{q})/x}dx. \tag{29}$$

The last step follows from the identity

$$\sum_{j=-\infty}^{\infty}\delta(x-j)=\sum_{l=-\infty}^{\infty}e^{-2\pi ilx}, \tag{30}$$

which forms the backbone of the Poisson summation formula. The integral in (29) is a tabulated Laplace transform; consequently

$$\begin{aligned}\rho_1(|\vec{r}-\vec{r}'|)&=\frac{\pi^{1/2}}{\lambda^3}\sum_{q_{1,2,3}=-\infty}^{\infty}\sum_{l=-\infty}^{\infty}\frac{\exp\{-2[\gamma(\vec{q})]^{1/2}(\alpha+2\pi il)^{1/2}\}}{[\gamma(\vec{q})]^{1/2}}\\ &=\frac{\pi^{1/2}\alpha^{1/2}}{\lambda^3}\sum_{q_{1,2,3}=-\infty}^{\infty}\frac{\exp\{-2[y_1^2(q_1+a_1)^2+y_2^2(q_2+a_2)^2+y_3^2(q_3+a_3)^2]^{1/2}\}}{[y_1^2(q_1+a_1)^2+y_2^2(q_2+a_2)^2+y_3^2(q_3+a_3)^2]^{1/2}}+\frac{2}{R\lambda^2}\sum_{l=1}^{\infty}e^{-2\pi l^{1/2}R/\lambda}\cos\left(2\pi l^{1/2}\frac{R}{\lambda}\right)\\ &\quad+\frac{2}{\lambda^2}\sum_{q_{1,2,3}=-\infty}^{\infty}{}'\sum_{l=1}^{\infty}\frac{\exp\{-2\pi(l^{1/2}/\lambda)[L_1^2(q_1+a_1)^2+L_2^2(q_2+a_2)^2+L_3^2(q_3+a_3)^2]^{1/2}\}}{[L_1^2(q_1+a_1)^2+L_2^2(q_2+a_2)^2+L_3^2(q_3+a_3)^2]^{1/2}}\\ &\qquad\times\cos\left(\frac{2\pi l^{1/2}}{\lambda}[L_1^2(q_1+a_1)^2+L_2^2(q_2+a_2)^2+L_3^2(q_3+a_3)^2]^{1/2}\right),\end{aligned}$$

where

$$R=(L_1^2a_1^2+L_2^2a_2^2+L_3^2a_3^2)^{1/2}$$
$$=(\bar{x}_1^2+\bar{x}_2^2+\bar{x}_3^2)^{1/2}=|\vec{r}'-\vec{r}|. \quad (31)$$

The first term here corresponds to $l=0$ and is precisely the result one would obtain by integrating (27) over j. The second and third terms correspond to $l\neq 0, q=0$ and $l\neq 0, q\neq 0$, respectively, and determine the relevant corrections as functions of the parameters λ/R and λ/L_i. For $R/\lambda \gg 1$ and $L_i/\lambda \gg 1$, these corrections are clearly negligible. The first of these conditions is consistent with the fact that we are primarily interested in the growth of *long-range* correlations; the second one is quite generally satisfied by systems of practical interest. Hence under these conditions the two-point correlation function may be written in the form

$$\rho_1(|\vec{r}-\vec{r}'|)=\frac{\pi^{1/2}\alpha^{1/2}}{\lambda^3}\sum_{q_{1,2,3}=-\infty}^{\infty}\frac{\exp\{-2[y_1^2(q_1+a_1)^2+y_2^2(q_2+a_2)^2+y_3^2(q_3+a_3)^2]^{1/2}\}}{[y_1^2(q_1+a_1)^2+y_2^2(q_2+a_2)^2+y_3^2(q_3+a_3)^2]^{1/2}}, \quad |\vec{a}|\neq 0, \quad (32)$$

which possesses the expected properties of reflection symmetry $[\rho_1(a_i)=\rho_1(-a_i)]$, of periodicity $[\rho_1(a_i)=\rho_1(1+a_i)]$, and of vanishing slope at integral and half-integral values of a_i. These properties are in accord with the imposition of periodic boundary conditions and allow us to confine our consideration of a_i to the range $(0,\frac{1}{2})$. In passing we note that the special case $R=0$, which determines the condensate, cannot be recovered from the foregoing expression; for that, one must go back to Eqs. (27) and (28), which give

$$\rho_1(0)=\frac{1}{\lambda^3}\sum_{j=1}^{\infty}j^{-3/2}e^{-j\alpha}e^{-\gamma^0(\vec{q})/j},$$

where

$$\gamma^0(\vec{q})=\pi\left[\left(\frac{L_1}{\lambda}\right)^2q_1^2+\left(\frac{L_2}{\lambda}\right)^2q_2^2+\left(\frac{L_3}{\lambda}\right)^2q_3^2\right]$$
$$=\frac{1}{\alpha}(y_1^2q_1^2+y_2^2q_2^2+y_3^2q_3^2).$$

Subsequent analysis then leads to the desired result (1), for $L_i/\lambda \gg 1$.

