Bose-Einstein condensation in finite noninteracting systems: A new law of corresponding states*

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We have carried out a rigorous asymptotic analysis of the thermodynamic behavior of an ideal Bose gas confined to an arbitrary, finite cuboidal geometry under periodic boundary conditions. Our investigation, which is based on the grand canonical ensemble, leads to the construction of an abstract, thermogeometric space in which the process of Bose-Einstein condensation appears as a "collapse" of the lattice points of the space towards its origin. In an infinite geometry, the collapse is accomplished in an infinitesimally small interval of temperature; this results in the appearance of mathematical singularities in the thermodynamic functions of the system. In a finite geometry, the "collapse" proceeds gradually and is spread over a temperature range ΔT such that $\Delta T/T_0 = O(\bar{l}/L_<)$, where $\bar{l}$ is the mean interatomic distance while $L_<$ is the length of the shortest side of the assembly; accordingly, the thermodynamic functions of the system remain smooth throughout. Special events, such as the specific-heat maximum, occur when the "lattice parameters" of our thermogeometric space acquire certain characteristic values which depend only on the shape of the system and not on its actual size. This leads to a new law of corresponding states for Bose-Einstein systems of finite size.

I. INTRODUCTION

Following the work of Osborne,[1] de Groot *et al.*,[2] and Ziman,[3] several authors have investigated the behavior of ideal Bose-Einstein systems confined to restricted geometries.[4-17] The motivation for these investigations stemmed mainly from the following considerations.

Firstly, one hoped that the study of finite Bose-Einstein systems would provide insight into the behavior of actual samples of liquid He^4 confined to restricted geometries. Ziman,[3] for instance, found that the so-called accumulation temperature of a finite Bose-Einstein system was a function of its dimensions and approached 0°K when some of the dimensions were infinite and at least one dimension finite. This finding, however, was in disagreement with the experimental data on liquid He^4 films.[18] To remove this discrepancy, Ziman proposed that the system under study be regarded as composed of a large number of noninteracting, finite cubic assemblies—the so-called *minimal* assemblies—whose physical dimensions were chosen to yield the best agreement with experiment. The physical significance of the proposed dimension (~700 Å) has, however, remained obscure. In any case, the relevance of an ideal Bose-Einstein gas to the problem of liquid He^4 is, from the very beginning, limited. At the same time, one cannot ignore the rôle played by the phenomenon of Bose-Einstein condensation in providing an understanding of the behavior of liquid He^4, *whatever the geometry of the container.*

Secondly, Bose-Einstein systems constitute a class of their own, for they exhibit a phase transition in which interparticle interactions do not play a decisive rôle. Consequently, these systems are amenable to analysis by rigorous analytical means, leading to a general theory for finite-size effects in such systems. Progress in this direction has been rather slow. However, we have now developed a formulation, based on the grand canonical ensemble, which treats the problem in considerable generality and throws an altogether new light on the phenomenon of Bose-Einstein condensation.

In our previous papers[14,17] we analyzed the critical behavior of an ideal Bose gas confined to a thin-film geometry ($\infty \times \infty \times D$) in the asymptotic region $D >> \lambda$, where λ is the mean thermal wavelength of the particles. We now report a substantial generalization of that analysis so as to encompass an arbitrarily finite cuboidal geometry ($L_1 \times L_2 \times L_3$), with $L_j >> \lambda$. A distinctive feature of the new analysis is that it is correct to *all* powers of the variables (λ/L_j); the errors involved are only of the order of $e^{-(L_j/\lambda)^2}$ which, in the asymptotic region, would be completely negligible.

The mathematical form of the various expressions obtained in this analysis leads us to the construction of an abstract *thermogeometric space*, with a lattice structure whose "lattice paramters" y_j are determined by the thermodynamics of the system as well as by its physical dimensions. The phenomenon of Bose-Einstein condensation then appears as a "collapse" of the lattice points of the thermogeometric space towards its origin, such that the relevant y_j's in the critical region are of the order of unity. If we consider an infinite system, the collapse is abrupt and takes place over an infinitesimally small range of temperatures—essentially at a unique temperature $T_0(\infty)$. For a finite system, on the other hand, the "collapse" proceeds gradually, extending over a finite range of temperatures. Special events associated with the phenomenon of condensation, such as the specific-heat maximum, occur over this range and are characterized by values of y_j which are unique for a given shape of the system, *independently of its actual size*. This behavior can be viewed as a "law of corresponding states" for finite-sized Bose-Einstein systems and is intimately related to the Fisher-Barber[19] scaling theory for finite-size effects.