To obtain a more tractable form we again apply Poisson's summation formula to Eq. (32) and obtain a remarkably simple result:

$$\rho_1(a_1,a_2,a_3)=\frac{N_0}{V}\sum_{q_{1,2,3}=-\infty}^{\infty}\frac{e^{-2\pi i(\vec{q}\cdot\vec{a})}}{1+\pi^2(q_1^2/y_1^2+q_2^2/y_2^2+q_3^2/y_3^2)}, \quad |\vec{a}|\neq 0 \quad (33)$$

where $N_0=1/\alpha$. The most striking feature of this result is that it is precisely the same as the original expression (21) except that the mean occupation numbers $\langle n_{\vec{k}}\rangle$ in the summand have been replaced by their low-energy approximation $(\alpha+\beta\epsilon)^{-1}$. This can be understood by noting that for $R=|\vec{r}'-\vec{r}|\gg\lambda$ the oscillatory factor in the numerator of (21) destroys contributions from most wave vectors except the ones for which $k\ll 2\pi/\lambda$. Accordingly, the replacement of $\langle n_{\vec{k}}\rangle$ by $(\alpha+\beta\epsilon)^{-1}$ causes errors in $\rho_1(|\vec{r}-\vec{r}'|)$ which are of a negligible magnitude; in explicit terms, these errors are given by the second and third terms of Eq. (31).

IV. DISCUSSION OF SPECIAL CASES

We first examine the case of a system confined to a cuboidal geometry with $L_1\gg L_2\gg L_3$ and hence $y_1\gg y_2\gg y_3$. For this we write Eq. (33) in the form

$$\rho_1(a_1,a_2,a_3)$$
$$=\frac{N_0}{V}+\frac{\pi^{3/2}\alpha^{1/2}}{\lambda^3y_1y_2y_3}\times\sum_{q_{1,2,3}=-\infty}^{\infty}{}'\frac{e^{-2\pi i(\vec{q}\cdot\vec{a})}}{1+\pi^2(q_1^2/y_1^2+q_2^2/y_2^2+q_3^2/y_3^2)}, \quad (34)$$

and, in view of the relative sizes of the various y's, calculate the sum over $\vec{q}$ as follows (see Fig. 4): (i) for $q_2=q_3=0$, we sum over q_1; (ii) for $q_3=0$, $q_2\neq 0$, we sum over q_2 but integrate over q_1; and (iii) for $q_3\neq 0$, we sum over q_3 but integrate over q_1 and q_2. This gives

$$\rho_1(a_1,a_2,a_3)=\frac{N_0}{V}+\frac{\pi^{3/2}\alpha^{1/2}}{\lambda^3y_1y_2y_3}\left[\left(\frac{y_1\cosh[y_1(1-2a_1)]}{\sinh y_1}-1\right)+2y_1\sum_{q_2=1}^{\infty}\left(\cos(2\pi q_2a_2)\frac{\exp\{-2a_1y_1[1+(\pi q_2/y_2)^2]^{1/2}\}}{[1+(\pi q_2/y_2)^2]^{1/2}}\right)\right.$$
$$\left.+\frac{4y_1y_2}{\pi}\sum_{q_3=1}^{\infty}\cos(2\pi q_3a_3)K_0(2(a_1^2y_1^2+a_2^2y_2^2)^{1/2}[1+(\pi q_3/y_3)^2]^{1/2})\right], \quad (35)$$

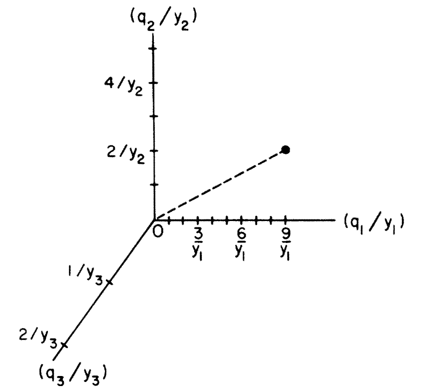

FIG. 4. Relative lattice spacings in the "reciprocal thermogeometric space" for a cuboidal geometry ($L_1 \gg L_2 \gg L_3$); this provides the motivation for a method of evaluation of the sum appearing in Eq. (34).

where $K_0(x)$ is the zero-order modified Bessel function; the last step requires that either a_1 or a_2 be nonzero. If we now proceed to the limit of a thin-film geometry, for which L_1, L_2 and hence $y_1, y_2 \to \infty$, the first part on the right-hand side vanishes while the second part can be approximated by integrating over q_2, provided that a_2 $[=\bar{x}_2/L_2]$ is taken small enough to make the cosine factor sufficiently slowly varying. However, this is not a severe restriction, because L_2 is infinitely large. The second part in (35) then becomes

$$2y_1 \sum_{q_2=1}^{\infty} (\;) \to \frac{2y_1y_2}{\pi} \int_0^{\infty} \cos(2a_2y_2u) \times \frac{\exp[-2a_1y_1(1+u^2)^{1/2}]}{(1+u^2)^{1/2}}\,du$$