II. FORMULATION OF PROBLEM

We consider a Bose-Einstein system of noninteracting particles with mean occupation numbers $\langle n_i \rangle$ for the single-particle energy levels ϵ_i. It has been shown previously[14] that the various thermodynamic quantities pertaining to this system can be expresssed in terms of the functions G_s, G_s', etc., where

$$G_s = \sum_i \left(\frac{\epsilon_i}{kT}\right)^s \left[\langle n_i\rangle + \langle n_i\rangle^2\right] = -\left(\frac{\partial Z_s}{\partial \alpha}\right)_{T,L_j}, \qquad (1)$$

$$Z_s = \sum_i \left(\frac{\epsilon_i}{kT}\right)^s \langle n_i\rangle, \qquad (2)$$

$$\langle n_i\rangle = (e^{\alpha+\epsilon_i/kT} - 1)^{-1},$$

$$G_s' = -\left(\frac{\partial G_s}{\partial \alpha}\right)_{T,L_j}, \qquad (3)$$

$$G_s'' = -\left(\frac{\partial G_s'}{\partial \alpha}\right)_{T,L_j}, \qquad (4)$$

and

$$\alpha = -\mu/kT, \qquad (5)$$

μ being the chemical potential of the system. For instance, the specific heat C_V and its first derivative with respect to temperature are given by

$$C_V = k(G_2 - G_1^2/G_0) \qquad (6)$$

and

$$\left(\frac{\partial C_V}{\partial T}\right)_{N,L_j} = \frac{k}{T}\left\{-2\left(G_2 - \frac{G_1^2}{G_0}\right) + \left[G_3' - 3\left(\frac{G_1}{G_0}\right)G_2' + 3\left(\frac{G_1}{G_0}\right)^2 G_1' - \left(\frac{G_1}{G_0}\right)^3 G_0'\right]\right\}. \qquad (7)$$

In addition, we have for the relevant temperature derivatives of the chemical potential

$$\left(\frac{\partial^2 \mu}{\partial T^2}\right)_{N,L_j} = \frac{k}{T}\left(2\frac{G_1 G_1'}{G_0^2} - \frac{G_1^2 G_0'}{G_0^3} - \frac{G_2'}{G_0}\right) \qquad (8)$$

and

$$\left(\frac{\partial^3 \mu}{\partial T^3}\right)_{N,L_j} = \frac{k}{T^2}\left(3\frac{G_2'}{G_0} + 3\frac{G_1^2 G_0'}{G_0^3} - 6\frac{G_1 G_1'}{G_0^2} + 3\frac{G_1 G_2''}{G_0^2} - 3\frac{G_1^2 G_1''}{G_0^3} + 3\frac{G_1' G_2'}{G_0^2} - 6\frac{G_1 G_1'^2}{G_0^3} + 9\frac{G_1^2 G_0' G_1'}{G_0^4} + \frac{G_1^3 G_0''}{G_0^4} - 3\frac{G_1 G_0' G_2'}{G_0^3} - 3\frac{G_1^3 G_0'^2}{G_0^5} - \frac{G_3''}{G_0}\right). \qquad (9)$$

It is important to note that the foregoing formulas hold irrespective of the dimensionality of the system, its size and shape, and the nature of the boundary conditions imposed on the wave functions. The characteristic influence of these factors enters through the functions Z_s whose evaluation constitues the central problem of our investigation. This evaluation, in the case of an arbitrary cuboidal assembly (of sides L_1, L_2, and L_3) has been carried out by a proper use of the Poisson summation formula; see Appendix A. The result, for periodic boundary conditions, turns out to be

$$Z_s = \frac{L_1 L_2 L_3}{\lambda^3}\left(\frac{\Gamma(s+\frac{3}{2})}{\Gamma(\frac{3}{2})} g_{s+3/2}(\alpha) + \pi^{1/2}(-1)^s \alpha^{s+1/2} \mathcal{S}_1(y_j)\right), \qquad (10)$$

where $\lambda\ [=\hbar(2\pi\beta/M)^{1/2}]$ is the mean thermal wavelength of the particles, $\Gamma(x)$ is the Γ function of x, while $g_n(\delta)$ are the familiar Bose-Einstein functions[20]

$$g_n(\delta)=\frac{1}{\Gamma(n)}\int_0^\infty \frac{x^{n-1}dx}{e^{x+\delta}-1}; \tag{11}$$

the new function $\mathcal{S}_1(y_j)$ is given by

$$\mathcal{S}_1(y_j)=\sum_{q_{1,2,3}=-\infty}^{\infty}{}' \frac{e^{-2R(\vec{q})}}{R(\vec{q})} \tag{12}$$

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

the parameters y_j being defined as

$$y_j=\pi^{1/2}\alpha^{1/2}(L_j/\lambda)\quad (j=1,2,3). \tag{13}$$

The primed summation in (12) implies that the term with $\vec{q}=0$ is excluded.