$$= \frac{2y_1y_2}{\pi} K_0\left(\frac{R'}{\xi}\right), \tag{36}$$

where $R' = (\bar{x}_1^2 + \bar{x}_2^2)^{1/2}$ is the magnitude of the projection of $\vec{r}' - \vec{r}$ on the (x,y) plane, while $\xi = L_i/2y_i = \lambda/(2\pi^{1/2}\alpha^{1/2})$ is the bulk correlation length. Combining this with the third part of (35) yields, for a thin-film geometry, the axially symmetric result

$$\rho_1(a_1,a_2,a_3) = \frac{N_0}{V} + \frac{2}{\lambda^3}\left(\frac{\lambda}{L_3}\right) \sum_{l=-\infty}^{\infty} \cos(2\pi l a_3) K_0\left(\frac{R'}{\xi}\left(1+\frac{\pi^2 l^2}{y_3^2}\right)^{1/2}\right), \quad R' \neq 0. \tag{37}$$

The $l=0$ term here corresponds to (36) and is precisely the result obtained earlier by Krueger[19] for the thin-film correlation function; the remaining terms provide an improvement over that result.

As a check we consider the limit of Eq. (37) as the film becomes increasingly thick and approaches the bulk system. For the latter, the two-point correlation function is given by[16]

$$\rho_1^{\text{bulk}}(a_1,a_2,a_3) = N_0/V + (1/\lambda^2 R)e^{-R/\xi}, \quad R \neq 0, \tag{38}$$

which is of the same form as the Ornstein-Zernike density-density correlation function for a classical fluid. Now, in the limit $L_3 \to \infty$, we may convert the summation in (37) into an integration, with the result

$$\rho_1(\vec{a}) \to \frac{N_0}{V} + \frac{4}{\lambda^3}\left(\frac{\lambda}{L_3}\right)\frac{y_3}{\pi} \int_0^{\infty} \cos(2a_3y_3u) K_0\left(\frac{R'}{\xi}(1+u^2)^{1/2}\right) du$$

$$= \frac{N_0}{V} + \frac{2^{3/2}\alpha^{1/2}}{\lambda^3}\left(\frac{R'^2}{\xi^2} + 4a_3^2y_3^2\right)^{-1/4} K_{1/2}\left(\frac{R'^2}{\xi^2} + 4a_3^2y_3^2\right)^{1/2}$$

$$= \frac{N_0}{V} + \frac{1}{\lambda^2 R} e^{-R/\xi},$$

with

$$R = (R'^2 + 4a_3^2y_3^2\xi^2)^{1/2} = (\bar{x}_1^2 + \bar{x}_2^2 + \bar{x}_3^2)^{1/2},$$

which is identical with (38). Quite expectedly, this result possesses spherical symmetry, for when we pass over to the bulk limit there are no surfaces left to define any special direction(s) in the system.

In the low-temperature regime, where $y_3 \ll 1$, the $l \neq 0$ terms in Eq. (37) become negligible and, except for the factor $1/L_3$, the correlation function becomes exactly the same as for a strictly two-dimensional infinite Bose gas (see Appendix B). In the three-dimensional case, the function acquires cylindrical symmetry.

A case that deserves special consideration is the one for which $R'=0$, i.e., where one considers correlations between points along a straight line normal to the surface. We then have, directly from (32),

$$\rho_1(0,0,a_3) = \frac{1}{\lambda^3}\left(\frac{\lambda}{L_3}\right) \sum_{q=-\infty}^{\infty} \frac{e^{-2y|q+a_3|}}{|q+a_3|} = \frac{1}{\lambda^3}\left(\frac{\lambda}{L_3}\right)\left(\frac{e^{-2ya_3}}{a_3}F(a_3,1,1+a_3;e^{-2y}) + \frac{e^{-2y(1-a_3)}}{(1-a_3)}F(1-a_3,1,2-a_3;e^{-2y})\right), \quad a_3 \neq 0, \tag{39}$$

where $F(a,b,c;z)$ is the hypergeometric function. Expression (39) does not contain any condensate term, because in a thin-film geometry a non-negligible condensate fraction cannot exist except at $T \simeq 0\,^\circ\mathrm{K}$. Specifically, for the condensate to be significant, we require

$$\alpha \sim 1/N \quad \text{or} \quad y_3 \sim (L_3/\lambda)(1/N^{1/2}).$$

Together with the thin-film result[16]

$$\sinh y_3 = \frac{1}{2}\exp\left[\frac{L_3}{\lambda}\left(\frac{\lambda_c^3(\infty) - \lambda^3}{\bar{l}^3}\right)\right], \quad T < T_c(\infty), \tag{40}$$

this requires that

$$[T/T_c(\infty)]\ln[(T_c(\infty)/T)N] \sim 1, \tag{41}$$

which can be satisfied only if $T/T_c(\infty) \sim 1/\ln N$. The bulk limit clearly implies that a condensate can only exist at $T = 0\,^\circ\mathrm{K}$. It may be noted that the foregoing result is analogous to that of Osborne,[1] who found an "accumulation temperature" $T_a \sim T_c(\infty)/\ln L$, where L denotes the lateral dimension of the film.

Since we are operating under periodic boundary conditions we may, without loss of generality, fix our origin at one of the points in the median plane of the film and vary the other point along the z axis (from $a_3 \gg \lambda/L_3$ to $a_3 = \frac{1}{2}$). For $a_3 = \frac{1}{2}$, which determines the degree of correlation between a point on the surface of the film and a point lying directly below it in the median plane, Eq. (39) becomes

$$\rho_1(0,0,\tfrac{1}{2}) = \frac{2}{\lambda^3}\left(\frac{\lambda}{L_3}\right)\ln\coth(\tfrac{1}{2}y)$$

$$\simeq \begin{cases} (2/\lambda^2 L_3)\ln(2/y), & \text{for } y \ll 1, \\ (4/\lambda^2 L_3)e^{-y}, & \text{for } y \gg 1. \end{cases} \tag{42}$$

In the asymptotic regime, where $y \gg 1$, $F(a,b,c;z) \simeq F(a,b,c;0) = 1$, so that

$$\rho_1(0,0,a_3) \simeq \frac{1}{\lambda^3}\left(\frac{\lambda}{L_3}\right)\left(\frac{e^{-2y a_3}}{a_3} + \frac{e^{-2y(1-a_3)}}{1-a_3}\right). \tag{43}$$

For $a_3 = \frac{1}{2}$, Eq. (43) agrees with the corresponding limit of Eq. (42). For values of a_3 which are not too close to $\frac{1}{2}$ the first term in (43) will dominate over the second, so we may further approximate by writing

$$\rho_1(0,0,a_3) \simeq (1/\lambda^2 L_3 a_3)e^{-2y a_3} = (1/\lambda^2 z)e^{-z/\xi}. \tag{44}$$

Note that this again is an Ornstein-Zernike type of result which can be obtained from the bulk result (38) by putting $a_1 = a_2 = 0$ (except for the background contribution N_0/V, which is absent in the case under study). This is indeed expected because when y is large finite-size effects generally disappear, although this will not be the case for $a_3 \simeq \frac{1}{2}$. It may be pointed out here that Eq. (44) can also be obtained by simply retaining the $q = 0$ term of Eq. (39), which is quite appropriate for $y \gg 1$ and for a_3 not too close to $\frac{1}{2}$.

In the other regime, where $y \ll 1$, we may use the approximation

$$F(a_3, 1, 1 + a_3; e^{-2y}) \simeq a_3[\ln(1/2y) + \psi(1) - \psi(a_3)],$$

with the result

$$\rho_1(0,0,a_3) \simeq \frac{1}{\lambda^2 L_3}\left[2\ln\left(\frac{1}{2y}\right) + 2\psi(1) - \psi(a_3) - \psi(1-a_3)\right]; \tag{45}$$

here, $\psi(z) = d[\ln\Gamma(z)]/dz$ is the digamma function. For $a_3 = \frac{1}{2}$, this reduces to [since $\psi(1) - \psi(\frac{1}{2}) = 2\ln 2$]

$$\rho_1(0,0,\tfrac{1}{2}) = (2/\lambda^2 L_3)\ln(2/y),$$

which agrees with the corresponding limit of Eq. (42).

We now turn our attention to the problem of correlations in the cubic geometry ($L_i = L$, $y_i = y$). In this case Eq. (33) takes the form

$$\rho_1(a_1,a_2,a_3) = \frac{\pi}{\lambda^2 L}\left(\frac{1}{y^2} + {\sum_{q_{1,2,3}=-\infty}^{\infty}}' \frac{e^{-2\pi i(\vec{q}\cdot\vec{a})}}{y^2 + \pi^2 q^2}\right), \tag{46}$$

where $q^2 = q_1^2 + q_2^2 + q_3^2$. Expanding in powers of y^2 we obtain, say,

$$\rho_1(a_1,a_2,a_3) = \frac{\pi}{\lambda^2 L}\left[\frac{1}{y^2} + \frac{1}{y^2}\sum_{j=0}^{\infty}(-1)^j\left(\frac{y}{\pi}\right)^{2j+2}\beta_{j+1}(a_1,a_2,a_3)\right] = \frac{N_0}{V} + \rho_1^*(\vec{a}), \tag{47}$$

with

$$\beta_k(a_1,a_2,a_3) = {\sum_{q_{1,2,3}=-\infty}^{\infty}}' \frac{e^{-2\pi i\vec{q}\cdot\vec{a}}}{q^{2k}}. \tag{48}$$