From Z_s we obtain

$$G_s=\frac{L_1L_2L_3}{\lambda^3}\left(\frac{\Gamma(s+\frac{3}{2})}{\Gamma(\frac{3}{2})}g_{s+1/2}(\alpha)+\pi^{1/2}(-1)^s\alpha^{s-1/2}(\mathcal{S}_0-s\mathcal{S}_1)\right), \tag{14}$$

and

$$G_s'=\frac{L_1L_2L_3}{\lambda^3}\left(\frac{\Gamma(s+\frac{3}{2})}{\Gamma(\frac{3}{2})}g_{s-1/2}(\alpha)+\pi^{1/2}(-1)^s\alpha^{s-3/2}\times[\mathcal{S}_{-1}^{+}(\tfrac{1}{2}-2s)\mathcal{S}_0+s(s-1)\mathcal{S}_1]\right), \tag{15}$$

where

$$\mathcal{S}_n(y_j)=\sum_{q_{1,2,3}=-\infty}^{\infty}{}' \frac{e^{-2R(\vec{q})}}{R^n(\vec{q})}. \tag{16}$$

The special case $Z_0=N$ deserves a closer scrutiny. We have

$$Z_0\equiv N=\frac{L_1L_2L_3}{\lambda^3}[g_{3/2}(\alpha)+\pi^{1/2}\alpha^{1/2}\mathcal{S}_1]. \tag{17}$$

The first term, $(V/\lambda^3)\,g_{3/2}(\alpha)$, corresponds to the customary bulk results, *exclusive* of the condensate; the second term, therefore, includes *all* characteristic effects arising from the finiteness of the geometry as well as the contribution from the condensate! The behavior of this term is governed by the function $\mathcal{S}_1$, defined in (12), which formally resembles the expression for the "screened Coulomb potential, at the origin, owing to an infinitely extended lattice distribution of point charges, with lattice constants y_1, y_2, and y_3." This resemblance prompts us to construct an abstract, *thermogeometric space*, with a lattice structure characterized by the *thermogeometric parameters* y_1, y_2, and y_3; see Fig. 1. As the temperature of the system decreases, these parameters decrease monotonically and, as a result, the lattice points of our structure in the thermogeometric space move progressively towards the origin ($\vec{q}=0$). The onset of Bose-Einstein condensation is characterized by a "collapse" of the lattice points onto the origin, which occurs over a temperature range determined by the geometry of the system.

In an infinite system, say a cube with $L(=L_{1,2,3})\to\infty$, the paramter $y(=y_{1,2,3})$ displays a *singular* behavior as T passes through the critical temperature $T_0(\infty)$, which is given by the expression[14]

$$T_0(\infty)=h^2(2\pi mk\bar{l}^{\,2})^{-1}[\zeta(\tfrac{3}{2})]^{-2/3}; \tag{18}$$

here, $\zeta(\frac{3}{2})$ is the Riemann ζ function of order $\frac{3}{2}$. Defining $\epsilon=[T-T_0(\infty)]/T_0(\infty)$, we obtain, see Appendix B,

$$y=\tfrac{3}{4}[\zeta(\tfrac{3}{2})]^{2/3}N^{1/3}\epsilon\quad (1\gg\epsilon\gg N^{-1/3}) \tag{19}$$

$$=0.973\ldots\qquad (\epsilon=0) \tag{20}$$

$$=(\tfrac{2}{3}\pi)^{1/2}[\zeta(\tfrac{3}{2})]^{-1/3}N^{-1/6}|\epsilon|^{-1/2}\quad (\epsilon<0,\ 1\gg|\epsilon|\gg N^{-1/3}). \tag{21}$$

Clearly, the transition from $y=O(N^{1/3})$ to $y=O(N^{-1/6})$ takes place over a temperature range ΔT such that

$$\Delta T/T_0(\infty)=O(N^{-1/3}); \tag{22}$$

in this range, the value of y has to be obtained numerically. For an infinite system, the transition is indeed sharp and appears literally as a *collapse* of the lattice points of the thermogeometric space toward its origin; at the same time,