These sums converge rather slowly; however, by using Poisson's summation formula they can be expressed in terms of other sums which converge rapidly. As shown in Appendix A,

$$\beta_k(a_1,a_2,a_3) = \frac{4\pi^k}{\Gamma(k)}\sum_{q_1=1}^{\infty}\sum_{q_{2,3}=-\infty}^{\infty}\cos(2\pi q_1 a_1)\left(\frac{[(q_2+a_2)^2+(q_3+a_3)^2]^{1/2}}{q_1}\right)^{k-1}K_{k-1}(2\pi q_1[(q_2+a_2)^2+(q_3+a_3)^2]^{1/2})$$

$$+\frac{4\pi^k}{\Gamma(k)}\sum_{q_2=1}^{\infty}\sum_{q_3=-\infty}^{\infty}\cos(2\pi q_2 a_2)\left(\frac{|q_3+a_3|}{q_2}\right)^{k-1/2}K_{k-1/2}(2\pi q_2|q_3+a_3|) + (-1)^{k-1}\frac{(2\pi)^{2k}}{(2k)!}B_{2k}(a_3), \tag{49}$$

where $K_\nu(x)$ and $B_n(x)$ are the modified Bessel functions and Bernoulli polynomials, respectively. The asymptotic behavior of the β's is given by

$$\beta_k(a_1,a_2,a_3) \xrightarrow[k\to\infty]{} 2\sum_{q=1}^{\infty} \frac{\cos(2\pi q a_1)+\cos(2\pi q a_2)+\cos(2\pi q a_3)}{q^{2k}}$$

$$= (-1)^{k-1}\frac{(2\pi)^{2k}}{(2k)!}\left[B_{2k}(a_1)+B_{2k}(a_2)+B_{2k}(a_3)\right] \simeq 2[\cos(2\pi a_1)+\cos(2\pi a_2)+\cos(2\pi a_3)]. \quad (50)$$

Numerical values of the β_k's, for selected a's, are given in Table I.

Since we are primarily interested in the onset of long-range order in the system we must consider correlations over distances of the order of L. For simplicity, we choose the center of the cube as origin and examine correlations between this point and (i) points at the centers of the faces of the container, say for $a=(0,0,\frac{1}{2})$, (ii) points bisecting the edges, say for $a=(0,\frac{1}{2},\frac{1}{2})$, and (iii) points at the corners, for which $a=(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. The appropriate coefficients β_k, along with the temperature dependence of the parameter y, as determined in Sec. II, are now sufficient to evaluate the quantity $\rho_1(\vec{x})$ as a function of temperature for cubes of different sizes. As in the study of the condensate fraction, we consider two specific sizes, viz., $L/\bar{l}=40$ and 100.

The resulting correlations are shown in Fig. 5, where we have plotted the correlation functions $\rho_1(\vec{a})$, with the background N_0/V subtracted. For a vivid demonstration of the scaling properties of these functions, we have preferred to plot the quantity $\rho_1^*(\vec{a})\bar{l}^3\times L/\bar{l}$ as a function of the reduced temperature $T/T_c(\infty)$. The leading temperature dependence turns out to be

$$\rho_1^*(\vec{a})\bar{l}^3\left(\frac{L}{\bar{l}}\right) \simeq \frac{\beta_1(\vec{a})}{\pi}[\zeta(\tfrac{3}{2})]^{-2/3}\left(\frac{T}{T_c(\infty)}\right). \quad (51)$$

That this quantity is independent of the actual size of the enclosure is precisely what one expects on the basis of the scaling theory for finite-size effects.[7,15] The presence of the coefficients $\beta_1(\vec{a})$ shows that this quantity is still shape dependent.

As expected on physical grounds, the temperature dependence of $\rho_1^*(\vec{a})$ between the origin and the corner is larger than that between the origin and the midpoint of an edge, which in turn is larger than that between the origin and the center of a face. This is quite reasonable, for a point at the corner of the cube "senses" the finiteness of the system much more strongly than a point in the middle of an edge, and so on.

Since in Fig. 5 we subtracted from $\rho_1(\vec{a})$ the background N_0/V corresponding to the finite system, we essentially excluded some of the finite-size effects. It may therefore be more appropriate to examine a quantity obtained by subtracting the condensate background corresponding to the bulk system instead. This is shown in Fig. 6, again for the three cases of interest. The leading temperature dependence remains of the same form as in (51), except that $\beta_1(\vec{a})$, which is negative, is now replaced by $\beta_1(\vec{a})-C_3$, which is positive [cf. Eq. (18)]. Finite-size corrections are now progressively larger in magnitude for the corner, the

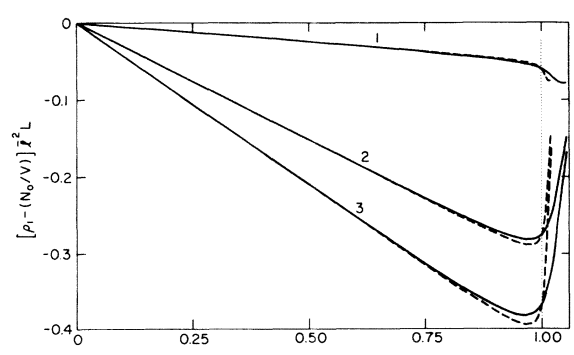

FIG. 5. Temperature dependence of the scaled correlation function $\rho_1\bar{l}^2L$, with condensate background corresponding to the finite system subtracted. Dashed curves are for $L/\bar{l}=100$, solid ones for $L/\bar{l}=40$. Furthermore, curve 1 is for $\vec{a}=(0,0,\frac{1}{2})$, 2 for $\vec{a}=(0,\frac{1}{2},\frac{1}{2})$, and 3 for $\vec{a}=(\frac{1}{2},\frac{1}{2},\frac{1}{2})$.