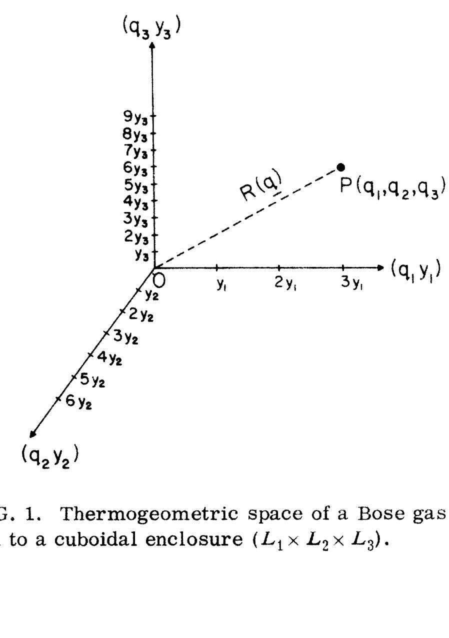

FIG. 1. Thermogeometric space of a Bose gas confined to a cuboidal enclosure ($L_1\times L_2\times L_3$).

the thermodynamic functions of the system encounter singularities characteristic of a phase transition. In this connection, we observe that for $T < T_0(\infty)$, when $y_j \ll 1$, the function $\mathcal{S}_1$ may be evaluated by replacing the summation over $q_{1,2,3}$ by an integration, with the result

$$\mathcal{S}_1 \simeq \int \frac{e^{-2R(\vec{q})}}{R(\vec{q})} d^3q = \int_0^\infty \frac{e^{-2R}}{R} \frac{4\pi R^2 dR}{y_1 y_2 y_3} = \frac{\pi}{y_1 y_2 y_3}, \tag{12'}$$

and hence

$$N \simeq \frac{V}{\lambda^3} g_{3/2}(\alpha) + \frac{1}{\alpha}, \tag{17'}$$

as is indeed expected. It is instructive to note that in the usual formulation the first term in (17′), which accounts for the particles in the excited states, arises as a result of an integration over states instead of a summation; in our formulation it arises from the single term corresponding to the origin ($q_{1,2,3} = 0$) of the thermogeometric space. Conversely, the second term, which accounts for the particles in the ground state, customarily arises from the expression for the mean occupation number $\langle n_0 \rangle$, with $\alpha \ll 1$; here, it results from an integration over the thermogeometric space, *excluding the origin*.

In a finite system the transition from $y_j \gg 1$ to $y_j \ll 1$ is spread over a finite temperature range,

$$|\Delta T| / T_0(\infty) = O(\lambda / L_<), \tag{23}$$

where $L_<$ is the length of the shortest side of the container; the thermodynamic functions of the system in this case remain *smooth* throughout. The "onset" of Bose-Einstein condensation can now be defined in a variety of ways, some of which will be considered in the sequel; in each case, the phenomenon of condensation takes place when $y_< \,[= \pi^{1/2}\alpha^{1/2}(L_</\lambda)]$ is of the order of unity.

III. SPECIAL CASES

First of all we consider the case $L_1 \gg L_2 \gg L_3$ for which, obviously, $y_1 \gg y_2 \gg y_3$. Referring to Fig. 1, and keeping in mind the functional form of the variable $R(\vec{q})$ appearing in the definition of $\mathcal{S}_1$, see Eq. (12), we observe that the summation over $\vec{q}$ in this case may be approximated as follows: (i) for $q_1 = q_2 = 0$, we sum over q_3, (ii) for $q_1 = 0$ and $q_2 \neq 0$, we sum over q_2 but integrate over q_3, and (iii) for $q_1 \neq 0$, we sum over q_1 but integrate over q_2 and q_3. We thereby obtain

$$N = \frac{L_1 L_2 L_3}{\lambda^3} \left[g_{3/2}(\alpha) + \frac{\lambda}{L_3} \left(2 g_1(2y_3) + 4 \sum_{l=1}^{\infty} K_0(2 l y_2) \right) + \frac{2\pi^{1/2}}{\alpha^{1/2}} \frac{\lambda^2}{L_2 L_3} \frac{1}{e^{2y_1} - 1} \right], \tag{24}$$

where $K_0(x)$ is a modified Bessel function of order zero. Expression (24) is identical with a corresponding result obtained earlier by Krueger[11] following different mathematical techniques. It is, however, important to note that this result is valid *only* for $L_1 \gg L_2 \gg L_3$, and *not for* $L_1 \geqslant L_2 \geqslant L_3$, as claimed by Krueger. Accordingly, this result cannot be applied to the case of a narrow channel for which $L_1 \to \infty$, L_2 and L_3 are generally comparable in magnitude. In that case, we must go back to Eq. (17) to obtain

$$N = \frac{V}{\lambda^3} \left(g_{3/2}(\alpha) + \pi^{1/2} \alpha^{1/2} \times \sum_{q_{2,3}=-\infty}^{\infty}{}' \frac{e^{-2(q_2^2 y_2^2 + q_3^2 y_3^2)^{1/2}}}{(q_2^2 y_2^2 + q_3^2 y_3^2)^{1/2}} \right). \tag{25}$$

The special case of a thin-film geometry can likewise be obtained from Eq. (17) as

$$N = \frac{V}{\lambda^3} \left(g_{3/2}(\alpha) + \pi^{1/2} \alpha^{1/2} \sum_{q_3=-\infty}^{\infty}{}' \frac{e^{-2q_3 y_3}}{q_3 y_3} \right) = \frac{V}{\lambda^3} \left(g_{3/2}(\alpha) + 2 \frac{\lambda}{L_3} g_1(2y_3) \right), \tag{26}$$

which is identical with Eq. (17) of I. This result, of course, can be obtained legitimately from Eq. (24) as well by letting $L_{1,2} \to \infty$.