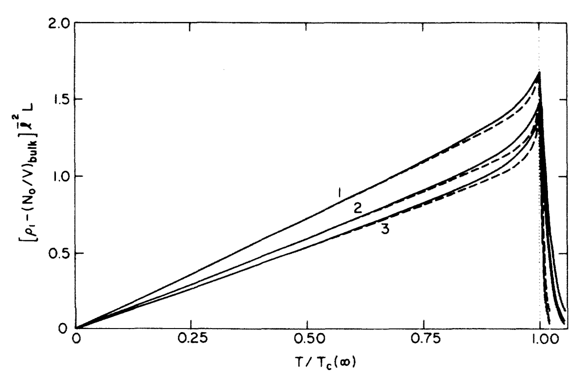

FIG. 6. Temperature dependence of the scaled correlation function $\rho_1\bar{l}^2L$, with condensate background corresponding to the bulk system subtracted. Dashed curves are for $L/\bar{l}=100$, solid ones for $L/\bar{l}=40$. Furthermore, curve 1 is for $\vec{a}=(0,0,\frac{1}{2})$, 2 for $\vec{a}=(0,\frac{1}{2},\frac{1}{2})$, and 3 for $\vec{a}=(\frac{1}{2},\frac{1}{2},\frac{1}{2})$.

edge, and the face of the enclosure, which may be understood in terms of the relative separations of these points from the origin. The minor influence of the actual size of the enclosure, which is expected over and above the dictates of the scaling hypothesis, is evident in both Figs. 5 and 6.

APPENDIX A

We propose to establish the expression (49) for the coefficients $\beta_k(\vec{a})$. For this we employ a method developed by Van der Hoff and Benson[12] which also makes use of the Poisson summation formula. First of all we have

$$\beta_k(\vec{a})=\sum_{\vec{q}=-\infty}^{\infty}{}' \frac{e^{-2\pi i\vec{q}\cdot\vec{a}}}{(q_1^2+q_2^2+q_3^2)^k}=\sum_{\vec{q}=-\infty}^{\infty}{}' \frac{\cos(2\pi q_1a_1)\cos(2\pi q_2a_2)\cos(2\pi q_3a_3)}{(q_1^2+q_2^2+q_3^2)^k}$$
$$=2\sum_{q_1=1}^{\infty}\sum_{q_2=-\infty}^{\infty}\sum_{q_3=-\infty}^{\infty}\frac{\cos(2\pi q_1a_1)\cos(2\pi q_2a_2)\cos(2\pi q_3a_3)}{(q_1^2+q_2^2+q_3^2)^k}+2\sum_{q_2=1}^{\infty}\sum_{q_3=-\infty}^{\infty}\frac{\cos(2\pi q_2a_2)\cos(2\pi q_3a_3)}{(q_2^2+q_3^2)^k}+2\sum_{q_3=1}^{\infty}\frac{\cos(2\pi q_3a_3)}{q_3^{2k}}. \tag{A1}$$

Using the integral representation

$$\frac{1}{q^n}=\frac{1}{\Gamma(n)}\int_0^\infty t^{n-1}e^{-qt}\,dt \tag{A2}$$

and the Poisson identity

$$\sum_{l=-\infty}^{\infty}e^{-(l+a)^2t}=\left(\frac{\pi}{t}\right)^{1/2}\sum_{q=-\infty}^{\infty}\cos(2\pi qa)e^{-\pi^2q^2/t}, \tag{A3}$$

we can write

$$\beta_k(\vec{a})=\frac{2\pi^{2k-1}}{\Gamma(k)}\sum_{q_1=1}^{\infty}\sum_{q_2=-\infty}^{\infty}\sum_{q_3=-\infty}^{\infty}\cos(2\pi q_1a_1)\int_0^\infty u^{k-2}e^{-\pi^2q_1^2u}\exp\left(-\frac{(q_2+a_2)^2+(q_3+a_3)^2}{u}\right)du$$
$$+\frac{2\pi^{2k-1/2}}{\Gamma(k)}\sum_{q_2=1}^{\infty}\sum_{q_3=-\infty}^{\infty}\cos(2\pi q_2a_2)\int_0^\infty u^{k-3/2}e^{-\pi^2q_2^2u}e^{-(q_3+a_3)^2/u}du+(-1)^{k-1}\frac{(2\pi)^{2k}}{(2k)!}B_{2k}(a_3). \tag{A4}$$