IV. RESULTS AND DISCUSSION

Of the various criteria that can be invoked for the onset of Bose-Einstein condensation in a finite system,[9,11,12] we consider here two which are based on the intensive quantites C_V/Nk and $(\partial^2 \mu / \partial T^2)_{N, L_j}$. In an infinite system, C_V/Nk possesses a sharp maximum (with a discontinuous temperature derivative) at the critical temperature $T_0(\infty)$, while $(\partial^2 \mu / \partial T^2)_{N, L_j}$ possesses a sharp minimum accompanied by a discontinuity in value. In a finite system, where no discontinuities can occur, one intuitively looks for the (smooth) *maximum* of C_V/Nk or the (smooth) minimum of $(\partial^2 \mu / \partial T^2)_{N, L_j}$. Starting from Eqs. (7) and (9), we obtain, after some straightforward but tedious calculation, equations involving the lattice sums $\mathcal{S}_n$ (over the thermogeometric space), which determine the *characteristic* values of the thermogeometric parameters y_j pertaining to the criterion employed.

For $(C_V/Nk)_{max}$ we obtain, to the *lowest* order in λ/L_j,

$$\frac{1+\mathcal{S}_0+2\mathcal{S}_{-1}}{(1+\mathcal{S}_0)^3}-\frac{10\pi}{3}\frac{\zeta(\frac{5}{2})}{[\zeta(\frac{3}{2})]^3}=0\ , \tag{27}$$

and for $(\partial^2\mu/\partial T^2)_{min}$

$$2\mathcal{S}_{-2}(1+\mathcal{S}_0)-3\mathcal{S}_{-1}(1+\mathcal{S}_0+2\mathcal{S}_{-1})=0\ . \tag{28}$$

It may be mentioned here that, for the case of a thin-film geometry, the characteristic equation (27) reduces to Eq. (31) of I.

Equations (27) and (28) have been solved for a variety of cuboidal shapes—in particular, a thin film ($\infty\times\infty\times L$), a square channel ($\infty\times L\times L$), and a cube ($L\times L\times L$). The relevant results for $y_<$ are displayed in Table I; for comparison, the respective values of $y_<$ at $T=T_0(\infty)$ are also included. These results can be converted into the *characteristic temperatures* $T_0(L_j)$ with the help of the basic relation (17) or, preferably, (B6).

The most important thing to observe here is that the actual size of the given system does not appear explicitly in the characteristic equations (27) and (28); it appears only implicitly through the thermogeometric parameters y_j. Once the shape of the system, as given by the ratios L_3/L_1 ($\equiv y_3/y_1$) and L_3/L_2 ($\equiv y_3/y_2$), is specified, the characteristic equations involve only y_3 (which we have preferred to denote by the symbol $y_<$). Now, the fact that special events, such as the maximum of C_V/Nk or the minimum of $(\partial^2\mu/\partial T^2)_{N,L_j}$, take place at certain characteristic values of the parameter $y_<$ (which, apart from the criterion employed, depends *only* on the shape of the system and *not* on its actual size) enables us to establish a thermodynamic correspondence between Bose-Einstein systems of similar shape but different sizes. We thus obtain a new *law of corresponding states*, according to which "two Bose-Einstein systems A and B, similar in shape but different in size, are in corresponding states when $(y_<)_A=(y_<)_B$." A reference to Eq. (13) reveals that when the y's of A are equal to the y's of B the respective temperatures, T_A and T_B, of the two systems are generally different; they depend upon the actual sizes as well.

TABLE I. Characteristic values of the thermogeometric parameter $y_<$ for various shapes of the cuboidal assembly.

	Thin film ($\infty\times\infty\times L$)	Square Channel ($\infty\times L\times L$)	Cube ($L\times L\times L$)
$y_<[T_0(\infty)]$	0.48[a]	0.76	0.97
$y_<(C_V/Nk)_{max}$	0.85[b]	1.14	1.35
$y_<(\partial^2\mu/\partial T^2)_{min}$	1.72	1.86	1.99

[a]This result may be stated explicitly as $\sinh^{-1}\frac{1}{2}\equiv\ln[\frac{1}{2}(\sqrt{5}+1)]=0.4812\ldots$.