Next, using the integral representation

$$\int_0^\infty t^{n-1}e^{-k^2t-\pi^2q^2/t}\,dt=2\left(\frac{\pi q}{k}\right)^nK_n(2\pi kq), \tag{A5}$$

we obtain the desired result:

$$\beta_k(\vec{a})=\frac{4\pi^k}{\Gamma(k)}\sum_{q_1=1}^{\infty}\sum_{q_2=-\infty}^{\infty}\sum_{q_3=-\infty}^{\infty}\cos(2\pi q_1a_1)\left(\frac{[(q_2+a_2)^2+(q_3+a_3)^2]^{1/2}}{q_1}\right)^{k-1}K_{k-1}(2\pi q_1[(q_2+a_2)^2+(q_3+a_3)^2]^{1/2})$$
$$+\frac{4\pi^k}{\Gamma(k)}\sum_{q_2=1}^{\infty}\sum_{q_3=-\infty}^{\infty}\cos(2\pi q_2a_2)\left(\frac{|q_3+a_3|}{q_2}\right)^{k-1/2}K_{k-1/2}(2\pi q_2|q_3+a_3|)+(-1)^{k-1}\frac{(2\pi)^{2k}}{(2k)!}B_{2k}(a_3). \tag{A6}$$

The asymptotic behavior of the $\beta_k(\vec{a})$, for large k, can be obtained from (A6) with several summations replaced by integrations, whence

$$\beta_k(\vec{a})\simeq\frac{4\pi^k}{\Gamma(k)}\sum_{q_1=1}^{\infty}\frac{\cos(2\pi q_1a_1)}{q_1^{k-1}}\int_{-\infty}^{\infty}d(q_2+a_2)\int_{-\infty}^{\infty}d(q_3+a_3)[(q_2+a_2)^2+(q_3+a_3)^2]^{(k-1)/2}K_{k-1}(2\pi q_1[(q_2+a_2)^2+(q_3+a_3)^2]^{1/2})$$
$$+\frac{8\pi^k}{\Gamma(k)}\sum_{q_2=1}^{\infty}\frac{\cos(2\pi q_2a_2)}{q_2^{k-1/2}}\int_0^\infty dl_3\,l_3^{k-1/2}K_{k-1/2}(2\pi q_2l_3)+(-1)^{k-1}\frac{(2\pi)^{2k}}{(2k)!}B_{2k}(a_3). \tag{A7}$$

Expressing the double integral in terms of plane polar coordinates and using the formula

$$\int_0^\infty x^\mu K_\nu(ax)\,dx=\frac{2^{\mu-1}}{a^{\mu+1}}\Gamma(\tfrac{1}{2}(\mu+\nu+1))\Gamma(\tfrac{1}{2}(\mu-\nu+1)),$$

we find, for large k,

$$\beta_k(\vec{a}) \simeq 2\sum_{q_1=1}^{\infty} \frac{\cos(2\pi q_1 a_1)}{q_1^{2k}} + 2\sum_{q_2=1}^{\infty} \frac{\cos(2\pi q_2 a_2)}{q_2^{2k}} + (-1)^{k-1}\frac{(2\pi)^{2k}}{(2k)!} B_{2k}(a_3)$$

$$= (-1)^{k-1}\frac{(2\pi)^{2k}}{(2k)!}[B_{2k}(a_1)+B_{2k}(a_2)+B_{2k}(a_3)] = 2\sum_{q=1}^{\infty} \frac{\cos(2\pi q a_1)+\cos(2\pi q a_2)+\cos(2\pi q a_3)}{q^{2k}}$$

$$\simeq 2[\cos(2\pi a_1) + \cos(2\pi a_2) + \cos(2\pi a_3)]. \tag{A8}$$

The special cases required for our analysis of the condensate fraction and correlation functions can be written after some rearrangement of terms, with the result

$$\beta_k(0,0,0) \equiv (-1)^k b_k = \frac{16\pi^k}{\Gamma(k)} \sum_{l,m,n=1}^{\infty} \left(\frac{[l^2+(m-1)^2]^{1/2}}{n}\right)^{k-1} K_{k-1}(2\pi n[l^2+(m-1)^2]^{1/2})$$

$$+ \frac{8\pi^k}{\Gamma(k)} \sum_{i,j=1}^{\infty} \left(\frac{i}{j}\right)^{k-1/2} K_{k-1/2}(2\pi ij) + \frac{2\pi}{k-1}\zeta(2k-2) + 2\zeta(2k) + 2\pi^{1/2}\frac{\Gamma(k-\frac{1}{2})}{\Gamma(k)}\zeta(2k-1), \quad k > \tfrac{3}{2}, \tag{A9}$$

$$\beta_k(0,0,\tfrac{1}{2}) = \frac{16\pi^k}{\Gamma(k)} 2^{-k+1} \sum_{l=1}^{\infty} \sum_{\substack{m=2\\ \text{even}}}^{\infty} \sum_{\substack{n=1\\ \text{odd}}}^{\infty} \left(\frac{(m^2+n^2)^{1/2}}{l}\right)^{k-1} K_{k-1}(\pi l(m^2+n^2)^{1/2})$$

$$+ \frac{8\pi^k}{\Gamma(k)} 2^{-k+1} \sum_{i=1}^{\infty} \sum_{\substack{j=1\\ \text{odd}}}^{\infty} \left[K_{k-1}(\pi ij) + 2^{-1/2}\left(\frac{j}{i}\right)^{1/2} K_{k-1/2}(\pi ij)\right]\left(\frac{j}{i}\right)^{k-1} - 2(1-2^{-2k+1})\zeta(2k), \tag{A10}$$

$$\beta_k(0,\tfrac{1}{2},\tfrac{1}{2}) = \frac{16\pi^k}{\Gamma(k)} 2^{-k+1} \sum_{l=1}^{\infty} \sum_{\substack{m,n=1\\ \text{odd}}}^{\infty} \left(\frac{(m^2+n^2)^{1/2}}{l}\right)^{k-1} K_{k-1}(\pi l(m^2+n^2)^{1/2})$$

$$+ \frac{8\pi^k}{\Gamma(k)} 2^{-k+1/2} \sum_{i=1}^{\infty} \sum_{\substack{j=1\\ \text{odd}}}^{\infty} (-1)^i \left(\frac{j}{i}\right)^{k-1/2} K_{k-1/2}(\pi ij) - 2(1-2^{-2k+1})\zeta(2k), \tag{A11}$$

$$\beta_k(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}) = \frac{16\pi^k}{\Gamma(k)} 2^{-k+1} \sum_{l=1}^{\infty} \sum_{\substack{m,n=1\\ \text{odd}}}^{\infty} (-1)^l \left(\frac{(m^2+n^2)^{1/2}}{l}\right)^{k-1} K_{k-1}(\pi l(m^2+n^2)^{1/2})$$

$$+ \frac{8\pi^k}{\Gamma(k)} 2^{-k+1/2} \sum_{i=1}^{\infty} \sum_{\substack{j=1\\ \text{odd}}}^{\infty} (-1)^i \left(\frac{j}{i}\right)^{k-1/2} K_{k-1/2}(\pi ij) - 2(1-2^{-2k+1})\zeta(2k). \tag{A12}$$

For asymptotic considerations, we note that

$$\sum_{q=1}^{\infty} \frac{\cos(2\pi q a_i)}{q^{2k}} = \begin{cases} \zeta(2k), & a_i = 0, \\ -(1-2^{1-2k})\zeta(2k), & a_i = \tfrac{1}{2}. \end{cases}$$

Since $\lim_{k\to\infty}\zeta(2k) = 1$, the asymptotic values of the foregoing coefficients turn out to be 6, 2, -2, and -6, respectively. Table I shows the manner in which the actual values of these coefficients approach their asymptotic limits.

APPENDIX B

For a strictly two-dimensional Bose gas, the correlation function is given by

$$\rho_1^{(2)}(\vec{r}-\vec{r}\,') = \frac{1}{L_1L_2} \sum_{k_{1,2}} e^{-i[\vec{k}\cdot(\vec{r}\,'-\vec{r})]} \sum_{j=1}^{\infty} e^{-j\alpha - j\beta\epsilon}. \tag{B1}$$

In the bulk limit

$$\sum_{k_{1,2}} \to \frac{L_1L_2}{4\pi^2} \int d^2k,$$

whence

$$\rho_1^{(2)}(\vec{r}-\vec{r}\,') \to \frac{1}{4\pi^2}\sum_{j=1}^{\infty} e^{-j\alpha}\int_0^{\infty} e^{-j\lambda^2 k^2/4\pi} k\,dk \int_0^{2\pi} e^{ik|\vec{r}-\vec{r}\,'|\cos\phi}\,d\phi = \frac{1}{2\pi}\sum_{j=1}^{\infty} e^{-j\alpha}\int_0^{\infty} e^{-j\lambda^2 k^2/4\pi} J_0(k\,|\vec{r}-\vec{r}\,'|)\,dk$$

$$= \frac{1}{\lambda^2}\sum_{j=1}^{\infty}\frac{e^{-j\alpha}}{j}\exp\left[-\pi\,\frac{(\vec{r}-\vec{r}\,')^2}{\lambda^2}\,j^{-1}\right]. \tag{B2}$$

Now, applying the Poisson summation formula to the sum over j, we get

$$\rho_1^{(2)}(\vec{r}-\vec{r}\,') = \frac{2}{\lambda^2}\sum_{j=-\infty}^{\infty} K_0(2(\pi^{1/2}/\lambda)(\alpha+2\pi i j)^{1/2}(\tilde{x}_1^2+\tilde{x}_2^2)^{1/2})$$

$$= \frac{2}{\lambda^2}K_0(R'/\xi) + \frac{2}{\lambda^2}\sum_{j=-\infty}^{\infty}{}' K_0(2(\pi^{1/2}/\lambda)\,|\vec{r}-\vec{r}\,'|\,(\alpha+2\pi i j)^{1/2}). \tag{B3}$$

The second term is negligible if $R' \gg \lambda$. Therefore to all intents and purposes

$$\rho_1^{(2)}(\vec{r}-\vec{r}\,') = (2/\lambda^2)K_0(R'/\xi). \tag{B4}$$

It may be noted that in the two-dimensional case the condensate term N_0/L_1L_2 is negligibly small for the whole temperature range of interest.

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