[b]This result was first reported in I.

We note that the foregoing statement (of correspondence) may be expressed in terms of the *reduced chemical potentials* of the two systems,[17] i.e.,

$$\left(\frac{\mu(L_3,T)}{h^2/ML_3^2}\right)_A=\left(\frac{\mu(L_3,T)}{h^2/ML_3^2}\right)_B\ . \tag{29}$$

The physical nature of this equality suggests that a similar result may be valid for establishing thermodynamic correspondence between two similar systems which are not necessarily cuboidal and in which interparticle interactions are not necessarily negligible. We propose to investigate this matter in detail in a subsequent communication.

In II, we discussed the relationship between our parameter $y_<$ for a thin-film geometry and the corresponding scaling variable z of Barber and Fisher,[16] namely,

$$z=(L_3/\bar{l})\,\mathring{t}\ , \tag{30}$$

where

$$\mathring{t}=[T-T_{max}(L_3)]/T_0(\infty)\ , \tag{31}$$

$T_{max}(L_3)$ being the temperature corresponding to the specific-heat maximum. Such relationships can also be established in the more general case being studied here. However, we shall avoid being repetitive and simply state that (i) the law of corresponding states emerging in our formulation and (ii) the Fisher-Barber scaling theory for finite-size effects[19] both stem from a common physical origin.

APPENDIX A

We shall first evaluate the function Z_0, from which Z_s can be derived in a surprisingly simple manner. In this evaluation we shall assume *periodic* boundary conditions; generalization to other boundary conditions is straightforward,[21] though the resulting formulas would be rather cumbersome.

By definition,

$$Z_0\equiv N=\sum_\epsilon(e^{\alpha+\beta\epsilon}-1)^{-1}=\sum_\epsilon\sum_{j=1}^{\infty}e^{-j(\alpha+\beta\epsilon)}$$

$$=\sum_{j=1}^{\infty}e^{-j\alpha}\sum_{n_1}e^{-jw_1n_1^2}\sum_{n_2}e^{-jw_2n_2^2}\sum_{n_3}e^{-jw_3n_3^2}\ , \tag{A1}$$

where

$$\epsilon=\frac{\hbar^2}{2M}(k_1^2+k_2^2+k_3^2)\ , \tag{A2}$$

with

$$k_i = (2\pi/L_i)n_i \quad (n_i = 0, \pm 1, \pm 2, \dots); \tag{A3}$$

the parameters w_i are given by

$$w_i = \frac{2\beta\hbar^2\pi^2}{ML_i^2} = \pi\left(\frac{\lambda}{L_i}\right)^2, \tag{A4}$$

where $\lambda\ [=\hbar(2\pi\beta/M)^{1/2}]$ is the mean thermal wavelength of the particles. Now, by Poisson's summation formula,[22]

$$\sum_{n=-\infty}^{\infty} F(n) = \sum_{q=-\infty}^{\infty} \mathfrak{F}(q)\ , \tag{A5}$$

where $\mathfrak{F}(q)$ is the Fourier transform of $F(n)$.

Choosing $F(n)$ to be e^{-jwn^2}, we obtain the remarkable identity

$$\sum_{n=-\infty}^{\infty} e^{-jwn^2} = 2\sum_{q=-\infty}^{\infty}\int_0^\infty \cos(2\pi q n)\, e^{-jwn^2} dn \tag{A6}$$

$$= \sum_{q=-\infty}^{\infty}\left(\frac{\pi}{jw}\right)^{1/2} e^{-\pi^2 q^2/jw}\ . \tag{A7}$$

It is instructive to note that the $q=0$ term in (A7) is precisely the result one would obtain if the summation over n were replaced by an integration, as is normally done for an infinite system; the $q\neq 0$ terms, therefore, represent corrections arising from the discreteness of the single-particle states. Using (A7), we obtain

$$Z_0 = \sum_{j=1}^{\infty} e^{-j\alpha} \prod_{i=1,2,3}\left[\left(\frac{\pi}{jw_i}\right)^{1/2}\sum_{q_i=-\infty}^{\infty}\exp\left(-\frac{\pi^2 q_i^2}{jw_i}\right)\right]$$

$$= \frac{\pi^{3/2}}{(w_1w_2w_3)^{1/2}}\sum_{q_{1,2,3}=-\infty}^{\infty}\sum_{j=1}^{\infty}\frac{e^{-j\alpha}}{j^{3/2}}\exp\left[-\left(\frac{\pi^2q_1^2}{jw_1}+\frac{\pi^2q_2^2}{jw_2}+\frac{\pi^2q_3^2}{jw_3}\right)\right] \tag{A8}$$

$$= \frac{L_1L_2L_3}{\lambda^3}\left\{\sum_{j=1}^{\infty}\frac{e^{-j\alpha}}{j^{3/2}} + \sum_{q_{1,2,3}=-\infty}^{\infty}{}'\sum_{j=1}^{\infty}\frac{e^{-j\alpha}}{j^{3/2}}\exp\left[-\left(\frac{\pi^2q_1^2}{jw_1}+\frac{\pi^2q_2^2}{jw_2}+\frac{\pi^2q_3^2}{jw_3}\right)\right]\right\}, \tag{A9}$$

where the primed summation in the second set of terms implies that the term with $\vec{q}=0$ is excluded. Now, setting $p=j\alpha$ and $y_i=\pi^{1/2}\alpha^{1/2}(L_i/\lambda)$, we may write

$$Z_0 = \frac{L_1L_2L_3}{\lambda^3}\left(g_{3/2}(\alpha) + \alpha^{1/2}\sum_{q_{1,2,3}=-\infty}^{\infty}{}'\int_0^\infty dp\, \frac{e^{-p}\exp[-(1/p)(q_1^2y_1^2+q_2^2y_2^2+q_3^2y_3^2)]}{p^{3/2}}\right); \tag{A10}$$

the replacement of the summation over j by an integration over p introduces errors of the order of $e^{-(L_i^2/\lambda^2)}$ which, for $L_i \gg \lambda$, are negligible. At this point it is important to note that no errors of order $(\lambda/L_i)^n$ are committed here.

We now make use of the tabulated Laplace transform[23]

$$\mathfrak{L}\left(\frac{1}{t^{3/2}}\, e^{-k^2/4t}\right) = \frac{2\pi^{1/2}}{k}\, e^{-k\sqrt{s}}, \tag{A11}$$

with $s=1$, to obtain the desired result

$$Z_0 = \frac{L_1L_2L_3}{\lambda^3}\left[g_{3/2}(\alpha) + \pi^{1/2}\alpha^{1/2}\mathcal{S}_1(y_1, y_2, y_3)\right], \tag{A12}$$

where

$$\mathcal{S}_1(y_1,y_2,y_3) = \sum_{q_{1,2,3}=-\infty}^{\infty}{}'\ \frac{\exp[-2(q_1^2y_1^2+q_2^2y_2^2+q_3^2y_3^2)^{1/2}]}{(q_1^2y_1^2+q_2^2y_2^2+q_3^2y_3^2)^{1/2}}\ . \tag{A13}$$

To derive Z_s, we observe that, since

$$Z_s = \sum_{j=1}^{\infty}\sum_{\epsilon} e^{-j\alpha}(\beta\epsilon)^s e^{-j\beta\epsilon} \tag{A14}$$

and

$$Z_0 = \sum_{j=1}^{\infty}\sum_{\epsilon} e^{-j\alpha}e^{-j\beta\epsilon}\ , \tag{A15}$$

we have the following mathematical relationship:

$$\left(\frac{\partial^s Z_s}{\partial\alpha^s}\right)_\beta = \beta^s\left(\frac{\partial^s Z_0}{\partial\beta^s}\right)_\alpha\ . \tag{A16}$$

Consequently, the desired expression for Z_s may be derived by differentiating the expression (A12) for Z_0 with respect to β (s times), integrating with respect to α (s times), and finally multiplying by β^s. Performing this calculation, and making use of the fact that $\mathcal{S}_1$ is an explicit function of the ratio α/β alone, we obtain

$$Z_s = \frac{L_1L_2L_3}{\lambda^3}\left(\frac{\Gamma(s+\frac{3}{2})}{\Gamma(\frac{3}{2})}\, g_{s+3/2}(\alpha) + \pi^{1/2}(-1)^s\alpha^{s+1/2}\mathcal{S}_1\right), \qquad \text{(A17)}$$

as quoted in Eq. (10) of Sec. II.

APPENDIX B

To establish relations (19)–(21), we start with (17), namely,

$$N = \frac{L_1L_2L_3}{\lambda^3}\left[g_{3/2}(\alpha) + \pi^{1/2}\alpha^{1/2}\mathcal{S}_1\right]. \qquad \text{(B1)}$$

For $\alpha \ll 1$, we may write

$$g_{3/2}(\alpha) \simeq \zeta(\tfrac{3}{2}) - 2\pi^{1/2}\alpha^{1/2}, \qquad \text{(B2)}$$

whereby Eq. (B1) becomes

$$N \simeq \frac{L_1L_2L_3}{\lambda^3}\left[\zeta(\tfrac{3}{2}) - \pi^{1/2}\alpha^{1/2}(2-\mathcal{S}_1)\right] \qquad \text{(B3)}$$

or, equivalently,

$$(\lambda/\bar{l})^3 \simeq \zeta(\tfrac{3}{2}) - \pi^{1/2}\alpha^{1/2}(2-\mathcal{S}_1), \qquad \text{(B4)}$$

where $\bar{l}$ is the mean interparticle distance. Now, if $\lambda_0(\infty)$ corresponds to the bulk transition temperature $T_0(\infty)$, then[14,20]

$$(\lambda_0(\infty)/\bar{l})^3 = \zeta(\tfrac{3}{2}). \qquad \text{(B5)}$$

Combining (B4) and (B5), we obtain (to first order in $\bar{l}/L_j$)

$$\frac{T}{T_0(\infty)} = 1 + \tfrac{2}{3}\left[\zeta(\tfrac{3}{2})\right]^{-2/3}\left(\frac{\bar{l}}{L_j}\, y_j\right)(2-\mathcal{S}_1). \qquad \text{(B6)}$$

Restricting ourselves to a *cubic* geometry and denoting the y_j's by a common symbol y, we note that, for T sufficiently below $T_0(\infty)$, $y \ll 1$ and the function $\mathcal{S}_1$ approaches the functional form π/y^3; see Eq. (12′). Consequently, letting $[T - T_0(\infty)]/T_0(\infty) = \epsilon$, Eq. (B6) yields the relation

$$y \simeq (\tfrac{2}{3}\pi)^{1/2}\left[\zeta(\tfrac{3}{2})\right]^{-1/3}N^{-1/6}|\epsilon|^{-1/2}, \qquad \text{(B7)}$$

with the condition

$$1 \gg |\epsilon| \gg N^{-1/3}. \qquad \text{(B8)}$$

We observe that, for a specific value of T in this region,

$$y \sim N^{-1/6}, \quad \alpha \sim N^{-1}, \qquad \text{(B9)}$$

as expected in the region of Bose-Einstein condensation.

To locate the value of y at $T = T_0(\infty)$, we must solve the characteristic equation

$$\mathcal{S}_1(y) = 2. \qquad \text{(B10)}$$

For a cubic geometry, the solution is $y \simeq 0.973$; solutions for some other geometries are included in Table I. It follows that for a given class of systems, similar in shape but different in size, the $y(T)$ curves (for various sizes) pass through the unique point $y\{T_0(\infty)\}$, which is the solution of Eq. (B10). In passing, we observe that at $T = T_0(\infty)$,

$$y \sim N^0, \quad \alpha \sim N^{-2/3}. \qquad \text{(B11)}$$

Returning to the cubic geometry, we further note that, for T sufficiently above $T_0(\infty)$, $y \gg 1$ and we may neglect $\mathcal{S}_1$, in comparison with 2, in Eq. (B6). We then obtain

$$y \simeq \tfrac{3}{4}\left[\zeta(\tfrac{3}{2})\right]^{2/3}N^{1/3}\epsilon, \qquad \text{(B12)}$$

with the condition

$$1 \gg \epsilon \gg N^{-1/3}. \qquad \text{(B13)}$$

In this case, for a specific value of T,

$$y \sim N^{1/3}, \quad \alpha \sim N^0, \qquad \text{(B14)}$$

that is, α now becomes a truly intensive variable.

Previous authors[24,25] have attempted to evaluate α at, or close to, $T_0(\infty)$ by solving the relation (17′), namely,

$$N \simeq \frac{V}{\lambda^3}\, g_{3/2}(\alpha) + \frac{1}{\alpha}, \qquad \text{(17′)}$$

with the help of the approximation (B2)—disregarding the fact that this relation is in error by terms $O(N^{2/3})$. In the customary treatment this error arises from the replacement of the summation over states in Eq. (A1) by an integration, leading to the familiar function $g_{3/2}(\alpha)$; in our approach, it arises from the replacement of the lattice sum $\mathcal{S}_1$ by the functional form π/y^3, as in (12′). Now, at $T = T_0(\infty)$, the term $1/\alpha$ in (17′) is itself $O(N^{2/3})$; consequently, α cannot be evaluated accurately from this relation, except to an order of magnitude. We finally note that the (erroneous) value of $y\{T_0(\infty)\}$ resulting from the expression for α obtained by these authors is $(\frac{1}{2}\pi)^{1/3}$; this is tantamount to replacing $\mathcal{S}_1$, in Eq. (B10), by the functional form π/y^3, *which is valid only for* $y \ll 1$, to obtain a value of y which is $O(1)$!

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